



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:53 PM UTC

PDB ID : 7QYA / pdb_00007qya
EMDB ID : EMD-14210
Title : Proteasome-ZFAND5 Complex Z-B state
Authors : Zhu, Y.; Lu, Y.
Deposited on : 2022-01-27
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

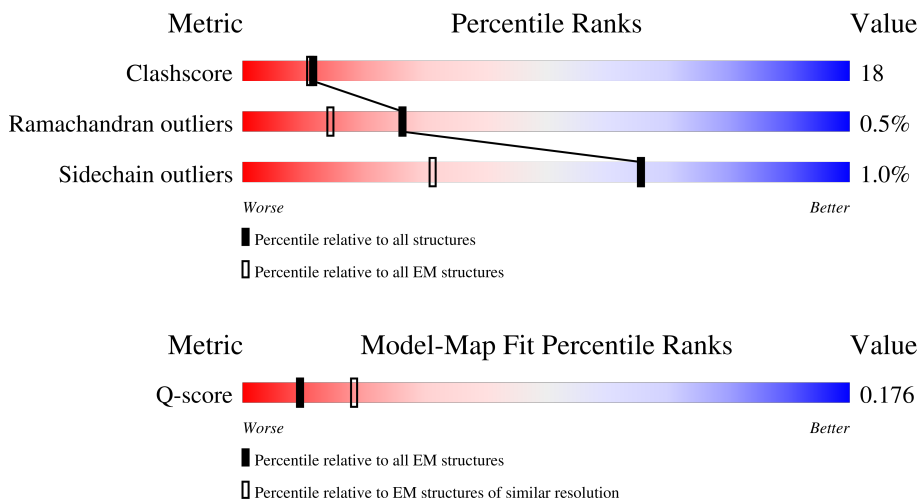
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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

Mol	Chain	Length	Quality of chain
1	a	376	
2	b	377	
3	c	309	
4	d	349	

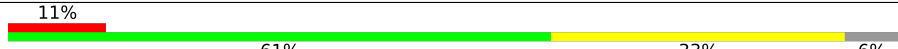
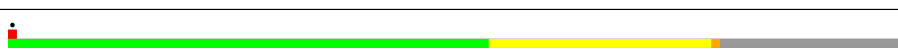
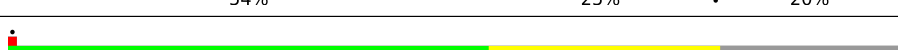
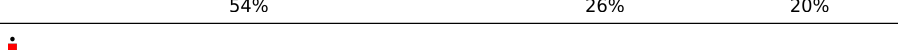
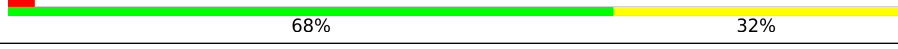
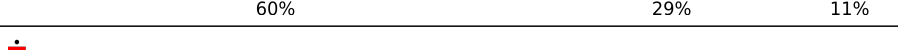
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	70	
6	f	908	
7	U	953	
8	V	533	
9	W	456	
10	X	422	
11	Y	389	
12	Z	324	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	
27	O	276	
27	o	276	
28	P	204	
28	p	204	
29	Q	201	
29	q	201	
30	R	262	
30	r	262	
31	S	240	
31	s	240	
32	T	263	
32	t	263	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 101325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	191	Total	C	N	O	S	0	0
			1457	910	260	279	8		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	278	Total	C	N	O	S	0	0
			2186	1389	373	406	18		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	257	Total	C	N	O	S	0	0
			2115	1371	345	390	9		

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	40	Total	C	N	O	S	0	0
			333	200	54	77	2		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	689	Total	C	N	O	S	0	0
			5318	3343	903	1037	35		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	806	Total	C	N	O	S	0	0
			6286	3990	1074	1178	44		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	473	Total	C	N	O	S	0	0
			3807	2418	675	700	14		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	456	Total	C	N	O	S	0	0
			3702	2339	634	704	25		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	380	Total	C	N	O	S	0	0
			3008	1918	508	570	12		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	378	Total	C	N	O	S	0	0
			3114	1987	532	578	17		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	286	Total	C	N	O	S	0	0
			2280	1457	391	427	5		

- Molecule 13 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	380	Total	C	N	O	S	0	0
			2892	1817	514	543	18		

- Molecule 14 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	370	Total	C	N	O	S	0	0
			2805	1763	477	553	12		

- Molecule 15 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	363	Total	C	N	O	S	0	0
			2858	1804	512	525	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3039	1923	523	580	13		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	375	Total	C	N	O	S	0	0
			2859	1796	511	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	376	Total	C	N	O	S	0	0
			2858	1802	495	546	15		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 24 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 26 is a protein called Proteasome subunit beta type-6.

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

- Molecule 27 is a protein called Proteasome subunit beta type-7.

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

- Molecule 28 is a protein called Proteasome subunit beta type-3.

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

- Molecule 29 is a protein called Proteasome subunit beta type-2.

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

- Molecule 30 is a protein called Proteasome subunit beta type-5.

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

- Molecule 31 is a protein called Proteasome subunit beta type-1.

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

Continued on next page...

Continued from previous page...

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

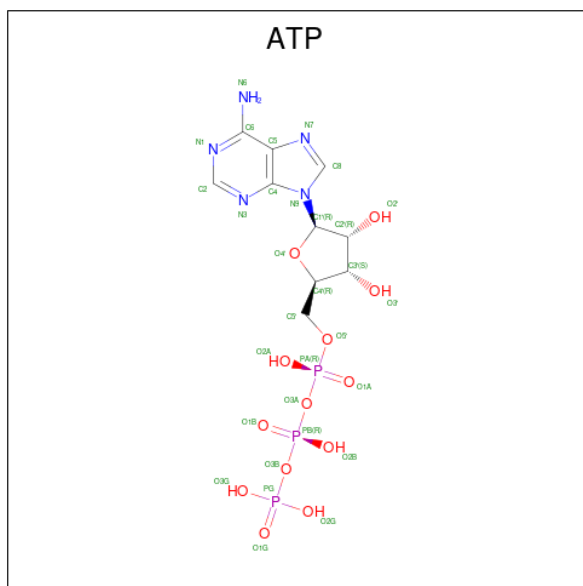
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- 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	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

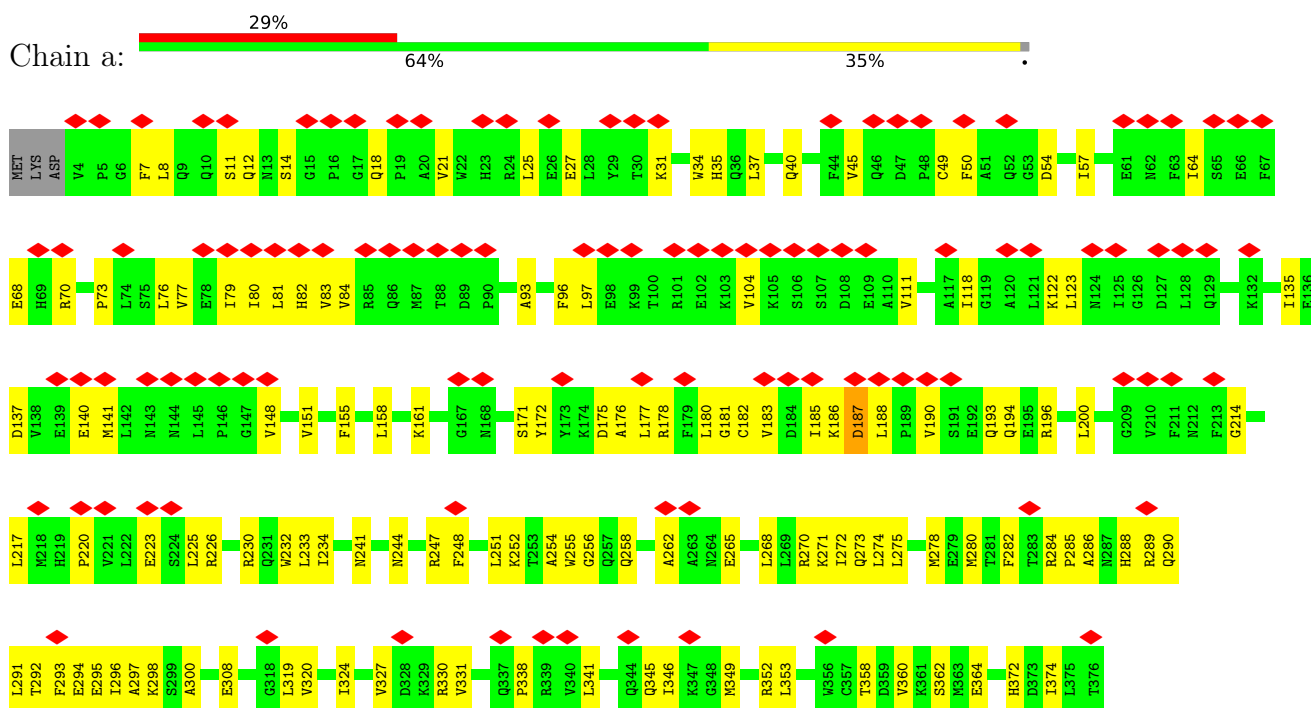
Continued from previous page...

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

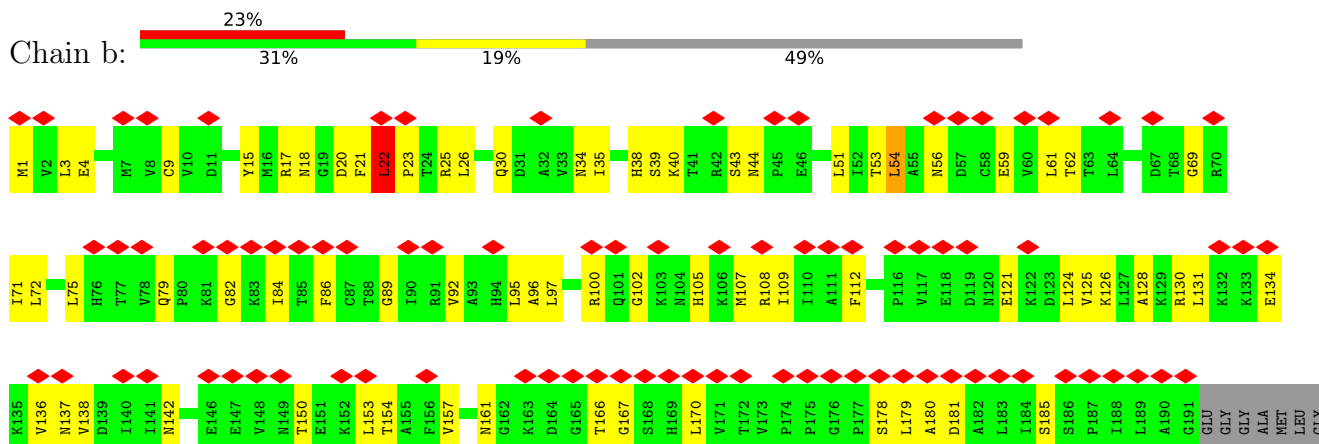
3 Residue-property plots

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

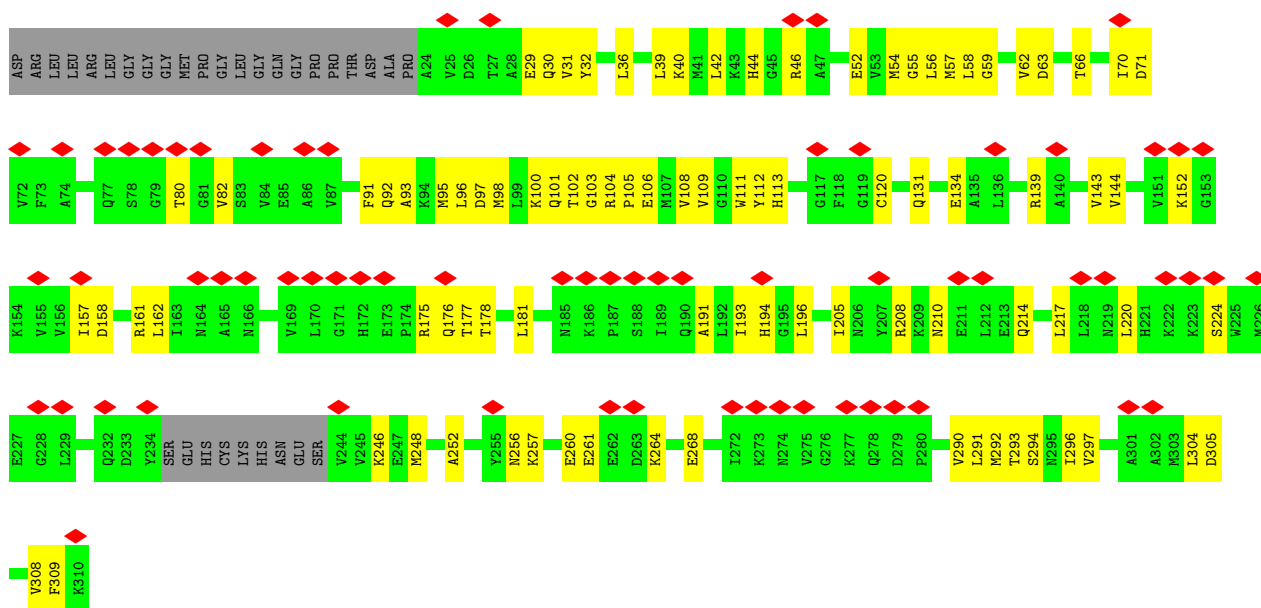
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 13



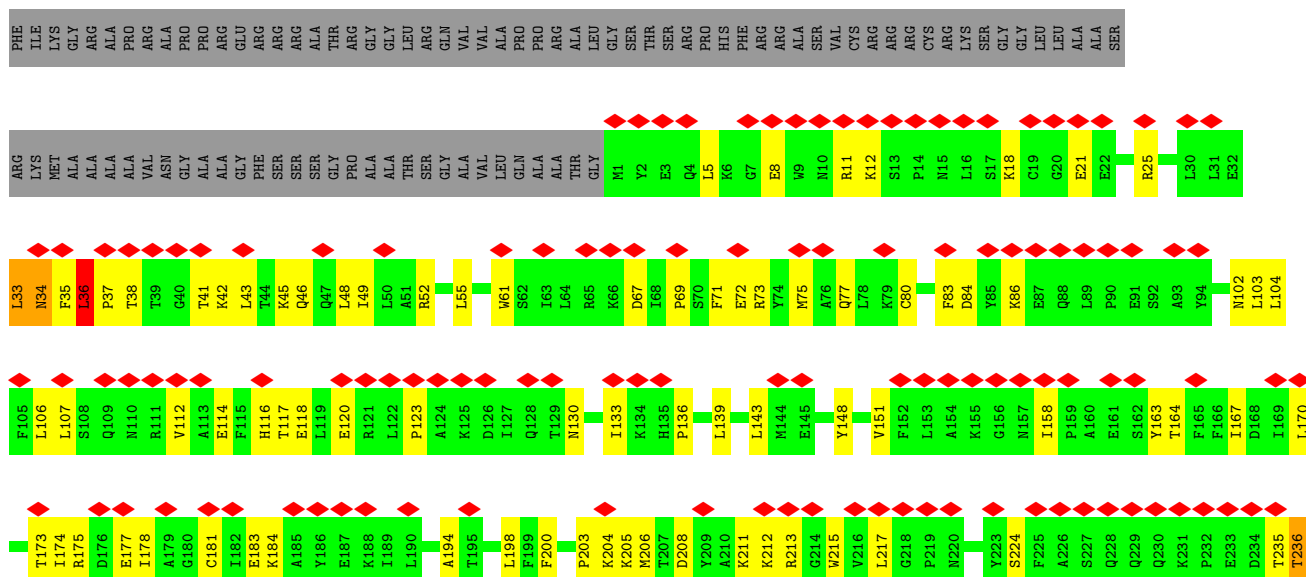
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 4

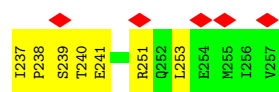


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 14

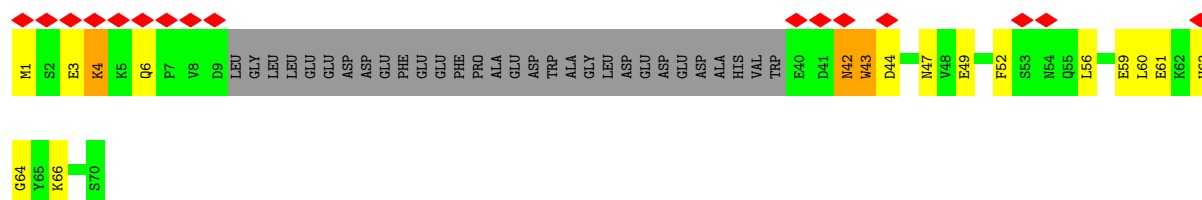
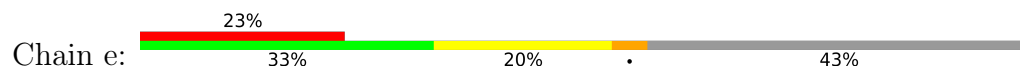


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 8

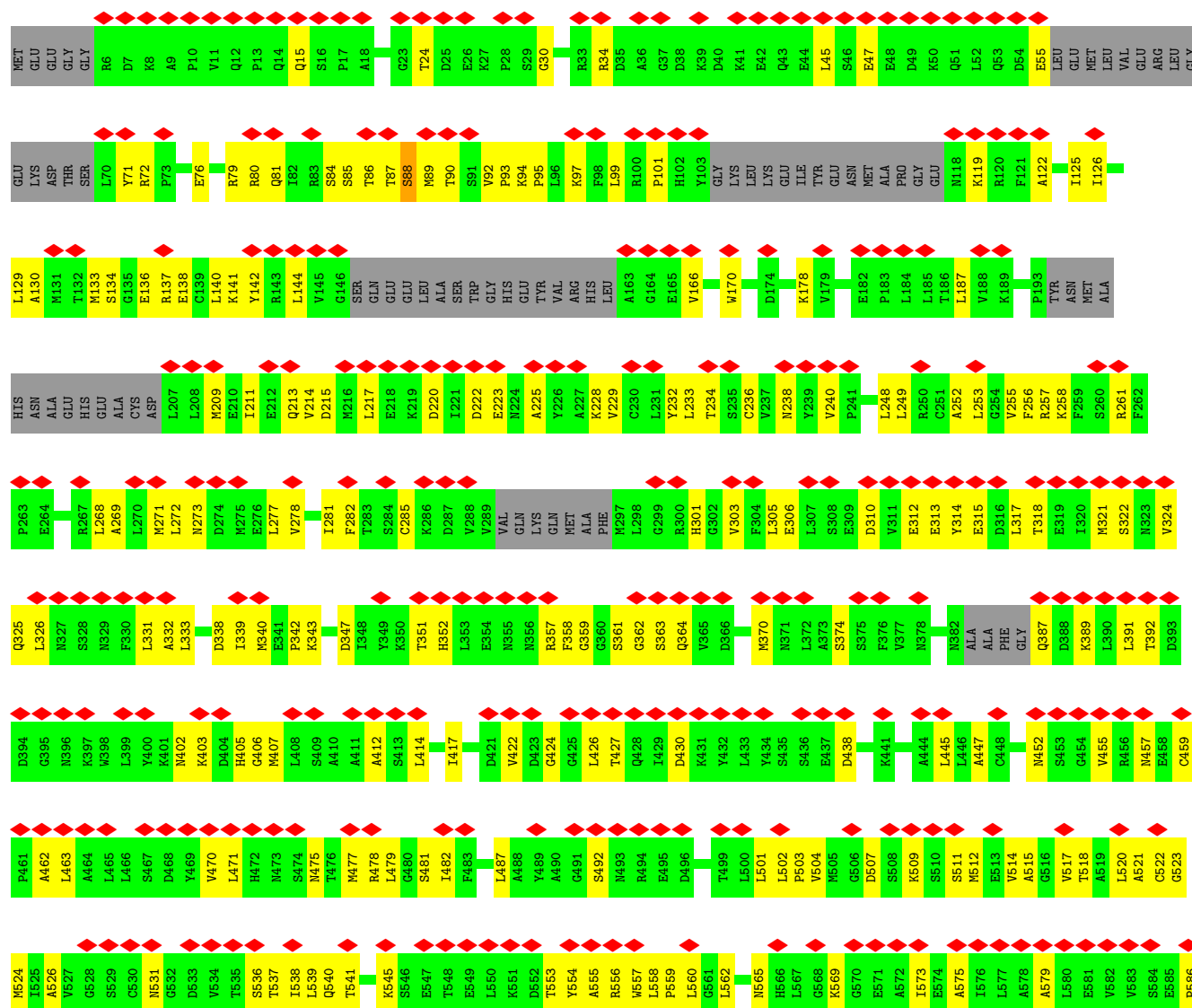
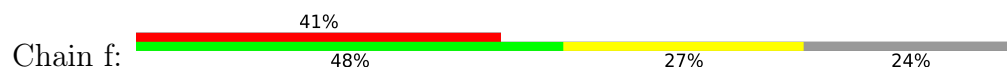


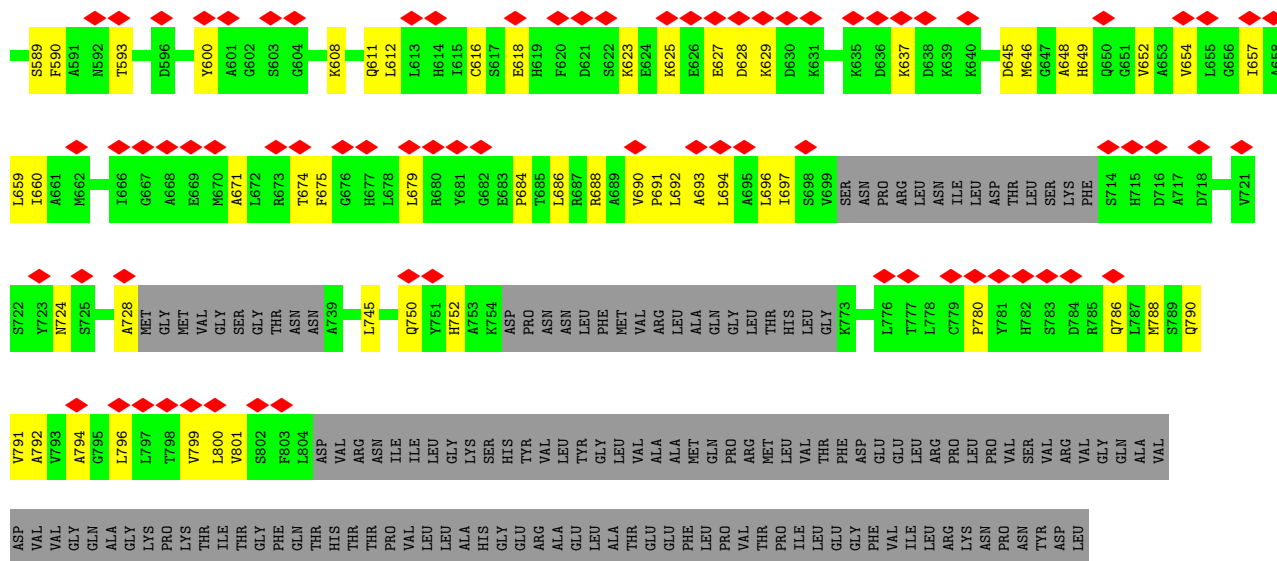


• Molecule 5: 26S proteasome complex subunit SEM1

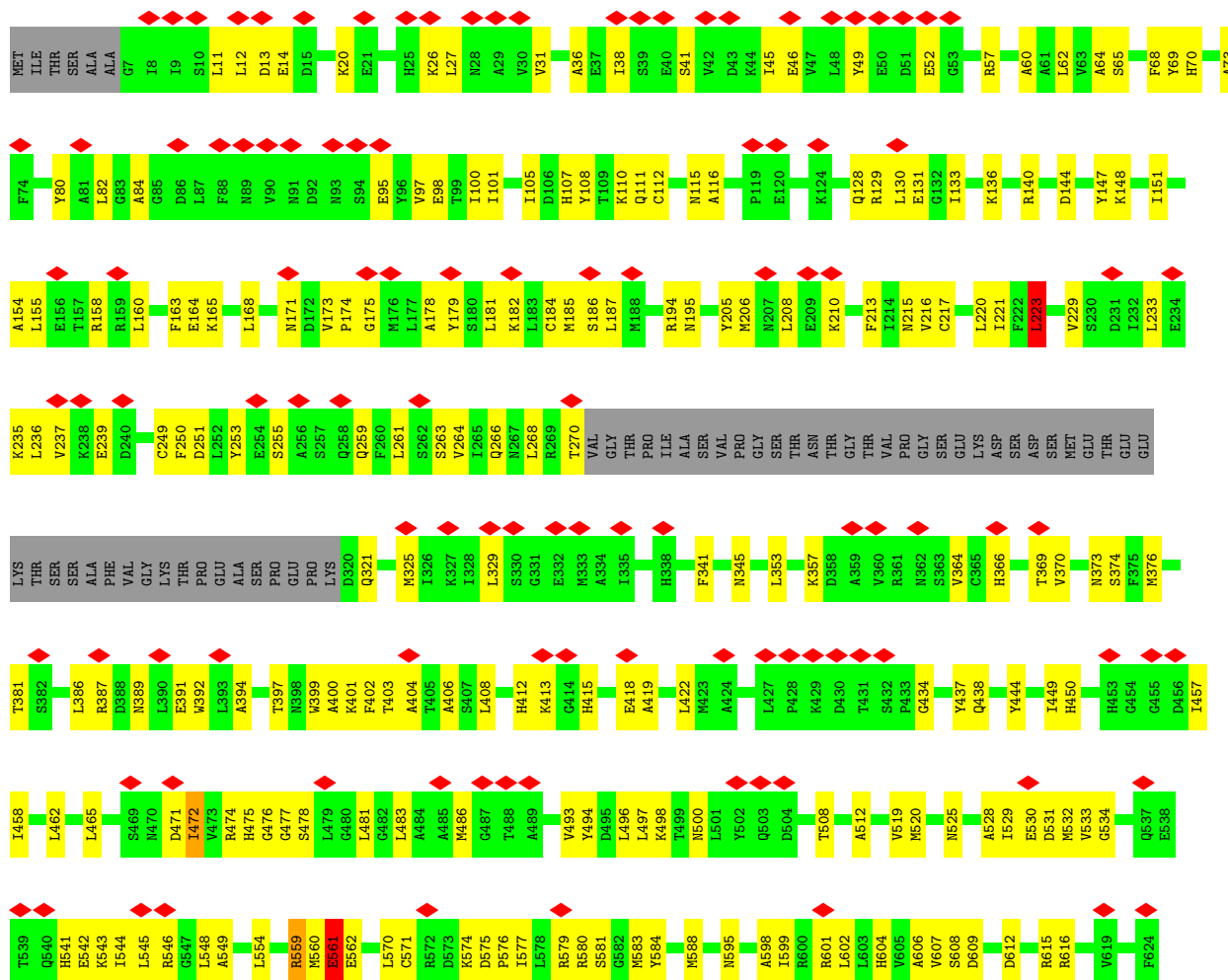


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 2

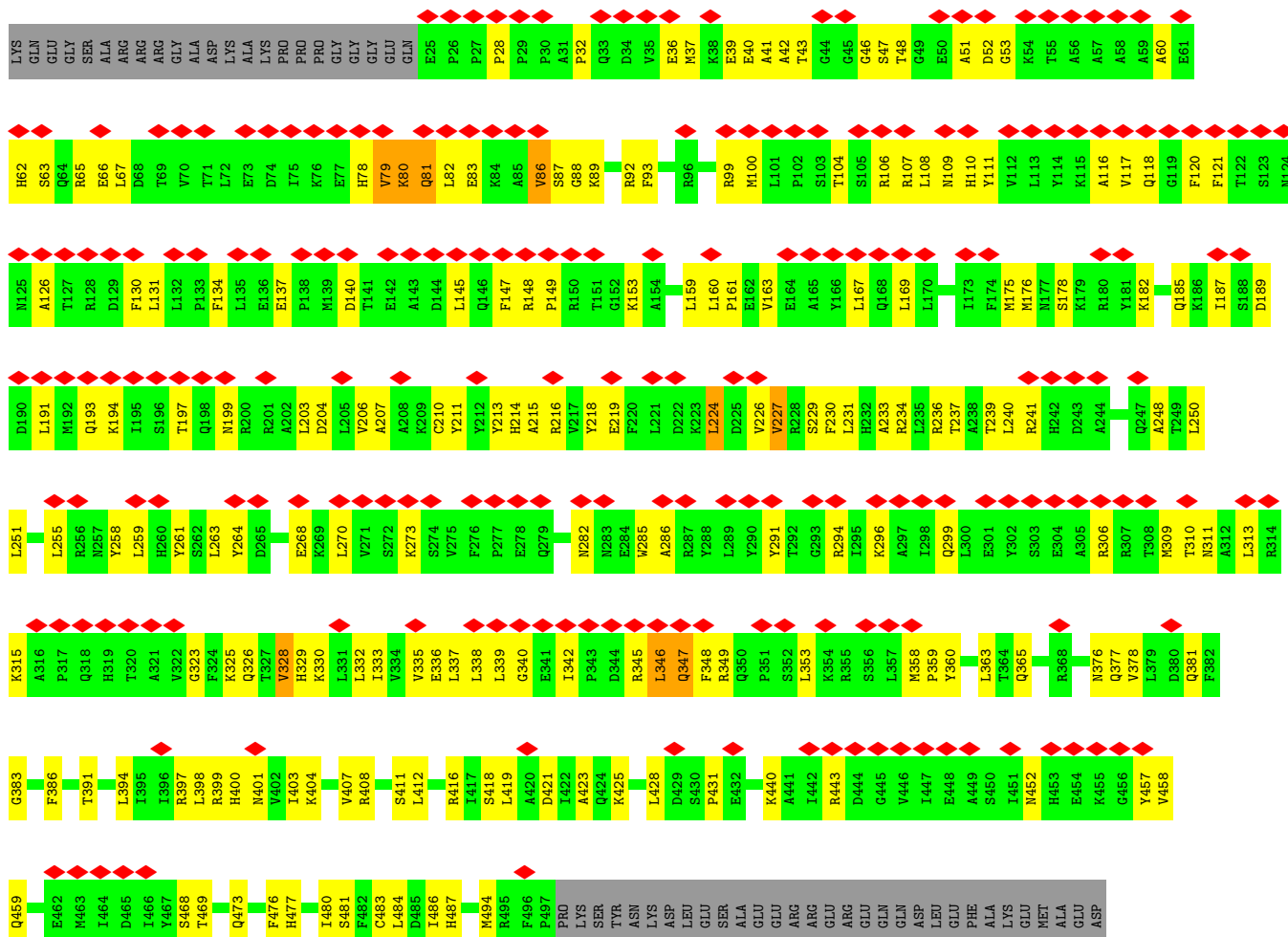




• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



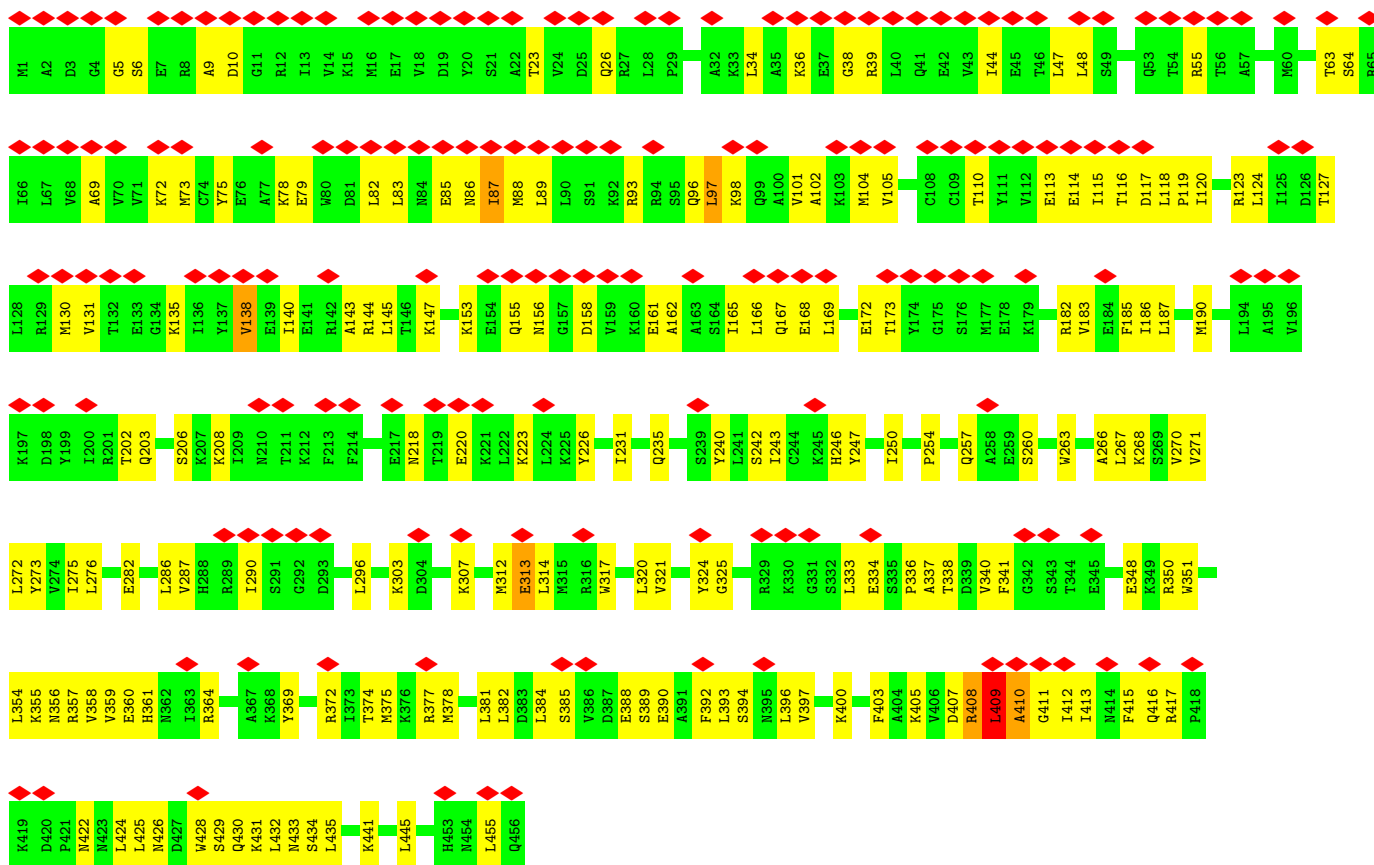
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 3



ASP
ASP
ASP
SER
PHE
PRO

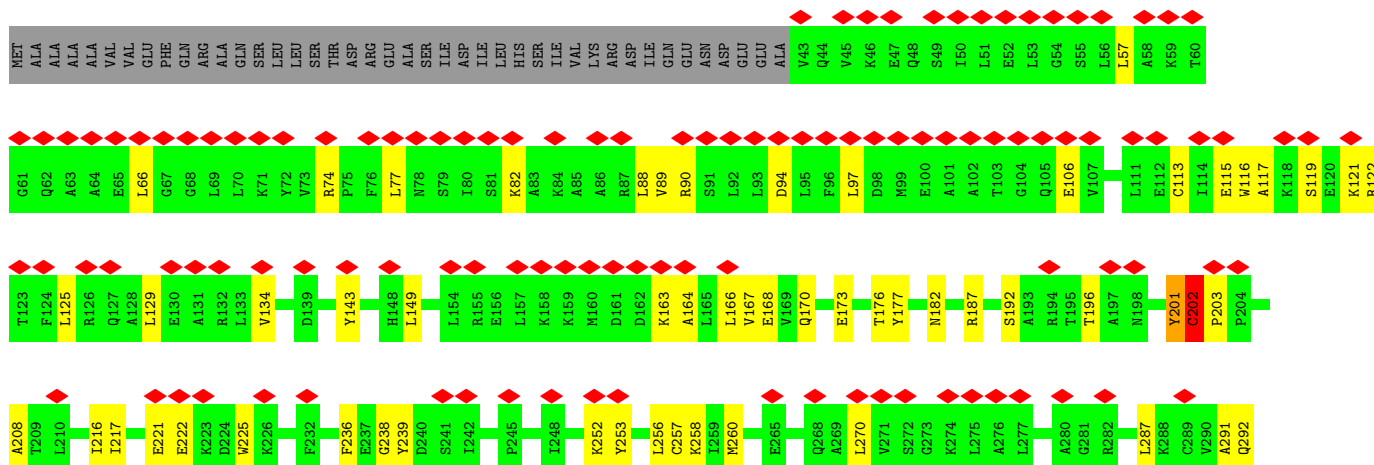
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

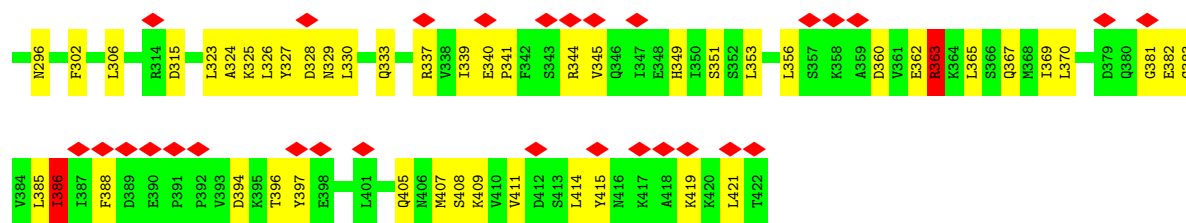
Chain W: 



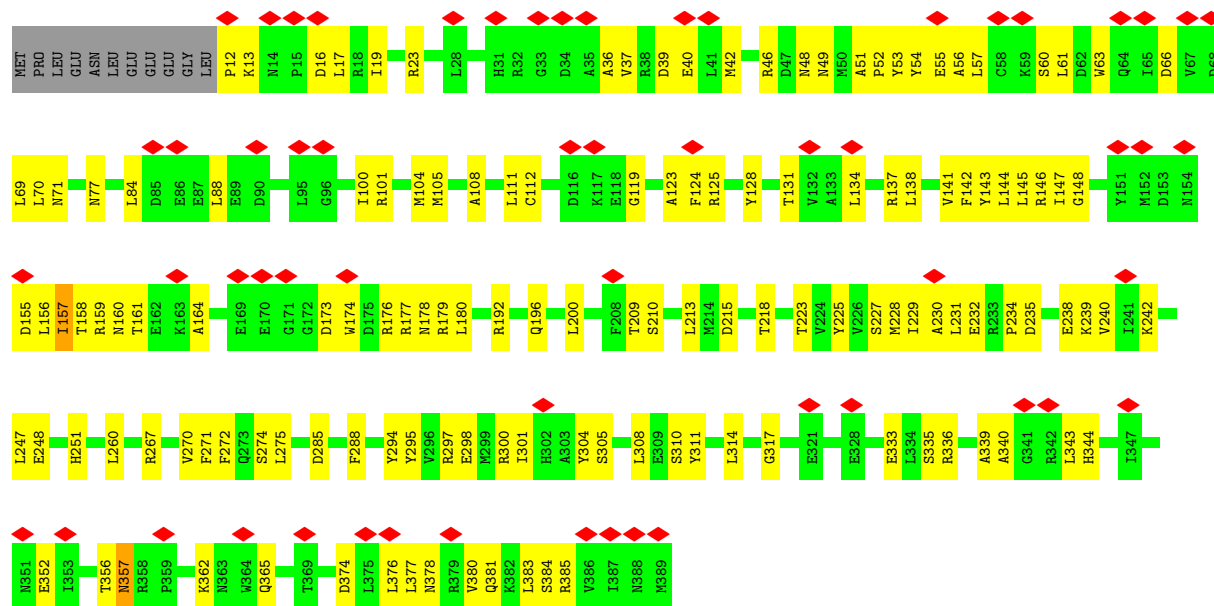
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 

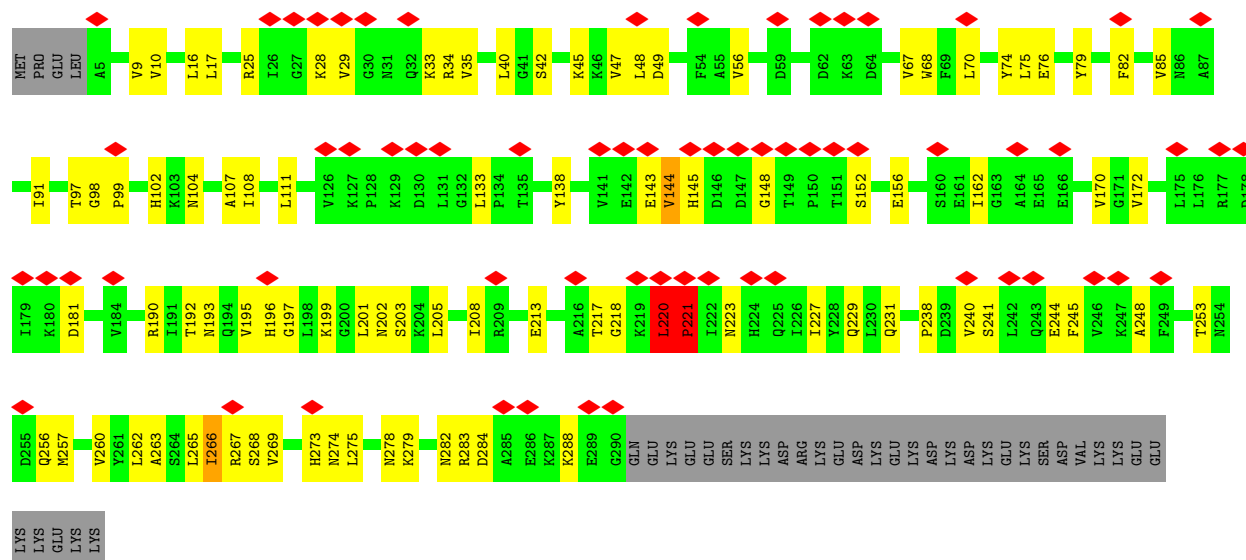




- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

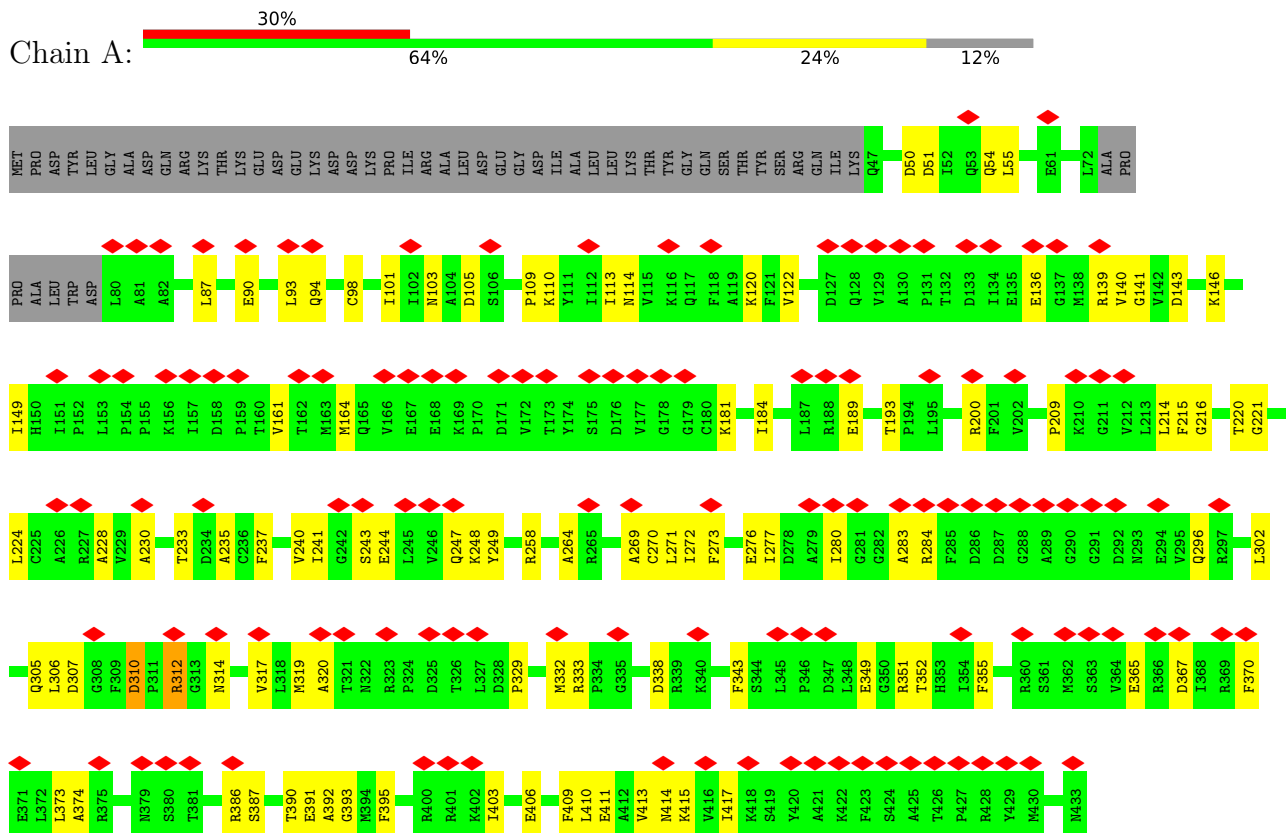


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7



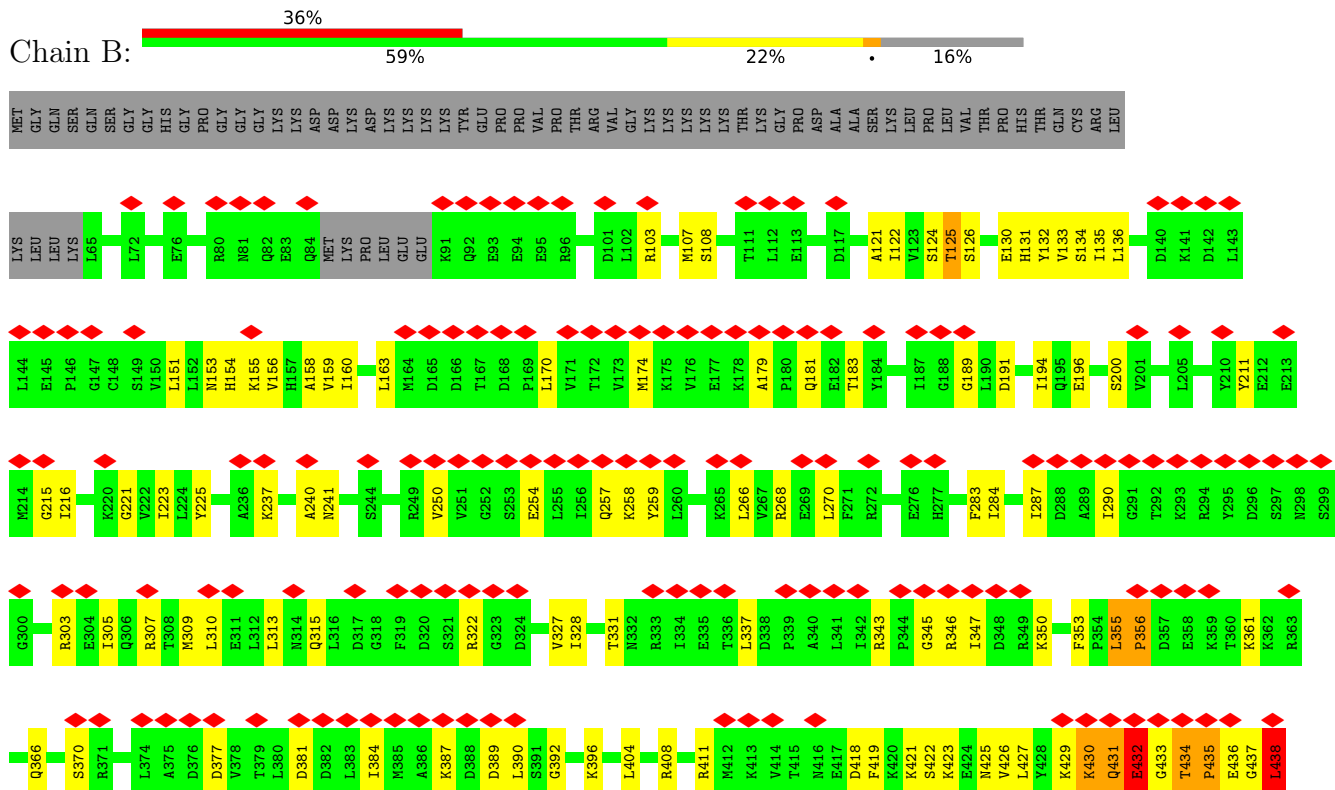
- Molecule 13: 26S protease regulatory subunit 7

Chain A:



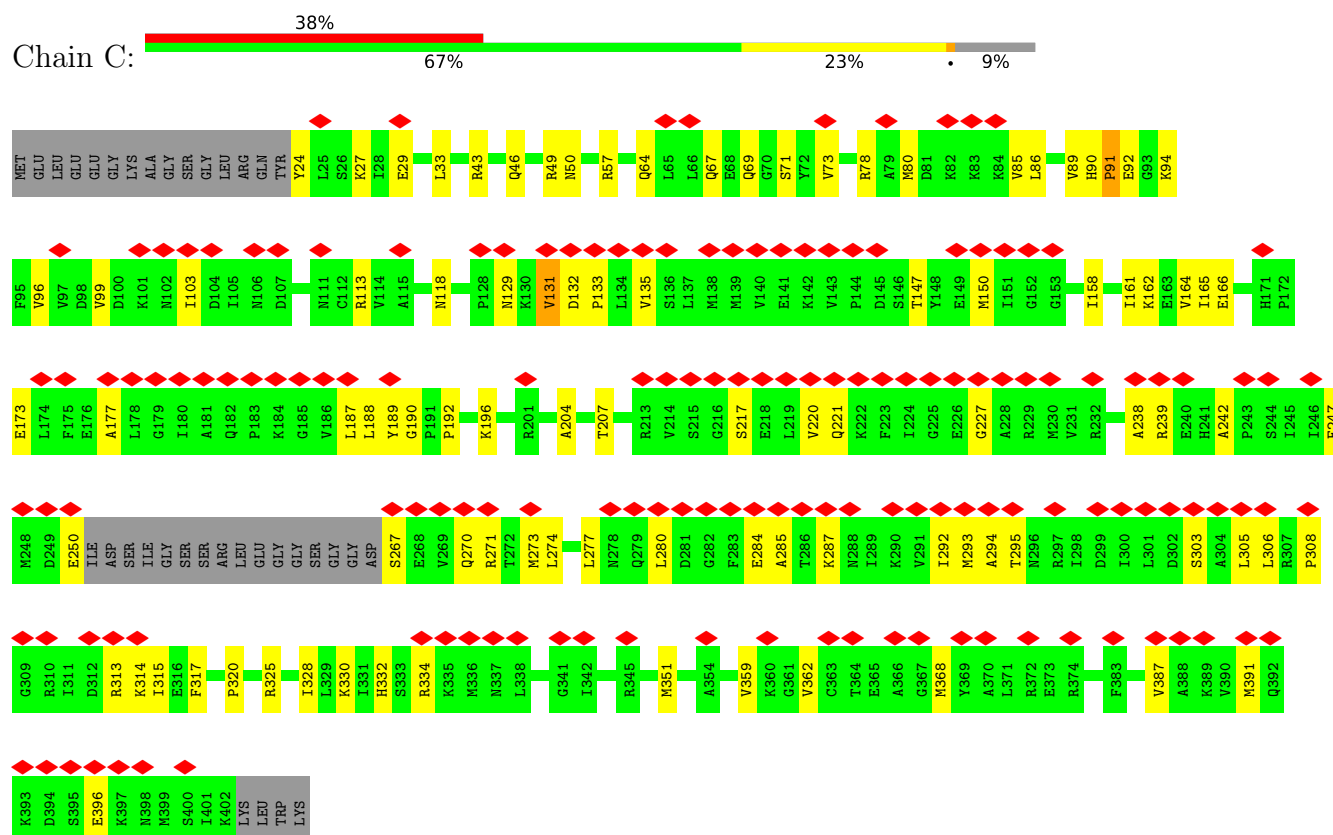
- Molecule 14: 26S protease regulatory subunit 4

Chain B:

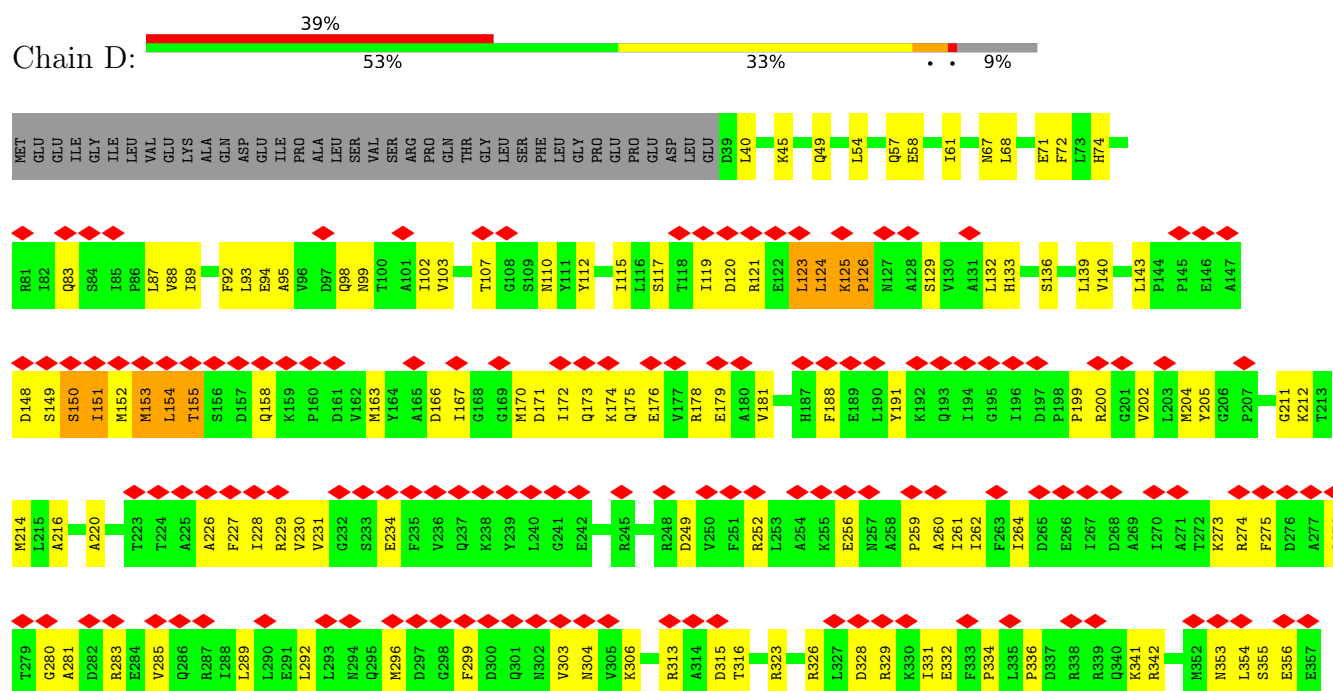


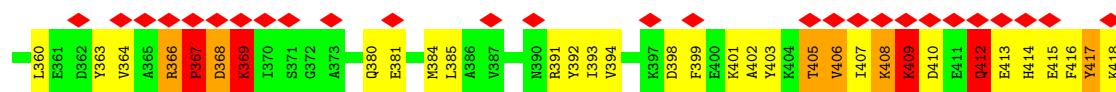


• Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8

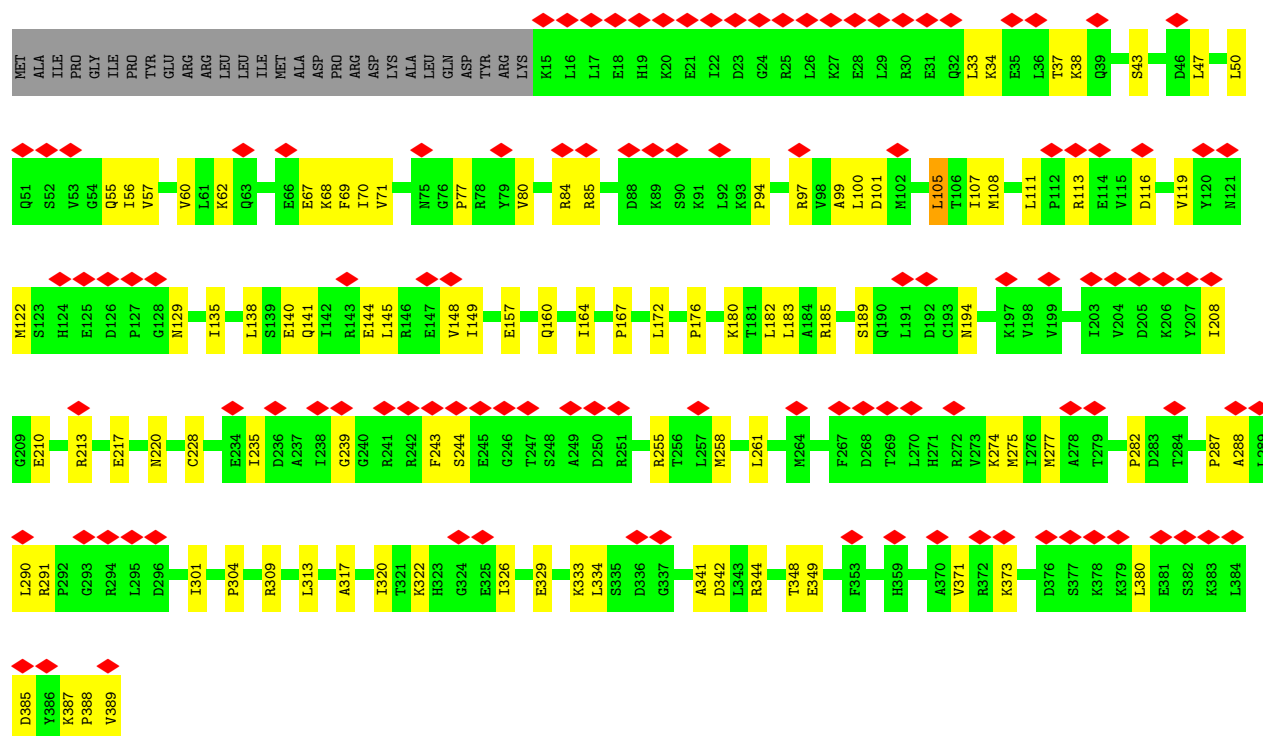


• Molecule 16: 26S protease regulatory subunit 6B

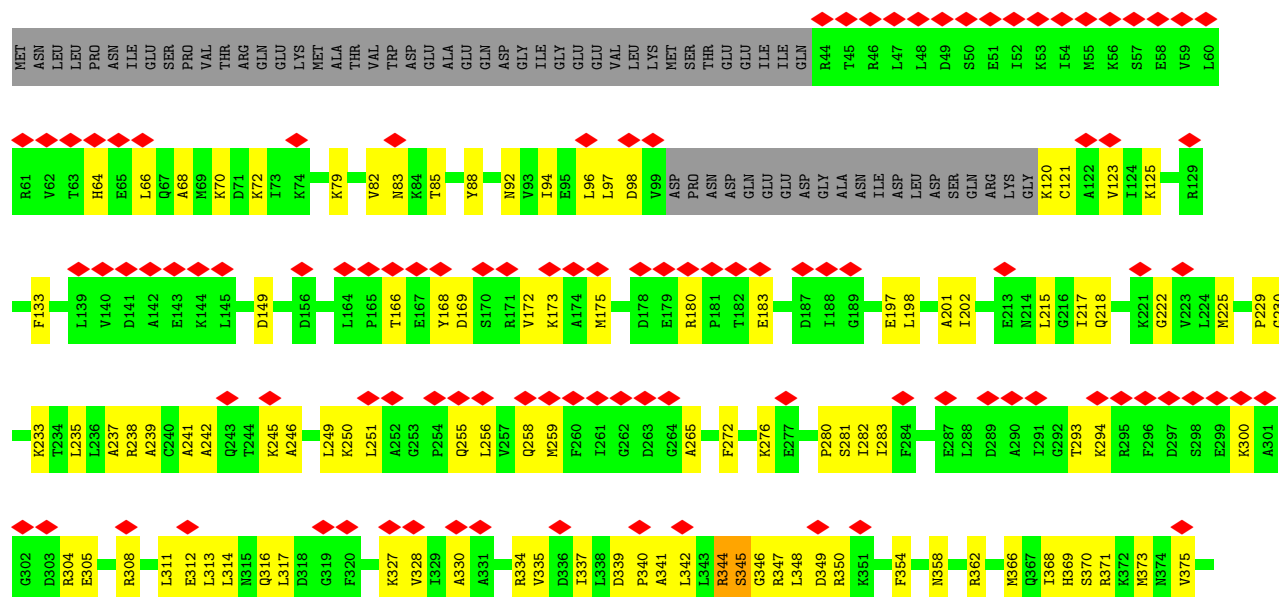


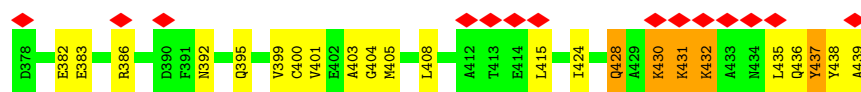


• Molecule 17: 26S proteasome regulatory subunit 10B

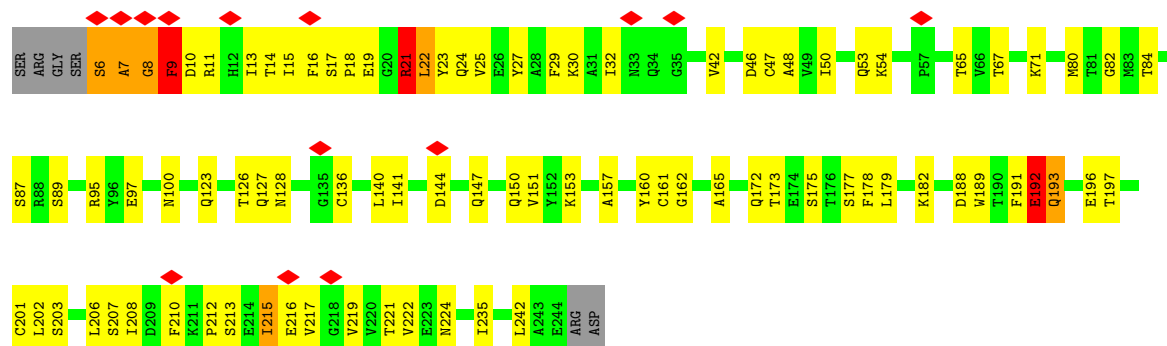


• Molecule 18: 26S protease regulatory subunit 6A

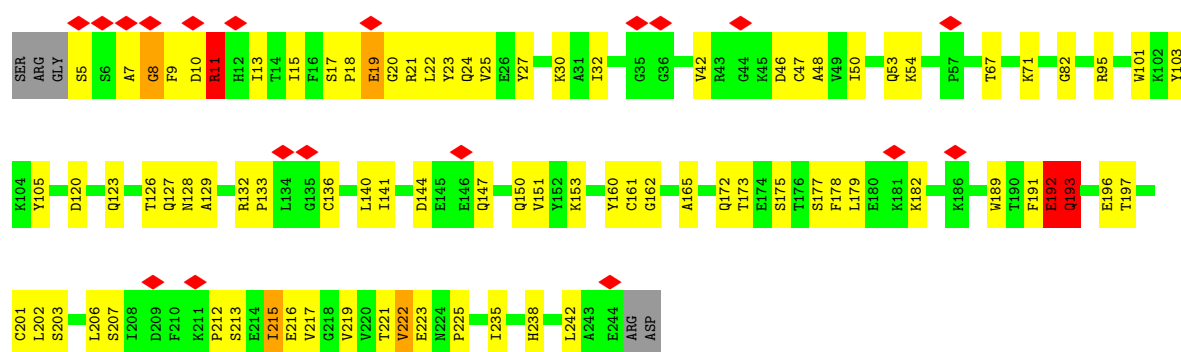




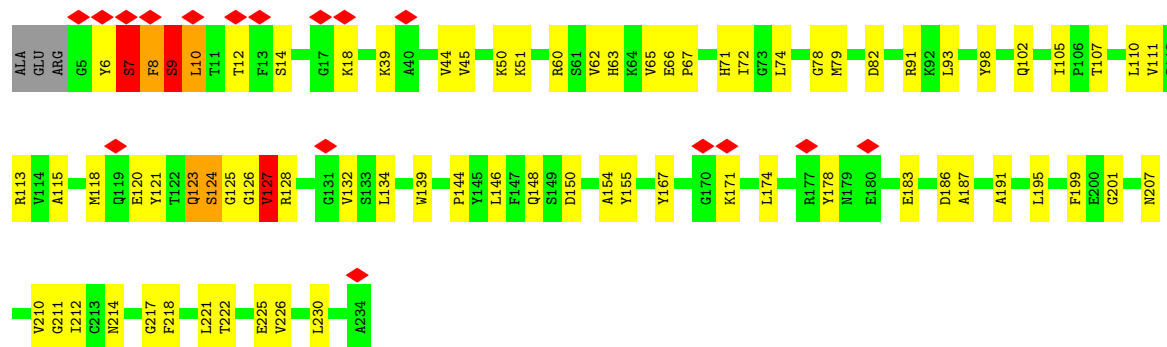
• Molecule 19: Proteasome subunit alpha type-6



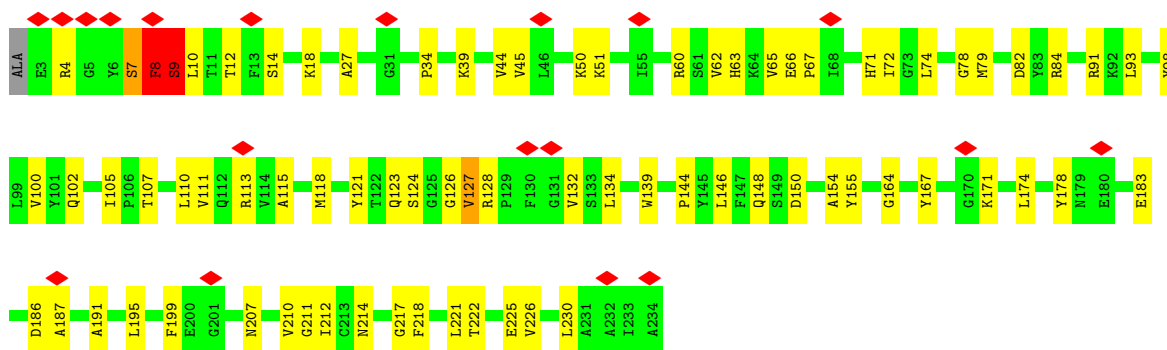
• Molecule 19: Proteasome subunit alpha type-6



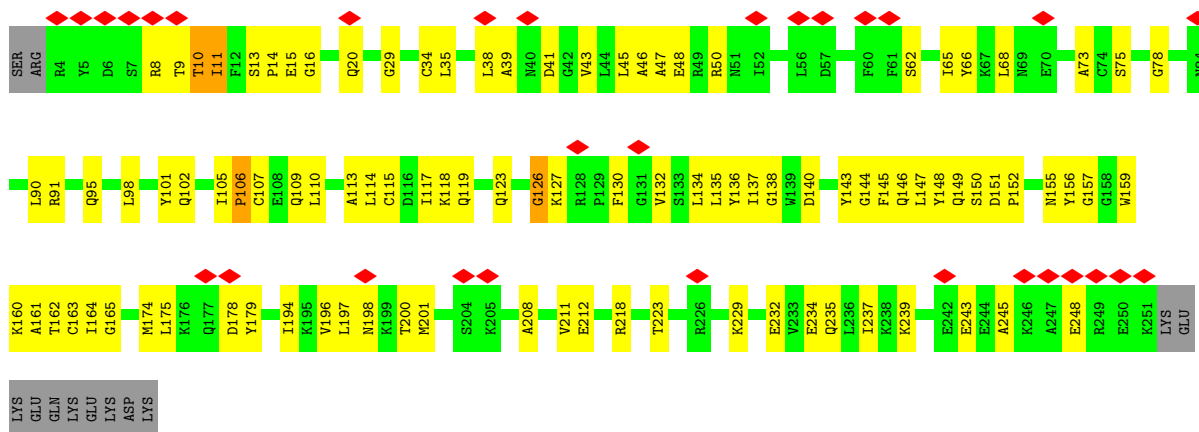
• Molecule 20: Proteasome subunit alpha type-2



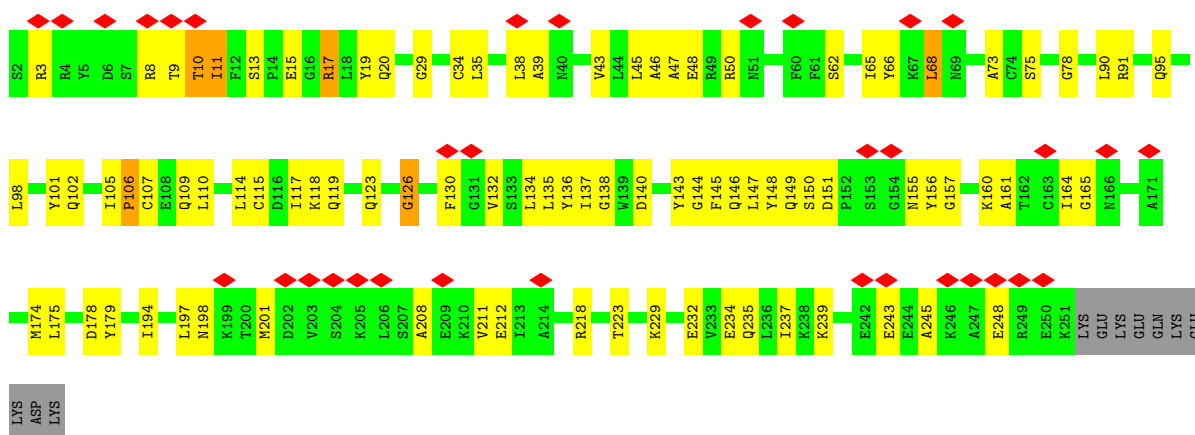
• Molecule 20: Proteasome subunit alpha type-2



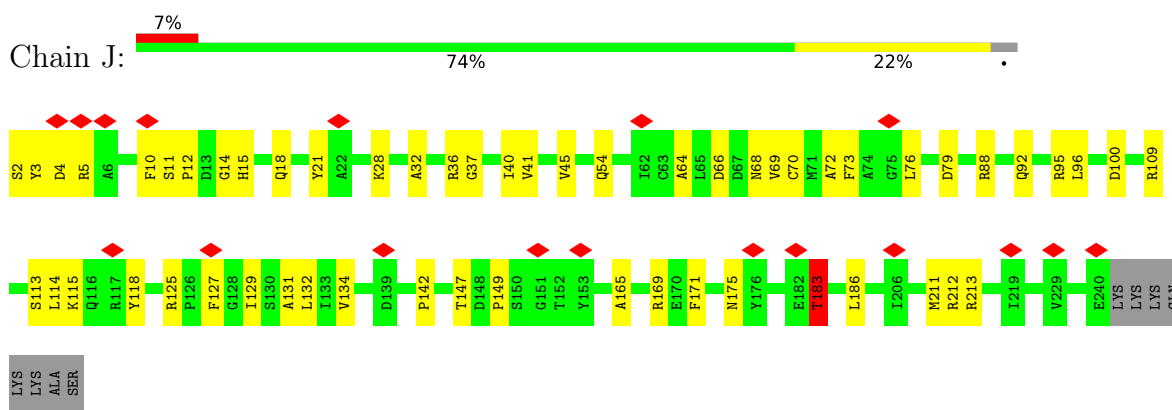
• Molecule 21: Proteasome subunit alpha type-4



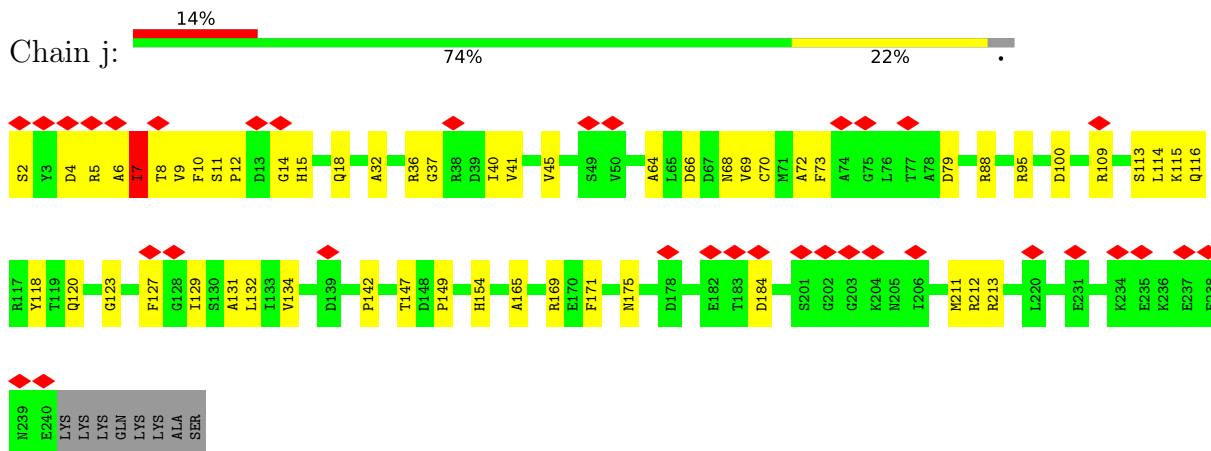
• Molecule 21: Proteasome subunit alpha type-4



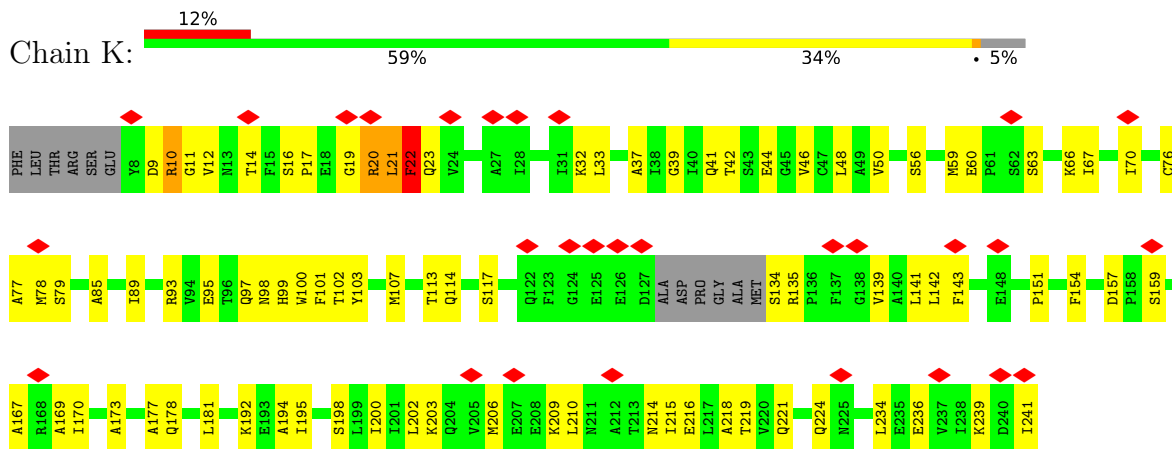
• Molecule 22: Proteasome subunit alpha type-7



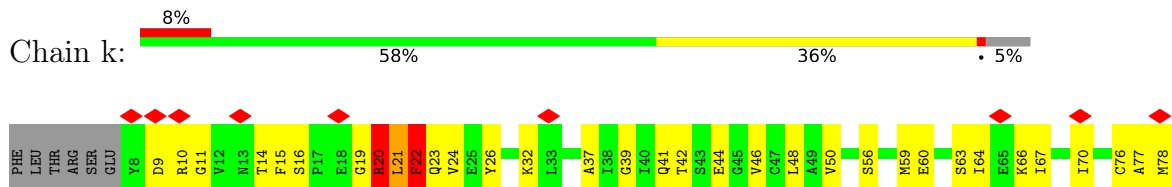
- Molecule 22: Proteasome subunit alpha type-7

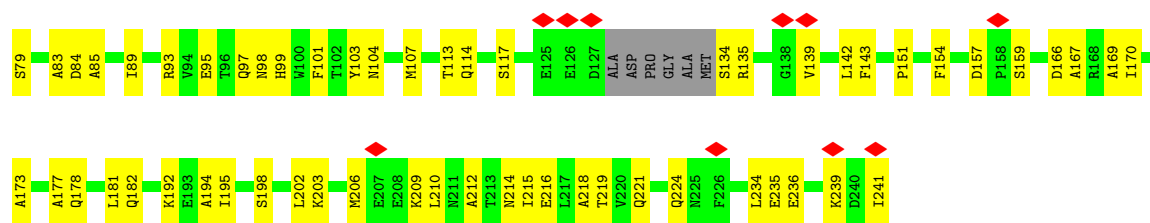


- Molecule 23: Proteasome subunit alpha type-5

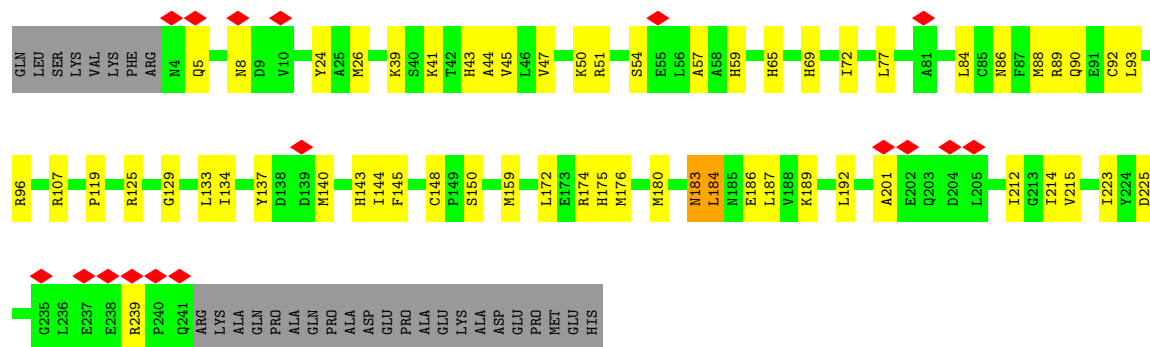


- Molecule 23: Proteasome subunit alpha type-5

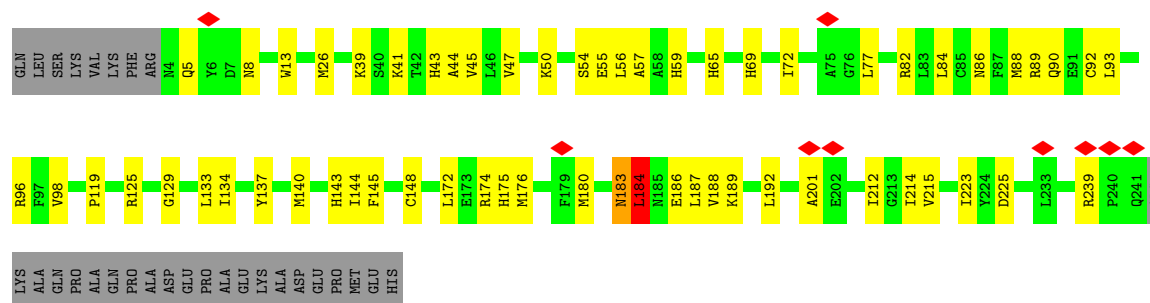




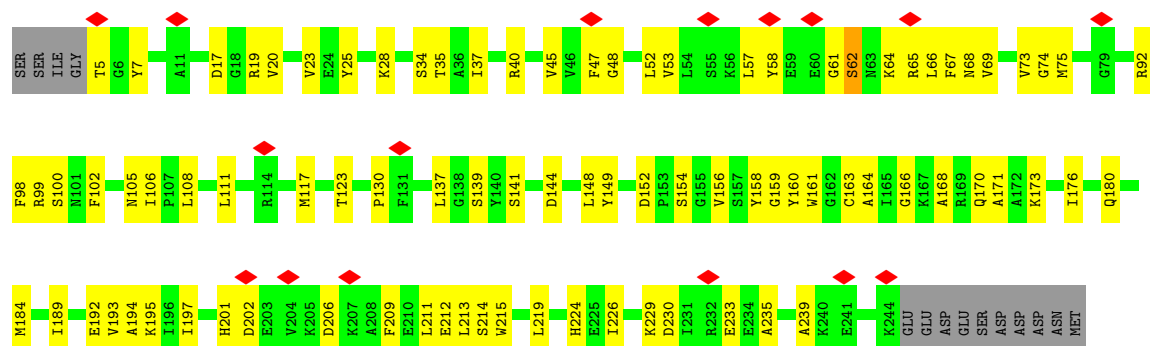
• Molecule 24: Isoform Long of Proteasome subunit alpha type-1



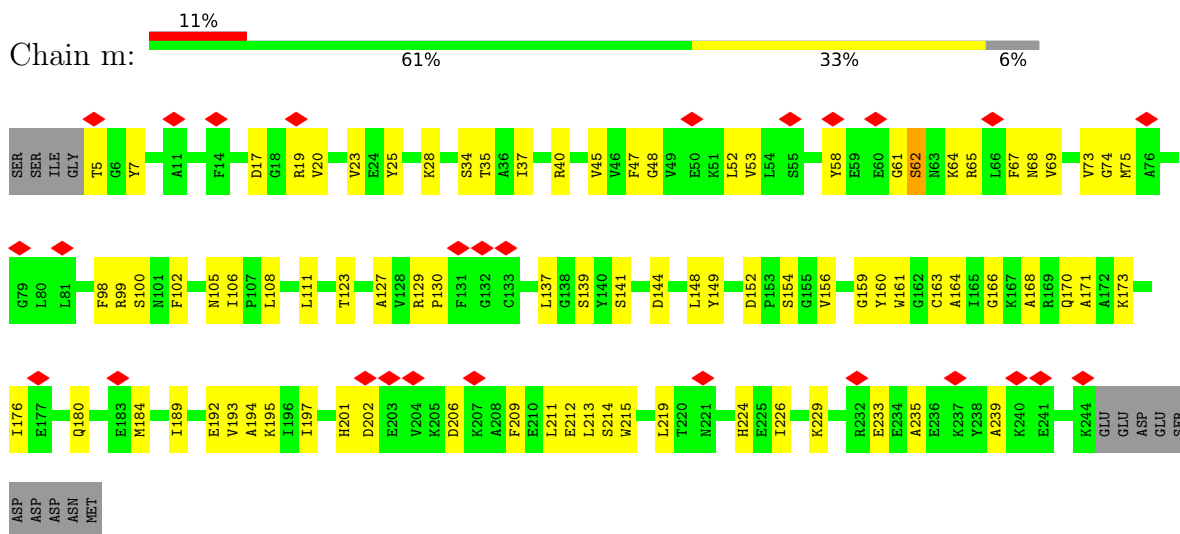
• Molecule 24: Isoform Long of Proteasome subunit alpha type-1



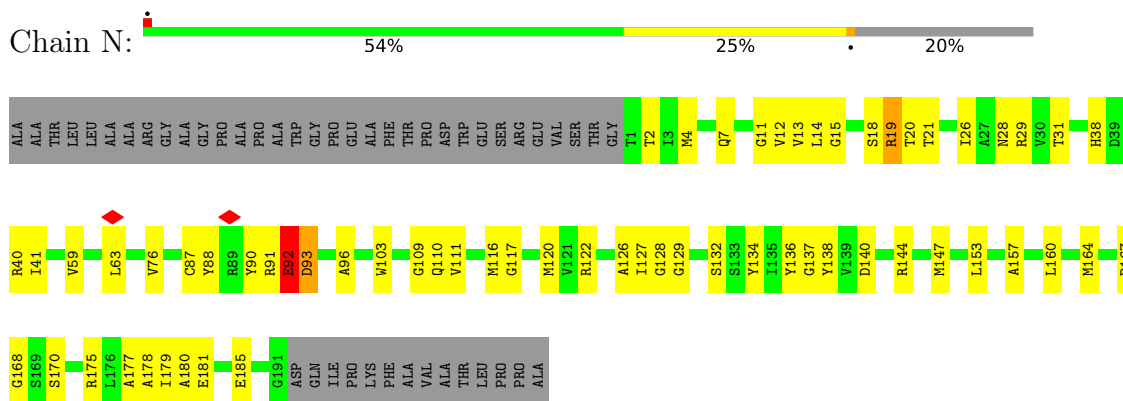
• Molecule 25: Proteasome subunit alpha type-3



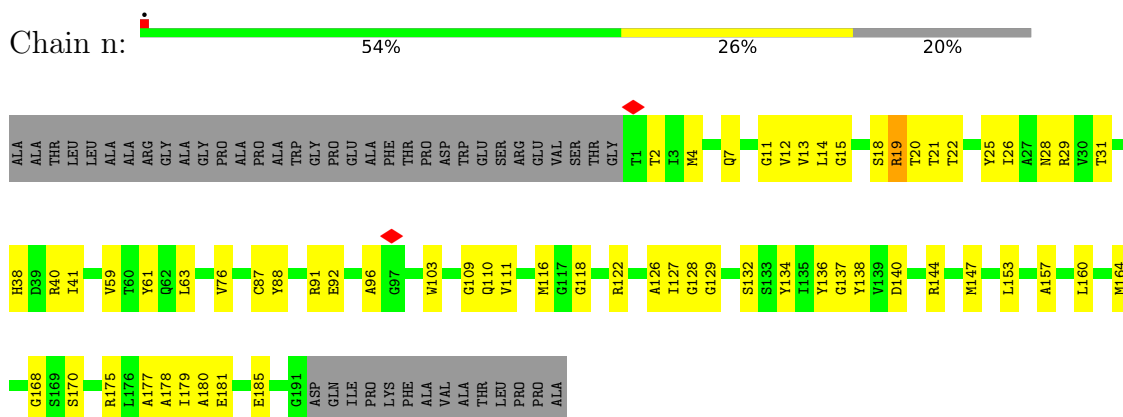
- Molecule 25: Proteasome subunit alpha type-3



- Molecule 26: Proteasome subunit beta type-6



- Molecule 26: Proteasome subunit beta type-6



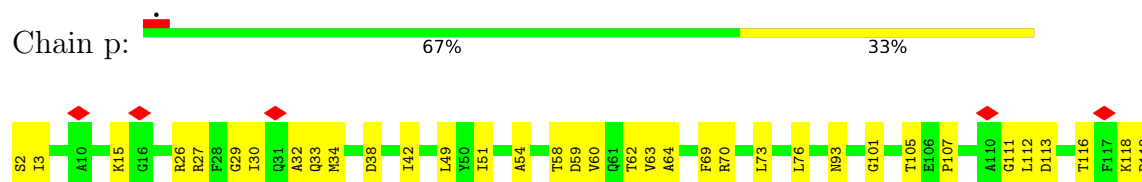
- Molecule 27: Proteasome subunit beta type-7

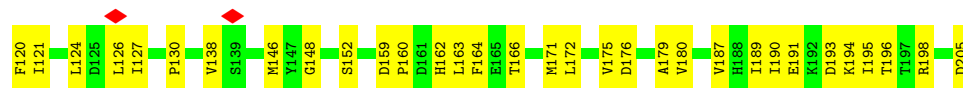


- Molecule 27: Proteasome subunit beta type-7

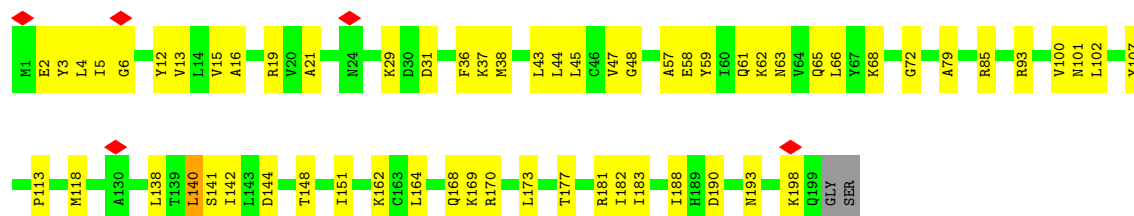
- Molecule 28: Proteasome subunit beta type-3

- Molecule 28: Proteasome subunit beta type-3

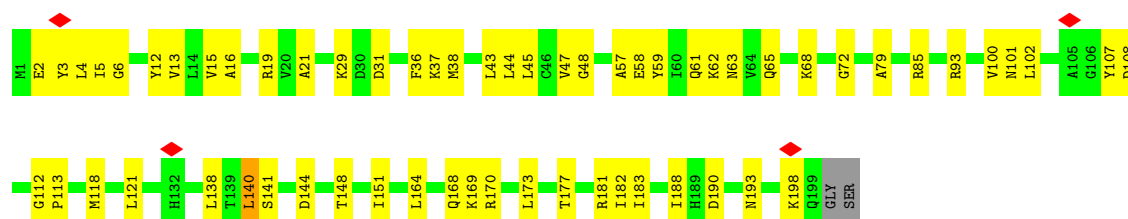




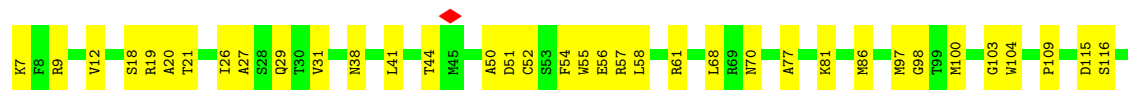
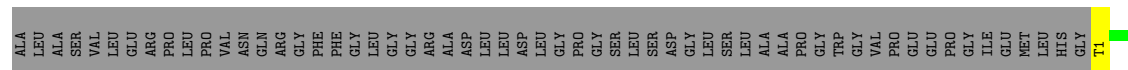
• Molecule 29: Proteasome subunit beta type-2



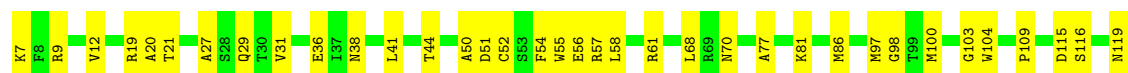
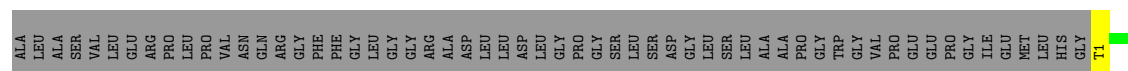
• Molecule 29: Proteasome subunit beta type-2

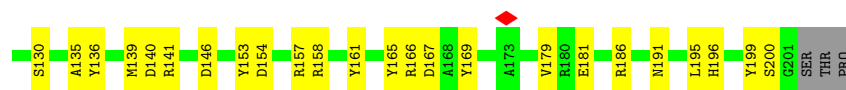


• Molecule 30: Proteasome subunit beta type-5

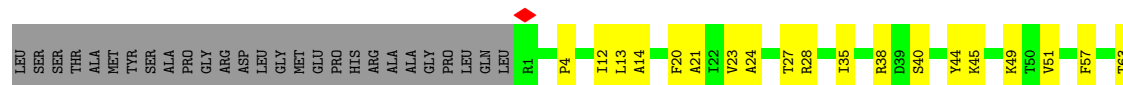


• Molecule 30: Proteasome subunit beta type-5

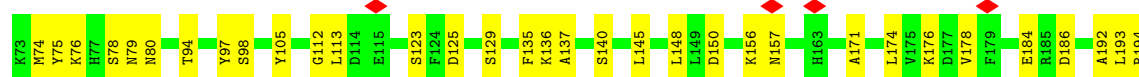
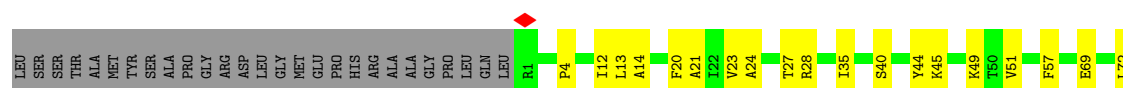




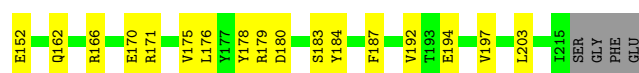
• Molecule 31: Proteasome subunit beta type-1



• Molecule 31: Proteasome subunit beta type-1

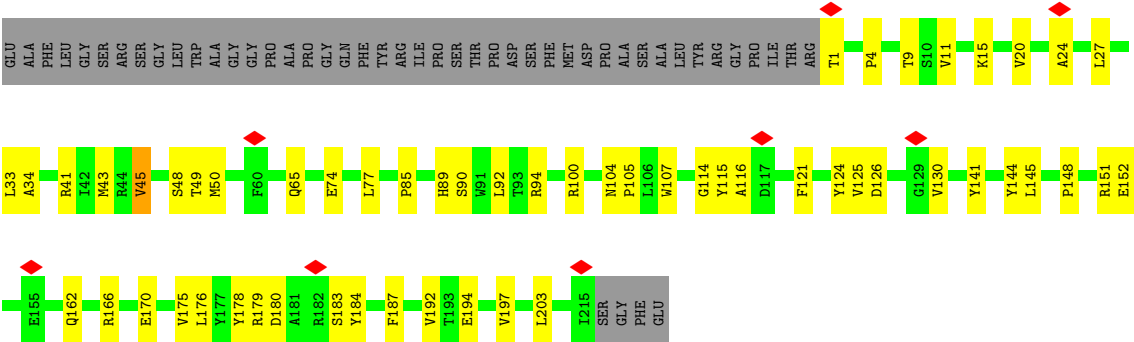


• Molecule 32: Proteasome subunit beta type-4



• Molecule 32: Proteasome subunit beta type-4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.26	0/3053	0.69	0/4133
2	b	0.26	0/1477	0.68	2/1999 (0.1%)
3	c	0.27	0/2225	0.71	0/3005
4	d	0.29	0/2161	0.79	6/2917 (0.2%)
5	e	0.34	0/337	0.94	1/448 (0.2%)
6	f	0.29	0/5392	0.76	7/7269 (0.1%)
7	U	0.27	1/6395 (0.0%)	0.66	5/8645 (0.1%)
8	V	0.30	0/3882	0.76	6/5245 (0.1%)
9	W	0.27	0/3750	0.74	5/5040 (0.1%)
10	X	0.26	0/3052	0.69	4/4113 (0.1%)
11	Y	0.28	0/3171	0.70	0/4269
12	Z	0.30	0/2323	0.80	8/3148 (0.3%)
13	A	0.24	0/2938	0.63	3/3968 (0.1%)
14	B	0.23	0/2843	0.75	6/3844 (0.2%)
15	C	0.25	0/2895	0.65	1/3893 (0.0%)
16	D	0.28	0/3089	0.79	8/4166 (0.2%)
17	E	0.24	0/2903	0.58	0/3922
18	F	0.24	0/2896	0.59	0/3910
19	G	0.29	0/1853	0.64	4/2515 (0.2%)
19	g	0.25	0/1859	0.65	3/2523 (0.1%)
20	H	0.25	0/1723	0.63	4/2346 (0.2%)
20	h	0.25	0/1743	0.62	4/2372 (0.2%)
21	I	0.25	0/1925	0.69	6/2606 (0.2%)
21	i	0.25	0/1942	0.64	4/2628 (0.2%)
22	J	0.25	0/1728	0.60	1/2358 (0.0%)
22	j	0.24	0/1728	0.57	1/2358 (0.0%)
23	K	0.26	0/1755	0.62	1/2375 (0.0%)
23	k	0.25	0/1747	0.62	2/2364 (0.1%)
24	L	0.25	0/1885	0.59	2/2552 (0.1%)
24	l	0.25	0/1885	0.59	2/2552 (0.1%)
25	M	0.25	0/1891	0.61	2/2552 (0.1%)
25	m	0.25	0/1891	0.61	2/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.24	0/1454	0.60	0/1967
26	n	0.25	0/1454	0.58	0/1967
27	O	0.23	0/1670	0.57	1/2265 (0.0%)
27	o	0.23	0/1670	0.57	1/2265 (0.0%)
28	P	0.24	0/1614	0.50	0/2177
28	p	0.24	0/1614	0.50	0/2177
29	Q	0.27	0/1603	0.59	0/2174
29	q	0.27	0/1603	0.59	0/2174
30	R	0.25	0/1579	0.49	0/2134
30	r	0.25	0/1579	0.49	0/2134
31	S	0.24	0/1671	0.54	0/2253
31	s	0.24	0/1671	0.54	0/2253
32	T	0.25	0/1700	0.53	1/2305 (0.0%)
32	t	0.25	0/1700	0.53	1/2305 (0.0%)
All	All	0.26	1/102919 (0.0%)	0.65	104/139137 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	773	PHE	C-N	5.87	1.39	1.34

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	434	THR	CA-C-N	14.60	138.09	119.84
14	B	434	THR	C-N-CA	14.60	138.09	119.84
16	D	366	ARG	CA-C-N	14.30	137.72	119.84
16	D	366	ARG	C-N-CA	14.30	137.72	119.84
12	Z	220	LEU	CA-C-N	9.39	131.58	119.84
12	Z	220	LEU	C-N-CA	9.39	131.58	119.84
10	X	202	CYS	CA-C-N	-8.92	111.19	120.38
10	X	202	CYS	C-N-CA	-8.92	111.19	120.38
14	B	355	LEU	CA-C-N	8.71	130.72	119.84
14	B	355	LEU	C-N-CA	8.71	130.72	119.84
16	D	409	LYS	N-CA-C	8.45	128.79	110.80
20	H	8	PHE	N-CA-C	-8.44	92.82	110.80
13	A	310	ASP	CA-C-N	8.37	130.31	119.84
13	A	310	ASP	C-N-CA	8.37	130.31	119.84
21	I	13	SER	CA-C-N	8.33	130.25	119.84
21	I	13	SER	C-N-CA	8.33	130.25	119.84
6	f	573	ILE	N-CA-C	-8.29	104.50	112.29
20	h	8	PHE	N-CA-C	-8.28	93.16	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	363	ARG	N-CA-C	-8.02	93.71	110.80
13	A	312	ARG	N-CA-C	7.96	121.94	111.75
22	J	183	THR	N-CA-C	-7.89	94.00	110.80
12	Z	221	PRO	N-CA-C	-7.58	96.84	112.47
7	U	364	VAL	N-CA-C	-7.43	105.48	112.83
12	Z	143	GLU	N-CA-C	-7.35	101.50	111.87
19	G	192	GLU	N-CA-C	-7.20	102.45	112.45
2	b	22	LEU	CA-C-N	7.03	128.63	119.84
2	b	22	LEU	C-N-CA	7.03	128.63	119.84
20	h	9	SER	CA-C-N	6.93	134.78	121.54
20	h	9	SER	C-N-CA	6.93	134.78	121.54
23	K	22	PHE	N-CA-C	-6.91	104.84	113.20
23	k	22	PHE	N-CA-C	-6.83	104.94	113.20
19	g	192	GLU	N-CA-C	-6.77	103.36	111.69
20	H	9	SER	CA-C-N	6.73	134.39	121.54
20	H	9	SER	C-N-CA	6.73	134.39	121.54
23	k	20	ARG	N-CA-C	6.30	117.60	108.34
9	W	313	GLU	CA-C-N	6.29	133.55	121.54
9	W	313	GLU	C-N-CA	6.29	133.55	121.54
14	B	355	LEU	N-CA-C	-6.25	96.33	108.59
14	B	156	VAL	N-CA-C	-6.11	107.03	112.90
24	l	184	LEU	N-CA-C	6.02	118.80	111.82
6	f	87	THR	N-CA-C	5.96	117.46	108.46
24	L	184	LEU	N-CA-C	5.95	118.72	111.82
21	I	68	LEU	CA-C-N	-5.91	114.45	121.90
21	I	68	LEU	C-N-CA	-5.91	114.45	121.90
19	G	6	SER	CA-C-N	5.91	132.82	121.54
19	G	6	SER	C-N-CA	5.91	132.82	121.54
16	D	367	PRO	N-CA-C	5.88	124.59	112.47
21	i	68	LEU	CA-C-N	-5.86	114.51	121.90
21	i	68	LEU	C-N-CA	-5.86	114.51	121.90
24	L	183	ASN	N-CA-C	5.85	118.55	109.60
6	f	324	VAL	CA-C-N	5.78	132.59	121.54
6	f	324	VAL	C-N-CA	5.78	132.59	121.54
12	Z	241	SER	CA-C-N	5.77	132.55	121.54
12	Z	241	SER	C-N-CA	5.77	132.55	121.54
19	g	8	GLY	N-CA-C	5.76	126.84	113.18
24	l	183	ASN	N-CA-C	5.74	118.38	109.60
4	d	200	PHE	CA-C-N	5.70	132.42	121.54
4	d	200	PHE	C-N-CA	5.70	132.42	121.54
10	X	386	ILE	N-CA-C	5.62	121.02	109.34
20	H	7	SER	N-CA-C	5.55	122.62	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	9	PHE	CA-C-O	-5.53	112.61	120.51
5	e	6	GLN	N-CA-C	5.51	122.00	109.81
7	U	223	LEU	CA-C-N	5.51	130.23	122.46
7	U	223	LEU	C-N-CA	5.51	130.23	122.46
4	d	33	LEU	CA-C-N	5.49	132.03	121.54
4	d	33	LEU	C-N-CA	5.49	132.03	121.54
4	d	236	THR	CA-C-N	5.49	124.72	120.33
4	d	236	THR	C-N-CA	5.49	124.72	120.33
21	I	106	PRO	CA-C-N	5.48	132.01	121.54
21	I	106	PRO	C-N-CA	5.48	132.01	121.54
21	i	106	PRO	CA-C-N	5.46	131.97	121.54
21	i	106	PRO	C-N-CA	5.46	131.97	121.54
9	W	97	LEU	N-CA-C	-5.42	108.45	114.62
19	g	193	GLN	N-CA-C	-5.41	105.28	111.07
9	W	87	ILE	CA-C-N	5.34	131.74	121.54
9	W	87	ILE	C-N-CA	5.34	131.74	121.54
8	V	79	VAL	N-CA-C	-5.31	105.20	110.62
8	V	323	GLY	CA-C-N	5.27	131.61	121.54
8	V	323	GLY	C-N-CA	5.27	131.61	121.54
20	h	7	SER	N-CA-C	5.24	121.95	110.80
6	f	460	ASP	N-CA-C	5.22	121.36	109.81
22	j	7	ILE	N-CA-C	-5.20	106.24	113.00
7	U	559	ARG	CA-C-N	5.19	131.45	121.54
7	U	559	ARG	C-N-CA	5.19	131.45	121.54
32	t	45	VAL	N-CA-C	-5.17	104.42	110.05
12	Z	256	GLN	CA-C-N	5.15	127.45	120.65
12	Z	256	GLN	C-N-CA	5.15	127.45	120.65
32	T	45	VAL	N-CA-C	-5.14	104.44	110.05
8	V	53	GLY	CA-C-N	5.14	127.89	120.38
8	V	53	GLY	C-N-CA	5.14	127.89	120.38
25	m	62	SER	CA-C-N	5.13	129.70	122.46
25	m	62	SER	C-N-CA	5.13	129.70	122.46
25	M	62	SER	CA-C-N	5.12	129.68	122.46
25	M	62	SER	C-N-CA	5.12	129.68	122.46
16	D	154	LEU	CA-C-N	5.10	131.29	121.54
16	D	154	LEU	C-N-CA	5.10	131.29	121.54
8	V	28	PRO	N-CA-C	5.10	116.92	110.70
15	C	396	GLU	CA-CB-CG	5.09	124.28	114.10
27	o	37	ILE	N-CA-C	-5.08	107.60	111.62
6	f	261	ARG	CA-C-N	5.08	126.11	120.06
6	f	261	ARG	C-N-CA	5.08	126.11	120.06
16	D	153	MET	CA-C-N	5.04	131.16	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	153	MET	C-N-CA	5.04	131.16	121.54
27	O	37	ILE	N-CA-C	-5.03	107.65	111.62

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	a	2995	0	3012	110	0
2	b	1457	0	1501	77	0
3	c	2186	0	2210	67	0
4	d	2115	0	2142	72	0
5	e	333	0	290	31	0
6	f	5318	0	5328	208	0
7	U	6286	0	6336	213	0
8	V	3807	0	3854	196	0
9	W	3702	0	3818	183	0
10	X	3008	0	3112	106	0
11	Y	3114	0	3117	108	0
12	Z	2280	0	2308	91	0
13	A	2892	0	2842	83	0
14	B	2805	0	2769	110	0
15	C	2858	0	2970	90	0
16	D	3039	0	3075	209	0
17	E	2859	0	2827	89	0
18	F	2858	0	2851	161	0
19	G	1820	0	1791	105	0
19	g	1826	0	1796	107	0
20	H	1688	0	1575	70	0
20	h	1708	0	1594	64	0
21	I	1895	0	1833	79	0
21	i	1912	0	1851	107	0
22	J	1704	0	1517	54	0
22	j	1704	0	1517	54	0
23	K	1729	0	1680	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	k	1722	0	1673	96	0
24	L	1850	0	1822	50	0
24	l	1850	0	1822	51	0
25	M	1856	0	1814	65	0
25	m	1856	0	1814	62	0
26	N	1430	0	1398	49	0
26	n	1430	0	1396	69	0
27	O	1643	0	1644	64	0
27	o	1643	0	1644	60	0
28	P	1585	0	1598	47	0
28	p	1585	0	1598	50	0
29	Q	1570	0	1547	46	0
29	q	1570	0	1547	41	0
30	R	1548	0	1499	43	0
30	r	1548	0	1499	45	0
31	S	1641	0	1618	51	0
31	s	1641	0	1618	47	0
32	T	1667	0	1628	45	0
32	t	1667	0	1628	42	0
33	c	1	0	0	0	0
34	A	31	0	12	4	0
34	D	31	0	12	2	0
34	E	31	0	12	6	0
34	F	31	0	12	2	0
All	All	101325	0	100371	3568	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 18.

