



Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 03:43 PM EDT

PDB ID : 9BW4 / pdb_00009bw4
EMDB ID : EMD-44952
Title : TXNL1-bound proteasome
Authors : Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on : 2024-05-20
Resolution : 3.30 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

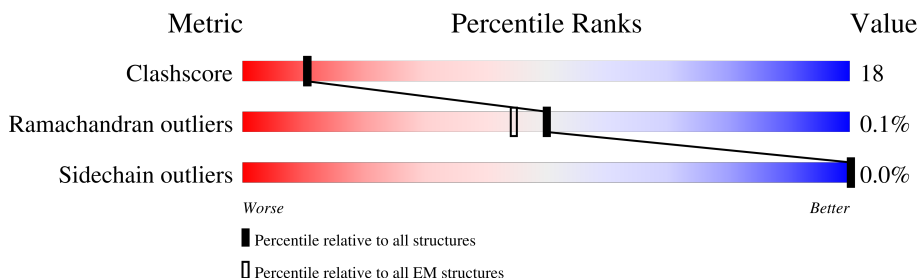
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.





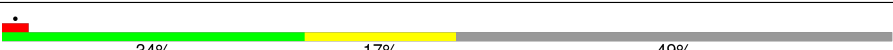

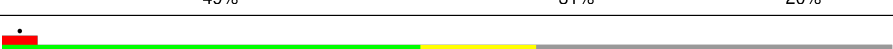
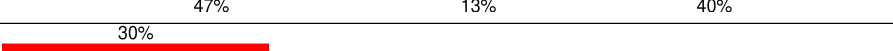
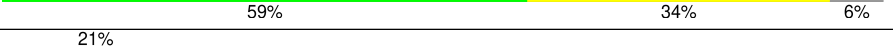





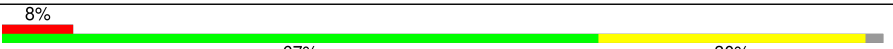


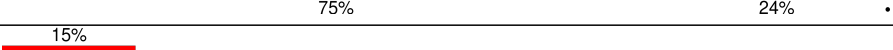






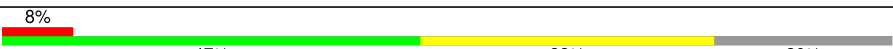

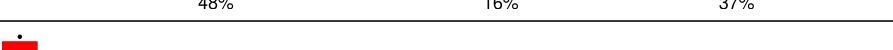
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	U	953	
2	V	534	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	c	310	
10	d	350	
11	e	70	
12	f	908	
13	x	289	
14	A	433	
15	B	440	
16	C	406	
17	D	418	
18	E	389	
19	F	439	
20	G	246	
21	H	234	
22	I	261	
23	J	248	
24	K	241	
25	L	263	
26	M	255	
27	N	239	
27	n	239	
28	O	277	
28	o	277	
29	P	205	
29	p	205	
30	Q	201	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	q	201	
31	R	263	
31	r	263	
32	S	241	
32	s	241	
33	T	264	
33	t	264	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90418 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	857	Total	C	N	O	S	0	0
			6685	4243	1136	1261	45		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	421	Total	C	N	O	S	0	0
			3434	2192	613	617	12		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	424	Total	C	N	O	S	0	0
			3465	2194	595	653	23		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	421	Total	C	N	O	S	0	0
			3327	2111	566	638	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	379	Total	C	N	O	S	0	0
			3123	1993	534	579	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	277	Total	C	N	O	S	0	0
			2184	1382	375	408	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	258	Total	C	N	O	S	0	0
			2099	1362	341	387	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	36	Total	C	N	O	0	0
			314	193	50	71		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	727	Total	C	N	O	S	0	0
			5633	3561	958	1069	45		

- Molecule 13 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	x	172	Total	C	N	O	S	0	0
			1376	865	226	276	9		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	405	Total	C	N	O	S	0	0
			3183	2002	561	602	18		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	390	Total	C	N	O	S	0	0
			3065	1931	521	598	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	389	Total	C	N	O	S	0	0
			3071	1932	550	571	18		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	373	Total	C	N	O	S	0	0
			2990	1894	517	567	12		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	296	Total	C	N	O	S	0	0
			2353	1481	414	442	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	368	Total	C	N	O	S	0	0
			2881	1821	496	547	17		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	241	Total	C	N	O	S	0	0
			1885	1196	314	362	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	233	Total	C	N	O	S	0	0
			1818	1161	308	343	6		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	258	Total	C	N	O	S	0	0
			2044	1290	350	394	10		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	232	Total	C	N	O	S	0	0
			1778	1116	295	356	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	245	Total	C	N	O	S	0	0
			1920	1214	326	369	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
27	n	179	Total	C	N	O	S	0	0
			1336	836	230	258	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
28	o	175	Total	C	N	O	S	0	0
			1307	817	227	252	11		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
29	p	164	Total	C	N	O	S	0	0
			1264	802	210	235	17		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
30	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
31	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
32	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		

Continued on next page...

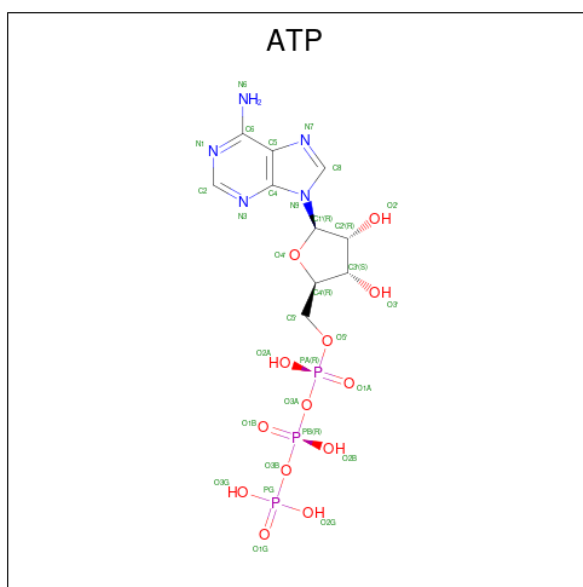
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

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

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

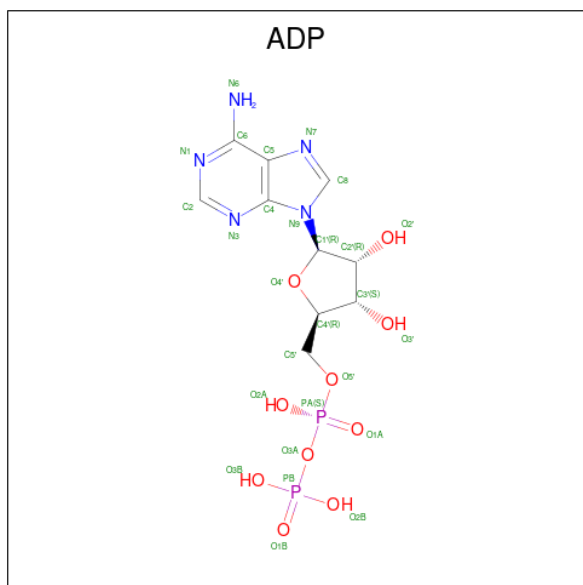
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

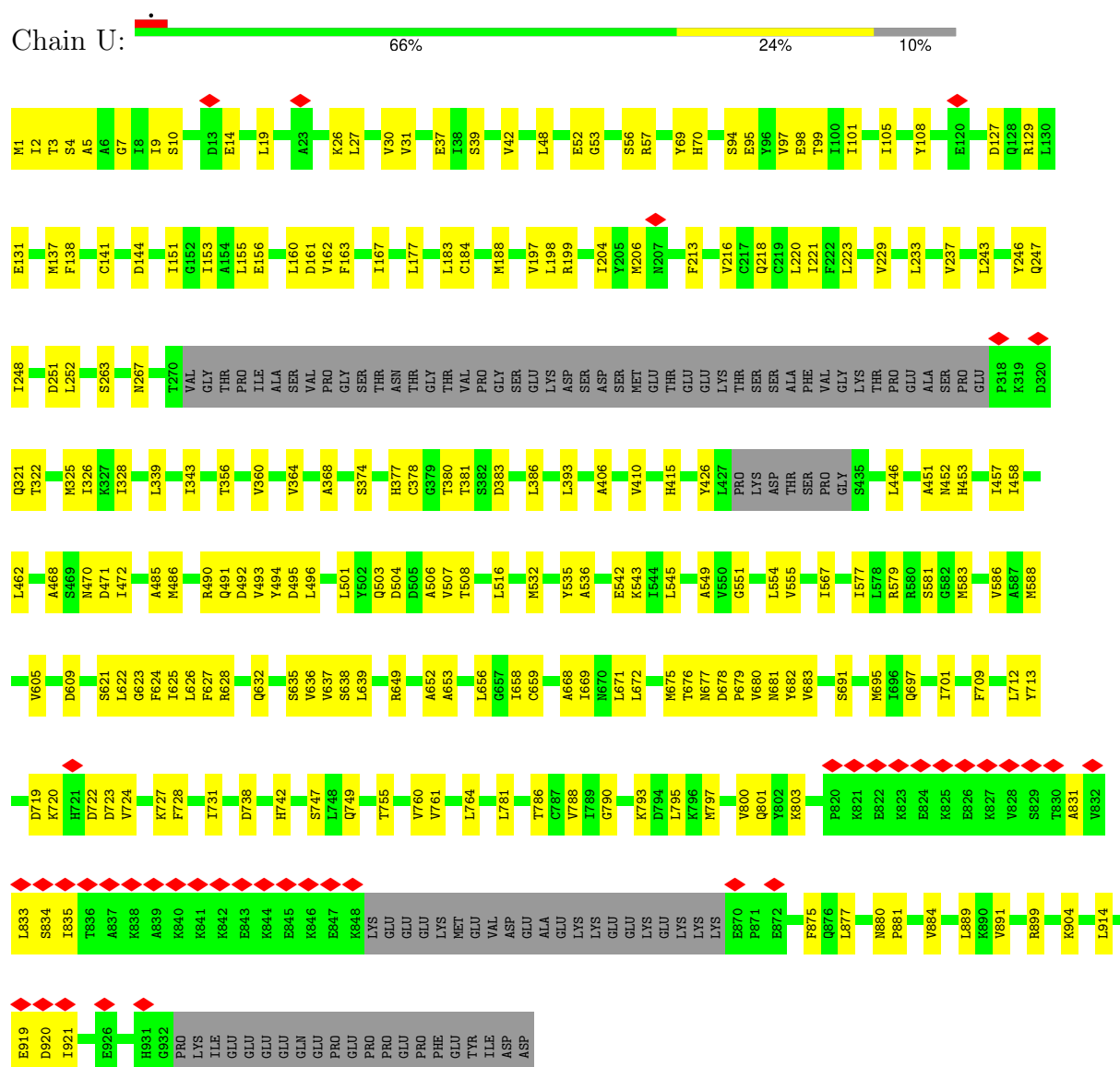


Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

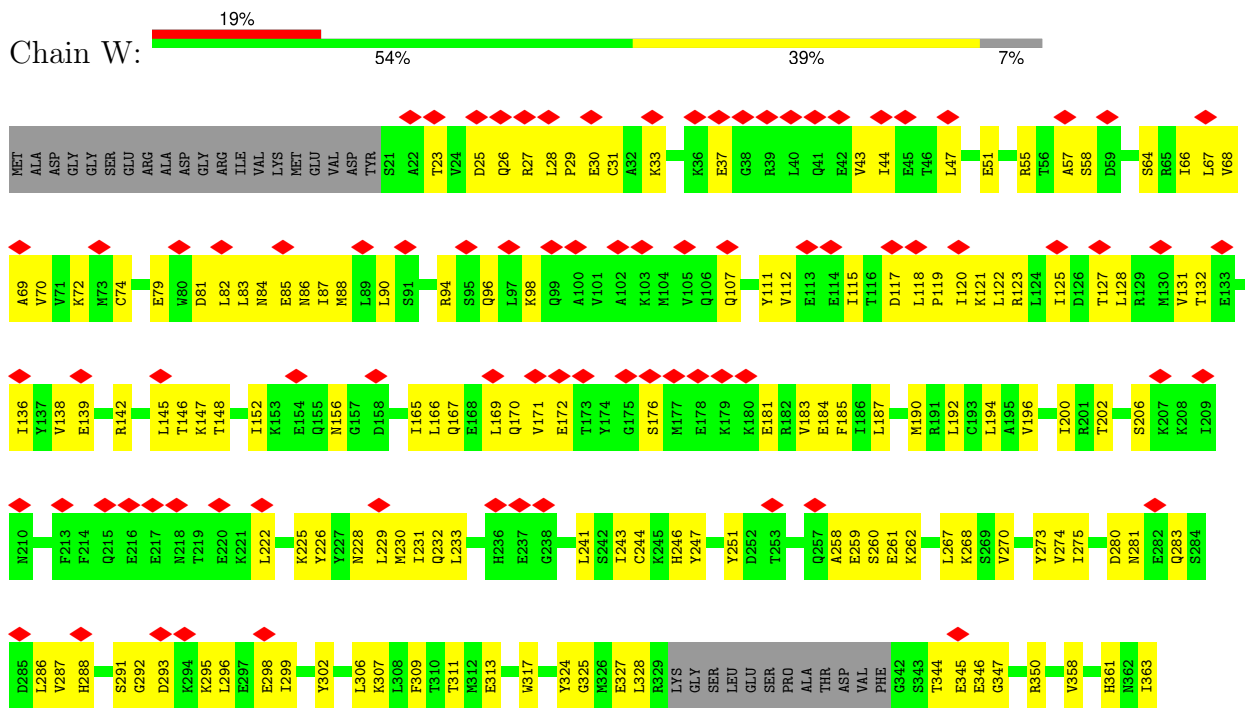
3 Residue-property plots

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

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

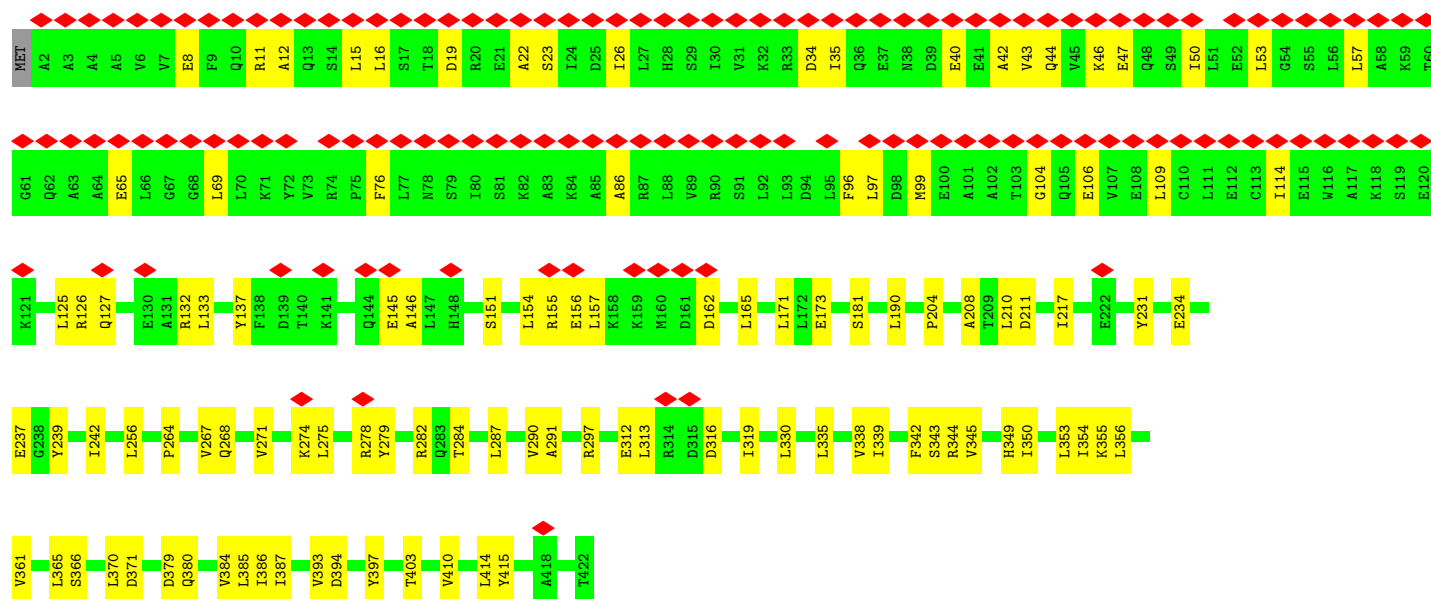
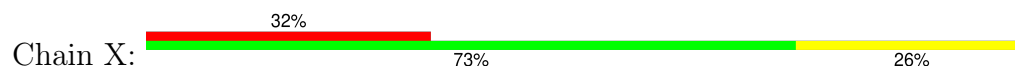


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

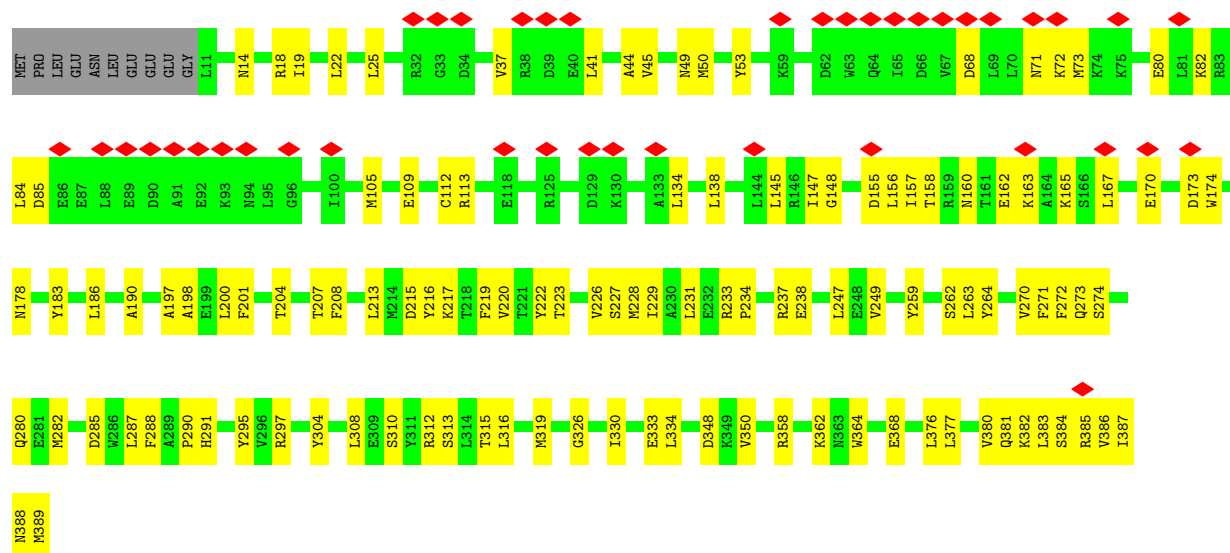




- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

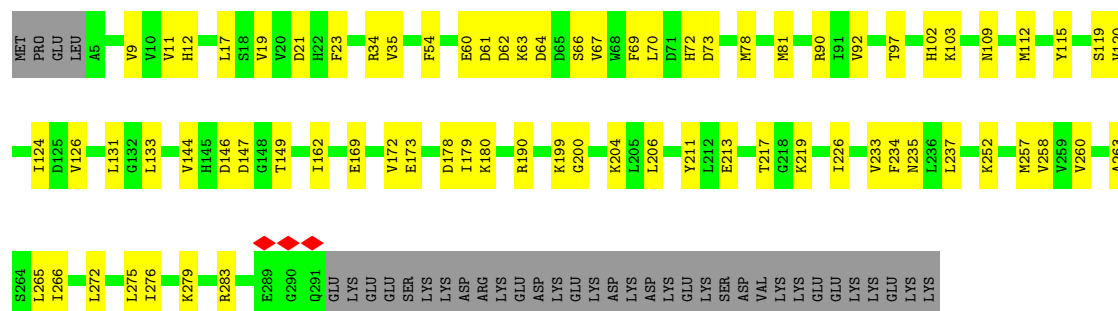


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

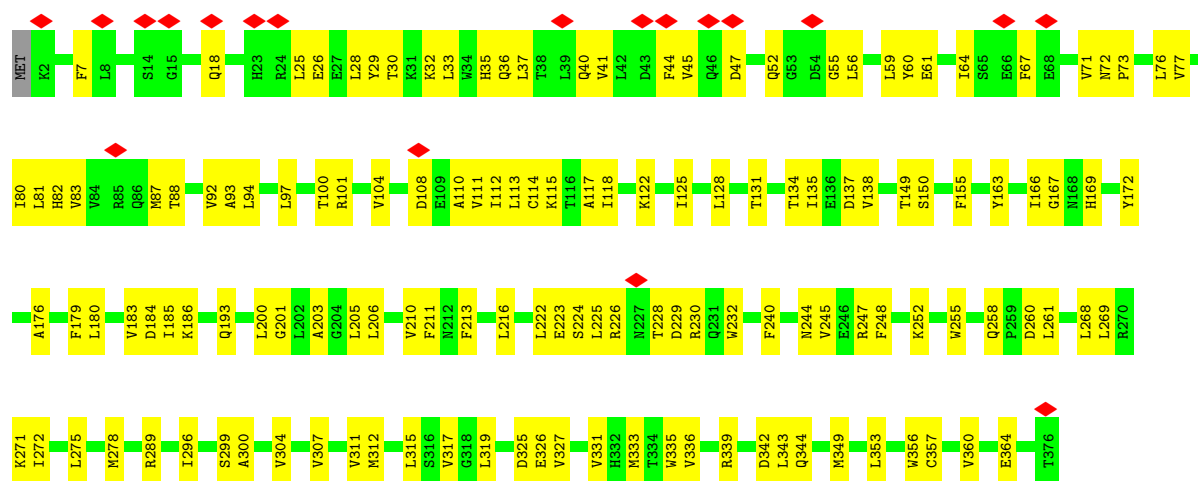


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

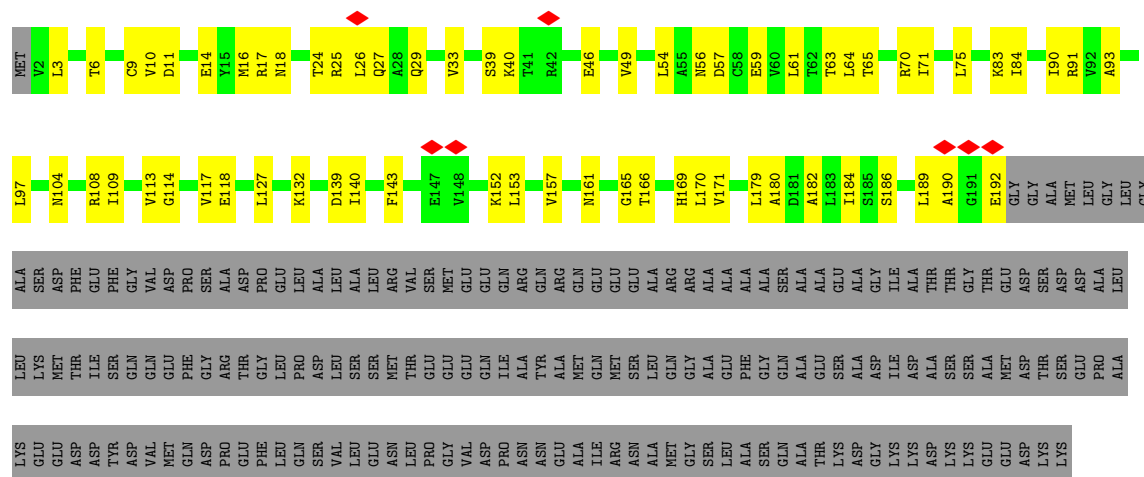
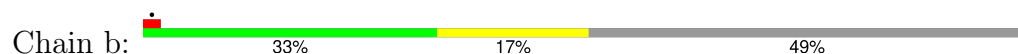




• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

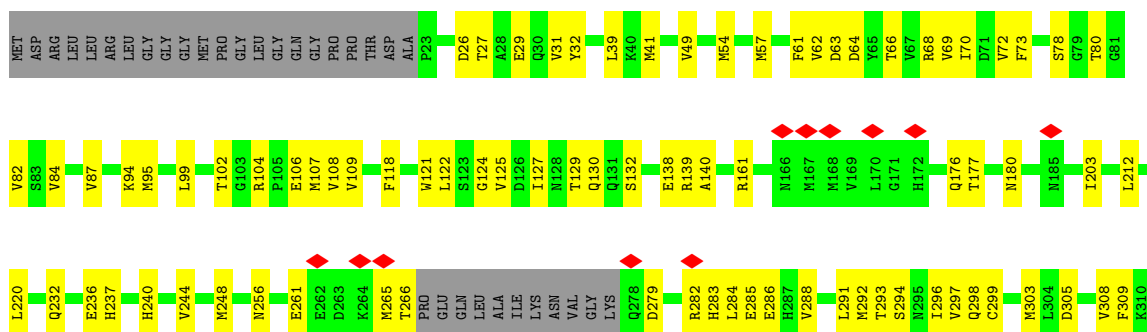


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

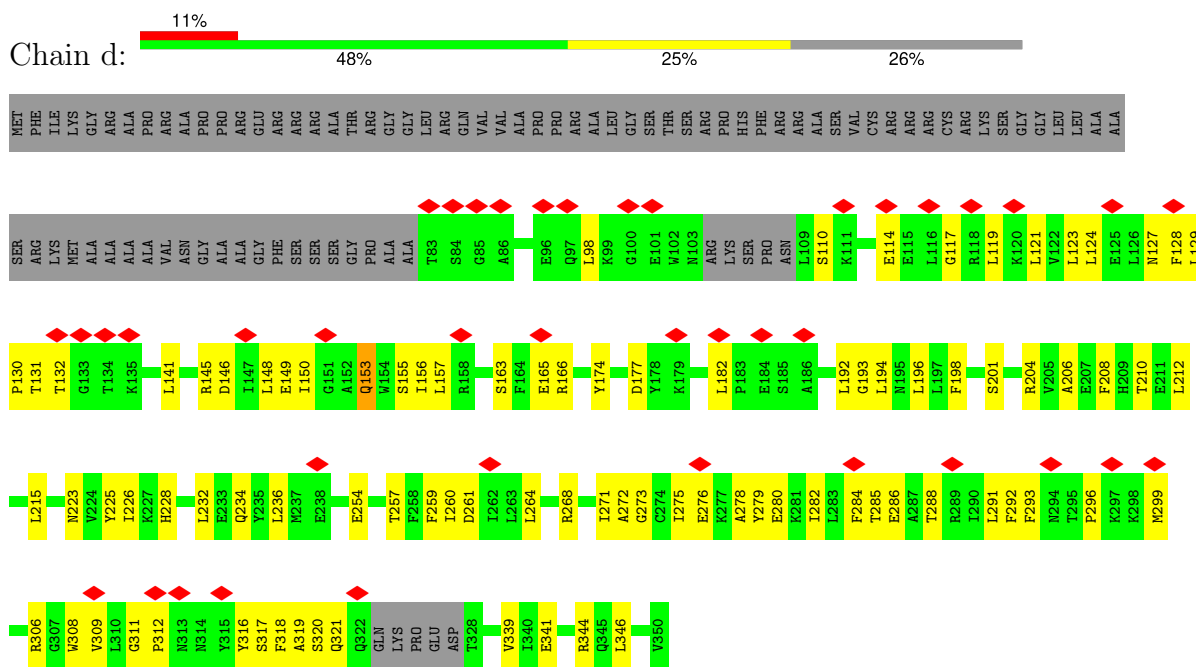


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

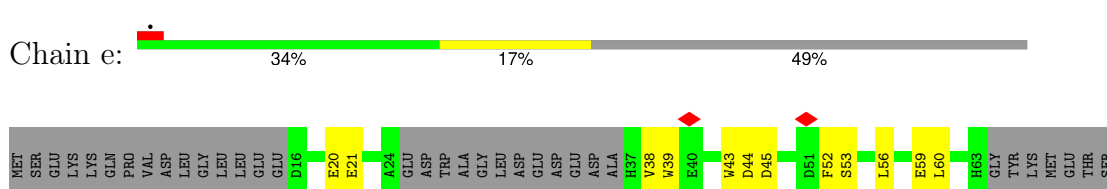




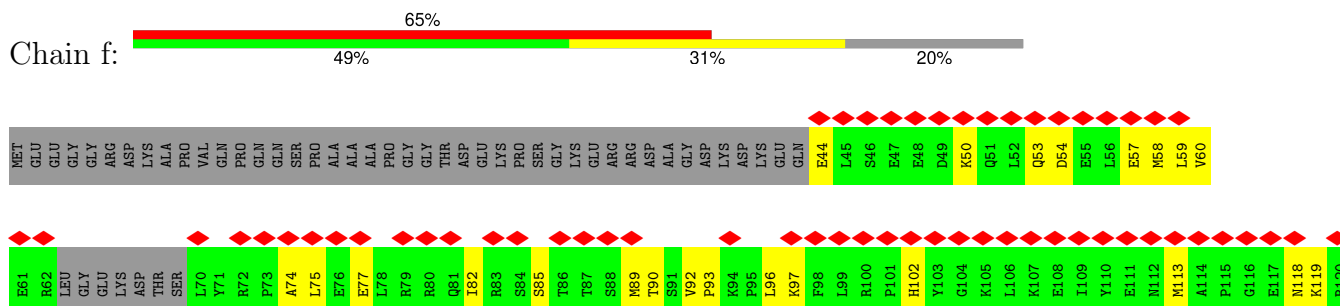
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 11: 26S proteasome complex subunit SEM1