All (3568) 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)
26:n:88:TYR:HA	26:n:91:ARG:CD	1.22	1.69
16:D:403:TYR:CD2	16:D:407:ILE:CD1	1.85	1.59
15:C:73:VAL:CG1	15:C:90:HIS:CE1	1.88	1.52
16:D:403:TYR:CG	16:D:407:ILE:HD11	1.02	1.52
16:D:403:TYR:CG	16:D:407:ILE:CD1	1.89	1.49
19:g:46:ASP:CB	19:g:222:VAL:HG21	1.39	1.47
19:g:46:ASP:CB	19:g:222:VAL:CG2	1.93	1.47
15:C:90:HIS:CD2	16:D:110:ASN:O	1.65	1.46
19:G:7:ALA:HA	19:G:11:ARG:NH2	1.31	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:176:PRO:CB	18:F:344:ARG:HD3	1.45	1.45
15:C:90:HIS:CE1	16:D:110:ASN:HB3	1.50	1.43
19:g:128:ASN:HA	20:h:127:VAL:CG1	1.29	1.42
19:g:128:ASN:CA	20:h:127:VAL:CG1	1.78	1.42
18:F:341:ALA:HB1	18:F:344:ARG:NH2	1.22	1.41
9:W:408:ARG:CG	10:X:349:HIS:HE1	1.31	1.41
14:B:387:LYS:CE	14:B:431:GLN:HG3	1.48	1.41
22:j:6:ALA:CB	22:j:9:VAL:CG2	1.99	1.41
15:C:73:VAL:HG13	15:C:90:HIS:CE1	1.49	1.40
16:D:121:ARG:O	16:D:124:LEU:CD2	1.66	1.40
14:B:427:LEU:O	14:B:431:GLN:CB	1.70	1.39
22:J:4:ASP:OD2	22:J:21:TYR:CE2	1.76	1.38
22:j:6:ALA:CB	22:j:9:VAL:HG22	1.52	1.38
17:E:176:PRO:HB2	18:F:344:ARG:CD	1.53	1.37
22:J:4:ASP:OD2	22:J:21:TYR:CZ	1.78	1.36
16:D:403:TYR:CD2	16:D:407:ILE:HD11	1.52	1.35
2:b:22:LEU:CD1	2:b:179:LEU:HA	1.56	1.35
12:Z:220:LEU:CG	12:Z:221:PRO:HD3	1.56	1.35
15:C:90:HIS:ND1	16:D:110:ASN:HB3	1.06	1.34
21:i:13:SER:CB	21:i:17:ARG:HG3	1.56	1.34
12:Z:220:LEU:CB	12:Z:221:PRO:HD3	1.47	1.33
18:F:341:ALA:CB	18:F:344:ARG:HH21	1.42	1.33
9:W:408:ARG:HG3	10:X:349:HIS:CE1	1.64	1.33
21:i:13:SER:CB	21:i:17:ARG:NH1	1.90	1.33
14:B:387:LYS:HE3	14:B:431:GLN:CG	1.59	1.32
26:n:88:TYR:CA	26:n:91:ARG:HD3	1.58	1.31
5:e:43:TRP:NE1	8:V:349:ARG:HA	1.45	1.31
12:Z:220:LEU:HG	12:Z:221:PRO:CD	1.60	1.31
26:n:91:ARG:NH1	26:n:118:GLY:HA3	1.37	1.31
22:j:6:ALA:HB1	22:j:9:VAL:CG2	1.55	1.30
19:g:10:ASP:CB	25:m:7:TYR:OH	1.79	1.30
27:O:201:ARG:NH1	27:O:203:ARG:NH2	1.79	1.30
20:H:121:TYR:HA	20:H:124:SER:OG	1.12	1.29
2:b:22:LEU:HD11	2:b:179:LEU:CA	1.60	1.29
18:F:344:ARG:NH1	18:F:347:ARG:CZ	1.95	1.29
6:f:88:SER:CB	6:f:92:VAL:HG23	1.63	1.28
9:W:409:LEU:HD23	10:X:381:GLY:O	1.13	1.28
20:H:121:TYR:CA	20:H:124:SER:OG	1.82	1.28
18:F:341:ALA:CB	18:F:344:ARG:NH2	1.96	1.28
8:V:329:HIS:CD2	8:V:346:LEU:HD21	1.66	1.27
15:C:90:HIS:NE2	16:D:110:ASN:O	1.64	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:437:TYR:CD2	23:K:20:ARG:HD2	1.66	1.27
7:U:561:GLU:OE2	7:U:562:GLU:HG2	1.28	1.27
26:n:87:CYS:O	26:n:91:ARG:CG	1.84	1.26
5:e:43:TRP:CD1	8:V:349:ARG:CA	2.17	1.25
19:G:10:ASP:CB	25:M:7:TYR:OH	1.84	1.25
34:E:401:ATP:O1G	18:F:344:ARG:CZ	1.83	1.25
19:g:128:ASN:CA	20:h:127:VAL:HG13	1.48	1.25
5:e:43:TRP:CD1	8:V:349:ARG:HA	1.71	1.24
16:D:403:TYR:CB	16:D:407:ILE:HD11	1.66	1.24
15:C:90:HIS:ND1	16:D:110:ASN:CB	2.01	1.24
19:G:203:SER:O	19:G:207:SER:HA	1.32	1.24
14:B:387:LYS:NZ	14:B:431:GLN:HG3	1.54	1.23
19:g:203:SER:O	19:g:207:SER:HA	1.32	1.22
9:W:408:ARG:CD	10:X:349:HIS:CE1	2.21	1.22
19:G:10:ASP:CG	25:M:7:TYR:OH	1.82	1.21
8:V:333:ILE:HD13	8:V:345:ARG:NE	1.54	1.21
19:G:10:ASP:HB3	25:M:7:TYR:OH	1.36	1.20
21:i:13:SER:CB	21:i:17:ARG:CG	2.19	1.20
24:l:183:ASN:OD1	24:l:186:GLU:OE1	1.55	1.20
16:D:121:ARG:C	16:D:124:LEU:CD2	2.15	1.19
26:n:91:ARG:NH1	26:n:118:GLY:CA	2.03	1.19
16:D:120:ASP:O	16:D:123:LEU:HG	1.39	1.19
22:J:4:ASP:OD2	22:J:21:TYR:OH	1.59	1.18
12:Z:220:LEU:HG	12:Z:221:PRO:HD2	1.18	1.18
27:O:201:ARG:HH12	27:O:203:ARG:NH2	1.38	1.18
14:B:427:LEU:O	14:B:431:GLN:HB2	1.02	1.17
15:C:90:HIS:CE1	16:D:110:ASN:CB	2.25	1.17
21:i:13:SER:CB	21:i:17:ARG:CZ	2.21	1.17
5:e:43:TRP:CD1	8:V:349:ARG:N	2.12	1.17
21:i:8:ARG:O	21:i:11:ILE:HD11	1.43	1.17
18:F:344:ARG:NH1	18:F:347:ARG:NH2	1.92	1.17
19:G:189:TRP:HA	19:G:193:GLN:HG2	1.27	1.16
20:h:9:SER:OG	20:h:123:GLN:O	1.60	1.16
9:W:408:ARG:CG	10:X:349:HIS:CE1	2.20	1.15
16:D:403:TYR:CE2	16:D:407:ILE:HD13	1.80	1.15
26:n:87:CYS:O	26:n:91:ARG:CB	1.93	1.15
14:B:437:GLY:O	14:B:440:LEU:CD1	1.94	1.15
16:D:403:TYR:CD2	16:D:407:ILE:HD13	1.60	1.15
12:Z:220:LEU:CG	12:Z:221:PRO:CD	2.21	1.15
24:L:43:HIS:CG	24:L:184:LEU:HD11	1.81	1.15
21:I:8:ARG:O	21:I:11:ILE:HD11	1.45	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:6:ALA:HB2	22:j:9:VAL:CG2	1.71	1.14
9:W:455:LEU:HD11	12:Z:220:LEU:CD1	1.76	1.13
19:G:22:LEU:HD12	19:G:24:GLN:H	1.04	1.13
18:F:341:ALA:HA	18:F:344:ARG:HG3	1.19	1.12
24:L:43:HIS:CB	24:L:184:LEU:HD11	1.79	1.13
17:E:176:PRO:HB3	18:F:344:ARG:HD3	1.29	1.12
34:E:401:ATP:O1G	18:F:344:ARG:NH1	1.82	1.12
9:W:408:ARG:CD	10:X:349:HIS:HE1	1.57	1.11
16:D:120:ASP:CB	16:D:123:LEU:HD21	1.79	1.11
19:g:10:ASP:HB3	25:m:7:TYR:OH	0.96	1.11
15:C:73:VAL:HG11	15:C:90:HIS:HE1	1.13	1.10
19:g:189:TRP:CZ3	19:g:193:GLN:OE1	2.05	1.10
12:Z:220:LEU:HB2	12:Z:221:PRO:HD3	1.25	1.10
14:B:427:LEU:C	14:B:431:GLN:HB2	1.75	1.10
16:D:120:ASP:O	16:D:123:LEU:CG	1.99	1.10
16:D:121:ARG:HA	16:D:124:LEU:HD21	1.12	1.10
18:F:437:TYR:HD2	23:K:20:ARG:CD	1.63	1.10
12:Z:220:LEU:HD23	12:Z:220:LEU:H	1.17	1.09
22:j:6:ALA:CB	22:j:9:VAL:HG23	1.81	1.09
15:C:73:VAL:CG1	15:C:90:HIS:NE2	2.13	1.09
16:D:401:LYS:O	16:D:405:THR:OG1	1.67	1.09
10:X:362:GLU:HG2	10:X:365:LEU:HD13	1.32	1.09
16:D:121:ARG:CA	16:D:124:LEU:HD21	1.83	1.09
9:W:407:ASP:OD2	9:W:409:LEU:HG	1.49	1.08
26:n:87:CYS:O	26:n:91:ARG:HB3	1.53	1.08
15:C:90:HIS:NE2	16:D:110:ASN:C	2.11	1.08
6:f:306:GLU:HB3	6:f:339:ILE:CD1	1.82	1.07
8:V:337:LEU:HD11	8:V:345:ARG:HH21	1.11	1.07
26:n:88:TYR:CA	26:n:91:ARG:CD	2.18	1.07
9:W:455:LEU:HD11	12:Z:220:LEU:HD13	1.21	1.07
19:g:127:GLN:HG3	20:h:127:VAL:HG21	1.24	1.07
5:e:43:TRP:HD1	8:V:349:ARG:N	1.45	1.07
6:f:358:PHE:O	6:f:362:GLY:HA3	1.55	1.06
16:D:120:ASP:HB3	16:D:123:LEU:HD21	1.09	1.06
16:D:121:ARG:C	16:D:124:LEU:HD23	1.76	1.06
26:n:87:CYS:O	26:n:91:ARG:HG2	1.51	1.05
6:f:88:SER:HB2	6:f:92:VAL:HG23	1.06	1.05
12:Z:220:LEU:CB	12:Z:221:PRO:CD	2.34	1.05
9:W:407:ASP:OD1	10:X:382:GLU:O	1.75	1.04
18:F:437:TYR:HD2	23:K:20:ARG:HD2	0.90	1.04
15:C:73:VAL:HG12	15:C:90:HIS:NE2	1.70	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:341:ALA:HA	18:F:344:ARG:CG	1.87	1.04
2:b:22:LEU:HG	2:b:180:ALA:N	1.72	1.04
20:H:6:TYR:CE2	20:H:126:GLY:HA2	1.93	1.04
23:k:10:ARG:HB3	23:k:14:THR:HB	1.40	1.04
16:D:125:LYS:HB3	16:D:126:PRO:CD	1.87	1.03
23:k:14:THR:O	23:k:22:PHE:HE2	1.40	1.03
6:f:306:GLU:HB3	6:f:339:ILE:HD13	1.39	1.03
18:F:424:ILE:HG22	18:F:428:GLN:HE21	1.22	1.03
8:V:333:ILE:CD1	8:V:345:ARG:CZ	2.36	1.03
19:G:17:SER:HB2	19:G:18:PRO:HD2	1.41	1.03
19:G:46:ASP:CB	19:G:222:VAL:CG2	2.36	1.02
23:k:14:THR:O	23:k:22:PHE:CE2	2.11	1.02
8:V:329:HIS:CD2	8:V:346:LEU:CD2	2.30	1.02
8:V:333:ILE:HD13	8:V:345:ARG:CZ	1.90	1.02
14:B:437:GLY:O	14:B:440:LEU:HD11	1.55	1.02
16:D:120:ASP:HB3	16:D:123:LEU:CD2	1.90	1.02
19:G:7:ALA:CA	19:G:11:ARG:NH2	2.22	1.02
16:D:120:ASP:O	16:D:123:LEU:CD2	2.08	1.02
7:U:561:GLU:OE2	7:U:562:GLU:CG	2.07	1.01
19:g:128:ASN:C	20:h:127:VAL:CG1	2.32	1.01
9:W:407:ASP:CG	10:X:382:GLU:O	2.04	1.01
5:e:43:TRP:HD1	8:V:349:ARG:CA	1.65	1.01
8:V:329:HIS:CG	8:V:346:LEU:HD21	1.95	1.01
17:E:176:PRO:CB	18:F:344:ARG:CD	2.18	1.01
21:i:8:ARG:O	21:i:11:ILE:CD1	2.08	1.01
6:f:333:LEU:HA	6:f:338:ASP:OD2	1.61	1.00
2:b:22:LEU:HD11	2:b:179:LEU:HA	1.07	1.00
9:W:428:TRP:O	9:W:432:LEU:HB2	1.60	1.00
17:E:176:PRO:HB2	18:F:344:ARG:HD2	1.40	1.00
9:W:409:LEU:CD2	10:X:381:GLY:O	2.10	1.00
10:X:201:TYR:HD2	20:H:201:GLY:HA3	1.25	1.00
16:D:409:LYS:HA	16:D:409:LYS:NZ	1.77	1.00
9:W:441:LYS:O	9:W:445:LEU:HB2	1.60	1.00
26:n:91:ARG:HH11	26:n:118:GLY:HA3	0.87	1.00
11:Y:374:ASP:O	11:Y:378:ASN:HB2	1.62	0.99
20:H:8:PHE:HB3	21:I:126:GLY:O	1.60	0.99
8:V:394:LEU:O	8:V:398:LEU:HB2	1.61	0.99
6:f:321:MET:O	6:f:325:GLN:HB3	1.61	0.99
21:i:3:ARG:NH2	23:k:10:ARG:HH21	1.60	0.99
21:i:17:ARG:NH2	21:i:19:TYR:HB2	1.77	0.99
26:n:88:TYR:HA	26:n:91:ARG:HD2	1.43	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:386:ILE:HG22	10:X:388:PHE:HD1	1.27	0.98
16:D:121:ARG:O	16:D:124:LEU:HD23	0.81	0.98
19:G:22:LEU:HD12	19:G:24:GLN:N	1.78	0.98
9:W:408:ARG:HG3	10:X:349:HIS:HE1	1.03	0.98
16:D:124:LEU:H	16:D:124:LEU:HD22	1.28	0.98
17:E:176:PRO:HB2	18:F:344:ARG:HD3	1.06	0.98
21:I:8:ARG:O	21:I:11:ILE:CD1	2.11	0.98
3:c:305:ASP:O	3:c:309:PHE:HB3	1.63	0.97
14:B:387:LYS:HE3	14:B:431:GLN:HG3	1.12	0.97
6:f:88:SER:HB2	6:f:92:VAL:CG2	1.93	0.97
21:i:8:ARG:C	21:i:11:ILE:CD1	2.38	0.97
7:U:496:LEU:O	7:U:500:ASN:HB2	1.63	0.97
19:g:223:GLU:O	19:g:225:PRO:HD3	1.65	0.97
2:b:22:LEU:HG	2:b:180:ALA:H	1.26	0.96
9:W:408:ARG:HD3	10:X:349:HIS:CE1	1.98	0.96
9:W:97:LEU:O	9:W:101:VAL:HB	1.65	0.96
19:G:46:ASP:CB	19:G:222:VAL:HG23	1.96	0.96
24:l:183:ASN:OD1	24:l:186:GLU:CD	2.08	0.96
12:Z:195:VAL:O	12:Z:199:LYS:HB2	1.66	0.96
14:B:387:LYS:HE3	14:B:431:GLN:HG2	1.45	0.95
8:V:227:VAL:O	8:V:231:LEU:HB2	1.66	0.95
21:I:8:ARG:C	21:I:11:ILE:CD1	2.39	0.95
12:Z:262:LEU:O	12:Z:266:ILE:HB	1.65	0.95
16:D:148:ASP:HA	16:D:152:MET:SD	2.06	0.95
5:e:43:TRP:HE1	8:V:349:ARG:HA	1.14	0.95
23:k:10:ARG:CZ	23:k:10:ARG:HA	1.96	0.95
18:F:344:ARG:HH12	18:F:347:ARG:CZ	1.66	0.94
22:J:4:ASP:OD2	22:J:21:TYR:HE2	1.48	0.94
22:j:6:ALA:HB1	22:j:9:VAL:HG22	1.11	0.94
4:d:194:ALA:O	4:d:198:LEU:HB2	1.67	0.94
2:b:22:LEU:HD11	2:b:178:SER:O	1.66	0.94
15:C:90:HIS:CE1	16:D:110:ASN:C	2.46	0.94
19:g:11:ARG:HG3	19:g:23:TYR:HB2	1.48	0.94
19:G:128:ASN:HA	20:H:127:VAL:HG13	1.49	0.94
2:b:22:LEU:CD1	2:b:178:SER:O	2.16	0.93
22:J:4:ASP:CG	22:J:21:TYR:CE2	2.44	0.93
27:o:15:GLY:HA2	27:o:174:ASP:O	1.69	0.93
16:D:403:TYR:CD1	16:D:407:ILE:HD11	2.03	0.93
2:b:22:LEU:HD11	2:b:178:SER:C	1.93	0.92
18:F:341:ALA:CA	18:F:344:ARG:HH21	1.82	0.92
19:G:46:ASP:CB	19:G:222:VAL:HG21	1.98	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:362:GLU:OE2	10:X:365:LEU:HD22	1.68	0.92
1:a:248:PHE:O	1:a:252:LYS:HB2	1.69	0.92
15:C:90:HIS:HD1	16:D:110:ASN:HB3	1.16	0.92
27:O:15:GLY:HA2	27:O:174:ASP:O	1.69	0.92
20:h:9:SER:HG	20:h:123:GLN:C	1.78	0.92
26:n:88:TYR:HA	26:n:91:ARG:CG	2.00	0.92
3:c:220:LEU:O	3:c:224:SER:HB2	1.70	0.92
20:H:7:SER:OG	20:H:125:GLY:HA3	1.69	0.92
9:W:455:LEU:CD1	12:Z:220:LEU:HD13	1.99	0.91
23:K:10:ARG:HB2	23:K:14:THR:HB	1.50	0.91
26:n:15:GLY:HA2	26:n:175:ARG:O	1.69	0.91
18:F:344:ARG:HH11	18:F:347:ARG:NH2	1.59	0.91
11:Y:101:ARG:O	11:Y:105:MET:HB3	1.69	0.91
19:g:10:ASP:O	25:m:7:TYR:OH	1.84	0.91
14:B:225:TYR:O	14:B:353:PHE:HB2	1.71	0.91
15:C:330:LYS:O	15:C:334:ARG:HB2	1.70	0.91
21:i:17:ARG:HG3	21:i:17:ARG:HH11	1.34	0.91
9:W:426:ASN:O	9:W:430:GLN:HB3	1.70	0.91
19:G:7:ALA:CA	19:G:11:ARG:HH22	1.80	0.91
26:N:15:GLY:HA2	26:N:175:ARG:O	1.69	0.91
6:f:95:PRO:O	6:f:99:LEU:HB2	1.71	0.90
7:U:761:VAL:O	7:U:765:VAL:HB	1.71	0.90
8:V:328:VAL:O	8:V:332:LEU:HB2	1.71	0.90
18:F:344:ARG:HH12	18:F:347:ARG:NH1	1.69	0.90
19:g:46:ASP:CB	19:g:222:VAL:HG23	2.01	0.90
6:f:503:PRO:O	6:f:507:ASP:HB2	1.71	0.90
22:j:7:ILE:HD12	22:j:8:THR:HG23	1.53	0.90
10:X:201:TYR:CD2	20:H:201:GLY:HA3	2.06	0.90
18:F:424:ILE:HG22	18:F:428:GLN:NE2	1.85	0.90
21:i:3:ARG:NH2	23:k:10:ARG:NH2	2.19	0.90
7:U:27:LEU:O	7:U:31:VAL:HB	1.72	0.90
8:V:187:ILE:O	8:V:191:LEU:HB2	1.72	0.90
16:D:292:LEU:O	16:D:296:MET:HB2	1.71	0.90
7:U:646:PRO:O	7:U:650:TYR:HB2	1.72	0.90
12:Z:278:ASN:O	12:Z:282:ASN:HB2	1.71	0.90
18:F:435:LEU:HD22	24:L:51:ARG:HH12	1.35	0.89
9:W:389:SER:O	9:W:393:LEU:HB2	1.70	0.89
1:a:171:SER:O	1:a:175:ASP:HB2	1.72	0.89
8:V:345:ARG:NH1	8:V:359:PRO:HB2	1.88	0.89
7:U:559:ARG:HD2	7:U:562:GLU:HB2	1.54	0.89
16:D:129:SER:O	16:D:143:LEU:HB2	1.71	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:43:HIS:HB2	24:L:184:LEU:HD11	1.55	0.89
23:K:16:SER:CA	23:K:22:PHE:CE2	2.56	0.88
18:F:341:ALA:HB1	18:F:344:ARG:HH22	1.06	0.88
20:H:121:TYR:C	20:H:124:SER:OG	2.16	0.88
21:i:194:ILE:O	21:i:198:ASN:HB2	1.73	0.88
8:V:185:GLN:O	8:V:189:ASP:HB2	1.74	0.88
14:B:440:LEU:HD22	14:B:440:LEU:H	1.38	0.88
21:I:194:ILE:O	21:I:198:ASN:HB2	1.73	0.88
6:f:232:TYR:O	6:f:236:CYS:HB2	1.74	0.88
5:e:43:TRP:HD1	8:V:349:ARG:H	1.21	0.88
23:K:16:SER:HA	23:K:22:PHE:CZ	2.08	0.88
21:i:13:SER:N	21:i:17:ARG:HH12	1.70	0.88
16:D:121:ARG:HA	16:D:124:LEU:CD2	2.02	0.88
18:F:430:LYS:HZ2	18:F:430:LYS:H	1.16	0.88
6:f:333:LEU:CA	6:f:338:ASP:OD2	2.22	0.88
21:i:3:ARG:CZ	23:k:10:ARG:NH2	2.37	0.87
6:f:332:ALA:C	6:f:338:ASP:OD2	2.18	0.87
9:W:243:ILE:O	9:W:247:TYR:HB2	1.73	0.87
11:Y:119:GLY:O	11:Y:123:ALA:HB3	1.75	0.87
16:D:369:LYS:O	16:D:369:LYS:NZ	2.08	0.87
19:g:11:ARG:NH1	19:g:27:TYR:OH	2.07	0.87
13:A:306:LEU:HD12	13:A:312:ARG:HD2	1.55	0.87
14:B:387:LYS:CE	14:B:431:GLN:CG	2.30	0.87
27:O:11:GLY:HA3	27:O:178:ILE:O	1.75	0.87
22:j:6:ALA:HB1	22:j:9:VAL:HG23	1.45	0.87
21:i:3:ARG:CZ	23:k:10:ARG:HH21	1.88	0.87
24:l:43:HIS:CD2	24:l:184:LEU:HD21	2.10	0.86
16:D:416:PHE:CZ	19:G:157:ALA:HB1	2.09	0.86
1:a:118:ILE:O	1:a:122:LYS:HB2	1.74	0.86
9:W:407:ASP:OD2	9:W:409:LEU:CG	2.22	0.86
16:D:125:LYS:HB3	16:D:126:PRO:HD3	1.55	0.86
21:i:13:SER:N	21:i:17:ARG:NH1	2.23	0.86
18:F:341:ALA:CA	18:F:344:ARG:HG3	2.02	0.86
10:X:386:ILE:HG22	10:X:388:PHE:CD1	2.10	0.86
7:U:216:VAL:O	7:U:220:LEU:HB2	1.76	0.85
23:K:16:SER:N	23:K:22:PHE:HE2	1.74	0.85
27:O:136:ALA:O	27:O:140:ASP:HB2	1.76	0.85
4:d:208:ASP:O	4:d:212:LYS:HB2	1.75	0.85
14:B:427:LEU:O	14:B:431:GLN:CA	2.24	0.85
27:O:201:ARG:HH11	27:O:203:ARG:CZ	1.89	0.85
10:X:324:ALA:O	10:X:328:ASP:HB2	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:o:11:GLY:HA3	27:o:178:ILE:O	1.75	0.85
27:o:136:ALA:O	27:o:140:ASP:HB2	1.76	0.85
2:b:22:LEU:HD22	2:b:22:LEU:H	1.39	0.85
13:A:312:ARG:HH22	13:A:317:VAL:HG23	1.40	0.85
6:f:88:SER:HB3	6:f:92:VAL:HG23	1.58	0.85
15:C:73:VAL:CG1	15:C:90:HIS:HE1	1.51	0.85
18:F:344:ARG:HH11	18:F:347:ARG:CZ	1.83	0.85
19:g:11:ARG:CG	19:g:23:TYR:HB2	2.07	0.85
6:f:301:HIS:O	6:f:305:LEU:HB2	1.76	0.84
8:V:337:LEU:HD11	8:V:345:ARG:NH2	1.91	0.84
16:D:402:ALA:O	16:D:406:VAL:HG23	1.76	0.84
19:G:7:ALA:HA	19:G:11:ARG:HH22	1.05	0.84
19:G:127:GLN:HG3	20:H:127:VAL:HG21	1.58	0.84
23:K:16:SER:HA	23:K:22:PHE:CE2	2.11	0.84
21:i:8:ARG:CA	21:i:11:ILE:CD1	2.56	0.84
1:a:8:LEU:O	1:a:12:GLN:HB3	1.78	0.84
8:V:80:LYS:HE2	8:V:118:GLN:HE22	1.42	0.84
4:d:204:LYS:O	4:d:208:ASP:HB2	1.77	0.84
7:U:598:ALA:O	7:U:602:LEU:HB2	1.78	0.84
25:M:235:ALA:O	25:M:239:ALA:HB2	1.78	0.84
16:D:409:LYS:HD3	17:E:387:LYS:NZ	1.93	0.83
14:B:437:GLY:O	14:B:440:LEU:HD13	1.77	0.83
15:C:267:SER:O	15:C:271:ARG:HB2	1.78	0.83
21:I:8:ARG:CA	21:I:11:ILE:CD1	2.56	0.83
7:U:251:ASP:O	7:U:255:SER:HB3	1.78	0.83
15:C:90:HIS:HB2	15:C:91:PRO:HD3	1.60	0.83
6:f:122:ALA:O	6:f:126:ILE:HB	1.79	0.83
18:F:430:LYS:H	18:F:430:LYS:NZ	1.75	0.83
2:b:22:LEU:CG	2:b:180:ALA:N	2.42	0.83
22:J:4:ASP:CG	22:J:21:TYR:HE2	1.84	0.83
19:g:203:SER:O	19:g:207:SER:CA	2.24	0.83
25:m:235:ALA:O	25:m:239:ALA:HB2	1.78	0.83
7:U:325:MET:O	7:U:329:LEU:HB2	1.79	0.83
21:i:13:SER:H	21:i:17:ARG:NH1	1.76	0.83
13:A:306:LEU:O	13:A:312:ARG:HG3	1.79	0.83
6:f:306:GLU:HB3	6:f:339:ILE:HD12	1.60	0.82
11:Y:336:ARG:O	11:Y:340:ALA:HB2	1.79	0.82
23:k:21:LEU:HD12	23:k:24:VAL:HG23	1.59	0.82
20:H:121:TYR:HA	20:H:124:SER:HG	1.44	0.82
23:k:10:ARG:O	23:k:22:PHE:CD2	2.31	0.82
27:O:138:PHE:O	27:O:142:PHE:HB2	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:407:ASP:OD1	10:X:382:GLU:C	2.22	0.82
22:j:40:ILE:CB	22:j:184:ASP:OD1	2.26	0.82
30:R:136:TYR:O	30:R:140:ASP:HB2	1.80	0.82
8:V:333:ILE:HD11	8:V:345:ARG:CZ	2.08	0.82
5:e:60:LEU:O	5:e:64:GLY:HA3	1.79	0.82
7:U:341:PHE:O	7:U:345:ASN:HB2	1.79	0.81
19:g:127:GLN:HG3	20:h:127:VAL:CG2	2.09	0.81
21:i:3:ARG:HH22	23:k:10:ARG:HH21	1.28	0.81
13:A:312:ARG:HH12	13:A:317:VAL:CG2	1.93	0.81
21:i:8:ARG:CA	21:i:11:ILE:HD13	2.10	0.81
30:r:136:TYR:O	30:r:140:ASP:HB2	1.80	0.81
1:a:93:ALA:O	1:a:97:LEU:HB2	1.80	0.81
2:b:22:LEU:HD21	2:b:179:LEU:C	2.05	0.81
4:d:34:ASN:HD21	7:U:26:LYS:HG3	1.43	0.81
18:F:431:LYS:HA	18:F:431:LYS:CE	2.11	0.81
26:n:88:TYR:C	26:n:91:ARG:HG2	2.05	0.81
27:o:138:PHE:O	27:o:142:PHE:HB2	1.80	0.81
21:i:13:SER:CB	21:i:17:ARG:HH11	1.92	0.81
14:B:366:GLN:O	14:B:370:SER:HB3	1.81	0.81
19:G:203:SER:O	19:G:207:SER:CA	2.24	0.81
21:i:17:ARG:HH21	21:i:19:TYR:HD1	1.27	0.81
23:K:16:SER:CA	23:K:22:PHE:HE2	1.93	0.81
2:b:22:LEU:HD11	2:b:179:LEU:N	1.96	0.81
14:B:387:LYS:HZ2	14:B:431:GLN:HG3	1.43	0.81
14:B:439:TYR:HB2	22:J:76:LEU:HA	1.60	0.80
23:K:10:ARG:CD	23:K:10:ARG:H	1.94	0.80
6:f:211:ILE:O	6:f:215:ASP:HB2	1.81	0.80
26:N:87:CYS:O	26:N:91:ARG:HB3	1.80	0.80
21:i:13:SER:CA	21:i:17:ARG:NH1	2.43	0.80
27:o:198:ARG:NH2	27:o:200:GLY:O	2.14	0.80
1:a:176:ALA:O	1:a:180:LEU:HB3	1.81	0.80
16:D:408:LYS:NZ	17:E:389:VAL:HG12	1.95	0.80
5:e:43:TRP:CD1	8:V:349:ARG:CG	2.65	0.80
27:O:198:ARG:NH2	27:O:200:GLY:O	2.15	0.80
21:i:148:TYR:HA	21:i:157:GLY:O	1.82	0.80
2:b:22:LEU:HD12	2:b:179:LEU:HA	1.63	0.80
15:C:73:VAL:HG13	15:C:90:HIS:NE2	1.89	0.80
21:I:148:TYR:HA	21:I:157:GLY:O	1.82	0.80
14:B:425:ASN:O	14:B:429:LYS:HB2	1.82	0.80
16:D:403:TYR:CD1	16:D:407:ILE:CD1	2.61	0.80
18:F:225:MET:HB2	18:F:330:ALA:O	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:10:ASP:HB3	25:M:7:TYR:CZ	2.17	0.80
19:g:10:ASP:HB3	25:m:7:TYR:CZ	2.15	0.80
6:f:333:LEU:N	6:f:338:ASP:OD2	2.15	0.79
10:X:363:ARG:O	10:X:367:GLN:HB2	1.81	0.79
23:k:10:ARG:HA	23:k:10:ARG:NE	1.96	0.79
19:G:10:ASP:CG	25:M:7:TYR:HH	1.82	0.79
19:G:11:ARG:O	19:G:24:GLN:NE2	2.13	0.79
15:C:90:HIS:CD2	16:D:110:ASN:C	2.56	0.79
18:F:431:LYS:O	18:F:431:LYS:HD3	1.82	0.79
21:I:11:ILE:H	21:I:11:ILE:HD12	1.48	0.79
16:D:408:LYS:HD2	16:D:409:LYS:HD2	1.65	0.79
19:g:192:GLU:HA	19:g:192:GLU:OE1	1.82	0.79
30:r:135:ALA:O	30:r:139:MET:HB3	1.82	0.79
24:L:84:LEU:O	24:L:88:MET:HB2	1.83	0.79
27:O:201:ARG:HH11	27:O:203:ARG:NH2	1.73	0.79
16:D:409:LYS:HD3	17:E:387:LYS:HZ2	1.46	0.79
19:G:128:ASN:HA	20:H:127:VAL:CG1	2.13	0.79
9:W:357:ARG:O	9:W:361:HIS:HB2	1.83	0.78
14:B:437:GLY:C	14:B:440:LEU:HD11	2.08	0.78
24:l:84:LEU:O	24:l:88:MET:HB2	1.83	0.78
23:K:10:ARG:H	23:K:10:ARG:HD2	1.48	0.78
21:i:8:ARG:HA	21:i:11:ILE:HD13	1.63	0.78
29:q:59:TYR:O	29:q:63:ASN:HB2	1.82	0.78
5:e:43:TRP:HB3	8:V:347:GLN:HA	1.65	0.78
29:Q:59:TYR:O	29:Q:63:ASN:HB2	1.82	0.78
30:R:135:ALA:O	30:R:139:MET:HB3	1.82	0.78
6:f:684:PRO:O	6:f:688:ARG:HB2	1.83	0.78
16:D:412:GLN:O	16:D:412:GLN:NE2	2.17	0.78
20:H:6:TYR:HE2	20:H:126:GLY:HA2	1.48	0.78
21:i:11:ILE:H	21:i:11:ILE:HD12	1.48	0.78
9:W:407:ASP:O	9:W:412:ILE:O	2.01	0.78
19:g:10:ASP:C	25:m:7:TYR:HH	1.91	0.78
8:V:345:ARG:NH1	8:V:359:PRO:O	2.16	0.78
21:I:8:ARG:CA	21:I:11:ILE:HD13	2.13	0.78
9:W:408:ARG:NH2	9:W:408:ARG:HB2	1.97	0.78
21:I:8:ARG:HA	21:I:11:ILE:HD13	1.66	0.78
9:W:431:LYS:O	9:W:435:LEU:HB2	1.84	0.78
19:g:10:ASP:CA	25:m:7:TYR:OH	2.31	0.78
7:U:458:ILE:O	7:U:462:LEU:HB2	1.85	0.77
5:e:59:GLU:O	5:e:63:HIS:HB2	1.84	0.77
27:O:201:ARG:NH1	27:O:203:ARG:CZ	2.46	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:138:TYR:HA	12:Z:156:GLU:O	1.83	0.77
16:D:408:LYS:HZ1	17:E:389:VAL:HG12	1.49	0.77
16:D:417:TYR:CZ	19:G:21:ARG:HG2	2.20	0.77
27:o:213:THR:O	28:p:198:ARG:HA	1.84	0.77
20:H:120:GLU:O	20:H:124:SER:CB	2.33	0.77
16:D:409:LYS:HA	16:D:409:LYS:HZ1	1.45	0.77
9:W:455:LEU:HD11	12:Z:220:LEU:HD12	1.67	0.77
16:D:408:LYS:HZ3	17:E:389:VAL:CG1	1.98	0.77
27:o:18:THR:HB	27:o:31:CYS:H	1.50	0.77
1:a:151:VAL:O	1:a:155:PHE:HB2	1.86	0.76
16:D:121:ARG:CA	16:D:124:LEU:CD2	2.51	0.76
19:G:21:ARG:H	19:G:21:ARG:CD	1.97	0.76
31:s:20:PHE:HA	31:s:198:VAL:O	1.85	0.76
12:Z:220:LEU:H	12:Z:220:LEU:CD2	1.95	0.76
14:B:431:GLN:OE1	14:B:431:GLN:HA	1.85	0.76
7:U:174:PRO:O	7:U:178:ALA:HB2	1.86	0.76
19:g:189:TRP:CE3	19:g:193:GLN:OE1	2.37	0.76
31:S:20:PHE:HA	31:S:198:VAL:O	1.85	0.75
31:s:193:LEU:O	31:s:207:THR:HA	1.86	0.75
18:F:431:LYS:HA	18:F:431:LYS:NZ	2.02	0.75
19:G:6:SER:N	19:G:18:PRO:HG3	2.00	0.75
27:O:18:THR:HB	27:O:31:CYS:H	1.50	0.75
7:U:559:ARG:O	7:U:561:GLU:OE1	2.03	0.75
16:D:409:LYS:HA	16:D:409:LYS:CE	2.13	0.75
31:S:193:LEU:O	31:S:207:THR:HA	1.86	0.75
9:W:408:ARG:HD2	10:X:349:HIS:CE1	2.19	0.75
14:B:121:ALA:O	14:B:132:TYR:HA	1.87	0.75
15:C:73:VAL:HG12	15:C:90:HIS:CE1	2.01	0.75
19:G:50:ILE:O	19:G:217:VAL:HA	1.87	0.75
20:H:120:GLU:O	20:H:124:SER:OG	2.05	0.75
8:V:477:HIS:O	8:V:481:SER:HB3	1.86	0.75
23:k:20:ARG:HG2	23:k:20:ARG:HH21	1.50	0.75
24:l:134:ILE:O	24:l:144:ILE:HA	1.87	0.75
20:h:210:VAL:O	20:h:221:LEU:HB2	1.86	0.74
23:k:20:ARG:HG2	23:k:20:ARG:NH2	2.02	0.74
13:A:224:LEU:O	13:A:228:ALA:HB2	1.87	0.74
16:D:125:LYS:CB	16:D:126:PRO:CD	2.64	0.74
28:P:203:ARG:HH12	30:r:191:ASN:HD21	1.33	0.74
2:b:22:LEU:HD22	2:b:22:LEU:N	2.02	0.74
16:D:123:LEU:HD23	16:D:123:LEU:H	1.51	0.74
24:L:134:ILE:O	24:L:144:ILE:HA	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:90:HIS:CG	16:D:110:ASN:H	2.05	0.74
16:D:204:MET:HA	16:D:331:ILE:O	1.87	0.74
26:n:88:TYR:HA	26:n:91:ARG:HD3	0.75	0.74
26:n:88:TYR:CA	26:n:91:ARG:CG	2.63	0.74
13:A:240:VAL:HB	13:A:273:PHE:O	1.86	0.74
15:C:90:HIS:CG	16:D:110:ASN:HB3	2.16	0.74
12:Z:284:ASP:O	12:Z:288:LYS:HB2	1.87	0.74
18:F:341:ALA:CA	18:F:344:ARG:NH2	2.43	0.74
20:H:210:VAL:O	20:H:221:LEU:HB2	1.86	0.74
16:D:120:ASP:O	16:D:123:LEU:HD21	1.87	0.74
21:I:8:ARG:C	21:I:11:ILE:HD11	2.07	0.74
28:p:111:GLY:O	28:p:120:PHE:HB3	1.88	0.74
10:X:362:GLU:O	10:X:363:ARG:HG3	1.88	0.74
22:J:4:ASP:O	22:J:18:GLN:NE2	2.21	0.74
21:I:8:ARG:HA	21:I:11:ILE:CD1	2.18	0.73
13:A:302:LEU:O	13:A:306:LEU:HB2	1.88	0.73
19:g:50:ILE:O	19:g:217:VAL:HA	1.87	0.73
14:B:440:LEU:HD22	14:B:440:LEU:N	2.04	0.73
12:Z:220:LEU:HB2	12:Z:221:PRO:CD	2.11	0.73
6:f:88:SER:CB	6:f:92:VAL:CG2	2.57	0.73
17:E:69:PHE:O	17:E:80:VAL:HA	1.88	0.73
19:g:17:SER:OG	19:g:21:ARG:O	2.07	0.73
23:k:99:HIS:O	23:k:103:TYR:HB2	1.88	0.73
24:l:184:LEU:HD12	24:l:184:LEU:N	2.04	0.73
6:f:625:LYS:O	6:f:629:LYS:HB2	1.88	0.73
6:f:675:PHE:O	6:f:679:LEU:HB2	1.89	0.73
28:P:111:GLY:O	28:P:120:PHE:HB3	1.88	0.73
27:o:14:LEU:O	27:o:175:LEU:HA	1.89	0.73
1:a:349:MET:O	1:a:353:LEU:HB2	1.89	0.72
23:K:16:SER:HB2	23:K:22:PHE:CE2	2.24	0.72
21:i:13:SER:CB	21:i:17:ARG:HG2	2.16	0.72
29:q:21:ALA:HB3	29:q:29:LYS:HB3	1.71	0.72
4:d:34:ASN:ND2	7:U:26:LYS:HG3	2.03	0.72
3:c:91:PHE:O	3:c:95:MET:HB3	1.90	0.72
7:U:213:PHE:O	7:U:217:CYS:HB2	1.89	0.72
23:K:11:GLY:O	23:K:21:LEU:HD21	1.89	0.72
28:p:187:VAL:HB	28:p:198:ARG:O	1.89	0.72
14:B:439:TYR:HB2	22:J:76:LEU:CA	2.18	0.72
16:D:124:LEU:CD2	16:D:124:LEU:H	2.02	0.72
16:D:408:LYS:NZ	17:E:389:VAL:CG1	2.52	0.72
27:O:14:LEU:O	27:O:175:LEU:HA	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:99:HIS:O	23:K:103:TYR:HB2	1.88	0.72
1:a:247:ARG:O	1:a:251:LEU:HB3	1.89	0.72
1:a:278:MET:O	1:a:282:PHE:HB3	1.90	0.72
6:f:129:LEU:O	6:f:133:MET:HB3	1.90	0.72
6:f:318:THR:O	6:f:322:SER:HB3	1.89	0.72
14:B:438:LEU:HD13	14:B:438:LEU:N	2.04	0.72
16:D:124:LEU:HD22	16:D:124:LEU:N	2.03	0.72
18:F:428:GLN:CD	18:F:428:GLN:H	1.98	0.72
21:i:8:ARG:HA	21:i:11:ILE:CD1	2.18	0.72
27:o:214:GLU:HA	28:p:198:ARG:HG2	1.71	0.72
16:D:148:ASP:CA	16:D:152:MET:SD	2.76	0.71
9:W:82:LEU:O	9:W:86:ASN:HB2	1.90	0.71
12:Z:218:GLY:HA2	12:Z:220:LEU:HD21	1.72	0.71
16:D:123:LEU:HD23	16:D:123:LEU:N	2.04	0.71
16:D:403:TYR:CA	16:D:407:ILE:HD11	2.09	0.71
28:P:187:VAL:HB	28:P:198:ARG:O	1.90	0.71
29:Q:21:ALA:HB3	29:Q:29:LYS:HB3	1.71	0.71
2:b:22:LEU:CD2	2:b:180:ALA:N	2.54	0.71
7:U:762:GLY:O	7:U:766:PHE:HB2	1.89	0.71
19:g:11:ARG:O	19:g:24:GLN:NE2	2.18	0.71
16:D:417:TYR:CE1	19:G:21:ARG:HG2	2.26	0.71
26:n:2:THR:HA	26:n:128:GLY:O	1.90	0.71
9:W:359:VAL:HG21	9:W:392:PHE:HB3	1.73	0.70
19:g:128:ASN:C	20:h:127:VAL:HG12	2.14	0.70
30:r:195:LEU:O	30:r:199:TYR:HB2	1.91	0.70
30:R:195:LEU:O	30:R:199:TYR:HB2	1.91	0.70
21:i:17:ARG:HG3	21:i:17:ARG:NH1	1.97	0.70
16:D:125:LYS:HB3	16:D:126:PRO:HD2	1.73	0.70
26:N:2:THR:HA	26:N:128:GLY:O	1.90	0.70
8:V:419:LEU:O	8:V:423:ALA:HB3	1.91	0.70
18:F:431:LYS:HA	18:F:431:LYS:HZ3	1.55	0.70
14:B:427:LEU:O	14:B:431:GLN:N	2.25	0.70
1:a:360:VAL:O	1:a:364:GLU:HB2	1.91	0.70
6:f:228:LYS:O	6:f:232:TYR:HB3	1.90	0.70
16:D:120:ASP:C	16:D:123:LEU:HD21	2.17	0.70
16:D:408:LYS:HE3	16:D:409:LYS:HB2	1.73	0.70
19:G:128:ASN:CA	20:H:127:VAL:CG1	2.70	0.70
26:n:88:TYR:CA	26:n:91:ARG:HG2	2.22	0.70
19:g:11:ARG:HD3	19:g:11:ARG:N	2.06	0.70
9:W:372:ARG:H	9:W:415:PHE:HB2	1.57	0.69
10:X:325:LYS:O	10:X:329:ASN:HB2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:252:ARG:O	16:D:256:GLU:HB2	1.92	0.69
20:H:121:TYR:C	20:H:124:SER:HG	1.97	0.69
24:L:43:HIS:CD2	24:L:184:LEU:HD21	2.27	0.69
31:s:49:LYS:O	31:s:112:GLY:HA3	1.92	0.69
14:B:437:GLY:O	14:B:440:LEU:CD2	2.41	0.69
23:k:21:LEU:HD13	23:k:23:GLN:HB3	1.73	0.69
8:V:353:LEU:HD11	8:V:359:PRO:HD3	1.74	0.69
16:D:416:PHE:HZ	19:G:157:ALA:HB1	1.56	0.69
4:d:69:PRO:O	4:d:73:ARG:HB2	1.92	0.69
13:A:269:ALA:HA	13:A:314:ASN:O	1.91	0.69
31:S:49:LYS:O	31:S:112:GLY:HA3	1.92	0.69
21:i:3:ARG:NH1	23:k:10:ARG:NH2	2.39	0.69
2:b:108:ARG:HA	2:b:137:ASN:O	1.92	0.69
3:c:98:MET:HG2	3:c:101:GLN:HE21	1.55	0.69
14:B:434:THR:HB	14:B:435:PRO:HD2	1.75	0.69
21:i:11:ILE:HD12	21:i:11:ILE:N	2.07	0.69
16:D:227:PHE:HA	16:D:261:ILE:O	1.93	0.69
21:i:3:ARG:NH1	23:k:10:ARG:HH21	1.91	0.69
6:f:252:ALA:O	6:f:256:PHE:HB2	1.93	0.69
6:f:478:ARG:O	6:f:482:ILE:HB	1.92	0.69
18:F:424:ILE:CG2	18:F:428:GLN:NE2	2.55	0.69
27:O:201:ARG:HH12	27:O:203:ARG:HH21	1.34	0.69
19:g:46:ASP:O	19:g:222:VAL:HG22	1.92	0.69
11:Y:100:ILE:O	11:Y:104:MET:HB3	1.93	0.68
24:l:183:ASN:CG	24:l:186:GLU:OE1	2.36	0.68
14:B:439:TYR:HB2	22:J:76:LEU:CB	2.23	0.68
24:l:69:HIS:HB2	24:l:137:TYR:HB2	1.74	0.68
6:f:541:THR:O	6:f:545:LYS:HB2	1.93	0.68
19:g:189:TRP:HZ3	19:g:193:GLN:OE1	1.69	0.68
6:f:281:ILE:O	6:f:285:CYS:HB2	1.94	0.68
26:n:87:CYS:O	26:n:91:ARG:CD	2.41	0.68
10:X:302:PHE:O	10:X:306:LEU:HB2	1.94	0.68
12:Z:220:LEU:CD1	12:Z:221:PRO:HD3	2.24	0.68
18:F:436:GLN:O	18:F:438:TYR:CD2	2.47	0.68
21:i:8:ARG:C	21:i:11:ILE:HD11	2.08	0.68
9:W:408:ARG:C	9:W:410:ALA:H	2.00	0.68
12:Z:227:ILE:O	12:Z:231:GLN:HB2	1.93	0.68
23:k:219:THR:HB	23:k:221:GLN:HE22	1.58	0.68
3:c:42:LEU:O	3:c:46:ARG:HB2	1.94	0.68
4:d:102:ASN:O	4:d:106:LEU:HB3	1.94	0.68
6:f:426:LEU:O	6:f:430:ASP:HB3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:188:LEU:O	15:C:294:ALA:HA	1.93	0.68
17:E:342:ASP:OD1	18:F:345:SER:HB3	1.92	0.68
31:s:75:TYR:O	31:s:79:ASN:HB2	1.94	0.68
17:E:176:PRO:HB3	18:F:344:ARG:CD	2.08	0.68
19:g:129:ALA:N	20:h:127:VAL:CG1	2.56	0.68
7:U:530:GLU:O	7:U:534:GLY:HA3	1.93	0.68
17:E:194:ASN:ND2	17:E:228:CYS:SG	2.67	0.68
21:I:11:ILE:HD12	21:I:11:ILE:N	2.07	0.68
24:L:69:HIS:HB2	24:L:137:TYR:HB2	1.74	0.68
9:W:203:GLN:HA	9:W:206:SER:HB3	1.76	0.67
11:Y:384:SER:HB2	12:Z:279:LYS:HE3	1.75	0.67
15:C:189:TYR:HA	15:C:295:THR:O	1.94	0.67
16:D:408:LYS:HZ3	17:E:389:VAL:HB	1.59	0.67
23:K:219:THR:HB	23:K:221:GLN:HE22	1.58	0.67
7:U:559:ARG:HB3	7:U:562:GLU:HB2	1.74	0.67
8:V:333:ILE:CD1	8:V:345:ARG:NH2	2.57	0.67
10:X:383:GLY:O	10:X:385:LEU:HD13	1.95	0.67
15:C:190:GLY:HA3	15:C:317:PHE:HB2	1.77	0.67
10:X:360:ASP:OD2	10:X:362:GLU:O	2.11	0.67
21:i:8:ARG:C	21:i:11:ILE:HD12	2.17	0.67
4:d:8:GLU:HB3	4:d:11:ARG:HB3	1.77	0.67
6:f:358:PHE:O	6:f:362:GLY:CA	2.39	0.67
16:D:87:LEU:HB2	17:E:80:VAL:HB	1.76	0.67
10:X:362:GLU:CD	10:X:365:LEU:HD22	2.20	0.67
14:B:355:LEU:HD22	14:B:390:LEU:O	1.95	0.67
20:H:6:TYR:CZ	20:H:126:GLY:HA2	2.28	0.67
32:T:162:GLN:O	32:T:166:ARG:HB2	1.95	0.67
11:Y:247:LEU:O	11:Y:251:HIS:HB2	1.93	0.67
21:i:13:SER:H	21:i:17:ARG:HH12	1.34	0.67
29:q:57:ALA:O	29:q:61:GLN:HB3	1.95	0.67
19:g:127:GLN:NE2	20:h:128:ARG:O	2.28	0.67
16:D:120:ASP:CA	16:D:123:LEU:HD21	2.24	0.67
16:D:259:PRO:HB3	16:D:304:ASN:HB2	1.77	0.67
19:G:46:ASP:O	19:G:222:VAL:HG23	1.94	0.67
19:g:10:ASP:HB3	25:m:7:TYR:HH	1.37	0.67
6:f:586:PRO:O	6:f:590:PHE:HB2	1.94	0.67
8:V:255:LEU:HD22	8:V:291:TYR:HB3	1.77	0.67
22:J:2:SER:HA	22:J:12:PRO:HD3	1.77	0.67
21:I:143:TYR:HB2	21:I:146:GLN:HE21	1.60	0.66
31:S:75:TYR:O	31:S:79:ASN:HB2	1.94	0.66
22:j:120:GLN:NE2	23:k:84:ASP:OD1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:27:GLU:O	1:a:31:LYS:HB2	1.95	0.66
16:D:409:LYS:CD	17:E:387:LYS:NZ	2.58	0.66
16:D:413:GLU:OE1	16:D:413:GLU:HA	1.95	0.66
21:i:149:GLN:O	21:i:156:TYR:HA	1.96	0.66
22:j:2:SER:HA	22:j:12:PRO:HD3	1.77	0.66
2:b:22:LEU:HD13	2:b:178:SER:O	1.95	0.66
30:R:52:CYS:O	30:R:56:GLU:HB2	1.95	0.66
5:e:43:TRP:CD1	8:V:349:ARG:CB	2.77	0.66
6:f:313:GLU:O	6:f:317:LEU:HB2	1.96	0.66
7:U:65:SER:O	7:U:69:TYR:HB2	1.94	0.66
9:W:124:LEU:HD22	9:W:147:LYS:HD2	1.77	0.66
16:D:409:LYS:CD	17:E:387:LYS:HZ1	2.07	0.66
21:I:8:ARG:C	21:I:11:ILE:HD12	2.18	0.66
21:I:175:LEU:O	21:I:179:TYR:HB2	1.96	0.66
26:n:88:TYR:C	26:n:91:ARG:CG	2.69	0.66
6:f:359:GLY:O	6:f:363:SER:HB3	1.96	0.66
10:X:202:CYS:H	10:X:203:PRO:HD3	1.60	0.66
10:X:287:LEU:O	10:X:291:ALA:HB2	1.95	0.66
29:Q:57:ALA:O	29:Q:61:GLN:HB3	1.95	0.66
3:c:292:MET:O	3:c:296:ILE:HB	1.96	0.66
19:g:141:ILE:HA	19:g:150:GLN:O	1.96	0.66
21:i:143:TYR:HB2	21:i:146:GLN:HE21	1.60	0.66
16:D:92:PHE:HA	16:D:103:VAL:HG12	1.77	0.66
1:a:73:PRO:HG3	1:a:104:VAL:HG11	1.78	0.66
29:Q:102:LEU:HB2	29:Q:118:MET:HB2	1.78	0.66
7:U:353:LEU:O	7:U:357:LYS:HB2	1.96	0.65
18:F:424:ILE:CG2	18:F:428:GLN:HE21	2.04	0.65
19:g:46:ASP:CB	19:g:222:VAL:HG22	2.16	0.65
30:r:52:CYS:O	30:r:56:GLU:HB2	1.95	0.65
8:V:330:LYS:HG3	8:V:358:MET:HB3	1.78	0.65
11:Y:271:PHE:O	11:Y:275:LEU:HB2	1.95	0.65
14:B:439:TYR:OH	22:J:28:LYS:HB2	1.97	0.65
24:l:184:LEU:HD12	24:l:184:LEU:H	1.60	0.65
13:A:122:VAL:HB	18:F:88:TYR:HB2	1.79	0.65
32:t:162:GLN:O	32:t:166:ARG:HB2	1.95	0.65
7:U:185:MET:SD	7:U:194:ARG:NH2	2.69	0.65
19:g:11:ARG:HG3	19:g:23:TYR:CD2	2.30	0.65
6:f:140:LEU:O	6:f:144:LEU:HB2	1.96	0.65
7:U:549:ALA:HB1	7:U:581:SER:HB2	1.79	0.65
7:U:561:GLU:OE2	7:U:562:GLU:OE2	2.15	0.65
19:g:10:ASP:C	25:m:7:TYR:OH	2.36	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:129:ALA:N	20:h:127:VAL:HG12	2.11	0.65
19:G:141:ILE:HA	19:G:150:GLN:O	1.96	0.65
19:g:11:ARG:HG3	19:g:23:TYR:CB	2.24	0.65
20:h:167:TYR:O	20:h:171:LYS:HB2	1.97	0.65
21:i:175:LEU:O	21:i:179:TYR:HB2	1.96	0.65
23:k:76:CYS:SG	23:k:77:ALA:N	2.69	0.65
2:b:22:LEU:CD1	2:b:179:LEU:CA	2.38	0.65
9:W:6:SER:O	9:W:10:ASP:HB3	1.96	0.65
23:K:76:CYS:SG	23:K:77:ALA:N	2.69	0.65
26:n:88:TYR:O	26:n:91:ARG:CG	2.44	0.65
6:f:654:VAL:HA	6:f:657:ILE:HD12	1.78	0.65
8:V:78:HIS:H	8:V:81:GLN:HG3	1.62	0.65
8:V:360:TYR:HB3	8:V:363:LEU:HB3	1.77	0.65
18:F:68:ALA:O	18:F:72:LYS:HB2	1.96	0.65
19:G:22:LEU:CD1	19:G:24:GLN:H	1.95	0.65
28:P:26:ARG:HH21	28:P:38:ASP:HA	1.62	0.65
21:i:17:ARG:HH11	21:i:17:ARG:C	2.04	0.65
1:a:64:ILE:O	1:a:68:GLU:HB3	1.97	0.65
14:B:427:LEU:CA	14:B:431:GLN:HB2	2.26	0.65
21:i:119:GLN:HE21	21:i:123:GLN:HE22	1.45	0.65
22:j:73:PHE:HA	22:j:131:ALA:HA	1.79	0.65
25:m:192:GLU:HA	25:m:195:LYS:HE3	1.79	0.65
6:f:30:GLY:O	6:f:34:ARG:HB2	1.97	0.65
6:f:166:VAL:O	6:f:170:TRP:HB2	1.97	0.65
7:U:12:LEU:HB3	7:U:20:LYS:HE3	1.79	0.65
7:U:807:LYS:HA	7:U:836:THR:HB	1.79	0.65
16:D:380:GLN:O	16:D:384:MET:HB2	1.97	0.65
19:G:17:SER:CB	19:G:18:PRO:HD2	2.19	0.65
25:M:192:GLU:HA	25:M:195:LYS:HE3	1.79	0.65
19:g:153:LYS:O	19:g:160:TYR:HA	1.97	0.65
6:f:268:LEU:O	6:f:272:LEU:HB2	1.97	0.64
9:W:110:THR:O	9:W:114:GLU:HB3	1.97	0.64
18:F:435:LEU:HD22	24:L:51:ARG:NH1	2.10	0.64
1:a:178:ARG:O	1:a:182:CYS:HB3	1.96	0.64
5:e:43:TRP:HD1	8:V:349:ARG:CB	2.10	0.64
13:A:284:ARG:HD2	18:F:334:ARG:HD3	1.78	0.64
19:g:17:SER:CB	19:g:21:ARG:O	2.45	0.64
21:i:47:ALA:HB3	21:i:212:GLU:HB3	1.80	0.64
22:j:131:ALA:H	22:j:147:THR:HG1	1.43	0.64
1:a:14:SER:H	1:a:18:GLN:HG2	1.60	0.64
15:C:90:HIS:CE1	16:D:110:ASN:CG	2.74	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:128:ASN:CA	20:H:127:VAL:HG13	2.23	0.64
22:J:73:PHE:HA	22:J:131:ALA:HA	1.79	0.64
19:g:82:GLY:HA3	19:g:136:CYS:HA	1.80	0.64
13:A:141:GLY:O	13:A:149:ILE:HA	1.97	0.64
16:D:94:GLU:HB2	16:D:102:ILE:HB	1.78	0.64
19:G:82:GLY:HA3	19:G:136:CYS:HA	1.80	0.64
19:g:11:ARG:NH1	19:g:27:TYR:CE2	2.63	0.64
21:i:17:ARG:NH1	21:i:17:ARG:O	2.30	0.64
6:f:618:GLU:HG2	6:f:623:LYS:HD2	1.80	0.64
19:G:153:LYS:O	19:G:160:TYR:HA	1.97	0.64
7:U:70:HIS:HA	8:V:236:ARG:HH12	1.62	0.64
18:F:435:LEU:HD13	24:L:51:ARG:HH11	1.63	0.64
21:I:149:GLN:O	21:I:156:TYR:HA	1.96	0.64
26:n:144:ARG:H	26:n:147:MET:HE3	1.62	0.64
9:W:408:ARG:HG2	10:X:345:VAL:HG13	1.79	0.64
15:C:24:TYR:HB3	15:C:27:LYS:HB2	1.80	0.64
27:O:201:ARG:NH1	27:O:203:ARG:HH21	1.86	0.64
29:q:102:LEU:HB2	29:q:118:MET:HB2	1.78	0.64
10:X:163:LYS:HG3	10:X:196:THR:HG23	1.80	0.64
23:k:77:ALA:HB3	23:k:142:LEU:HB2	1.80	0.64
11:Y:134:LEU:O	11:Y:138:LEU:HB2	1.97	0.63
15:C:78:ARG:HH12	15:C:80:MET:HE3	1.62	0.63
6:f:501:LEU:HD22	6:f:518:THR:HG23	1.79	0.63
20:H:167:TYR:O	20:H:171:LYS:HB2	1.97	0.63
21:I:29:GLY:HA2	21:I:165:GLY:HA3	1.80	0.63
21:I:47:ALA:HB3	21:I:212:GLU:HB3	1.80	0.63
22:J:183:THR:O	22:J:186:LEU:N	2.30	0.63
26:N:144:ARG:H	26:N:147:MET:HE3	1.62	0.63
25:m:48:GLY:HA2	25:m:212:GLU:O	1.98	0.63
4:d:75:MET:HE2	4:d:102:ASN:HB2	1.79	0.63
8:V:149:PRO:O	8:V:153:LYS:HB2	1.97	0.63
8:V:333:ILE:CD1	8:V:345:ARG:NE	2.42	0.63
12:Z:45:LYS:HB3	12:Z:47:VAL:HG12	1.80	0.63
31:S:35:ILE:HB	32:T:151:ARG:HH12	1.63	0.63
31:S:123:SER:HB3	31:S:136:LYS:HG3	1.80	0.63
7:U:477:GLY:O	7:U:481:LEU:HB2	1.99	0.63
10:X:77:LEU:HD12	10:X:88:LEU:HD22	1.81	0.63
24:l:50:LYS:HB3	24:l:59:HIS:HB3	1.80	0.63
31:s:123:SER:HB3	31:s:136:LYS:HG3	1.80	0.63
1:a:70:ARG:HH22	2:b:79:GLN:HE22	1.45	0.63
7:U:80:TYR:O	7:U:84:ALA:HB2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:418:SER:HA	8:V:458:VAL:HB	1.81	0.63
14:B:426:VAL:O	14:B:429:LYS:HB3	1.99	0.63
18:F:430:LYS:H	18:F:430:LYS:CE	2.10	0.63
23:K:16:SER:CB	23:K:22:PHE:CE2	2.81	0.63
23:K:77:ALA:HB3	23:K:142:LEU:HB2	1.80	0.63
19:g:11:ARG:HG3	19:g:23:TYR:HD2	1.63	0.63
7:U:528:ALA:O	7:U:532:MET:HB2	1.99	0.63
23:K:16:SER:HA	23:K:22:PHE:HZ	1.61	0.63
6:f:692:LEU:O	6:f:696:LEU:HB2	1.97	0.63
7:U:583:MET:SD	7:U:601:ARG:NH1	2.72	0.63
11:Y:173:ASP:OD2	11:Y:176:ARG:NH2	2.32	0.63
13:A:103:ASN:HA	13:A:136:GLU:HG2	1.80	0.63
15:C:192:PRO:HA	15:C:196:LYS:HE3	1.81	0.63
22:J:109:ARG:NH2	30:R:70:ASN:OD1	2.32	0.63
27:O:201:ARG:HH12	27:O:203:ARG:HH22	1.39	0.63
26:n:18:SER:HB2	26:n:31:THR:H	1.64	0.63
12:Z:274:ASN:O	12:Z:278:ASN:HB2	1.99	0.63
13:A:114:ASN:HB3	13:A:120:LYS:HG2	1.81	0.63
16:D:417:TYR:OH	19:G:21:ARG:HD2	1.99	0.63
21:I:151:ASP:HB2	21:I:155:ASN:O	1.99	0.63
20:h:4:ARG:HD3	25:m:127:ALA:HB2	1.79	0.63
7:U:576:PRO:HG2	7:U:577:ILE:HG12	1.80	0.62
15:C:90:HIS:CE1	16:D:110:ASN:CA	2.82	0.62
23:k:10:ARG:HG3	23:k:14:THR:HG21	1.81	0.62
32:t:126:ASP:HB2	32:t:130:VAL:O	1.99	0.62
7:U:643:SER:O	7:U:649:ARG:NH1	2.32	0.62
19:g:103:TYR:O	27:o:81:ARG:NH1	2.30	0.62
19:g:128:ASN:HA	20:h:127:VAL:HG13	0.64	0.62
8:V:106:ARG:O	8:V:110:HIS:ND1	2.32	0.62
14:B:266:LEU:O	14:B:270:LEU:HB2	1.98	0.62
14:B:283:PHE:HA	14:B:328:ILE:O	1.99	0.62
17:E:182:LEU:HD22	34:E:401:ATP:H2'	1.81	0.62
31:S:4:PRO:O	32:T:100:ARG:NH2	2.32	0.62
21:i:34:CYS:H	21:i:164:ILE:HG13	1.64	0.62
25:m:149:TYR:HA	25:m:159:GLY:HA2	1.81	0.62
8:V:239:THR:HG22	8:V:240:LEU:HG	1.81	0.62
8:V:248:ALA:HA	8:V:251:LEU:HB3	1.81	0.62
24:L:183:ASN:O	24:L:187:LEU:HB2	2.00	0.62
25:M:149:TYR:HA	25:M:159:GLY:HA2	1.81	0.62
26:N:18:SER:HB2	26:N:31:THR:H	1.64	0.62
24:l:183:ASN:O	24:l:187:LEU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:26:ARG:HH21	28:p:38:ASP:HA	1.62	0.62
16:D:45:LYS:O	16:D:49:GLN:NE2	2.32	0.62
18:F:341:ALA:HA	18:F:344:ARG:CD	2.29	0.62
21:i:13:SER:CB	21:i:17:ARG:NE	2.63	0.62
21:i:29:GLY:HA2	21:i:165:GLY:HA3	1.80	0.62
21:i:98:LEU:O	21:i:102:GLN:HA	1.99	0.62
8:V:117:VAL:HA	8:V:121:PHE:HB2	1.80	0.62
21:I:119:GLN:HE21	21:I:123:GLN:HE22	1.45	0.62
21:i:151:ASP:HB2	21:i:155:ASN:O	1.99	0.62
25:M:47:PHE:HB2	25:M:214:SER:HB3	1.82	0.62
1:a:176:ALA:O	1:a:180:LEU:CB	2.48	0.62
5:e:56:LEU:HB2	5:e:59:GLU:HB2	1.82	0.62
10:X:369:ILE:HG22	11:Y:310:SER:HB3	1.81	0.62
20:h:111:VAL:O	20:h:115:ALA:HB3	2.00	0.62
5:e:43:TRP:CD1	8:V:349:ARG:H	2.01	0.62
6:f:536:SER:O	6:f:540:GLN:HB2	2.00	0.62
19:G:203:SER:C	19:G:207:SER:HA	2.22	0.62
7:U:559:ARG:HD2	7:U:562:GLU:CB	2.27	0.62
9:W:407:ASP:H	9:W:413:ILE:HG22	1.64	0.62
16:D:408:LYS:HZ3	17:E:389:VAL:CB	2.12	0.62
18:F:180:ARG:HH12	18:F:245:LYS:HG2	1.65	0.62
21:i:17:ARG:NH2	21:i:19:TYR:CD1	2.68	0.62
1:a:247:ARG:HE	1:a:251:LEU:HB2	1.65	0.61
6:f:136:GLU:O	6:f:140:LEU:HB2	1.99	0.61
6:f:459:CYS:O	6:f:463:LEU:HB2	2.00	0.61
19:g:5:SER:HA	19:g:18:PRO:HB2	1.81	0.61
2:b:22:LEU:CD2	2:b:179:LEU:C	2.73	0.61
6:f:80:ARG:O	6:f:84:SER:HB3	1.99	0.61
7:U:742:HIS:O	7:U:883:ARG:NH2	2.33	0.61
21:I:98:LEU:O	21:I:102:GLN:HA	1.99	0.61
25:M:48:GLY:HA2	25:M:212:GLU:O	1.98	0.61
26:N:21:THR:HG22	26:N:26:ILE:HG13	1.82	0.61
18:F:437:TYR:CD2	23:K:20:ARG:CD	2.51	0.61
32:T:126:ASP:HB2	32:T:130:VAL:O	1.99	0.61
21:i:8:ARG:CB	21:i:11:ILE:HD13	2.30	0.61
6:f:253:LEU:O	6:f:257:ARG:HB2	1.99	0.61
8:V:251:LEU:O	8:V:255:LEU:HB2	2.00	0.61
10:X:82:LYS:HB3	10:X:122:ARG:HH12	1.64	0.61
12:Z:263:ALA:O	12:Z:267:ARG:HB2	2.00	0.61
15:C:161:ILE:HG23	15:C:165:ILE:HD12	1.81	0.61
21:I:34:CYS:H	21:I:164:ILE:HG13	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:163:ILE:HA	27:O:168:GLY:HA3	1.82	0.61
6:f:455:VAL:HG12	6:f:457:ASN:H	1.65	0.61
6:f:502:LEU:HG	6:f:540:GLN:HE22	1.65	0.61
24:L:50:LYS:HB3	24:L:59:HIS:HB3	1.80	0.61
26:N:178:ALA:HB3	26:N:185:GLU:HB2	1.83	0.61
32:t:180:ASP:HB3	32:t:183:SER:HB3	1.83	0.61
1:a:349:MET:O	1:a:353:LEU:CB	2.48	0.61
7:U:801:GLN:HA	7:U:841:LYS:HB2	1.82	0.61
11:Y:53:TYR:O	11:Y:57:LEU:HB2	2.00	0.61
14:B:419:PHE:O	14:B:423:LYS:HB2	2.00	0.61
21:I:8:ARG:CB	21:I:11:ILE:HD13	2.31	0.61
23:k:21:LEU:CD1	23:k:24:VAL:HG23	2.29	0.61
4:d:36:LEU:CD1	4:d:84:ASP:HB2	2.30	0.61
15:C:57:ARG:NH2	16:D:71:GLU:OE1	2.33	0.61
16:D:403:TYR:CG	16:D:407:ILE:CG1	2.81	0.61
24:L:43:HIS:CG	24:L:184:LEU:CD1	2.71	0.61
4:d:80:CYS:HA	4:d:83:PHE:HB3	1.83	0.61
7:U:561:GLU:OE2	7:U:562:GLU:CD	2.44	0.61
17:E:334:LEU:HB3	17:E:371:VAL:HG11	1.82	0.61
23:K:48:LEU:HB3	23:K:218:ALA:HB3	1.83	0.61
24:L:43:HIS:HB2	24:L:184:LEU:CD1	2.30	0.61
24:l:65:HIS:O	24:l:89:ARG:NH2	2.34	0.61
31:s:24:ALA:HA	31:s:194:ARG:O	2.01	0.61
7:U:112:CYS:O	7:U:116:ALA:HB2	2.01	0.61
20:H:111:VAL:O	20:H:115:ALA:HB3	2.00	0.61
22:j:72:ALA:HB3	22:j:132:LEU:HB2	1.83	0.61
25:m:47:PHE:HB2	25:m:214:SER:HB3	1.82	0.61
26:n:88:TYR:CB	26:n:91:ARG:HD3	2.28	0.61
27:o:163:ILE:HA	27:o:168:GLY:HA3	1.82	0.61
1:a:345:GLN:O	1:a:349:MET:HB2	2.00	0.60
6:f:236:CYS:HA	6:f:240:VAL:HB	1.83	0.60
7:U:235:LYS:O	7:U:239:GLU:HB2	2.01	0.60
10:X:386:ILE:CG2	10:X:388:PHE:CD1	2.83	0.60
13:A:306:LEU:O	13:A:312:ARG:CG	2.48	0.60
16:D:368:ASP:N	16:D:368:ASP:OD1	2.30	0.60
20:H:139:TRP:HA	20:H:144:PRO:HA	1.83	0.60
21:I:123:GLN:NE2	22:J:79:ASP:OD1	2.33	0.60
23:k:20:ARG:HH21	23:k:20:ARG:CG	2.14	0.60
6:f:359:GLY:O	6:f:363:SER:CB	2.49	0.60
18:F:432:LYS:HZ3	18:F:432:LYS:HB2	1.65	0.60
24:L:183:ASN:O	24:L:187:LEU:CB	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:139:TRP:HA	20:h:144:PRO:HA	1.83	0.60
26:n:21:THR:HG22	26:n:26:ILE:HG13	1.82	0.60
4:d:177:GLU:O	4:d:181:CYS:HB2	2.01	0.60
8:V:80:LYS:HE3	8:V:83:GLU:HB3	1.82	0.60
19:G:22:LEU:CD1	19:G:24:GLN:HB2	2.32	0.60
27:O:204:CYS:HB2	27:O:208:THR:HG21	1.83	0.60
2:b:51:LEU:HD11	2:b:61:LEU:HB2	1.84	0.60
2:b:157:VAL:HG21	2:b:170:LEU:HB2	1.84	0.60
8:V:237:THR:OG1	8:V:241:ARG:NH2	2.34	0.60
8:V:345:ARG:HH12	8:V:359:PRO:C	2.09	0.60
9:W:429:SER:O	9:W:433:ASN:HB3	2.02	0.60
13:A:94:GLN:NE2	13:A:143:ASP:OD1	2.35	0.60
26:n:178:ALA:HB3	26:n:185:GLU:HB2	1.82	0.60
11:Y:297:ARG:HA	11:Y:300:ARG:HG2	1.83	0.60
15:C:164:VAL:HG13	15:C:165:ILE:HG13	1.84	0.60
16:D:119:ILE:HG23	16:D:123:LEU:HD12	1.83	0.60
20:H:39:LYS:HE2	20:H:144:PRO:HG2	1.84	0.60
23:K:16:SER:CA	23:K:22:PHE:CZ	2.82	0.60
31:S:24:ALA:HA	31:S:194:ARG:O	2.01	0.60
6:f:370:MET:O	6:f:374:SER:HB2	2.02	0.60
27:o:204:CYS:HB2	27:o:208:THR:HG21	1.83	0.60
29:q:6:GLY:HA2	29:q:15:VAL:HG12	1.83	0.60
32:t:1:THR:N	32:t:105:PRO:O	2.35	0.60
7:U:173:VAL:HG22	7:U:175:GLY:H	1.66	0.60
16:D:408:LYS:NZ	17:E:389:VAL:HB	2.16	0.60
29:Q:48:GLY:HA3	29:Q:100:VAL:HA	1.84	0.60
32:T:180:ASP:HB3	32:T:183:SER:HB3	1.82	0.60
27:o:13:VAL:HA	27:o:176:CYS:O	2.02	0.60
16:D:416:PHE:O	16:D:418:LYS:N	2.34	0.60
27:O:7:VAL:HG22	27:O:12:ILE:HG12	1.82	0.60
29:Q:6:GLY:HA2	29:Q:15:VAL:HG12	1.83	0.60
29:Q:198:LYS:H	29:q:198:LYS:H	1.49	0.60
22:j:10:PHE:HB2	23:k:26:TYR:HB3	1.84	0.60
23:k:32:LYS:HZ3	23:k:173:ALA:H	1.48	0.60
25:m:17:ASP:OD2	25:m:19:ARG:NH2	2.35	0.60
1:a:70:ARG:HG2	2:b:17:ARG:HB3	1.84	0.60
2:b:9:CYS:O	2:b:112:PHE:HB2	2.01	0.60
4:d:12:LYS:HB3	4:d:61:TRP:HE1	1.67	0.60
17:E:180:LYS:HG2	17:E:301:ILE:HD12	1.83	0.60
19:G:65:THR:HB	25:M:158:TYR:HB2	1.83	0.60
32:T:1:THR:N	32:T:105:PRO:O	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:19:GLU:OE1	19:g:19:GLU:HA	2.01	0.60
21:I:161:ALA:HB1	21:I:175:LEU:HD13	1.83	0.60
25:M:68:ASN:ND2	25:M:224:HIS:O	2.35	0.60
20:h:39:LYS:HE2	20:h:144:PRO:HG2	1.84	0.60
25:m:68:ASN:ND2	25:m:224:HIS:O	2.35	0.60
6:f:234:THR:O	6:f:238:ASN:HB2	2.02	0.59
6:f:333:LEU:HA	6:f:338:ASP:CG	2.27	0.59
9:W:243:ILE:HD12	9:W:273:TYR:HB2	1.82	0.59
13:A:312:ARG:NH2	13:A:317:VAL:HG23	2.13	0.59
16:D:119:ILE:O	16:D:121:ARG:NH1	2.35	0.59
16:D:385:LEU:HD23	16:D:398:ASP:HA	1.84	0.59
19:G:22:LEU:HD11	19:G:25:VAL:H	1.66	0.59
25:M:67:PHE:HB2	25:M:75:MET:HB2	1.84	0.59
27:O:174:ASP:OD2	27:O:187:ARG:NH1	2.35	0.59
2:b:124:LEU:O	2:b:128:ALA:HB2	2.01	0.59
4:d:36:LEU:N	4:d:36:LEU:HD23	2.18	0.59
10:X:415:TYR:O	10:X:419:LYS:HB2	2.03	0.59
23:K:209:LYS:O	23:K:214:ASN:ND2	2.35	0.59
24:L:65:HIS:O	24:L:89:ARG:NH2	2.34	0.59
30:R:19:ARG:HE	30:R:29:GLN:HE22	1.50	0.59
3:c:103:GLY:HA3	12:Z:25:ARG:HB3	1.84	0.59
6:f:130:ALA:O	6:f:134:SER:HB3	2.01	0.59
8:V:333:ILE:HD13	8:V:345:ARG:HE	1.58	0.59
11:Y:225:TYR:HA	11:Y:228:MET:HE3	1.83	0.59
15:C:320:PRO:O	15:C:325:ARG:NH1	2.35	0.59
32:T:171:ARG:NH2	27:o:140:ASP:OD1	2.35	0.59
19:g:9:PHE:O	19:g:9:PHE:HD1	1.85	0.59
3:c:42:LEU:O	3:c:46:ARG:CB	2.51	0.59
8:V:226:VAL:O	8:V:230:PHE:HB3	2.02	0.59
8:V:345:ARG:NH2	8:V:359:PRO:O	2.34	0.59
15:C:43:ARG:HH21	16:D:57:GLN:HB2	1.67	0.59
25:M:17:ASP:OD2	25:M:19:ARG:NH2	2.35	0.59
21:i:161:ALA:HB1	21:i:175:LEU:HD13	1.83	0.59
6:f:625:LYS:HA	6:f:657:ILE:HD11	1.84	0.59
7:U:14:GLU:O	7:U:20:LYS:NZ	2.35	0.59
7:U:740:GLY:O	7:U:743:ASN:ND2	2.36	0.59
9:W:187:LEU:HA	9:W:190:MET:HE3	1.85	0.59
10:X:337:ARG:NH1	10:X:340:GLU:OE1	2.35	0.59
11:Y:13:LYS:O	11:Y:17:LEU:HB2	2.03	0.59
21:I:118:LYS:NZ	21:I:132:VAL:O	2.35	0.59
6:f:628:ASP:HB2	6:f:657:ILE:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:86:ASN:ND2	9:W:96:GLN:OE1	2.35	0.59
9:W:169:LEU:O	9:W:208:LYS:NZ	2.36	0.59
18:F:98:ASP:OD1	18:F:120:LYS:N	2.35	0.59
27:O:13:VAL:HA	27:O:176:CYS:O	2.02	0.59
20:h:9:SER:OG	20:h:123:GLN:C	2.38	0.59
21:i:138:GLY:O	21:i:145:PHE:HA	2.02	0.59
23:k:209:LYS:O	23:k:214:ASN:ND2	2.35	0.59
24:l:183:ASN:O	24:l:187:LEU:CB	2.50	0.59
27:o:7:VAL:HG22	27:o:12:ILE:HG12	1.82	0.59
4:d:178:ILE:O	4:d:213:ARG:NH2	2.34	0.59
6:f:586:PRO:HA	6:f:589:SER:HB2	1.83	0.59
6:f:790:GLN:HG3	6:f:792:ALA:H	1.68	0.59
8:V:126:ALA:HB1	8:V:130:PHE:HB2	1.84	0.59
9:W:78:LYS:O	9:W:82:LEU:HB2	2.02	0.59
10:X:385:LEU:N	10:X:385:LEU:HD12	2.17	0.59
17:E:141:GLN:HG2	17:E:301:ILE:HG12	1.84	0.59
22:J:72:ALA:HB3	22:J:132:LEU:HB2	1.83	0.59
21:i:174:MET:O	21:i:178:ASP:HB2	2.03	0.59
26:n:19:ARG:NH2	26:n:168:GLY:O	2.35	0.59
27:o:174:ASP:OD2	27:o:187:ARG:NH1	2.35	0.59
7:U:646:PRO:O	7:U:650:TYR:CB	2.49	0.59
9:W:422:ASN:HD21	9:W:425:LEU:HB3	1.68	0.59
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.83	0.59
17:E:349:GLU:OE1	17:E:373:LYS:NZ	2.36	0.59
34:E:401:ATP:O1G	18:F:344:ARG:NE	2.34	0.59
1:a:294:GLU:O	1:a:298:LYS:HB3	2.03	0.59
3:c:112:TYR:HA	3:c:143:VAL:HB	1.83	0.59
6:f:691:PRO:HG2	6:f:745:LEU:HB2	1.85	0.59
10:X:370:LEU:HD23	11:Y:310:SER:HB2	1.84	0.59
21:I:174:MET:O	21:I:178:ASP:HB2	2.03	0.59
30:R:77:ALA:O	30:R:81:LYS:HB2	2.02	0.59
21:i:118:LYS:NZ	21:i:132:VAL:O	2.35	0.59
4:d:33:LEU:HD23	4:d:48:LEU:HD21	1.84	0.59
26:N:19:ARG:NH2	26:N:168:GLY:O	2.35	0.59
30:R:51:ASP:O	30:R:55:TRP:HB2	2.03	0.59
31:S:185:ARG:NH1	27:o:26:VAL:O	2.35	0.59
25:m:67:PHE:HB2	25:m:75:MET:HB2	1.84	0.59
29:q:48:GLY:HA3	29:q:100:VAL:HA	1.84	0.59
7:U:155:LEU:O	7:U:158:ARG:NH1	2.32	0.58
9:W:183:VAL:HG21	9:W:223:LYS:HE3	1.84	0.58
11:Y:142:PHE:HA	11:Y:145:LEU:HD12	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:89:ILE:HD11	17:E:80:VAL:HG23	1.85	0.58
18:F:341:ALA:HA	18:F:344:ARG:HH21	1.65	0.58
23:K:100:TRP:O	30:R:57:ARG:NH2	2.36	0.58
28:p:15:LYS:HE3	28:p:121:ILE:HG12	1.84	0.58
7:U:164:GLU:O	7:U:168:LEU:HB2	2.03	0.58
11:Y:16:ASP:HB3	11:Y:146:ARG:HH21	1.69	0.58
23:k:48:LEU:HB3	23:k:218:ALA:HB3	1.83	0.58
4:d:158:ILE:HG21	4:d:163:TYR:HB2	1.85	0.58
16:D:98:GLN:HE22	16:D:121:ARG:HE	1.50	0.58
26:N:120:MET:H	32:T:61:GLN:HE22	1.49	0.58
30:R:21:THR:HA	30:R:27:ALA:H	1.69	0.58
25:m:137:LEU:HB2	25:m:149:TYR:HB2	1.85	0.58
29:q:140:LEU:O	29:q:144:ASP:HB2	2.03	0.58
1:a:196:ARG:O	1:a:200:LEU:HB2	2.03	0.58
6:f:80:ARG:HB3	6:f:95:PRO:HB2	1.84	0.58
6:f:471:LEU:HG	6:f:509:LYS:HE3	1.85	0.58
11:Y:66:ASP:O	11:Y:71:ASN:N	2.32	0.58
25:M:100:SER:O	32:T:65:GLN:NE2	2.36	0.58
19:g:203:SER:C	19:g:207:SER:HA	2.22	0.58
26:n:41:ILE:HG12	26:n:76:VAL:HG22	1.85	0.58
18:F:344:ARG:NH1	18:F:347:ARG:NH1	2.37	0.58
19:G:54:LYS:NZ	19:G:213:SER:O	2.36	0.58
21:I:101:TYR:HB3	29:Q:79:ALA:HB1	1.85	0.58
21:I:138:GLY:O	21:I:145:PHE:HA	2.02	0.58
23:K:32:LYS:HZ3	23:K:173:ALA:H	1.51	0.58
29:Q:140:LEU:O	29:Q:144:ASP:HB2	2.03	0.58
21:i:239:LYS:NZ	21:i:243:GLU:OE2	2.37	0.58
30:r:77:ALA:O	30:r:81:LYS:HB2	2.02	0.58
8:V:338:LEU:HD11	8:V:394:LEU:HA	1.84	0.58
9:W:187:LEU:HB3	9:W:226:TYR:HE1	1.67	0.58
13:A:413:VAL:HG13	13:A:417:ILE:HD12	1.85	0.58
14:B:315:GLN:OE1	14:B:322:ARG:NH1	2.37	0.58
18:F:436:GLN:O	18:F:438:TYR:N	2.37	0.58
19:g:54:LYS:NZ	19:g:213:SER:O	2.36	0.58
30:r:51:ASP:O	30:r:55:TRP:HB2	2.03	0.58
31:s:210:LEU:O	31:s:212:LYS:NZ	2.37	0.58
9:W:408:ARG:HB2	9:W:408:ARG:HH21	1.68	0.58
11:Y:36:ALA:O	11:Y:40:GLU:HB2	2.04	0.58
16:D:174:LYS:O	16:D:178:ARG:HB2	2.04	0.58
19:G:22:LEU:CD1	19:G:24:GLN:N	2.62	0.58
28:P:15:LYS:HE3	28:P:121:ILE:HG12	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:17:ARG:HH22	21:i:19:TYR:HB2	1.65	0.58
26:n:87:CYS:C	26:n:91:ARG:HG2	2.25	0.58
28:p:60:VAL:O	28:p:64:ALA:HB2	2.04	0.58
5:e:43:TRP:CD1	8:V:349:ARG:HG3	2.38	0.58
7:U:147:TYR:OH	7:U:171:ASN:OD1	2.21	0.58
7:U:519:VAL:HG23	7:U:520:MET:HG2	1.86	0.58
11:Y:141:VAL:HG13	11:Y:160:ASN:HB2	1.84	0.58
13:A:386:ARG:HH22	14:B:345:GLY:HA2	1.68	0.58
16:D:199:PRO:HB3	16:D:328:ASP:HB2	1.86	0.58
18:F:305:GLU:HA	18:F:308:ARG:HB2	1.86	0.58
31:s:35:ILE:HB	32:t:151:ARG:HH12	1.69	0.58
2:b:26:LEU:O	2:b:30:GLN:HB2	2.03	0.58
6:f:556:ARG:NH1	6:f:786:GLN:OE1	2.37	0.58
7:U:895:PRO:HG2	7:U:901:GLN:HG2	1.84	0.58
8:V:452:ASN:HB3	8:V:457:TYR:HB2	1.85	0.58
14:B:440:LEU:HD13	14:B:440:LEU:N	2.19	0.58
19:G:6:SER:N	19:G:18:PRO:CG	2.65	0.58
26:N:41:ILE:HG12	26:N:76:VAL:HG22	1.85	0.58
23:k:143:PHE:HB2	23:k:154:PHE:HB2	1.86	0.58
4:d:102:ASN:O	4:d:106:LEU:CB	2.51	0.58
6:f:269:ALA:HB2	6:f:277:LEU:HD22	1.85	0.58
13:A:351:ARG:HE	13:A:374:ALA:HB1	1.68	0.58
14:B:438:LEU:HD13	14:B:438:LEU:H	1.68	0.58
25:M:137:LEU:HB2	25:M:149:TYR:HB2	1.85	0.58
19:g:17:SER:HB3	19:g:21:ARG:O	2.04	0.58
2:b:22:LEU:CG	2:b:179:LEU:C	2.77	0.57
4:d:175:ARG:HD3	4:d:178:ILE:HD12	1.85	0.57
6:f:129:LEU:O	6:f:133:MET:CB	2.51	0.57
8:V:227:VAL:HA	8:V:230:PHE:HB3	1.86	0.57
9:W:317:TRP:HD1	9:W:358:VAL:HG11	1.68	0.57
28:P:60:VAL:O	28:P:64:ALA:HB2	2.04	0.57
30:r:58:LEU:HD12	30:r:61:ARG:HD3	1.86	0.57
4:d:143:LEU:O	8:V:440:LYS:NZ	2.36	0.57
5:e:63:HIS:HA	5:e:66:LYS:HG3	1.85	0.57
14:B:439:TYR:CB	22:J:76:LEU:HB3	2.33	0.57
21:I:239:LYS:NZ	21:I:243:GLU:OE2	2.37	0.57
24:L:77:LEU:HD12	24:L:129:GLY:H	1.69	0.57
30:R:44:THR:HG21	30:R:100:MET:HE3	1.86	0.57
19:g:11:ARG:O	19:g:11:ARG:HG2	2.03	0.57
30:r:19:ARG:HE	30:r:29:GLN:HE22	1.50	0.57
6:f:332:ALA:O	6:f:338:ASP:OD2	2.23	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:470:VAL:HG22	6:f:471:LEU:HB2	1.86	0.57
8:V:477:HIS:O	8:V:481:SER:CB	2.51	0.57
9:W:172:GLU:OE1	9:W:182:ARG:NH2	2.37	0.57
11:Y:51:ALA:HA	11:Y:54:TYR:HB3	1.86	0.57
12:Z:9:VAL:HA	12:Z:48:LEU:HB3	1.85	0.57
14:B:250:VAL:HB	14:B:284:ILE:HG12	1.86	0.57
22:J:92:GLN:HG2	29:Q:66:LEU:HB2	1.86	0.57
30:R:58:LEU:HD12	30:R:61:ARG:HD3	1.86	0.57
8:V:82:LEU:HA	8:V:87:SER:HB2	1.86	0.57
8:V:259:LEU:HD13	8:V:294:ARG:HH21	1.70	0.57
9:W:428:TRP:HA	9:W:432:LEU:HD13	1.86	0.57
17:E:344:ARG:NH1	34:E:401:ATP:O2'	2.37	0.57
24:L:41:LYS:NZ	24:L:180:MET:O	2.37	0.57
31:S:14:ALA:O	31:S:135:PHE:HA	2.05	0.57
8:V:345:ARG:HH12	8:V:359:PRO:HB2	1.69	0.57
14:B:387:LYS:NZ	14:B:431:GLN:CG	2.48	0.57
15:C:161:ILE:HA	15:C:164:VAL:HG12	1.87	0.57
15:C:173:GLU:O	15:C:177:ALA:HB2	2.04	0.57
16:D:68:LEU:O	16:D:72:PHE:HB2	2.04	0.57
23:K:93:ARG:HD3	30:R:68:LEU:HD13	1.86	0.57
28:p:62:THR:OG1	29:q:85:ARG:NH2	2.38	0.57
5:e:60:LEU:C	5:e:64:GLY:H	2.12	0.57
11:Y:66:ASP:HB2	11:Y:70:LEU:HB2	1.87	0.57
13:A:411:GLU:O	13:A:415:LYS:HB2	2.04	0.57
30:R:50:ALA:O	30:R:54:PHE:HB3	2.04	0.57
31:S:210:LEU:O	31:S:212:LYS:NZ	2.37	0.57
24:l:41:LYS:NZ	24:l:180:MET:O	2.37	0.57
1:a:49:CYS:SG	1:a:50:PHE:N	2.78	0.57
9:W:231:ILE:O	9:W:235:GLN:HB2	2.04	0.57
11:Y:36:ALA:O	11:Y:40:GLU:CB	2.52	0.57
2:b:22:LEU:CG	2:b:179:LEU:HA	2.31	0.57
6:f:281:ILE:O	6:f:285:CYS:CB	2.53	0.57
7:U:400:ALA:O	7:U:404:ALA:HB2	2.05	0.57
8:V:227:VAL:O	8:V:231:LEU:CB	2.48	0.57
10:X:74:ARG:HH22	10:X:116:TRP:HB2	1.70	0.57
13:A:90:GLU:HA	13:A:93:LEU:HD23	1.86	0.57
15:C:132:ASP:HB3	15:C:135:VAL:HB	1.87	0.57
20:H:45:VAL:HG22	20:H:212:ILE:HG22	1.87	0.57
31:s:14:ALA:O	31:s:135:PHE:HA	2.05	0.57
31:s:192:ALA:HA	31:s:209:SER:HA	1.87	0.57
3:c:93:ALA:O	3:c:97:ASP:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:104:ARG:HE	3:c:106:GLU:HB3	1.69	0.57
6:f:575:ALA:O	6:f:579:ALA:HB2	2.04	0.57
8:V:159:LEU:HB3	8:V:175:MET:HG2	1.87	0.57
8:V:337:LEU:O	8:V:401:ASN:ND2	2.38	0.57
11:Y:267:ARG:HB2	11:Y:270:VAL:HG12	1.87	0.57
13:A:237:PHE:HA	13:A:271:LEU:HB2	1.86	0.57
15:C:73:VAL:HG11	15:C:90:HIS:CE1	1.92	0.57
26:N:90:TYR:HA	26:N:92:GLU:OE2	2.05	0.57
20:h:8:PHE:CD1	20:h:8:PHE:N	2.73	0.57
30:r:21:THR:HA	30:r:27:ALA:H	1.69	0.57
6:f:422:VAL:HA	6:f:452:ASN:HD21	1.70	0.57
9:W:5:GLY:O	9:W:9:ALA:HB3	2.05	0.57
11:Y:124:PHE:O	11:Y:128:TYR:CB	2.53	0.57
13:A:302:LEU:O	13:A:306:LEU:CB	2.53	0.57
13:A:329:PRO:HA	13:A:332:MET:HB2	1.87	0.57
14:B:439:TYR:HB2	22:J:76:LEU:HB3	1.85	0.57
28:P:54:ALA:O	28:P:105:THR:HA	2.05	0.57
22:j:11:SER:H	22:j:15:HIS:H	1.52	0.57
24:l:77:LEU:HD12	24:l:129:GLY:H	1.69	0.57
3:c:91:PHE:O	3:c:95:MET:CB	2.52	0.56
9:W:218:ASN:HD22	9:W:223:LYS:H	1.52	0.56
9:W:390:GLU:HB3	10:X:344:ARG:HD3	1.86	0.56
18:F:339:ASP:HB2	18:F:342:LEU:HG	1.86	0.56
29:Q:164:LEU:O	29:Q:168:GLN:NE2	2.38	0.56
32:T:179:ARG:HD2	26:n:29:ARG:HH21	1.70	0.56
20:h:45:VAL:HG22	20:h:212:ILE:HG22	1.87	0.56
25:m:108:LEU:HD11	25:m:137:LEU:HB3	1.87	0.56
26:n:88:TYR:CD1	26:n:91:ARG:HD3	2.40	0.56
8:V:468:SER:OG	11:Y:362:LYS:NZ	2.38	0.56
9:W:348:GLU:HA	9:W:351:TRP:HD1	1.69	0.56
12:Z:35:VAL:H	12:Z:97:THR:HG22	1.70	0.56
16:D:403:TYR:CD1	16:D:407:ILE:HG12	2.40	0.56
17:E:116:ASP:HB2	17:E:217:GLU:HG2	1.87	0.56
26:N:132:SER:O	26:N:136:TYR:CB	2.53	0.56
6:f:412:ALA:HA	6:f:447:ALA:HB2	1.87	0.56
6:f:692:LEU:O	6:f:696:LEU:CB	2.53	0.56
7:U:216:VAL:O	7:U:220:LEU:CB	2.52	0.56
7:U:249:CYS:O	7:U:253:TYR:HB2	2.05	0.56
7:U:678:ASP:O	7:U:684:ARG:NH1	2.37	0.56
8:V:376:ASN:OD1	8:V:399:ARG:NH1	2.38	0.56
10:X:143:TYR:OH	11:Y:248:GLU:O	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:174:TRP:O	11:Y:178:ASN:ND2	2.39	0.56
12:Z:213:GLU:O	12:Z:217:THR:C	2.47	0.56
13:A:387:SER:O	13:A:391:GLU:CB	2.54	0.56
15:C:238:ALA:O	15:C:242:ALA:HA	2.05	0.56
22:J:11:SER:H	22:J:15:HIS:H	1.52	0.56
23:K:143:PHE:HB2	23:K:154:PHE:HB2	1.86	0.56
29:Q:36:PHE:HB2	29:Q:44:LEU:HB3	1.88	0.56
32:T:114:GLY:O	32:T:121:PHE:HB3	2.05	0.56
21:i:10:THR:H	21:i:11:ILE:HD12	1.70	0.56
27:o:20:ALA:HB3	27:o:28:ASP:HB3	1.87	0.56
28:p:54:ALA:O	28:p:105:THR:HA	2.05	0.56
29:q:47:VAL:O	29:q:101:ASN:HB2	2.06	0.56
32:t:114:GLY:O	32:t:121:PHE:HB3	2.05	0.56
1:a:372:HIS:HA	12:Z:190:ARG:HH22	1.71	0.56
14:B:122:ILE:HD11	14:B:130:GLU:HB3	1.87	0.56
14:B:133:VAL:HB	14:B:158:ALA:HA	1.86	0.56
15:C:187:LEU:O	15:C:314:LYS:HA	2.04	0.56
19:g:46:ASP:O	19:g:222:VAL:CG2	2.52	0.56
21:i:17:ARG:NH2	21:i:19:TYR:CB	2.61	0.56
26:n:132:SER:O	26:n:136:TYR:CB	2.53	0.56
28:p:107:PRO:HG2	28:p:124:LEU:HB2	1.87	0.56
7:U:174:PRO:O	7:U:178:ALA:CB	2.54	0.56
7:U:602:LEU:O	7:U:606:ALA:HB2	2.06	0.56
8:V:104:THR:HA	8:V:107:ARG:HD3	1.86	0.56
8:V:494:MET:HG2	15:C:49:ARG:HH22	1.71	0.56
9:W:273:TYR:HA	9:W:276:LEU:HD13	1.87	0.56
11:Y:100:ILE:O	11:Y:104:MET:CB	2.53	0.56
15:C:247:PHE:HA	15:C:292:ILE:O	2.05	0.56
16:D:149:SER:N	16:D:152:MET:SD	2.78	0.56
18:F:238:ARG:O	18:F:242:ALA:HB2	2.05	0.56
19:G:27:TYR:HA	19:G:30:LYS:HZ3	1.71	0.56
25:M:98:PHE:O	25:M:102:PHE:HB2	2.05	0.56
28:P:107:PRO:HG2	28:P:124:LEU:HB2	1.87	0.56
29:q:164:LEU:O	29:q:168:GLN:NE2	2.38	0.56
30:r:135:ALA:O	30:r:139:MET:CB	2.54	0.56
1:a:293:PHE:O	1:a:297:ALA:HB3	2.06	0.56
5:e:1:MET:O	8:V:216:ARG:NH2	2.39	0.56
7:U:584:TYR:OH	7:U:768:GLN:NE2	2.39	0.56
8:V:311:ASN:O	8:V:315:LYS:HB2	2.05	0.56
8:V:473:GLN:HE22	12:Z:253:THR:HG23	1.71	0.56
9:W:39:ARG:HB2	9:W:44:ILE:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:125:ARG:HA	11:Y:128:TYR:HB3	1.87	0.56
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.86	0.56
18:F:436:GLN:C	18:F:438:TYR:H	2.13	0.56
29:Q:47:VAL:O	29:Q:101:ASN:HB2	2.06	0.56
31:S:192:ALA:HA	31:S:209:SER:HA	1.87	0.56
30:r:50:ALA:O	30:r:54:PHE:HB3	2.04	0.56
16:D:54:LEU:O	16:D:58:GLU:HB2	2.05	0.56
16:D:280:GLY:HA2	16:D:283:ARG:HE	1.70	0.56
17:E:341:ALA:HB3	18:F:345:SER:OG	2.04	0.56
19:G:144:ASP:HB3	19:G:147:GLN:HB2	1.87	0.56
21:I:8:ARG:HB3	21:I:11:ILE:HD13	1.88	0.56
22:J:114:LEU:O	22:J:118:TYR:HB2	2.06	0.56
23:k:182:GLN:NE2	24:l:55:GLU:OE1	2.39	0.56
7:U:802:TYR:HE2	7:U:892:LEU:HB2	1.71	0.56
8:V:32:PRO:O	8:V:36:GLU:HB2	2.06	0.56
12:Z:253:THR:O	12:Z:257:MET:HB2	2.06	0.56
14:B:392:GLY:O	14:B:396:LYS:CB	2.54	0.56
14:B:440:LEU:H	14:B:440:LEU:CD2	2.05	0.56
15:C:71:SER:HB2	16:D:112:TYR:HD2	1.70	0.56
19:g:144:ASP:HB3	19:g:147:GLN:HB2	1.86	0.56
29:q:68:LYS:O	29:q:72:GLY:HA2	2.06	0.56
30:r:44:THR:HG21	30:r:100:MET:HE3	1.86	0.56
4:d:73:ARG:HD2	7:U:11:LEU:HA	1.87	0.56
5:e:43:TRP:HD1	8:V:349:ARG:CG	2.15	0.56
10:X:415:TYR:O	10:X:419:LYS:CB	2.54	0.56
12:Z:220:LEU:HD23	12:Z:220:LEU:N	2.02	0.56
16:D:228:ILE:HB	16:D:262:ILE:HG12	1.86	0.56
16:D:408:LYS:NZ	17:E:389:VAL:CB	2.68	0.56
17:E:322:LYS:HD3	17:E:326:ILE:HG13	1.88	0.56
18:F:255:GLN:O	18:F:258:GLN:NE2	2.39	0.56
18:F:436:GLN:O	18:F:438:TYR:HD2	1.89	0.56
25:M:61:GLY:O	25:M:64:LYS:NZ	2.39	0.56
25:M:99:ARG:NH2	25:M:105:ASN:OD1	2.39	0.56
27:O:20:ALA:HB3	27:O:28:ASP:HB3	1.87	0.56
24:l:172:LEU:O	24:l:176:MET:HB3	2.06	0.56
26:n:103:TRP:HA	26:n:109:GLY:HA2	1.88	0.56
7:U:471:ASP:HB2	7:U:508:THR:HG21	1.88	0.56
11:Y:124:PHE:O	11:Y:128:TYR:HB2	2.05	0.56
13:A:244:GLU:HA	14:B:268:ARG:HH12	1.71	0.56
14:B:266:LEU:O	14:B:270:LEU:CB	2.54	0.56
19:G:188:ASP:O	19:G:193:GLN:NE2	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:22:PHE:N	23:K:22:PHE:CD2	2.73	0.56
24:L:186:GLU:HA	24:L:189:LYS:HG2	1.87	0.56
25:M:197:ILE:HG21	25:M:211:LEU:HD13	1.89	0.56
21:i:75:SER:HB2	21:i:135:LEU:HD12	1.88	0.56
22:j:114:LEU:O	22:j:118:TYR:HB2	2.06	0.56
27:o:211:VAL:HG11	28:p:198:ARG:HD3	1.86	0.56
4:d:5:LEU:HD22	4:d:25:ARG:HG2	1.88	0.55
14:B:189:GLY:HA3	14:B:356:PRO:HB3	1.86	0.55
16:D:152:MET:O	16:D:154:LEU:N	2.39	0.55
18:F:249:LEU:HD23	18:F:283:ILE:HG12	1.89	0.55
19:G:128:ASN:OD1	20:H:6:TYR:OH	2.23	0.55
24:L:172:LEU:O	24:L:176:MET:HB3	2.06	0.55
27:O:138:PHE:O	27:O:142:PHE:CB	2.53	0.55
21:i:91:ARG:O	21:i:95:GLN:CB	2.54	0.55
21:i:101:TYR:HB3	29:q:79:ALA:HB1	1.87	0.55
1:a:252:LYS:HD3	1:a:255:TRP:HB2	1.88	0.55
3:c:58:LEU:HA	3:c:108:VAL:HA	1.88	0.55
6:f:477:MET:O	6:f:481:SER:CB	2.54	0.55
11:Y:304:TYR:O	11:Y:308:LEU:HB2	2.06	0.55
11:Y:335:SER:O	11:Y:339:ALA:HB3	2.06	0.55
12:Z:34:ARG:HE	12:Z:98:GLY:HA3	1.70	0.55
15:C:162:LYS:O	15:C:166:GLU:HB2	2.05	0.55
19:G:21:ARG:H	19:G:21:ARG:NE	2.04	0.55
23:K:79:SER:HB2	23:K:170:ILE:HD13	1.89	0.55
25:m:98:PHE:O	25:m:102:PHE:HB2	2.05	0.55
1:a:34:TRP:HD1	2:b:18:ASN:HB2	1.70	0.55
8:V:60:ALA:HB1	8:V:63:SER:HB2	1.89	0.55
9:W:268:LYS:HA	9:W:271:VAL:HG12	1.87	0.55
9:W:390:GLU:O	9:W:394:SER:OG	2.18	0.55
11:Y:294:TYR:HA	11:Y:297:ARG:HG3	1.88	0.55
18:F:272:PHE:O	18:F:276:LYS:HB2	2.05	0.55
21:I:91:ARG:O	21:I:95:GLN:HB2	2.07	0.55
25:M:108:LEU:HD11	25:M:137:LEU:HB3	1.87	0.55
25:M:214:SER:HA	25:M:226:ILE:HA	1.87	0.55
19:g:141:ILE:HG22	19:g:151:VAL:HG22	1.88	0.55
21:i:8:ARG:HB3	21:i:11:ILE:HD13	1.89	0.55
4:d:203:PRO:HB2	4:d:205:LYS:H	1.70	0.55
6:f:312:GLU:HG3	6:f:492:SER:HA	1.87	0.55
11:Y:66:ASP:HA	11:Y:69:LEU:HB2	1.88	0.55
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.88	0.55
15:C:351:MET:HE1	15:C:359:VAL:HG13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:151:ILE:CD1	16:D:229:ARG:NH2	2.70	0.55
16:D:417:TYR:CZ	19:G:21:ARG:CG	2.88	0.55
18:F:92:ASN:HA	18:F:149:ASP:O	2.07	0.55
30:R:161:TYR:O	30:R:165:TYR:HB2	2.06	0.55
24:l:186:GLU:HA	24:l:189:LYS:HG2	1.87	0.55
6:f:313:GLU:O	6:f:317:LEU:CB	2.54	0.55
8:V:137:GLU:HA	8:V:140:ASP:HB2	1.87	0.55
8:V:486:ILE:HG22	12:Z:275:LEU:HD21	1.89	0.55
9:W:388:GLU:O	9:W:392:PHE:HB2	2.05	0.55
9:W:430:GLN:O	9:W:434:SER:OG	2.25	0.55
18:F:265:ALA:HA	18:F:312:GLU:HG2	1.88	0.55
20:h:66:GLU:OE2	20:h:91:ARG:NH2	2.39	0.55
22:j:6:ALA:CA	22:j:9:VAL:HG22	2.32	0.55
1:a:247:ARG:O	1:a:251:LEU:CB	2.54	0.55
4:d:36:LEU:C	4:d:38:THR:H	2.14	0.55
15:C:131:VAL:HG13	15:C:133:PRO:HD3	1.88	0.55
21:I:10:THR:H	21:I:11:ILE:HD12	1.72	0.55
21:I:91:ARG:O	21:I:95:GLN:CB	2.54	0.55
30:R:1:THR:N	30:R:169:TYR:O	2.40	0.55
29:q:57:ALA:O	29:q:61:GLN:CB	2.55	0.55
3:c:248:MET:O	3:c:252:ALA:CB	2.55	0.55
6:f:93:PRO:HB2	6:f:137:ARG:HE	1.72	0.55
6:f:306:GLU:CB	6:f:339:ILE:HD13	2.24	0.55
8:V:421:ASP:O	8:V:425:LYS:CB	2.55	0.55
14:B:440:LEU:H	14:B:440:LEU:HD13	1.71	0.55
17:E:101:ASP:HB3	17:E:105:LEU:H	1.71	0.55
17:E:101:ASP:HB2	17:E:108:MET:HE3	1.87	0.55
17:E:258:MET:HG2	17:E:261:LEU:HD12	1.88	0.55
27:O:14:LEU:HB2	27:O:176:CYS:HB3	1.88	0.55
1:a:177:LEU:O	1:a:181:GLY:HA3	2.07	0.55
1:a:294:GLU:O	1:a:298:LYS:CB	2.55	0.55
8:V:329:HIS:CG	8:V:346:LEU:CD2	2.75	0.55
9:W:272:LEU:HD12	9:W:336:PRO:HB2	1.88	0.55
17:E:60:VAL:HA	17:E:71:VAL:HG12	1.89	0.55
18:F:293:THR:HA	18:F:337:ILE:HG22	1.89	0.55
20:H:66:GLU:OE2	20:H:91:ARG:NH2	2.39	0.55
20:H:71:HIS:HA	20:H:218:PHE:H	1.72	0.55
26:N:20:THR:HB	26:N:28:ASN:HB3	1.89	0.55
19:g:178:PHE:O	19:g:182:LYS:CB	2.55	0.55
20:h:222:THR:OG1	20:h:225:GLU:OE1	2.25	0.55
25:m:99:ARG:NH2	25:m:105:ASN:OD1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:214:SER:HA	25:m:226:ILE:HA	1.87	0.55
30:r:41:LEU:HD23	30:r:103:GLY:HA3	1.89	0.55
11:Y:46:ARG:O	11:Y:49:ASN:ND2	2.40	0.55
11:Y:144:LEU:HB2	11:Y:160:ASN:HB3	1.89	0.55
16:D:99:ASN:HA	16:D:115:ILE:HG13	1.88	0.55
19:g:192:GLU:O	19:g:196:GLU:N	2.31	0.55
21:i:91:ARG:O	21:i:95:GLN:HB2	2.07	0.55
23:k:10:ARG:HA	23:k:10:ARG:NH1	2.22	0.55
23:k:11:GLY:O	23:k:21:LEU:HD21	2.06	0.55
27:o:14:LEU:HB2	27:o:176:CYS:HB3	1.88	0.55
6:f:477:MET:O	6:f:481:SER:HB2	2.07	0.55
7:U:229:VAL:HG13	7:U:268:LEU:HD11	1.89	0.55
7:U:401:LYS:HE2	7:U:437:TYR:HB2	1.89	0.55
23:K:21:LEU:HD22	23:K:23:GLN:H	1.72	0.55
24:L:26:MET:HE1	24:L:148:CYS:HB2	1.88	0.55
20:h:71:HIS:HA	20:h:218:PHE:H	1.72	0.55
23:k:203:LYS:HA	23:k:206:MET:HG2	1.89	0.55
25:m:197:ILE:HG21	25:m:211:LEU:HD13	1.89	0.55
29:q:36:PHE:HB2	29:q:44:LEU:HB3	1.87	0.55
6:f:478:ARG:NH1	6:f:507:ASP:OD2	2.40	0.54
9:W:36:LYS:HE3	9:W:85:GLU:HB2	1.88	0.54
13:A:51:ASP:O	13:A:55:LEU:CB	2.55	0.54
18:F:358:ASN:O	18:F:362:ARG:NH1	2.40	0.54
20:H:105:ILE:HG12	20:H:110:LEU:HD12	1.90	0.54
21:I:115:CYS:O	21:I:119:GLN:HB2	2.07	0.54
30:R:98:GLY:HA2	30:R:115:ASP:HA	1.90	0.54
31:S:213:ASP:OD2	27:o:19:ARG:NH2	2.40	0.54
19:g:11:ARG:NH1	19:g:27:TYR:HE2	2.05	0.54
29:q:181:ARG:NH1	29:q:190:ASP:OD1	2.40	0.54
2:b:142:ASN:HD21	2:b:153:LEU:HD22	1.72	0.54
6:f:255:VAL:HA	6:f:258:LYS:HZ2	1.72	0.54
13:A:224:LEU:O	13:A:228:ALA:CB	2.55	0.54
17:E:329:GLU:O	17:E:333:LYS:HB2	2.07	0.54
25:M:168:ALA:HB1	25:M:171:ALA:HB3	1.89	0.54
27:O:21:THR:HG22	27:O:26:VAL:HA	1.90	0.54
28:P:34:MET:O	30:r:166:ARG:NH2	2.40	0.54
29:Q:68:LYS:O	29:Q:72:GLY:HA2	2.06	0.54
23:k:15:PHE:HD1	23:k:20:ARG:HA	1.71	0.54
26:n:20:THR:HB	26:n:28:ASN:HB3	1.89	0.54
30:r:1:THR:N	30:r:169:TYR:O	2.40	0.54
1:a:123:LEU:HG	1:a:161:LYS:HE2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:416:ARG:HE	8:V:459:GLN:HA	1.71	0.54
10:X:326:LEU:O	10:X:330:LEU:HB2	2.06	0.54
12:Z:144:VAL:HG12	12:Z:148:GLY:HA2	1.89	0.54
16:D:119:ILE:HG23	16:D:123:LEU:CD1	2.38	0.54
17:E:275:MET:HB3	17:E:277:MET:HE2	1.89	0.54
18:F:222:GLY:HA2	18:F:328:VAL:HB	1.90	0.54
18:F:251:LEU:HD11	18:F:256:LEU:HD21	1.88	0.54
18:F:344:ARG:HH12	18:F:347:ARG:NH2	1.76	0.54
19:G:141:ILE:HG22	19:G:151:VAL:HG22	1.88	0.54
30:R:135:ALA:O	30:R:139:MET:CB	2.54	0.54
23:k:79:SER:HB2	23:k:170:ILE:HD13	1.89	0.54
24:l:26:MET:HE1	24:l:148:CYS:HB2	1.88	0.54
30:r:98:GLY:HA2	30:r:115:ASP:HA	1.90	0.54
1:a:327:VAL:N	9:W:372:ARG:O	2.40	0.54
6:f:338:ASP:O	6:f:342:PRO:HD3	2.07	0.54
7:U:604:HIS:O	7:U:608:SER:OG	2.21	0.54
9:W:408:ARG:CB	9:W:408:ARG:CZ	2.86	0.54
18:F:79:LYS:O	18:F:83:ASN:HB2	2.08	0.54
19:G:178:PHE:O	19:G:182:LYS:CB	2.55	0.54
29:Q:173:LEU:HA	29:q:173:LEU:HA	1.90	0.54
20:h:105:ILE:HG12	20:h:110:LEU:HD12	1.90	0.54
23:k:42:THR:HG22	23:k:44:GLU:H	1.71	0.54
24:l:189:LYS:HA	24:l:192:LEU:HG	1.90	0.54
27:o:88:PHE:O	27:o:91:GLN:NE2	2.40	0.54
29:q:177:THR:HB	29:q:193:ASN:HD21	1.72	0.54
5:e:49:GLU:HA	5:e:52:PHE:HB2	1.90	0.54
7:U:213:PHE:O	7:U:217:CYS:CB	2.55	0.54
7:U:497:LEU:HD23	7:U:512:ALA:HA	1.90	0.54
7:U:681:ASN:HB2	7:U:723:ASP:HB2	1.89	0.54
9:W:242:SER:O	9:W:246:HIS:HB3	2.07	0.54
10:X:323:LEU:O	10:X:327:TYR:CB	2.56	0.54
11:Y:271:PHE:O	11:Y:275:LEU:CB	2.55	0.54
16:D:212:LYS:NZ	34:D:501:ATP:O3G	2.41	0.54
16:D:409:LYS:HD2	17:E:387:LYS:HZ1	1.72	0.54
20:h:98:TYR:O	20:h:102:GLN:HA	2.08	0.54
5:e:43:TRP:CD1	8:V:349:ARG:HG2	2.43	0.54
6:f:333:LEU:HD23	6:f:338:ASP:HB3	1.90	0.54
9:W:408:ARG:C	9:W:411:GLY:H	2.15	0.54
12:Z:269:VAL:O	12:Z:273:HIS:ND1	2.39	0.54
20:H:222:THR:OG1	20:H:225:GLU:OE1	2.25	0.54
25:M:235:ALA:O	25:M:239:ALA:CB	2.53	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:103:TRP:HA	26:N:109:GLY:HA2	1.88	0.54
32:t:192:VAL:HG12	32:t:197:VAL:HG22	1.90	0.54
1:a:64:ILE:O	1:a:68:GLU:CB	2.55	0.54
3:c:248:MET:O	3:c:252:ALA:HB3	2.08	0.54
6:f:232:TYR:O	6:f:236:CYS:CB	2.53	0.54
6:f:306:GLU:OE1	6:f:339:ILE:HD13	2.08	0.54
8:V:203:LEU:O	8:V:207:ALA:CB	2.56	0.54
8:V:391:THR:HG23	8:V:394:LEU:HD23	1.88	0.54
9:W:166:LEU:HD23	9:W:169:LEU:HD12	1.89	0.54
9:W:242:SER:O	9:W:246:HIS:CB	2.56	0.54
11:Y:156:LEU:HD23	11:Y:159:ARG:HD3	1.90	0.54
15:C:368:MET:HE1	16:D:191:TYR:HE1	1.73	0.54
16:D:151:ILE:HD13	16:D:229:ARG:NH2	2.23	0.54
16:D:416:PHE:CZ	19:G:157:ALA:CB	2.86	0.54
18:F:68:ALA:O	18:F:72:LYS:CB	2.56	0.54
19:G:202:LEU:O	19:G:206:LEU:HB2	2.08	0.54
23:K:203:LYS:HA	23:K:206:MET:HG2	1.89	0.54
29:Q:57:ALA:O	29:Q:61:GLN:CB	2.55	0.54
25:m:61:GLY:O	25:m:64:LYS:NZ	2.39	0.54
27:o:138:PHE:O	27:o:142:PHE:CB	2.53	0.54
28:p:112:LEU:HA	28:p:119:PRO:HA	1.89	0.54
1:a:214:GLY:O	1:a:241:ASN:ND2	2.41	0.54
1:a:280:MET:HB2	1:a:291:LEU:HD13	1.89	0.54
3:c:293:THR:O	3:c:297:VAL:HB	2.08	0.54
7:U:571:CYS:HA	7:U:579:ARG:HG2	1.90	0.54
8:V:296:LYS:HA	8:V:299:GLN:HB2	1.89	0.54
17:E:287:PRO:HA	17:E:290:LEU:HB2	1.89	0.54
18:F:230:GLY:HA3	18:F:392:ASN:HD22	1.71	0.54
20:H:98:TYR:O	20:H:102:GLN:HA	2.08	0.54
27:O:43:CYS:HA	27:O:99:VAL:O	2.08	0.54
21:i:123:GLN:NE2	22:j:79:ASP:OD1	2.41	0.54
27:o:43:CYS:HA	27:o:99:VAL:O	2.08	0.54
6:f:509:LYS:HG2	6:f:511:SER:H	1.73	0.54
7:U:206:MET:SD	7:U:235:LYS:NZ	2.81	0.54
10:X:362:GLU:OE2	10:X:365:LEU:CD2	2.49	0.54
16:D:188:PHE:HA	16:D:191:TYR:HD2	1.73	0.54
18:F:197:GLU:O	18:F:201:ALA:HB2	2.08	0.54
19:G:212:PRO:HB3	19:G:235:ILE:HG22	1.90	0.54
25:M:37:ILE:HD11	25:M:193:VAL:HG13	1.90	0.54
29:Q:181:ARG:NH1	29:Q:190:ASP:OD1	2.40	0.54
21:i:115:CYS:O	21:i:119:GLN:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:117:THR:HA	4:d:120:GLU:HB3	1.90	0.54
5:e:42:ASN:C	5:e:44:ASP:H	2.16	0.54
5:e:47:ASN:OD1	8:V:365:GLN:NE2	2.41	0.54
6:f:623:LYS:O	6:f:627:GLU:CB	2.55	0.54
9:W:55:ARG:HH11	9:W:75:TYR:HB3	1.72	0.54
9:W:385:SER:O	9:W:389:SER:N	2.41	0.54
16:D:93:LEU:HG	16:D:94:GLU:HG3	1.89	0.54
16:D:285:VAL:HG21	17:E:255:ARG:HH22	1.72	0.54
16:D:409:LYS:CE	16:D:409:LYS:CA	2.85	0.54
21:i:218:ARG:NH1	21:i:223:THR:OG1	2.36	0.54
11:Y:57:LEU:HD13	11:Y:63:TRP:HD1	1.73	0.53
18:F:430:LYS:HZ2	18:F:430:LYS:N	1.95	0.53
21:I:75:SER:HB2	21:I:135:LEU:HD12	1.89	0.53
22:j:2:SER:N	22:j:10:PHE:O	2.41	0.53
25:m:47:PHE:O	25:m:213:LEU:HA	2.08	0.53
30:r:161:TYR:O	30:r:165:TYR:HB2	2.06	0.53
1:a:244:ASN:HB3	1:a:275:LEU:HB3	1.90	0.53
6:f:81:GLN:O	6:f:85:SER:HB2	2.07	0.53
8:V:80:LYS:O	8:V:82:LEU:N	2.33	0.53
8:V:131:LEU:HD23	8:V:134:PHE:HD2	1.73	0.53
16:D:171:ASP:O	16:D:175:GLN:HB3	2.08	0.53
20:H:183:GLU:H	20:H:186:ASP:HB2	1.73	0.53
23:K:42:THR:HG22	23:K:44:GLU:H	1.71	0.53
26:N:40:ARG:NH1	26:N:180:ALA:O	2.41	0.53
31:S:125:ASP:OD1	31:S:129:SER:N	2.37	0.53
20:h:183:GLU:H	20:h:186:ASP:HB2	1.73	0.53
24:l:92:CYS:O	24:l:96:ARG:HB2	2.08	0.53
25:m:163:CYS:SG	25:m:164:ALA:N	2.81	0.53
25:m:168:ALA:HB1	25:m:171:ALA:HB3	1.89	0.53
3:c:100:LYS:HG2	3:c:105:PRO:HB3	1.88	0.53
4:d:181:CYS:SG	8:V:443:ARG:NH2	2.76	0.53
6:f:612:LEU:O	6:f:616:CYS:HB2	2.08	0.53
7:U:46:GLU:OE2	7:U:80:TYR:OH	2.26	0.53
7:U:105:ILE:HA	7:U:108:TYR:HB3	1.90	0.53
8:V:215:ALA:O	8:V:219:GLU:HB2	2.08	0.53
8:V:326:GLN:HB3	8:V:353:LEU:HD13	1.91	0.53
10:X:302:PHE:O	10:X:306:LEU:CB	2.57	0.53
15:C:273:MET:HE3	15:C:305:LEU:HD21	1.90	0.53
19:G:189:TRP:CE3	19:G:193:GLN:HG3	2.43	0.53
24:L:189:LYS:HA	24:L:192:LEU:HG	1.90	0.53
28:P:112:LEU:HA	28:P:119:PRO:HA	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:151:VAL:O	1:a:155:PHE:CB	2.54	0.53
1:a:308:GLU:HG2	9:W:381:LEU:HD21	1.90	0.53
3:c:120:CYS:HB2	3:c:144:VAL:HG12	1.90	0.53
8:V:62:HIS:HA	8:V:65:ARG:HB3	1.90	0.53
8:V:149:PRO:O	8:V:153:LYS:CB	2.57	0.53
9:W:397:VAL:HG22	10:X:339:ILE:HG22	1.89	0.53
17:E:157:GLU:HA	17:E:160:GLN:HB2	1.90	0.53
18:F:431:LYS:HA	18:F:431:LYS:HE2	1.89	0.53
24:L:43:HIS:CB	24:L:184:LEU:CD1	2.71	0.53
27:O:44:CYS:HB2	27:O:99:VAL:HB	1.91	0.53
27:O:88:PHE:O	27:O:91:GLN:NE2	2.40	0.53
19:g:27:TYR:HA	19:g:30:LYS:HZ3	1.73	0.53
23:k:10:ARG:HB3	23:k:14:THR:CB	2.26	0.53
25:m:37:ILE:HD11	25:m:193:VAL:HG13	1.90	0.53
27:o:35:HIS:NE2	27:o:53:ASP:OD1	2.42	0.53
7:U:38:ILE:HA	7:U:41:SER:HB3	1.90	0.53
7:U:82:LEU:O	7:U:129:ARG:NH1	2.41	0.53
16:D:92:PHE:HZ	16:D:95:ALA:HB2	1.74	0.53
23:K:167:ALA:HB3	23:K:181:LEU:HD21	1.91	0.53
27:O:35:HIS:NE2	27:O:53:ASP:OD1	2.42	0.53
21:i:105:ILE:HG12	21:i:110:LEU:HB2	1.90	0.53
21:i:197:LEU:O	21:i:201:MET:CB	2.57	0.53
23:k:16:SER:N	23:k:20:ARG:O	2.35	0.53
26:n:127:ILE:HB	26:n:132:SER:HB2	1.90	0.53
28:p:189:ILE:HG23	28:p:196:THR:HB	1.91	0.53
7:U:373:ASN:HA	7:U:376:MET:HG2	1.90	0.53
9:W:375:MET:HB2	9:W:413:ILE:HG23	1.90	0.53
10:X:258:LYS:HE3	10:X:270:LEU:HD12	1.88	0.53
11:Y:311:TYR:HB2	11:Y:314:LEU:HD12	1.91	0.53
14:B:303:ARG:O	14:B:307:ARG:NH2	2.42	0.53
19:g:212:PRO:HB3	19:g:235:ILE:HG22	1.90	0.53
26:n:40:ARG:NH1	26:n:180:ALA:O	2.41	0.53
6:f:608:LYS:HA	6:f:611:GLN:HB3	1.91	0.53
9:W:105:VAL:HG11	9:W:143:ALA:HB1	1.90	0.53
13:A:139:ARG:NH2	14:B:130:GLU:OE1	2.42	0.53
18:F:94:ILE:HD12	18:F:123:VAL:HG12	1.91	0.53
24:L:92:CYS:O	24:L:96:ARG:HB2	2.08	0.53
28:P:177:ARG:NH2	31:s:150:ASP:OD2	2.41	0.53
28:P:189:ILE:HG23	28:P:196:THR:HB	1.91	0.53
25:m:69:VAL:H	25:m:74:GLY:HA2	1.73	0.53
1:a:248:PHE:O	1:a:252:LYS:CB	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:268:LEU:HD23	1:a:271:LYS:HD3	1.90	0.53
1:a:286:ALA:HA	12:Z:238:PRO:HB2	1.91	0.53
3:c:40:LYS:O	3:c:44:HIS:HB2	2.09	0.53
7:U:107:HIS:HA	7:U:110:LYS:HE3	1.91	0.53
7:U:685:GLN:NE2	7:U:725:MET:O	2.41	0.53
7:U:713:TYR:O	7:U:717:ILE:HB	2.08	0.53
20:H:65:VAL:HG11	20:H:211:GLY:HA3	1.91	0.53
23:K:203:LYS:HZ1	23:K:241:ILE:HG12	1.71	0.53
29:Q:177:THR:HB	29:Q:193:ASN:HD21	1.72	0.53
30:R:41:LEU:HD23	30:R:103:GLY:HA3	1.89	0.53
25:m:235:ALA:O	25:m:239:ALA:CB	2.53	0.53
1:a:364:GLU:HG2	12:Z:197:GLY:HA3	1.90	0.53
3:c:92:GLN:O	3:c:96:LEU:HB2	2.08	0.53
6:f:15:GLN:NE2	6:f:47:GLU:OE1	2.42	0.53
10:X:134:VAL:HB	10:X:149:LEU:HD23	1.90	0.53
10:X:173:GLU:HA	10:X:176:THR:HG22	1.90	0.53
15:C:90:HIS:CG	16:D:110:ASN:N	2.77	0.53
16:D:403:TYR:CD1	16:D:407:ILE:CG1	2.91	0.53
18:F:382:GLU:O	18:F:386:ARG:HB2	2.09	0.53
20:H:121:TYR:CA	20:H:124:SER:HG	2.00	0.53
21:I:105:ILE:HG12	21:I:110:LEU:HB2	1.90	0.53
22:J:2:SER:N	22:J:10:PHE:O	2.41	0.53
24:L:201:ALA:O	24:L:239:ARG:NH1	2.42	0.53
2:b:15:TYR:O	2:b:25:ARG:NH1	2.42	0.53
6:f:178:LYS:NZ	6:f:215:ASP:O	2.37	0.53
6:f:229:VAL:O	6:f:233:LEU:CB	2.57	0.53
8:V:234:ARG:HG3	8:V:250:LEU:HD11	1.91	0.53
9:W:275:ILE:HG23	9:W:357:ARG:HG3	1.91	0.53
9:W:287:VAL:HA	9:W:290:ILE:HG12	1.91	0.53
11:Y:196:GLN:O	11:Y:200:LEU:HB2	2.08	0.53
13:A:411:GLU:O	13:A:415:LYS:CB	2.57	0.53
14:B:418:ASP:O	14:B:422:SER:HB3	2.09	0.53
18:F:432:LYS:HZ3	18:F:432:LYS:CB	2.22	0.53
29:Q:148:THR:HB	29:Q:151:ILE:HB	1.91	0.53
19:g:202:LEU:O	19:g:206:LEU:HB2	2.08	0.53
2:b:22:LEU:CD1	2:b:178:SER:C	2.73	0.52
6:f:253:LEU:O	6:f:257:ARG:CB	2.57	0.52
8:V:377:GLN:O	8:V:381:GLN:HB2	2.10	0.52
11:Y:177:ARG:HA	11:Y:180:LEU:HD13	1.91	0.52
13:A:241:ILE:HG22	13:A:243:SER:H	1.74	0.52
14:B:418:ASP:O	14:B:422:SER:CB	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:163:CYS:SG	25:M:164:ALA:N	2.81	0.52
26:N:14:LEU:HB2	26:N:177:ALA:HB3	1.91	0.52
23:k:104:ASN:OD1	30:r:57:ARG:NH2	2.42	0.52
26:n:132:SER:O	26:n:136:TYR:HB2	2.09	0.52
6:f:55:GLU:HB2	6:f:72:ARG:HH11	1.74	0.52
7:U:325:MET:HB2	7:U:329:LEU:HD12	1.91	0.52
7:U:728:PHE:O	7:U:732:LEU:HB2	2.08	0.52
8:V:80:LYS:HG3	8:V:87:SER:HA	1.91	0.52
8:V:337:LEU:HD23	8:V:342:ILE:HG21	1.91	0.52
9:W:110:THR:HA	9:W:113:GLU:HG2	1.92	0.52
10:X:167:VAL:HA	10:X:170:GLN:HB2	1.92	0.52
11:Y:333:GLU:HA	11:Y:336:ARG:HH21	1.74	0.52
11:Y:344:HIS:ND1	11:Y:357:ASN:OD1	2.39	0.52
19:G:165:ALA:HB1	19:G:179:LEU:HD13	1.91	0.52
21:I:197:LEU:O	21:I:201:MET:CB	2.57	0.52
29:Q:173:LEU:HD23	29:q:173:LEU:HD23	1.91	0.52
20:h:51:LYS:HG2	20:h:207:ASN:HD22	1.75	0.52
26:n:14:LEU:HB2	26:n:177:ALA:HB3	1.91	0.52
27:o:21:THR:HG22	27:o:26:VAL:HA	1.90	0.52
5:e:61:GLU:OE2	11:Y:300:ARG:NH2	2.41	0.52
7:U:612:ASP:HA	7:U:615:ARG:HD3	1.91	0.52
8:V:48:THR:O	8:V:52:ASP:HB2	2.08	0.52
13:A:312:ARG:HH12	13:A:317:VAL:HG21	1.72	0.52
23:K:41:GLN:NE2	23:K:151:PRO:O	2.42	0.52
24:L:93:LEU:HA	24:L:96:ARG:HB3	1.91	0.52
20:h:65:VAL:HG11	20:h:211:GLY:HA3	1.91	0.52
29:q:148:THR:HB	29:q:151:ILE:HB	1.91	0.52
1:a:273:GLN:HG2	1:a:300:ALA:HB1	1.91	0.52
6:f:209:MET:SD	6:f:213:GLN:NE2	2.82	0.52
6:f:645:ASP:O	6:f:649:HIS:ND1	2.43	0.52
7:U:62:LEU:HD12	7:U:84:ALA:HB1	1.90	0.52
7:U:68:PHE:HB3	7:U:73:ALA:HB3	1.91	0.52
7:U:625:ILE:HG13	7:U:626:LEU:HG	1.90	0.52
7:U:697:GLN:NE2	7:U:742:HIS:O	2.42	0.52
9:W:218:ASN:ND2	9:W:220:GLU:O	2.42	0.52
9:W:282:GLU:O	9:W:286:LEU:HB2	2.09	0.52
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.92	0.52
23:k:41:GLN:NE2	23:k:151:PRO:O	2.42	0.52
23:k:216:GLU:HA	23:k:234:LEU:HD11	1.92	0.52
6:f:80:ARG:O	6:f:84:SER:CB	2.58	0.52
7:U:575:ASP:OD1	7:U:579:ARG:NH2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:254:GLU:O	14:B:257:GLN:NE2	2.42	0.52
18:F:237:ALA:O	18:F:241:ALA:HB3	2.09	0.52
20:H:174:LEU:O	20:H:178:TYR:CB	2.58	0.52
20:H:226:VAL:O	20:H:230:LEU:CB	2.58	0.52
31:S:12:ILE:O	31:S:137:ALA:HA	2.09	0.52
32:T:192:VAL:HG12	32:T:197:VAL:HG22	1.90	0.52
22:j:6:ALA:C	22:j:8:THR:H	2.17	0.52
23:k:167:ALA:HB3	23:k:181:LEU:HD21	1.91	0.52
1:a:345:GLN:O	1:a:349:MET:CB	2.57	0.52
3:c:161:ARG:NH1	3:c:162:LEU:O	2.43	0.52
8:V:176:MET:HE1	8:V:214:HIS:HE1	1.74	0.52
8:V:230:PHE:HA	8:V:233:ALA:HB3	1.91	0.52
9:W:247:TYR:HA	9:W:250:ILE:HG23	1.92	0.52
9:W:429:SER:O	9:W:433:ASN:CB	2.56	0.52
13:A:244:GLU:O	13:A:247:GLN:NE2	2.43	0.52
14:B:437:GLY:O	14:B:440:LEU:HD21	2.10	0.52
18:F:435:LEU:HD13	24:L:51:ARG:NH1	2.24	0.52
22:J:3:TYR:HB3	22:J:5:ARG:HD2	1.92	0.52
23:K:221:GLN:HB2	23:K:224:GLN:HB3	1.91	0.52
26:N:127:ILE:HB	26:N:132:SER:HB2	1.90	0.52
22:j:70:CYS:HB2	22:j:134:VAL:HB	1.92	0.52
27:o:63:LEU:O	27:o:67:SER:HB3	2.10	0.52
28:p:2:SER:OG	28:p:3:ILE:N	2.43	0.52
28:p:160:PRO:O	28:p:164:PHE:HB2	2.09	0.52
4:d:49:ILE:HD12	4:d:52:ARG:HH11	1.75	0.52
4:d:67:ASP:O	4:d:71:PHE:HB2	2.09	0.52
9:W:407:ASP:O	9:W:412:ILE:C	2.52	0.52
10:X:253:TYR:O	10:X:257:CYS:HB2	2.10	0.52
11:Y:134:LEU:O	11:Y:138:LEU:CB	2.57	0.52
17:E:348:THR:OG1	18:F:218:GLN:NE2	2.43	0.52
25:M:47:PHE:O	25:M:213:LEU:HA	2.08	0.52
27:O:100:LEU:HB3	27:O:111:TYR:HB2	1.92	0.52
23:k:66:LYS:HA	23:k:78:MET:HE3	1.92	0.52
27:o:44:CYS:HB2	27:o:99:VAL:HB	1.91	0.52
32:t:145:LEU:HB3	32:t:179:ARG:HH21	1.74	0.52
6:f:724:ASN:O	6:f:728:ALA:C	2.53	0.52
7:U:542:GLU:O	7:U:546:ARG:HB2	2.10	0.52
12:Z:28:LYS:HG3	12:Z:29:VAL:HG13	1.91	0.52
12:Z:278:ASN:O	12:Z:282:ASN:CB	2.53	0.52
14:B:125:THR:OG1	14:B:126:SER:N	2.40	0.52
18:F:431:LYS:CE	18:F:431:LYS:CA	2.85	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:123:GLN:OE1	21:I:127:LYS:HD2	2.09	0.52
23:K:41:GLN:HA	23:K:46:VAL:HG22	1.91	0.52
25:M:69:VAL:H	25:M:74:GLY:HA2	1.73	0.52
1:a:226:ARG:HH21	1:a:234:ILE:HG21	1.75	0.52
4:d:77:GLN:HE21	7:U:11:LEU:HD22	1.75	0.52
6:f:303:VAL:O	6:f:339:ILE:HD12	2.10	0.52
6:f:333:LEU:HA	6:f:338:ASP:CB	2.40	0.52
6:f:347:ASP:O	6:f:351:THR:OG1	2.28	0.52
7:U:544:ILE:O	7:U:548:LEU:HB2	2.10	0.52
7:U:545:LEU:O	7:U:549:ALA:HB2	2.10	0.52
8:V:204:ASP:OD1	8:V:234:ARG:NH2	2.42	0.52
8:V:282:ASN:O	8:V:286:ALA:HB2	2.10	0.52
8:V:346:LEU:HD23	8:V:348:PHE:CZ	2.44	0.52
8:V:408:ARG:O	8:V:412:LEU:HB2	2.09	0.52
9:W:341:PHE:O	9:W:351:TRP:NE1	2.38	0.52
10:X:113:CYS:HB3	10:X:129:LEU:HD13	1.90	0.52
10:X:202:CYS:N	10:X:203:PRO:HD3	2.25	0.52
10:X:421:LEU:HD21	12:Z:283:ARG:HD2	1.90	0.52
11:Y:12:PRO:O	11:Y:146:ARG:NH1	2.38	0.52
11:Y:104:MET:O	11:Y:108:ALA:CB	2.58	0.52
13:A:224:LEU:HG	34:A:501:ATP:H5'1	1.92	0.52
14:B:404:LEU:O	14:B:408:ARG:HB2	2.10	0.52
16:D:281:ALA:HB2	17:E:208:ILE:HD12	1.92	0.52
18:F:383:GLU:HG2	18:F:386:ARG:HH22	1.74	0.52
27:O:63:LEU:O	27:O:67:SER:CB	2.58	0.52
27:O:63:LEU:O	27:O:67:SER:HB3	2.10	0.52
28:P:160:PRO:O	28:P:164:PHE:HB2	2.09	0.52
20:h:14:SER:OG	20:h:18:LYS:N	2.43	0.52
20:h:226:VAL:O	20:h:230:LEU:CB	2.58	0.52
22:j:68:ASN:HA	22:j:211:MET:HE1	1.92	0.52
23:k:41:GLN:HA	23:k:46:VAL:HG22	1.92	0.52
23:k:166:ASP:HB2	24:l:56:LEU:HB2	1.92	0.52
29:q:169:LYS:HG2	29:q:170:ARG:HG3	1.92	0.52
3:c:59:GLY:HA2	3:c:70:ILE:HG22	1.92	0.52
6:f:138:GLU:O	6:f:142:TYR:CB	2.57	0.52
6:f:403:LYS:O	6:f:407:MET:N	2.43	0.52
7:U:140:ARG:O	7:U:144:ASP:HB2	2.10	0.52
7:U:458:ILE:O	7:U:462:LEU:CB	2.57	0.52
7:U:638:SER:HB2	7:U:671:LEU:HD13	1.92	0.52
10:X:287:LEU:O	10:X:291:ALA:CB	2.58	0.52
15:C:99:VAL:HB	15:C:103:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:123:LEU:CD2	16:D:123:LEU:H	2.14	0.52
18:F:430:LYS:N	18:F:430:LYS:CD	2.73	0.52
20:H:120:GLU:O	20:H:124:SER:HB3	2.10	0.52
21:I:136:TYR:HB2	21:I:148:TYR:HB2	1.92	0.52
23:K:16:SER:N	23:K:22:PHE:CE2	2.65	0.52
23:K:22:PHE:N	23:K:22:PHE:HD2	2.07	0.52
7:U:494:TYR:OH	7:U:531:ASP:OD2	2.27	0.51
7:U:648:VAL:O	7:U:652:ALA:CB	2.58	0.51
10:X:177:TYR:O	10:X:182:ASN:N	2.43	0.51
15:C:29:GLU:O	15:C:33:LEU:HB2	2.10	0.51
16:D:172:ILE:O	16:D:176:GLU:HB2	2.10	0.51
17:E:119:VAL:HA	17:E:122:MET:HE2	1.91	0.51
17:E:317:ALA:HA	17:E:320:ILE:HD12	1.91	0.51
20:H:14:SER:OG	20:H:18:LYS:N	2.43	0.51
20:h:150:ASP:OD1	20:h:154:ALA:N	2.43	0.51
31:s:171:ALA:HA	31:s:174:LEU:HD12	1.92	0.51
1:a:7:PHE:HE2	1:a:57:ILE:HD12	1.73	0.51
7:U:237:VAL:HG22	7:U:321:GLN:HE21	1.75	0.51
7:U:792:ASN:HD21	7:U:796:LYS:HD3	1.73	0.51
8:V:187:ILE:HA	8:V:191:LEU:HD13	1.91	0.51
8:V:346:LEU:CD1	8:V:346:LEU:N	2.73	0.51
9:W:359:VAL:HG13	9:W:396:LEU:HD11	1.93	0.51
9:W:426:ASN:O	9:W:430:GLN:CB	2.53	0.51
11:Y:119:GLY:O	11:Y:123:ALA:CB	2.55	0.51
13:A:214:LEU:O	13:A:320:ALA:HA	2.09	0.51
13:A:235:ALA:HB1	13:A:270:CYS:HA	1.91	0.51
13:A:393:GLY:HA3	14:B:216:ILE:HD13	1.92	0.51
20:H:51:LYS:HG2	20:H:207:ASN:HD22	1.75	0.51
31:S:171:ALA:HA	31:S:174:LEU:HD12	1.92	0.51
32:T:145:LEU:HB3	32:T:179:ARG:HH21	1.74	0.51
20:h:174:LEU:O	20:h:178:TYR:CB	2.58	0.51
24:l:184:LEU:H	24:l:184:LEU:CD1	2.21	0.51
27:o:63:LEU:O	27:o:67:SER:CB	2.58	0.51
1:a:182:CYS:SG	1:a:183:VAL:N	2.83	0.51
3:c:268:GLU:HG3	10:X:409:LYS:HE3	1.92	0.51
3:c:291:LEU:HD22	12:Z:266:ILE:HG21	1.93	0.51
6:f:522:CYS:O	6:f:526:ALA:HB2	2.10	0.51
8:V:88:GLY:H	8:V:118:GLN:HE21	1.58	0.51
9:W:403:PHE:HD2	9:W:417:ARG:HD3	1.74	0.51
14:B:151:LEU:HD21	14:B:163:LEU:HD13	1.91	0.51
17:E:34:LYS:O	17:E:38:LYS:CB	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:129:ASN:HB3	17:E:189:SER:HB3	1.92	0.51
20:H:7:SER:OG	20:H:125:GLY:CA	2.51	0.51
22:J:70:CYS:HB2	22:J:134:VAL:HB	1.92	0.51
28:P:159:ASP:O	28:P:163:LEU:CB	2.58	0.51
22:j:40:ILE:HA	22:j:212:ARG:HA	1.92	0.51
23:k:221:GLN:HB2	23:k:224:GLN:HB3	1.91	0.51
28:p:172:LEU:O	28:p:176:ASP:HB2	2.10	0.51
31:s:12:ILE:O	31:s:137:ALA:HA	2.09	0.51
6:f:520:LEU:HD21	6:f:560:LEU:HD12	1.91	0.51
6:f:541:THR:O	6:f:545:LYS:CB	2.57	0.51
7:U:402:PHE:O	7:U:406:ALA:HB2	2.10	0.51
8:V:46:GLY:HA3	8:V:62:HIS:HD1	1.75	0.51
9:W:155:GLN:NE2	9:W:158:ASP:OD2	2.42	0.51
17:E:210:GLU:OE2	17:E:213:ARG:NH2	2.43	0.51
19:G:42:VAL:O	19:G:48:ALA:HA	2.11	0.51
20:H:150:ASP:OD1	20:H:154:ALA:N	2.43	0.51
21:I:35:LEU:O	21:I:45:LEU:HA	2.10	0.51
25:M:160:TYR:HD2	25:M:163:CYS:HB2	1.76	0.51
27:o:30:ASN:OD1	27:o:187:ARG:NH2	2.44	0.51
7:U:580:ARG:NH2	7:U:768:GLN:OE1	2.44	0.51
8:V:214:HIS:O	8:V:218:TYR:HB2	2.09	0.51
8:V:377:GLN:O	8:V:381:GLN:CB	2.58	0.51
13:A:241:ILE:HB	13:A:244:GLU:HG3	1.93	0.51
18:F:222:GLY:O	18:F:349:ASP:N	2.43	0.51
21:I:90:LEU:HD12	21:I:114:LEU:HD22	1.93	0.51
23:K:66:LYS:HA	23:K:78:MET:HE3	1.92	0.51
28:P:49:LEU:HG	28:P:111:GLY:HA3	1.93	0.51
21:i:35:LEU:O	21:i:45:LEU:HA	2.10	0.51
24:l:201:ALA:O	24:l:239:ARG:NH1	2.42	0.51
30:r:196:HIS:O	30:r:200:SER:CB	2.59	0.51
4:d:164:THR:HA	4:d:167:ILE:HG12	1.91	0.51
8:V:229:SER:O	8:V:233:ALA:HB2	2.10	0.51
9:W:384:LEU:HD22	9:W:392:PHE:HD2	1.75	0.51
10:X:383:GLY:O	10:X:385:LEU:CD1	2.57	0.51
24:L:92:CYS:O	24:L:96:ARG:CB	2.59	0.51
26:N:132:SER:O	26:N:136:TYR:HB2	2.09	0.51
28:P:29:GLY:HA3	28:P:34:MET:HA	1.93	0.51
21:i:90:LEU:HD12	21:i:114:LEU:HD22	1.93	0.51
21:i:91:ARG:NH1	28:p:76:LEU:O	2.43	0.51
28:p:159:ASP:O	28:p:163:LEU:CB	2.58	0.51
6:f:222:ASP:HA	6:f:225:ALA:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:250:PHE:HA	7:U:253:TYR:HB3	1.93	0.51
7:U:402:PHE:HB2	7:U:437:TYR:HB3	1.93	0.51
7:U:646:PRO:HA	7:U:649:ARG:HB2	1.92	0.51
9:W:82:LEU:O	9:W:86:ASN:CB	2.57	0.51
13:A:387:SER:O	13:A:391:GLU:HB2	2.11	0.51
17:E:55:GLN:N	18:F:133:PHE:O	2.38	0.51
18:F:235:LEU:O	18:F:239:ALA:HB2	2.11	0.51
18:F:430:LYS:CE	18:F:430:LYS:N	2.73	0.51
20:H:93:LEU:HD11	20:H:113:ARG:HB3	1.93	0.51
28:P:172:LEU:O	28:P:176:ASP:HB2	2.10	0.51
31:S:187:VAL:HG21	27:o:24:MET:HE3	1.93	0.51
27:o:216:ILE:HG23	28:p:194:LYS:HD2	1.92	0.51
1:a:21:VAL:O	1:a:25:LEU:HB2	2.10	0.51
2:b:22:LEU:HD11	2:b:179:LEU:C	2.30	0.51
2:b:30:GLN:HG3	2:b:75:LEU:HD22	1.92	0.51
6:f:79:ARG:HE	6:f:95:PRO:HG3	1.76	0.51
8:V:99:ARG:NH2	8:V:147:PHE:O	2.44	0.51
9:W:267:LEU:HA	9:W:270:VAL:HG12	1.93	0.51
18:F:197:GLU:O	18:F:201:ALA:CB	2.59	0.51
27:O:30:ASN:OD1	27:O:187:ARG:NH2	2.44	0.51
28:P:2:SER:OG	28:P:3:ILE:N	2.43	0.51
20:h:187:ALA:O	20:h:191:ALA:HB2	2.10	0.51
27:o:106:THR:OG1	27:o:109:HIS:NE2	2.39	0.51
2:b:22:LEU:HD21	2:b:180:ALA:N	2.23	0.51
6:f:370:MET:O	6:f:374:SER:CB	2.59	0.51
9:W:356:ASN:O	9:W:360:GLU:CB	2.59	0.51
11:Y:192:ARG:HH12	11:Y:295:TYR:HB2	1.75	0.51
11:Y:234:PRO:O	11:Y:238:GLU:HB2	2.10	0.51
12:Z:190:ARG:HA	12:Z:193:ASN:HB2	1.93	0.51
17:E:167:PRO:O	17:E:274:LYS:NZ	2.42	0.51
18:F:313:LEU:O	18:F:317:LEU:CB	2.59	0.51
29:Q:13:VAL:HB	29:Q:183:ILE:HD12	1.93	0.51
29:Q:169:LYS:HG2	29:Q:170:ARG:HG3	1.92	0.51
30:R:196:HIS:O	30:R:200:SER:CB	2.59	0.51
20:h:93:LEU:HD11	20:h:113:ARG:HB3	1.93	0.51
23:k:169:ALA:N	23:k:178:GLN:OE1	2.43	0.51
29:q:13:VAL:HB	29:q:183:ILE:HD12	1.93	0.51
1:a:292:THR:HG23	1:a:295:GLU:H	1.76	0.51
2:b:100:ARG:NH1	2:b:102:GLY:O	2.44	0.51
2:b:126:LYS:O	2:b:130:ARG:HB2	2.11	0.51
3:c:58:LEU:HB3	3:c:71:ASP:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:140:LEU:O	6:f:144:LEU:CB	2.59	0.51
11:Y:301:ILE:HG13	11:Y:343:LEU:HD12	1.93	0.51
20:H:187:ALA:O	20:H:191:ALA:HB2	2.10	0.51
25:M:152:ASP:OD2	25:M:154:SER:OG	2.28	0.51
29:Q:4:LEU:HD22	29:Q:45:LEU:HD13	1.93	0.51
21:i:118:LYS:HE3	21:i:130:PHE:HB2	1.93	0.51
24:l:93:LEU:HA	24:l:96:ARG:HB3	1.91	0.51
1:a:54:ASP:HA	1:a:57:ILE:HG22	1.93	0.50
1:a:346:ILE:HA	1:a:349:MET:HE2	1.93	0.50
5:e:43:TRP:HZ3	8:V:345:ARG:HB2	1.76	0.50
6:f:478:ARG:HD3	6:f:504:VAL:HG13	1.93	0.50
7:U:205:TYR:HD2	7:U:215:ASN:HB3	1.76	0.50
7:U:229:VAL:HG22	7:U:268:LEU:HD21	1.93	0.50
12:Z:227:ILE:O	12:Z:231:GLN:CB	2.59	0.50
16:D:103:VAL:HG11	16:D:139:LEU:HD21	1.93	0.50
16:D:416:PHE:CD2	19:G:29:PHE:HZ	2.29	0.50
18:F:431:LYS:NZ	18:F:431:LYS:CA	2.73	0.50
22:J:40:ILE:HA	22:J:212:ARG:HA	1.93	0.50
22:J:115:LYS:HE3	22:J:127:PHE:HB2	1.93	0.50
28:P:113:ASP:OD2	28:P:116:THR:N	2.43	0.50
19:g:42:VAL:O	19:g:48:ALA:HA	2.11	0.50
21:i:134:LEU:N	21:i:150:SER:OG	2.44	0.50
26:n:96:ALA:H	26:n:116:MET:HG2	1.76	0.50
1:a:93:ALA:HA	1:a:96:PHE:HB3	1.92	0.50
3:c:32:TYR:HB3	3:c:208:ARG:HE	1.75	0.50
6:f:138:GLU:O	6:f:142:TYR:HB2	2.11	0.50
7:U:598:ALA:O	7:U:602:LEU:CB	2.54	0.50
7:U:637:VAL:HG11	7:U:655:ALA:HB3	1.93	0.50
8:V:187:ILE:HG23	8:V:191:LEU:HD22	1.93	0.50
9:W:407:ASP:OD1	10:X:382:GLU:CA	2.59	0.50
10:X:396:THR:HG23	12:Z:265:LEU:HD21	1.93	0.50
15:C:147:THR:HG22	15:C:150:MET:HE3	1.94	0.50
16:D:172:ILE:O	16:D:176:GLU:CB	2.58	0.50
19:G:17:SER:HB2	19:G:18:PRO:CD	2.26	0.50
26:N:96:ALA:H	26:N:116:MET:HG2	1.76	0.50
21:i:62:SER:OG	21:i:65:ILE:O	2.29	0.50
21:i:106:PRO:HD2	21:i:109:GLN:HE21	1.76	0.50
24:l:92:CYS:O	24:l:96:ARG:CB	2.59	0.50
31:s:27:THR:O	31:s:40:SER:N	2.43	0.50
3:c:252:ALA:O	3:c:256:ASN:ND2	2.44	0.50
7:U:345:ASN:HD21	7:U:883:ARG:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:439:TYR:O	14:B:439:TYR:CD1	2.65	0.50
19:G:17:SER:CB	19:G:18:PRO:CD	2.88	0.50
21:I:8:ARG:O	21:I:11:ILE:HD12	2.07	0.50
22:j:114:LEU:O	22:j:118:TYR:CB	2.59	0.50
24:l:45:VAL:HG22	24:l:214:ILE:HG23	1.93	0.50
26:n:29:ARG:NH1	27:o:139:GLU:OE1	2.44	0.50
28:p:42:ILE:HA	28:p:51:ILE:O	2.12	0.50
29:q:4:LEU:HD22	29:q:45:LEU:HD13	1.93	0.50
3:c:220:LEU:O	3:c:224:SER:CB	2.52	0.50
7:U:588:MET:HG2	7:U:764:LEU:HD22	1.94	0.50
8:V:80:LYS:CE	8:V:83:GLU:HB3	2.41	0.50
9:W:320:LEU:HD21	9:W:354:LEU:HD21	1.93	0.50
13:A:98:CYS:HA	13:A:140:VAL:O	2.11	0.50
16:D:416:PHE:C	16:D:418:LYS:H	2.18	0.50
19:G:14:THR:OG1	20:H:127:VAL:HG12	2.12	0.50
23:K:169:ALA:N	23:K:178:GLN:OE1	2.43	0.50
23:K:216:GLU:HA	23:K:234:LEU:HD11	1.92	0.50
7:U:408:LEU:O	7:U:412:HIS:ND1	2.38	0.50
8:V:404:LYS:HA	8:V:407:VAL:HG12	1.92	0.50
10:X:117:ALA:O	10:X:121:LYS:HA	2.11	0.50
13:A:220:THR:HG21	13:A:343:PHE:HB3	1.93	0.50
14:B:361:LYS:HD2	14:B:384:ILE:HG12	1.93	0.50
16:D:151:ILE:CD1	16:D:229:ARG:CZ	2.90	0.50
16:D:231:VAL:HB	16:D:234:GLU:HB2	1.92	0.50
18:F:437:TYR:CD2	23:K:20:ARG:CG	2.94	0.50
19:G:161:CYS:SG	19:G:162:GLY:N	2.84	0.50
22:J:68:ASN:HA	22:J:211:MET:HE1	1.92	0.50
31:s:125:ASP:OD1	31:s:129:SER:N	2.37	0.50
6:f:538:ILE:HA	6:f:541:THR:HG22	1.93	0.50
7:U:345:ASN:O	7:U:743:ASN:ND2	2.36	0.50
7:U:397:THR:HG23	7:U:399:TRP:H	1.75	0.50
7:U:418:GLU:HG2	7:U:422:LEU:HB2	1.93	0.50
8:V:421:ASP:O	8:V:425:LYS:HB2	2.12	0.50
14:B:439:TYR:CB	22:J:76:LEU:CB	2.88	0.50
16:D:353:ASN:HD22	16:D:392:TYR:HB2	1.77	0.50
28:P:190:ILE:HG22	28:P:195:ILE:HG23	1.94	0.50
32:T:162:GLN:O	32:T:166:ARG:CB	2.59	0.50
21:i:105:ILE:HG13	21:i:107:CYS:H	1.77	0.50
25:m:160:TYR:HD2	25:m:163:CYS:HB2	1.76	0.50
27:o:100:LEU:HB3	27:o:111:TYR:HB2	1.92	0.50
6:f:119:LYS:HB2	6:f:122:ALA:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:248:LEU:O	6:f:252:ALA:CB	2.60	0.50
6:f:273:ASN:ND2	6:f:310:ASP:OD2	2.44	0.50
8:V:32:PRO:O	8:V:36:GLU:CB	2.58	0.50
8:V:78:HIS:ND1	8:V:161:PRO:O	2.43	0.50
8:V:116:ALA:O	8:V:120:PHE:N	2.37	0.50
8:V:340:GLY:O	8:V:408:ARG:NH1	2.44	0.50
9:W:430:GLN:O	9:W:434:SER:CB	2.59	0.50
18:F:340:PRO:O	18:F:344:ARG:CG	2.60	0.50
19:G:84:THR:HB	25:M:156:VAL:HG22	1.94	0.50
20:H:111:VAL:O	20:H:115:ALA:CB	2.59	0.50
27:O:174:ASP:HA	27:O:186:LEU:O	2.12	0.50
31:S:27:THR:O	31:S:40:SER:N	2.43	0.50
20:h:111:VAL:O	20:h:115:ALA:CB	2.59	0.50
21:i:136:TYR:HB2	21:i:148:TYR:HB2	1.92	0.50
28:p:190:ILE:HG22	28:p:195:ILE:HG23	1.94	0.50
31:s:35:ILE:O	32:t:151:ARG:NH2	2.39	0.50
32:t:89:HIS:NE2	32:t:124:TYR:O	2.43	0.50
4:d:45:LYS:HE3	4:d:86:LYS:HG3	1.93	0.50
19:G:71:LYS:O	19:G:95:ARG:NH2	2.44	0.50
21:I:62:SER:OG	21:I:65:ILE:O	2.29	0.50
25:M:189:ILE:HA	25:M:192:GLU:HB2	1.94	0.50
6:f:213:GLN:O	6:f:217:LEU:HB2	2.12	0.50
6:f:278:VAL:HA	6:f:281:ILE:HG22	1.94	0.50
6:f:338:ASP:C	6:f:340:MET:H	2.20	0.50
6:f:357:ARG:O	6:f:361:SER:HB2	2.12	0.50
6:f:536:SER:HA	6:f:539:LEU:HB3	1.93	0.50
8:V:203:LEU:O	8:V:207:ALA:HB2	2.11	0.50
9:W:158:ASP:OD1	9:W:158:ASP:N	2.44	0.50
17:E:84:ARG:O	17:E:85:ARG:NE	2.44	0.50
21:I:11:ILE:CD1	21:I:11:ILE:N	2.73	0.50
22:J:10:PHE:HB3	22:J:14:GLY:HA2	1.94	0.50
22:J:115:LYS:HE2	22:J:149:PRO:HA	1.94	0.50
23:K:16:SER:CB	23:K:22:PHE:CZ	2.95	0.50
24:L:45:VAL:HG22	24:L:214:ILE:HG23	1.93	0.50
19:g:161:CYS:SG	19:g:162:GLY:N	2.84	0.50
30:r:153:TYR:O	30:r:157:ARG:HB2	2.12	0.50
7:U:415:HIS:CE1	7:U:418:GLU:HB3	2.47	0.49
8:V:469:THR:HA	12:Z:257:MET:HE1	1.94	0.49
14:B:122:ILE:HA	14:B:131:HIS:O	2.12	0.49
17:E:140:GLU:O	17:E:144:GLU:CB	2.60	0.49
18:F:97:LEU:O	18:F:120:LYS:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:313:LEU:O	18:F:317:LEU:HB2	2.12	0.49
21:I:118:LYS:HE3	21:I:130:PHE:HB2	1.94	0.49
22:J:79:ASP:HB3	22:J:127:PHE:HD1	1.77	0.49
26:N:7:GLN:HA	26:N:12:VAL:HA	1.94	0.49
27:O:213:THR:O	28:P:198:ARG:HA	2.12	0.49
28:P:42:ILE:HA	28:P:51:ILE:O	2.12	0.49
26:n:4:MET:HA	26:n:126:ALA:O	2.12	0.49
27:o:174:ASP:HA	27:o:186:LEU:O	2.12	0.49
30:r:115:ASP:HB2	30:r:119:ASN:HB2	1.93	0.49
30:r:130:SER:OG	30:r:167:ASP:OD2	2.31	0.49
1:a:308:GLU:OE2	9:W:377:ARG:NH2	2.44	0.49
6:f:94:LYS:HA	6:f:97:LYS:HG2	1.93	0.49
6:f:487:LEU:HD23	6:f:524:MET:HE1	1.93	0.49
7:U:98:GLU:HA	7:U:101:ILE:HG12	1.93	0.49
7:U:187:LEU:HD13	16:D:45:LYS:HE3	1.94	0.49
7:U:599:ILE:HD12	7:U:602:LEU:HD22	1.94	0.49
8:V:51:ALA:HB2	8:V:199:ASN:HD21	1.77	0.49
9:W:124:LEU:HD13	9:W:147:LYS:HB2	1.94	0.49
9:W:355:LYS:HA	9:W:358:VAL:HG22	1.94	0.49
16:D:211:GLY:HA3	16:D:214:MET:HE2	1.93	0.49
21:I:106:PRO:HD2	21:I:109:GLN:HE21	1.76	0.49
23:K:194:ALA:O	23:K:198:SER:HB3	2.12	0.49
25:M:123:THR:HG22	25:M:130:PRO:HB3	1.95	0.49
26:N:4:MET:HA	26:N:126:ALA:O	2.12	0.49
25:m:180:GLN:HB3	25:m:184:MET:HE3	1.94	0.49
28:p:29:GLY:HA3	28:p:34:MET:HA	1.93	0.49
32:t:162:GLN:O	32:t:166:ARG:CB	2.59	0.49
6:f:253:LEU:HD12	6:f:277:LEU:HD12	1.94	0.49
7:U:574:LYS:HG3	7:U:576:PRO:HD2	1.93	0.49
7:U:648:VAL:O	7:U:652:ALA:HB2	2.12	0.49
8:V:345:ARG:CZ	8:V:359:PRO:O	2.60	0.49
13:A:161:VAL:HA	13:A:164:MET:HE3	1.94	0.49
16:D:176:GLU:OE2	16:D:329:ARG:NH1	2.45	0.49
17:E:380:LEU:HD22	18:F:335:VAL:HG11	1.93	0.49
21:I:134:LEU:N	21:I:150:SER:OG	2.44	0.49
22:J:95:ARG:NH1	22:J:100:ASP:O	2.45	0.49
30:R:115:ASP:HB2	30:R:119:ASN:HB2	1.93	0.49
19:g:120:ASP:OD1	20:h:84:ARG:NH1	2.45	0.49
23:k:22:PHE:CD2	23:k:22:PHE:N	2.73	0.49
4:d:148:TYR:HE1	4:d:174:ILE:HG23	1.78	0.49
7:U:370:VAL:O	7:U:374:SER:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:231:LEU:HD21	11:Y:239:LYS:HB2	1.93	0.49
22:J:114:LEU:O	22:J:118:TYR:CB	2.60	0.49
19:g:173:THR:O	19:g:177:SER:HB3	2.13	0.49
22:j:95:ARG:NH1	22:j:100:ASP:O	2.45	0.49
23:k:194:ALA:O	23:k:198:SER:HB3	2.12	0.49
31:s:211:ARG:NH2	31:s:213:ASP:OD2	2.43	0.49
1:a:270:ARG:HH22	1:a:274:LEU:HB3	1.76	0.49
3:c:56:LEU:HA	3:c:111:TRP:HA	1.94	0.49
6:f:343:LYS:O	6:f:347:ASP:N	2.42	0.49
6:f:531:ASN:HA	6:f:569:LYS:HA	1.93	0.49
7:U:45:ILE:HG23	7:U:60:ALA:HB1	1.93	0.49
9:W:186:ILE:HD11	9:W:208:LYS:HG3	1.95	0.49
15:C:91:PRO:HG2	15:C:92:GLU:HG3	1.94	0.49
21:I:105:ILE:HG13	21:I:107:CYS:H	1.77	0.49
30:R:130:SER:OG	30:R:167:ASP:OD2	2.31	0.49
20:h:50:LYS:NZ	20:h:62:VAL:O	2.36	0.49
25:m:34:SER:OG	25:m:65:ARG:NH2	2.45	0.49
1:a:137:ASP:HA	1:a:140:GLU:HB2	1.94	0.49
1:a:285:PRO:HG2	1:a:288:HIS:CE1	2.48	0.49
1:a:291:LEU:O	1:a:331:VAL:N	2.42	0.49
6:f:684:PRO:O	6:f:688:ARG:CB	2.56	0.49
8:V:42:ALA:O	8:V:62:HIS:ND1	2.42	0.49
8:V:80:LYS:NZ	8:V:83:GLU:HB3	2.28	0.49
10:X:163:LYS:HA	10:X:166:LEU:HD13	1.95	0.49
18:F:246:ALA:HB1	18:F:280:PRO:HB2	1.94	0.49
19:G:123:GLN:NE2	20:H:82:ASP:OD1	2.45	0.49
20:H:107:THR:HA	20:H:110:LEU:HD13	1.94	0.49
27:O:56:THR:O	27:O:60:SER:HB3	2.12	0.49
20:h:79:MET:H	20:h:132:VAL:HG22	1.78	0.49
22:j:79:ASP:HB3	22:j:127:PHE:HD1	1.77	0.49
26:n:7:GLN:HA	26:n:12:VAL:HA	1.94	0.49
8:V:476:PHE:HD2	12:Z:260:VAL:HG12	1.78	0.49
9:W:144:ARG:HA	9:W:147:LYS:HG2	1.95	0.49
11:Y:144:LEU:HA	11:Y:147:ILE:HG22	1.95	0.49
13:A:105:ASP:HB2	13:A:110:LYS:HB2	1.95	0.49
13:A:333:ARG:HH21	18:F:230:GLY:HA2	1.77	0.49
16:D:88:VAL:HG23	16:D:132:LEU:HB2	1.94	0.49
19:G:7:ALA:HA	19:G:11:ARG:CZ	2.27	0.49
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.36	0.49
29:Q:142:ILE:HG21	30:r:141:ARG:HH21	1.78	0.49
30:R:7:LYS:HD2	30:R:109:PRO:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:211:ARG:NH2	31:S:213:ASP:OD2	2.43	0.49
19:g:71:LYS:O	19:g:95:ARG:NH2	2.44	0.49
22:j:154:HIS:CE1	23:k:59:MET:HG3	2.47	0.49
24:l:184:LEU:N	24:l:184:LEU:CD1	2.73	0.49
26:n:21:THR:HA	26:n:26:ILE:HA	1.95	0.49
28:p:49:LEU:HG	28:p:111:GLY:HA3	1.93	0.49
1:a:252:LYS:HA	1:a:255:TRP:HD1	1.77	0.49
1:a:296:ILE:O	1:a:300:ALA:CB	2.61	0.49
2:b:35:ILE:O	2:b:39:SER:HB2	2.13	0.49
2:b:54:LEU:HD13	2:b:84:ILE:HG13	1.95	0.49
2:b:161:ASN:HD22	2:b:166:THR:HA	1.78	0.49
9:W:83:LEU:HA	9:W:86:ASN:HB3	1.94	0.49
9:W:130:MET:SD	9:W:130:MET:N	2.86	0.49
19:G:9:PHE:C	19:G:11:ARG:H	2.21	0.49
19:G:53:GLN:HA	19:G:215:ILE:HA	1.95	0.49
31:S:113:LEU:HG	31:S:198:VAL:HG12	1.94	0.49
19:g:10:ASP:O	25:m:7:TYR:CZ	2.65	0.49
30:r:38:ASN:HD22	30:r:41:LEU:HD12	1.78	0.49
32:t:187:PHE:O	32:t:203:LEU:N	2.46	0.49
1:a:148:VAL:HB	1:a:151:VAL:HG12	1.95	0.49
5:e:42:ASN:C	5:e:44:ASP:N	2.70	0.49
30:R:153:TYR:O	30:R:157:ARG:HB2	2.12	0.49
22:j:6:ALA:C	22:j:8:THR:N	2.70	0.49
26:n:59:VAL:O	26:n:63:LEU:HB3	2.13	0.49
2:b:22:LEU:H	2:b:22:LEU:HD13	1.78	0.49
6:f:537:THR:OG1	6:f:538:ILE:N	2.44	0.49
9:W:135:LYS:HA	9:W:140:ILE:HB	1.95	0.49
10:X:222:GLU:HA	10:X:225:TRP:HE1	1.78	0.49
18:F:432:LYS:CB	18:F:432:LYS:NZ	2.73	0.49
19:G:67:THR:HG23	19:G:216:GLU:HG2	1.95	0.49
25:M:40:ARG:HA	25:M:45:VAL:HA	1.95	0.49
32:T:48:SER:HB2	32:T:116:ALA:HB2	1.95	0.49
32:T:74:GLU:HG3	32:T:77:LEU:HD12	1.95	0.49
22:j:131:ALA:N	22:j:147:THR:OG1	2.39	0.49
27:o:56:THR:O	27:o:60:SER:HB3	2.12	0.49
28:p:138:VAL:HB	28:p:146:MET:HE3	1.95	0.49
32:t:43:MET:HE3	32:t:45:VAL:HG22	1.95	0.49
1:a:214:GLY:HA2	1:a:217:LEU:HD13	1.94	0.48
3:c:98:MET:HA	3:c:101:GLN:HG2	1.94	0.48
7:U:366:HIS:O	7:U:369:THR:OG1	2.30	0.48
7:U:413:LYS:HD2	7:U:780:SER:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:476:PHE:O	8:V:480:ILE:HB	2.13	0.48
10:X:385:LEU:N	10:X:385:LEU:CD1	2.75	0.48
11:Y:270:VAL:O	11:Y:274:SER:OG	2.28	0.48
13:A:221:GLY:N	34:A:501:ATP:O2A	2.46	0.48
16:D:151:ILE:HD13	16:D:229:ARG:CZ	2.43	0.48
16:D:200:ARG:NH1	16:D:303:VAL:O	2.46	0.48
27:O:201:ARG:NH1	27:O:203:ARG:HH22	1.94	0.48
30:r:196:HIS:O	30:r:200:SER:OG	2.27	0.48
31:s:145:LEU:HD22	31:s:178:VAL:HB	1.95	0.48
1:a:278:MET:O	1:a:282:PHE:CB	2.59	0.48
1:a:360:VAL:O	1:a:364:GLU:CB	2.60	0.48
9:W:336:PRO:O	9:W:340:VAL:HB	2.13	0.48
9:W:337:ALA:O	9:W:341:PHE:HB2	2.13	0.48
11:Y:53:TYR:O	11:Y:57:LEU:CB	2.61	0.48
14:B:392:GLY:O	14:B:396:LYS:HB2	2.13	0.48
16:D:133:HIS:HD2	16:D:136:SER:H	1.59	0.48
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.46	0.48
19:G:173:THR:O	19:G:177:SER:HB3	2.13	0.48
26:N:59:VAL:O	26:N:63:LEU:HB3	2.13	0.48
19:g:129:ALA:N	20:h:127:VAL:HG13	2.26	0.48
22:j:6:ALA:HB2	22:j:9:VAL:HG21	1.80	0.48
22:j:115:LYS:HE3	22:j:127:PHE:HB2	1.93	0.48
22:j:115:LYS:HE2	22:j:149:PRO:HA	1.95	0.48
28:p:148:GLY:O	28:p:152:SER:OG	2.27	0.48
30:r:7:LYS:HD2	30:r:109:PRO:HB2	1.95	0.48
1:a:70:ARG:HG3	2:b:17:ARG:HH11	1.78	0.48
8:V:407:VAL:O	8:V:411:SER:OG	2.30	0.48
8:V:440:LYS:HA	8:V:443:ARG:HB3	1.95	0.48
13:A:355:PHE:HD2	13:A:370:PHE:HB3	1.79	0.48
17:E:194:ASN:HB3	17:E:228:CYS:HA	1.95	0.48
20:H:79:MET:H	20:H:132:VAL:HG22	1.78	0.48
30:R:7:LYS:HA	30:R:12:VAL:HA	1.95	0.48
31:S:176:LYS:HE2	31:S:208:VAL:HG21	1.95	0.48
31:S:197:ILE:O	31:S:203:ILE:HA	2.13	0.48
31:S:199:THR:OG1	31:S:202:GLY:O	2.30	0.48
21:i:13:SER:CB	21:i:17:ARG:CD	2.90	0.48
21:i:66:TYR:O	21:i:73:ALA:HA	2.13	0.48
22:j:154:HIS:HE1	23:k:64:ILE:HD11	1.79	0.48
28:p:27:ARG:NH1	28:p:180:VAL:O	2.46	0.48
7:U:465:LEU:O	7:U:474:ARG:NH1	2.47	0.48
9:W:408:ARG:NH2	9:W:408:ARG:CB	2.73	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:124:SER:HA	14:B:130:GLU:HG2	1.93	0.48
16:D:412:GLN:HE21	16:D:412:GLN:C	2.22	0.48
17:E:385:ASP:OD1	17:E:385:ASP:N	2.45	0.48
24:L:5:GLN:O	24:L:8:ASN:ND2	2.47	0.48
25:M:34:SER:OG	25:M:65:ARG:NH2	2.45	0.48
26:N:21:THR:HA	26:N:26:ILE:HA	1.95	0.48
28:P:138:VAL:HB	28:P:146:MET:HE3	1.95	0.48
19:g:20:GLY:O	19:g:21:ARG:HG3	2.13	0.48
19:g:53:GLN:HA	19:g:215:ILE:HA	1.95	0.48
21:i:17:ARG:CG	21:i:17:ARG:HH11	2.13	0.48
26:n:87:CYS:O	26:n:91:ARG:HD2	2.12	0.48
32:t:115:TYR:HE2	32:t:194:GLU:HB3	1.79	0.48
1:a:284:ARG:HB3	1:a:285:PRO:HD2	1.96	0.48
4:d:235:THR:HG22	4:d:236:THR:HG23	1.94	0.48
21:I:196:VAL:O	21:I:200:THR:OG1	2.29	0.48
23:K:12:VAL:HA	23:K:21:LEU:HD11	1.95	0.48
25:M:99:ARG:HB3	32:T:69:GLN:HE22	1.78	0.48
25:M:180:GLN:HB3	25:M:184:MET:HE3	1.94	0.48
28:P:30:ILE:N	28:P:33:GLN:O	2.44	0.48
19:g:123:GLN:NE2	20:h:82:ASP:OD1	2.47	0.48
22:j:10:PHE:HB3	22:j:14:GLY:HA2	1.94	0.48
22:j:115:LYS:NZ	22:j:129:ILE:O	2.47	0.48
23:k:93:ARG:HD3	30:r:68:LEU:HB3	1.95	0.48
1:a:186:LYS:O	1:a:193:GLN:NE2	2.46	0.48
3:c:176:GLN:HG3	3:c:177:THR:HG23	1.94	0.48
4:d:106:LEU:HD11	4:d:114:GLU:HB3	1.95	0.48
6:f:586:PRO:O	6:f:590:PHE:CB	2.61	0.48
6:f:600:TYR:HB3	6:f:608:LYS:HE2	1.96	0.48
13:A:248:LYS:HE2	14:B:259:TYR:HB3	1.96	0.48
15:C:113:ARG:NH2	15:C:129:ASN:O	2.47	0.48
16:D:369:LYS:HB2	16:D:369:LYS:HE2	1.49	0.48
18:F:96:LEU:HA	18:F:121:CYS:O	2.13	0.48
18:F:237:ALA:O	18:F:241:ALA:CB	2.62	0.48
22:J:40:ILE:HA	22:J:211:MET:O	2.14	0.48
26:N:91:ARG:NH1	26:N:117:GLY:O	2.47	0.48
27:O:38:SER:OG	27:O:40:ASN:OD1	2.23	0.48
28:P:27:ARG:NH1	28:P:180:VAL:O	2.46	0.48
30:R:196:HIS:O	30:R:200:SER:OG	2.27	0.48
25:m:123:THR:HG22	25:m:130:PRO:HB3	1.95	0.48
3:c:144:VAL:O	3:c:157:ILE:HA	2.14	0.48
6:f:24:THR:HG22	6:f:71:TYR:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:166:VAL:O	6:f:170:TRP:CB	2.62	0.48
6:f:438:ASP:N	6:f:438:ASP:OD1	2.43	0.48
6:f:623:LYS:O	6:f:627:GLU:HB3	2.13	0.48
9:W:72:LYS:HD2	9:W:123:ARG:HD3	1.94	0.48
10:X:90:ARG:O	10:X:94:ASP:HB2	2.13	0.48
10:X:407:MET:HB3	11:Y:376:LEU:HD13	1.95	0.48
11:Y:23:ARG:HH22	11:Y:55:GLU:HB2	1.78	0.48
12:Z:220:LEU:CD1	12:Z:221:PRO:CD	2.87	0.48
15:C:90:HIS:CG	16:D:110:ASN:CB	2.88	0.48
15:C:387:VAL:O	15:C:391:MET:HB2	2.14	0.48
18:F:314:LEU:HD21	18:F:342:LEU:HD23	1.95	0.48
22:J:36:ARG:NH1	22:J:142:PRO:O	2.46	0.48
27:O:177:VAL:HB	27:O:184:ASP:HB2	1.96	0.48
31:S:49:LYS:O	31:S:112:GLY:CA	2.61	0.48
32:T:187:PHE:O	32:T:203:LEU:N	2.46	0.48
22:j:40:ILE:HA	22:j:211:MET:O	2.14	0.48
23:k:37:ALA:HB2	23:k:50:VAL:HG23	1.96	0.48
24:l:5:GLN:O	24:l:8:ASN:ND2	2.47	0.48
31:s:113:LEU:HG	31:s:198:VAL:HG12	1.94	0.48
32:t:49:THR:OG1	32:t:50:MET:N	2.46	0.48
1:a:34:TRP:HZ3	1:a:64:ILE:HG12	1.79	0.48
2:b:3:LEU:HB3	2:b:105:HIS:HA	1.96	0.48
3:c:30:GLN:HB3	3:c:66:THR:HG22	1.95	0.48
3:c:144:VAL:HB	3:c:158:ASP:HB3	1.95	0.48
4:d:36:LEU:HD13	4:d:84:ASP:HB2	1.94	0.48
4:d:238:PRO:HA	4:d:241:GLU:HG2	1.96	0.48
7:U:195:ASN:HB2	7:U:223:LEU:HD23	1.94	0.48
9:W:87:ILE:HG22	9:W:89:LEU:H	1.79	0.48
9:W:320:LEU:O	9:W:324:TYR:HB2	2.14	0.48
11:Y:232:GLU:O	11:Y:235:ASP:N	2.46	0.48
15:C:86:LEU:HD21	15:C:94:LYS:HB3	1.95	0.48
18:F:366:MET:O	18:F:370:SER:OG	2.29	0.48
21:I:38:LEU:HG	21:I:160:LYS:HB3	1.96	0.48
24:L:54:SER:H	24:L:57:ALA:HB3	1.79	0.48
25:M:106:ILE:HG12	25:M:111:LEU:HD13	1.96	0.48
20:h:78:GLY:HA3	20:h:132:VAL:HG22	1.95	0.48
2:b:40:LYS:HA	2:b:43:SER:HB3	1.96	0.48
6:f:89:MET:HG2	6:f:90:THR:HG23	1.95	0.48
7:U:45:ILE:HG21	7:U:64:ALA:HB2	1.94	0.48
9:W:254:PRO:HA	9:W:257:GLN:HG2	1.96	0.48
10:X:362:GLU:O	10:X:363:ARG:CG	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:411:VAL:HA	10:X:414:LEU:HD12	1.96	0.48
11:Y:56:ALA:O	11:Y:60:SER:HB3	2.14	0.48
14:B:181:GLN:O	14:B:241:ASN:ND2	2.47	0.48
16:D:171:ASP:O	16:D:175:GLN:CB	2.62	0.48
18:F:175:MET:HA	18:F:250:LYS:HE3	1.96	0.48
18:F:346:GLY:HA2	18:F:349:ASP:HA	1.95	0.48
23:K:85:ALA:HB2	23:K:139:VAL:HG21	1.95	0.48
30:R:26:ILE:HG13	28:p:179:ALA:HB2	1.96	0.48
31:S:184:GLU:OE1	31:S:211:ARG:NH1	2.47	0.48
31:S:184:GLU:OE1	27:o:29:LYS:NZ	2.47	0.48
19:g:140:LEU:O	19:g:151:VAL:HA	2.14	0.48
20:h:107:THR:HA	20:h:110:LEU:HD13	1.94	0.48
21:i:136:TYR:O	21:i:147:LEU:HA	2.13	0.48
25:m:189:ILE:HA	25:m:192:GLU:HB2	1.94	0.48
26:n:134:TYR:O	26:n:137:GLY:N	2.47	0.48
31:s:197:ILE:O	31:s:203:ILE:HA	2.13	0.48
6:f:575:ALA:O	6:f:579:ALA:CB	2.62	0.48
14:B:421:LYS:O	14:B:425:ASN:HB2	2.14	0.48
17:E:140:GLU:O	17:E:144:GLU:HB2	2.14	0.48
26:N:19:ARG:NH1	26:N:170:SER:O	2.47	0.48
26:N:87:CYS:O	26:N:91:ARG:CB	2.58	0.48
32:T:166:ARG:NH1	32:T:170:GLU:OE2	2.47	0.48
19:g:67:THR:HG23	19:g:216:GLU:HG2	1.95	0.48
24:l:54:SER:H	24:l:57:ALA:HB3	1.79	0.48
25:m:152:ASP:OD2	25:m:154:SER:OG	2.28	0.48
27:o:177:VAL:HB	27:o:184:ASP:HB2	1.96	0.48
30:r:7:LYS:HA	30:r:12:VAL:HA	1.95	0.48
31:s:4:PRO:O	32:t:100:ARG:NH2	2.46	0.48
1:a:35:HIS:CE1	2:b:17:ARG:HB2	2.49	0.47
6:f:229:VAL:O	6:f:233:LEU:HB3	2.14	0.47
6:f:322:SER:HA	6:f:331:LEU:HD11	1.96	0.47
7:U:904:LYS:HB3	7:U:913:ILE:HG12	1.95	0.47
8:V:291:TYR:HD1	8:V:294:ARG:HH22	1.62	0.47
15:C:90:HIS:CB	16:D:110:ASN:H	2.25	0.47
15:C:284:GLU:OE1	15:C:287:LYS:NZ	2.37	0.47
17:E:33:LEU:O	17:E:37:THR:CB	2.62	0.47
23:K:101:PHE:HA	30:R:57:ARG:HH21	1.80	0.47
25:M:202:ASP:N	25:M:202:ASP:OD1	2.47	0.47
26:N:153:LEU:O	26:N:157:ALA:HB2	2.14	0.47
28:P:160:PRO:O	28:P:164:PHE:CB	2.62	0.47
32:T:115:TYR:HE2	32:T:194:GLU:HB3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:35:LEU:HG	21:i:46:ALA:HB3	1.96	0.47
21:i:38:LEU:HG	21:i:160:LYS:HB3	1.96	0.47
24:l:39:LYS:HA	24:l:44:ALA:HA	1.96	0.47
26:n:19:ARG:NH1	26:n:170:SER:O	2.47	0.47
32:t:1:THR:N	32:t:104:ASN:OD1	2.46	0.47
1:a:244:ASN:HB2	1:a:272:ILE:HB	1.95	0.47
2:b:22:LEU:HD23	2:b:180:ALA:HB2	1.96	0.47
7:U:208:LEU:HD23	7:U:210:LYS:H	1.78	0.47
9:W:403:PHE:O	9:W:417:ARG:NH1	2.47	0.47
13:A:50:ASP:O	13:A:54:GLN:CB	2.62	0.47
13:A:283:ALA:O	13:A:296:GLN:NE2	2.43	0.47
16:D:355:SER:HB3	16:D:393:ILE:HG23	1.96	0.47
19:G:32:ILE:HA	19:G:82:GLY:HA2	1.96	0.47
20:H:67:PRO:HA	20:H:72:ILE:O	2.13	0.47
21:I:66:TYR:O	21:I:73:ALA:HA	2.13	0.47
23:K:37:ALA:HB2	23:K:50:VAL:HG23	1.95	0.47
27:O:161:ALA:O	27:O:165:ASN:HB2	2.13	0.47
28:P:148:GLY:O	28:P:152:SER:OG	2.27	0.47
32:T:1:THR:N	32:T:104:ASN:OD1	2.46	0.47
23:k:56:SER:HB3	23:k:59:MET:HB2	1.96	0.47
27:o:161:ALA:O	27:o:165:ASN:HB2	2.13	0.47
32:t:74:GLU:HG3	32:t:77:LEU:HD12	1.95	0.47
2:b:131:LEU:HD22	2:b:136:VAL:HB	1.95	0.47
6:f:559:PRO:HA	6:f:562:LEU:HB2	1.95	0.47
10:X:252:LYS:HE2	10:X:315:ASP:HB2	1.96	0.47
12:Z:245:PHE:HB3	12:Z:248:ALA:HB3	1.97	0.47
14:B:392:GLY:O	14:B:396:LYS:HB3	2.15	0.47
17:E:135:ILE:HD12	17:E:138:LEU:HD11	1.94	0.47
18:F:235:LEU:O	18:F:239:ALA:CB	2.62	0.47
26:N:140:ASP:OD1	26:N:140:ASP:N	2.47	0.47
27:O:56:THR:O	27:O:60:SER:CB	2.62	0.47
31:S:38:ARG:HH12	32:T:151:ARG:HD3	1.78	0.47
31:S:145:LEU:HD22	31:S:178:VAL:HB	1.95	0.47
23:k:85:ALA:HB2	23:k:139:VAL:HG21	1.96	0.47
25:m:40:ARG:HA	25:m:45:VAL:HA	1.95	0.47
26:n:153:LEU:O	26:n:157:ALA:HB2	2.14	0.47
31:s:176:LYS:HE2	31:s:208:VAL:HG21	1.95	0.47
31:s:184:GLU:OE1	31:s:211:ARG:NH1	2.47	0.47
32:t:166:ARG:NH1	32:t:170:GLU:OE2	2.47	0.47
4:d:114:GLU:O	4:d:118:GLU:HB2	2.14	0.47
7:U:165:LYS:HA	7:U:168:LEU:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:530:GLU:O	7:U:534:GLY:CA	2.60	0.47
7:U:723:ASP:HB3	7:U:726:ALA:HB2	1.97	0.47
9:W:405:LYS:HE3	9:W:417:ARG:HA	1.97	0.47
9:W:407:ASP:OD1	10:X:382:GLU:CG	2.62	0.47
18:F:373:MET:HE1	18:F:401:VAL:HA	1.96	0.47
20:H:214:ASN:HB2	20:H:217:GLY:O	2.14	0.47
21:I:136:TYR:O	21:I:147:LEU:HA	2.13	0.47
23:K:56:SER:HB3	23:K:59:MET:HB2	1.96	0.47
23:K:102:THR:HG22	31:S:94:THR:HG21	1.96	0.47
24:L:47:VAL:HG13	24:L:212:ILE:HG13	1.95	0.47
24:L:134:ILE:HB	24:L:145:PHE:HB2	1.96	0.47
26:N:93:ASP:OD2	26:N:93:ASP:N	2.31	0.47
19:g:32:ILE:HA	19:g:82:GLY:HA2	1.96	0.47
25:m:52:LEU:HA	25:m:209:PHE:HA	1.97	0.47
25:m:53:VAL:HG13	25:m:58:TYR:HB3	1.97	0.47
26:n:88:TYR:O	26:n:91:ARG:HG3	2.12	0.47
28:p:58:THR:O	29:q:85:ARG:NH2	2.47	0.47
28:p:113:ASP:OD2	28:p:116:THR:N	2.43	0.47
4:d:69:PRO:O	4:d:73:ARG:CB	2.62	0.47
4:d:114:GLU:HA	4:d:117:THR:HG22	1.95	0.47
6:f:522:CYS:O	6:f:526:ALA:CB	2.63	0.47
6:f:645:ASP:HB3	6:f:648:ALA:HB3	1.95	0.47
7:U:128:GLN:HA	7:U:131:GLU:HG2	1.95	0.47
8:V:167:LEU:HD12	8:V:169:LEU:H	1.79	0.47
8:V:285:TRP:HD1	8:V:315:LYS:HE2	1.80	0.47
10:X:57:LEU:HB3	10:X:66:LEU:HB2	1.96	0.47
11:Y:223:THR:O	11:Y:227:SER:HB3	2.14	0.47
13:A:249:TYR:OH	16:D:278:GLN:OE1	2.33	0.47
14:B:411:ARG:NH2	14:B:418:ASP:OD2	2.47	0.47
16:D:125:LYS:CB	16:D:126:PRO:HD2	2.39	0.47
18:F:439:ALA:OXT	24:L:51:ARG:NE	2.46	0.47
26:N:13:VAL:HA	26:N:177:ALA:O	2.15	0.47
30:R:38:ASN:HD22	30:R:41:LEU:HD12	1.78	0.47
28:p:160:PRO:O	28:p:164:PHE:CB	2.62	0.47
32:t:48:SER:HB2	32:t:116:ALA:HB2	1.95	0.47
3:c:55:GLY:HA3	3:c:112:TYR:CZ	2.50	0.47
3:c:177:THR:HG22	7:U:399:TRP:HE1	1.79	0.47
8:V:43:THR:O	8:V:47:SER:OG	2.32	0.47
9:W:202:THR:O	9:W:206:SER:CB	2.63	0.47
9:W:257:GLN:HE21	9:W:263:TRP:HB2	1.79	0.47
16:D:103:VAL:HG21	16:D:132:LEU:HD21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:78:GLY:HA3	20:H:132:VAL:HG22	1.95	0.47
22:J:131:ALA:N	22:J:147:THR:OG1	2.39	0.47
20:h:214:ASN:HB2	20:h:217:GLY:O	2.14	0.47
21:i:3:ARG:NH2	23:k:10:ARG:CZ	2.76	0.47
21:i:245:ALA:HA	21:i:248:GLU:HG2	1.97	0.47
24:l:137:TYR:HE2	24:l:215:VAL:HG13	1.80	0.47
28:p:30:ILE:N	28:p:33:GLN:O	2.44	0.47
3:c:80:THR:HA	18:F:85:THR:HG22	1.97	0.47
6:f:125:ILE:HA	6:f:129:LEU:HB2	1.97	0.47
7:U:36:ALA:HB2	8:V:268:GLU:HG2	1.97	0.47
7:U:45:ILE:O	7:U:49:TYR:HB2	2.14	0.47
7:U:52:GLU:HA	7:U:57:ARG:HH11	1.79	0.47
7:U:444:TYR:HB2	7:U:476:GLY:HA3	1.97	0.47
8:V:43:THR:OG1	8:V:66:GLU:OE1	2.33	0.47
8:V:336:GLU:HA	8:V:339:LEU:HG	1.95	0.47
8:V:346:LEU:N	8:V:346:LEU:HD12	2.30	0.47
9:W:86:ASN:OD1	9:W:93:ARG:NE	2.48	0.47
9:W:110:THR:O	9:W:114:GLU:CB	2.61	0.47
9:W:115:ILE:HD13	9:W:119:PRO:HG2	1.96	0.47
11:Y:23:ARG:HH21	11:Y:52:PRO:HA	1.79	0.47
11:Y:104:MET:O	11:Y:108:ALA:HB3	2.15	0.47
11:Y:131:THR:O	11:Y:137:ARG:NH1	2.45	0.47
11:Y:157:ILE:H	11:Y:157:ILE:HG13	1.49	0.47
11:Y:179:ARG:HH22	11:Y:210:SER:HB3	1.78	0.47
11:Y:381:GLN:HB3	11:Y:385:ARG:HH12	1.80	0.47
12:Z:10:VAL:O	12:Z:49:ASP:HA	2.14	0.47
13:A:103:ASN:ND2	18:F:166:THR:OG1	2.48	0.47
13:A:215:PHE:O	13:A:343:PHE:HB2	2.15	0.47
15:C:90:HIS:HD1	16:D:110:ASN:CB	1.98	0.47
15:C:303:SER:HA	15:C:306:LEU:HB2	1.97	0.47
17:E:235:ILE:HD11	17:E:277:MET:HB3	1.96	0.47
18:F:64:HIS:O	18:F:68:ALA:CB	2.62	0.47
18:F:294:LYS:N	18:F:337:ILE:O	2.47	0.47
18:F:375:VAL:HG22	18:F:415:LEU:HD12	1.96	0.47
18:F:401:VAL:HG12	18:F:405:MET:HE2	1.97	0.47
19:G:21:ARG:NE	19:G:21:ARG:N	2.62	0.47
19:G:140:LEU:O	19:G:151:VAL:HA	2.14	0.47
22:J:211:MET:HG2	22:J:213:ARG:H	1.79	0.47
24:L:137:TYR:HE2	24:L:215:VAL:HG13	1.80	0.47
24:L:148:CYS:SG	24:L:150:SER:OG	2.66	0.47
25:M:53:VAL:HG13	25:M:58:TYR:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:195:LYS:HE3	31:s:184:GLU:HG3	1.97	0.47
29:Q:37:LYS:HA	29:Q:43:LEU:HD23	1.96	0.47
32:T:43:MET:HE3	32:T:45:VAL:HG22	1.95	0.47
19:g:189:TRP:CE3	19:g:193:GLN:HG3	2.50	0.47
20:h:67:PRO:HA	20:h:72:ILE:O	2.13	0.47
23:k:15:PHE:O	23:k:22:PHE:HZ	1.97	0.47
24:l:183:ASN:CG	24:l:186:GLU:CD	2.79	0.47
25:m:202:ASP:N	25:m:202:ASP:OD1	2.48	0.47
26:n:31:THR:O	26:n:175:ARG:NE	2.48	0.47
27:o:175:LEU:HB2	27:o:186:LEU:HB2	1.97	0.47
2:b:121:GLU:HA	2:b:124:LEU:HG	1.95	0.47
6:f:80:ARG:HE	6:f:99:LEU:HD13	1.80	0.47
6:f:352:HIS:HA	6:f:387:GLN:HG2	1.97	0.47
6:f:553:THR:HA	6:f:556:ARG:HE	1.80	0.47
7:U:710:ARG:HG2	7:U:737:LEU:HD21	1.95	0.47
7:U:808:PRO:HA	7:U:811:PHE:HD2	1.79	0.47
14:B:189:GLY:HA3	14:B:356:PRO:CB	2.44	0.47
16:D:152:MET:O	16:D:155:THR:HG23	2.15	0.47
17:E:235:ILE:O	17:E:239:GLY:N	2.42	0.47
17:E:304:PRO:O	17:E:309:ARG:NH1	2.48	0.47
20:H:50:LYS:NZ	20:H:62:VAL:O	2.36	0.47
26:N:11:GLY:HA3	26:N:179:ILE:O	2.15	0.47
26:N:134:TYR:O	26:N:137:GLY:N	2.47	0.47
23:k:117:SER:HB3	24:l:82:ARG:HH12	1.79	0.47
24:l:47:VAL:HG13	24:l:212:ILE:HG13	1.95	0.47
25:m:106:ILE:HG12	25:m:111:LEU:HD13	1.96	0.47
26:n:88:TYR:CG	26:n:91:ARG:HD3	2.50	0.47
9:W:303:LYS:O	9:W:307:LYS:HB2	2.15	0.47
16:D:167:ILE:HG12	16:D:214:MET:HE3	1.97	0.47
24:l:134:ILE:HB	24:l:145:PHE:HB2	1.96	0.47
31:s:13:LEU:O	31:s:23:VAL:HA	2.15	0.47
31:s:57:PHE:N	31:s:105:TYR:O	2.43	0.47
2:b:109:ILE:HB	2:b:138:VAL:HG22	1.97	0.47
8:V:80:LYS:HG2	8:V:89:LYS:HG2	1.96	0.47
16:D:170:MET:HB3	16:D:173:GLN:HB2	1.96	0.47
17:E:67:GLU:HG3	17:E:68:LYS:HG3	1.97	0.47
19:G:8:GLY:C	19:G:10:ASP:H	2.23	0.47
23:K:169:ALA:HB3	23:K:178:GLN:HG2	1.97	0.47
27:O:6:VAL:HG23	27:O:124:TYR:HB3	1.96	0.47
32:T:148:PRO:O	32:T:152:GLU:HB2	2.15	0.47
19:g:22:LEU:HD11	19:g:25:VAL:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:324:ILE:HD13	9:W:369:TYR:HB3	1.97	0.46
2:b:86:PHE:O	2:b:89:GLY:N	2.47	0.46
3:c:93:ALA:O	3:c:97:ASP:CB	2.63	0.46
9:W:356:ASN:O	9:W:360:GLU:HB3	2.15	0.46
11:Y:285:ASP:HB3	11:Y:288:PHE:HB2	1.97	0.46
12:Z:107:ALA:O	12:Z:111:LEU:HB2	2.15	0.46
13:A:269:ALA:CA	13:A:314:ASN:O	2.63	0.46
13:A:392:ALA:HA	13:A:395:PHE:HD2	1.80	0.46
34:D:501:ATP:O2A	34:D:501:ATP:O1B	2.33	0.46
18:F:169:ASP:HB2	18:F:172:VAL:HG23	1.97	0.46
22:J:32:ALA:HB2	22:J:45:VAL:HG23	1.97	0.46
22:j:32:ALA:HB2	22:j:45:VAL:HG23	1.97	0.46
27:o:56:THR:O	27:o:60:SER:CB	2.62	0.46
32:t:148:PRO:O	32:t:152:GLU:HB2	2.15	0.46
7:U:607:VAL:O	16:D:67:ASN:ND2	2.48	0.46
8:V:335:VAL:HA	8:V:338:LEU:HB2	1.98	0.46
9:W:153:LYS:HA	9:W:156:ASN:HA	1.97	0.46
9:W:408:ARG:C	9:W:410:ALA:N	2.72	0.46
11:Y:380:VAL:O	11:Y:384:SER:HB2	2.15	0.46
14:B:153:ASN:HD21	14:B:155:LYS:HE3	1.81	0.46
19:G:8:GLY:C	19:G:10:ASP:N	2.73	0.46
26:N:31:THR:O	26:N:175:ARG:NE	2.48	0.46
31:S:13:LEU:O	31:S:23:VAL:HA	2.15	0.46
20:h:9:SER:CB	20:h:123:GLN:O	2.59	0.46
22:j:36:ARG:HB2	22:j:142:PRO:HB2	1.97	0.46
23:k:10:ARG:O	23:k:22:PHE:HD2	1.93	0.46
23:k:15:PHE:C	23:k:22:PHE:CZ	2.93	0.46
23:k:177:ALA:O	23:k:181:LEU:HB2	2.15	0.46
28:p:113:ASP:N	28:p:118:LYS:O	2.48	0.46
29:q:43:LEU:HD21	29:q:188:ILE:HG12	1.98	0.46
1:a:45:VAL:HG13	1:a:82:HIS:HE1	1.81	0.46
6:f:479:LEU:HA	6:f:517:VAL:HG21	1.97	0.46
8:V:86:VAL:HG12	8:V:118:GLN:HG2	1.96	0.46
9:W:97:LEU:HD11	9:W:130:MET:HB3	1.96	0.46
9:W:394:SER:OG	10:X:340:GLU:OE2	2.33	0.46
13:A:312:ARG:HH12	13:A:317:VAL:HG23	1.76	0.46
15:C:217:SER:HB3	15:C:220:VAL:HG23	1.96	0.46
16:D:120:ASP:N	16:D:123:LEU:HD11	2.31	0.46
18:F:311:LEU:HD23	18:F:314:LEU:HD12	1.97	0.46
26:N:59:VAL:O	26:N:63:LEU:CB	2.63	0.46
26:n:13:VAL:HA	26:n:177:ALA:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:o:136:ALA:O	27:o:140:ASP:CB	2.56	0.46
1:a:25:LEU:HD11	1:a:37:LEU:HD13	1.97	0.46
3:c:246:LYS:HD2	9:W:424:LEU:HA	1.96	0.46
4:d:36:LEU:C	4:d:38:THR:N	2.72	0.46
4:d:170:LEU:HA	4:d:173:THR:HG22	1.95	0.46
6:f:130:ALA:O	6:f:134:SER:CB	2.63	0.46
6:f:338:ASP:C	6:f:340:MET:N	2.74	0.46
9:W:382:LEU:HB3	9:W:384:LEU:HG	1.98	0.46
10:X:252:LYS:O	10:X:256:LEU:CB	2.62	0.46
10:X:292:GLN:OE1	10:X:296:ASN:ND2	2.49	0.46
12:Z:75:LEU:O	12:Z:79:TYR:HB2	2.15	0.46
12:Z:218:GLY:HA2	12:Z:220:LEU:CD2	2.43	0.46
16:D:407:ILE:HG22	16:D:408:LYS:O	2.15	0.46
18:F:431:LYS:NZ	18:F:431:LYS:C	2.73	0.46
18:F:432:LYS:HB2	18:F:432:LYS:NZ	2.30	0.46
19:G:126:THR:HG22	20:H:128:ARG:HH22	1.80	0.46
21:I:245:ALA:HA	21:I:248:GLU:HG2	1.97	0.46
23:K:60:GLU:OE1	23:K:63:SER:N	2.48	0.46
23:K:134:SER:OG	23:K:135:ARG:N	2.47	0.46
27:O:96:ALA:H	27:O:115:PRO:HB3	1.81	0.46
28:P:113:ASP:HB2	28:P:118:LYS:HB3	1.97	0.46
31:S:195:ILE:O	31:S:205:GLU:HA	2.16	0.46
32:T:175:VAL:HA	32:T:178:TYR:HD2	1.80	0.46
20:h:12:THR:OG1	21:i:20:GLN:NE2	2.37	0.46
24:l:140:MET:HE2	24:l:143:HIS:HE1	1.80	0.46
27:o:38:SER:OG	27:o:40:ASN:OD1	2.23	0.46
13:A:224:LEU:HD11	34:A:501:ATP:C4	2.51	0.46
16:D:152:MET:C	16:D:154:LEU:H	2.24	0.46
19:G:21:ARG:H	19:G:21:ARG:HD3	1.77	0.46
20:H:12:THR:OG1	21:I:20:GLN:NE2	2.41	0.46
23:K:177:ALA:O	23:K:181:LEU:HB2	2.15	0.46
27:O:1:THR:O	27:O:129:SER:N	2.44	0.46
27:O:46:ALA:HB3	27:O:97:ALA:O	2.16	0.46
28:P:62:THR:OG1	29:Q:85:ARG:NH2	2.48	0.46
28:P:101:GLY:O	29:Q:93:ARG:NH1	2.46	0.46
31:S:150:ASP:HB3	31:S:156:LYS:HD2	1.97	0.46
31:S:195:ILE:HB	31:S:206:GLU:O	2.15	0.46
19:g:196:GLU:HA	19:g:242:LEU:HD22	1.98	0.46
24:l:72:ILE:HG22	24:l:134:ILE:HA	1.98	0.46
27:o:6:VAL:HG23	27:o:124:TYR:HB3	1.96	0.46
29:q:12:TYR:HB2	29:q:182:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:s:150:ASP:HB3	31:s:156:LYS:HD2	1.97	0.46
2:b:56:ASN:HB2	2:b:82:GLY:HA3	1.96	0.46
2:b:181:ASP:O	2:b:185:SER:HB2	2.15	0.46
7:U:148:LYS:HA	7:U:151:ILE:HG22	1.97	0.46
8:V:483:CYS:O	8:V:487:HIS:ND1	2.48	0.46
12:Z:40:LEU:HA	12:Z:91:ILE:HA	1.97	0.46
12:Z:75:LEU:O	12:Z:79:TYR:CB	2.63	0.46
15:C:64:GLN:HA	15:C:67:GLN:HB2	1.98	0.46
21:I:35:LEU:HG	21:I:46:ALA:HB3	1.96	0.46
23:K:200:ILE:HA	23:K:203:LYS:HZ3	1.80	0.46
27:O:175:LEU:HB2	27:O:186:LEU:HB2	1.97	0.46
29:Q:43:LEU:HD21	29:Q:188:ILE:HG12	1.98	0.46
23:k:21:LEU:CD1	23:k:23:GLN:HB3	2.45	0.46
28:p:60:VAL:O	28:p:64:ALA:CB	2.64	0.46
29:q:31:ASP:OD1	29:q:31:ASP:N	2.49	0.46
29:q:138:LEU:O	29:q:141:SER:OG	2.32	0.46
31:s:49:LYS:O	31:s:112:GLY:CA	2.61	0.46
1:a:289:ARG:NH1	12:Z:244:GLU:O	2.49	0.46
1:a:296:ILE:O	1:a:300:ALA:HB3	2.15	0.46
1:a:352:ARG:HD3	12:Z:240:VAL:HG12	1.96	0.46
7:U:401:LYS:HD3	7:U:434:GLY:H	1.81	0.46
9:W:408:ARG:HG2	10:X:345:VAL:CG1	2.45	0.46
16:D:181:VAL:HG22	16:D:306:LYS:HD2	1.97	0.46
17:E:313:LEU:O	17:E:317:ALA:CB	2.64	0.46
18:F:222:GLY:HA3	18:F:348:LEU:HA	1.98	0.46
18:F:437:TYR:CD2	23:K:20:ARG:HG3	2.51	0.46
19:G:189:TRP:CE3	19:G:193:GLN:CG	2.98	0.46
28:P:113:ASP:N	28:P:118:LYS:O	2.48	0.46
23:k:93:ARG:NH1	30:r:68:LEU:O	2.48	0.46
26:n:88:TYR:O	26:n:91:ARG:HG2	2.11	0.46
31:s:195:ILE:O	31:s:205:GLU:HA	2.16	0.46
1:a:80:ILE:HD12	1:a:83:VAL:HB	1.98	0.46
6:f:515:ALA:HB1	6:f:558:LEU:HD21	1.98	0.46
7:U:561:GLU:CD	7:U:561:GLU:N	2.73	0.46
9:W:441:LYS:HA	9:W:445:LEU:HD13	1.98	0.46
10:X:323:LEU:O	10:X:327:TYR:HB2	2.15	0.46
14:B:191:ASP:HA	14:B:194:ILE:HB	1.98	0.46
18:F:251:LEU:HD21	18:F:256:LEU:HD11	1.97	0.46
22:J:115:LYS:NZ	22:J:129:ILE:O	2.46	0.46
31:S:209:SER:OG	31:S:212:LYS:NZ	2.35	0.46
21:i:10:THR:HG21	22:j:123:GLY:HA2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:109:ARG:O	22:j:113:SER:HB3	2.16	0.46
22:j:211:MET:HG2	22:j:213:ARG:H	1.79	0.46
23:k:203:LYS:HZ1	23:k:241:ILE:HG12	1.81	0.46
29:q:37:LYS:HA	29:q:43:LEU:HD23	1.96	0.46
32:t:175:VAL:HA	32:t:178:TYR:HD2	1.80	0.46
3:c:178:THR:HA	3:c:181:LEU:HB2	1.97	0.46
7:U:151:ILE:HA	7:U:154:ALA:HB3	1.98	0.46
7:U:249:CYS:O	7:U:253:TYR:CB	2.64	0.46
7:U:636:VAL:HG11	15:C:43:ARG:HH22	1.81	0.46
7:U:655:ALA:O	7:U:659:CYS:CB	2.64	0.46
9:W:124:LEU:HA	9:W:127:THR:HG22	1.98	0.46
17:E:70:ILE:HG12	17:E:80:VAL:HG22	1.97	0.46
17:E:145:LEU:HD22	17:E:183:LEU:HD21	1.98	0.46
18:F:431:LYS:HD3	18:F:431:LYS:C	2.36	0.46
22:J:36:ARG:HB2	22:J:142:PRO:HB2	1.97	0.46
25:M:52:LEU:HA	25:M:209:PHE:HA	1.97	0.46
26:N:90:TYR:C	26:N:92:GLU:OE2	2.58	0.46
28:P:60:VAL:O	28:P:64:ALA:CB	2.64	0.46
29:Q:12:TYR:HB2	29:Q:182:ILE:HD11	1.97	0.46
30:R:104:TRP:CD2	30:R:181:GLU:HA	2.51	0.46
31:S:74:MET:O	31:S:78:SER:HB3	2.16	0.46
32:T:49:THR:HA	32:T:114:GLY:HA2	1.97	0.46
1:a:185:ILE:HD12	1:a:187:ASP:HB3	1.97	0.46
6:f:652:VAL:HG22	6:f:686:LEU:HG	1.97	0.46
13:A:143:ASP:OD2	13:A:146:LYS:N	2.37	0.46
14:B:103:ARG:HG2	14:B:160:ILE:HG23	1.98	0.46
19:G:178:PHE:O	19:G:182:LYS:HB3	2.16	0.46
30:R:12:VAL:HB	30:R:179:VAL:HB	1.97	0.46
20:h:195:LEU:O	20:h:199:PHE:CB	2.64	0.46
21:i:232:GLU:HA	21:i:235:GLN:HG2	1.98	0.46
23:k:113:THR:O	23:k:117:SER:OG	2.29	0.46
23:k:169:ALA:HB3	23:k:178:GLN:HG2	1.97	0.46
26:n:59:VAL:O	26:n:63:LEU:CB	2.63	0.46
31:s:209:SER:HG	31:s:212:LYS:HZ1	1.58	0.46
3:c:193:ILE:HD13	3:c:196:LEU:HD12	1.98	0.45
8:V:191:LEU:O	8:V:194:LYS:NZ	2.42	0.45
9:W:34:LEU:HD22	9:W:47:LEU:HD13	1.98	0.45
9:W:408:ARG:HG3	10:X:349:HIS:NE2	2.21	0.45
11:Y:356:THR:OG1	11:Y:357:ASN:N	2.49	0.45
17:E:113:ARG:HH22	17:E:220:ASN:HB3	1.81	0.45
17:E:172:LEU:HD11	17:E:183:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:140:MET:HE2	24:L:143:HIS:HE1	1.80	0.45
28:P:172:LEU:HD13	31:s:157:ASN:HB3	1.98	0.45
20:h:8:PHE:CB	21:i:126:GLY:O	2.64	0.45
23:k:60:GLU:OE1	23:k:63:SER:N	2.48	0.45
24:l:39:LYS:HD3	24:l:144:ILE:HG12	1.98	0.45
30:r:12:VAL:HB	30:r:179:VAL:HB	1.97	0.45
2:b:34:ASN:O	2:b:38:HIS:ND1	2.35	0.45
3:c:113:HIS:CE1	3:c:144:VAL:HG22	2.51	0.45
7:U:97:VAL:HA	7:U:100:ILE:HG12	1.97	0.45
7:U:386:LEU:HB3	7:U:387:ARG:HD2	1.99	0.45
7:U:602:LEU:O	7:U:606:ALA:CB	2.63	0.45
8:V:39:GLU:O	8:V:43:THR:OG1	2.30	0.45
9:W:173:THR:HG23	9:W:182:ARG:HH11	1.81	0.45
10:X:325:LYS:O	10:X:329:ASN:CB	2.64	0.45
13:A:209:PRO:HB3	13:A:338:ASP:HB2	1.97	0.45
22:J:165:ALA:O	22:J:169:ARG:CB	2.65	0.45
23:K:203:LYS:HB3	23:K:210:LEU:HD22	1.98	0.45
19:g:47:CYS:HB3	19:g:221:THR:HG23	1.98	0.45
28:p:113:ASP:HB2	28:p:118:LYS:HB3	1.97	0.45
31:s:195:ILE:HB	31:s:206:GLU:O	2.15	0.45
2:b:150:THR:O	2:b:154:THR:OG1	2.26	0.45
4:d:237:ILE:O	4:d:240:THR:OG1	2.31	0.45
6:f:696:LEU:HD13	6:f:752:HIS:HD2	1.81	0.45
7:U:45:ILE:O	7:U:49:TYR:CB	2.64	0.45
7:U:160:LEU:HA	7:U:163:PHE:HB3	1.97	0.45
9:W:407:ASP:OD1	10:X:382:GLU:HG3	2.16	0.45
16:D:107:THR:HG22	17:E:77:PRO:HG3	1.98	0.45
20:H:195:LEU:O	20:H:199:PHE:CB	2.64	0.45
21:I:229:LYS:N	21:I:232:GLU:OE2	2.49	0.45
21:I:232:GLU:HA	21:I:235:GLN:HG2	1.98	0.45
23:k:203:LYS:HB3	23:k:210:LEU:HD22	1.98	0.45
26:n:11:GLY:HA3	26:n:179:ILE:O	2.15	0.45
2:b:124:LEU:O	2:b:128:ALA:CB	2.65	0.45
3:c:63:ASP:O	3:c:139:ARG:NH2	2.39	0.45
7:U:403:THR:HA	7:U:406:ALA:HB3	1.98	0.45
8:V:89:LYS:HD2	8:V:93:PHE:HE2	1.82	0.45
8:V:306:ARG:O	8:V:310:THR:OG1	2.26	0.45
11:Y:223:THR:O	11:Y:227:SER:CB	2.65	0.45
14:B:309:MET:O	14:B:313:LEU:HB2	2.16	0.45
16:D:216:ALA:O	16:D:220:ALA:CB	2.65	0.45
19:G:192:GLU:O	19:G:196:GLU:N	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:96:LEU:HG	29:Q:58:GLU:HB3	1.99	0.45
23:K:157:ASP:OD2	23:K:159:SER:OG	2.35	0.45
24:L:39:LYS:HA	24:L:44:ALA:HA	1.96	0.45
19:g:178:PHE:O	19:g:182:LYS:HB3	2.17	0.45
21:i:78:GLY:HA3	21:i:132:VAL:HG22	1.98	0.45
22:j:165:ALA:O	22:j:169:ARG:CB	2.65	0.45
32:t:27:LEU:HD22	32:t:184:TYR:HB2	1.98	0.45
3:c:57:MET:HE3	3:c:109:VAL:HG23	1.99	0.45
3:c:217:LEU:HD21	12:Z:172:VAL:HG13	1.99	0.45
5:e:3:GLU:HG2	5:e:4:LYS:H	1.80	0.45
5:e:59:GLU:O	5:e:63:HIS:CB	2.61	0.45
6:f:249:LEU:HD21	6:f:271:MET:HG3	1.97	0.45
7:U:475:HIS:O	7:U:478:SER:OG	2.30	0.45
7:U:559:ARG:CD	7:U:562:GLU:HB2	2.36	0.45
7:U:655:ALA:O	7:U:659:CYS:HB2	2.16	0.45
9:W:63:THR:OG1	9:W:64:SER:N	2.50	0.45
11:Y:112:CYS:HB2	11:Y:119:GLY:HA3	1.97	0.45
16:D:416:PHE:C	16:D:418:LYS:N	2.74	0.45
17:E:145:LEU:HA	17:E:148:VAL:HG12	1.99	0.45
18:F:64:HIS:O	18:F:68:ALA:HB3	2.17	0.45
28:P:159:ASP:O	28:P:163:LEU:HB3	2.17	0.45
29:Q:2:GLU:HG2	29:Q:3:TYR:H	1.82	0.45
24:l:225:ASP:OD1	24:l:225:ASP:N	2.49	0.45
27:o:46:ALA:HB3	27:o:97:ALA:O	2.16	0.45
28:p:70:ARG:HA	28:p:73:LEU:HD12	1.98	0.45
31:s:74:MET:O	31:s:78:SER:HB3	2.16	0.45
6:f:314:TYR:HA	6:f:317:LEU:HB3	1.97	0.45
7:U:184:CYS:HA	7:U:187:LEU:HG	1.98	0.45
7:U:389:ASN:HB3	7:U:392:TRP:HE3	1.80	0.45
8:V:148:ARG:NH1	8:V:193:GLN:OE1	2.49	0.45
11:Y:53:TYR:HB2	11:Y:63:TRP:HE1	1.81	0.45
11:Y:272:PHE:HA	11:Y:275:LEU:HB3	1.99	0.45
13:A:373:LEU:HD22	13:A:413:VAL:HG21	1.98	0.45
16:D:163:MET:SD	16:D:163:MET:N	2.90	0.45
17:E:57:VAL:HG13	17:E:97:ARG:HD3	1.99	0.45
24:L:72:ILE:HA	24:L:133:LEU:O	2.17	0.45
24:L:183:ASN:O	24:L:187:LEU:HB3	2.17	0.45
24:L:225:ASP:OD1	24:L:225:ASP:N	2.49	0.45
27:O:87:LEU:HD13	27:O:115:PRO:HA	1.98	0.45
29:Q:107:TYR:HA	29:Q:113:PRO:HA	1.98	0.45
31:S:74:MET:O	31:S:78:SER:CB	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:13:ILE:HG13	19:g:15:ILE:HG23	1.99	0.45
21:i:9:THR:HB	21:i:126:GLY:C	2.42	0.45
21:i:47:ALA:N	21:i:212:GLU:O	2.49	0.45
21:i:229:LYS:N	21:i:232:GLU:OE2	2.50	0.45
29:q:107:TYR:HA	29:q:113:PRO:HA	1.98	0.45
32:t:49:THR:HA	32:t:114:GLY:HA2	1.97	0.45
3:c:36:LEU:HB3	12:Z:17:LEU:HD22	1.99	0.45
3:c:304:LEU:O	3:c:308:VAL:HB	2.17	0.45
6:f:392:THR:HA	6:f:414:LEU:HD22	1.99	0.45
7:U:111:GLN:OE1	7:U:115:ASN:ND2	2.50	0.45
7:U:400:ALA:O	7:U:404:ALA:CB	2.64	0.45
7:U:609:ASP:O	7:U:615:ARG:NH1	2.42	0.45
8:V:80:LYS:HD2	8:V:80:LYS:HA	1.34	0.45
8:V:270:LEU:HD23	8:V:273:LYS:HD2	1.98	0.45
12:Z:145:HIS:HB3	12:Z:148:GLY:H	1.82	0.45
13:A:312:ARG:NH1	13:A:317:VAL:CG2	2.70	0.45
18:F:437:TYR:CE2	23:K:20:ARG:HG3	2.52	0.45
25:M:35:THR:HA	25:M:166:GLY:HA3	1.98	0.45
31:S:157:ASN:HB3	28:p:172:LEU:HD13	1.99	0.45
24:l:72:ILE:HA	24:l:133:LEU:O	2.17	0.45
28:p:159:ASP:O	28:p:163:LEU:HB3	2.17	0.45
28:p:162:HIS:O	28:p:166:THR:OG1	2.31	0.45
30:r:154:ASP:OD1	30:r:157:ARG:NH1	2.50	0.45
31:s:76:LYS:O	31:s:80:ASN:N	2.40	0.45
1:a:135:ILE:HG12	1:a:158:LEU:HD13	1.97	0.45
2:b:131:LEU:HA	2:b:134:GLU:HB2	1.98	0.45
6:f:538:ILE:HD13	6:f:565:ASN:HB3	1.98	0.45
8:V:363:LEU:HB2	8:V:378:VAL:HG11	1.99	0.45
9:W:119:PRO:O	9:W:123:ARG:HB2	2.17	0.45
10:X:394:ASP:HA	10:X:397:TYR:HB2	1.99	0.45
11:Y:240:VAL:HB	11:Y:260:LEU:HD13	1.99	0.45
12:Z:76:GLU:HA	12:Z:79:TYR:HB3	1.99	0.45
13:A:276:GLU:HG2	14:B:310:LEU:HD11	1.99	0.45
14:B:387:LYS:HZ2	14:B:431:GLN:CG	2.19	0.45
15:C:27:LYS:HG3	16:D:40:LEU:HG	1.98	0.45
18:F:430:LYS:N	18:F:430:LYS:HD3	2.29	0.45
21:I:78:GLY:HA3	21:I:132:VAL:HG22	1.98	0.45
19:g:132:ARG:HA	19:g:133:PRO:HD3	1.78	0.45
19:g:189:TRP:HA	19:g:193:GLN:CG	2.47	0.45
20:h:187:ALA:O	20:h:191:ALA:CB	2.65	0.45
28:p:124:LEU:HG	28:p:130:PRO:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:55:TRP:NE1	31:s:97:TYR:OH	2.50	0.45
32:t:176:LEU:O	32:t:180:ASP:HB3	2.17	0.45
2:b:20:ASP:OD2	2:b:25:ARG:NH2	2.46	0.45
4:d:151:VAL:HG21	4:d:174:ILE:HD11	1.99	0.45
8:V:383:GLY:HA2	8:V:386:PHE:HB2	1.99	0.45
10:X:177:TYR:HB3	10:X:182:ASN:HB3	1.98	0.45
16:D:121:ARG:C	16:D:124:LEU:HD22	2.29	0.45
18:F:399:VAL:O	18:F:403:ALA:HB2	2.16	0.45
22:J:109:ARG:O	22:J:113:SER:HB3	2.16	0.45
24:L:119:PRO:HA	24:L:125:ARG:HB3	1.99	0.45
27:O:100:LEU:HB2	27:O:113:ILE:HD11	1.98	0.45
28:P:162:HIS:O	28:P:166:THR:OG1	2.31	0.45
32:T:89:HIS:NE2	32:T:124:TYR:O	2.43	0.45
23:k:15:PHE:O	23:k:22:PHE:CZ	2.70	0.45
23:k:16:SER:HA	23:k:22:PHE:CE1	2.52	0.45
24:l:43:HIS:CG	24:l:184:LEU:HD21	2.50	0.45
31:s:74:MET:O	31:s:78:SER:CB	2.65	0.45
2:b:22:LEU:CD2	2:b:180:ALA:CA	2.95	0.45
4:d:183:GLU:HG3	4:d:224:SER:HA	1.99	0.45
4:d:203:PRO:HG2	4:d:205:LYS:HE2	1.99	0.45
6:f:671:ALA:O	6:f:674:THR:OG1	2.31	0.45
7:U:181:LEU:HD11	7:U:205:TYR:HE2	1.82	0.45
7:U:221:ILE:HD13	7:U:754:HIS:HB2	1.99	0.45
8:V:229:SER:O	8:V:233:ALA:CB	2.65	0.45
8:V:419:LEU:HD22	8:V:431:PRO:HB3	1.98	0.45
11:Y:335:SER:O	11:Y:339:ALA:CB	2.64	0.45
15:C:274:LEU:HD23	15:C:305:LEU:HD13	1.98	0.45
16:D:163:MET:HB2	16:D:166:ASP:HB2	1.99	0.45
18:F:436:GLN:C	18:F:438:TYR:N	2.71	0.45
19:G:84:THR:HG21	25:M:156:VAL:HG13	1.98	0.45
19:G:196:GLU:HA	19:G:242:LEU:HD22	1.97	0.45
20:H:187:ALA:O	20:H:191:ALA:CB	2.65	0.45
23:k:95:GLU:HA	23:k:98:ASN:HD22	1.82	0.45
25:m:35:THR:HA	25:m:166:GLY:HA3	1.98	0.45
25:m:58:TYR:OH	25:m:62:SER:O	2.29	0.45
27:o:87:LEU:HD13	27:o:115:PRO:HA	1.98	0.45
27:o:96:ALA:H	27:o:115:PRO:HB3	1.81	0.45
31:s:140:SER:OG	31:s:186:ASP:OD2	2.33	0.45
1:a:374:ILE:HG22	4:d:251:ARG:HB2	1.98	0.44
3:c:191:ALA:HA	3:c:194:HIS:HB3	1.99	0.44
4:d:55:LEU:HD23	4:d:55:LEU:HA	1.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:333:LEU:HA	6:f:338:ASP:HB2	1.99	0.44
6:f:445:LEU:HG	6:f:462:ALA:HB2	1.98	0.44
7:U:370:VAL:O	7:U:374:SER:CB	2.65	0.44
7:U:714:SER:HA	7:U:717:ILE:HG22	1.98	0.44
7:U:755:THR:OG1	7:U:756:HIS:N	2.49	0.44
9:W:260:SER:HA	9:W:263:TRP:HB3	1.99	0.44
12:Z:181:ASP:OD1	12:Z:181:ASP:N	2.49	0.44
13:A:349:GLU:O	13:A:352:THR:OG1	2.28	0.44
14:B:221:GLY:HA2	14:B:327:VAL:O	2.18	0.44
18:F:312:GLU:O	18:F:316:GLN:HB2	2.17	0.44
19:G:47:CYS:HB3	19:G:221:THR:HG23	1.98	0.44
23:K:97:GLN:O	23:K:101:PHE:HB2	2.17	0.44
27:O:45:GLY:HA2	27:O:98:LEU:HD23	1.99	0.44
27:O:136:ALA:O	27:O:140:ASP:CB	2.56	0.44
19:g:193:GLN:OE1	19:g:197:THR:CG2	2.65	0.44
23:k:97:GLN:O	23:k:101:PHE:HB2	2.17	0.44
23:k:134:SER:OG	23:k:135:ARG:N	2.47	0.44
25:m:20:VAL:HG12	25:m:23:VAL:H	1.82	0.44
1:a:319:LEU:HD12	1:a:320:VAL:HB	1.99	0.44
3:c:291:LEU:HD23	3:c:291:LEU:HA	1.84	0.44
4:d:21:GLU:O	4:d:25:ARG:CB	2.65	0.44
6:f:517:VAL:O	6:f:521:ALA:CB	2.65	0.44
7:U:391:GLU:HA	7:U:394:ALA:HB3	1.99	0.44
10:X:345:VAL:HG11	10:X:383:GLY:HA3	2.00	0.44
13:A:101:ILE:HA	13:A:113:ILE:HG12	1.99	0.44
14:B:427:LEU:HD22	14:B:431:GLN:HG2	1.98	0.44
16:D:403:TYR:CZ	16:D:407:ILE:HD13	2.42	0.44
16:D:417:TYR:OH	19:G:21:ARG:CD	2.65	0.44
17:E:62:LYS:HA	17:E:94:PRO:HB3	1.99	0.44
19:G:178:PHE:O	19:G:182:LYS:HB2	2.17	0.44
21:I:159:TRP:HA	22:J:54:GLN:HA	1.99	0.44
21:I:162:THR:OG1	21:I:163:CYS:N	2.49	0.44
26:N:160:LEU:O	26:N:164:MET:HB2	2.17	0.44
19:g:193:GLN:CD	19:g:193:GLN:C	2.85	0.44
23:k:21:LEU:HB3	23:k:24:VAL:H	1.82	0.44
27:o:100:LEU:HB2	27:o:113:ILE:HD11	1.98	0.44
29:q:2:GLU:HG2	29:q:3:TYR:H	1.81	0.44
30:r:104:TRP:CD2	30:r:181:GLU:HA	2.51	0.44
1:a:285:PRO:HG2	1:a:288:HIS:NE2	2.32	0.44
2:b:26:LEU:O	2:b:30:GLN:CB	2.64	0.44
3:c:102:THR:OG1	12:Z:74:TYR:OH	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:639:LEU:HD21	15:C:50:ASN:HB3	2.00	0.44
9:W:48:LEU:HD12	9:W:93:ARG:HD2	1.99	0.44
12:Z:192:THR:O	12:Z:196:HIS:ND1	2.36	0.44
13:A:200:ARG:HB3	18:F:408:LEU:HD11	2.00	0.44
13:A:387:SER:O	13:A:391:GLU:HB3	2.17	0.44
14:B:196:GLU:O	14:B:200:SER:OG	2.33	0.44
14:B:432:GLU:HB3	14:B:433:GLY:H	1.55	0.44
18:F:168:TYR:HB2	18:F:173:LYS:HE2	1.99	0.44
21:I:9:THR:HB	21:I:126:GLY:C	2.43	0.44
21:I:47:ALA:N	21:I:212:GLU:O	2.49	0.44
24:L:72:ILE:HG22	24:L:134:ILE:HA	1.98	0.44
26:N:138:TYR:HB3	26:n:138:TYR:HB3	1.99	0.44
19:g:172:GLN:HA	19:g:175:SER:HB3	1.99	0.44
23:k:70:ILE:HD11	23:k:89:ILE:HD12	2.00	0.44
24:l:119:PRO:HA	24:l:125:ARG:HB3	1.99	0.44
2:b:18:ASN:OD1	2:b:25:ARG:NE	2.50	0.44
6:f:659:LEU:HD11	6:f:690:VAL:HG23	2.00	0.44
11:Y:148:GLY:HA3	11:Y:157:ILE:HG23	2.00	0.44
13:A:258:ARG:HG2	13:A:305:GLN:HE22	1.83	0.44
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.48	0.44
23:K:39:GLY:HA2	23:K:48:LEU:HA	1.99	0.44
27:O:98:LEU:O	27:O:113:ILE:HB	2.18	0.44
28:P:58:THR:O	29:Q:85:ARG:NH2	2.50	0.44
32:T:49:THR:OG1	32:T:50:MET:N	2.46	0.44
32:T:176:LEU:O	32:T:180:ASP:HB3	2.17	0.44
26:n:160:LEU:O	26:n:164:MET:HB2	2.17	0.44
2:b:89:GLY:HA2	2:b:92:VAL:HG12	1.98	0.44
4:d:43:LEU:HA	4:d:46:GLN:HG2	2.00	0.44
8:V:108:LEU:HD23	8:V:111:TYR:HD2	1.82	0.44
8:V:148:ARG:HH22	8:V:197:THR:HG21	1.83	0.44
8:V:226:VAL:O	8:V:230:PHE:CB	2.63	0.44
9:W:407:ASP:OD1	10:X:382:GLU:CD	2.61	0.44
10:X:330:LEU:HA	10:X:333:GLN:HB2	1.99	0.44
10:X:397:TYR:HD1	11:Y:365:GLN:HE22	1.64	0.44
11:Y:143:TYR:HA	11:Y:146:ARG:HG2	2.00	0.44
14:B:429:LYS:HG3	15:C:308:PRO:HG3	2.00	0.44
23:K:11:GLY:C	23:K:21:LEU:HD21	2.41	0.44
25:M:58:TYR:OH	25:M:62:SER:O	2.29	0.44
25:M:73:VAL:HG22	25:M:139:SER:HB2	1.99	0.44
22:j:36:ARG:NH1	22:j:142:PRO:O	2.46	0.44
23:k:39:GLY:HA2	23:k:48:LEU:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:173:LYS:HA	25:m:176:ILE:HB	1.99	0.44
26:n:87:CYS:C	26:n:91:ARG:CG	2.81	0.44
27:o:45:GLY:HA2	27:o:98:LEU:HD23	1.99	0.44
27:o:98:LEU:O	27:o:113:ILE:HB	2.18	0.44
1:a:111:VAL:HG21	1:a:141:MET:HE2	1.99	0.44
2:b:21:PHE:HB3	2:b:22:LEU:HD22	1.99	0.44
2:b:69:GLY:HA2	2:b:72:LEU:HD12	2.00	0.44
7:U:266:GLN:O	7:U:270:THR:OG1	2.29	0.44
7:U:533:VAL:HG21	7:U:570:LEU:HD11	1.98	0.44
7:U:561:GLU:CD	7:U:561:GLU:C	2.85	0.44
12:Z:202:ASN:OD1	12:Z:203:SER:N	2.51	0.44
15:C:85:VAL:O	15:C:96:VAL:HA	2.17	0.44
16:D:154:LEU:HB3	16:D:158:GLN:HB2	1.99	0.44
19:G:172:GLN:HA	19:G:175:SER:HB3	1.99	0.44
24:L:39:LYS:HD3	24:L:144:ILE:HG12	1.98	0.44
25:M:20:VAL:HG12	25:M:23:VAL:H	1.82	0.44
26:N:29:ARG:HH21	32:t:179:ARG:HB3	1.83	0.44
30:R:154:ASP:OD1	30:R:157:ARG:NH1	2.50	0.44
20:h:44:VAL:HG11	20:h:146:LEU:HD13	2.00	0.44
6:f:523:GLY:HA2	6:f:526:ALA:HB3	2.00	0.44
7:U:259:GLN:O	7:U:263:SER:CB	2.66	0.44
8:V:67:LEU:HD21	8:V:206:VAL:HG22	1.99	0.44
9:W:162:ALA:HA	9:W:165:ILE:HG22	2.00	0.44
9:W:162:ALA:HB1	9:W:166:LEU:HG	2.00	0.44
12:Z:265:LEU:O	12:Z:268:SER:OG	2.30	0.44
14:B:258:LYS:HD2	16:D:274:ARG:HH12	1.83	0.44
15:C:204:ALA:HA	15:C:207:THR:HG22	1.99	0.44
17:E:243:PHE:HZ	18:F:304:ARG:HE	1.66	0.44
21:I:114:LEU:HA	21:I:117:ILE:HD12	2.00	0.44
23:K:19:GLY:HA3	23:K:20:ARG:NH1	2.33	0.44
31:S:44:TYR:O	31:S:51:VAL:HA	2.18	0.44
32:T:15:LYS:HG2	32:T:20:VAL:HG22	1.99	0.44
19:g:11:ARG:HH22	25:m:7:TYR:HE2	1.64	0.44
24:l:13:TRP:HE1	25:m:129:ARG:HB2	1.82	0.44
25:m:73:VAL:HG22	25:m:139:SER:HB2	1.99	0.44
29:q:59:TYR:O	29:q:63:ASN:CB	2.60	0.44
1:a:25:LEU:HD13	1:a:40:GLN:HG2	2.00	0.44
2:b:1:MET:HB3	2:b:44:ASN:HB2	1.99	0.44
3:c:54:MET:HB2	3:c:82:VAL:HG13	1.99	0.44
3:c:292:MET:HE2	4:d:253:LEU:HD21	1.98	0.44
6:f:92:VAL:HG12	6:f:133:MET:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:229:VAL:O	6:f:233:LEU:HB2	2.18	0.44
6:f:477:MET:O	6:f:481:SER:OG	2.36	0.44
6:f:512:MET:HE2	6:f:557:TRP:HB2	1.99	0.44
7:U:261:LEU:HA	7:U:264:VAL:HG12	1.99	0.44
9:W:104:MET:SD	9:W:123:ARG:NH2	2.91	0.44
9:W:334:GLU:O	9:W:338:THR:OG1	2.32	0.44
11:Y:84:LEU:HD11	11:Y:111:LEU:HD21	2.00	0.44
18:F:83:ASN:O	18:F:88:TYR:OH	2.36	0.44
22:J:109:ARG:O	22:J:113:SER:CB	2.66	0.44
23:K:17:PRO:HA	24:L:24:TYR:CG	2.53	0.44
28:P:70:ARG:HA	28:P:73:LEU:HD12	1.98	0.44
19:g:19:GLU:OE1	20:h:27:ALA:HB1	2.17	0.44
20:h:148:GLN:O	20:h:155:TYR:HA	2.18	0.44
22:j:109:ARG:NH2	30:r:70:ASN:OD1	2.51	0.44
23:k:157:ASP:OD2	23:k:159:SER:OG	2.35	0.44
29:q:108:ASP:N	29:q:112:GLY:O	2.43	0.44
31:s:28:ARG:NH2	31:s:213:ASP:O	2.51	0.44
1:a:194:GLN:HA	1:a:225:LEU:HB3	2.00	0.44
2:b:97:LEU:HD23	2:b:107:MET:HG2	2.00	0.44
3:c:264:LYS:NZ	10:X:405:GLN:OE1	2.33	0.44
6:f:536:SER:O	6:f:540:GLN:CB	2.65	0.44
6:f:796:LEU:HD12	6:f:799:VAL:HG11	2.00	0.44
7:U:402:PHE:O	7:U:406:ALA:CB	2.66	0.44
8:V:258:TYR:HA	8:V:261:TYR:HB3	1.99	0.44
8:V:282:ASN:O	8:V:286:ALA:CB	2.66	0.44
9:W:407:ASP:O	9:W:413:ILE:HG22	2.18	0.44
9:W:415:PHE:HB3	9:W:416:GLN:H	1.66	0.44
11:Y:39:ASP:HA	11:Y:42:MET:HB3	1.99	0.44
12:Z:193:ASN:HA	12:Z:196:HIS:CE1	2.53	0.44
13:A:410:LEU:O	13:A:414:ASN:HB2	2.17	0.44
16:D:120:ASP:H	16:D:123:LEU:HD11	1.83	0.44
17:E:99:ALA:HB2	17:E:111:LEU:HD11	1.99	0.44
26:N:132:SER:O	26:N:136:TYR:HB3	2.17	0.44
31:S:28:ARG:NH2	31:S:213:ASP:O	2.51	0.44
19:g:189:TRP:CE3	19:g:193:GLN:CD	2.96	0.44
21:i:3:ARG:HH12	23:k:10:ARG:HH21	1.65	0.44
22:j:109:ARG:O	22:j:113:SER:CB	2.66	0.44
24:l:98:VAL:HA	32:t:94:ARG:HG3	2.00	0.44
27:o:41:ILE:HG12	27:o:102:GLY:HA3	2.00	0.44
29:q:58:GLU:O	29:q:62:LYS:HB2	2.17	0.44
4:d:103:LEU:O	4:d:107:LEU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:184:LYS:N	4:d:224:SER:OG	2.51	0.43
6:f:234:THR:HG23	6:f:637:LYS:HE2	2.00	0.43
7:U:726:ALA:O	7:U:730:ALA:HB2	2.18	0.43
8:V:224:LEU:HD13	8:V:227:VAL:HB	1.99	0.43
9:W:378:MET:HE1	9:W:415:PHE:HZ	1.83	0.43
13:A:386:ARG:O	13:A:390:THR:OG1	2.34	0.43
16:D:275:PHE:HZ	16:D:289:LEU:HD12	1.83	0.43
16:D:384:MET:HE1	17:E:164:ILE:HB	1.99	0.43
20:H:118:MET:HA	20:H:121:TYR:HD2	1.83	0.43
21:I:8:ARG:HB3	21:I:11:ILE:CD1	2.48	0.43
21:I:39:ALA:HB3	21:I:43:VAL:HA	2.00	0.43
23:K:95:GLU:HA	23:K:98:ASN:HD22	1.82	0.43
31:S:140:SER:OG	31:S:186:ASP:OD2	2.33	0.43
32:T:27:LEU:HD22	32:T:184:TYR:HB2	1.98	0.43
1:a:171:SER:O	1:a:175:ASP:CB	2.57	0.43
1:a:186:LYS:HB3	1:a:193:GLN:HE22	1.82	0.43
2:b:92:VAL:O	2:b:96:ALA:HB2	2.18	0.43
7:U:650:TYR:HA	7:U:683:VAL:HG23	2.00	0.43
9:W:5:GLY:O	9:W:9:ALA:CB	2.66	0.43
9:W:98:LYS:O	9:W:102:ALA:CB	2.67	0.43
9:W:161:GLU:CD	9:W:162:ALA:H	2.27	0.43
9:W:271:VAL:HG11	9:W:296:LEU:HD11	2.01	0.43
13:A:181:LYS:HA	13:A:184:ILE:HD12	2.00	0.43
14:B:108:SER:HB3	14:B:154:HIS:CE1	2.54	0.43
14:B:170:LEU:O	14:B:174:MET:HB2	2.18	0.43
16:D:313:ARG:HG3	16:D:315:ASP:H	1.84	0.43
16:D:323:ARG:HB2	16:D:326:ARG:HD2	1.99	0.43
16:D:403:TYR:HA	16:D:407:ILE:HG13	1.73	0.43
34:E:401:ATP:O2G	34:E:401:ATP:O2B	2.33	0.43
25:M:173:LYS:HA	25:M:176:ILE:HB	1.99	0.43
25:M:214:SER:OG	25:M:224:HIS:NE2	2.51	0.43
29:Q:19:ARG:HH21	29:Q:31:ASP:HB2	1.83	0.43
19:g:178:PHE:O	19:g:182:LYS:HB2	2.17	0.43
20:h:118:MET:HA	20:h:121:TYR:HD2	1.83	0.43
1:a:7:PHE:O	1:a:11:SER:OG	2.35	0.43
3:c:152:LYS:HA	12:Z:170:VAL:HA	2.00	0.43
4:d:203:PRO:HD2	4:d:206:MET:HG2	1.99	0.43
9:W:98:LYS:HG2	9:W:138:VAL:HG21	2.00	0.43
10:X:323:LEU:O	10:X:327:TYR:HB3	2.18	0.43
11:Y:336:ARG:O	11:Y:340:ALA:CB	2.59	0.43
12:Z:10:VAL:HB	12:Z:48:LEU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:90:HIS:CB	15:C:91:PRO:HD3	2.38	0.43
16:D:381:GLU:O	16:D:385:LEU:HB2	2.17	0.43
23:K:157:ASP:OD1	23:K:157:ASP:N	2.50	0.43
26:N:91:ARG:HG3	26:N:92:GLU:H	1.83	0.43
30:R:169:TYR:HE2	28:p:32:ALA:HA	1.83	0.43
32:t:15:LYS:HG2	32:t:20:VAL:HG22	1.99	0.43
32:t:141:TYR:O	32:t:144:TYR:N	2.51	0.43
1:a:188:LEU:O	1:a:193:GLN:NE2	2.52	0.43
1:a:338:PRO:HG3	12:Z:229:GLN:HA	1.99	0.43
2:b:22:LEU:N	2:b:22:LEU:HD13	2.33	0.43
4:d:36:LEU:N	4:d:37:PRO:CD	2.82	0.43
6:f:141:LYS:HA	6:f:144:LEU:HB3	1.99	0.43
7:U:418:GLU:O	7:U:422:LEU:HB3	2.18	0.43
10:X:115:GLU:O	10:X:119:SER:HB2	2.18	0.43
10:X:236:PHE:HA	10:X:239:TYR:HB2	2.01	0.43
12:Z:82:PHE:HA	12:Z:85:VAL:HG12	2.00	0.43
14:B:211:TYR:O	14:B:215:GLY:HA2	2.19	0.43
14:B:434:THR:CB	14:B:435:PRO:HD2	2.28	0.43
16:D:273:LYS:HE3	16:D:316:THR:HA	1.98	0.43
19:G:13:ILE:HG13	19:G:15:ILE:HG23	1.99	0.43
20:H:74:LEU:HD21	20:H:134:LEU:HD22	2.00	0.43
22:J:96:LEU:HA	29:Q:62:LYS:HE3	2.01	0.43
22:J:171:PHE:O	22:J:175:ASN:HB2	2.18	0.43
27:O:136:ALA:HB2	32:t:179:ARG:HH22	1.83	0.43
28:P:124:LEU:HG	28:P:130:PRO:HA	1.99	0.43
31:s:21:ALA:HB3	31:s:198:VAL:HB	2.00	0.43
1:a:254:ALA:O	1:a:258:GLN:NE2	2.51	0.43
4:d:33:LEU:HB3	4:d:34:ASN:H	1.62	0.43
7:U:450:HIS:CG	7:U:457:ILE:HG13	2.54	0.43
11:Y:155:ASP:O	11:Y:158:THR:OG1	2.34	0.43
15:C:270:GLN:HA	15:C:273:MET:HE2	2.01	0.43
16:D:230:VAL:HB	16:D:264:ILE:HG12	2.01	0.43
26:N:88:TYR:OH	32:T:59:ASP:OD1	2.30	0.43
31:S:63:THR:HG23	32:T:94:ARG:HH12	1.83	0.43
32:T:92:LEU:HD23	32:T:125:VAL:HG21	2.01	0.43
19:g:19:GLU:C	19:g:19:GLU:CD	2.85	0.43
23:k:21:LEU:HD22	23:k:23:GLN:H	1.83	0.43
30:r:9:ARG:NH2	30:r:146:ASP:OD1	2.39	0.43
1:a:286:ALA:HB2	12:Z:240:VAL:HG22	2.00	0.43
3:c:52:GLU:HG2	3:c:82:VAL:HG21	2.00	0.43
4:d:120:GLU:HA	4:d:123:PRO:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:72:ARG:O	6:f:76:GLU:HG2	2.18	0.43
6:f:657:ILE:HA	6:f:660:ILE:HD12	2.01	0.43
15:C:221:GLN:HB3	15:C:227:GLY:HA2	2.00	0.43
16:D:336:PRO:HB2	16:D:341:LYS:HG3	2.00	0.43
16:D:399:PHE:HA	16:D:402:ALA:HB3	2.00	0.43
24:L:159:MET:HE1	25:M:57:LEU:HD13	1.99	0.43
29:Q:38:MET:O	29:Q:65:GLN:NE2	2.52	0.43
29:Q:162:LYS:C	30:r:141:ARG:HH22	2.26	0.43
30:R:18:SER:OG	30:R:29:GLN:O	2.27	0.43
31:S:76:LYS:O	31:S:80:ASN:N	2.40	0.43
31:S:94:THR:O	31:S:98:SER:HB3	2.19	0.43
22:j:7:ILE:H	22:j:7:ILE:HG13	1.47	0.43
24:l:183:ASN:O	24:l:187:LEU:HB3	2.18	0.43
31:s:94:THR:O	31:s:98:SER:HB3	2.19	0.43
1:a:341:LEU:HD21	1:a:349:MET:HE1	1.99	0.43
4:d:73:ARG:HH12	7:U:13:ASP:HB2	1.82	0.43
6:f:321:MET:O	6:f:325:GLN:CB	2.48	0.43
7:U:541:HIS:HB2	7:U:544:ILE:HG22	2.00	0.43
8:V:326:GLN:O	8:V:330:LYS:HB2	2.18	0.43
8:V:421:ASP:O	8:V:425:LYS:HB3	2.19	0.43
11:Y:37:VAL:HA	11:Y:40:GLU:HB3	2.00	0.43
14:B:355:LEU:HD13	14:B:389:ASP:HB2	2.01	0.43
16:D:366:ARG:HA	16:D:367:PRO:HD2	1.74	0.43
23:K:70:ILE:HD11	23:K:89:ILE:HD12	2.00	0.43
32:T:141:TYR:O	32:T:144:TYR:N	2.51	0.43
19:g:223:GLU:C	19:g:225:PRO:HD3	2.37	0.43
21:i:39:ALA:HB3	21:i:43:VAL:HA	2.00	0.43
23:k:15:PHE:HD1	23:k:20:ARG:CA	2.31	0.43
26:n:132:SER:O	26:n:136:TYR:HB3	2.17	0.43
26:n:140:ASP:OD1	26:n:140:ASP:N	2.47	0.43
2:b:95:LEU:HD23	12:Z:67:VAL:HG12	2.00	0.43
3:c:63:ASP:OD1	3:c:66:THR:OG1	2.26	0.43
6:f:424:GLY:HA2	6:f:427:THR:HG22	2.01	0.43
7:U:82:LEU:HD11	7:U:130:LEU:HD23	2.01	0.43
9:W:131:VAL:HG13	9:W:140:ILE:HG22	2.00	0.43
13:A:230:ALA:HA	13:A:233:THR:HB	2.01	0.43
14:B:437:GLY:HA2	14:B:440:LEU:HD21	2.01	0.43
14:B:439:TYR:OH	22:J:28:LYS:CB	2.67	0.43
16:D:98:GLN:OE1	16:D:121:ARG:NH2	2.52	0.43
17:E:288:ALA:HA	17:E:291:ARG:HH12	1.83	0.43
18:F:202:ILE:HG23	18:F:327:LYS:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:501:ATP:O1B	34:F:501:ATP:O2G	2.36	0.43
23:K:50:VAL:HG11	23:K:66:LYS:HB2	2.01	0.43
26:N:92:GLU:CD	26:N:92:GLU:N	2.76	0.43
29:Q:58:GLU:O	29:Q:62:LYS:HB2	2.17	0.43
31:S:112:GLY:HA2	31:S:198:VAL:HG11	2.00	0.43
22:j:37:GLY:H	22:j:41:VAL:HA	1.84	0.43
22:j:171:PHE:O	22:j:175:ASN:HB2	2.18	0.43
23:k:157:ASP:N	23:k:157:ASP:OD1	2.50	0.43
25:m:25:TYR:HD1	25:m:28:LYS:HE3	1.83	0.43
7:U:60:ALA:O	7:U:64:ALA:CB	2.67	0.43
7:U:65:SER:O	7:U:69:TYR:CB	2.63	0.43
7:U:95:GLU:HA	7:U:98:GLU:HG2	2.01	0.43
7:U:233:LEU:HA	7:U:236:LEU:HG	2.00	0.43
7:U:415:HIS:CE1	7:U:422:LEU:HD13	2.54	0.43
9:W:321:VAL:O	9:W:325:GLY:HA3	2.19	0.43
15:C:90:HIS:ND1	16:D:110:ASN:CA	2.79	0.43
15:C:239:ARG:HH21	15:C:284:GLU:HG3	1.84	0.43
16:D:342:ARG:HG3	16:D:364:VAL:HG11	2.01	0.43
18:F:229:PRO:O	34:F:501:ATP:O2G	2.36	0.43
18:F:341:ALA:HA	18:F:344:ARG:NH2	2.28	0.43
20:H:148:GLN:O	20:H:155:TYR:HA	2.18	0.43
28:P:171:MET:O	28:P:175:VAL:HB	2.18	0.43
29:Q:59:TYR:O	29:Q:63:ASN:CB	2.60	0.43
23:k:67:ILE:HG12	23:k:218:ALA:HB2	2.01	0.43
25:m:194:ALA:HB1	25:m:235:ALA:HA	2.01	0.43
29:q:19:ARG:HH21	29:q:31:ASP:HB2	1.84	0.43
29:q:38:MET:O	29:q:65:GLN:NE2	2.52	0.43
1:a:77:VAL:HA	1:a:80:ILE:HG22	2.01	0.43
2:b:22:LEU:HD21	2:b:179:LEU:O	2.18	0.43
4:d:34:ASN:ND2	7:U:26:LYS:CG	2.76	0.43
6:f:405:HIS:CG	6:f:792:ALA:HA	2.54	0.43
7:U:235:LYS:O	7:U:239:GLU:CB	2.66	0.43
8:V:213:TYR:HA	8:V:216:ARG:HB2	2.01	0.43
11:Y:238:GLU:HA	11:Y:242:LYS:HB2	2.01	0.43
14:B:135:ILE:HA	14:B:159:VAL:HB	2.00	0.43
14:B:438:LEU:HB2	14:B:439:TYR:H	1.68	0.43
16:D:173:GLN:HE21	16:D:334:PRO:HD2	1.84	0.43
18:F:314:LEU:HD22	18:F:347:ARG:HH11	1.84	0.43
25:M:229:LYS:O	25:M:233:GLU:HA	2.19	0.43
27:O:201:ARG:O	27:O:201:ARG:HG3	2.19	0.43
29:Q:19:ARG:HE	29:Q:31:ASP:HA	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Q:31:ASP:OD1	29:Q:31:ASP:N	2.48	0.43
31:S:45:LYS:HA	31:S:51:VAL:HG22	2.01	0.43
25:m:229:LYS:O	25:m:233:GLU:HA	2.19	0.43
31:s:112:GLY:HA2	31:s:198:VAL:HG11	2.00	0.43
4:d:21:GLU:O	4:d:25:ARG:HB2	2.19	0.42
4:d:112:VAL:O	4:d:116:HIS:ND1	2.45	0.42
6:f:187:LEU:HD13	6:f:228:LYS:HD3	2.00	0.42
6:f:623:LYS:O	6:f:627:GLU:HB2	2.17	0.42
7:U:890:LYS:HG3	7:U:891:VAL:HG13	2.01	0.42
8:V:62:HIS:O	8:V:66:GLU:HB2	2.19	0.42
8:V:99:ARG:HG3	8:V:145:LEU:HB2	2.01	0.42
8:V:106:ARG:HA	8:V:109:ASN:HB2	2.01	0.42
9:W:317:TRP:CD1	9:W:320:LEU:HD22	2.55	0.42
11:Y:158:THR:O	11:Y:161:THR:OG1	2.30	0.42
11:Y:160:ASN:O	11:Y:164:ALA:HB2	2.19	0.42
11:Y:301:ILE:O	11:Y:305:SER:HB3	2.18	0.42
15:C:46:GLN:HB3	16:D:61:ILE:HG21	2.01	0.42
18:F:249:LEU:N	18:F:282:ILE:O	2.43	0.42
20:H:123:GLN:NE2	20:H:123:GLN:HA	2.33	0.42
23:K:113:THR:O	23:K:117:SER:OG	2.29	0.42
25:M:5:THR:C	25:M:7:TYR:H	2.27	0.42
25:M:25:TYR:HD1	25:M:28:LYS:HE3	1.83	0.42
27:O:219:LEU:HD11	28:P:195:ILE:HG13	2.00	0.42
29:Q:138:LEU:O	29:Q:141:SER:OG	2.32	0.42
31:S:21:ALA:HB3	31:S:198:VAL:HB	2.00	0.42
19:g:127:GLN:CG	20:h:127:VAL:HG21	2.18	0.42
23:k:202:LEU:HD13	23:k:215:ILE:HG21	2.01	0.42
24:l:174:ARG:HG3	24:l:175:HIS:ND1	2.34	0.42
29:q:5:ILE:HG22	29:q:16:ALA:HB3	2.01	0.42
29:q:19:ARG:HE	29:q:31:ASP:HA	1.84	0.42
32:t:49:THR:HB	32:t:85:PRO:HG3	2.00	0.42
32:t:92:LEU:HD23	32:t:125:VAL:HG21	2.01	0.42
3:c:39:LEU:HD23	3:c:42:LEU:HD21	2.01	0.42
4:d:42:LYS:NZ	4:d:46:GLN:OE1	2.51	0.42
6:f:315:GLU:HA	6:f:318:THR:HG22	2.00	0.42
8:V:37:MET:O	8:V:41:ALA:HB2	2.19	0.42
8:V:46:GLY:HA3	8:V:62:HIS:ND1	2.34	0.42
8:V:333:ILE:HD11	8:V:345:ARG:NH2	2.31	0.42
11:Y:374:ASP:O	11:Y:378:ASN:CB	2.49	0.42
13:A:216:GLY:HA3	13:A:343:PHE:HB2	2.00	0.42
14:B:134:SER:O	14:B:159:VAL:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:216:ALA:O	16:D:220:ALA:HB2	2.18	0.42
16:D:354:LEU:HD23	16:D:356:GLU:HA	2.00	0.42
22:J:64:ALA:O	22:J:88:ARG:NH1	2.52	0.42
24:L:86:ASN:O	24:L:90:GLN:HB2	2.19	0.42
29:Q:37:LYS:O	29:Q:61:GLN:NE2	2.51	0.42
30:r:196:HIS:O	30:r:200:SER:HB3	2.19	0.42
1:a:290:GLN:HG2	1:a:330:ARG:HB3	2.00	0.42
4:d:215:TRP:CZ3	4:d:217:LEU:HA	2.54	0.42
7:U:259:GLN:O	7:U:263:SER:HB3	2.19	0.42
7:U:528:ALA:HB1	7:U:532:MET:HE2	2.02	0.42
7:U:575:ASP:HA	7:U:579:ARG:HH21	1.84	0.42
7:U:749:GLN:HA	7:U:755:THR:HA	2.00	0.42
9:W:408:ARG:HB2	9:W:408:ARG:CZ	2.50	0.42
14:B:381:ASP:HA	14:B:384:ILE:HB	2.01	0.42
15:C:164:VAL:HG21	15:C:313:ARG:HG3	2.01	0.42
17:E:148:VAL:HG13	17:E:149:ILE:HG13	2.01	0.42
18:F:281:SER:O	18:F:327:LYS:HB2	2.20	0.42
30:R:196:HIS:O	30:R:200:SER:HB3	2.19	0.42
32:T:97:TYR:O	32:T:101:SER:OG	2.26	0.42
21:i:114:LEU:HA	21:i:117:ILE:HD12	2.00	0.42
23:k:19:GLY:HA3	23:k:20:ARG:NH1	2.33	0.42
25:m:141:SER:HB3	25:m:144:ASP:HB2	2.01	0.42
28:p:171:MET:O	28:p:175:VAL:HB	2.18	0.42
2:b:4:GLU:OE2	2:b:40:LYS:NZ	2.42	0.42
4:d:104:LEU:HD21	4:d:167:ILE:HG23	2.01	0.42
4:d:203:PRO:HB2	4:d:205:LYS:HB3	2.01	0.42
6:f:211:ILE:HA	6:f:214:VAL:HG22	2.00	0.42
6:f:282:PHE:HE2	6:f:317:LEU:HD21	1.85	0.42
8:V:159:LEU:HD12	8:V:178:SER:HB3	2.00	0.42
8:V:484:LEU:HA	8:V:487:HIS:HD1	1.84	0.42
10:X:256:LEU:O	10:X:260:MET:HB2	2.19	0.42
10:X:405:GLN:O	10:X:408:SER:OG	2.28	0.42
11:Y:48:ASN:HD21	11:Y:77:ASN:HA	1.83	0.42
11:Y:57:LEU:HD13	11:Y:63:TRP:CD1	2.54	0.42
14:B:337:LEU:HD13	14:B:337:LEU:HA	1.89	0.42
23:K:16:SER:HB2	23:K:22:PHE:CZ	2.54	0.42
23:K:67:ILE:HG12	23:K:218:ALA:HB2	2.01	0.42
24:L:174:ARG:HG3	24:L:175:HIS:ND1	2.34	0.42
26:N:129:GLY:O	26:N:132:SER:OG	2.35	0.42
32:T:49:THR:HB	32:T:85:PRO:HG3	2.00	0.42
20:h:100:VAL:HG13	28:p:93:ASN:HD22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:o:103:VAL:HA	27:o:108:PRO:HA	2.01	0.42
31:s:44:TYR:O	31:s:51:VAL:HA	2.18	0.42
31:s:199:THR:OG1	31:s:202:GLY:O	2.30	0.42
4:d:18:LYS:HA	4:d:21:GLU:HB3	2.00	0.42
6:f:99:LEU:HD22	6:f:101:PRO:HA	2.02	0.42
7:U:472:ILE:H	7:U:472:ILE:HG13	1.63	0.42
7:U:494:TYR:O	7:U:498:LYS:NZ	2.49	0.42
8:V:182:LYS:HB3	8:V:182:LYS:HE3	1.77	0.42
8:V:345:ARG:NH1	8:V:359:PRO:CB	2.72	0.42
9:W:182:ARG:O	9:W:186:ILE:HB	2.19	0.42
15:C:277:LEU:HA	15:C:280:LEU:HG	2.01	0.42
18:F:404:GLY:HA2	18:F:415:LEU:HD21	2.01	0.42
20:H:127:VAL:HB	20:H:128:ARG:H	1.46	0.42
21:I:140:ASP:OD1	21:I:144:GLY:N	2.53	0.42
27:O:41:ILE:HG12	27:O:102:GLY:HA3	2.00	0.42
24:l:98:VAL:O	32:t:90:SER:OG	2.33	0.42
26:n:129:GLY:O	26:n:132:SER:OG	2.35	0.42
27:o:1:THR:O	27:o:129:SER:N	2.44	0.42
31:s:45:LYS:HA	31:s:51:VAL:HG22	2.01	0.42
1:a:172:TYR:O	1:a:176:ALA:HB2	2.19	0.42
1:a:220:PRO:HA	1:a:223:GLU:HG2	2.01	0.42
5:e:59:GLU:HG3	5:e:60:LEU:HD22	2.02	0.42
7:U:381:THR:HG22	7:U:412:HIS:HA	2.02	0.42
7:U:419:ALA:HB2	7:U:449:ILE:HG21	2.02	0.42
7:U:477:GLY:O	7:U:481:LEU:CB	2.68	0.42
7:U:661:ALA:HB3	7:U:746:ILE:HD11	2.00	0.42
9:W:266:ALA:O	9:W:270:VAL:HB	2.19	0.42
18:F:183:GLU:HB3	18:F:239:ALA:HA	2.01	0.42
19:G:21:ARG:H	19:G:21:ARG:CZ	2.33	0.42
20:H:44:VAL:HG11	20:H:146:LEU:HD13	2.00	0.42
25:M:201:HIS:HE1	25:M:206:ASP:HB2	1.84	0.42
19:g:10:ASP:CB	25:m:7:TYR:HH	2.02	0.42
19:g:10:ASP:C	19:g:11:ARG:HD3	2.44	0.42
21:i:8:ARG:NH2	22:j:5:ARG:NH1	2.67	0.42
21:i:48:GLU:OE2	21:i:50:ARG:NH2	2.52	0.42
27:o:110:LEU:HD21	27:o:125:VAL:HG22	2.02	0.42
1:a:262:ALA:HA	1:a:265:GLU:HB2	2.02	0.42
1:a:293:PHE:O	1:a:297:ALA:CB	2.67	0.42
7:U:69:TYR:HE2	8:V:236:ARG:HD2	1.85	0.42
7:U:154:ALA:HB1	7:U:163:PHE:HA	2.02	0.42
8:V:80:LYS:C	8:V:82:LEU:H	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:229:ILE:HG22	11:Y:230:ALA:H	1.85	0.42
14:B:343:ARG:HE	14:B:346:ARG:HG3	1.85	0.42
21:I:135:LEU:HD23	21:I:135:LEU:HA	1.87	0.42
22:J:37:GLY:H	22:J:41:VAL:HA	1.84	0.42
24:L:107:ARG:NH2	32:T:79:ASP:OD2	2.32	0.42
25:M:215:TRP:HZ2	25:M:219:LEU:HB3	1.85	0.42
20:h:74:LEU:HD21	20:h:134:LEU:HD22	2.00	0.42
23:k:21:LEU:HD23	23:k:21:LEU:HA	1.81	0.42
24:l:86:ASN:O	24:l:90:GLN:HB2	2.19	0.42
25:m:201:HIS:HE1	25:m:206:ASP:HB2	1.84	0.42
2:b:22:LEU:CG	2:b:179:LEU:CA	2.96	0.42
2:b:62:THR:HG21	2:b:71:ILE:HG13	2.02	0.42
6:f:389:LYS:HG3	6:f:417:ILE:HG22	2.01	0.42
7:U:895:PRO:HD2	7:U:902:PRO:HD2	2.02	0.42
8:V:234:ARG:HA	8:V:237:THR:HG22	2.01	0.42
9:W:23:THR:HA	9:W:26:GLN:HB2	2.02	0.42
11:Y:179:ARG:NH2	11:Y:210:SER:HB3	2.35	0.42
12:Z:205:LEU:HA	12:Z:208:ILE:HG22	2.01	0.42
13:A:189:GLU:O	13:A:193:THR:OG1	2.37	0.42
14:B:290:ILE:HG12	14:B:305:ILE:HG23	2.01	0.42
14:B:430:LYS:HA	14:B:430:LYS:HD3	1.26	0.42
16:D:117:SER:HA	16:D:121:ARG:HH22	1.84	0.42
16:D:360:LEU:HA	16:D:363:TYR:HD2	1.83	0.42
17:E:373:LYS:HZ1	18:F:350:ARG:HH22	1.67	0.42
19:G:11:ARG:HE	19:G:23:TYR:HB2	1.85	0.42
19:G:15:ILE:HG22	20:H:10:LEU:HD11	2.00	0.42
20:H:120:GLU:O	20:H:124:SER:N	2.52	0.42
25:M:141:SER:HB3	25:M:144:ASP:HB2	2.01	0.42
27:O:201:ARG:HE	27:O:201:ARG:HB2	1.53	0.42
19:g:192:GLU:OE1	19:g:238:HIS:CE1	2.73	0.42
20:h:34:PRO:HA	20:h:164:GLY:HA3	2.02	0.42
25:m:45:VAL:HG11	25:m:148:LEU:HD13	2.01	0.42
25:m:215:TRP:HZ2	25:m:219:LEU:HB3	1.85	0.42
32:t:9:THR:O	32:t:41:ARG:NH2	2.51	0.42
4:d:211:LYS:HZ1	4:d:217:LEU:HD22	1.84	0.42
6:f:688:ARG:HH22	6:f:788:MET:HA	1.84	0.42
8:V:37:MET:HE3	8:V:41:ALA:HB2	2.01	0.42
8:V:325:LYS:HA	8:V:328:VAL:HG12	2.01	0.42
11:Y:88:LEU:HD23	11:Y:104:MET:HE3	2.02	0.42
12:Z:33:LYS:HE3	12:Z:102:HIS:CE1	2.55	0.42
12:Z:98:GLY:HA2	12:Z:99:PRO:HD3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:277:ILE:HG22	13:A:280:ILE:HD12	2.01	0.42
16:D:226:ALA:HB3	16:D:260:ALA:HB1	2.02	0.42
18:F:66:LEU:O	18:F:70:LYS:CB	2.68	0.42
18:F:217:ILE:HG13	18:F:218:GLN:H	1.85	0.42
18:F:430:LYS:HD3	18:F:430:LYS:HA	1.80	0.42
18:F:431:LYS:C	18:F:431:LYS:HZ2	2.27	0.42
19:G:89:SER:OG	25:M:117:MET:SD	2.68	0.42
20:H:9:SER:HA	20:H:125:GLY:CA	2.50	0.42
21:I:208:ALA:HA	21:I:211:VAL:HG22	2.02	0.42
25:M:40:ARG:HE	25:M:161:TRP:CD1	2.38	0.42
30:R:9:ARG:NH2	30:R:146:ASP:OD1	2.39	0.42
30:R:97:MET:O	30:R:116:SER:N	2.53	0.42
31:S:35:ILE:O	32:T:151:ARG:NH2	2.46	0.42
19:g:103:TYR:HB2	26:n:61:TYR:CD1	2.55	0.42
27:o:163:ILE:HD13	27:o:192:PRO:HG3	2.02	0.42
28:p:58:THR:OG1	29:q:121:LEU:O	2.34	0.42
3:c:291:LEU:O	12:Z:267:ARG:NH1	2.50	0.42
4:d:130:ASN:ND2	4:d:133:ILE:HG12	2.35	0.42
6:f:45:LEU:HD22	6:f:86:THR:HG21	2.01	0.42
8:V:347:GLN:HG2	8:V:347:GLN:O	2.19	0.42
8:V:419:LEU:HD23	8:V:458:VAL:HG23	2.01	0.42
10:X:351:SER:HA	10:X:362:GLU:OE1	2.19	0.42
12:Z:56:VAL:HG13	12:Z:70:LEU:HD22	2.02	0.42
12:Z:133:LEU:HD23	12:Z:162:ILE:HG12	2.01	0.42
13:A:406:GLU:HA	13:A:409:PHE:HD2	1.84	0.42
14:B:223:ILE:HD12	14:B:350:LYS:HG3	2.00	0.42
15:C:90:HIS:CG	16:D:110:ASN:CA	3.03	0.42
21:I:118:LYS:HE2	21:I:152:PRO:HA	2.02	0.42
22:J:4:ASP:H	22:J:5:ARG:HH11	1.68	0.42
22:J:66:ASP:H	22:J:69:VAL:HG12	1.85	0.42
32:T:28:GLY:N	32:T:36:PHE:O	2.47	0.42
22:j:66:ASP:H	22:j:69:VAL:HG12	1.85	0.42
25:m:40:ARG:HE	25:m:161:TRP:CD1	2.38	0.42
30:r:97:MET:O	30:r:116:SER:N	2.53	0.42
1:a:327:VAL:HA	9:W:374:THR:HG23	2.02	0.41
2:b:22:LEU:CD1	2:b:179:LEU:C	2.93	0.41
3:c:29:GLU:OE2	3:c:175:ARG:NH2	2.53	0.41
4:d:45:LYS:HG2	4:d:48:LEU:HD12	2.02	0.41
6:f:125:ILE:HD12	6:f:126:ILE:HG13	2.02	0.41
6:f:646:MET:HA	6:f:649:HIS:HD1	1.84	0.41
7:U:418:GLU:O	7:U:422:LEU:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:483:LEU:HD12	7:U:486:MET:HE3	2.02	0.41
9:W:116:THR:HG23	9:W:118:LEU:H	1.84	0.41
10:X:187:ARG:NH2	10:X:221:GLU:OE2	2.53	0.41
12:Z:42:SER:N	12:Z:49:ASP:O	2.44	0.41
13:A:312:ARG:HH12	13:A:317:VAL:CB	2.32	0.41
14:B:107:MET:HG2	14:B:160:ILE:HD13	2.01	0.41
16:D:313:ARG:HD2	16:D:315:ASP:HB2	2.01	0.41
17:E:43:SER:O	17:E:47:LEU:CB	2.67	0.41
18:F:369:HIS:HD2	18:F:400:CYS:HB3	1.84	0.41
19:G:22:LEU:HD11	19:G:24:GLN:HB2	2.01	0.41
21:I:8:ARG:CA	21:I:11:ILE:HD11	2.43	0.41
25:M:45:VAL:HG11	25:M:148:LEU:HD13	2.01	0.41
27:O:103:VAL:HA	27:O:108:PRO:HA	2.01	0.41
27:O:110:LEU:HD21	27:O:125:VAL:HG22	2.02	0.41
28:P:164:PHE:O	28:P:168:SER:OG	2.30	0.41
21:i:8:ARG:O	21:i:11:ILE:HD12	2.04	0.41
21:i:140:ASP:OD1	21:i:144:GLY:N	2.53	0.41
22:j:64:ALA:O	22:j:88:ARG:NH1	2.52	0.41
25:m:170:GLN:HA	25:m:173:LYS:HE2	2.02	0.41
28:p:126:LEU:HD12	28:p:127:ILE:HG23	2.02	0.41
1:a:172:TYR:O	1:a:176:ALA:CB	2.68	0.41
6:f:220:ASP:HB3	6:f:223:GLU:HB2	2.02	0.41
7:U:182:LYS:O	7:U:186:SER:CB	2.68	0.41
7:U:520:MET:HG3	7:U:525:ASN:ND2	2.36	0.41
10:X:192:SER:O	10:X:196:THR:OG1	2.26	0.41
11:Y:19:ILE:HG21	11:Y:52:PRO:HB3	2.02	0.41
11:Y:383:LEU:O	12:Z:283:ARG:NH1	2.52	0.41
21:I:48:GLU:OE2	21:I:50:ARG:NH2	2.52	0.41
21:I:234:GLU:HA	21:I:237:ILE:HD12	2.02	0.41
27:O:163:ILE:HD13	27:O:192:PRO:HG3	2.02	0.41
19:g:101:TRP:O	19:g:105:TYR:HB2	2.20	0.41
3:c:210:ASN:O	3:c:214:GLN:N	2.42	0.41
6:f:545:LYS:HE2	6:f:555:ALA:HA	2.01	0.41
7:U:164:GLU:O	7:U:168:LEU:CB	2.69	0.41
8:V:100:MET:H	8:V:104:THR:HG21	1.84	0.41
8:V:211:TYR:HD1	8:V:214:HIS:HD2	1.68	0.41
9:W:38:GLY:H	9:W:44:ILE:HD11	1.85	0.41
12:Z:68:TRP:CD1	12:Z:104:ASN:HD21	2.37	0.41
12:Z:144:VAL:HB	12:Z:145:HIS:H	1.50	0.41
13:A:249:TYR:HB3	18:F:259:MET:HG3	2.02	0.41
15:C:188:LEU:HD23	15:C:315:ILE:HB	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:391:ARG:HD2	16:D:393:ILE:HD12	2.02	0.41
19:G:21:ARG:N	19:G:21:ARG:CZ	2.83	0.41
27:O:135:MET:C	32:t:179:ARG:HH12	2.28	0.41
27:O:172:ASN:ND2	27:O:188:PRO:HA	2.36	0.41
30:R:19:ARG:NH2	28:p:205:ASP:O	2.46	0.41
30:R:158:ARG:HH12	30:R:199:TYR:HB3	1.85	0.41
27:o:18:THR:OG1	27:o:29:LYS:O	2.38	0.41
30:r:55:TRP:CZ3	30:r:86:MET:HB3	2.55	0.41
1:a:76:LEU:HA	1:a:79:ILE:HG22	2.03	0.41
3:c:40:LYS:O	3:c:44:HIS:CB	2.68	0.41
3:c:257:LYS:HA	3:c:260:GLU:HB2	2.02	0.41
6:f:80:ARG:HD2	6:f:133:MET:HE1	2.01	0.41
6:f:553:THR:OG1	6:f:556:ARG:NH2	2.49	0.41
7:U:560:MET:SD	7:U:595:ASN:ND2	2.88	0.41
8:V:40:GLU:HA	8:V:43:THR:HB	2.02	0.41
8:V:309:MET:HE3	8:V:332:LEU:HG	2.03	0.41
9:W:202:THR:O	9:W:206:SER:HB2	2.21	0.41
10:X:89:VAL:HG21	10:X:125:LEU:HD21	2.01	0.41
13:A:87:LEU:HD22	14:B:136:LEU:HD23	2.02	0.41
13:A:214:LEU:HB2	13:A:319:MET:O	2.20	0.41
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.84	0.41
16:D:148:ASP:CB	16:D:152:MET:SD	3.08	0.41
18:F:238:ARG:O	18:F:242:ALA:CB	2.67	0.41
19:G:7:ALA:C	19:G:11:ARG:NH2	2.75	0.41
23:K:99:HIS:HB2	23:K:107:MET:HE3	2.02	0.41
27:O:153:ASN:O	27:O:157:GLU:HB2	2.21	0.41
28:P:102:PRO:O	29:Q:93:ARG:NH2	2.49	0.41
30:R:20:ALA:HB3	30:R:31:VAL:HG21	2.03	0.41
19:g:191:PHE:HE1	19:g:219:VAL:HG21	1.85	0.41
23:k:99:HIS:HB2	23:k:107:MET:HE3	2.02	0.41
23:k:192:LYS:HA	23:k:195:ILE:HD12	2.03	0.41
30:r:20:ALA:HB3	30:r:31:VAL:HG21	2.03	0.41
3:c:220:LEU:HD21	12:Z:16:LEU:HD13	2.03	0.41
4:d:236:THR:O	4:d:239:SER:OG	2.32	0.41
9:W:88:MET:HG2	9:W:93:ARG:HB3	2.02	0.41
11:Y:209:THR:HA	11:Y:213:LEU:HD12	2.02	0.41
11:Y:215:ASP:O	11:Y:218:THR:OG1	2.29	0.41
14:B:419:PHE:O	14:B:423:LYS:CB	2.68	0.41
15:C:284:GLU:HG2	15:C:285:ALA:H	1.84	0.41
19:G:80:MET:HE2	19:G:87:SER:HA	2.03	0.41
20:H:6:TYR:HE2	20:H:126:GLY:CA	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:202:LEU:HD13	23:K:215:ILE:HG21	2.01	0.41
26:N:167:ASP:HB3	26:N:170:SER:HB2	2.03	0.41
28:P:61:GLN:HB2	29:Q:85:ARG:NH2	2.36	0.41
29:Q:5:ILE:HG22	29:Q:16:ALA:HB3	2.01	0.41
31:S:148:LEU:HD23	31:S:178:VAL:HG12	2.03	0.41
32:T:176:LEU:O	32:T:180:ASP:CB	2.68	0.41
23:k:10:ARG:HB2	23:k:22:PHE:CE2	2.56	0.41
23:k:50:VAL:HG11	23:k:66:LYS:HB2	2.01	0.41
25:m:152:ASP:OD1	25:m:156:VAL:N	2.54	0.41
26:n:40:ARG:NH2	26:n:181:GLU:O	2.53	0.41
27:o:153:ASN:O	27:o:157:GLU:HB2	2.21	0.41
30:r:55:TRP:HZ3	30:r:86:MET:HB3	1.86	0.41
32:t:27:LEU:HD11	32:t:34:ALA:HB1	2.02	0.41
32:t:176:LEU:O	32:t:180:ASP:CB	2.68	0.41
3:c:131:GLN:HA	3:c:134:GLU:HG2	2.02	0.41
6:f:509:LYS:HB3	6:f:514:VAL:HG21	2.03	0.41
7:U:341:PHE:O	7:U:345:ASN:CB	2.59	0.41
8:V:403:ILE:HD11	8:V:428:LEU:HD11	2.03	0.41
10:X:345:VAL:HG23	10:X:353:LEU:HD21	2.03	0.41
13:A:224:LEU:HD21	34:A:501:ATP:H2'	2.02	0.41
14:B:183:THR:OG1	14:B:241:ASN:ND2	2.54	0.41
15:C:57:ARG:HG2	16:D:68:LEU:HD22	2.01	0.41
19:G:21:ARG:HB2	19:G:22:LEU:H	1.48	0.41
21:I:41:ASP:OD1	21:I:41:ASP:N	2.49	0.41
23:K:10:ARG:CB	23:K:14:THR:HB	2.35	0.41
23:K:33:LEU:H	23:K:33:LEU:HG	1.76	0.41
23:K:114:GLN:HA	23:K:117:SER:HB2	2.03	0.41
30:R:153:TYR:O	30:R:157:ARG:CB	2.69	0.41
31:S:91:MET:O	31:S:94:THR:OG1	2.32	0.41
23:k:212:ALA:HB2	23:k:235:GLU:HG2	2.03	0.41
27:o:11:GLY:CA	27:o:178:ILE:O	2.59	0.41
30:r:36:GLU:OE2	30:r:186:ARG:NH2	2.54	0.41
31:s:209:SER:OG	31:s:212:LYS:NZ	2.35	0.41
6:f:364:GLN:HG3	6:f:750:GLN:HE22	1.84	0.41
6:f:512:MET:HE1	6:f:554:TYR:HA	2.02	0.41
7:U:401:LYS:HB3	7:U:438:GLN:N	2.35	0.41
9:W:69:ALA:HB1	9:W:73:MET:HE3	2.03	0.41
11:Y:88:LEU:HB3	11:Y:104:MET:HE3	2.03	0.41
12:Z:221:PRO:C	12:Z:223:ASN:N	2.76	0.41
15:C:328:ILE:HG23	15:C:332:HIS:HD2	1.85	0.41
16:D:202:VAL:HG23	16:D:329:ARG:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:191:PHE:HE1	19:G:219:VAL:HG21	1.85	0.41
25:M:152:ASP:OD1	25:M:156:VAL:N	2.54	0.41
25:M:170:GLN:HA	25:M:173:LYS:HE2	2.02	0.41
25:M:230:ASP:OD1	25:M:230:ASP:N	2.53	0.41
32:T:179:ARG:HB3	26:n:29:ARG:HE	1.84	0.41
28:p:159:ASP:O	28:p:163:LEU:HB2	2.21	0.41
29:q:37:LYS:O	29:q:61:GLN:NE2	2.51	0.41
30:r:158:ARG:HH12	30:r:199:TYR:HB3	1.85	0.41
32:t:11:VAL:HG13	32:t:24:ALA:HB2	2.03	0.41
1:a:230:ARG:HE	1:a:233:LEU:HD22	1.85	0.41
3:c:290:VAL:O	3:c:294:SER:HB2	2.21	0.41
6:f:301:HIS:O	6:f:305:LEU:CB	2.59	0.41
6:f:402:ASN:ND2	6:f:406:GLY:O	2.53	0.41
7:U:179:TYR:HB2	7:U:182:LYS:HE2	2.02	0.41
8:V:80:LYS:C	8:V:82:LEU:N	2.79	0.41
9:W:101:VAL:HA	9:W:104:MET:HG2	2.03	0.41
9:W:407:ASP:OD2	10:X:382:GLU:O	2.35	0.41
10:X:202:CYS:H	10:X:203:PRO:CD	2.26	0.41
11:Y:317:GLY:N	11:Y:352:GLU:OE2	2.54	0.41
12:Z:201:LEU:HD23	12:Z:201:LEU:HA	1.90	0.41
15:C:158:ILE:HG22	15:C:162:LYS:HE3	2.02	0.41
18:F:215:LEU:HD22	18:F:217:ILE:HG12	2.02	0.41
19:G:6:SER:OG	19:G:7:ALA:N	2.53	0.41
23:K:236:GLU:HA	23:K:239:LYS:HE3	2.02	0.41
30:R:55:TRP:HZ3	30:R:86:MET:HB3	1.86	0.41
19:g:197:THR:O	19:g:201:CYS:HB3	2.21	0.41
21:i:8:ARG:HA	21:i:11:ILE:HD11	2.01	0.41
23:k:114:GLN:HA	23:k:117:SER:HB2	2.03	0.41
1:a:45:VAL:HG13	1:a:82:HIS:CE1	2.56	0.41
2:b:92:VAL:HA	12:Z:67:VAL:HG13	2.02	0.41
6:f:693:ALA:O	6:f:697:ILE:HB	2.21	0.41
8:V:78:HIS:CD2	8:V:81:GLN:HE21	2.38	0.41
8:V:89:LYS:HD3	8:V:92:ARG:NH1	2.35	0.41
8:V:211:TYR:HA	8:V:214:HIS:HD2	1.86	0.41
9:W:145:LEU:HD22	9:W:185:PHE:CZ	2.55	0.41
9:W:276:LEU:HD11	9:W:350:ARG:HD3	2.01	0.41
9:W:282:GLU:O	9:W:286:LEU:CB	2.68	0.41
10:X:252:LYS:O	10:X:256:LEU:HB2	2.20	0.41
10:X:405:GLN:O	10:X:409:LYS:HG2	2.21	0.41
13:A:264:ALA:HB2	13:A:272:ILE:HD11	2.03	0.41
13:A:306:LEU:HD11	13:A:312:ARG:HH11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:307:ASP:OD1	13:A:312:ARG:HG3	2.21	0.41
14:B:179:ALA:HB1	14:B:241:ASN:HA	2.02	0.41
14:B:237:LYS:HA	14:B:240:ALA:HB3	2.03	0.41
15:C:351:MET:HE2	15:C:362:VAL:HG21	2.02	0.41
16:D:205:TYR:O	16:D:332:GLU:HA	2.21	0.41
16:D:355:SER:OG	16:D:394:VAL:O	2.28	0.41
17:E:244:SER:HB2	18:F:300:LYS:HA	2.03	0.41
18:F:438:TYR:CE2	23:K:20:ARG:NE	2.89	0.41
25:M:194:ALA:HB1	25:M:235:ALA:HA	2.01	0.41
26:N:110:GLN:HG2	26:N:122:ARG:CZ	2.51	0.41
28:P:59:ASP:O	28:P:63:VAL:HB	2.21	0.41
28:P:159:ASP:O	28:P:163:LEU:HB2	2.21	0.41
28:P:191:GLU:HG3	28:P:193:ASP:H	1.85	0.41
30:R:55:TRP:CZ3	30:R:86:MET:HB3	2.55	0.41
31:S:27:THR:HB	31:S:40:SER:H	1.86	0.41
31:S:57:PHE:N	31:S:105:TYR:O	2.43	0.41
19:g:11:ARG:CG	19:g:23:TYR:HD2	2.32	0.41
19:g:20:GLY:O	19:g:21:ARG:CG	2.69	0.41
21:i:8:ARG:HB3	21:i:11:ILE:CD1	2.50	0.41
21:i:234:GLU:HA	21:i:237:ILE:HD12	2.02	0.41
22:j:116:GLN:HG2	23:k:83:ALA:HB3	2.03	0.41
25:m:5:THR:C	25:m:7:TYR:H	2.28	0.41
26:n:22:THR:N	26:n:25:TYR:O	2.40	0.41
30:r:153:TYR:O	30:r:157:ARG:CB	2.69	0.41
1:a:232:TRP:CZ2	1:a:256:GLY:HA3	2.56	0.41
3:c:261:GLU:HA	3:c:264:LYS:HG2	2.02	0.41
6:f:76:GLU:OE1	6:f:79:ARG:NH2	2.54	0.41
6:f:391:LEU:HD12	6:f:417:ILE:HD11	2.02	0.41
6:f:675:PHE:CG	6:f:694:LEU:HD23	2.56	0.41
6:f:791:VAL:HA	6:f:794:ALA:HB3	2.03	0.41
7:U:493:VAL:HA	7:U:497:LEU:HD13	2.02	0.41
9:W:240:TYR:HD1	9:W:276:LEU:HB3	1.86	0.41
10:X:164:ALA:O	10:X:168:GLU:HB2	2.20	0.41
10:X:208:ALA:HB2	10:X:238:GLY:HA3	2.02	0.41
11:Y:36:ALA:O	11:Y:40:GLU:HB3	2.21	0.41
16:D:71:GLU:HA	16:D:74:HIS:HD2	1.86	0.41
16:D:83:GLN:HB3	16:D:140:VAL:HG11	2.02	0.41
18:F:233:LYS:HG2	18:F:354:PHE:CE2	2.56	0.41
18:F:340:PRO:O	18:F:344:ARG:HG3	2.21	0.41
24:L:212:ILE:O	24:L:223:ILE:HA	2.21	0.41
25:M:92:ARG:NH1	32:T:76:LEU:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:129:ALA:H	20:h:127:VAL:CG1	2.34	0.41
20:h:8:PHE:HB2	21:i:126:GLY:O	2.21	0.41
20:h:60:ARG:O	20:h:63:HIS:NE2	2.54	0.41
21:i:95:GLN:HG3	28:p:69:PHE:CE1	2.55	0.41
24:l:45:VAL:HG11	24:l:188:VAL:HG22	2.03	0.41
24:l:212:ILE:O	24:l:223:ILE:HA	2.21	0.41
25:m:100:SER:O	32:t:65:GLN:NE2	2.53	0.41
26:n:7:GLN:HB3	26:n:111:VAL:HG23	2.03	0.41
32:t:9:THR:H	32:t:41:ARG:NH2	2.19	0.41
2:b:125:VAL:HA	2:b:128:ALA:HB3	2.02	0.40
4:d:72:GLU:HA	4:d:75:MET:HB3	2.03	0.40
4:d:136:PRO:HA	4:d:139:LEU:HB3	2.02	0.40
6:f:460:ASP:OD1	6:f:460:ASP:N	2.54	0.40
6:f:475:ASN:HA	6:f:478:ARG:HB3	2.03	0.40
6:f:691:PRO:HA	6:f:694:LEU:HB3	2.02	0.40
7:U:133:ILE:HA	7:U:136:LYS:HB3	2.03	0.40
8:V:263:LEU:HB3	8:V:264:TYR:H	1.72	0.40
9:W:117:ASP:HA	9:W:120:ILE:HG22	2.03	0.40
9:W:408:ARG:O	9:W:410:ALA:N	2.54	0.40
9:W:430:GLN:O	9:W:434:SER:HB3	2.21	0.40
12:Z:195:VAL:HG13	12:Z:199:LYS:HG3	2.02	0.40
13:A:365:GLU:HG2	13:A:367:ASP:H	1.86	0.40
14:B:287:ILE:HG13	14:B:331:THR:HG22	2.02	0.40
17:E:288:ALA:O	17:E:291:ARG:NH2	2.54	0.40
19:G:21:ARG:NE	19:G:21:ARG:CA	2.84	0.40
19:G:197:THR:O	19:G:201:CYS:HB3	2.21	0.40
19:G:208:ILE:HB	19:G:210:PHE:HD1	1.86	0.40
21:I:73:ALA:HB3	21:I:137:ILE:HD11	2.03	0.40
26:N:40:ARG:NH2	26:N:181:GLU:O	2.53	0.40
27:O:63:LEU:O	27:O:67:SER:OG	2.39	0.40
22:j:4:ASP:O	22:j:18:GLN:NE2	2.38	0.40
23:k:236:GLU:HA	23:k:239:LYS:HE3	2.02	0.40
26:n:110:GLN:HG2	26:n:122:ARG:CZ	2.51	0.40
27:o:172:ASN:ND2	27:o:188:PRO:HA	2.36	0.40
1:a:190:VAL:HA	1:a:193:GLN:HB2	2.01	0.40
6:f:333:LEU:HD23	6:f:338:ASP:CB	2.51	0.40
7:U:493:VAL:HG11	7:U:519:VAL:HG11	2.01	0.40
8:V:160:LEU:HA	8:V:163:VAL:HG23	2.02	0.40
9:W:303:LYS:O	9:W:307:LYS:CB	2.69	0.40
9:W:357:ARG:O	9:W:361:HIS:CB	2.63	0.40
10:X:97:LEU:HD22	10:X:106:GLU:HG2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:294:TYR:O	11:Y:298:GLU:HB2	2.21	0.40
17:E:313:LEU:O	17:E:317:ALA:HB2	2.21	0.40
18:F:392:ASN:OD1	18:F:395:GLN:N	2.48	0.40
20:H:120:GLU:C	20:H:124:SER:OG	2.63	0.40
23:K:78:MET:HA	23:K:141:LEU:HD23	2.03	0.40
23:K:236:GLU:HA	23:K:239:LYS:HG2	2.04	0.40
26:N:7:GLN:HB3	26:N:111:VAL:HG23	2.03	0.40
26:N:90:TYR:CA	26:N:92:GLU:OE2	2.69	0.40
20:h:167:TYR:O	20:h:171:LYS:CB	2.67	0.40
21:i:68:LEU:HA	21:i:91:ARG:HE	1.87	0.40
21:i:208:ALA:HA	21:i:211:VAL:HG22	2.02	0.40
23:k:236:GLU:HA	23:k:239:LYS:HG2	2.04	0.40
28:p:59:ASP:O	28:p:63:VAL:HB	2.20	0.40
28:p:191:GLU:HG3	28:p:193:ASP:H	1.85	0.40
1:a:81:LEU:HA	1:a:84:VAL:HG12	2.03	0.40
3:c:31:VAL:HB	3:c:205:ILE:HG13	2.02	0.40
4:d:36:LEU:N	4:d:37:PRO:HD2	2.36	0.40
6:f:629:LYS:HE2	6:f:660:ILE:HG21	2.04	0.40
6:f:780:PRO:HB2	6:f:800:LEU:HG	2.02	0.40
9:W:79:GLU:HB3	9:W:130:MET:HE2	2.03	0.40
9:W:167:GLN:HG3	9:W:168:GLU:HG3	2.04	0.40
9:W:312:MET:HE1	9:W:364:ARG:HB2	2.03	0.40
9:W:400:LYS:HB2	10:X:339:ILE:HD13	2.03	0.40
11:Y:60:SER:OG	11:Y:61:LEU:N	2.53	0.40
11:Y:298:GLU:HA	11:Y:301:ILE:HG22	2.03	0.40
12:Z:144:VAL:O	12:Z:152:SER:HB3	2.21	0.40
15:C:250:GLU:HA	15:C:293:MET:HE3	2.03	0.40
16:D:151:ILE:HD11	16:D:229:ARG:CZ	2.52	0.40
16:D:369:LYS:HZ3	16:D:369:LYS:C	2.14	0.40
17:E:100:LEU:HD23	17:E:107:ILE:HA	2.02	0.40
17:E:182:LEU:HA	17:E:185:ARG:HB2	2.02	0.40
18:F:368:ILE:HG12	18:F:371:ARG:HH22	1.86	0.40
20:H:60:ARG:O	20:H:63:HIS:NE2	2.55	0.40
25:M:66:LEU:HD13	25:M:214:SER:HB2	2.03	0.40
27:O:18:THR:OG1	27:O:29:LYS:O	2.38	0.40
28:P:126:LEU:HD12	28:P:127:ILE:HG23	2.02	0.40
32:T:9:THR:O	32:T:41:ARG:NH2	2.51	0.40
32:T:27:LEU:HD11	32:T:34:ALA:HB1	2.02	0.40
23:k:70:ILE:HA	23:k:93:ARG:HE	1.87	0.40
31:s:148:LEU:HD23	31:s:178:VAL:HG12	2.03	0.40
2:b:53:THR:HG22	2:b:59:GLU:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:137:ASN:HB3	2:b:167:GLY:HA3	2.03	0.40
6:f:590:PHE:HA	6:f:593:THR:HG22	2.04	0.40
7:U:543:LYS:HG2	7:U:546:ARG:HH22	1.86	0.40
7:U:616:ARG:HH21	7:U:647:HIS:HA	1.86	0.40
8:V:400:HIS:HA	8:V:403:ILE:HG22	2.03	0.40
9:W:183:VAL:HA	9:W:186:ILE:HG22	2.03	0.40
11:Y:377:LEU:O	11:Y:381:GLN:HG3	2.21	0.40
15:C:188:LEU:HD13	15:C:317:PHE:HZ	1.86	0.40
17:E:50:LEU:HB3	18:F:82:VAL:HG21	2.03	0.40
17:E:282:PRO:HB2	17:E:388:PRO:HB3	2.04	0.40
19:G:16:PHE:CE2	20:H:128:ARG:HB2	2.56	0.40
21:I:109:GLN:O	21:I:113:ALA:HB2	2.22	0.40
26:N:38:HIS:HB3	26:N:41:ILE:HB	2.03	0.40
19:g:193:GLN:OE1	19:g:197:THR:HG21	2.21	0.40
26:n:38:HIS:HB3	26:n:41:ILE:HB	2.03	0.40
26:n:136:TYR:HE2	32:t:33:LEU:HD11	1.87	0.40
28:p:101:GLY:O	29:q:93:ARG:NH1	2.51	0.40
31:s:69:GLU:HA	31:s:72:LEU:HD12	2.04	0.40
1:a:358:THR:O	1:a:362:SER:CB	2.69	0.40
1:a:358:THR:O	1:a:362:SER:HB3	2.22	0.40
6:f:517:VAL:O	6:f:521:ALA:HB2	2.22	0.40
8:V:210:CYS:HA	8:V:213:TYR:HD2	1.86	0.40
8:V:313:LEU:HD13	8:V:332:LEU:HD13	2.03	0.40
8:V:338:LEU:HD22	8:V:397:ARG:HG3	2.02	0.40
11:Y:84:LEU:HD22	11:Y:104:MET:SD	2.61	0.40
17:E:101:ASP:HB3	17:E:105:LEU:N	2.36	0.40
19:G:97:GLU:HA	19:G:100:ASN:HD22	1.87	0.40
21:I:123:GLN:NE2	22:J:125:ARG:HH21	2.19	0.40
23:K:192:LYS:HA	23:K:195:ILE:HD12	2.02	0.40
25:M:99:ARG:HH21	25:M:105:ASN:HA	1.86	0.40
19:g:126:THR:O	20:h:128:ARG:NH1	2.41	0.40
21:i:73:ALA:HB3	21:i:137:ILE:HD11	2.03	0.40
32:t:4:PRO:HG3	32:t:107:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	371/376 (99%)	334 (90%)	36 (10%)	1 (0%)	36	71
2	b	189/377 (50%)	165 (87%)	23 (12%)	1 (0%)	24	63
3	c	274/309 (89%)	230 (84%)	44 (16%)	0	100	100
4	d	255/349 (73%)	220 (86%)	32 (12%)	3 (1%)	10	42
5	e	36/70 (51%)	27 (75%)	8 (22%)	1 (3%)	4	24
6	f	669/908 (74%)	582 (87%)	86 (13%)	1 (0%)	48	83
7	U	798/953 (84%)	721 (90%)	76 (10%)	1 (0%)	48	83
8	V	471/533 (88%)	400 (85%)	70 (15%)	1 (0%)	43	78
9	W	454/456 (100%)	392 (86%)	58 (13%)	4 (1%)	14	49
10	X	378/422 (90%)	336 (89%)	38 (10%)	4 (1%)	11	45
11	Y	376/389 (97%)	329 (88%)	47 (12%)	0	100	100
12	Z	284/324 (88%)	245 (86%)	37 (13%)	2 (1%)	18	55
13	A	376/433 (87%)	328 (87%)	46 (12%)	2 (0%)	24	63
14	B	366/440 (83%)	324 (88%)	36 (10%)	6 (2%)	7	37
15	C	359/398 (90%)	317 (88%)	40 (11%)	2 (1%)	21	58
16	D	378/418 (90%)	324 (86%)	41 (11%)	13 (3%)	3	20
17	E	373/403 (93%)	330 (88%)	43 (12%)	0	100	100
18	F	372/439 (85%)	329 (88%)	41 (11%)	2 (0%)	24	63
19	G	237/245 (97%)	204 (86%)	29 (12%)	4 (2%)	7	35
19	g	238/245 (97%)	207 (87%)	28 (12%)	3 (1%)	9	41
20	H	228/233 (98%)	213 (93%)	12 (5%)	3 (1%)	9	41
20	h	230/233 (99%)	213 (93%)	14 (6%)	3 (1%)	9	41
21	I	246/260 (95%)	220 (89%)	22 (9%)	4 (2%)	7	37
21	i	248/260 (95%)	222 (90%)	24 (10%)	2 (1%)	16	52
22	J	237/247 (96%)	219 (92%)	17 (7%)	1 (0%)	30	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	j	237/247 (96%)	221 (93%)	16 (7%)	0	100	100
23	K	224/240 (93%)	202 (90%)	22 (10%)	0	100	100
23	k	224/240 (93%)	202 (90%)	22 (10%)	0	100	100
24	L	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
24	l	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
25	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
25	m	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
26	N	189/238 (79%)	174 (92%)	13 (7%)	2 (1%)	11	45
26	n	189/238 (79%)	176 (93%)	12 (6%)	1 (0%)	24	63
27	O	218/276 (79%)	208 (95%)	10 (5%)	0	100	100
27	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	P	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
28	p	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
29	Q	197/201 (98%)	179 (91%)	18 (9%)	0	100	100
29	q	197/201 (98%)	179 (91%)	18 (9%)	0	100	100
30	R	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
30	r	199/262 (76%)	188 (94%)	11 (6%)	0	100	100
31	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
31	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
32	T	213/263 (81%)	200 (94%)	13 (6%)	0	100	100
32	t	213/263 (81%)	200 (94%)	13 (6%)	0	100	100
All	All	12934/14859 (87%)	11629 (90%)	1238 (10%)	67 (0%)	26	63

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	23	PRO
4	d	34	ASN
9	W	410	ALA
10	X	363	ARG
10	X	386	ILE
12	Z	221	PRO
14	B	435	PRO
15	C	91	PRO
16	D	125	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	153	MET
16	D	367	PRO
16	D	409	LYS
16	D	410	ASP
16	D	417	TYR
18	F	344	ARG
18	F	437	TYR
19	G	7	ALA
20	H	10	LEU
21	I	126	GLY
22	J	183	THR
26	N	92	GLU
19	g	8	GLY
19	g	11	ARG
20	h	10	LEU
21	i	126	GLY
12	Z	144	VAL
14	B	438	LEU
19	G	8	GLY
19	G	9	PHE
20	H	9	SER
20	H	127	VAL
19	g	7	ALA
20	h	9	SER
20	h	126	GLY
1	a	187	ASP
6	f	326	LEU
8	V	81	GLN
9	W	313	GLU
10	X	202	CYS
14	B	432	GLU
16	D	369	LYS
16	D	412	GLN
16	D	414	HIS
19	G	21	ARG
7	U	561	GLU
9	W	314	LEU
9	W	409	LEU
14	B	356	PRO
16	D	126	PRO
16	D	150	SER
16	D	299	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	I	14	PRO
26	n	19	ARG
4	d	35	PHE
10	X	201	TYR
14	B	377	ASP
21	I	10	THR
26	N	19	ARG
21	i	10	THR
5	e	4	LYS
13	A	109	PRO
14	B	436	GLU
16	D	155	THR
21	I	16	GLY
4	d	36	LEU
15	C	89	VAL
13	A	310	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	333/336 (99%)	333 (100%)	0	100	100
2	b	166/312 (53%)	164 (99%)	2 (1%)	63	73
3	c	243/267 (91%)	242 (100%)	1 (0%)	84	83
4	d	230/293 (78%)	228 (99%)	2 (1%)	70	77
5	e	37/63 (59%)	35 (95%)	2 (5%)	20	42
6	f	579/763 (76%)	577 (100%)	2 (0%)	86	84
7	U	685/816 (84%)	678 (99%)	7 (1%)	68	76
8	V	409/459 (89%)	401 (98%)	8 (2%)	48	66
9	W	415/416 (100%)	411 (99%)	4 (1%)	68	76
10	X	326/362 (90%)	322 (99%)	4 (1%)	63	73
11	Y	333/344 (97%)	331 (99%)	2 (1%)	78	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	257/295 (87%)	254 (99%)	3 (1%)	63	73
13	A	297/372 (80%)	296 (100%)	1 (0%)	86	84
14	B	300/385 (78%)	294 (98%)	6 (2%)	48	66
15	C	314/346 (91%)	313 (100%)	1 (0%)	86	84
16	D	332/366 (91%)	319 (96%)	13 (4%)	28	50
17	E	298/353 (84%)	297 (100%)	1 (0%)	86	84
18	F	296/379 (78%)	290 (98%)	6 (2%)	48	66
19	G	192/209 (92%)	185 (96%)	7 (4%)	31	52
19	g	193/209 (92%)	187 (97%)	6 (3%)	35	56
20	H	162/190 (85%)	157 (97%)	5 (3%)	35	56
20	h	164/190 (86%)	159 (97%)	5 (3%)	36	57
21	I	191/220 (87%)	189 (99%)	2 (1%)	68	76
21	i	193/220 (88%)	190 (98%)	3 (2%)	55	69
22	J	152/210 (72%)	152 (100%)	0	100	100
22	j	152/210 (72%)	151 (99%)	1 (1%)	76	79
23	K	187/202 (93%)	182 (97%)	5 (3%)	39	60
23	k	186/202 (92%)	182 (98%)	4 (2%)	45	64
24	L	198/229 (86%)	198 (100%)	0	100	100
24	l	198/229 (86%)	197 (100%)	1 (0%)	81	82
25	M	192/211 (91%)	192 (100%)	0	100	100
25	m	192/211 (91%)	192 (100%)	0	100	100
26	N	148/180 (82%)	146 (99%)	2 (1%)	59	71
26	n	148/180 (82%)	147 (99%)	1 (1%)	76	79
27	O	177/227 (78%)	176 (99%)	1 (1%)	78	81
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	172/173 (99%)	172 (100%)	0	100	100
28	p	172/173 (99%)	172 (100%)	0	100	100
29	Q	164/171 (96%)	163 (99%)	1 (1%)	78	81
29	q	164/171 (96%)	163 (99%)	1 (1%)	78	81
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	S	174/198 (88%)	174 (100%)	0	100	100
31	s	174/198 (88%)	174 (100%)	0	100	100
32	T	175/214 (82%)	175 (100%)	0	100	100
32	t	175/214 (82%)	175 (100%)	0	100	100
All	All	10728/12597 (85%)	10618 (99%)	110 (1%)	65	76