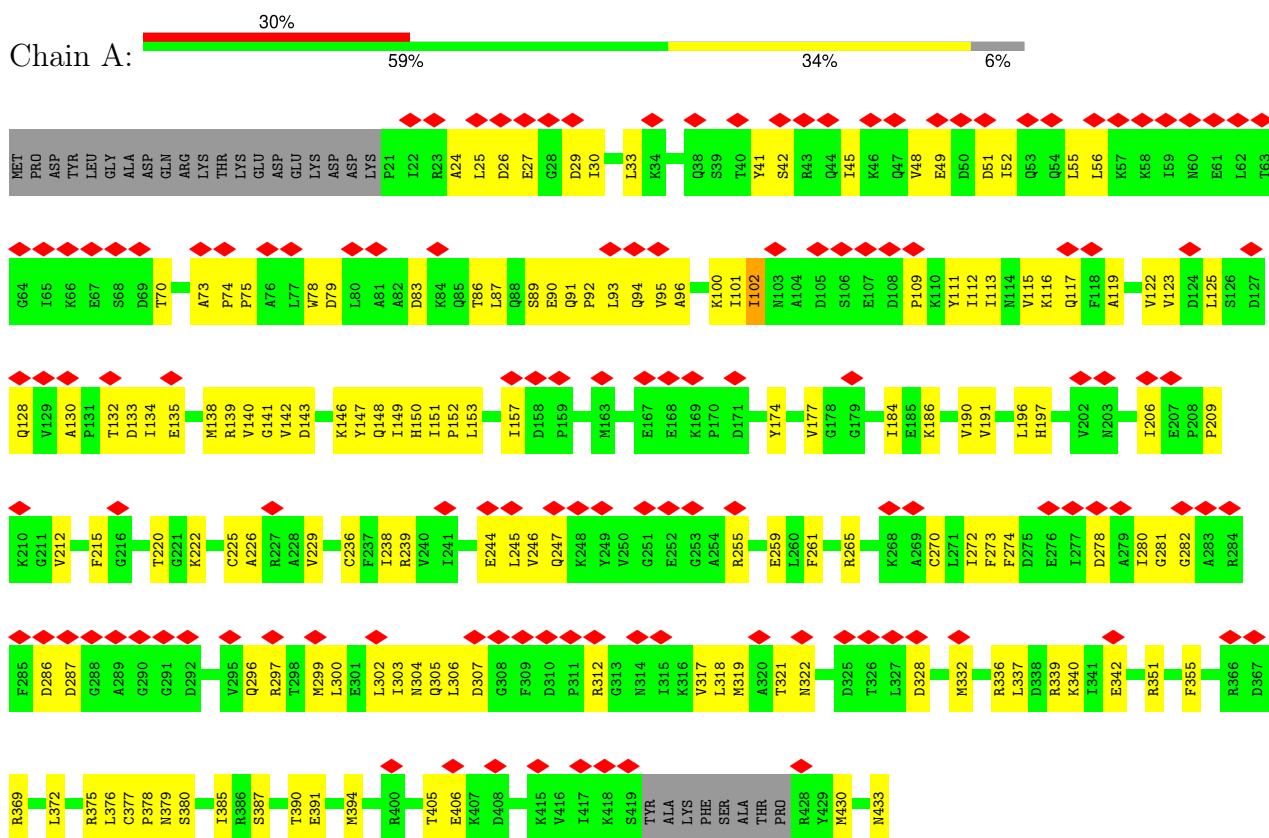


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

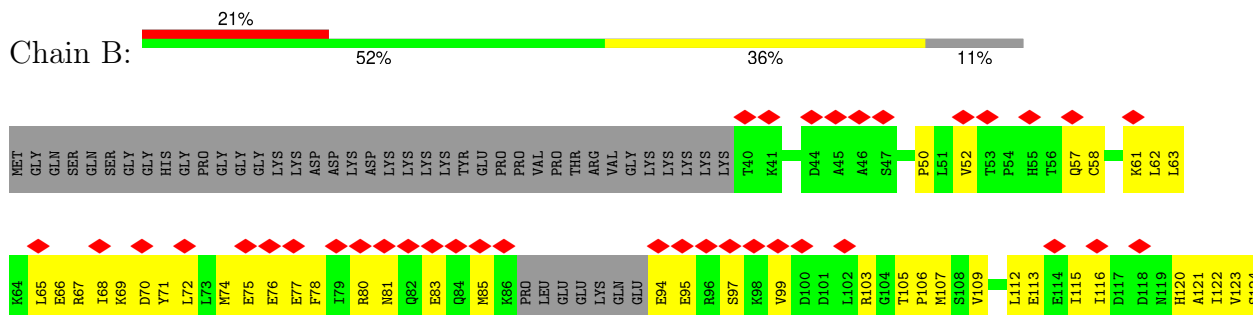


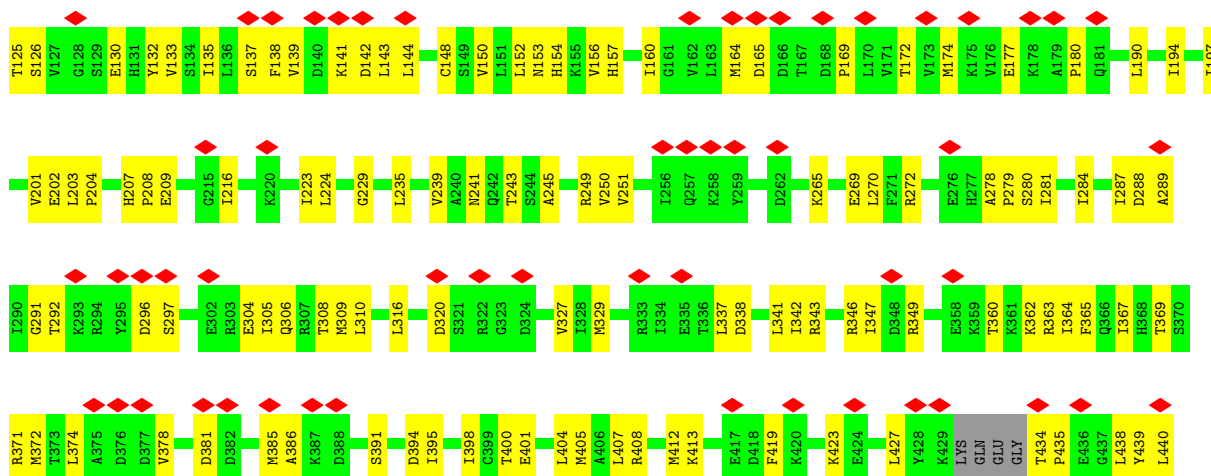


- Molecule 14: 26S proteasome regulatory subunit 7

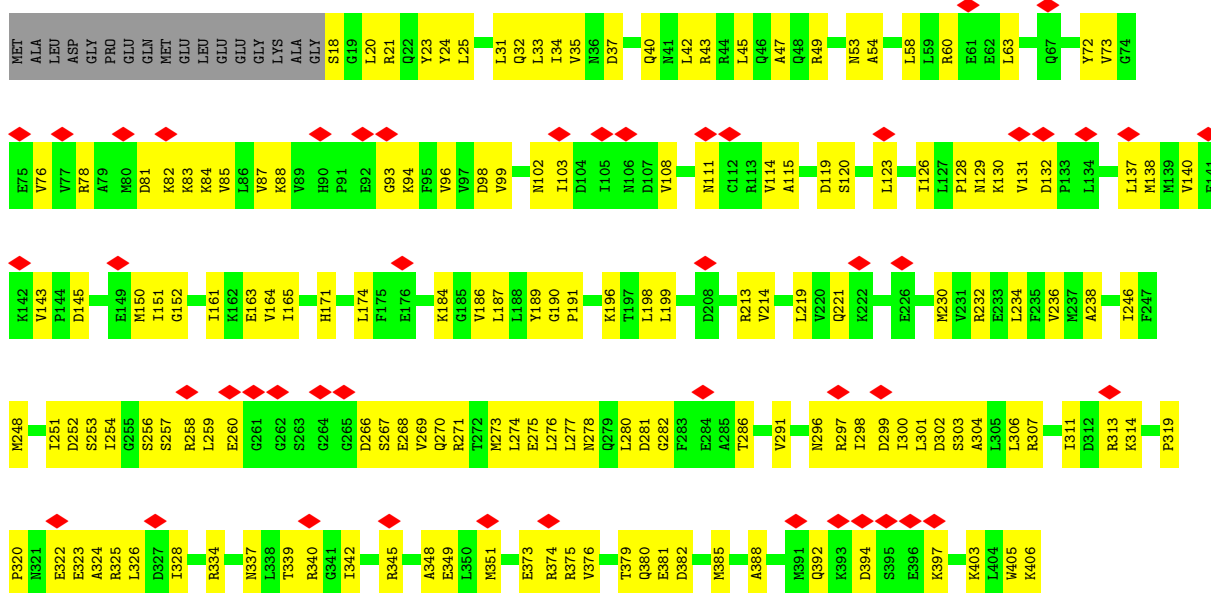


- Molecule 15: 26S proteasome regulatory subunit 4

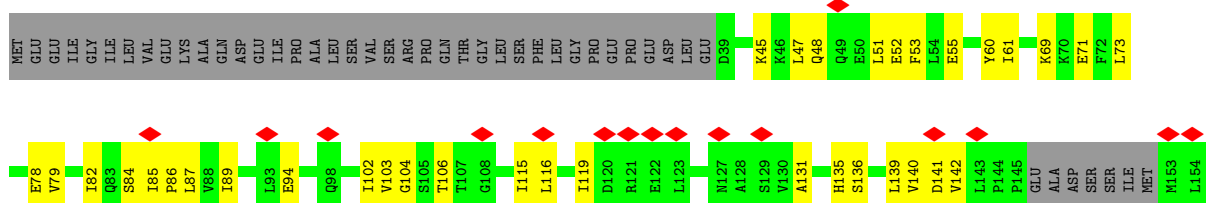


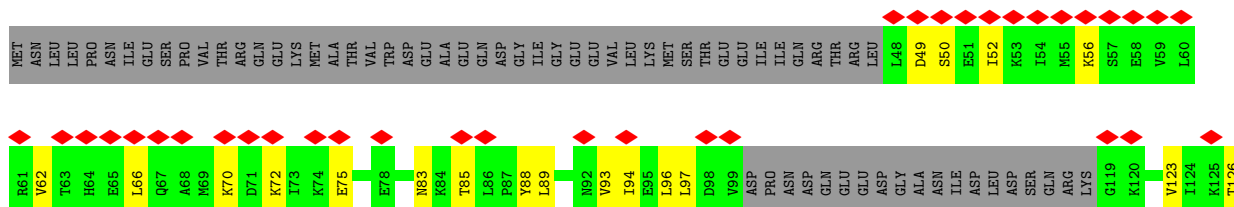


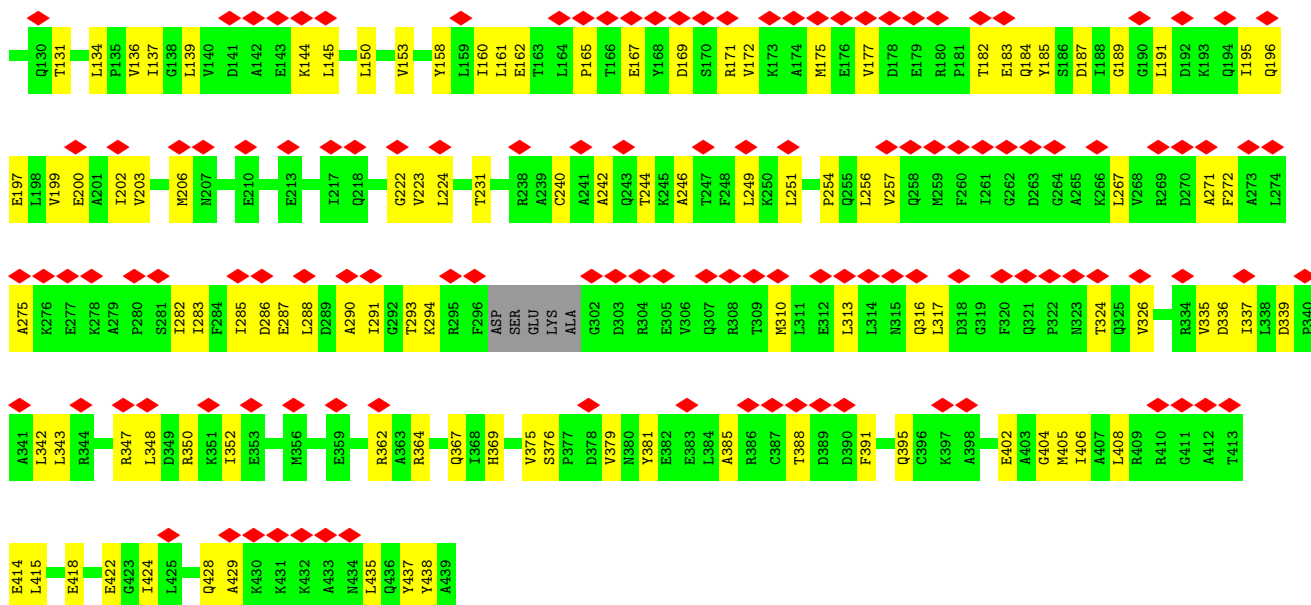
• Molecule 16: 26S protease regulatory subunit 8



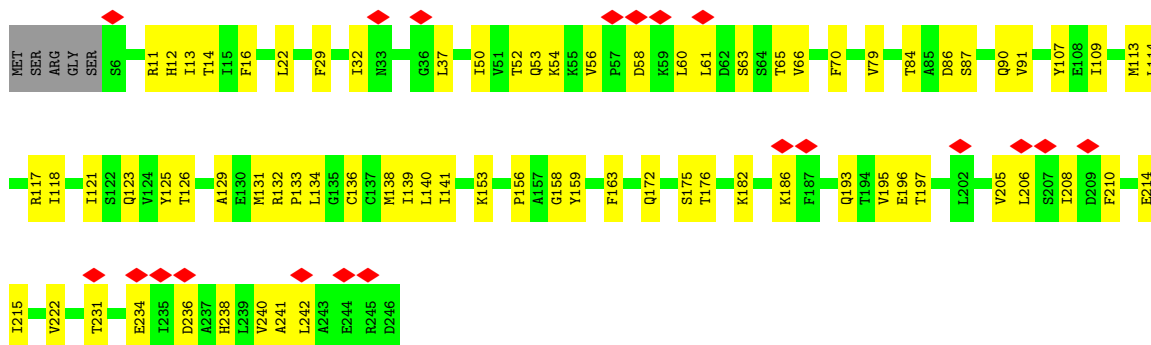
• Molecule 17: 26S proteasome regulatory subunit 6B



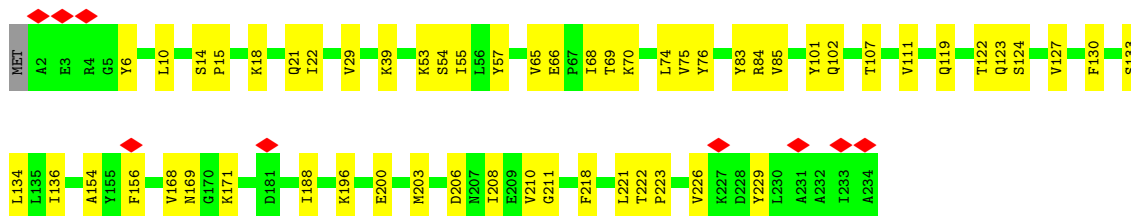




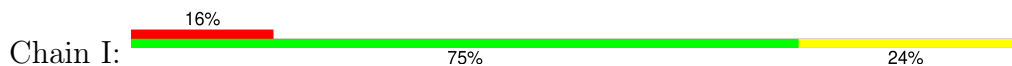
• Molecule 20: Proteasome subunit alpha type-6

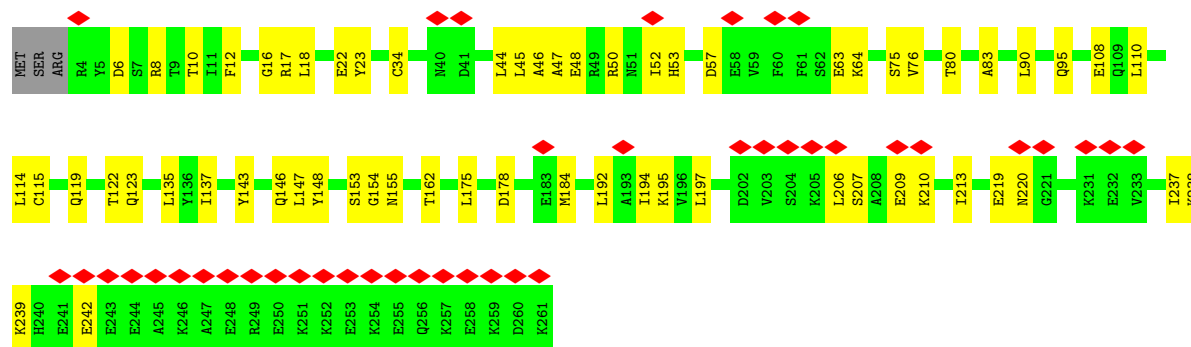


• Molecule 21: Proteasome subunit alpha type-2

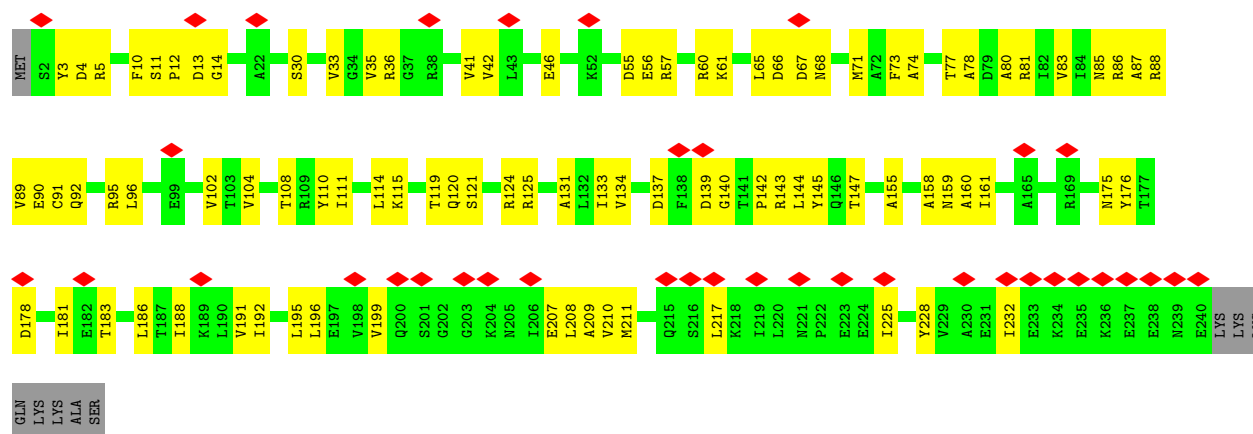


• Molecule 22: Proteasome subunit alpha type-4

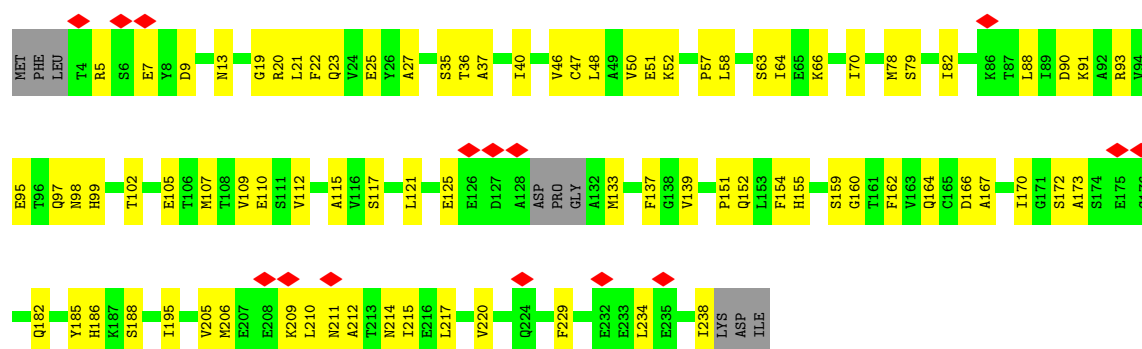




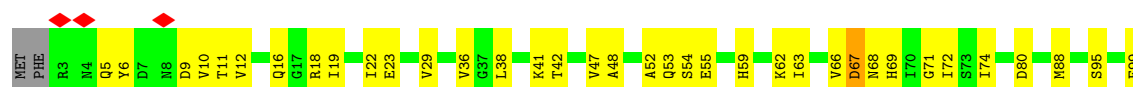
• Molecule 23: Proteasome subunit alpha type-7

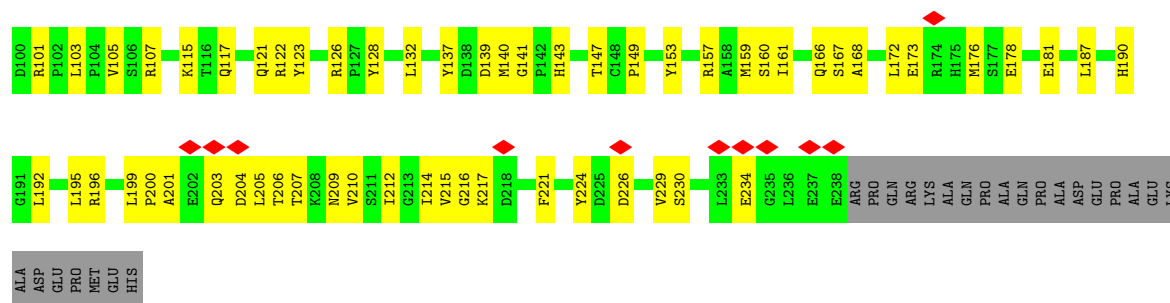


• Molecule 24: Proteasome subunit alpha type-5

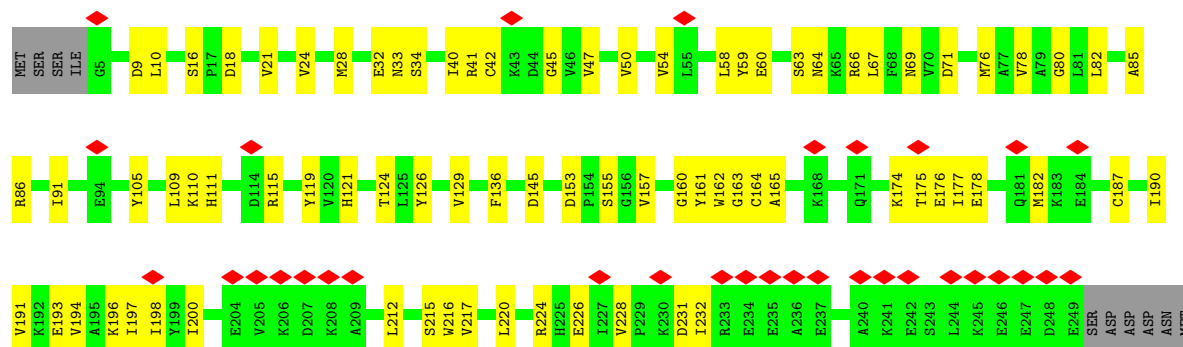


• Molecule 25: Proteasome subunit alpha type-1

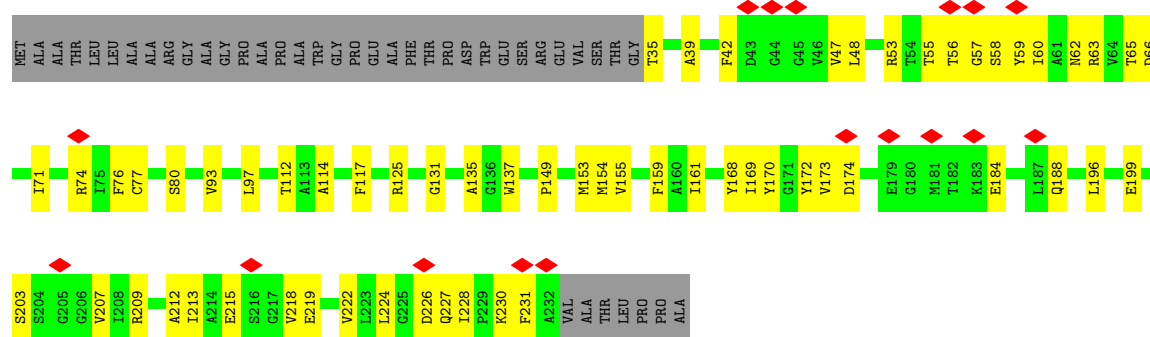




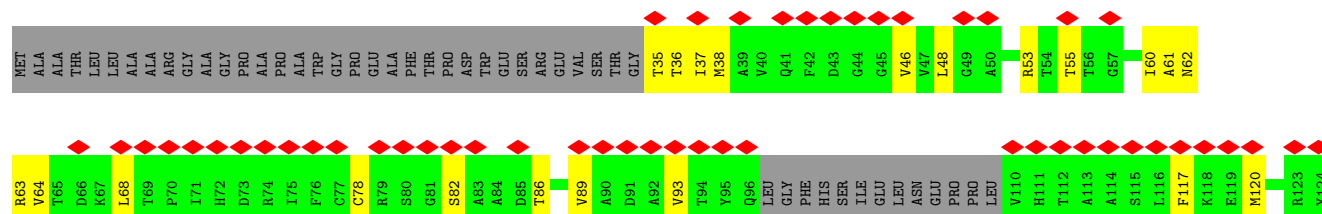
• Molecule 26: Proteasome subunit alpha type-3

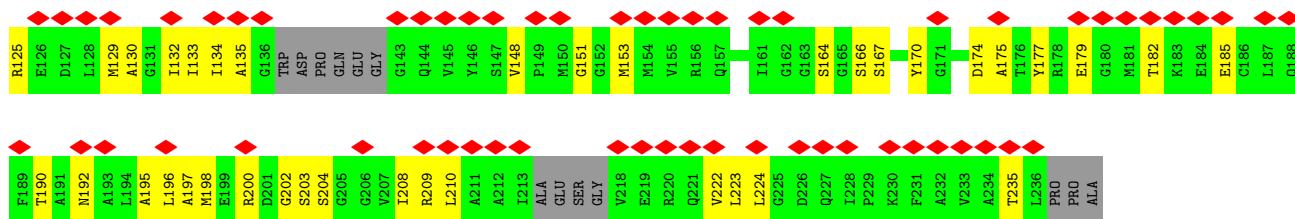


• Molecule 27: Proteasome subunit beta type-6

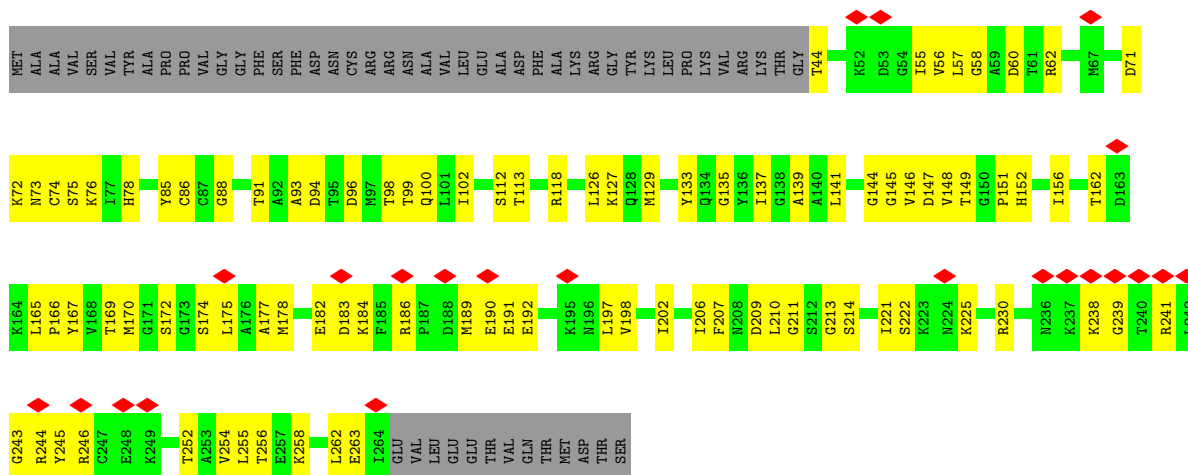


• Molecule 27: Proteasome subunit beta type-6

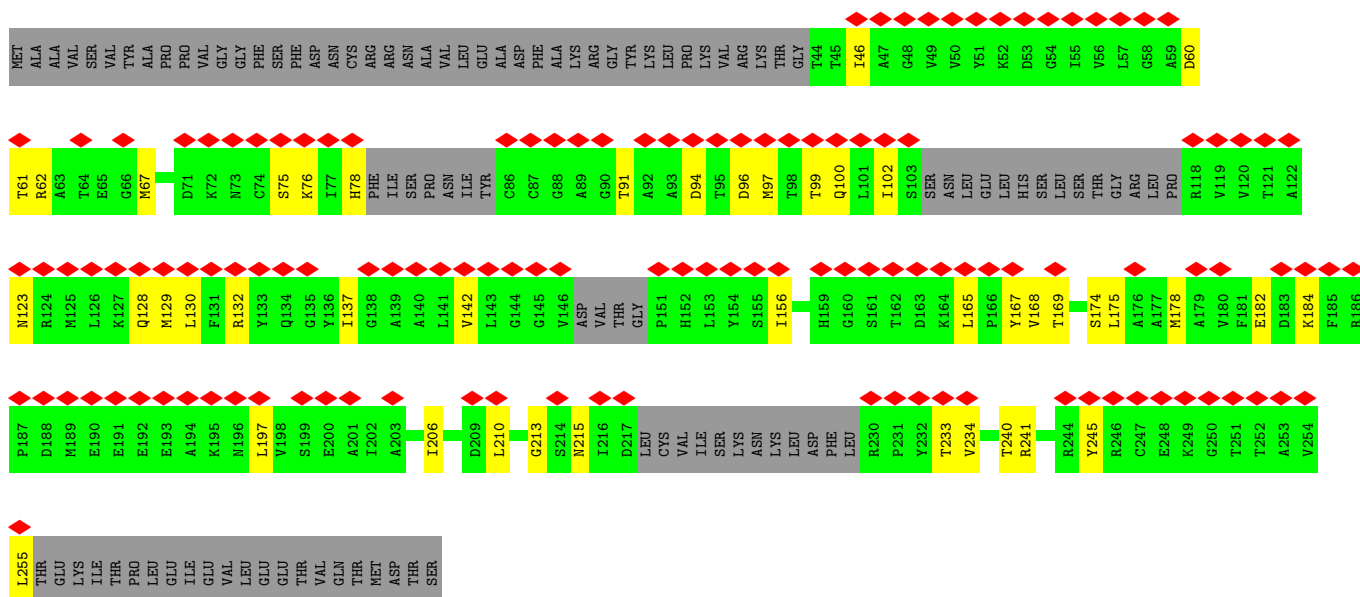




• Molecule 28: Proteasome subunit beta type-7

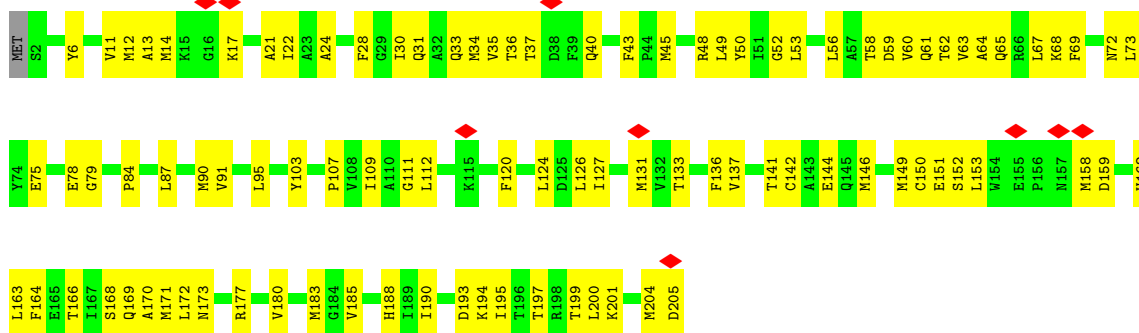


• Molecule 28: Proteasome subunit beta type-7



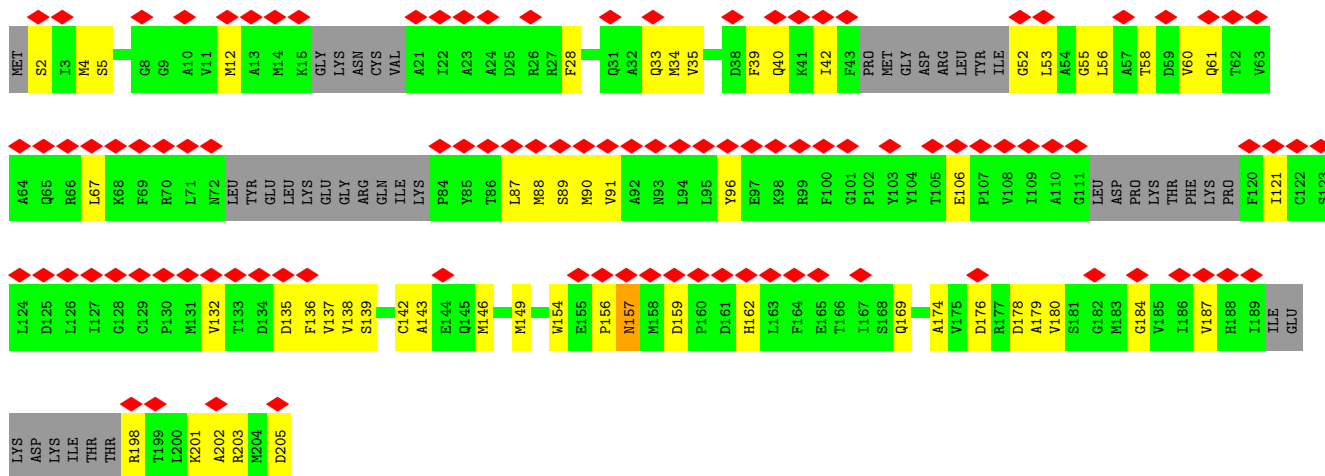
• Molecule 29: Proteasome subunit beta type-3

Chain P: 



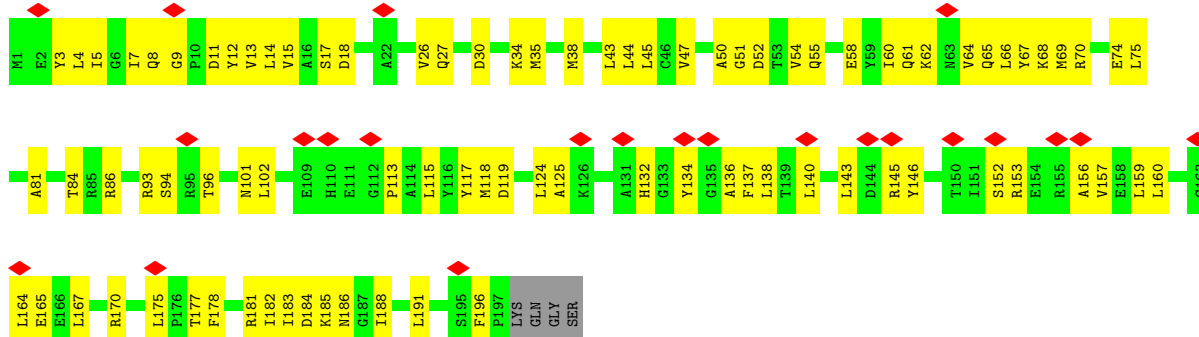
• Molecule 29: Proteasome subunit beta type-3

Chain p: 



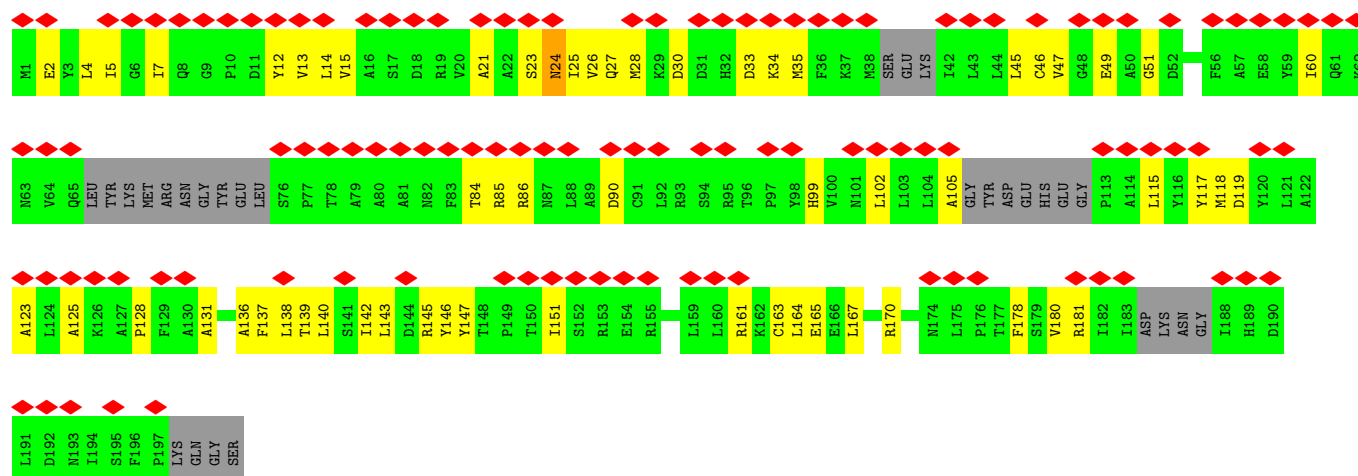
• Molecule 30: Proteasome subunit beta type-2

Chain Q: 



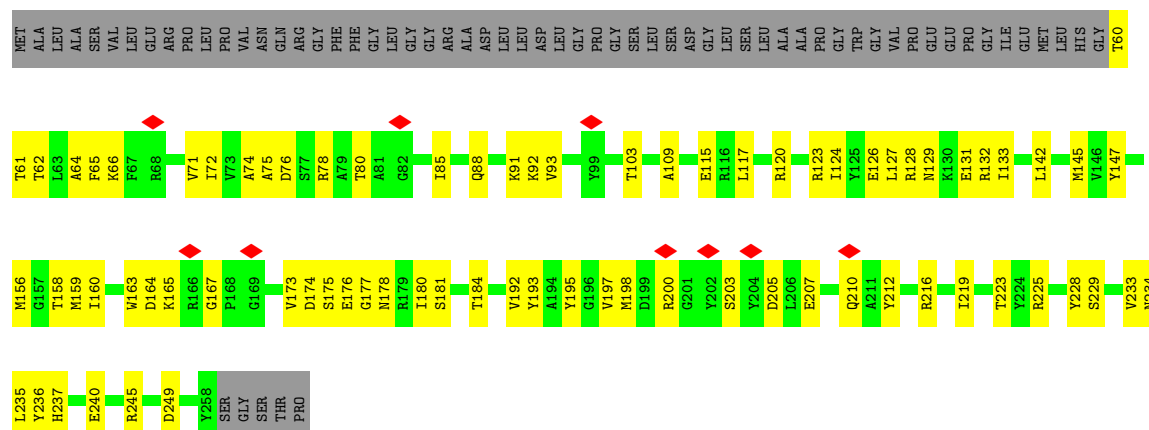
• Molecule 30: Proteasome subunit beta type-2

Chain q: 



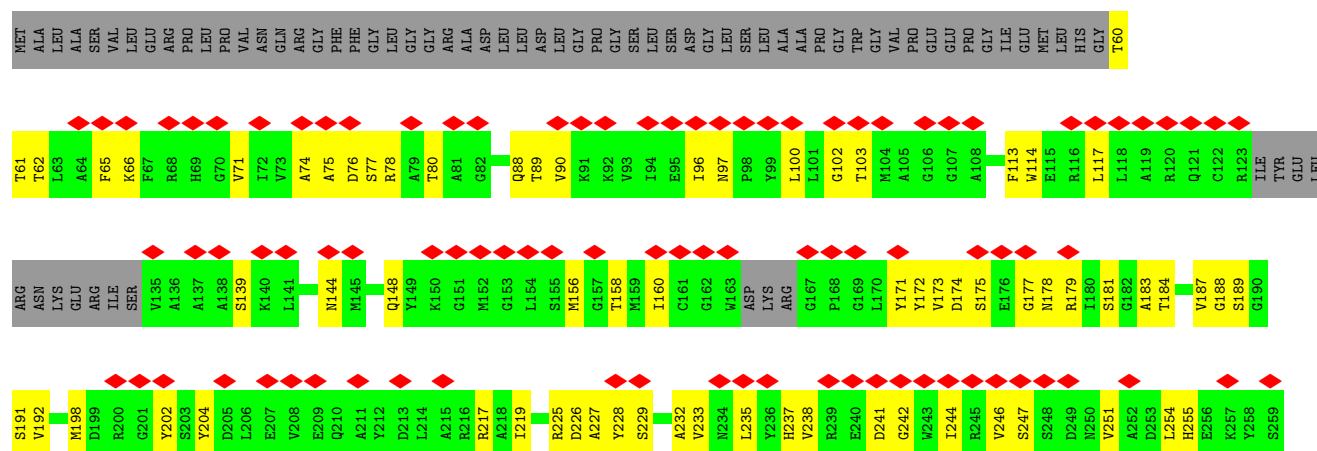
• Molecule 31: Proteasome subunit beta type-5

Chain R: 46% 29% 24%



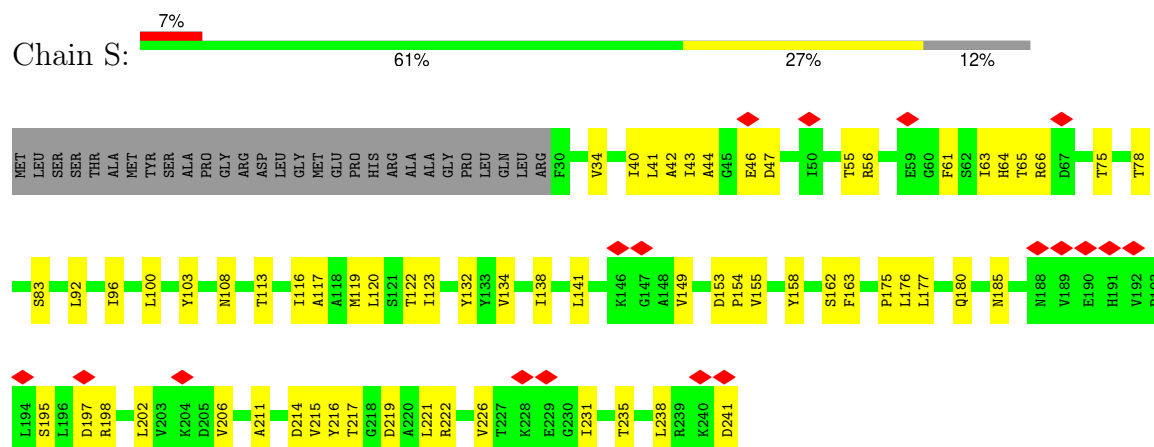
• Molecule 31: Proteasome subunit beta type-5

Chain r: 35% 45% 26% 29%





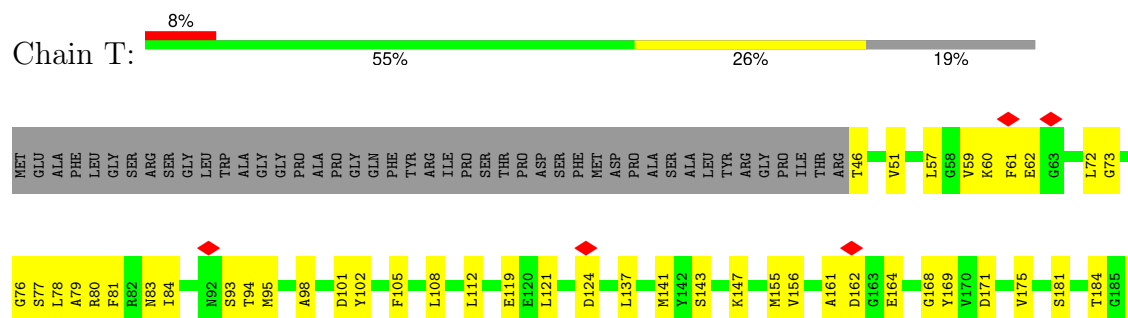
• Molecule 32: Proteasome subunit beta type-1



• Molecule 32: Proteasome subunit beta type-1

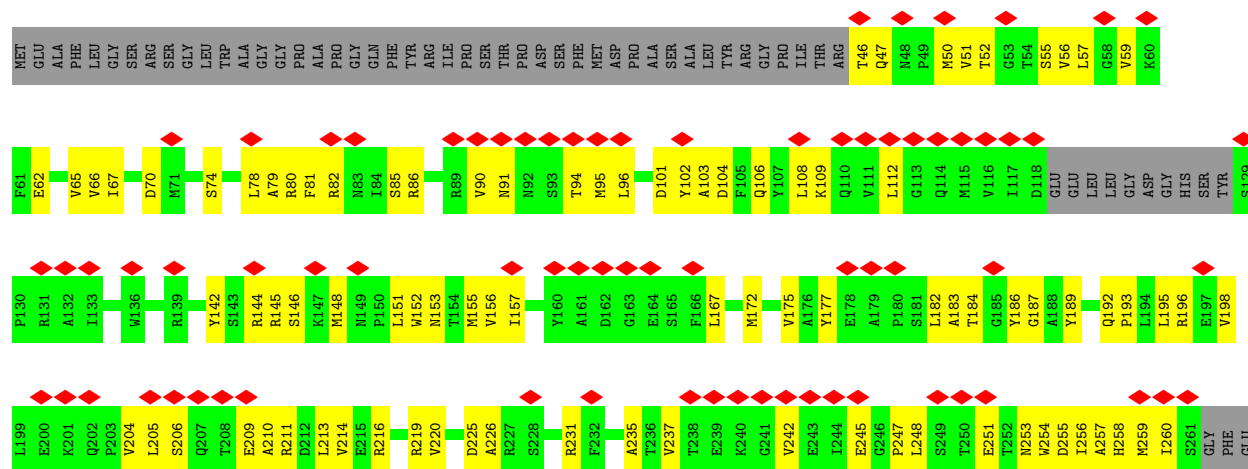
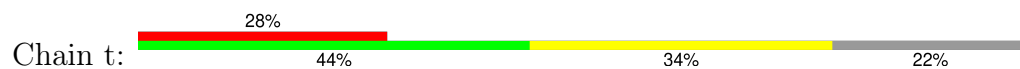


• Molecule 33: Proteasome subunit beta type-4





• Molecule 33: 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	103163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.642	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	U	0.27	0/6800	0.36	0/9192
2	V	0.27	0/3499	0.43	0/4722
3	W	0.21	0/3509	0.37	0/4716
4	X	0.21	0/3373	0.34	0/4548
5	Y	0.26	0/3181	0.38	0/4285
6	Z	0.30	0/2333	0.38	0/3162
7	a	0.23	0/3070	0.39	0/4155
8	b	0.21	0/1479	0.34	0/2003
9	c	0.30	0/2225	0.40	0/3005
10	d	0.22	0/2141	0.42	0/2891
11	e	0.22	0/322	0.40	0/436
12	f	0.16	0/5724	0.39	0/7735
13	x	0.20	0/1403	0.30	0/1892
14	A	0.23	0/3233	0.41	1/4362 (0.0%)
15	B	0.23	0/3109	0.39	0/4193
16	C	0.25	0/3112	0.41	0/4182
17	D	0.24	0/3039	0.42	0/4098
18	E	0.17	0/2380	0.38	0/3192
19	F	0.20	0/2919	0.39	0/3931
20	G	0.26	0/1919	0.42	0/2593
21	H	0.31	0/1857	0.38	0/2514
22	I	0.26	0/2074	0.34	0/2786
23	J	0.26	0/1913	0.38	0/2581
24	K	0.32	0/1804	0.46	0/2435
25	L	0.27	0/1891	0.39	0/2555
26	M	0.26	0/1955	0.39	0/2632
27	N	0.26	0/1513	0.41	0/2047
27	n	0.19	0/1352	0.35	0/1822
28	O	0.27	0/1694	0.40	0/2293
28	o	0.17	0/1323	0.37	0/1780
29	P	0.28	0/1620	0.42	0/2184
29	p	0.15	0/1282	0.37	0/1722