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	22	LEU
2	b	54	LEU
3	c	62	VAL
4	d	36	LEU
4	d	41	THR
5	e	42	ASN
5	e	43	TRP
6	f	88	SER
6	f	801	VAL
7	U	223	LEU
7	U	472	ILE
7	U	529	ILE
7	U	554	LEU
7	U	561	GLU
7	U	629	THR
7	U	765	VAL
8	V	79	VAL
8	V	80	LYS
8	V	86	VAL
8	V	224	LEU
8	V	227	VAL
8	V	328	VAL
8	V	346	LEU
8	V	347	GLN
9	W	138	VAL
9	W	333	LEU
9	W	408	ARG
9	W	409	LEU
10	X	216	ILE
10	X	217	ILE
10	X	341	PRO
10	X	356	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	157	ILE
11	Y	357	ASN
12	Z	108	ILE
12	Z	220	LEU
12	Z	266	ILE
13	A	403	ILE
14	B	125	THR
14	B	430	LYS
14	B	431	GLN
14	B	432	GLU
14	B	438	LEU
14	B	440	LEU
15	C	131	VAL
16	D	123	LEU
16	D	124	LEU
16	D	150	SER
16	D	151	ILE
16	D	367	PRO
16	D	368	ASP
16	D	369	LYS
16	D	405	THR
16	D	406	VAL
16	D	408	LYS
16	D	409	LYS
16	D	412	GLN
16	D	415	GLU
17	E	105	LEU
18	F	198	LEU
18	F	345	SER
18	F	428	GLN
18	F	430	LYS
18	F	431	LYS
18	F	432	LYS
19	G	19	GLU
19	G	21	ARG
19	G	22	LEU
19	G	192	GLU
19	G	193	GLN
19	G	215	ILE
19	G	224	ASN
20	H	7	SER
20	H	9	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	H	123	GLN
20	H	124	SER
20	H	127	VAL
21	I	11	ILE
21	I	15	GLU
23	K	9	ASP
23	K	10	ARG
23	K	20	ARG
23	K	21	LEU
23	K	22	PHE
26	N	92	GLU
26	N	93	ASP
27	O	201	ARG
29	Q	140	LEU
19	g	11	ARG
19	g	19	GLU
19	g	192	GLU
19	g	193	GLN
19	g	215	ILE
19	g	222	VAL
20	h	7	SER
20	h	8	PHE
20	h	9	SER
20	h	124	SER
20	h	127	VAL
21	i	11	ILE
21	i	15	GLU
21	i	17	ARG
22	j	7	ILE
23	k	9	ASP
23	k	20	ARG
23	k	21	LEU
23	k	22	PHE
24	l	184	LEU
26	n	92	GLU
29	q	140	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	9	GLN
1	a	35	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	46	GLN
1	a	62	ASN
1	a	86	GLN
1	a	168	ASN
1	a	193	GLN
1	a	227	ASN
1	a	231	GLN
1	a	257	GLN
1	a	370	GLN
2	b	79	GLN
2	b	161	ASN
3	c	101	GLN
3	c	176	GLN
3	c	214	GLN
3	c	219	ASN
3	c	254	ASN
3	c	256	ASN
4	d	4	GLN
4	d	96	HIS
4	d	102	ASN
4	d	135	HIS
6	f	102	HIS
6	f	180	GLN
6	f	213	GLN
6	f	325	GLN
6	f	327	ASN
6	f	428	GLN
6	f	452	ASN
6	f	457	ASN
6	f	493	ASN
6	f	540	GLN
6	f	565	ASN
6	f	650	GLN
7	U	111	GLN
7	U	115	ASN
7	U	192	GLN
7	U	345	ASN
7	U	346	ASN
7	U	355	ASN
7	U	452	ASN
7	U	491	GLN
7	U	768	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	880	ASN
8	V	81	GLN
8	V	118	GLN
8	V	199	ASN
8	V	347	GLN
8	V	365	GLN
8	V	453	HIS
8	V	473	GLN
9	W	106	GLN
9	W	107	GLN
9	W	235	GLN
9	W	257	GLN
9	W	283	GLN
9	W	440	ASN
9	W	454	ASN
10	X	127	GLN
10	X	148	HIS
10	X	170	GLN
10	X	296	ASN
10	X	349	HIS
11	Y	136	HIS
11	Y	363	ASN
11	Y	367	GLN
12	Z	243	GLN
13	A	150	HIS
13	A	197	HIS
13	A	247	GLN
13	A	293	ASN
13	A	305	GLN
14	B	241	ASN
14	B	277	HIS
15	C	48	GLN
15	C	171	HIS
15	C	288	ASN
15	C	332	HIS
16	D	49	GLN
16	D	74	HIS
16	D	83	GLN
16	D	133	HIS
16	D	173	GLN
16	D	353	ASN
16	D	412	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	D	414	HIS
17	E	86	GLN
17	E	194	ASN
17	E	263	GLN
17	E	323	HIS
17	E	339	ASN
17	E	364	GLN
18	F	83	ASN
18	F	218	GLN
19	G	100	ASN
19	G	123	GLN
19	G	127	GLN
20	H	95	GLN
20	H	119	GLN
20	H	123	GLN
20	H	166	ASN
21	I	69	ASN
21	I	119	GLN
21	I	146	GLN
22	J	54	GLN
22	J	154	HIS
22	J	175	ASN
23	K	41	GLN
23	K	98	ASN
23	K	114	GLN
23	K	152	GLN
23	K	164	GLN
23	K	214	ASN
23	K	224	GLN
24	L	8	ASN
24	L	53	GLN
24	L	117	GLN
25	M	32	ASN
25	M	110	HIS
26	N	66	HIS
27	O	62	ASN
27	O	91	GLN
29	Q	101	ASN
29	Q	168	GLN
30	R	38	ASN
30	R	119	ASN
31	S	159	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	T	69	GLN
32	T	188	GLN
19	g	224	ASN
20	h	119	GLN
20	h	123	GLN
20	h	166	ASN
21	i	69	ASN
21	i	119	GLN
21	i	146	GLN
21	i	149	GLN
22	j	85	ASN
22	j	92	GLN
22	j	122	ASN
22	j	154	HIS
22	j	175	ASN
23	k	114	GLN
23	k	152	GLN
23	k	164	GLN
23	k	214	ASN
23	k	224	GLN
24	l	8	ASN
24	l	53	GLN
24	l	90	GLN
24	l	117	GLN
24	l	152	ASN
25	m	32	ASN
27	o	62	ASN
27	o	91	GLN
27	o	193	ASN
28	p	93	ASN
29	q	101	ASN
29	q	132	HIS
29	q	168	GLN
30	r	38	ASN
31	s	159	GLN
32	t	2	GLN
32	t	69	GLN
32	t	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	ATP	E	401	-	32,33,33	2.65	3 (9%)	48,52,52	0.44	0
34	ATP	D	501	-	32,33,33	2.60	1 (3%)	48,52,52	0.44	0
34	ATP	A	501	-	32,33,33	2.60	1 (3%)	48,52,52	0.52	0
34	ATP	F	501	-	32,33,33	2.60	1 (3%)	48,52,52	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	E	401	-	-	7/22/38/38	0/3/3/3
34	ATP	D	501	-	-	6/22/38/38	0/3/3/3
34	ATP	A	501	-	-	7/22/38/38	0/3/3/3
34	ATP	F	501	-	-	9/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	ATP	PG-O1G	14.44	1.95	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	501	ATP	PG-O1G	14.38	1.95	1.50
34	A	501	ATP	PG-O1G	14.37	1.95	1.50
34	E	401	ATP	PG-O1G	14.35	1.95	1.50
34	E	401	ATP	PB-O3A	-2.76	1.56	1.59
34	E	401	ATP	PB-O3B	-2.13	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