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	Q	0.28	0/1611	0.43	0/2180
30	q	0.18	0/1405	0.34	0/1899
31	R	0.25	0/1580	0.36	0/2134
31	r	0.26	0/1460	0.44	0/1972
32	S	0.25	0/1673	0.37	0/2254
32	s	0.18	0/1625	0.35	0/2188
33	T	0.25	0/1698	0.39	0/2299
33	t	0.18	0/1639	0.34	0/2217
All	All	0.24	0/91739	0.39	1/123787 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	75	PRO	CA-N-CD	-5.33	104.55	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6685	0	6748	180	0
2	V	3434	0	3503	134	0
3	W	3465	0	3591	153	0
4	X	3327	0	3423	103	0
5	Y	3123	0	3130	102	0
6	Z	2290	0	2320	76	0
7	a	3012	0	3029	119	0
8	b	1459	0	1499	53	0
9	c	2184	0	2191	85	0
10	d	2099	0	2127	77	0
11	e	314	0	247	14	0
12	f	5633	0	5648	262	0
13	x	1376	0	1324	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	3183	0	3242	163	0
15	B	3065	0	3130	165	0
16	C	3071	0	3193	156	0
17	D	2990	0	3029	152	0
18	E	2353	0	2404	135	0
19	F	2881	0	2973	116	0
20	G	1885	0	1889	76	0
21	H	1818	0	1811	51	0
22	I	2044	0	2069	62	0
23	J	1887	0	1905	93	0
24	K	1778	0	1761	78	0
25	L	1857	0	1845	81	0
26	M	1920	0	1893	79	0
27	N	1487	0	1452	66	0
27	n	1336	0	1324	62	0
28	O	1667	0	1689	100	0
28	o	1307	0	1310	39	0
29	P	1591	0	1609	100	0
29	p	1264	0	1255	44	0
30	Q	1578	0	1580	92	0
30	q	1380	0	1399	61	0
31	R	1549	0	1512	66	0
31	r	1432	0	1384	75	0
32	S	1643	0	1640	62	0
32	s	1597	0	1597	82	0
33	T	1665	0	1638	66	0
33	t	1609	0	1597	91	0
34	c	1	0	0	0	0
35	A	31	0	12	3	0
35	B	31	0	12	1	0
35	C	31	0	12	3	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
37	D	27	0	12	6	0
37	E	27	0	12	2	0
37	F	27	0	12	2	0
All	All	90418	0	90982	3336	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 (3336) 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)
14:A:339:ARG:NH2	19:F:405:MET:SD	2.27	1.07
29:P:67:LEU:HD11	29:P:91:VAL:HG22	1.37	1.06
24:K:91:LYS:NZ	24:K:95:GLU:OE2	1.87	1.06
12:f:171:GLN:NE2	12:f:210:GLU:OE2	1.93	1.02
19:F:251:LEU:HD22	19:F:285:ILE:HG23	1.41	1.02
12:f:771:LEU:HD21	12:f:825:MET:HE3	1.40	1.00
4:X:414:LEU:HD22	5:Y:383:LEU:HD11	1.43	0.98
21:H:66:GLU:OE1	21:H:83:TYR:OH	1.78	0.98
1:U:653:ALA:HB2	1:U:675:MET:HE1	1.46	0.98
16:C:405:TRP:O	22:I:50:ARG:NH2	1.97	0.98
10:d:128:PHE:O	10:d:174:TYR:OH	1.81	0.97
28:O:189:MET:HE1	28:O:197:LEU:HD22	1.46	0.97
30:q:139:THR:HG23	30:q:167:LEU:HD21	1.45	0.96
5:Y:319:MET:HE1	5:Y:334:LEU:HD11	1.46	0.96
14:A:95:VAL:O	14:A:115:VAL:HA	1.66	0.95
17:D:219:VAL:O	17:D:223:THR:OG1	1.84	0.95
23:J:87:ALA:HB2	23:J:111:ILE:HD11	1.50	0.94
33:t:90:VAL:HG13	33:t:112:LEU:HD21	1.50	0.94
2:V:223:LYS:O	2:V:261:TYR:OH	1.84	0.94
30:Q:3:TYR:N	30:Q:18:ASP:OD2	2.01	0.93
23:J:120:GLN:NE2	24:K:133:MET:SD	2.43	0.91
13:x:286:GLY:O	14:A:146:LYS:NZ	2.04	0.91
18:E:195:PHE:O	18:E:196:LEU:HD22	1.71	0.90
29:p:159:ASP:OD1	29:p:162:HIS:ND1	2.04	0.90
14:A:222:LYS:NZ	14:A:322:ASN:OD1	2.04	0.90
1:U:691:SER:HG	1:U:713:TYR:HH	1.19	0.89
31:R:225:ARG:NH1	29:p:34:MET:O	2.05	0.89
31:R:225:ARG:NH2	30:q:140:LEU:HD23	1.87	0.89
27:N:170:TYR:OH	33:T:79:ALA:O	1.91	0.88
33:t:46:THR:HG23	33:t:50:MET:HE1	1.55	0.88
30:q:131:ALA:HB3	30:q:140:LEU:HD11	1.56	0.88
14:A:190:VAL:HG21	14:A:212:VAL:HG21	1.53	0.88
17:D:89:ILE:HD11	18:E:80:VAL:HG13	1.54	0.87
33:t:47:GLN:NE2	33:t:148:MET:O	2.07	0.87
3:W:280:ASP:OD1	3:W:281:ASN:N	2.07	0.87
12:f:505:MET:SD	12:f:541:THR:OG1	2.31	0.87
3:W:422:ASN:OD1	6:Z:252:LYS:NZ	2.07	0.87
18:E:171:LEU:HD11	18:E:295:LEU:HD21	1.57	0.86
22:I:146:GLN:NE2	22:I:148:TYR:OH	2.07	0.86
12:f:250:ARG:NH1	12:f:251:CYS:SG	2.48	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:94:GLN:OE1	14:A:139:ARG:NH2	2.09	0.86
16:C:337:ASN:ND2	16:C:376:VAL:O	2.09	0.86
23:J:155:ALA:N	24:K:63:SER:OG	2.10	0.85
7:a:52:GLN:OE1	7:a:52:GLN:N	2.10	0.85
15:B:107:MET:HE3	15:B:160:ILE:HG23	1.58	0.85
30:Q:164:LEU:HD22	30:Q:178:PHE:CD2	2.11	0.85
29:p:58:THR:O	30:q:85:ARG:NH2	2.09	0.85
2:V:199:ASN:OD1	2:V:241:ARG:NH2	2.11	0.84
12:f:113:MET:SD	12:f:118:ASN:ND2	2.50	0.84
15:B:83:GLU:OE1	15:B:83:GLU:N	2.10	0.84
14:A:300:LEU:HA	14:A:303:ILE:HD12	1.59	0.84
5:Y:387:ILE:O	6:Z:279:LYS:NZ	2.10	0.84
19:F:288:LEU:HD21	19:F:342:LEU:HD21	1.60	0.84
24:K:35:SER:O	24:K:66:LYS:NZ	2.10	0.83
18:E:348:THR:HG22	18:E:352:MET:HE3	1.59	0.83
24:K:133:MET:HE2	24:K:133:MET:HA	1.61	0.83
3:W:172:GLU:O	18:E:146:ARG:NH2	2.12	0.83
30:Q:84:THR:HG22	30:Q:118:MET:HE1	1.60	0.82
32:S:55:THR:OG1	32:S:219:ASP:O	1.95	0.82
9:c:49:VAL:HG22	18:E:103:THR:HG21	1.60	0.82
2:V:259:LEU:HD11	2:V:295:ILE:HD11	1.61	0.82
9:c:248:MET:HE1	9:c:291:LEU:HD12	1.60	0.82
27:n:35:THR:N	27:n:204:SER:HG	1.78	0.81
14:A:299:MET:SD	14:A:303:ILE:HD11	2.20	0.81
17:D:79:VAL:O	17:D:82:ILE:HG22	1.80	0.81
3:W:440:ASN:OD1	6:Z:204:LYS:NZ	2.12	0.81
10:d:223:ASN:OD1	10:d:225:TYR:N	2.13	0.81
20:G:231:THR:OG1	20:G:234:GLU:OE1	1.99	0.81
25:L:67:ASP:OD1	25:L:68:ASN:N	2.13	0.81
16:C:268:GLU:OE1	16:C:271:ARG:NH2	2.14	0.81
10:d:312:PRO:O	10:d:317:SER:OG	1.97	0.81
2:V:181:TYR:HB2	2:V:221:LEU:HD21	1.63	0.81
30:Q:68:LYS:NZ	30:Q:74:GLU:OE2	2.13	0.81
1:U:377:HIS:O	1:U:380:THR:OG1	1.98	0.81
33:T:202:GLN:NE2	33:T:204:VAL:O	2.14	0.81
31:R:60:THR:N	31:R:228:TYR:O	2.14	0.80
10:d:141:LEU:HD22	10:d:182:LEU:HB2	1.62	0.80
29:P:21:ALA:HB2	29:P:163:LEU:HD21	1.63	0.80
25:L:157:ARG:NH2	25:L:176:MET:O	2.15	0.80
16:C:40:GLN:OE1	16:C:43:ARG:NH2	2.14	0.80
21:H:154:ALA:HB2	22:I:80:THR:HG21	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:251:ILE:HG23	16:C:301:LEU:HD11	1.63	0.80
30:Q:5:ILE:HD11	30:Q:143:LEU:HD11	1.63	0.80
27:n:36:THR:HG21	27:n:197:ALA:CB	2.11	0.80
26:M:42:CYS:SG	26:M:45:GLY:N	2.55	0.80
12:f:609:VAL:HG12	12:f:660:ILE:HG21	1.64	0.80
4:X:371:ASP:OD1	5:Y:233:ARG:NH1	2.15	0.79
7:a:223:GLU:OE1	7:a:226:ARG:NH1	2.15	0.79
9:c:265:MET:SD	9:c:266:THR:HG23	2.23	0.79
28:O:133:TYR:HD2	28:O:137:ILE:HD11	1.46	0.79
2:V:243:ASP:OD1	2:V:244:ALA:N	2.14	0.79
3:W:170:GLN:OE1	3:W:170:GLN:N	2.15	0.79
14:A:196:LEU:O	14:A:197:HIS:ND1	2.15	0.79
32:S:214:ASP:O	32:S:217:THR:OG1	1.98	0.79
1:U:7:GLY:O	1:U:10:SER:OG	2.00	0.79
1:U:27:LEU:O	1:U:31:VAL:HG23	1.82	0.79
3:W:260:SER:OG	3:W:261:GLU:OE1	1.99	0.79
12:f:666:ILE:HD11	15:B:68:ILE:CG1	2.12	0.79
2:V:353:LEU:HD23	2:V:357:LEU:HD11	1.63	0.79
4:X:415:TYR:CD1	5:Y:383:LEU:HD12	2.18	0.79
5:Y:297:ARG:NE	11:e:44:ASP:OD2	2.16	0.79
8:b:83:LYS:NZ	8:b:118:GLU:OE1	2.16	0.79
29:p:187:VAL:O	29:p:198:ARG:N	2.16	0.79
5:Y:222:TYR:OH	5:Y:285:ASP:OD2	2.00	0.78
27:N:48:LEU:HD21	27:N:135:ALA:HB3	1.63	0.78
17:D:258:ALA:HB3	17:D:259:PRO:HD3	1.64	0.78
22:I:46:ALA:HB1	22:I:197:LEU:HD11	1.66	0.78
6:Z:21:ASP:OD2	9:c:104:ARG:NH2	2.16	0.78
14:A:191:VAL:HG11	14:A:229:VAL:HG21	1.65	0.78
15:B:103:ARG:NH2	15:B:160:ILE:O	2.16	0.78
19:F:224:LEU:HD13	19:F:343:LEU:HD21	1.63	0.78
29:P:13:ALA:HB3	29:P:137:VAL:CG2	2.13	0.78
32:S:216:TYR:CE2	28:o:67:MET:HE1	2.19	0.78
5:Y:387:ILE:HG21	6:Z:276:ILE:CD1	2.14	0.78
12:f:482:ILE:HG21	12:f:518:THR:HA	1.66	0.78
2:V:67:LEU:O	2:V:71:THR:HG23	1.84	0.77
32:S:195:SER:OG	32:S:197:ASP:OD1	2.01	0.77
26:M:216:TRP:CE3	26:M:228:VAL:HG22	2.19	0.77
12:f:545:LYS:HZ1	12:f:583:VAL:HG22	1.47	0.77
12:f:552:ASP:O	12:f:553:THR:OG1	2.03	0.77
30:q:117:TYR:N	30:q:125:ALA:O	2.18	0.77
7:a:72:ASN:OD1	8:b:17:ARG:NH1	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:327:ASN:ND2	12:f:420:TRP:O	2.17	0.77
17:D:135:HIS:O	17:D:136:SER:OG	2.02	0.77
28:o:123:ASN:OD1	28:o:156:ILE:HD11	1.83	0.77
2:V:167:LEU:O	2:V:171:VAL:HG23	1.85	0.77
5:Y:183:TYR:CE1	5:Y:213:LEU:HD11	2.19	0.76
9:c:29:GLU:OE2	9:c:139:ARG:NH2	2.17	0.76
18:E:310:LEU:HD11	18:E:329:GLU:HG3	1.67	0.76
19:F:254:PRO:O	19:F:257:VAL:HG22	1.85	0.76
27:n:46:VAL:HG11	27:n:135:ALA:HB1	1.67	0.76
1:U:835:ILE:HD11	12:f:606:VAL:HG22	1.67	0.76
7:a:37:LEU:O	7:a:41:VAL:HG23	1.86	0.76
31:R:176:GLU:OE1	31:R:176:GLU:N	2.18	0.76
12:f:520:LEU:HD23	12:f:560:LEU:HD22	1.68	0.76
21:H:6:TYR:OH	22:I:6:ASP:OD2	2.02	0.76
5:Y:262:SER:HB2	5:Y:270:VAL:HG23	1.68	0.76
14:A:265:ARG:NH2	14:A:305:GLN:OE1	2.18	0.76
19:F:424:ILE:O	19:F:428:GLN:NE2	2.18	0.76
27:N:60:ILE:HD11	28:O:175:LEU:HD23	1.67	0.76
24:K:98:ASN:OD1	31:R:120:ARG:NE	2.19	0.76
29:P:53:LEU:HD13	29:P:63:VAL:HG23	1.68	0.76
7:a:35:HIS:NE2	8:b:14:GLU:OE1	2.19	0.75
14:A:297:ARG:HD2	19:F:257:VAL:HG21	1.68	0.75
31:r:233:VAL:HG21	31:r:254:LEU:CD1	2.16	0.75
33:T:76:GLY:O	33:T:77:SER:OG	2.04	0.75
23:J:88:ARG:NE	30:Q:69:MET:O	2.19	0.75
18:E:74:THR:HG21	19:F:131:THR:HB	1.68	0.75
26:M:78:VAL:HG21	26:M:85:ALA:CB	2.16	0.75
32:s:202:LEU:O	32:s:206:VAL:HG23	1.85	0.75
9:c:232:GLN:NE2	9:c:236:GLU:OE1	2.19	0.75
31:R:212:TYR:OH	31:R:237:HIS:ND1	2.19	0.75
2:V:171:VAL:HG12	2:V:175:MET:HE1	1.69	0.75
24:K:79:SER:OG	24:K:170:ILE:HD12	1.86	0.75
31:R:193:TYR:OH	29:p:33:GLN:NE2	2.19	0.75
3:W:345:GLU:OE1	3:W:346:GLU:N	2.20	0.75
18:E:175:PRO:O	18:E:177:GLY:N	2.20	0.75
18:E:180:LYS:NZ	37:E:401:ADP:O2B	2.19	0.75
24:K:117:SER:OG	24:K:160:GLY:O	2.03	0.75
2:V:176:MET:CE	2:V:217:VAL:HG22	2.17	0.75
12:f:502:LEU:HD11	12:f:534:VAL:HG22	1.69	0.75
14:A:405:THR:OG1	14:A:406:GLU:OE1	2.05	0.75
29:P:34:MET:O	31:r:225:ARG:NH1	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:s:214:ASP:OD1	32:s:216:TYR:N	2.20	0.75
2:V:282:ASN:OD1	5:Y:385:ARG:NE	2.20	0.74
6:Z:34:ARG:NH1	6:Z:60:GLU:OE1	2.20	0.74
16:C:60:ARG:NH2	17:D:71:GLU:OE2	2.20	0.74
28:O:241:ARG:NH2	29:P:151:GLU:O	2.21	0.74
12:f:666:ILE:HD11	15:B:68:ILE:HG13	1.70	0.74
17:D:181:VAL:HG11	17:D:219:VAL:HG21	1.69	0.74
23:J:33:VAL:HG22	23:J:160:ALA:HB2	1.70	0.74
8:b:180:ALA:O	8:b:184:ILE:HD12	1.86	0.74
9:c:129:THR:O	9:c:132:SER:OG	2.06	0.74
27:N:60:ILE:CD1	28:O:175:LEU:HD23	2.18	0.74
3:W:307:LYS:O	3:W:311:THR:HG23	1.87	0.74
29:p:203:ARG:NH2	29:p:205:ASP:OD2	2.21	0.74
1:U:583:MET:CE	1:U:605:VAL:HG21	2.18	0.74
14:A:117:GLN:N	14:A:117:GLN:OE1	2.21	0.74
27:n:164:SER:OG	27:n:203:SER:OG	2.02	0.74
2:V:300:LEU:O	2:V:300:LEU:HD23	1.88	0.73
30:q:49:GLU:OE1	30:q:99:HIS:ND1	2.21	0.73
32:s:120:LEU:HD23	32:s:152:PHE:CE2	2.23	0.73
14:A:138:MET:HE2	14:A:152:PRO:HB2	1.69	0.73
17:D:387:VAL:HG11	18:E:159:PHE:HE1	1.53	0.73
2:V:482:PHE:O	2:V:486:ILE:HD12	1.88	0.73
29:P:67:LEU:CD1	29:P:91:VAL:HG22	2.16	0.73
30:Q:164:LEU:HD22	30:Q:178:PHE:CE2	2.24	0.73
30:Q:170:ARG:NH2	30:q:27:GLN:O	2.21	0.73
33:t:62:GLU:N	33:t:62:GLU:OE1	2.21	0.73
2:V:467:TYR:OH	4:X:397:TYR:OH	2.06	0.73
2:V:213:TYR:O	2:V:217:VAL:HG23	1.89	0.73
17:D:202:VAL:HG12	17:D:329:ARG:HB3	1.70	0.73
32:S:176:LEU:HD23	32:S:206:VAL:HG12	1.71	0.73
30:q:51:GLY:N	31:r:177:GLY:O	2.22	0.73
30:Q:153:ARG:NH2	30:Q:184:ASP:OD2	2.21	0.73
28:O:56:VAL:HG12	28:O:198:VAL:HG11	1.68	0.73
1:U:899:ARG:NH2	1:U:920:ASP:OD1	2.21	0.73
12:f:346:ASP:O	12:f:349:TYR:C	2.32	0.73
32:S:197:ASP:OD1	32:S:198:ARG:N	2.21	0.73
29:p:106:GLU:OE1	29:p:139:SER:OG	2.07	0.73
12:f:377:VAL:HG23	12:f:767:GLY:HA2	1.71	0.72
22:I:154:GLY:O	23:J:81:ARG:NH2	2.22	0.72
7:a:206:LEU:HD11	7:a:261:LEU:HD23	1.69	0.72
23:J:42:VAL:CG1	23:J:191:VAL:HG21	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:54:VAL:HG12	30:Q:58:GLU:OE2	1.88	0.72
5:Y:219:PHE:O	5:Y:223:THR:HG23	1.90	0.72
29:P:171:MET:HE2	29:P:185:VAL:HG13	1.70	0.72
30:Q:35:MET:SD	30:Q:45:LEU:HD21	2.29	0.72
27:N:196:LEU:HD22	27:n:174:ASP:OD1	1.90	0.72
29:P:59:ASP:OD1	30:Q:93:ARG:NH2	2.22	0.72
12:f:187:LEU:O	12:f:191:ILE:HD12	1.88	0.72
14:A:297:ARG:HD3	19:F:257:VAL:HG11	1.71	0.72
27:N:48:LEU:HD21	27:N:135:ALA:CB	2.18	0.72
31:r:188:GLY:O	31:r:191:SER:OG	2.04	0.72
2:V:212:TYR:OH	11:e:21:GLU:OE1	2.04	0.72
12:f:782:HIS:O	12:f:785:ARG:NH2	2.22	0.72
33:T:232:PHE:CE1	33:T:250:THR:HG23	2.24	0.72
12:f:53:GLN:NE2	12:f:57:GLU:OE2	2.22	0.72
7:a:333:MET:HE2	7:a:333:MET:HA	1.71	0.72
16:C:281:ASP:OD2	16:C:307:ARG:NH2	2.23	0.71
33:T:78:LEU:O	33:T:78:LEU:HD23	1.90	0.71
31:r:89:THR:O	32:s:159:GLN:NE2	2.23	0.71
5:Y:304:TYR:OH	5:Y:333:GLU:OE2	2.08	0.71
12:f:416:MET:SD	12:f:822:VAL:HG11	2.29	0.71
25:L:195:LEU:HD23	25:L:205:LEU:HD11	1.72	0.71
27:n:153:MET:SD	33:t:51:VAL:HG11	2.30	0.71
1:U:144:ASP:OD2	16:C:18:SER:N	2.23	0.71
15:B:250:VAL:HG22	15:B:270:LEU:HD11	1.71	0.71
16:C:151:ILE:HG12	16:C:198:LEU:HD22	1.72	0.71
24:K:125:GLU:OE1	24:K:125:GLU:N	2.22	0.71
28:O:60:ASP:O	28:O:76:LYS:NZ	2.23	0.71
31:r:233:VAL:O	31:r:233:VAL:HG12	1.90	0.71
8:b:11:ASP:O	8:b:16:MET:HE3	1.90	0.71
24:K:195:ILE:HD12	24:K:217:LEU:HD21	1.71	0.71
2:V:330:LYS:NZ	2:V:389:ASP:OD2	2.22	0.71
14:A:317:VAL:HG11	14:A:319:MET:HE2	1.73	0.71
15:B:365:PHE:O	15:B:369:THR:HG22	1.90	0.71
23:J:188:ILE:O	23:J:192:ILE:HD12	1.90	0.71
28:O:86:CYS:SG	28:O:141:LEU:HD22	2.31	0.71
29:p:149:MET:N	29:p:149:MET:HE2	2.05	0.71
12:f:274:ASP:OD2	12:f:277:LEU:N	2.24	0.71
17:D:291:GLU:OE2	17:D:295:GLN:NE2	2.23	0.71
22:I:153:SER:OG	22:I:155:ASN:OD1	2.07	0.71
18:E:236:ASP:OD1	18:E:281:ARG:NH2	2.24	0.70
28:O:55:ILE:HD11	28:O:221:ILE:HD12	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:92:LEU:HD22	32:S:134:VAL:HG21	1.71	0.70
29:p:67:LEU:HD12	29:p:90:MET:HE1	1.73	0.70
3:W:81:ASP:OD1	3:W:123:ARG:NH1	2.24	0.70
27:N:53:ARG:HG2	27:N:55:THR:HG23	1.72	0.70
1:U:579:ARG:NH1	1:U:609:ASP:OD1	2.24	0.70
1:U:583:MET:HE1	1:U:605:VAL:HG21	1.73	0.70
1:U:738:ASP:OD1	1:U:742:HIS:NE2	2.23	0.70
12:f:44:GLU:OE2	14:A:24:ALA:N	2.24	0.70
23:J:195:LEU:O	23:J:199:VAL:HG22	1.91	0.70
25:L:140:MET:HE1	33:T:124:ASP:O	1.91	0.70
2:V:192:MET:HE1	2:V:211:TYR:HA	1.73	0.70
3:W:445:LEU:CB	6:Z:226:ILE:HD11	2.22	0.70
12:f:137:ARG:HH12	12:f:168:LYS:HZ1	1.38	0.70
23:J:11:SER:OG	23:J:13:ASP:OD1	2.06	0.70
28:O:78:HIS:HB2	28:O:99:THR:HG21	1.73	0.70
32:S:141:LEU:HD13	32:S:226:VAL:HG12	1.72	0.70
28:O:175:LEU:HD13	33:t:189:TYR:HB3	1.72	0.70
29:P:37:THR:HG22	29:P:37:THR:O	1.92	0.70
10:d:268:ARG:NH1	10:d:292:PHE:O	2.24	0.70
27:N:169:ILE:O	27:N:173:VAL:HG23	1.92	0.70
4:X:415:TYR:HD1	5:Y:383:LEU:HD12	1.55	0.70
15:B:269:GLU:OE1	15:B:272:ARG:NH2	2.25	0.70
15:B:288:ASP:OD1	16:C:274:LEU:HD21	1.90	0.70
18:E:144:GLU:O	18:E:148:VAL:HG23	1.91	0.70
28:O:214:SER:OG	32:s:239:ARG:NH1	2.24	0.70
1:U:95:GLU:OE2	2:V:237:THR:OG1	2.09	0.70
1:U:622:LEU:HD21	1:U:636:VAL:HG11	1.74	0.70
12:f:416:MET:SD	12:f:822:VAL:HG21	2.31	0.70
15:B:440:LEU:O	23:J:77:THR:OG1	2.10	0.70
32:s:41:LEU:HD11	32:s:177:LEU:HD11	1.74	0.70
5:Y:280:GLN:OE1	11:e:53:SER:OG	2.08	0.69
12:f:528:GLY:N	12:f:564:LEU:O	2.25	0.69
23:J:228:TYR:O	23:J:232:ILE:HD12	1.92	0.69
31:r:139:SER:CB	31:r:179:ARG:HE	2.05	0.69
6:Z:263:ALA:HB1	9:c:288:VAL:HG23	1.72	0.69
29:P:95:LEU:HD11	29:P:107:PRO:HG2	1.75	0.69
32:S:66:ARG:NH1	32:S:219:ASP:OD1	2.25	0.69
32:S:75:THR:HG1	32:S:78:THR:HG1	1.30	0.69
3:W:369:TYR:CD2	7:a:312:MET:HE1	2.27	0.69
4:X:343:SER:O	4:X:345:VAL:HG23	1.91	0.69
12:f:346:ASP:O	12:f:349:TYR:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:154:ALA:HB1	21:H:156:PHE:HE2	1.55	0.69
33:T:171:ASP:OD1	33:T:175:VAL:N	2.26	0.69
15:B:112:LEU:HD21	15:B:115:ILE:HG13	1.74	0.69
35:C:501:ATP:O3G	17:D:323:ARG:NH2	2.25	0.69
21:H:154:ALA:HB1	21:H:156:PHE:CE2	2.27	0.69
23:J:104:VAL:HG11	23:J:143:ARG:HB2	1.74	0.69
25:L:72:ILE:HD11	25:L:132:LEU:HD22	1.74	0.69
15:B:337:LEU:HD12	15:B:342:ILE:HD11	1.75	0.69
1:U:237:VAL:HG21	1:U:325:MET:HE1	1.74	0.69
1:U:919:GLU:OE1	1:U:919:GLU:N	2.25	0.69
12:f:429:ILE:HG21	12:f:448:CYS:SG	2.33	0.69
27:N:47:VAL:HG12	27:N:212:ALA:HB2	1.75	0.69
27:N:125:ARG:NH2	33:T:101:ASP:OD2	2.25	0.69
32:S:180:GLN:O	32:S:198:ARG:NH2	2.25	0.69
3:W:112:VAL:HA	3:W:115:ILE:HD12	1.73	0.69
9:c:84:VAL:HG13	13:x:278:PHE:CE2	2.28	0.69
2:V:440:LYS:NZ	10:d:236:LEU:O	2.24	0.69
7:a:240:PHE:HZ	7:a:268:LEU:HD22	1.56	0.69
12:f:398:TRP:O	12:f:401:LYS:NZ	2.26	0.69
14:A:101:ILE:O	14:A:102:ILE:HG22	1.93	0.69
27:n:148:VAL:HG22	27:n:153:MET:O	1.93	0.69
10:d:98:LEU:HD21	10:d:150:ILE:HG21	1.75	0.68
12:f:659:LEU:HD13	12:f:797:LEU:HD21	1.75	0.68
12:f:456:ARG:NH2	12:f:492:SER:OG	2.26	0.68
18:E:57:VAL:O	18:E:74:THR:HG23	1.92	0.68
27:n:125:ARG:NH1	33:t:50:MET:SD	2.66	0.68
2:V:289:LEU:HB3	2:V:312:ALA:HB2	1.74	0.68
18:E:294:ARG:NE	18:E:296:ASP:OD2	2.25	0.68
20:G:196:GLU:HG2	20:G:242:LEU:HD13	1.74	0.68
26:M:71:ASP:O	33:T:121:LEU:HD21	1.94	0.68
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.76	0.68
2:V:131:LEU:HD23	2:V:171:VAL:HG21	1.74	0.68
15:B:329:MET:SD	15:B:347:ILE:HD11	2.34	0.68
15:B:407:LEU:HD11	16:C:174:LEU:HD23	1.75	0.68
16:C:214:VAL:HG21	16:C:234:LEU:HD21	1.74	0.68
23:J:42:VAL:HG13	23:J:191:VAL:HG21	1.76	0.68
22:I:45:LEU:HD12	22:I:137:ILE:HD13	1.75	0.68
27:n:62:ASN:CG	28:o:165:LEU:HD21	2.18	0.68
1:U:1:MET:SD	1:U:2:ILE:N	2.66	0.68
2:V:181:TYR:CB	2:V:221:LEU:HD21	2.24	0.68
3:W:183:VAL:O	3:W:187:LEU:HD23	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:117:VAL:O	8:b:152:LYS:NZ	2.24	0.68
28:O:94:ASP:HB3	28:O:137:ILE:HG23	1.74	0.68
29:P:12:MET:HE2	29:P:14:MET:HE1	1.76	0.68
1:U:52:GLU:OE2	1:U:57:ARG:NH2	2.26	0.68
2:V:334:VAL:O	2:V:338:LEU:HD23	1.93	0.68
12:f:89:MET:O	12:f:90:THR:OG1	2.09	0.68
28:O:73:ASN:OD1	28:O:230:ARG:NH1	2.24	0.68
6:Z:73:ASP:OD2	8:b:63:THR:OG1	2.10	0.68
16:C:388:ALA:O	16:C:392:GLN:NE2	2.27	0.68
19:F:288:LEU:HD12	19:F:291:ILE:HD12	1.76	0.68
32:s:181:VAL:CG2	32:s:194:LEU:HD22	2.24	0.68
16:C:81:ASP:OD1	16:C:82:LYS:N	2.26	0.68
19:F:385:ALA:O	19:F:388:THR:OG1	2.12	0.68
5:Y:273:GLN:OE1	11:e:60:LEU:HD11	1.93	0.68
10:d:309:VAL:O	10:d:309:VAL:HG12	1.94	0.68
12:f:233:LEU:O	12:f:237:VAL:HG23	1.94	0.68
28:O:133:TYR:CD2	28:O:137:ILE:HD11	2.28	0.68
22:I:17:ARG:NH1	22:I:22:GLU:OE2	2.27	0.67
31:R:129:ASN:O	31:R:131:GLU:N	2.26	0.67
30:q:4:LEU:HD13	30:q:45:LEU:HB3	1.76	0.67
1:U:161:ASP:OD1	1:U:162:VAL:N	2.27	0.67
4:X:354:ILE:HG22	4:X:356:LEU:HD23	1.76	0.67
4:X:414:LEU:HD21	6:Z:276:ILE:HG13	1.76	0.67
6:Z:23:PHE:CE2	6:Z:126:VAL:HG21	2.29	0.67
9:c:32:TYR:CE2	9:c:66:THR:HG23	2.30	0.67
29:p:2:SER:O	29:p:5:SER:OG	2.11	0.67
1:U:834:SER:OG	15:B:66:GLU:OE2	2.09	0.67
2:V:162:GLU:OE2	2:V:200:ARG:NH1	2.27	0.67
3:W:241:LEU:HD11	3:W:286:LEU:HD22	1.74	0.67
10:d:341:GLU:OE2	10:d:344:ARG:NH2	2.27	0.67
22:I:175:LEU:HD23	22:I:192:LEU:HD21	1.76	0.67
22:I:178:ASP:OD2	22:I:195:LYS:NZ	2.14	0.67
15:B:197:ILE:HD13	15:B:235:LEU:HG	1.76	0.67
12:f:219:LYS:O	12:f:258:LYS:NZ	2.24	0.67
15:B:70:ASP:OD1	15:B:71:TYR:N	2.27	0.67
2:V:131:LEU:CD2	2:V:171:VAL:HG21	2.25	0.67
16:C:221:GLN:NE2	16:C:230:MET:HE1	2.10	0.67
16:C:375:ARG:NH2	16:C:382:ASP:OD2	2.28	0.67
23:J:104:VAL:HG12	23:J:137:ASP:OD1	1.95	0.67
3:W:445:LEU:HB3	6:Z:226:ILE:HD11	1.77	0.67
22:I:119:GLN:NE2	22:I:123:GLN:OE1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:216:TYR:CZ	28:o:67:MET:HE1	2.30	0.67
1:U:622:LEU:HD21	1:U:636:VAL:CG1	2.25	0.67
5:Y:228:MET:HE1	5:Y:259:TYR:CE2	2.30	0.67
14:A:297:ARG:CD	19:F:257:VAL:HG21	2.25	0.67
29:P:172:LEU:HD11	29:P:201:LYS:O	1.94	0.67
2:V:497:PRO:O	16:C:43:ARG:NH1	2.28	0.67
25:L:199:LEU:HD11	25:L:205:LEU:HD22	1.77	0.67
1:U:446:LEU:HD22	1:U:457:ILE:CD1	2.25	0.66
2:V:309:MET:HE2	2:V:331:LEU:HB3	1.75	0.66
9:c:279:ASP:OD1	9:c:282:ARG:NH2	2.27	0.66
18:E:117:PRO:O	18:E:121:ASN:ND2	2.27	0.66
24:K:47:CYS:SG	24:K:195:ILE:HD13	2.35	0.66
33:T:223:TYR:O	27:n:60:ILE:HD11	1.96	0.66
3:W:112:VAL:O	3:W:121:LYS:NZ	2.18	0.66
12:f:408:LEU:HD11	12:f:446:LEU:HD12	1.76	0.66
17:D:254:ALA:HB2	17:D:262:ILE:HD11	1.77	0.66
25:L:38:LEU:HD13	25:L:187:LEU:HD11	1.77	0.66
27:N:125:ARG:NH1	33:T:46:THR:OG1	2.28	0.66
18:E:235:ILE:HD12	18:E:279:THR:HB	1.77	0.66
22:I:90:LEU:HD22	22:I:110:LEU:HD21	1.78	0.66
15:B:121:ALA:HB2	15:B:135:ILE:HD11	1.77	0.66
29:P:205:ASP:OXT	31:r:78:ARG:NH1	2.27	0.66
5:Y:319:MET:CE	5:Y:334:LEU:HD11	2.23	0.66
18:E:325:GLU:O	18:E:328:TYR:N	2.28	0.66
26:M:32:GLU:O	26:M:33:ASN:ND2	2.26	0.66
29:P:35:VAL:HG12	29:P:36:THR:HG23	1.77	0.66
3:W:132:THR:O	3:W:142:ARG:NH1	2.28	0.66
9:c:305:ASP:HA	9:c:308:VAL:HG12	1.78	0.66
12:f:679:LEU:HD22	12:f:713:PHE:CE2	2.31	0.66
13:x:273:THR:HG23	13:x:273:THR:O	1.94	0.66
24:K:151:PRO:O	24:K:152:GLN:NE2	2.28	0.66
31:r:78:ARG:NE	31:r:88:GLN:OE1	2.25	0.66
15:B:341:LEU:O	15:B:347:ILE:HD12	1.96	0.66
7:a:360:VAL:HG22	9:c:308:VAL:CG2	2.25	0.66
19:F:376:SER:OG	19:F:414:GLU:OE1	2.13	0.66
22:I:45:LEU:CD1	22:I:137:ILE:HD13	2.25	0.66
27:n:82:SER:OG	27:n:129:MET:O	2.14	0.66
1:U:156:GLU:OE2	17:D:45:LYS:NZ	2.28	0.66
1:U:206:MET:HE3	1:U:216:VAL:HG21	1.78	0.66
12:f:195:ASN:CG	12:f:204:ALA:HB2	2.21	0.66
16:C:322:GLU:O	16:C:323:GLU:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:387:VAL:HG11	18:E:159:PHE:CE1	2.31	0.66
18:E:295:LEU:HD23	18:E:295:LEU:O	1.96	0.66
22:I:76:VAL:HG21	22:I:83:ALA:HB1	1.78	0.66
33:t:104:ASP:O	33:t:108:LEU:HD23	1.97	0.66
14:A:191:VAL:HG22	14:A:318:LEU:HD21	1.77	0.65
16:C:219:LEU:HD12	16:C:254:ILE:HD12	1.77	0.65
31:r:139:SER:HB3	31:r:179:ARG:HE	1.61	0.65
31:r:241:ASP:OD1	31:r:242:GLY:N	2.29	0.65
7:a:224:SER:C	7:a:225:LEU:HD12	2.21	0.65
12:f:825:MET:O	12:f:826:GLN:NE2	2.30	0.65
17:D:89:ILE:O	17:D:106:THR:HG23	1.96	0.65
25:L:196:ARG:HG2	25:L:205:LEU:HD23	1.76	0.65
7:a:137:ASP:OD1	7:a:138:VAL:N	2.29	0.65
7:a:258:GLN:OE1	7:a:260:ASP:N	2.28	0.65
28:O:175:LEU:HD13	33:t:189:TYR:CB	2.26	0.65
7:a:88:THR:HG22	7:a:88:THR:O	1.97	0.65
22:I:47:ALA:HB1	22:I:64:LYS:HD2	1.79	0.65
29:P:21:ALA:CB	29:P:163:LEU:HD21	2.26	0.65
29:p:178:ASP:OD1	29:p:179:ALA:N	2.28	0.65
32:s:165:ALA:HB1	32:s:173:LEU:HD12	1.77	0.65
33:t:90:VAL:CG1	33:t:112:LEU:HD21	2.26	0.65
3:W:74:CYS:SG	3:W:86:ASN:ND2	2.69	0.65
4:X:96:PHE:HA	4:X:99:MET:HE1	1.79	0.65
6:Z:90:ARG:O	6:Z:92:VAL:HG13	1.95	0.65
17:D:229:ARG:NH2	17:D:265:ASP:OD2	2.30	0.65
19:F:288:LEU:CD1	19:F:291:ILE:HD12	2.26	0.65
22:I:119:GLN:CG	23:J:78:ALA:HB1	2.27	0.65
1:U:2:ILE:HD11	10:d:131:THR:HA	1.79	0.65
24:K:164:GLN:NE2	24:K:166:ASP:OD1	2.29	0.65
20:G:11:ARG:O	20:G:12:HIS:ND1	2.29	0.65
21:H:210:VAL:HG23	21:H:221:LEU:HD12	1.79	0.65
27:N:47:VAL:HG12	27:N:212:ALA:CB	2.27	0.65
4:X:35:ILE:HD11	4:X:46:LYS:HD2	1.78	0.65
16:C:260:GLU:OE1	16:C:260:GLU:N	2.29	0.65
18:E:342:ASP:OD1	18:E:343:LEU:N	2.29	0.65
12:f:50:LYS:NZ	12:f:54:ASP:OD1	2.30	0.65
12:f:541:THR:HG22	12:f:558:LEU:HD21	1.79	0.65
12:f:794:ALA:O	12:f:798:THR:HG23	1.96	0.65
15:B:362:LYS:NZ	15:B:381:ASP:OD1	2.26	0.65
15:B:439:TYR:OH	22:I:16:GLY:O	2.14	0.65
16:C:191:PRO:O	16:C:196:LYS:NZ	2.19	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:268:ASP:OD1	17:D:311:THR:OG1	2.15	0.65
28:o:184:LYS:HG3	28:o:197:LEU:HD13	1.79	0.65
1:U:624:PHE:CE1	1:U:658:ILE:HD13	2.31	0.64
23:J:159:ASN:OD1	23:J:160:ALA:N	2.27	0.64
5:Y:158:THR:O	5:Y:162:GLU:OE1	2.15	0.64
8:b:56:ASN:OD1	8:b:57:ASP:N	2.30	0.64
12:f:369:ARG:NH1	12:f:756:PRO:O	2.30	0.64
12:f:545:LYS:NZ	12:f:583:VAL:HG22	2.12	0.64
17:D:384:MET:HE1	18:E:167:PRO:HB3	1.78	0.64
2:V:113:LEU:HD22	2:V:174:PHE:CD2	2.32	0.64
31:R:236:TYR:CE1	31:R:245:ARG:HG3	2.31	0.64
2:V:236:ARG:O	2:V:240:LEU:HD23	1.98	0.64
31:r:60:THR:N	31:r:189:SER:HG	1.95	0.64
21:H:39:LYS:NZ	22:I:57:ASP:OD2	2.21	0.64
31:R:103:THR:O	31:R:158:THR:OG1	2.15	0.64
31:r:174:ASP:OD2	31:r:178:ASN:ND2	2.30	0.64
15:B:81:ASN:O	15:B:85:MET:N	2.30	0.64
26:M:78:VAL:HG21	26:M:85:ALA:HB2	1.79	0.64
27:N:168:TYR:CZ	33:t:78:LEU:HD13	2.33	0.64
3:W:231:ILE:HD13	3:W:247:TYR:CD1	2.33	0.64
12:f:776:LEU:HD23	12:f:827:PRO:HA	1.78	0.64
14:A:306:LEU:HD21	14:A:317:VAL:HG21	1.77	0.64
1:U:108:TYR:OH	1:U:131:GLU:OE2	2.09	0.64
3:W:145:LEU:O	3:W:148:THR:OG1	2.15	0.64
14:A:174:TYR:CD1	14:A:184:ILE:HD11	2.33	0.64
14:A:306:LEU:O	14:A:312:ARG:NH1	2.30	0.64
15:B:94:GLU:O	15:B:97:SER:OG	2.12	0.64
16:C:280:LEU:CD2	16:C:291:VAL:HG21	2.28	0.64
33:T:169:TYR:CE1	33:T:184:THR:HG22	2.33	0.64
28:o:206:ILE:HG23	28:o:213:GLY:HA2	1.78	0.64
32:s:173:LEU:CD2	32:s:206:VAL:HG12	2.28	0.64
27:N:184:GLU:O	27:N:188:GLN:OE1	2.16	0.64
33:t:219:ARG:NE	33:t:251:GLU:O	2.31	0.64
2:V:83:GLU:O	2:V:87:SER:OG	2.09	0.63
12:f:399:LEU:CD1	12:f:410:ALA:HB3	2.28	0.63
20:G:113:MET:HE2	28:O:113:THR:HA	1.79	0.63
22:I:95:GLN:HG3	29:P:73:LEU:HD22	1.80	0.63
27:n:93:VAL:HG21	27:n:117:PHE:CD1	2.33	0.63
32:s:39:THR:CG2	32:s:173:LEU:HD11	2.28	0.63
2:V:176:MET:HE3	2:V:217:VAL:HG22	1.79	0.63
7:a:77:VAL:O	7:a:81:LEU:HD23	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:27:THR:HG23	9:c:176:GLN:O	1.98	0.63
18:E:142:ILE:HD13	18:E:183:LEU:CD1	2.29	0.63
30:Q:43:LEU:HD11	30:Q:188:ILE:HG21	1.80	0.63
32:S:46:GLU:OE1	32:S:46:GLU:N	2.31	0.63
6:Z:131:LEU:HD11	6:Z:200:GLY:HA2	1.80	0.63
12:f:195:ASN:ND2	12:f:200:ALA:O	2.30	0.63
12:f:505:MET:HA	12:f:518:THR:HG21	1.80	0.63
21:H:68:ILE:O	21:H:69:THR:OG1	2.13	0.63
24:K:36:THR:HG22	24:K:51:GLU:CD	2.23	0.63
28:O:166:PRO:HB3	33:t:259:MET:HE1	1.79	0.63
30:Q:51:GLY:N	31:R:177:GLY:O	2.32	0.63
31:R:85:ILE:HD12	31:R:88:GLN:OE1	1.98	0.63
13:x:148:ASN:ND2	13:x:156:PHE:O	2.31	0.63
18:E:305:ASN:OD1	18:E:306:GLU:N	2.32	0.63
24:K:105:GLU:OE2	32:S:103:TYR:OH	2.15	0.63
29:p:67:LEU:HD11	29:p:87:LEU:HD11	1.80	0.63
16:C:267:SER:O	16:C:271:ARG:NE	2.31	0.63
17:D:233:SER:HB2	18:E:260:LEU:HD13	1.80	0.63
17:D:274:ARG:NE	17:D:318:ASP:OD1	2.32	0.63
18:E:89:LYS:O	18:E:90:SER:OG	2.13	0.63
9:c:32:TYR:CD2	9:c:66:THR:HG23	2.34	0.63
17:D:357:GLU:OE1	17:D:357:GLU:N	2.32	0.63
20:G:52:THR:OG1	20:G:79:VAL:HG21	1.99	0.63
7:a:37:LEU:HD11	7:a:67:PHE:CE2	2.34	0.63
19:F:175:MET:SD	19:F:249:LEU:HD11	2.39	0.63
29:P:87:LEU:O	29:P:91:VAL:HG23	1.98	0.63
31:R:203:SER:OG	31:R:205:ASP:O	2.17	0.63
27:n:177:TYR:OH	27:n:179:GLU:OE1	2.14	0.63
12:f:674:THR:HG22	15:B:75:GLU:CG	2.29	0.63
35:A:501:ATP:O1G	15:B:346:ARG:NH1	2.30	0.63
16:C:119:ASP:O	16:C:120:SER:OG	2.14	0.63
1:U:722:ASP:O	1:U:727:LYS:NZ	2.32	0.63
7:a:81:LEU:HD11	7:a:117:ALA:HB2	1.80	0.63
21:H:74:LEU:HD11	21:H:134:LEU:HD23	1.80	0.63
28:O:44:THR:N	28:O:211:GLY:O	2.32	0.63
33:t:46:THR:CG2	33:t:50:MET:HE1	2.28	0.63
1:U:669:ILE:HD12	1:U:695:MET:HE3	1.79	0.62
1:U:678:ASP:OD2	1:U:683:VAL:HG11	1.99	0.62
15:B:76:GLU:OE2	15:B:80:ARG:NE	2.28	0.62
17:D:87:LEU:HD21	17:D:140:VAL:HG23	1.80	0.62
17:D:135:HIS:C	17:D:136:SER:HG	2.04	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:358:VAL:O	17:D:358:VAL:HG22	1.99	0.62
33:T:190:LEU:HD11	33:T:221:LEU:HD23	1.81	0.62
33:T:211:ARG:O	33:T:215:GLU:OE1	2.17	0.62
17:D:413:GLU:O	21:H:53:LYS:NZ	2.32	0.62
28:O:262:LEU:HD11	29:P:193:ASP:HA	1.80	0.62
6:Z:78:MET:HE1	9:c:95:MET:CE	2.29	0.62
14:A:307:ASP:OD1	14:A:336:ARG:NE	2.32	0.62
15:B:202:GLU:N	15:B:202:GLU:OE2	2.32	0.62
1:U:5:ALA:O	1:U:9:ILE:HD12	1.99	0.62
3:W:268:LYS:O	3:W:302:TYR:OH	2.17	0.62
25:L:117:GLN:NE2	25:L:121:GLN:OE1	2.32	0.62
14:A:79:ASP:N	15:B:137:SER:OG	2.33	0.62
16:C:302:ASP:OD1	16:C:303:SER:N	2.33	0.62
17:D:115:ILE:HG22	17:D:139:LEU:HB3	1.82	0.62
18:E:72:LYS:NZ	18:E:76:GLY:O	2.23	0.62
22:I:76:VAL:HG21	22:I:83:ALA:CB	2.30	0.62
27:n:48:LEU:HD11	27:n:135:ALA:CB	2.29	0.62
1:U:723:ASP:OD1	1:U:724:VAL:N	2.31	0.62
4:X:15:LEU:HD13	4:X:22:ALA:CB	2.30	0.62
4:X:96:PHE:CE2	4:X:109:LEU:HD13	2.34	0.62
5:Y:228:MET:HE1	5:Y:259:TYR:CD2	2.34	0.62
16:C:161:ILE:HG21	16:C:199:LEU:HD21	1.80	0.62
19:F:418:GLU:OE2	25:L:167:SER:OG	2.17	0.62
33:T:211:ARG:O	33:T:214:VAL:HG22	1.99	0.62
14:A:272:ILE:HG21	14:A:274:PHE:CE2	2.35	0.62
27:n:89:VAL:HG23	27:n:120:MET:SD	2.40	0.62
15:B:169:PRO:HA	15:B:172:THR:HG22	1.82	0.62
15:B:337:LEU:CD1	15:B:342:ILE:HD11	2.30	0.62
18:E:310:LEU:HG	18:E:332:VAL:HG21	1.81	0.62
31:R:200:ARG:CZ	30:q:142:ILE:HG23	2.29	0.62
31:r:77:SER:OG	31:r:232:ALA:N	2.33	0.62
1:U:637:VAL:HG13	1:U:652:ALA:HB1	1.82	0.61
3:W:225:LYS:O	3:W:229:LEU:HD23	2.00	0.61
6:Z:64:ASP:OD2	8:b:91:ARG:NH2	2.30	0.61
12:f:275:MET:O	12:f:279:GLU:OE1	2.18	0.61
18:E:327:ASP:OD1	18:E:328:TYR:N	2.33	0.61
19:F:404:GLY:HA2	19:F:415:LEU:HD21	1.82	0.61
23:J:92:GLN:OE1	30:Q:66:LEU:N	2.33	0.61
28:O:262:LEU:HD13	29:P:48:ARG:NH1	2.15	0.61
3:W:94:ARG:O	3:W:96:GLN:N	2.33	0.61
10:d:192:LEU:HD21	10:d:215:LEU:CD2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:K:90:ASP:OD1	31:R:128:ARG:NH2	2.33	0.61
31:R:91:LYS:NZ	31:R:93:VAL:O	2.32	0.61
28:o:61:THR:OG1	28:o:215:ASN:OD1	2.08	0.61
29:p:138:VAL:HG11	29:p:146:MET:HG2	1.81	0.61
33:t:90:VAL:HG22	33:t:112:LEU:CD2	2.30	0.61
25:L:19:ILE:HG21	25:L:22:ILE:HD12	1.80	0.61
29:P:169:GLN:NE2	32:s:185:ASN:O	2.33	0.61
29:p:12:MET:HB2	29:p:138:VAL:HG12	1.81	0.61
30:q:4:LEU:HB3	30:q:45:LEU:HD23	1.80	0.61
30:q:164:LEU:HD23	30:q:167:LEU:HD12	1.80	0.61
1:U:542:GLU:OE1	9:c:32:TYR:OH	2.19	0.61
17:D:214:MET:HE1	37:D:501:ADP:C4	2.36	0.61
28:o:60:ASP:OD2	28:o:213:GLY:N	2.32	0.61
9:c:240:HIS:O	9:c:244:VAL:HG23	2.00	0.61
19:F:134:LEU:HD21	19:F:158:TYR:O	1.99	0.61
21:H:119:GLN:NE2	21:H:123:GLN:OE1	2.30	0.61
10:d:346:LEU:HD23	10:d:346:LEU:O	2.01	0.61
27:N:196:LEU:HD21	27:N:231:PHE:HD2	1.65	0.61
31:r:219:ILE:CG2	31:r:233:VAL:HG22	2.30	0.61
33:t:55:SER:OG	33:t:187:GLY:N	2.31	0.61
33:t:57:LEU:HD21	33:t:59:VAL:HG13	1.80	0.61
1:U:39:SER:O	1:U:42:VAL:HG12	2.01	0.61
12:f:59:LEU:HD13	12:f:77:GLU:OE2	2.00	0.61
22:I:90:LEU:HD21	22:I:114:LEU:HD22	1.81	0.61
33:t:91:ASN:OD1	33:t:94:THR:N	2.34	0.61
2:V:281:ASN:OD1	2:V:282:ASN:N	2.33	0.61
5:Y:71:ASN:OD1	5:Y:72:LYS:N	2.34	0.61
5:Y:308:LEU:O	5:Y:358:ARG:NH2	2.33	0.61
5:Y:388:ASN:OD1	5:Y:389:MET:N	2.33	0.61
33:T:169:TYR:CD1	33:T:184:THR:HG22	2.36	0.61
31:r:173:VAL:CG1	31:r:179:ARG:HD3	2.30	0.61
2:V:191:LEU:HD21	2:V:210:CYS:SG	2.40	0.61
5:Y:186:LEU:CD1	5:Y:213:LEU:HD13	2.31	0.61
6:Z:23:PHE:CD2	6:Z:126:VAL:HG21	2.36	0.61
17:D:388:ARG:NE	18:E:147:GLU:OE2	2.33	0.61
23:J:66:ASP:CA	30:Q:69:MET:HE1	2.30	0.61
26:M:69:ASN:O	33:T:121:LEU:HD22	2.01	0.61
2:V:79:VAL:O	2:V:83:GLU:OE1	2.19	0.61
18:E:228:CYS:HB2	18:E:273:VAL:HG13	1.82	0.61
30:q:13:VAL:HG12	30:q:115:LEU:HD21	1.81	0.61
4:X:397:TYR:CZ	6:Z:258:VAL:HG21	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:250:ARG:NH1	12:f:251:CYS:HG	1.99	0.60
27:N:153:MET:HE3	27:N:154:MET:H	1.65	0.60
32:s:176:LEU:HD22	32:s:206:VAL:CG2	2.31	0.60
7:a:184:ASP:OD1	7:a:185:ILE:N	2.34	0.60
18:E:71:VAL:CG1	18:E:100:LEU:HD11	2.31	0.60
2:V:102:PRO:O	2:V:105:SER:OG	2.17	0.60
17:D:89:ILE:HD11	18:E:80:VAL:CG1	2.29	0.60
25:L:53:GLN:O	25:L:54:SER:OG	2.16	0.60
32:S:92:LEU:CD2	32:S:134:VAL:HG21	2.31	0.60
33:T:211:ARG:NH1	33:T:215:GLU:OE2	2.34	0.60
32:s:173:LEU:HD22	32:s:206:VAL:HG12	1.83	0.60
1:U:691:SER:OG	1:U:713:TYR:OH	1.99	0.60
3:W:138:VAL:HG13	3:W:138:VAL:O	2.01	0.60
4:X:171:LEU:HD21	4:X:210:LEU:HD23	1.83	0.60
6:Z:178:ASP:OD1	6:Z:179:ILE:N	2.35	0.60
12:f:795:GLY:O	12:f:799:VAL:HG23	2.01	0.60
14:A:304:ASN:OD1	14:A:305:GLN:N	2.34	0.60
18:E:190:GLN:NE2	18:E:190:GLN:O	2.34	0.60
31:R:74:ALA:HB1	31:R:219:ILE:HD12	1.82	0.60
3:W:409:LEU:HD23	4:X:344:ARG:CZ	2.32	0.60
9:c:130:GLN:NE2	9:c:140:ALA:O	2.33	0.60
12:f:253:LEU:HD11	12:f:281:ILE:HD11	1.83	0.60
12:f:695:ALA:O	12:f:699:VAL:HG13	2.01	0.60
28:O:183:ASP:OD2	33:t:216:ARG:NH2	2.34	0.60
29:P:12:MET:HE1	29:P:170:ALA:HB1	1.84	0.60
33:T:189:TYR:HB2	28:o:175:LEU:HD13	1.84	0.60
12:f:268:LEU:O	12:f:268:LEU:HD23	2.02	0.60
14:A:100:LYS:O	14:A:112:ILE:HG22	2.01	0.60
17:D:340:GLN:O	17:D:344:ILE:HG12	2.02	0.60
25:L:5:GLN:O	26:M:10:LEU:HD21	2.02	0.60
28:O:175:LEU:HD13	33:t:189:TYR:CG	2.36	0.60
32:S:61:PHE:HA	28:o:210:LEU:HD13	1.84	0.60
11:e:38:VAL:HG22	11:e:38:VAL:O	2.01	0.60
12:f:699:VAL:HG12	12:f:731:MET:HE2	1.83	0.60
32:S:222:ARG:NE	32:S:235:THR:OG1	2.33	0.60
1:U:719:ASP:OD1	1:U:720:LYS:N	2.35	0.60
3:W:166:LEU:HD23	3:W:192:LEU:HD12	1.82	0.60
12:f:89:MET:SD	15:B:413:LYS:NZ	2.74	0.60
12:f:137:ARG:HE	12:f:169:GLU:HB3	1.67	0.60
12:f:771:LEU:CD2	12:f:825:MET:HE3	2.23	0.60
30:Q:146:TYR:O	30:Q:159:LEU:HD22	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:176:LEU:HB2	29:p:149:MET:HE1	1.84	0.60
3:W:412:ILE:HG22	3:W:412:ILE:O	2.01	0.60
7:a:245:VAL:HG21	7:a:300:ALA:HA	1.84	0.60
9:c:26:ASP:OD1	9:c:176:GLN:NE2	2.35	0.60
11:e:52:PHE:CZ	11:e:56:LEU:HD13	2.36	0.60
14:A:56:LEU:HD22	15:B:72:LEU:HD11	1.82	0.60
14:A:134:ILE:HG23	14:A:140:VAL:HG11	1.82	0.60
27:N:35:THR:N	27:N:203:SER:HG	2.00	0.60
33:t:85:SER:O	33:t:102:TYR:OH	2.11	0.60
5:Y:326:GLY:N	11:e:59:GLU:OE2	2.35	0.60
9:c:61:PHE:CZ	9:c:109:VAL:HG12	2.36	0.60
14:A:274:PHE:CZ	14:A:302:LEU:HD11	2.37	0.60
18:E:230:ILE:HG22	18:E:232:MET:SD	2.42	0.60
18:E:233:ASP:OD1	18:E:234:GLU:N	2.34	0.60
19:F:197:GLU:OE1	19:F:350:ARG:NH1	2.35	0.60
21:H:210:VAL:CG2	21:H:221:LEU:HD12	2.32	0.60
23:J:83:VAL:CG1	23:J:111:ILE:HD12	2.32	0.60
17:D:177:VAL:O	17:D:181:VAL:HG12	2.01	0.59
28:O:169:THR:O	28:O:174:SER:OG	2.20	0.59
2:V:216:ARG:NH1	11:e:20:GLU:OE1	2.34	0.59
4:X:190:LEU:HD22	4:X:217:ILE:HD12	1.83	0.59
7:a:360:VAL:HG22	9:c:308:VAL:HG23	1.82	0.59
13:x:190:GLY:N	13:x:251:ASN:OD1	2.35	0.59
23:J:55:ASP:OD1	23:J:56:GLU:N	2.34	0.59
29:P:177:ARG:NH1	32:s:174:GLN:OE1	2.35	0.59
32:S:41:LEU:HD11	32:S:177:LEU:CD1	2.32	0.59
33:T:73:GLY:O	33:T:80:ARG:N	2.35	0.59
32:s:172:MET:HE1	32:s:214:ASP:HB2	1.83	0.59
1:U:446:LEU:HD22	1:U:457:ILE:HD11	1.83	0.59
14:A:42:SER:O	14:A:45:ILE:HG22	2.02	0.59
22:I:108:GLU:OE2	23:J:60:ARG:NH2	2.32	0.59
23:J:73:PHE:CE1	23:J:80:ALA:HB2	2.37	0.59
3:W:275:ILE:HD11	3:W:306:LEU:HD12	1.84	0.59
8:b:182:ALA:O	8:b:186:SER:OG	2.19	0.59