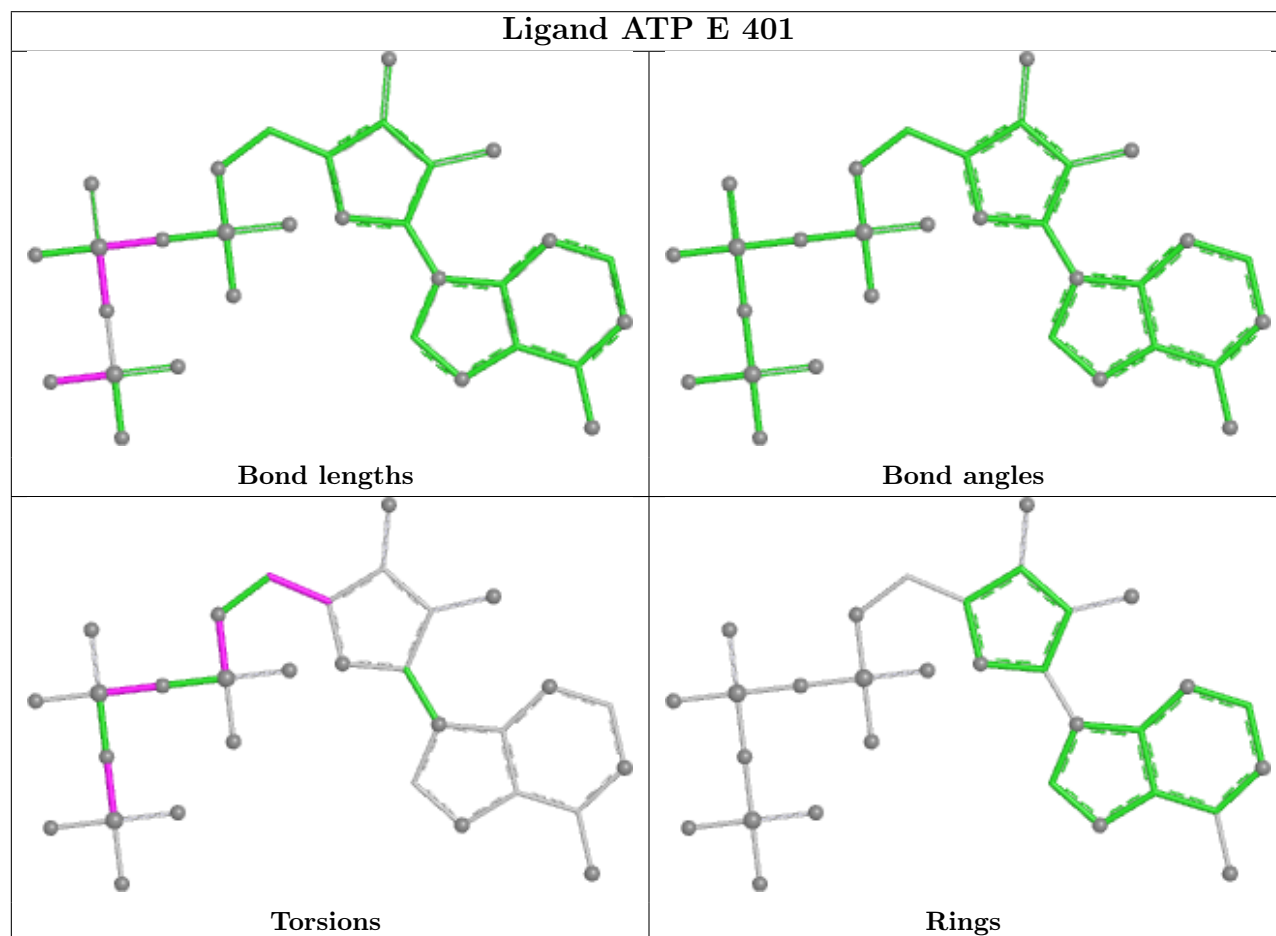
Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C5'-O5'-PA-O3A
34	D	501	ATP	C5'-O5'-PA-O1A
34	E	401	ATP	PB-O3B-PG-O2G
34	E	401	ATP	PB-O3B-PG-O3G
34	E	401	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	PB-O3B-PG-O2G
34	F	501	ATP	C5'-O5'-PA-O1A
34	F	501	ATP	C5'-O5'-PA-O3A
34	A	501	ATP	O4'-C4'-C5'-O5'
34	A	501	ATP	C3'-C4'-C5'-O5'
34	D	501	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	O4'-C4'-C5'-O5'
34	D	501	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	C3'-C4'-C5'-O5'
34	F	501	ATP	C4'-C5'-O5'-PA
34	D	501	ATP	C5'-O5'-PA-O2A
34	D	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	C5'-O5'-PA-O2A
34	A	501	ATP	C4'-C5'-O5'-PA
34	D	501	ATP	C4'-C5'-O5'-PA
34	E	401	ATP	PA-O3A-PB-O1B
34	F	501	ATP	PB-O3B-PG-O1G
34	F	501	ATP	PB-O3A-PA-O2A
34	A	501	ATP	PG-O3B-PB-O1B
34	A	501	ATP	PG-O3B-PB-O2B

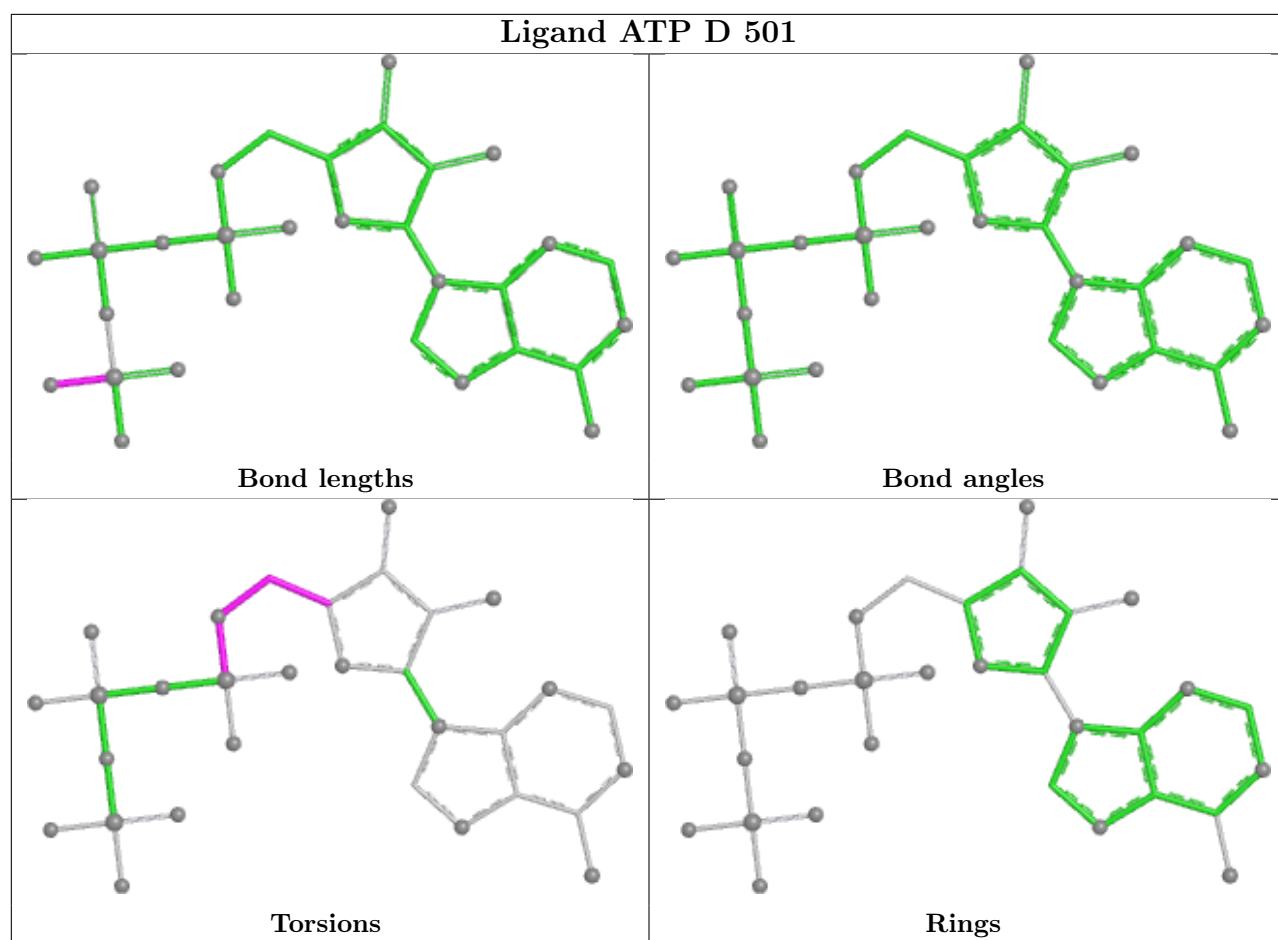
There are no ring outliers.