17:D:48:GLN:O	17:D:52:GLU:OE1	2.20	0.59
25:L:62:LYS:NZ	25:L:74:ILE:O	2.28	0.59
30:Q:64:VAL:HG22	30:Q:75:LEU:HD12	1.85	0.59
32:s:181:VAL:HG21	32:s:194:LEU:HD22	1.84	0.59
9:c:177:THR:HG23	9:c:177:THR:O	2.01	0.59
14:A:91:GLN:NE2	14:A:142:VAL:O	2.35	0.59
29:P:173:ASN:ND2	32:s:178:ASP:OD1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R:192:VAL:HG12	30:q:137:PHE:HB2	1.83	0.59
33:T:181:SER:O	33:T:192:GLN:NE2	2.35	0.59
4:X:145:GLU:OE1	4:X:145:GLU:N	2.36	0.59
14:A:433:ASN:H	24:K:82:ILE:HD11	1.67	0.59
16:C:49:ARG:NE	16:C:53:ASN:OD1	2.35	0.59
19:F:240:CYS:O	19:F:244:THR:OG1	2.19	0.59
19:F:435:LEU:HD11	24:K:20:ARG:NH1	2.18	0.59
25:L:95:SER:CB	25:L:103:LEU:HD13	2.33	0.59
28:O:183:ASP:OD2	28:O:184:LYS:NZ	2.36	0.59
31:R:62:THR:HG21	31:R:103:THR:HB	1.84	0.59
32:S:43:ILE:HD11	32:S:177:LEU:HD13	1.83	0.59
27:n:117:PHE:CE2	27:n:132:ILE:HG21	2.37	0.59
27:n:117:PHE:HD2	27:n:134:ILE:HD11	1.67	0.59
1:U:492:ASP:OD1	1:U:493:VAL:N	2.35	0.59
2:V:442:ILE:HG21	10:d:278:ALA:CB	2.32	0.59
5:Y:174:TRP:CZ2	5:Y:207:THR:HG21	2.38	0.59
10:d:127:ASN:O	10:d:128:PHE:C	2.45	0.59
12:f:408:LEU:CD1	12:f:446:LEU:HD12	2.32	0.59
12:f:457:ASN:OD1	12:f:458:GLU:N	2.36	0.59
3:W:288:HIS:O	3:W:291:SER:OG	2.20	0.59
4:X:256:LEU:HD13	4:X:319:ILE:HG13	1.85	0.59
5:Y:304:TYR:HH	5:Y:333:GLU:CD	2.10	0.59
17:D:394:VAL:C	17:D:395:LEU:HD12	2.27	0.59
26:M:71:ASP:C	33:T:121:LEU:HD21	2.27	0.59
27:N:65:THR:HG22	27:N:66:ASP:H	1.68	0.59
29:P:12:MET:HE2	29:P:14:MET:CE	2.31	0.59
32:s:89:CYS:O	32:s:93:THR:HG23	2.03	0.59
33:t:210:ALA:O	33:t:214:VAL:HG13	2.03	0.59
5:Y:215:ASP:OD1	5:Y:216:TYR:N	2.35	0.59
27:N:56:THR:O	27:N:56:THR:HG23	2.03	0.59
29:P:6:TYR:CD1	29:P:31:GLN:NE2	2.71	0.59
32:S:134:VAL:HG23	32:S:134:VAL:O	2.03	0.59
1:U:221:ILE:HD11	1:U:252:LEU:HD23	1.85	0.58
7:a:56:LEU:HD21	7:a:83:VAL:HG22	1.84	0.58
9:c:107:MET:HE2	13:x:273:THR:HG22	1.83	0.58
17:D:303:VAL:HG13	17:D:303:VAL:O	2.03	0.58
22:I:95:GLN:OE1	29:P:72:ASN:ND2	2.33	0.58
30:Q:7:ILE:HD12	30:Q:156:ALA:HB1	1.84	0.58
32:S:215:VAL:HG21	28:o:210:LEU:HB3	1.85	0.58
32:s:120:LEU:HD23	32:s:152:PHE:HE2	1.64	0.58
1:U:588:MET:HE1	1:U:760:VAL:HG12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:198:PHE:O	10:d:201:SER:OG	2.20	0.58
14:A:113:ILE:HD11	14:A:123:VAL:HG21	1.85	0.58
14:A:206:ILE:HD11	19:F:408:LEU:HD12	1.84	0.58
17:D:238:LYS:O	17:D:239:TYR:HB2	2.02	0.58
20:G:56:VAL:HG13	20:G:61:LEU:HD23	1.85	0.58
1:U:470:ASN:OD1	1:U:471:ASP:N	2.36	0.58
3:W:183:VAL:HG12	3:W:222:LEU:HD12	1.85	0.58
5:Y:263:LEU:HD12	5:Y:271:PHE:CE1	2.38	0.58
6:Z:17:LEU:HD12	9:c:39:LEU:HD12	1.85	0.58
8:b:10:VAL:HG13	8:b:29:GLN:CD	2.28	0.58
14:A:322:ASN:ND2	35:A:501:ATP:O3G	2.36	0.58
15:B:223:ILE:CG1	15:B:347:ILE:HD13	2.33	0.58
19:F:123:VAL:O	19:F:123:VAL:HG12	2.03	0.58
1:U:328:ILE:HD11	1:U:795:LEU:HD11	1.85	0.58
6:Z:9:VAL:HG21	6:Z:120:VAL:HG11	1.85	0.58
14:A:286:ASP:OD1	14:A:287:ASP:N	2.36	0.58
29:P:45:MET:HE3	29:P:67:LEU:HD22	1.85	0.58
32:S:202:LEU:O	32:S:206:VAL:HG13	2.04	0.58
33:t:216:ARG:O	33:t:220:VAL:HG23	2.02	0.58
2:V:294:ARG:NH2	2:V:390:GLY:O	2.33	0.58
5:Y:25:LEU:HD22	5:Y:37:VAL:HG11	1.86	0.58
14:A:52:ILE:O	14:A:56:LEU:HD23	2.03	0.58
1:U:899:ARG:NH2	1:U:921:ILE:O	2.37	0.58
9:c:299:CYS:SG	9:c:303:MET:HE1	2.43	0.58
12:f:718:ASP:OD1	12:f:720:GLU:N	2.35	0.58
14:A:319:MET:HE3	14:A:337:LEU:HD21	1.84	0.58
15:B:235:LEU:O	15:B:239:VAL:HG23	2.02	0.58
15:B:385:MET:SD	15:B:386:ALA:N	2.76	0.58
23:J:209:ALA:HB1	23:J:217:LEU:HD21	1.84	0.58
25:L:157:ARG:HB2	26:M:60:GLU:OE1	2.04	0.58
3:W:455:LEU:HD21	6:Z:102:HIS:C	2.29	0.58
4:X:414:LEU:O	4:X:414:LEU:HD23	2.04	0.58
13:x:190:GLY:O	13:x:252:GLN:N	2.37	0.58
15:B:107:MET:HB2	16:C:96:VAL:HG22	1.83	0.58
27:N:153:MET:HE1	33:T:102:TYR:CD2	2.39	0.58
3:W:313:GLU:C	3:W:365:ILE:HD13	2.28	0.58
28:O:256:THR:HG22	29:P:199:THR:OG1	2.03	0.58
27:n:223:LEU:C	27:n:224:LEU:HD12	2.29	0.58
28:o:97:MET:HE2	29:p:96:TYR:CD2	2.39	0.58
9:c:87:VAL:HG21	13:x:278:PHE:CE2	2.39	0.58
12:f:237:VAL:HG13	12:f:249:LEU:HD22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:91:GLN:CG	14:A:93:LEU:HD23	2.33	0.58
17:D:275:PHE:O	17:D:286:GLN:NE2	2.37	0.58
20:G:113:MET:CE	28:O:113:THR:HA	2.34	0.58
20:G:114:LEU:O	20:G:118:ILE:HD12	2.03	0.58
22:I:219:GLU:OE1	22:I:220:ASN:ND2	2.37	0.58
24:K:110:GLU:OE2	32:S:108:ASN:ND2	2.36	0.58
26:M:198:ILE:HG21	26:M:212:LEU:CD1	2.34	0.58
27:N:153:MET:HE3	27:N:154:MET:N	2.18	0.58
32:S:34:VAL:HG13	32:S:34:VAL:O	2.03	0.58
30:q:139:THR:CG2	30:q:167:LEU:HD21	2.27	0.58
32:s:66:ARG:NH1	32:s:219:ASP:OD1	2.36	0.58
2:V:65:ARG:O	2:V:69:THR:HG23	2.03	0.58
12:f:502:LEU:HG	12:f:537:THR:HG21	1.85	0.58
12:f:512:MET:HE3	12:f:555:ALA:HB2	1.86	0.58
18:E:331:ILE:HG23	18:E:374:VAL:HG11	1.85	0.58
33:T:232:PHE:HE1	33:T:250:THR:HG23	1.68	0.58
30:q:33:ASP:OD1	30:q:34:LYS:N	2.36	0.58
1:U:26:LYS:O	1:U:30:VAL:HG22	2.04	0.57
5:Y:381:GLN:OE1	5:Y:385:ARG:NH1	2.36	0.57
7:a:37:LEU:HA	7:a:40:GLN:HG2	1.86	0.57
19:F:364:ARG:NH2	19:F:367:GLN:OE1	2.38	0.57
20:G:29:PHE:HA	20:G:32:ILE:HD12	1.86	0.57
20:G:61:LEU:HD21	20:G:66:VAL:HG21	1.86	0.57
33:t:96:LEU:HD12	33:t:156:VAL:O	2.04	0.57
7:a:261:LEU:HD22	7:a:268:LEU:HD11	1.84	0.57
15:B:400:THR:O	15:B:404:LEU:HD23	2.04	0.57
20:G:37:LEU:HD12	20:G:53:GLN:CB	2.33	0.57
27:n:125:ARG:NH2	27:n:151:GLY:O	2.36	0.57
30:q:139:THR:O	30:q:143:LEU:HD23	2.04	0.57
3:W:409:LEU:HD22	4:X:384:VAL:HG21	1.85	0.57
8:b:90:ILE:HD12	8:b:109:ILE:HG21	1.86	0.57
15:B:342:ILE:O	15:B:342:ILE:HG22	2.03	0.57
19:F:169:ASP:OD2	19:F:171:ARG:NH2	2.37	0.57
21:H:14:SER:OG	21:H:18:LYS:O	2.15	0.57
24:K:173:ALA:HB1	24:K:205:VAL:HG21	1.87	0.57
32:S:185:ASN:O	29:p:169:GLN:NE2	2.37	0.57
33:T:83:ASN:ND2	27:n:235:THR:O	2.37	0.57
30:q:139:THR:CG2	30:q:167:LEU:HD11	2.34	0.57
31:r:114:TRP:NE1	32:s:125:TYR:OH	2.36	0.57
31:r:219:ILE:HG21	31:r:233:VAL:HG22	1.86	0.57
33:t:209:GLU:OE1	33:t:209:GLU:N	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:400:HIS:O	2:V:403:ILE:HG22	2.04	0.57
3:W:228:ASN:O	3:W:232:GLN:NE2	2.37	0.57
6:Z:19:VAL:HG21	6:Z:124:ILE:CD1	2.33	0.57
12:f:82:ILE:HG21	12:f:154:TRP:CZ3	2.39	0.57
12:f:494:ARG:NH2	12:f:496:ASP:OD2	2.37	0.57
18:E:171:LEU:CD1	18:E:295:LEU:HD21	2.31	0.57
18:E:194:ASN:O	18:E:195:PHE:CG	2.58	0.57
25:L:147:THR:HG22	25:L:153:TYR:HB3	1.87	0.57
32:S:64:HIS:O	32:S:65:THR:OG1	2.20	0.57
29:p:180:VAL:HG23	29:p:180:VAL:O	2.04	0.57
31:r:173:VAL:HG13	31:r:179:ARG:HH11	1.68	0.57
1:U:462:LEU:HD12	1:U:496:LEU:HD23	1.85	0.57
12:f:700:SER:OG	12:f:734:SER:OG	2.15	0.57
19:F:251:LEU:HD11	19:F:256:LEU:HD21	1.87	0.57
19:F:406:ILE:HD13	19:F:422:GLU:HB3	1.86	0.57
20:G:138:MET:HE3	20:G:140:LEU:HG	1.86	0.57
3:W:435:LEU:HD11	6:Z:237:LEU:HD23	1.87	0.57
6:Z:266:ILE:HD13	9:c:284:LEU:HD11	1.86	0.57
8:b:186:SER:O	8:b:190:ALA:N	2.35	0.57
12:f:477:MET:HA	12:f:477:MET:HE3	1.87	0.57
18:E:70:ILE:HG13	18:E:80:VAL:HG12	1.87	0.57
31:r:74:ALA:HB1	31:r:219:ILE:CD1	2.35	0.57
4:X:15:LEU:HD13	4:X:22:ALA:HB1	1.85	0.57
12:f:130:ALA:HB1	12:f:135:GLY:HA3	1.85	0.57
12:f:416:MET:O	12:f:419:LEU:HG	2.04	0.57
14:A:96:ALA:HB2	14:A:142:VAL:CG2	2.35	0.57
16:C:63:LEU:HD22	17:D:78:GLU:OE1	2.05	0.57
17:D:323:ARG:O	17:D:325:GLY:N	2.32	0.57
18:E:214:LEU:O	18:E:218:MET:SD	2.62	0.57
19:F:286:ASP:OD1	19:F:287:GLU:N	2.37	0.57
20:G:50:ILE:HG23	20:G:141:ILE:HG21	1.86	0.57
28:O:254:VAL:HG12	28:O:255:LEU:N	2.20	0.57
31:r:156:MET:N	31:r:175:SER:OG	2.37	0.57
1:U:588:MET:HE1	1:U:760:VAL:CG1	2.34	0.57
4:X:397:TYR:OH	6:Z:258:VAL:HG21	2.04	0.57
19:F:191:LEU:HD12	19:F:191:LEU:O	2.05	0.57
1:U:2:ILE:HG22	1:U:4:SER:H	1.69	0.57
1:U:184:CYS:HA	1:U:188:MET:HE3	1.87	0.57
12:f:247:ALA:O	12:f:250:ARG:NH1	2.38	0.57
16:C:137:LEU:HD12	16:C:137:LEU:O	2.05	0.57
16:C:322:GLU:OE1	16:C:323:GLU:N	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:391:PHE:HE1	19:F:428:GLN:OE1	1.88	0.57
27:n:53:ARG:NH1	27:n:204:SER:O	2.38	0.57
3:W:406:VAL:HG23	3:W:406:VAL:O	2.04	0.57
7:a:44:PHE:O	7:a:47:ASP:N	2.31	0.57
12:f:168:LYS:HA	12:f:171:GLN:OE1	2.05	0.57
18:E:258:MET:O	18:E:258:MET:HG3	2.05	0.57
19:F:203:VAL:HG22	19:F:244:THR:HG23	1.85	0.57
25:L:38:LEU:HD13	25:L:187:LEU:CD1	2.35	0.57
5:Y:201:PHE:HB3	5:Y:223:THR:HG22	1.86	0.56
8:b:143:PHE:O	8:b:143:PHE:CD1	2.58	0.56
1:U:141:CYS:SG	16:C:20:LEU:HD13	2.44	0.56
1:U:218:GLN:NE2	1:U:251:ASP:OD2	2.38	0.56
4:X:126:ARG:NH2	4:X:156:GLU:OE1	2.37	0.56
10:d:278:ALA:O	10:d:279:TYR:CD1	2.58	0.56
15:B:306:GLN:O	15:B:310:LEU:HD23	2.05	0.56
1:U:48:LEU:HD23	1:U:56:SER:HB3	1.88	0.56
1:U:167:ILE:CD1	1:U:177:LEU:HD23	2.35	0.56
1:U:747:SER:OG	1:U:749:GLN:O	2.23	0.56
2:V:417:ILE:O	2:V:458:VAL:HG12	2.05	0.56
3:W:231:ILE:HD13	3:W:247:TYR:CE1	2.40	0.56
3:W:395:ASN:OD1	3:W:399:ASN:ND2	2.38	0.56
4:X:34:ASP:O	4:X:35:ILE:HD13	2.05	0.56
6:Z:169:GLU:HA	6:Z:172:VAL:HG22	1.87	0.56
7:a:149:THR:HG22	7:a:150:SER:H	1.70	0.56
7:a:163:TYR:HA	7:a:166:ILE:HG22	1.87	0.56
12:f:130:ALA:O	12:f:133:MET:N	2.38	0.56
12:f:208:LEU:HD21	12:f:217:LEU:CB	2.35	0.56
21:H:200:GLU:OE1	21:H:200:GLU:N	2.33	0.56
22:I:119:GLN:HG2	23:J:78:ALA:HB1	1.87	0.56
28:O:146:VAL:HG11	28:O:222:SER:C	2.31	0.56
29:P:67:LEU:HD21	29:P:87:LEU:HD11	1.87	0.56
27:n:68:LEU:HD11	27:n:209:ARG:O	2.06	0.56
31:r:65:PHE:CE2	31:r:202:TYR:CE1	2.93	0.56
33:t:96:LEU:HD13	33:t:157:ILE:HG12	1.87	0.56
8:b:113:VAL:O	8:b:113:VAL:HG12	2.04	0.56
8:b:166:THR:O	8:b:169:HIS:NE2	2.39	0.56
14:A:113:ILE:CD1	14:A:123:VAL:HG21	2.35	0.56
16:C:345:ARG:O	16:C:349:GLU:OE1	2.23	0.56
31:R:142:LEU:HD23	31:R:173:VAL:HG21	1.87	0.56
1:U:167:ILE:HD11	1:U:177:LEU:HD23	1.87	0.56
1:U:364:VAL:CG2	9:c:177:THR:HG21	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:84:ASN:OD1	3:W:85:GLU:N	2.38	0.56
23:J:183:THR:OG1	23:J:186:LEU:HD23	2.05	0.56
26:M:50:VAL:HG11	26:M:66:ARG:HB2	1.86	0.56
28:O:118:ARG:HG2	28:O:147:ASP:HB2	1.88	0.56
33:T:51:VAL:HG23	33:T:51:VAL:O	2.05	0.56
12:f:334:ALA:O	12:f:338:ASP:HA	2.06	0.56
23:J:11:SER:O	23:J:14:GLY:N	2.38	0.56
31:R:126:GLU:OE1	31:R:132:ARG:NH1	2.39	0.56
32:S:116:ILE:HD12	32:S:119:MET:HE2	1.87	0.56
14:A:220:THR:O	14:A:220:THR:HG22	2.05	0.56
17:D:116:LEU:N	17:D:119:ILE:HD11	2.21	0.56
25:L:6:TYR:OH	26:M:9:ASP:OD2	2.09	0.56
32:s:140:GLY:HA2	32:s:226:VAL:HG11	1.87	0.56
1:U:831:ALA:HB3	15:B:77:GLU:OE2	2.06	0.56
2:V:473:GLN:OE1	6:Z:257:MET:SD	2.64	0.56
15:B:291:GLY:HA2	15:B:309:MET:HE2	1.88	0.56
17:D:230:VAL:HG11	17:D:235:PHE:CE1	2.40	0.56
18:E:148:VAL:HG22	18:E:297:ARG:NE	2.20	0.56
18:E:303:LEU:HB3	18:E:304:PRO:HD3	1.88	0.56
25:L:159:MET:HE1	26:M:58:LEU:HD12	1.87	0.56
27:N:213:ILE:HG12	27:N:218:VAL:HG22	1.88	0.56
29:P:49:LEU:CD2	29:P:87:LEU:HD22	2.35	0.56
31:R:109:ALA:CB	32:S:155:VAL:HG23	2.35	0.56
27:n:36:THR:HG21	27:n:197:ALA:HB3	1.86	0.56
3:W:412:ILE:HD12	7:a:327:VAL:HG11	1.88	0.56
4:X:35:ILE:HG23	4:X:42:ALA:HB3	1.86	0.56
14:A:191:VAL:HG11	14:A:229:VAL:CG2	2.36	0.56
15:B:434:THR:HG23	22:I:17:ARG:HH11	1.70	0.56
25:L:212:ILE:HD12	25:L:229:VAL:HG23	1.88	0.56
32:S:117:ALA:HB1	32:S:158:TYR:CE1	2.41	0.56
33:T:223:TYR:OH	33:T:253:ASN:N	2.39	0.56
3:W:23:THR:O	3:W:26:GLN:NE2	2.39	0.56
12:f:204:ALA:HB1	12:f:217:LEU:HD21	1.88	0.56
14:A:143:ASP:OD2	14:A:150:HIS:NE2	2.39	0.56
15:B:250:VAL:CG2	15:B:270:LEU:HD11	2.34	0.56
23:J:175:ASN:OD1	23:J:175:ASN:O	2.23	0.56
27:N:172:TYR:CG	27:N:172:TYR:O	2.59	0.56
32:s:63:ILE:H	32:s:63:ILE:HD12	1.70	0.56
1:U:639:LEU:O	16:C:49:ARG:NH2	2.28	0.55
5:Y:233:ARG:NH2	5:Y:264:TYR:O	2.39	0.55
10:d:276:GLU:OE2	10:d:306:ARG:NH2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:208:LEU:HD21	12:f:217:LEU:HB3	1.88	0.55
12:f:799:VAL:HG21	12:f:821:LEU:HB2	1.88	0.55
28:O:55:ILE:HD13	28:O:145:GLY:N	2.21	0.55
33:T:57:LEU:HD11	33:T:221:LEU:HD11	1.88	0.55
31:r:238:VAL:HG23	31:r:238:VAL:O	2.06	0.55
33:t:59:VAL:HG11	33:t:195:LEU:HD22	1.87	0.55
1:U:676:THR:HG21	1:U:712:LEU:HD21	1.89	0.55
9:c:109:VAL:HG23	9:c:109:VAL:O	2.05	0.55
10:d:272:ALA:O	10:d:276:GLU:OE1	2.24	0.55
12:f:75:LEU:HD11	12:f:118:ASN:HA	1.87	0.55
12:f:674:THR:HG22	15:B:75:GLU:HG2	1.88	0.55
15:B:180:PRO:O	15:B:241:ASN:ND2	2.39	0.55
33:T:95:MET:CE	33:T:242:VAL:HG13	2.36	0.55
1:U:101:ILE:HD12	1:U:137:MET:HE3	1.88	0.55
2:V:442:ILE:HG21	10:d:278:ALA:HB2	1.88	0.55
2:V:442:ILE:HD13	2:V:449:ALA:O	2.06	0.55
19:F:437:TYR:OH	24:K:25:GLU:OE2	2.21	0.55
21:H:75:VAL:HG22	21:H:76:TYR:H	1.69	0.55
27:N:42:PHE:CE1	27:N:47:VAL:HG13	2.42	0.55
32:S:113:THR:O	32:S:116:ILE:HG22	2.06	0.55
33:T:137:LEU:HD11	33:T:155:MET:HE1	1.89	0.55
31:r:233:VAL:HG21	31:r:254:LEU:HD12	1.88	0.55
33:t:101:ASP:OD1	33:t:103:ALA:N	2.40	0.55
1:U:381:THR:HG21	1:U:415:HIS:ND1	2.21	0.55
4:X:86:ALA:HB1	4:X:125:LEU:HD13	1.88	0.55
4:X:234:GLU:OE2	17:D:342:ARG:NH2	2.40	0.55
15:B:249:ARG:O	15:B:250:VAL:HG23	2.06	0.55
18:E:373:LYS:O	18:E:376:ASP:N	2.39	0.55
19:F:139:LEU:HD13	19:F:161:LEU:HD23	1.88	0.55
26:M:110:LYS:NZ	26:M:145:ASP:OD2	2.39	0.55
32:s:33:TYR:OH	32:s:131:PRO:O	2.08	0.55
32:s:176:LEU:HD22	32:s:206:VAL:HG22	1.87	0.55
1:U:246:TYR:OH	1:U:321:GLN:OE1	2.23	0.55
2:V:398:LEU:O	2:V:399:ARG:C	2.49	0.55
3:W:346:GLU:OE2	3:W:350:ARG:NH2	2.39	0.55
4:X:12:ALA:O	4:X:23:SER:OG	2.15	0.55
12:f:802:SER:OG	12:f:817:VAL:HG11	2.06	0.55
14:A:70:THR:O	14:A:70:THR:HG22	2.06	0.55
14:A:102:ILE:HD11	19:F:165:PRO:HD3	1.89	0.55
16:C:198:LEU:HD23	16:C:198:LEU:O	2.05	0.55
17:D:119:ILE:O	17:D:119:ILE:HG22	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:402:ALA:O	17:D:406:VAL:HG22	2.05	0.55
30:Q:43:LEU:HD12	30:Q:183:ILE:HD11	1.88	0.55
7:a:296:ILE:HG21	7:a:307:VAL:HG13	1.88	0.55
15:B:126:SER:OG	16:C:93:GLY:N	2.39	0.55
18:E:65:THR:O	18:E:67:GLU:N	2.40	0.55
23:J:208:LEU:HD23	23:J:225:ILE:HD13	1.88	0.55
32:S:162:SER:HG	32:S:163:PHE:HD1	1.54	0.55
32:s:181:VAL:HG23	32:s:194:LEU:HD22	1.88	0.55
2:V:413:SER:O	2:V:414:TYR:CG	2.60	0.55
3:W:146:THR:HG23	3:W:169:LEU:HD11	1.89	0.55
14:A:122:VAL:HG11	19:F:88:TYR:HD2	1.72	0.55
29:P:56:LEU:O	29:P:60:VAL:HG23	2.07	0.55
33:t:74:SER:OG	33:t:78:LEU:O	2.16	0.55
1:U:632:GLN:O	1:U:635:SER:OG	2.13	0.55
7:a:77:VAL:HG12	7:a:113:LEU:HD22	1.88	0.55
14:A:96:ALA:HB1	14:A:140:VAL:HG23	1.88	0.55
15:B:280:SER:OG	15:B:281:ILE:N	2.38	0.55
16:C:63:LEU:HD21	17:D:79:VAL:CG2	2.36	0.55
18:E:97:ARG:NH1	18:E:112:PRO:O	2.40	0.55
31:R:78:ARG:HE	31:R:88:GLN:HG3	1.71	0.55
32:S:63:ILE:O	32:S:63:ILE:HG13	2.07	0.55
29:p:143:ALA:HA	29:p:146:MET:SD	2.46	0.55
7:a:149:THR:HG22	7:a:150:SER:N	2.22	0.55
8:b:33:VAL:HG11	8:b:75:LEU:HD22	1.88	0.55
12:f:239:TYR:HB3	15:B:63:LEU:HD21	1.89	0.55
13:x:191:PRO:O	13:x:252:GLN:NE2	2.39	0.55
16:C:130:LYS:NZ	17:D:94:GLU:OE2	2.28	0.55
16:C:151:ILE:CG1	16:C:198:LEU:HD22	2.37	0.55
27:N:199:GLU:OE2	33:t:82:ARG:NH1	2.40	0.55
30:q:119:ASP:OD1	30:q:123:ALA:N	2.39	0.55
33:t:90:VAL:HG22	33:t:112:LEU:HD21	1.87	0.55
14:A:52:ILE:HD12	15:B:65:LEU:HD21	1.88	0.55
16:C:45:LEU:HB3	17:D:61:ILE:HG21	1.89	0.55
18:E:29:LEU:HD12	18:E:30:ARG:N	2.22	0.55
19:F:136:VAL:HG13	19:F:136:VAL:O	2.06	0.55
23:J:4:ASP:OD1	23:J:5:ARG:N	2.37	0.55
26:M:109:LEU:O	26:M:109:LEU:HD23	2.07	0.55
32:S:56:ARG:NH2	32:S:219:ASP:OD1	2.40	0.55
29:p:40:GLN:NE2	29:p:42:ILE:O	2.40	0.55
31:r:60:THR:N	31:r:229:SER:HG	2.04	0.55
2:V:459:GLN:NE2	10:d:280:GLU:OE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:460:SER:OG	2:V:461:LYS:N	2.38	0.54
3:W:28:LEU:HD21	3:W:69:ALA:HB1	1.88	0.54
8:b:132:LYS:NZ	13:x:160:ASP:OD1	2.39	0.54
15:B:292:THR:O	15:B:309:MET:HE1	2.06	0.54
19:F:231:THR:O	37:F:501:ADP:N7	2.40	0.54
31:R:103:THR:HG21	31:R:159:MET:HE3	1.89	0.54
3:W:432:LEU:HD22	9:c:309:PHE:CD2	2.42	0.54
6:Z:199:LYS:HD3	7:a:364:GLU:OE2	2.07	0.54
9:c:82:VAL:HG23	9:c:82:VAL:O	2.07	0.54
17:D:85:ILE:HB	17:D:86:PRO:HD3	1.89	0.54
19:F:134:LEU:HD11	19:F:158:TYR:O	2.07	0.54
20:G:37:LEU:HD12	20:G:53:GLN:HB3	1.89	0.54
20:G:240:VAL:HG23	20:G:241:ALA:N	2.22	0.54
25:L:199:LEU:HD11	25:L:205:LEU:CD2	2.37	0.54
2:V:241:ARG:O	2:V:243:ASP:N	2.39	0.54
6:Z:234:PHE:HZ	7:a:353:LEU:HD22	1.72	0.54
12:f:615:ILE:HA	12:f:618:GLU:OE1	2.07	0.54
15:B:190:LEU:O	15:B:194:ILE:HG13	2.07	0.54
25:L:115:LYS:NZ	25:L:128:TYR:OH	2.38	0.54
26:M:215:SER:HA	26:M:228:VAL:HG23	1.88	0.54
28:o:178:MET:HE2	28:o:178:MET:HA	1.89	0.54
32:s:183:PHE:HA	32:s:186:MET:HE1	1.89	0.54
33:t:78:LEU:HD12	33:t:79:ALA:H	1.73	0.54
1:U:551:GLY:O	1:U:555:VAL:HG23	2.07	0.54
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.72	0.54
1:U:697:GLN:NE2	1:U:786:THR:OG1	2.36	0.54
12:f:482:ILE:HG22	12:f:521:ALA:CB	2.38	0.54
15:B:284:ILE:HG21	15:B:287:ILE:HD13	1.89	0.54
15:B:305:ILE:HD11	16:C:271:ARG:HH22	1.73	0.54
15:B:401:GLU:O	15:B:405:MET:HG2	2.08	0.54
18:E:119:VAL:HG23	18:E:120:TYR:N	2.23	0.54
24:K:210:LEU:HD13	24:K:215:ILE:HG21	1.90	0.54
26:M:216:TRP:CZ3	26:M:228:VAL:HG22	2.42	0.54
28:O:71:ASP:OD1	29:P:131:MET:HE1	2.08	0.54
30:Q:67:TYR:CD2	30:Q:75:LEU:HD21	2.43	0.54
32:s:41:LEU:CD1	32:s:177:LEU:HD11	2.36	0.54
9:c:99:LEU:HA	9:c:102:THR:HG22	1.90	0.54
12:f:420:TRP:NE1	12:f:453:SER:O	2.41	0.54
12:f:608:LYS:O	12:f:612:LEU:HD23	2.07	0.54
15:B:143:LEU:O	15:B:164:MET:HE3	2.06	0.54
24:K:186:HIS:NE2	24:K:188:SER:O	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:186:ASN:OD1	30:Q:186:ASN:O	2.26	0.54
27:n:53:ARG:NH1	27:n:202:GLY:O	2.40	0.54
31:r:139:SER:OG	31:r:179:ARG:NH2	2.32	0.54
33:t:253:ASN:OD1	33:t:253:ASN:O	2.25	0.54
4:X:35:ILE:HD12	4:X:42:ALA:HB1	1.90	0.54
7:a:167:GLY:O	7:a:169:HIS:ND1	2.36	0.54
7:a:278:MET:HE2	7:a:319:LEU:HB3	1.88	0.54
12:f:192:VAL:CG1	12:f:217:LEU:HD22	2.37	0.54
12:f:377:VAL:HG23	12:f:767:GLY:CA	2.37	0.54
14:A:375:ARG:HE	14:A:376:LEU:HD22	1.73	0.54
17:D:345:PHE:HB3	17:D:360:LEU:HD13	1.88	0.54
24:K:7:GLU:N	24:K:7:GLU:OE1	2.41	0.54
24:K:234:LEU:O	24:K:238:ILE:HD12	2.08	0.54
27:N:228:ILE:O	27:N:230:LYS:NZ	2.41	0.54
30:Q:38:MET:SD	30:Q:61:GLN:HA	2.48	0.54
32:S:132:TYR:HB3	32:S:134:VAL:HG22	1.90	0.54
32:S:141:LEU:CD1	32:S:226:VAL:HG12	2.37	0.54
4:X:386:ILE:HD13	5:Y:312:ARG:NH2	2.22	0.54
5:Y:22:LEU:CD1	5:Y:37:VAL:HG13	2.38	0.54
7:a:76:LEU:O	7:a:80:ILE:HG12	2.07	0.54
7:a:304:VAL:HG23	7:a:304:VAL:O	2.08	0.54
8:b:39:SER:OG	8:b:189:LEU:HD11	2.08	0.54
10:d:228:HIS:O	10:d:232:LEU:HD23	2.08	0.54
17:D:236:VAL:O	17:D:236:VAL:HG12	2.07	0.54
19:F:175:MET:O	19:F:249:LEU:HD12	2.08	0.54
23:J:3:TYR:OH	24:K:5:ARG:O	2.24	0.54
26:M:54:VAL:O	26:M:54:VAL:HG23	2.07	0.54
29:p:67:LEU:HD11	29:p:87:LEU:CD1	2.38	0.54
31:r:226:ASP:O	31:r:229:SER:N	2.32	0.54
3:W:445:LEU:HB2	6:Z:226:ILE:HD11	1.88	0.54
6:Z:190:ARG:HD3	9:c:297:VAL:HG21	1.90	0.54
12:f:408:LEU:HD12	12:f:443:GLY:HA2	1.90	0.54
14:A:177:VAL:HG11	14:A:225:CYS:SG	2.47	0.54
16:C:31:LEU:O	16:C:35:VAL:HG23	2.07	0.54
16:C:73:VAL:HG23	16:C:73:VAL:O	2.07	0.54
17:D:277:ALA:HB3	17:D:283:ARG:HE	1.72	0.54
19:F:196:GLN:O	19:F:200:GLU:OE1	2.24	0.54
20:G:132:ARG:NE	20:G:132:ARG:O	2.38	0.54
23:J:108:THR:HG23	23:J:147:THR:CG2	2.38	0.54
24:K:217:LEU:HD23	24:K:229:PHE:CD2	2.43	0.54
33:t:46:THR:HG23	33:t:50:MET:CE	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:51:GLU:HA	3:W:66:ILE:HD12	1.90	0.54
3:W:68:VAL:HG12	3:W:72:LYS:HD2	1.89	0.54
3:W:261:GLU:OE1	3:W:261:GLU:N	2.41	0.54
9:c:108:VAL:H	13:x:273:THR:HG21	1.72	0.54
12:f:97:LYS:NZ	14:A:29:ASP:OD1	2.32	0.54
12:f:143:ARG:NH1	12:f:158:TYR:OH	2.41	0.54
12:f:399:LEU:HD13	12:f:410:ALA:HB3	1.90	0.54
16:C:248:MET:HE1	16:C:276:LEU:HD22	1.89	0.54
18:E:61:LEU:N	18:E:70:ILE:O	2.41	0.54
20:G:186:LYS:O	20:G:186:LYS:HD2	2.08	0.54
26:M:153:ASP:OD1	26:M:157:VAL:HG22	2.08	0.54
29:P:61:GLN:O	29:P:65:GLN:OE1	2.25	0.54
30:Q:164:LEU:HD22	30:Q:178:PHE:HD2	1.69	0.54
31:r:74:ALA:HB1	31:r:219:ILE:HD12	1.89	0.54
32:s:44:ALA:HB1	32:s:147:GLY:HA3	1.90	0.54
1:U:160:LEU:O	1:U:163:PHE:N	2.41	0.54
12:f:805:ASP:O	12:f:809:ILE:HG22	2.07	0.54
13:x:210:GLU:OE1	13:x:210:GLU:N	2.41	0.54
14:A:239:ARG:NE	14:A:239:ARG:O	2.41	0.54
15:B:148:CYS:SG	15:B:164:MET:HE2	2.48	0.54
16:C:298:ILE:HD11	16:C:306:LEU:HD22	1.88	0.54
17:D:313:ARG:NH1	17:D:316:THR:OG1	2.41	0.54
17:D:337:ASP:OD1	17:D:338:ARG:N	2.37	0.54
18:E:119:VAL:HG23	18:E:120:TYR:H	1.73	0.54
20:G:32:ILE:HD11	20:G:156:PRO:CD	2.38	0.54
25:L:80:ASP:OD2	25:L:126:ARG:NH1	2.40	0.54
30:q:2:GLU:OE2	30:q:34:LYS:NZ	2.29	0.54
31:r:65:PHE:HE1	31:r:183:ALA:HB1	1.73	0.54
2:V:168:GLN:OE1	2:V:187:ILE:HD11	2.08	0.53
12:f:249:LEU:HB3	12:f:268:LEU:HD21	1.90	0.53
15:B:95:GLU:OE1	15:B:95:GLU:N	2.40	0.53
21:H:107:THR:O	21:H:111:VAL:HG23	2.07	0.53
24:K:109:VAL:HA	24:K:112:VAL:HG12	1.89	0.53
31:R:184:THR:HB	31:R:198:MET:HE3	1.89	0.53
29:p:132:VAL:O	29:p:132:VAL:HG13	2.09	0.53
1:U:198:LEU:HB3	1:U:223:LEU:HD11	1.90	0.53
1:U:237:VAL:CG2	1:U:325:MET:HE1	2.38	0.53
8:b:11:ASP:CG	8:b:84:ILE:HD12	2.34	0.53
12:f:419:LEU:HD21	12:f:450:ILE:HG12	1.90	0.53
12:f:590:PHE:CD2	12:f:652:VAL:HG21	2.43	0.53
12:f:594:LEU:HA	12:f:597:VAL:HG22	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:261:PHE:HE2	14:A:302:LEU:HD12	1.73	0.53
15:B:404:LEU:HB3	16:C:163:GLU:OE2	2.08	0.53
17:D:167:ILE:HD11	17:D:170:MET:CE	2.38	0.53
17:D:354:LEU:HB3	17:D:358:VAL:HG11	1.89	0.53
26:M:231:ASP:OD1	26:M:232:ILE:N	2.40	0.53
32:s:153:ASP:OD1	32:s:156:GLY:N	2.37	0.53
1:U:554:LEU:HD22	1:U:761:VAL:HG22	1.91	0.53
1:U:653:ALA:HB2	1:U:675:MET:CE	2.30	0.53
1:U:891:VAL:HG23	1:U:891:VAL:O	2.08	0.53
12:f:789:SER:O	12:f:793:VAL:HG23	2.08	0.53
15:B:107:MET:CE	15:B:160:ILE:HG23	2.37	0.53
32:s:72:TYR:CD2	32:s:93:THR:HG21	2.43	0.53
32:s:221:LEU:HD23	32:s:236:VAL:CG1	2.38	0.53
1:U:451:ALA:O	1:U:452:ASN:C	2.52	0.53
1:U:623:GLY:HA2	1:U:659:CYS:SG	2.48	0.53
2:V:458:VAL:HG13	2:V:458:VAL:O	2.07	0.53
13:x:148:ASN:OD1	13:x:151:ARG:NH2	2.41	0.53
14:A:140:VAL:CG2	14:A:149:ILE:HD12	2.39	0.53
14:A:339:ARG:NH1	19:F:402:GLU:OE1	2.41	0.53
27:N:60:ILE:H	27:N:60:ILE:HD12	1.73	0.53
32:s:64:HIS:O	33:t:196:ARG:NH2	2.41	0.53
33:t:96:LEU:HD13	33:t:157:ILE:CG1	2.38	0.53
5:Y:227:SER:HB3	5:Y:231:LEU:HD12	1.90	0.53
12:f:409:SER:O	12:f:819:TYR:OH	2.17	0.53
14:A:86:THR:HG23	15:B:156:VAL:CG2	2.39	0.53
21:H:119:GLN:HA	21:H:122:THR:HG22	1.90	0.53
23:J:104:VAL:HG23	23:J:133:ILE:HG22	1.90	0.53
26:M:78:VAL:HG21	26:M:85:ALA:HB1	1.89	0.53
26:M:111:HIS:O	26:M:115:ARG:HG3	2.09	0.53
28:O:91:THR:HG21	28:O:94:ASP:OD2	2.09	0.53
28:O:146:VAL:HG12	28:O:221:ILE:HG22	1.91	0.53
28:o:96:ASP:O	28:o:100:GLN:OE1	2.27	0.53
32:s:151:SER:C	32:s:152:PHE:HD1	2.15	0.53
5:Y:22:LEU:HD13	5:Y:37:VAL:HG13	1.90	0.53
7:a:278:MET:CE	7:a:319:LEU:HD13	2.39	0.53
7:a:289:ARG:HD3	7:a:333:MET:O	2.09	0.53
7:a:299:SER:O	7:a:300:ALA:C	2.50	0.53
12:f:247:ALA:O	12:f:250:ARG:HD3	2.09	0.53
18:E:261:LEU:HD23	18:E:261:LEU:O	2.09	0.53
18:E:316:HIS:ND1	18:E:316:HIS:O	2.41	0.53
19:F:195:ILE:O	19:F:199:VAL:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:66:VAL:HG12	25:L:67:ASP:H	1.73	0.53
28:O:202:ILE:O	28:O:206:ILE:HG12	2.08	0.53
29:P:24:ALA:N	29:P:171:MET:HE1	2.24	0.53
31:R:164:ASP:O	31:R:167:GLY:N	2.37	0.53
31:r:65:PHE:CE1	31:r:184:THR:HG22	2.44	0.53
7:a:331:VAL:CG1	7:a:333:MET:HE3	2.37	0.53
15:B:139:VAL:HG12	15:B:141:LYS:H	1.73	0.53
15:B:434:THR:HG23	22:I:17:ARG:NH1	2.23	0.53
28:O:189:MET:CE	28:O:197:LEU:HD22	2.29	0.53
29:P:28:PHE:CG	29:P:28:PHE:O	2.61	0.53
29:P:168:SER:OG	29:P:200:LEU:HD22	2.08	0.53
30:Q:4:LEU:HD13	30:Q:45:LEU:HB3	1.91	0.53
30:q:12:TYR:OH	30:q:151:ILE:O	2.17	0.53
6:Z:234:PHE:CZ	7:a:353:LEU:HD22	2.43	0.53
8:b:24:THR:OG1	8:b:27:GLN:OE1	2.27	0.53
12:f:192:VAL:HG23	12:f:193:PRO:HD3	1.91	0.53
14:A:96:ALA:HB2	14:A:142:VAL:HG23	1.90	0.53
16:C:267:SER:C	16:C:271:ARG:HE	2.15	0.53
20:G:114:LEU:HD23	20:G:118:ILE:HD13	1.91	0.53
2:V:290:TYR:CD1	2:V:309:MET:HE1	2.44	0.53
4:X:290:VAL:HG21	4:X:313:LEU:CD1	2.39	0.53
7:a:229:ASP:OD1	7:a:230:ARG:N	2.42	0.53
7:a:342:ASP:OD1	7:a:343:LEU:N	2.39	0.53
12:f:387:GLN:H	12:f:417:ILE:HG22	1.73	0.53
16:C:406:LYS:O	22:I:64:LYS:NZ	2.32	0.53
17:D:403:TYR:O	17:D:407:ILE:HG22	2.09	0.53
20:G:117:ARG:O	20:G:121:ILE:HG12	2.09	0.53
27:n:62:ASN:ND2	27:n:64:VAL:O	2.42	0.53
2:V:442:ILE:CG1	2:V:447:ILE:HD11	2.39	0.53
4:X:370:LEU:HD12	5:Y:310:SER:HB3	1.89	0.53
5:Y:183:TYR:CD1	5:Y:213:LEU:HD11	2.44	0.53
7:a:240:PHE:CZ	7:a:268:LEU:HD22	2.41	0.53
12:f:59:LEU:HD11	12:f:74:ALA:HA	1.91	0.53
15:B:296:ASP:OD1	15:B:297:SER:N	2.42	0.53
21:H:111:VAL:HG22	21:H:136:ILE:HD13	1.91	0.53
22:I:194:ILE:HG23	22:I:237:ILE:HD13	1.90	0.53
25:L:95:SER:HB2	25:L:103:LEU:HD13	1.90	0.53
31:R:233:VAL:O	31:R:233:VAL:HG12	2.09	0.53
33:T:169:TYR:CD2	33:T:169:TYR:O	2.62	0.53
31:r:61:THR:N	31:r:76:ASP:OD2	2.41	0.53
1:U:155:LEU:HD22	1:U:188:MET:HE1	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:361:HIS:CD2	3:W:365:ILE:HD11	2.44	0.52
5:Y:207:THR:O	5:Y:207:THR:HG22	2.09	0.52
7:a:35:HIS:C	7:a:37:LEU:H	2.17	0.52
10:d:145:ARG:O	10:d:146:ASP:C	2.51	0.52
12:f:343:LYS:HE2	12:f:348:ILE:HD11	1.91	0.52
12:f:512:MET:CE	12:f:555:ALA:HB2	2.39	0.52
17:D:214:MET:HE1	37:D:501:ADP:N3	2.24	0.52
17:D:351:LYS:HZ3	18:E:164:ILE:HG22	1.75	0.52
18:E:219:PHE:CZ	18:E:269:THR:HG21	2.43	0.52
18:E:348:THR:HG22	18:E:352:MET:CE	2.32	0.52
32:s:72:TYR:HD2	32:s:93:THR:HG21	1.74	0.52
4:X:278:ARG:NH2	4:X:279:TYR:OH	2.42	0.52
7:a:60:TYR:O	7:a:61:GLU:C	2.50	0.52
12:f:573:ILE:HG22	12:f:573:ILE:O	2.09	0.52
14:A:152:PRO:C	14:A:153:LEU:HD12	2.34	0.52
18:E:50:LEU:HD22	19:F:83:ASN:ND2	2.24	0.52
19:F:202:ILE:HG23	19:F:282:ILE:HD12	1.90	0.52
20:G:186:LYS:NZ	20:G:193:GLN:OE1	2.42	0.52
22:I:8:ARG:NH1	22:I:10:THR:OG1	2.42	0.52
28:O:88:GLY:HA2	28:O:141:LEU:HD23	1.92	0.52
28:O:98:THR:HG23	28:O:129:MET:HE1	1.91	0.52
27:n:125:ARG:CZ	33:t:50:MET:HE3	2.39	0.52
4:X:365:LEU:HD13	4:X:385:LEU:HD12	1.91	0.52
10:d:192:LEU:HD21	10:d:215:LEU:HD22	1.91	0.52
17:D:85:ILE:HG23	18:E:68:LYS:HD2	1.91	0.52
28:o:75:SER:O	28:o:78:HIS:NE2	2.43	0.52
1:U:788:VAL:HG13	1:U:788:VAL:O	2.09	0.52
4:X:35:ILE:HD12	4:X:42:ALA:CB	2.40	0.52
16:C:32:GLN:OE1	17:D:47:LEU:HD22	2.10	0.52
25:L:71:GLY:HA3	25:L:221:PHE:CE1	2.44	0.52
25:L:139:ASP:OD1	25:L:140:MET:N	2.42	0.52
33:T:72:LEU:HD11	33:T:79:ALA:HB1	1.91	0.52
27:n:38:MET:HG2	27:n:190:THR:HG23	1.90	0.52
31:r:65:PHE:CD1	31:r:184:THR:HG22	2.44	0.52
1:U:94:SER:O	1:U:98:GLU:OE1	2.27	0.52
9:c:248:MET:CE	9:c:291:LEU:HD12	2.36	0.52
10:d:131:THR:O	10:d:132:THR:OG1	2.23	0.52
12:f:82:ILE:HG21	12:f:154:TRP:CE3	2.44	0.52
12:f:270:LEU:HD22	12:f:787:LEU:HD13	1.92	0.52
14:A:86:THR:O	14:A:86:THR:HG22	2.10	0.52
16:C:140:VAL:HG22	16:C:213:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:254:ILE:HG13	16:C:254:ILE:O	2.08	0.52
26:M:91:ILE:HD13	26:M:119:TYR:CE1	2.44	0.52
30:Q:81:ALA:HB1	30:Q:124:LEU:HD21	1.91	0.52
28:o:255:LEU:HD11	29:p:201:LYS:HA	1.91	0.52
2:V:192:MET:HE1	2:V:211:TYR:HD1	1.74	0.52
4:X:355:LYS:C	4:X:356:LEU:HD22	2.35	0.52
8:b:59:GLU:OE1	8:b:61:LEU:HD22	2.10	0.52
12:f:659:LEU:CD1	12:f:797:LEU:HD21	2.40	0.52
14:A:74:PRO:O	14:A:78:TRP:NE1	2.42	0.52
15:B:201:VAL:HG11	15:B:239:VAL:CG1	2.38	0.52
17:D:84:SER:O	17:D:87:LEU:HD13	2.09	0.52
19:F:177:VAL:O	19:F:177:VAL:HG23	2.08	0.52
22:I:90:LEU:HG	22:I:114:LEU:HD13	1.92	0.52
22:I:119:GLN:HG3	23:J:78:ALA:HB1	1.91	0.52
23:J:120:GLN:HB3	24:K:133:MET:HE1	1.91	0.52
26:M:63:SER:OG	26:M:64:ASN:N	2.42	0.52
26:M:76:MET:HE3	26:M:136:PHE:CG	2.45	0.52
27:N:161:ILE:CD1	27:N:173:VAL:HG21	2.40	0.52
30:Q:8:GLN:NE2	30:Q:113:PRO:O	2.42	0.52
7:a:211:PHE:O	7:a:339:ARG:NH1	2.42	0.52
12:f:476:THR:OG1	12:f:477:MET:N	2.43	0.52
12:f:670:MET:O	12:f:674:THR:HG23	2.09	0.52
14:A:96:ALA:HB3	14:A:140:VAL:O	2.08	0.52
15:B:338:ASP:O	15:B:341:LEU:HD23	2.10	0.52
19:F:424:ILE:HG22	19:F:428:GLN:HE22	1.74	0.52
33:t:205:LEU:CD2	33:t:210:ALA:HB2	2.39	0.52
1:U:206:MET:HE2	1:U:206:MET:HA	1.92	0.52
4:X:355:LYS:O	4:X:356:LEU:HD22	2.10	0.52
12:f:196:MET:HE2	12:f:217:LEU:HD21	1.91	0.52
12:f:242:GLU:O	12:f:245:ASN:HB2	2.09	0.52
18:E:177:GLY:O	18:E:180:LYS:N	2.43	0.52
23:J:36:ARG:NE	23:J:142:PRO:O	2.42	0.52
23:J:134:VAL:HG12	23:J:144:LEU:HD12	1.92	0.52
25:L:66:VAL:HG12	25:L:67:ASP:N	2.24	0.52
28:O:55:ILE:HD12	28:O:57:LEU:HD13	1.92	0.52
29:P:62:THR:HG23	30:Q:86:ARG:HH12	1.75	0.52
32:S:43:ILE:HD13	32:S:163:PHE:HB2	1.91	0.52
27:n:153:MET:HE3	33:t:102:TYR:HD2	1.75	0.52
30:q:85:ARG:HB2	30:q:118:MET:HE1	1.92	0.52
3:W:146:THR:CG2	3:W:169:LEU:HD11	2.39	0.52
14:A:25:LEU:HD11	15:B:407:LEU:HD21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:223:ILE:HD11	15:B:347:ILE:HD13	1.92	0.52
16:C:258:ARG:HG3	16:C:258:ARG:O	2.09	0.52
19:F:183:GLU:O	19:F:184:GLN:HB2	2.10	0.52
30:Q:5:ILE:CD1	30:Q:143:LEU:HD11	2.34	0.52
32:S:41:LEU:HD12	32:S:42:ALA:H	1.75	0.52
33:T:186:TYR:OH	28:o:175:LEU:HD21	2.10	0.52
13:x:125:ASP:OD1	13:x:264:THR:OG1	2.28	0.52
18:E:221:TYR:O	18:E:225:HIS:ND1	2.43	0.52
23:J:71:MET:HE3	23:J:131:ALA:CB	2.40	0.52
24:K:205:VAL:HG22	24:K:205:VAL:O	2.10	0.52
24:K:211:ASN:O	24:K:212:ALA:HB3	2.09	0.52
28:O:71:ASP:CG	29:P:131:MET:HE1	2.35	0.52
28:O:102:ILE:HG13	28:O:126:LEU:HD23	1.91	0.52
27:n:93:VAL:HG21	27:n:117:PHE:HD1	1.75	0.52
33:t:50:MET:O	33:t:52:THR:HG23	2.10	0.52
2:V:395:ILE:HG22	2:V:395:ILE:O	2.10	0.51
7:a:60:TYR:CE1	7:a:64:ILE:HG21	2.46	0.51
15:B:112:LEU:HD11	15:B:115:ILE:CG1	2.40	0.51
16:C:277:LEU:HD21	16:C:304:ALA:HB3	1.91	0.51
28:O:252:THR:HG23	28:O:252:THR:O	2.10	0.51
29:P:69:PHE:O	29:P:73:LEU:HD23	2.10	0.51
32:S:96:ILE:O	32:S:100:LEU:HD23	2.09	0.51
32:s:62:SER:O	32:s:63:ILE:C	2.53	0.51
32:s:85:PHE:HD1	32:s:88:ASP:H	1.57	0.51
33:t:51:VAL:HG23	33:t:74:SER:C	2.35	0.51
4:X:271:VAL:HG22	4:X:284:THR:OG1	2.10	0.51
12:f:127:SER:HB3	12:f:143:ARG:HD2	1.92	0.51
12:f:471:LEU:O	12:f:478:ARG:NH2	2.44	0.51
31:R:76:ASP:OD1	31:R:92:LYS:NZ	2.44	0.51
30:q:13:VAL:HG11	30:q:105:ALA:HB1	1.92	0.51
1:U:506:ALA:HB2	9:c:63:ASP:OD2	2.10	0.51
4:X:282:ARG:NH1	4:X:312:GLU:OE2	2.43	0.51
7:a:184:ASP:OD1	7:a:186:LYS:N	2.43	0.51
11:e:52:PHE:CE1	11:e:56:LEU:HD13	2.45	0.51
27:N:55:THR:HG21	33:t:226:ALA:HB2	1.93	0.51
14:A:56:LEU:HD22	15:B:72:LEU:CD1	2.41	0.51
14:A:375:ARG:NH1	24:K:172:SER:OG	2.43	0.51
23:J:207:GLU:C	23:J:208:LEU:HD22	2.35	0.51
3:W:57:ALA:O	3:W:58:SER:OG	2.22	0.51
5:Y:82:LYS:O	5:Y:85:ASP:OD1	2.28	0.51
5:Y:186:LEU:HD12	5:Y:213:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:113:VAL:CG2	8:b:140:ILE:HG23	2.40	0.51
10:d:284:PHE:CD1	10:d:285:THR:HG23	2.45	0.51
19:F:182:THR:HG23	19:F:182:THR:O	2.10	0.51
20:G:123:GLN:O	20:G:126:THR:HG22	2.10	0.51
22:I:175:LEU:HD23	22:I:192:LEU:CD2	2.39	0.51
24:K:182:GLN:NE2	25:L:55:GLU:OE2	2.44	0.51
26:M:82:LEU:HD23	26:M:86:ARG:HH12	1.75	0.51
30:Q:13:VAL:HG13	30:Q:183:ILE:HB	1.92	0.51
1:U:5:ALA:HB3	1:U:37:GLU:OE1	2.11	0.51
1:U:880:ASN:HB3	1:U:881:PRO:HD3	1.93	0.51
2:V:287:ARG:NE	11:e:21:GLU:OE2	2.43	0.51
4:X:15:LEU:HD12	4:X:26:ILE:HD12	1.91	0.51
7:a:115:LYS:NZ	7:a:137:ASP:OD2	2.39	0.51
7:a:201:GLY:O	7:a:205:LEU:HD13	2.10	0.51
7:a:271:LYS:O	7:a:275:LEU:HD23	2.11	0.51
11:e:39:TRP:CD1	11:e:39:TRP:N	2.78	0.51
16:C:138:MET:CG	16:C:213:ARG:O	2.59	0.51
28:O:244:ARG:HD3	28:O:246:ARG:HG2	1.92	0.51
31:r:233:VAL:HG21	31:r:254:LEU:HD11	1.92	0.51
32:s:50:ILE:HG22	32:s:225:ILE:HA	1.92	0.51
2:V:345:ARG:NH1	11:e:45:ASP:OD2	2.39	0.51
3:W:346:GLU:OE2	3:W:350:ARG:NH1	2.44	0.51
4:X:15:LEU:O	4:X:19:ASP:C	2.54	0.51
4:X:264:PRO:O	4:X:267:VAL:HG12	2.11	0.51
4:X:339:ILE:HG13	4:X:387:ILE:HD11	1.92	0.51
5:Y:174:TRP:CG	16:C:337:ASN:OD1	2.64	0.51
14:A:317:VAL:CG1	14:A:319:MET:HE2	2.39	0.51
16:C:219:LEU:CD1	16:C:254:ILE:HD12	2.40	0.51
17:D:142:VAL:HG23	17:D:142:VAL:O	2.11	0.51
18:E:130:VAL:HG23	18:E:131:SER:N	2.25	0.51
18:E:172:LEU:HD12	18:E:183:LEU:HD23	1.92	0.51
25:L:201:ALA:O	25:L:203:GLN:N	2.42	0.51
26:M:40:ILE:HD12	26:M:194:VAL:CG2	2.41	0.51
30:Q:13:VAL:HG22	30:Q:13:VAL:O	2.10	0.51
31:R:200:ARG:CZ	30:q:146:TYR:CE2	2.94	0.51
32:S:221:LEU:O	32:S:235:THR:HG23	2.09	0.51
33:t:70:ASP:OD1	33:t:86:ARG:NH1	2.37	0.51
7:a:97:LEU:HA	7:a:100:THR:HG22	1.93	0.51
12:f:236:CYS:O	12:f:240:VAL:HG23	2.10	0.51
19:F:275:ALA:HB2	19:F:283:ILE:HD11	1.92	0.51
20:G:182:LYS:HG2	20:G:197:THR:HG23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J:139:ASP:OD1	23:J:140:GLY:N	2.43	0.51
31:R:115:GLU:OE2	31:R:158:THR:OG1	2.29	0.51
29:p:56:LEU:O	29:p:60:VAL:HG23	2.11	0.51
30:q:46:CYS:HA	30:q:102:LEU:HD23	1.92	0.51
2:V:164:GLU:OE1	2:V:164:GLU:N	2.42	0.51
3:W:409:LEU:HD23	4:X:344:ARG:NH1	2.26	0.51
5:Y:290:PRO:HB2	11:e:39:TRP:CH2	2.46	0.51
7:a:244:ASN:O	7:a:247:ARG:N	2.44	0.51
12:f:245:ASN:C	12:f:249:LEU:HD23	2.36	0.51
16:C:111:ASN:O	16:C:129:ASN:ND2	2.41	0.51
16:C:325:ARG:NH1	16:C:348:ALA:O	2.44	0.51
17:D:284:GLU:OE1	17:D:287:ARG:NE	2.43	0.51
19:F:335:VAL:HG23	19:F:335:VAL:O	2.11	0.51
27:N:74:ARG:O	27:N:213:ILE:HD13	2.11	0.51
30:Q:93:ARG:O	30:Q:94:SER:OG	2.25	0.51
32:s:64:HIS:CE1	33:t:177:TYR:CD2	2.99	0.51
2:V:476:PHE:CZ	6:Z:258:VAL:HG22	2.46	0.51
3:W:88:MET:HE3	3:W:127:THR:CG2	2.41	0.51
12:f:512:MET:HE2	12:f:553:THR:O	2.11	0.51
12:f:666:ILE:HD11	15:B:68:ILE:HG12	1.89	0.51
16:C:73:VAL:HG21	17:D:102:ILE:HD11	1.94	0.51
20:G:132:ARG:O	20:G:133:PRO:C	2.54	0.51
28:O:245:TYR:HH	29:P:152:SER:C	2.19	0.51
29:P:78:GLU:O	29:P:79:GLY:C	2.53	0.51
29:P:193:ASP:O	29:P:194:LYS:HE2	2.11	0.51