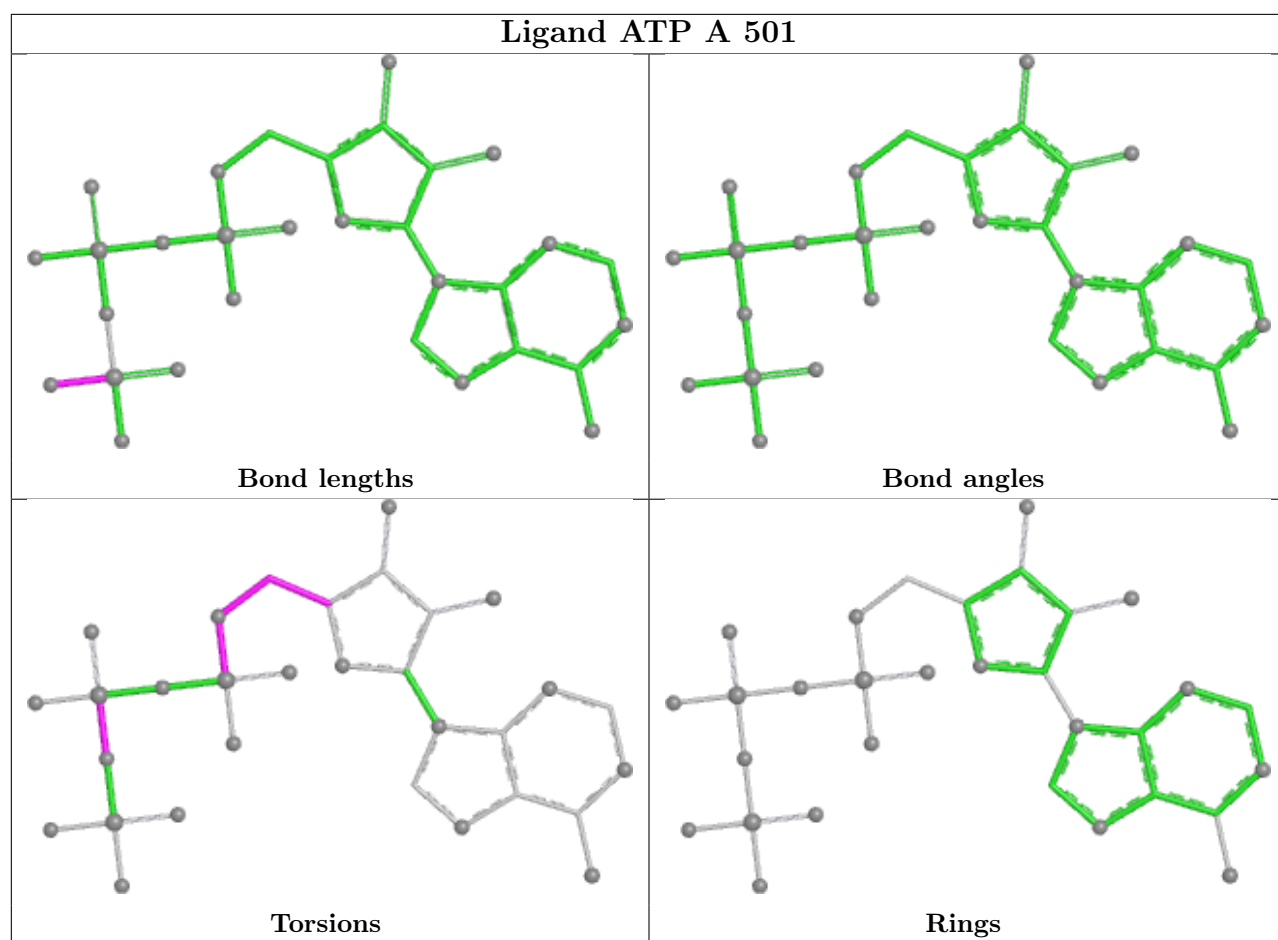
4 monomers are involved in 14 short contacts:

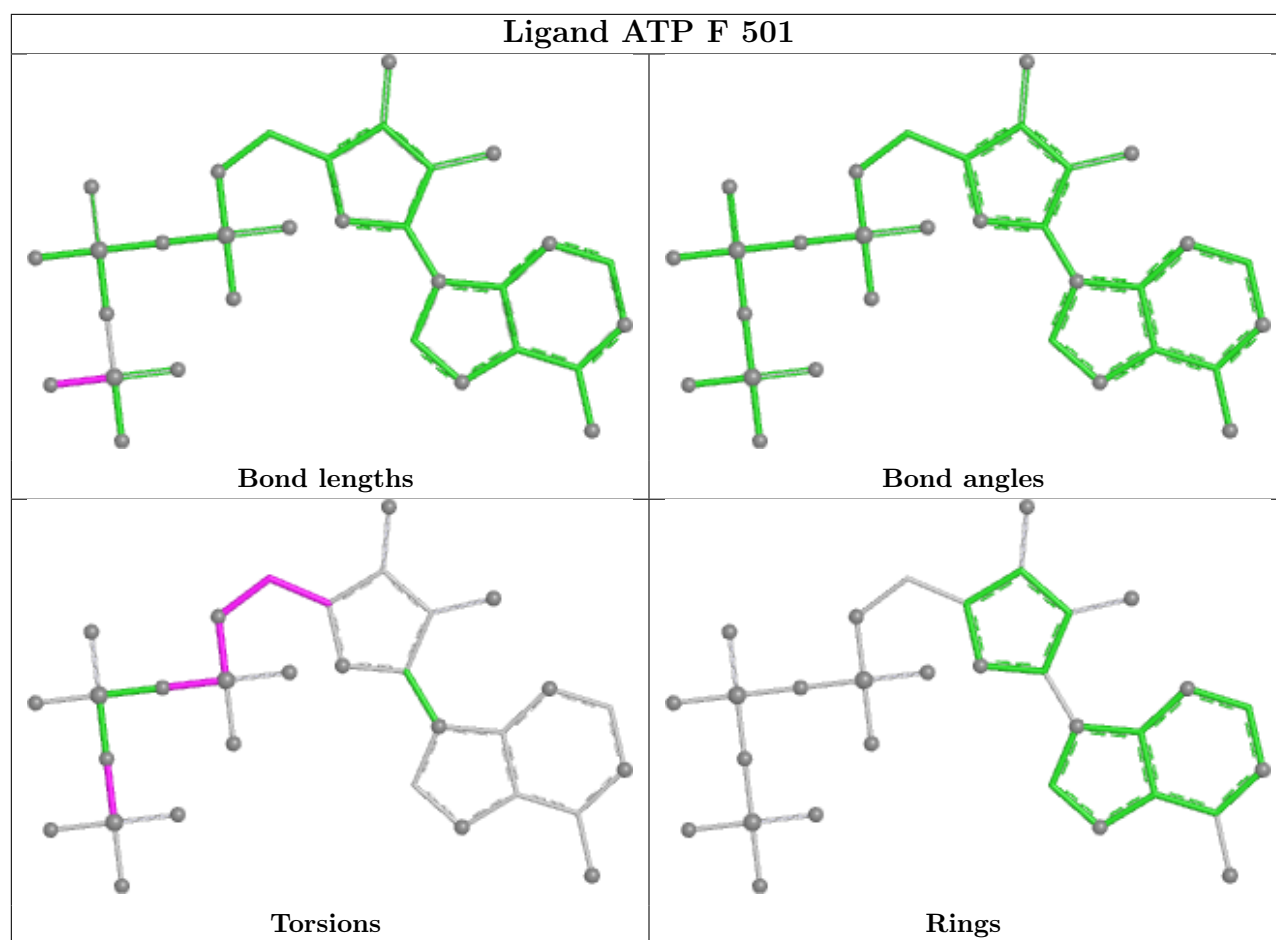
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	401	ATP	6	0
34	D	501	ATP	2	0
34	A	501	ATP	4	0
34	F	501	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

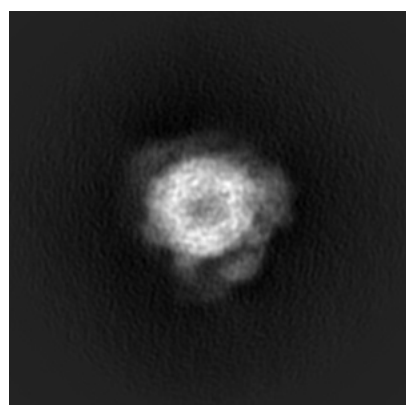
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14210. These allow visual inspection of the internal detail of the map and identification of artifacts.

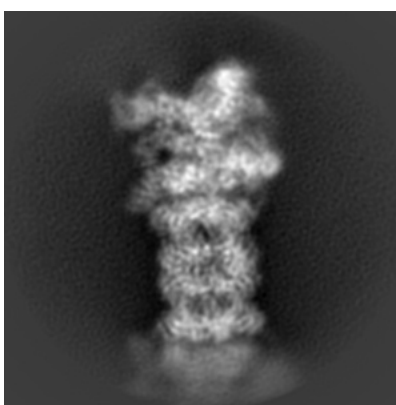
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

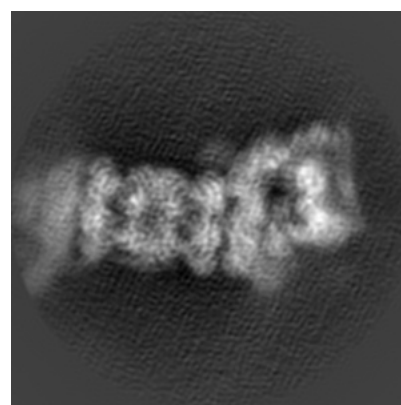
6.1.1 Primary map



X



Y

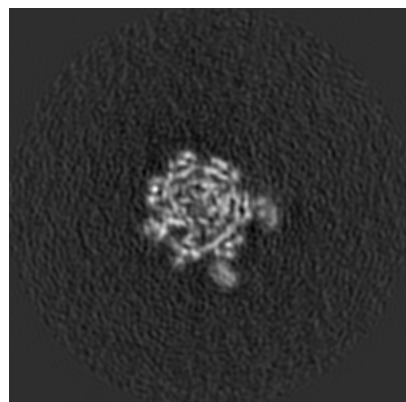


Z

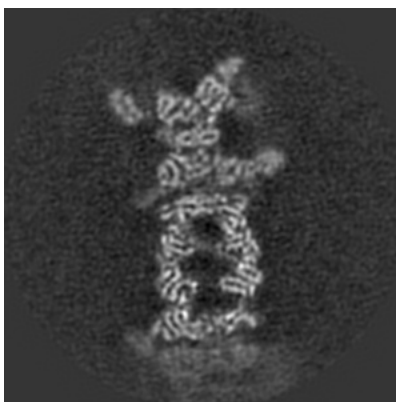
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

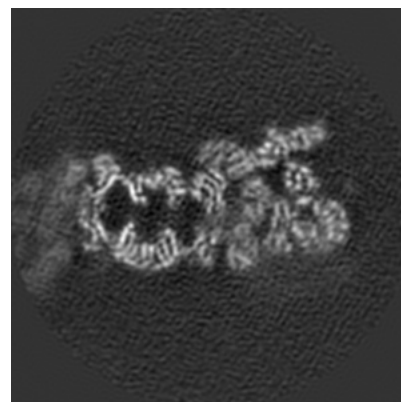
6.2.1 Primary map



X Index: 160



Y Index: 160

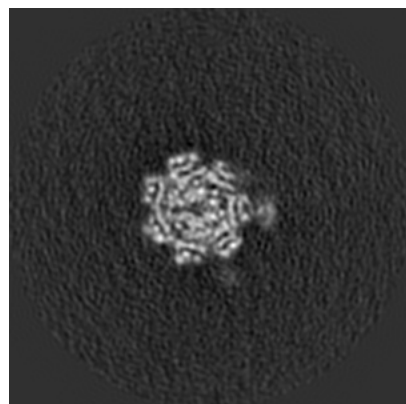


Z Index: 160

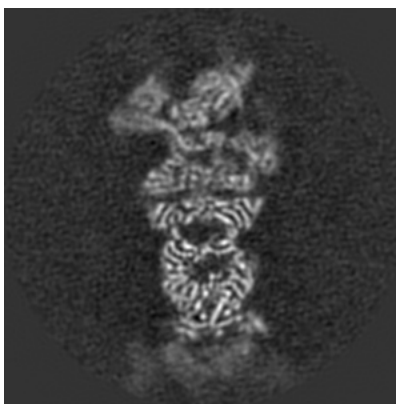
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

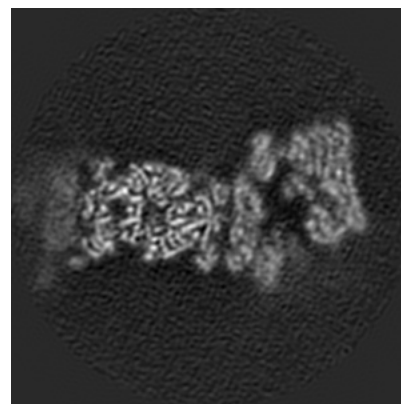
6.3.1 Primary map



X Index: 156



Y Index: 140

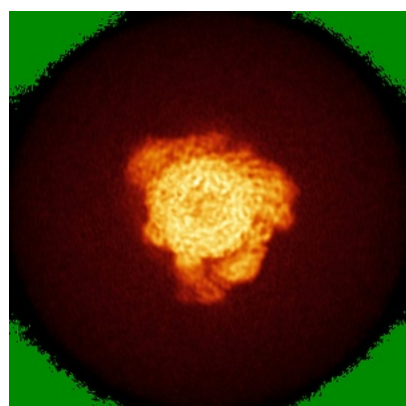


Z Index: 181

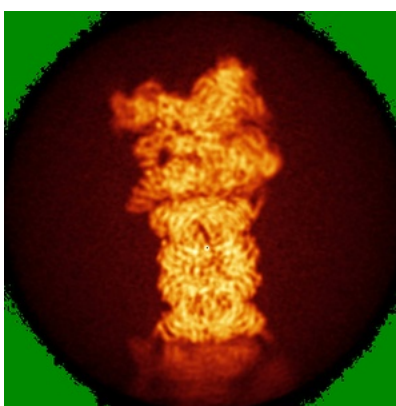
The images above show the largest variance slices of the map in three orthogonal directions.

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

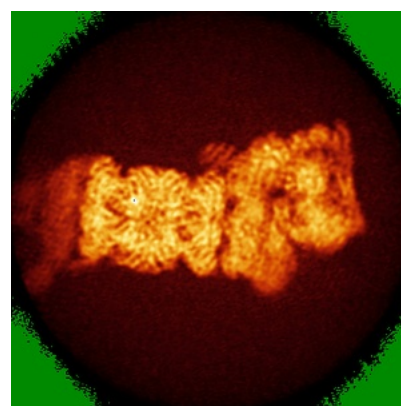
6.4.1 Primary map



X



Y

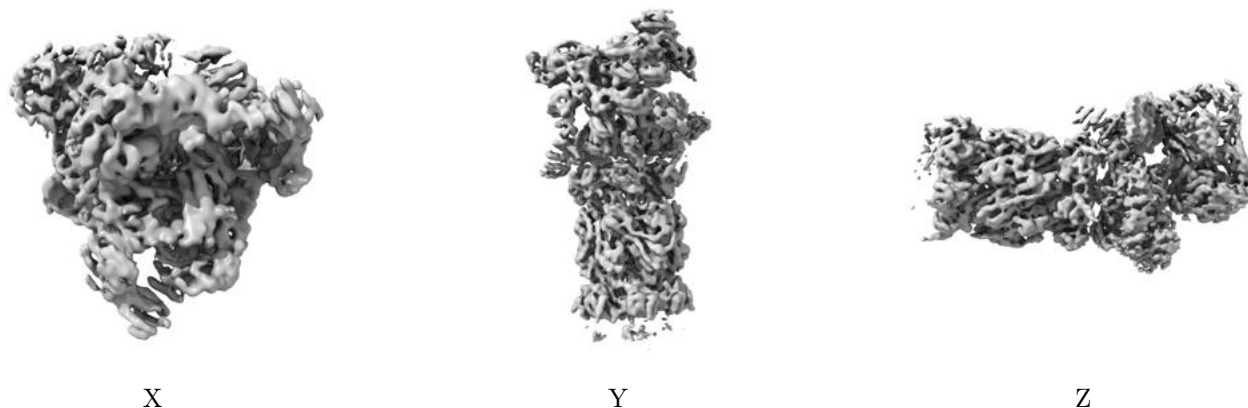


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

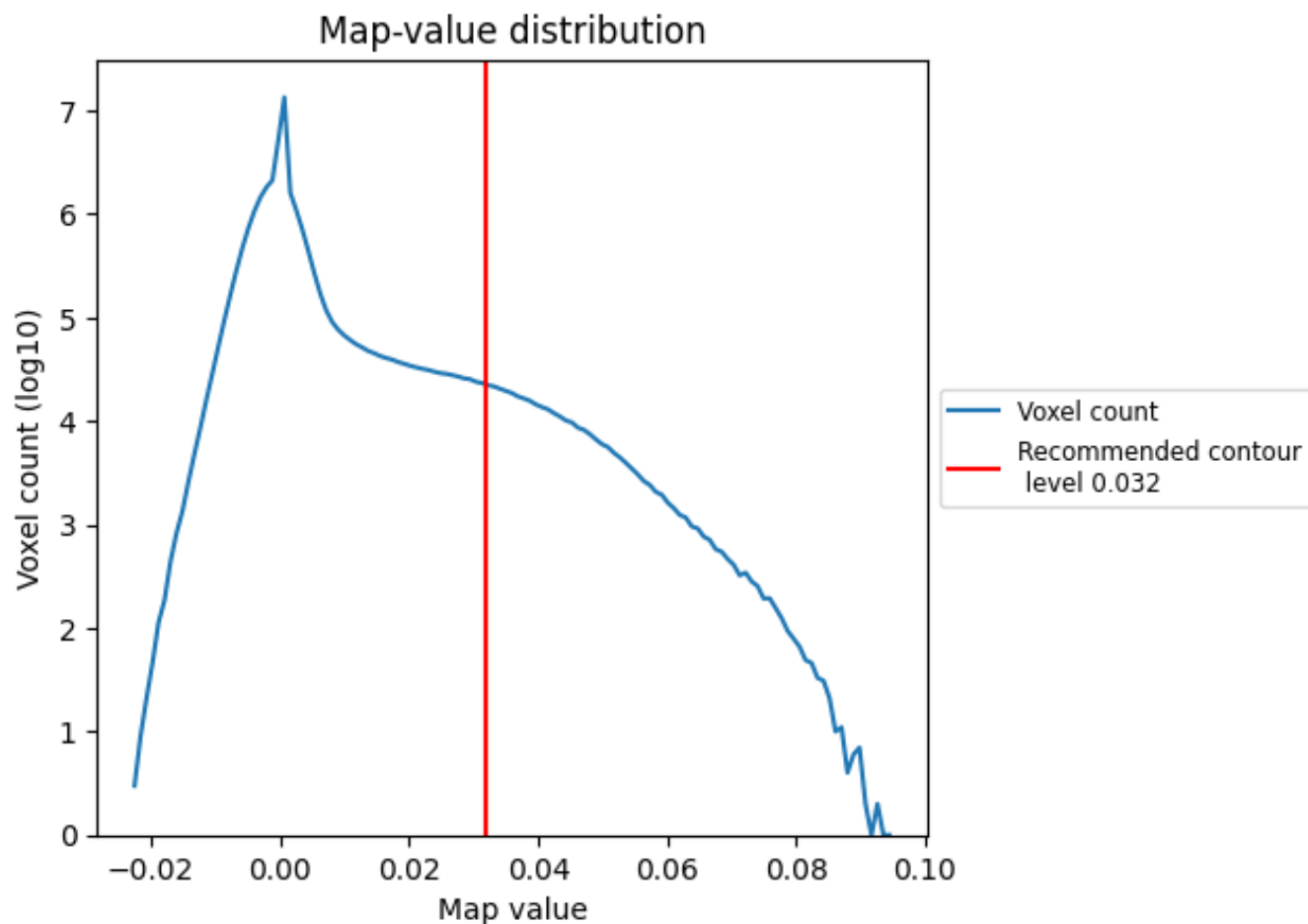
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

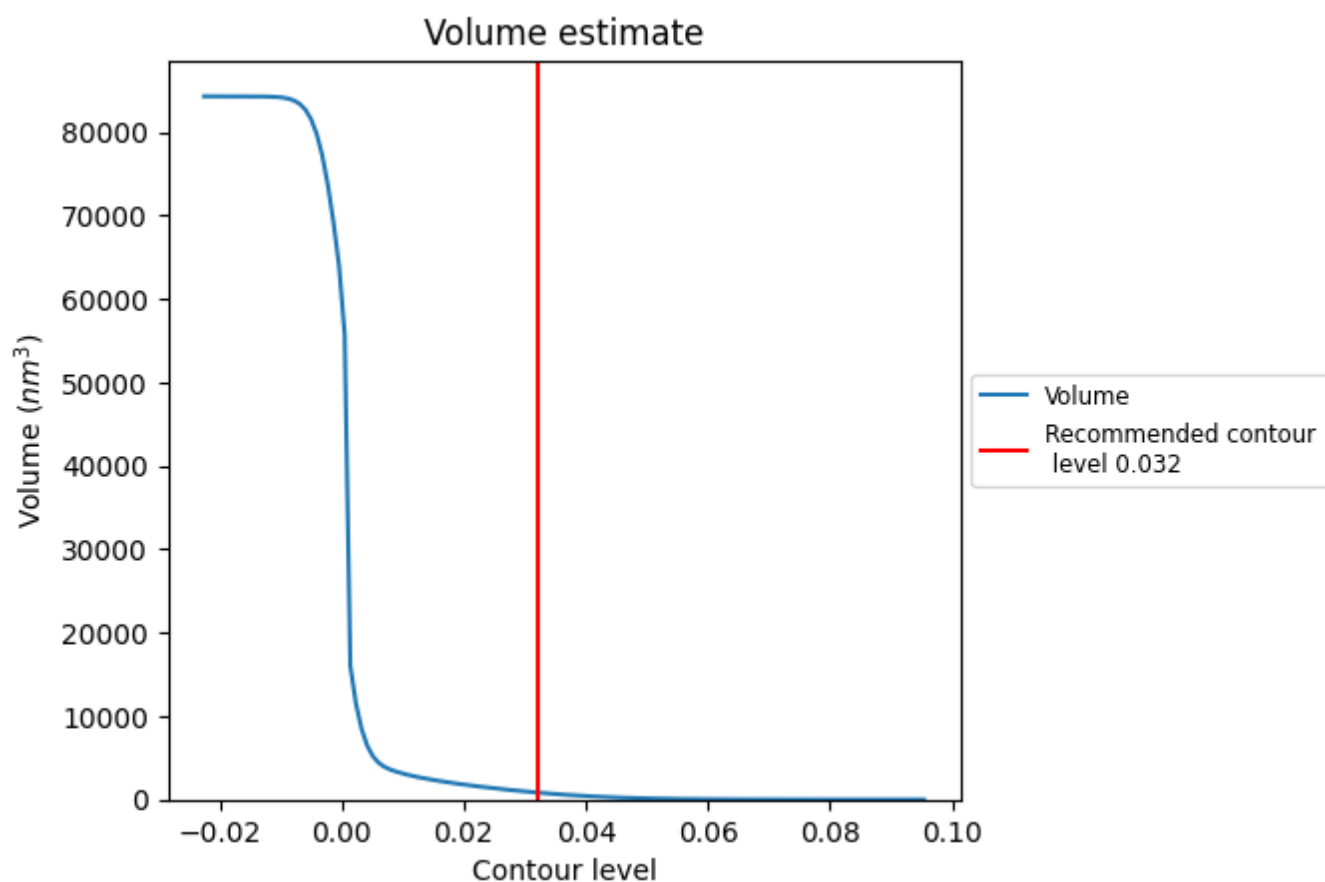
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

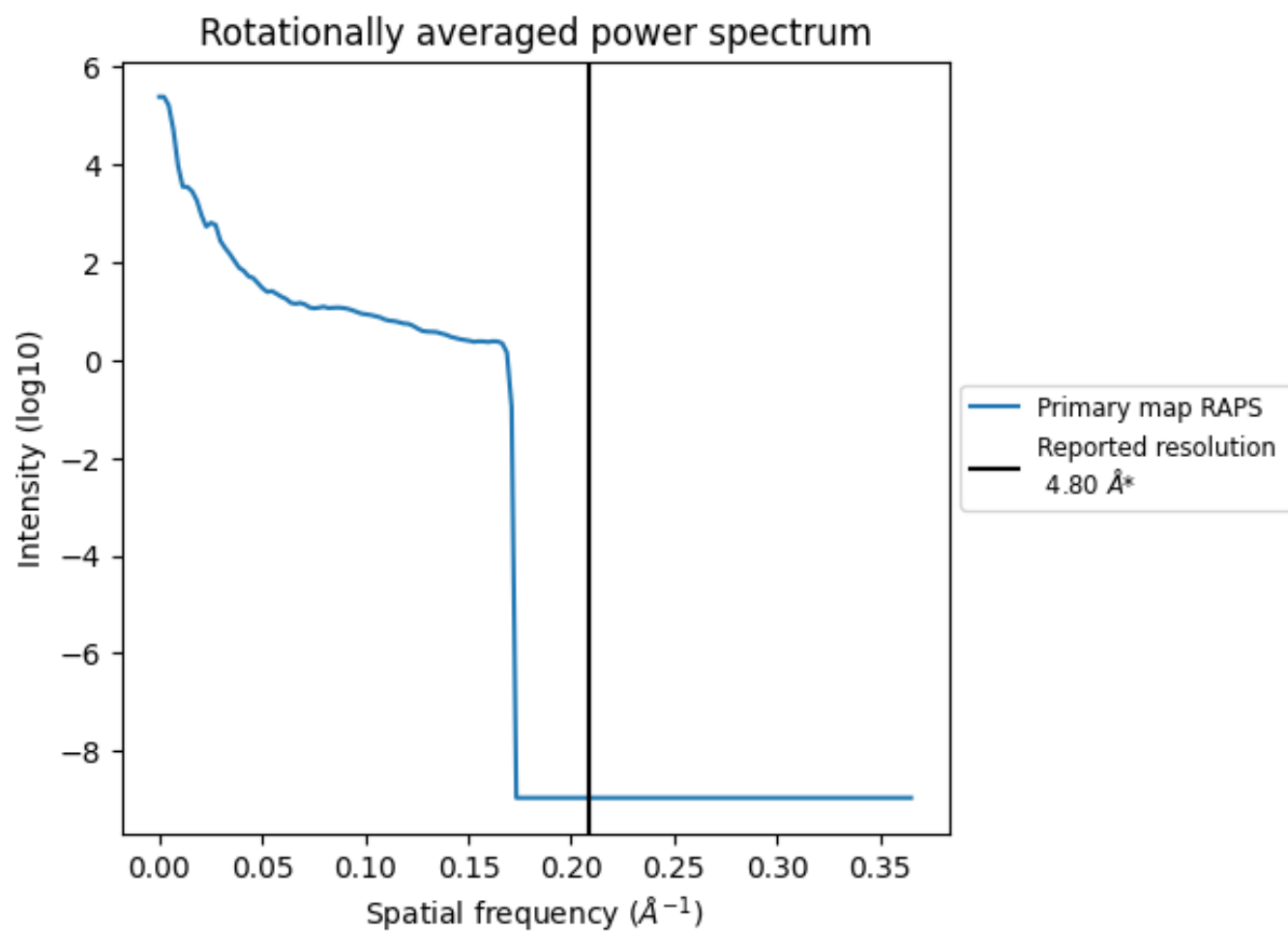
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 840 nm³; this corresponds to an approximate mass of 759 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 0.208 Å⁻¹

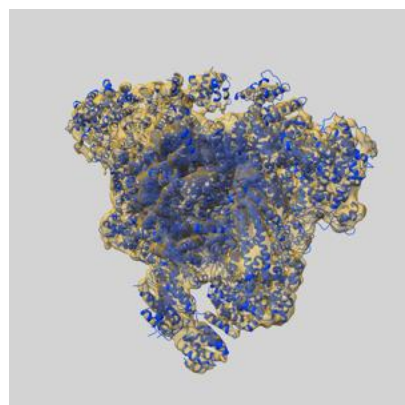
8 Fourier-Shell correlation

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

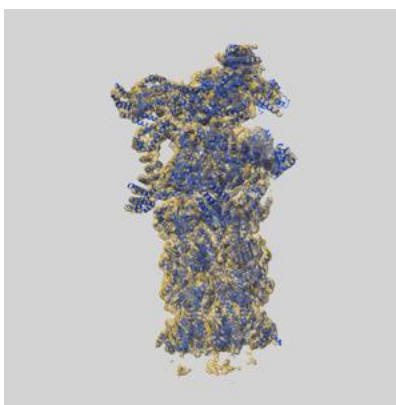
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14210 and PDB model 7QYA. Per-residue inclusion information can be found in section 3 on page 12.

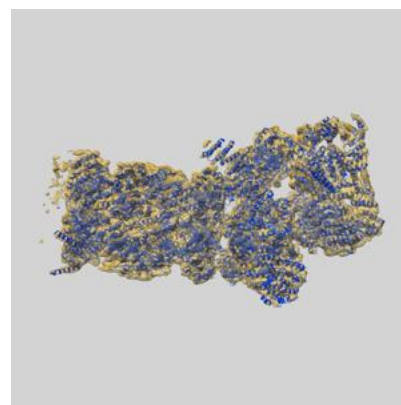
9.1 Map-model overlay [i](#)



X



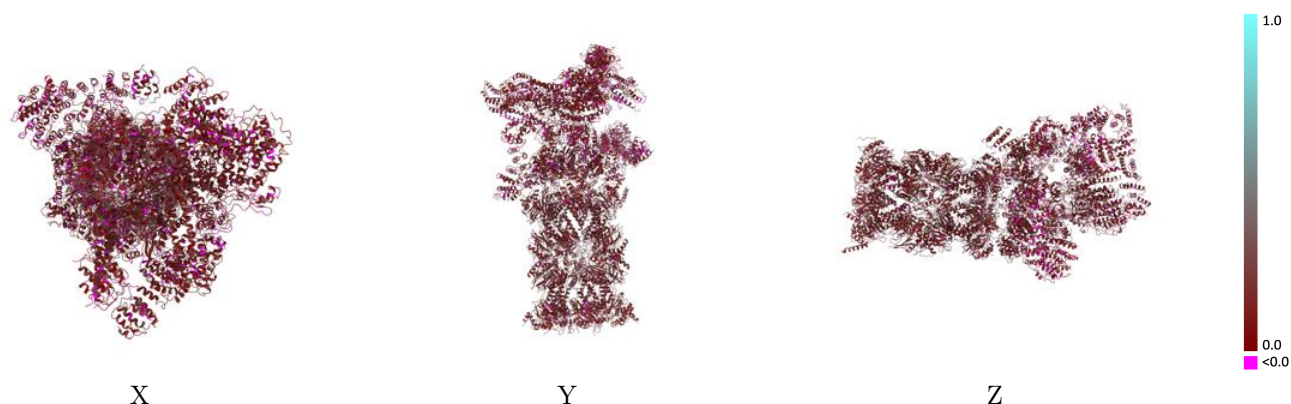
Y



Z

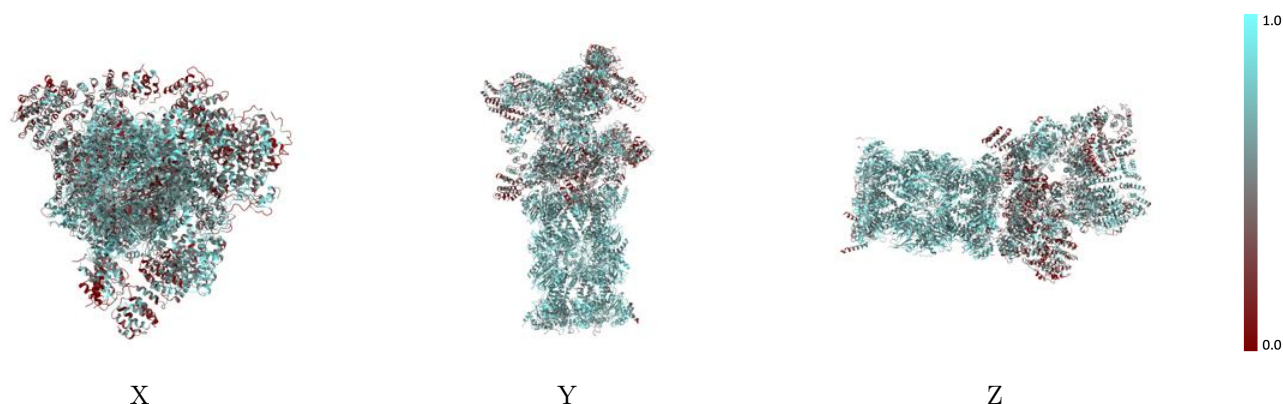
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



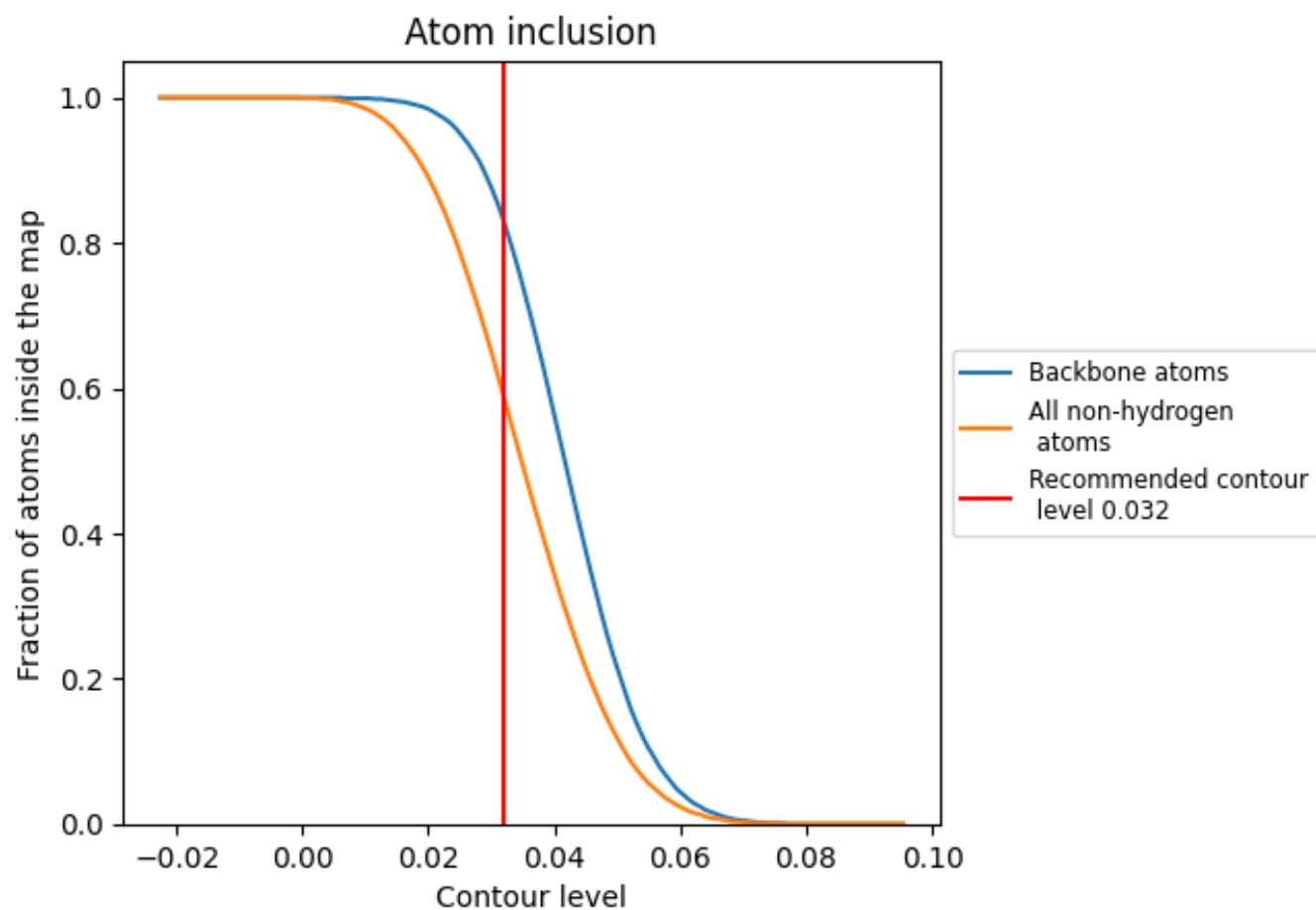
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 59% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.1760
A	 0.5090	 0.1800
B	 0.4240	 0.1710
C	 0.4500	 0.1670
D	 0.4330	 0.1680
E	 0.5330	 0.1740
F	 0.5370	 0.1730
G	 0.6810	 0.1990
H	 0.6750	 0.1950
I	 0.6250	 0.1920
J	 0.6850	 0.2140
K	 0.6280	 0.1850
L	 0.6960	 0.1940
M	 0.6800	 0.1930
N	 0.7300	 0.2040
O	 0.7310	 0.2110
P	 0.7010	 0.1940
Q	 0.7130	 0.2050
R	 0.7460	 0.2070
S	 0.7100	 0.2060
T	 0.7440	 0.2160
U	 0.6130	 0.1570
V	 0.4190	 0.1360
W	 0.4870	 0.1530
X	 0.4800	 0.1620
Y	 0.6400	 0.1500
Z	 0.5610	 0.1580
a	 0.5330	 0.1520
b	 0.4190	 0.1420
c	 0.5770	 0.1560
d	 0.4090	 0.1400
e	 0.4470	 0.0890
f	 0.3630	 0.1210
g	 0.6560	 0.2010
h	 0.6560	 0.2010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6210	 0.1940
j	 0.6430	 0.1980
k	 0.6560	 0.1980
l	 0.6960	 0.2070
m	 0.6580	 0.1830
n	 0.7470	 0.2070
o	 0.7390	 0.2140
p	 0.7060	 0.1930
q	 0.7240	 0.2090
r	 0.7580	 0.2070
s	 0.7290	 0.2110
t	 0.7330	 0.2130