1:U:681:ASN:OD1	1:U:682:TYR:N	2.44	0.50
2:V:367:VAL:HG22	2:V:402:VAL:HG22	1.93	0.50
4:X:237:GLU:OE1	17:D:338:ARG:NH2	2.39	0.50
10:d:288:THR:OG1	10:d:299:MET:HE2	2.11	0.50
12:f:82:ILE:HG22	12:f:85:SER:OG	2.11	0.50
12:f:818:LEU:O	12:f:822:VAL:HG23	2.11	0.50
16:C:20:LEU:N	16:C:20:LEU:HD12	2.26	0.50
16:C:214:VAL:O	16:C:214:VAL:HG12	2.12	0.50
17:D:216:ALA:O	17:D:219:VAL:HG12	2.10	0.50
19:F:62:VAL:O	19:F:66:LEU:HD23	2.11	0.50
20:G:196:GLU:O	20:G:197:THR:C	2.53	0.50
31:R:175:SER:OG	31:R:176:GLU:OE1	2.25	0.50
27:n:37:ILE:HD12	27:n:133:ILE:HD12	1.92	0.50
33:t:167:LEU:HG	33:t:182:LEU:HD12	1.91	0.50
2:V:466:ILE:O	2:V:466:ILE:HG13	2.11	0.50
5:Y:134:LEU:O	5:Y:138:LEU:HD23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:185:ILE:O	7:a:193:GLN:NE2	2.44	0.50
14:A:51:ASP:OD1	15:B:69:LYS:NZ	2.38	0.50
15:B:394:ASP:O	15:B:398:ILE:HG13	2.12	0.50
16:C:161:ILE:HD13	16:C:186:VAL:HG11	1.92	0.50
16:C:339:THR:HG22	16:C:340:ARG:N	2.25	0.50
23:J:66:ASP:OD1	23:J:67:ASP:N	2.44	0.50
27:N:65:THR:HG22	27:N:66:ASP:N	2.27	0.50
28:O:91:THR:HG23	28:O:91:THR:O	2.11	0.50
30:Q:38:MET:HE2	30:Q:44:LEU:HB2	1.93	0.50
33:T:141:MET:HE3	33:T:171:ASP:O	2.12	0.50
33:t:237:VAL:HG23	33:t:242:VAL:HG22	1.92	0.50
1:U:695:MET:HE1	1:U:709:PHE:CD2	2.46	0.50
6:Z:217:THR:HG21	6:Z:219:LYS:NZ	2.26	0.50
8:b:161:ASN:O	8:b:165:GLY:N	2.35	0.50
8:b:171:VAL:HG23	8:b:171:VAL:O	2.11	0.50
9:c:180:ASN:OD1	9:c:180:ASN:O	2.28	0.50
12:f:57:GLU:OE1	12:f:102:HIS:NE2	2.44	0.50
12:f:606:VAL:O	15:B:74:MET:HE1	2.12	0.50
17:D:320:ALA:O	17:D:327:LEU:HD12	2.11	0.50
27:N:153:MET:HE1	33:T:102:TYR:CE2	2.47	0.50
31:R:216:ARG:HG3	31:R:233:VAL:HG11	1.93	0.50
30:q:115:LEU:HD12	30:q:128:PRO:O	2.11	0.50
1:U:468:ALA:O	13:x:121:LYS:NZ	2.44	0.50
3:W:176:SER:HB2	3:W:181:GLU:OE2	2.12	0.50
7:a:232:TRP:CZ2	7:a:255:TRP:HA	2.47	0.50
10:d:129:LEU:O	10:d:131:THR:OG1	2.21	0.50
14:A:116:LYS:NZ	15:B:130:GLU:OE2	2.36	0.50
18:E:64:LEU:CD1	18:E:70:ILE:HD11	2.42	0.50
23:J:192:ILE:O	23:J:196:LEU:HD13	2.11	0.50
25:L:67:ASP:O	25:L:69:HIS:N	2.45	0.50
30:Q:26:VAL:HG12	30:q:170:ARG:HG3	1.93	0.50
31:r:65:PHE:CZ	31:r:202:TYR:CZ	2.98	0.50
4:X:316:ASP:HB3	4:X:319:ILE:HG22	1.94	0.50
10:d:254:GLU:O	10:d:257:THR:OG1	2.24	0.50
16:C:54:ALA:O	16:C:58:LEU:HD23	2.11	0.50
16:C:63:LEU:HD21	17:D:79:VAL:HG23	1.93	0.50
18:E:65:THR:O	18:E:68:LYS:N	2.45	0.50
27:n:68:LEU:HD23	27:n:78:CYS:SG	2.51	0.50
28:o:129:MET:HE2	28:o:129:MET:HA	1.92	0.50
5:Y:200:LEU:O	5:Y:204:THR:HG22	2.12	0.50
6:Z:61:ASP:HB3	6:Z:67:VAL:CG2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:781:TYR:HA	12:f:787:LEU:O	2.12	0.50
15:B:107:MET:HE3	15:B:160:ILE:CG2	2.37	0.50
16:C:76:VAL:HG13	16:C:85:VAL:CG1	2.42	0.50
16:C:150:MET:HE2	16:C:334:ARG:HH21	1.76	0.50
17:D:254:ALA:HB2	17:D:262:ILE:CD1	2.42	0.50
18:E:151:LEU:O	18:E:154:THR:O	2.30	0.50
19:F:224:LEU:CD1	19:F:343:LEU:HD21	2.37	0.50
22:I:135:LEU:HD21	22:I:162:THR:HG23	1.94	0.50
25:L:11:THR:HG22	25:L:11:THR:O	2.12	0.50
29:P:149:MET:HE1	32:s:176:LEU:HA	1.94	0.50
30:q:13:VAL:O	30:q:15:VAL:HG13	2.12	0.50
32:s:174:GLN:HA	32:s:177:LEU:HD12	1.94	0.50
33:t:225:ASP:OD1	33:t:226:ALA:N	2.44	0.50
2:V:64:GLN:OE1	2:V:109:ASN:ND2	2.44	0.50
3:W:324:TYR:O	3:W:327:GLU:HG3	2.11	0.50
6:Z:19:VAL:HG21	6:Z:124:ILE:HD13	1.93	0.50
12:f:658:ALA:HB2	12:f:693:ALA:HA	1.93	0.50
14:A:273:PHE:CG	14:A:273:PHE:O	2.64	0.50
15:B:289:ALA:HB2	16:C:274:LEU:HD23	1.94	0.50
16:C:140:VAL:HG22	16:C:213:ARG:HH11	1.76	0.50
20:G:70:PHE:CD2	20:G:91:VAL:HG21	2.47	0.50
20:G:113:MET:HE1	28:O:112:SER:O	2.12	0.50
24:K:95:GLU:OE1	24:K:115:ALA:HB3	2.12	0.50
27:N:155:VAL:HG11	33:T:81:PHE:CD1	2.47	0.50
29:P:75:GLU:O	29:P:79:GLY:HA2	2.11	0.50
33:T:161:ALA:O	33:T:164:GLU:N	2.44	0.50
31:r:233:VAL:O	31:r:233:VAL:CG1	2.59	0.50
4:X:96:PHE:HD1	4:X:99:MET:HE1	1.77	0.50
7:a:77:VAL:CG1	7:a:113:LEU:HD22	2.42	0.50
8:b:3:LEU:HD21	8:b:46:GLU:HG3	1.92	0.50
8:b:18:ASN:HB2	8:b:25:ARG:HE	1.77	0.50
12:f:170:TRP:HB3	12:f:211:ILE:HD13	1.94	0.50
16:C:198:LEU:HD23	16:C:198:LEU:C	2.37	0.50
17:D:417:TYR:OH	20:G:22:LEU:N	2.40	0.50
18:E:130:VAL:HG23	18:E:131:SER:H	1.77	0.50
32:S:226:VAL:HG22	32:S:231:ILE:HG12	1.94	0.50
33:t:257:ALA:O	33:t:260:ILE:HG22	2.11	0.50
1:U:588:MET:HA	1:U:588:MET:HE3	1.93	0.50
3:W:274:VAL:HG12	3:W:287:VAL:HG22	1.94	0.50
4:X:242:ILE:O	4:X:242:ILE:HG22	2.12	0.50
7:a:349:MET:O	7:a:353:LEU:HD23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:153:GLN:HA	10:d:153:GLN:HE21	1.76	0.50
12:f:460:ASP:OD1	12:f:489:TYR:OH	2.20	0.50
15:B:269:GLU:OE2	15:B:272:ARG:NH1	2.45	0.50
15:B:329:MET:HE1	15:B:341:LEU:HD12	1.94	0.50
16:C:266:ASP:OD2	17:D:283:ARG:NH1	2.45	0.50
18:E:170:CYS:C	18:E:171:LEU:HD12	2.37	0.50
19:F:310:MET:HE1	19:F:342:LEU:HD22	1.93	0.50
26:M:161:TYR:CD2	26:M:164:CYS:HB2	2.47	0.50
26:M:164:CYS:SG	26:M:165:ALA:N	2.84	0.50
28:O:73:ASN:O	28:O:230:ARG:NH2	2.45	0.50
1:U:206:MET:CE	1:U:216:VAL:HG21	2.42	0.49
1:U:503:GLN:O	1:U:535:TYR:OH	2.31	0.49
5:Y:173:ASP:N	5:Y:173:ASP:OD1	2.44	0.49
12:f:262:PHE:HB2	12:f:265:ALA:HB3	1.94	0.49
14:A:191:VAL:HG21	14:A:318:LEU:HD11	1.93	0.49
17:D:87:LEU:HD21	17:D:140:VAL:CG2	2.41	0.49
18:E:113:ARG:NH2	18:E:116:ASP:OD1	2.45	0.49
18:E:142:ILE:HD13	18:E:183:LEU:HD12	1.94	0.49
19:F:175:MET:HE2	19:F:251:LEU:HA	1.93	0.49
29:p:121:ILE:CG2	29:p:137:VAL:HG22	2.42	0.49
32:s:212:GLU:OE2	32:s:239:ARG:NH2	2.45	0.49
1:U:14:GLU:OE2	10:d:166:ARG:NE	2.45	0.49
4:X:380:GLN:O	5:Y:315:THR:OG1	2.29	0.49
5:Y:170:GLU:O	5:Y:170:GLU:CD	2.55	0.49
8:b:108:ARG:NH1	8:b:139:ASP:OD2	2.46	0.49
9:c:138:GLU:OE1	9:c:138:GLU:O	2.30	0.49
12:f:562:LEU:HD23	12:f:595:VAL:HG21	1.93	0.49
12:f:809:ILE:HG23	12:f:810:ILE:N	2.27	0.49
14:A:134:ILE:HG23	14:A:140:VAL:CG1	2.42	0.49
17:D:181:VAL:CG1	17:D:219:VAL:HG21	2.40	0.49
21:H:206:ASP:OD1	21:H:206:ASP:O	2.31	0.49
25:L:157:ARG:CB	26:M:60:GLU:OE1	2.60	0.49
25:L:178:GLU:OE1	25:L:190:HIS:NE2	2.45	0.49
27:n:48:LEU:HD11	27:n:135:ALA:HB3	1.94	0.49
1:U:155:LEU:CD2	1:U:188:MET:HE1	2.42	0.49
1:U:588:MET:SD	1:U:764:LEU:HD22	2.52	0.49
2:V:98:LEU:HD21	2:V:209:LYS:HG3	1.93	0.49
2:V:290:TYR:HD1	2:V:328:VAL:HG22	1.77	0.49
7:a:104:VAL:HG11	7:a:110:ALA:CB	2.42	0.49
7:a:125:ILE:O	7:a:125:ILE:HG22	2.11	0.49
8:b:11:ASP:OD2	8:b:84:ILE:HD12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:560:LEU:HD23	12:f:560:LEU:C	2.37	0.49
15:B:207:HIS:N	15:B:208:PRO:HD3	2.28	0.49
15:B:239:VAL:O	15:B:243:THR:HG22	2.12	0.49
15:B:316:LEU:CD2	15:B:327:VAL:HG21	2.41	0.49
16:C:406:LYS:NZ	22:I:63:GLU:O	2.33	0.49
19:F:251:LEU:HD21	19:F:291:ILE:HD11	1.93	0.49
22:I:238:LYS:O	22:I:239:LYS:C	2.55	0.49
23:J:90:GLU:HG2	23:J:110:TYR:CG	2.47	0.49
1:U:70:HIS:O	2:V:236:ARG:NH1	2.45	0.49
1:U:229:VAL:HG11	1:U:252:LEU:HD11	1.94	0.49
1:U:875:PHE:CD2	1:U:877:LEU:HD23	2.48	0.49
3:W:268:LYS:HA	3:W:302:TYR:OH	2.12	0.49
14:A:142:VAL:HG13	14:A:147:TYR:HB3	1.95	0.49
35:A:501:ATP:O3A	15:B:343:ARG:NH1	2.44	0.49
15:B:223:ILE:HG13	15:B:347:ILE:HD13	1.94	0.49
16:C:275:GLU:OE2	16:C:275:GLU:HA	2.12	0.49
18:E:98:VAL:HB	18:E:107:ILE:HG23	1.93	0.49
19:F:172:VAL:HG13	19:F:267:LEU:CD1	2.42	0.49
20:G:86:ASP:OD1	26:M:121:HIS:NE2	2.45	0.49
20:G:206:LEU:HB2	20:G:208:ILE:HG22	1.94	0.49
23:J:115:LYS:O	23:J:119:THR:HG23	2.12	0.49
24:K:48:LEU:O	24:K:217:LEU:HD12	2.13	0.49
24:K:88:LEU:HD12	24:K:139:VAL:CG1	2.43	0.49
27:N:222:VAL:HG21	33:t:258:HIS:CD2	2.47	0.49
29:P:188:HIS:CE1	29:P:197:THR:HG22	2.46	0.49
30:Q:64:VAL:HG13	30:Q:75:LEU:HD12	1.94	0.49
1:U:206:MET:HE1	1:U:213:PHE:CE1	2.47	0.49
1:U:494:TYR:CE1	1:U:516:LEU:HD22	2.48	0.49
3:W:259:GLU:OE1	3:W:262:LYS:N	2.36	0.49
3:W:378:MET:HE1	3:W:393:LEU:HD12	1.94	0.49
5:Y:290:PRO:O	5:Y:291:HIS:ND1	2.46	0.49
5:Y:376:LEU:HD21	6:Z:265:LEU:HD21	1.94	0.49
8:b:65:THR:HG21	8:b:70:ARG:HD3	1.93	0.49
9:c:41:MET:HE3	9:c:72:VAL:HG11	1.94	0.49
10:d:145:ARG:O	10:d:149:GLU:HG3	2.13	0.49
18:E:137:GLY:N	18:E:311:ASP:OD2	2.45	0.49
22:I:45:LEU:HD11	22:I:137:ILE:CG2	2.42	0.49
28:O:210:LEU:HD23	32:s:63:ILE:HD11	1.95	0.49
31:R:117:LEU:HD22	31:R:145:MET:SD	2.52	0.49
3:W:119:PRO:HA	3:W:122:LEU:HD23	1.94	0.49
7:a:108:ASP:O	7:a:112:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:270:GLN:O	16:C:274:LEU:HD13	2.12	0.49
16:C:306:LEU:O	16:C:314:LYS:NZ	2.36	0.49
22:I:206:LEU:O	22:I:207:SER:OG	2.26	0.49
23:J:66:ASP:N	30:Q:69:MET:HE1	2.28	0.49
24:K:22:PHE:HA	24:K:25:GLU:OE1	2.12	0.49
26:M:63:SER:O	26:M:64:ASN:C	2.56	0.49
26:M:187:CYS:O	26:M:191:VAL:HG23	2.13	0.49
12:f:498:LEU:O	12:f:502:LEU:HD13	2.12	0.49
12:f:714:SER:O	12:f:716:ASP:N	2.45	0.49
24:K:57:PRO:O	24:K:58:LEU:HB2	2.13	0.49
1:U:678:ASP:OD1	1:U:679:PRO:HD2	2.11	0.49
4:X:339:ILE:CG1	4:X:387:ILE:HD11	2.43	0.49
14:A:141:GLY:N	14:A:151:ILE:O	2.45	0.49
16:C:164:VAL:HG11	16:C:186:VAL:CG2	2.43	0.49
17:D:232:GLY:O	17:D:236:VAL:HG23	2.13	0.49
25:L:38:LEU:HD12	25:L:38:LEU:C	2.37	0.49
26:M:47:VAL:HG11	26:M:190:ILE:HG22	1.94	0.49
30:Q:61:GLN:OE1	30:Q:62:LYS:NZ	2.46	0.49
33:T:190:LEU:HD11	33:T:221:LEU:CD2	2.42	0.49
33:T:222:TYR:CD2	33:T:252:THR:HG21	2.48	0.49
2:V:176:MET:HE1	2:V:217:VAL:HG22	1.94	0.49
7:a:45:VAL:HG11	7:a:82:HIS:HB3	1.95	0.49
8:b:90:ILE:CD1	8:b:109:ILE:HG21	2.42	0.49
9:c:62:VAL:HB	9:c:66:THR:HB	1.93	0.49
10:d:110:SER:O	10:d:114:GLU:OE1	2.30	0.49
10:d:206:ALA:O	10:d:210:THR:HG23	2.13	0.49
12:f:576:ILE:O	12:f:580:LEU:HD23	2.12	0.49
18:E:28:GLU:OE1	18:E:28:GLU:N	2.46	0.49
18:E:305:ASN:CG	18:E:308:ALA:HB3	2.38	0.49
18:E:310:LEU:HD21	18:E:329:GLU:N	2.27	0.49
19:F:375:VAL:HG13	19:F:379:VAL:HG11	1.95	0.49
20:G:131:MET:CE	26:M:126:TYR:HE1	2.26	0.49
23:J:96:LEU:HD12	30:Q:62:LYS:HG3	1.95	0.49
32:s:39:THR:HG21	32:s:169:ALA:HB3	1.95	0.49
1:U:26:LYS:HE2	10:d:131:THR:OG1	2.12	0.49
3:W:243:ILE:HG21	3:W:273:TYR:CZ	2.48	0.49
4:X:133:LEU:HD11	4:X:137:TYR:CE1	2.48	0.49
5:Y:50:MET:HB3	5:Y:53:TYR:HB3	1.95	0.49
5:Y:148:GLY:O	5:Y:157:ILE:HD11	2.13	0.49
6:Z:260:VAL:HG13	9:c:292:MET:HE3	1.94	0.49
7:a:216:LEU:O	7:a:216:LEU:HD23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:148:LEU:CD1	10:d:174:TYR:CE2	2.96	0.49
14:A:206:ILE:HD11	19:F:408:LEU:CD1	2.43	0.49
14:A:303:ILE:HG23	14:A:336:ARG:NE	2.27	0.49
16:C:84:LYS:NZ	16:C:98:ASP:OD1	2.46	0.49
16:C:232:ARG:O	16:C:236:VAL:HG23	2.12	0.49
20:G:37:LEU:HD12	20:G:53:GLN:HB2	1.94	0.49
20:G:236:ASP:O	20:G:240:VAL:HG22	2.13	0.49
28:O:191:GLU:OE2	28:O:225:LYS:NZ	2.46	0.49
29:P:12:MET:HE1	29:P:170:ALA:CB	2.42	0.49
29:P:158:MET:HG3	29:P:162:HIS:HD1	1.78	0.49
8:b:93:ALA:O	8:b:97:LEU:HG	2.13	0.48
12:f:196:MET:HE3	12:f:217:LEU:HD11	1.93	0.48
12:f:487:LEU:CD2	12:f:823:ALA:HB2	2.43	0.48
12:f:599:ALA:O	12:f:600:TYR:C	2.55	0.48
17:D:205:TYR:CE1	17:D:314:ALA:HB1	2.48	0.48
18:E:92:LEU:HD13	18:E:107:ILE:HG21	1.95	0.48
25:L:141:GLY:O	25:L:143:HIS:CD2	2.66	0.48
28:O:93:ALA:HB3	29:P:127:ILE:HD12	1.94	0.48
29:P:87:LEU:HD23	29:P:109:ILE:HD13	1.95	0.48
30:Q:64:VAL:HG22	30:Q:75:LEU:CD1	2.43	0.48
33:T:108:LEU:HD13	33:T:155:MET:SD	2.52	0.48
1:U:356:THR:O	1:U:360:VAL:HG23	2.13	0.48
2:V:252:ASN:HD21	2:V:287:ARG:CD	2.26	0.48
2:V:423:ALA:O	2:V:424:GLN:HB3	2.13	0.48
2:V:492:LYS:O	2:V:493:ALA:HB3	2.13	0.48
3:W:258:ALA:O	3:W:262:LYS:NZ	2.33	0.48
10:d:272:ALA:O	10:d:275:ILE:N	2.46	0.48
12:f:647:GLY:HA2	12:f:685:THR:HG21	1.95	0.48
12:f:745:LEU:HD11	12:f:762:VAL:HG23	1.94	0.48
15:B:125:THR:HG22	15:B:126:SER:N	2.28	0.48
15:B:371:ARG:HG2	15:B:371:ARG:O	2.14	0.48
17:D:131:ALA:HB3	17:D:141:ASP:HB3	1.95	0.48
18:E:326:ILE:H	18:E:326:ILE:HD12	1.77	0.48
23:J:83:VAL:HG13	23:J:111:ILE:HD12	1.95	0.48
23:J:91:CYS:HA	23:J:102:VAL:HG11	1.94	0.48
27:N:212:ALA:HB3	27:N:219:GLU:OE2	2.14	0.48
28:O:151:PRO:O	28:O:152:HIS:ND1	2.46	0.48
29:P:164:PHE:CE1	29:P:200:LEU:HD21	2.48	0.48
33:T:80:ARG:O	33:T:81:PHE:C	2.56	0.48
2:V:211:TYR:CD2	2:V:250:LEU:HD21	2.49	0.48
5:Y:237:ARG:NH1	5:Y:238:GLU:OE2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:282:MET:HE2	5:Y:295:TYR:CD2	2.48	0.48
7:a:25:LEU:HA	7:a:40:GLN:HE22	1.78	0.48
12:f:613:LEU:HD21	15:B:78:PHE:HB2	1.95	0.48
16:C:326:LEU:HD22	16:C:345:ARG:HG2	1.95	0.48
18:E:177:GLY:HA3	18:E:180:LYS:HE3	1.94	0.48
25:L:166:GLN:O	25:L:167:SER:C	2.57	0.48
30:Q:3:TYR:HE1	30:Q:136:ALA:HA	1.78	0.48
6:Z:173:GLU:OE2	6:Z:180:LYS:NZ	2.37	0.48
12:f:92:VAL:O	12:f:92:VAL:HG12	2.12	0.48
14:A:246:VAL:HG23	14:A:280:ILE:HD11	1.95	0.48
22:I:143:TYR:HE2	23:J:57:ARG:NH2	2.12	0.48
23:J:178:ASP:O	23:J:181:ILE:C	2.56	0.48
27:N:80:SER:OG	27:N:131:GLY:O	2.22	0.48
30:Q:143:LEU:HD23	30:Q:159:LEU:HD21	1.95	0.48
1:U:151:ILE:H	1:U:151:ILE:HD12	1.78	0.48
2:V:337:LEU:HD22	2:V:367:VAL:HG11	1.96	0.48
3:W:128:LEU:HA	3:W:131:VAL:HG12	1.95	0.48
5:Y:50:MET:C	5:Y:73:MET:HE2	2.39	0.48
8:b:189:LEU:HD12	8:b:192:GLU:HB2	1.95	0.48
12:f:484:GLY:HA2	12:f:487:LEU:HD12	1.96	0.48
15:B:243:THR:HG23	15:B:243:THR:O	2.13	0.48
16:C:189:TYR:HE1	16:C:298:ILE:HD13	1.77	0.48
18:E:145:LEU:CD2	18:E:187:VAL:HG11	2.44	0.48
18:E:325:GLU:O	18:E:329:GLU:OE1	2.31	0.48
19:F:244:THR:O	19:F:244:THR:HG22	2.14	0.48
23:J:36:ARG:HA	23:J:41:VAL:HG12	1.95	0.48
25:L:214:ILE:HD12	25:L:224:TYR:CE1	2.48	0.48
3:W:98:LYS:HD3	3:W:98:LYS:N	2.28	0.48
4:X:342:PHE:CD1	4:X:345:VAL:HG22	2.48	0.48
14:A:33:LEU:HD13	15:B:412:MET:SD	2.53	0.48
14:A:78:TRP:HZ3	15:B:99:VAL:HG11	1.79	0.48
14:A:191:VAL:CG2	14:A:318:LEU:HD21	2.42	0.48
15:B:434:THR:N	15:B:435:PRO:CD	2.77	0.48
15:B:440:LEU:HD22	23:J:61:LYS:HE3	1.94	0.48
16:C:394:ASP:N	16:C:394:ASP:OD1	2.47	0.48
17:D:223:THR:HG22	17:D:225:ALA:H	1.79	0.48
17:D:388:ARG:NH2	18:E:151:LEU:HD23	2.27	0.48
19:F:206:MET:HE1	19:F:244:THR:HG22	1.94	0.48
20:G:210:PHE:CD1	20:G:215:ILE:HD11	2.49	0.48
22:I:34:CYS:SG	22:I:64:LYS:HD3	2.53	0.48
25:L:41:LYS:HG3	25:L:42:THR:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:161:ILE:HD11	27:N:173:VAL:HG21	1.96	0.48
30:Q:182:ILE:HD11	30:Q:191:LEU:HD22	1.95	0.48
1:U:19:LEU:HA	10:d:124:LEU:HD12	1.95	0.48
6:Z:126:VAL:O	9:c:212:LEU:HD11	2.13	0.48
7:a:278:MET:HE1	7:a:319:LEU:HD13	1.96	0.48
10:d:124:LEU:HD23	10:d:124:LEU:C	2.38	0.48
12:f:343:LYS:CE	12:f:348:ILE:HD11	2.44	0.48
14:A:93:LEU:CB	14:A:141:GLY:HA2	2.44	0.48
16:C:131:VAL:HG12	16:C:132:ASP:N	2.29	0.48
16:C:297:ARG:HH22	16:C:300:ILE:HD11	1.79	0.48
18:E:170:CYS:O	18:E:171:LEU:HD12	2.14	0.48
19:F:202:ILE:CG2	19:F:282:ILE:HD12	2.44	0.48
21:H:85:VAL:HG11	21:H:130:PHE:HZ	1.77	0.48
30:Q:17:SER:OG	30:Q:45:LEU:HD22	2.13	0.48
30:Q:134:TYR:C	30:Q:136:ALA:N	2.70	0.48
4:X:403:THR:HG21	6:Z:266:ILE:HD11	1.96	0.48
6:Z:81:MET:HE1	9:c:94:LYS:HB3	1.95	0.48
12:f:475:ASN:O	12:f:476:THR:OG1	2.25	0.48
12:f:750:GLN:OE1	12:f:750:GLN:HA	2.14	0.48
14:A:332:MET:O	14:A:340:LYS:NZ	2.36	0.48
18:E:180:LYS:HG3	18:E:181:THR:N	2.29	0.48
20:G:53:GLN:OE1	20:G:53:GLN:HA	2.14	0.48
26:M:50:VAL:HG23	26:M:67:LEU:HD21	1.96	0.48
28:O:62:ARG:CB	28:O:213:GLY:HA2	2.43	0.48
28:O:172:SER:C	28:O:209:ASP:OD2	2.56	0.48
30:Q:18:ASP:OD1	30:Q:178:PHE:CE1	2.67	0.48
3:W:79:GLU:HB2	3:W:83:LEU:HD22	1.96	0.48
16:C:256:SER:OG	16:C:257:SER:N	2.46	0.48
17:D:85:ILE:HG23	18:E:68:LYS:CG	2.44	0.48
18:E:81:VAL:HB	18:E:105:LEU:O	2.14	0.48
19:F:395:GLN:OE1	19:F:395:GLN:N	2.45	0.48
25:L:168:ALA:O	25:L:172:LEU:HG	2.14	0.48
25:L:181:GLU:HA	25:L:181:GLU:OE2	2.14	0.48
28:O:186:ARG:H	28:O:189:MET:HE3	1.79	0.48
31:R:184:THR:HB	31:R:198:MET:CE	2.44	0.48
28:o:62:ARG:O	28:o:76:LYS:NZ	2.35	0.48
31:r:172:TYR:CE1	31:r:187:VAL:HG11	2.49	0.48
33:t:56:VAL:N	33:t:184:THR:OG1	2.39	0.48
1:U:680:VAL:HG23	1:U:683:VAL:HB	1.95	0.48
1:U:884:VAL:HG11	1:U:889:LEU:HD23	1.95	0.48
2:V:400:HIS:NE2	10:d:234:GLN:HA	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:374:THR:HG22	3:W:376:LYS:H	1.79	0.48
4:X:114:ILE:CD1	4:X:133:LEU:HD22	2.44	0.48
14:A:91:GLN:HG2	14:A:93:LEU:HD23	1.94	0.48
14:A:157:ILE:HG13	14:A:157:ILE:O	2.14	0.48
14:A:215:PHE:CE2	14:A:342:GLU:HG3	2.49	0.48
14:A:238:ILE:HD13	14:A:270:CYS:SG	2.54	0.48
17:D:167:ILE:HD11	17:D:170:MET:SD	2.54	0.48
18:E:64:LEU:O	18:E:65:THR:C	2.57	0.48
18:E:185:ARG:HA	18:E:195:PHE:CZ	2.48	0.48
19:F:367:GLN:HG3	19:F:381:TYR:CD2	2.49	0.48
23:J:86:ARG:HA	23:J:89:VAL:HG22	1.96	0.48
26:M:216:TRP:CZ3	26:M:228:VAL:HG13	2.48	0.48
26:M:217:VAL:HG13	26:M:217:VAL:O	2.14	0.48
33:T:234:ILE:O	33:T:234:ILE:HG22	2.14	0.48
4:X:47:GLU:HA	4:X:50:ILE:HG12	1.96	0.47
4:X:343:SER:O	4:X:344:ARG:C	2.56	0.47
7:a:28:LEU:HD23	7:a:33:LEU:HD12	1.95	0.47
9:c:61:PHE:CE2	9:c:109:VAL:HG12	2.49	0.47
12:f:82:ILE:HG22	12:f:85:SER:HG	1.79	0.47
12:f:799:VAL:HA	12:f:817:VAL:HG13	1.95	0.47
14:A:372:LEU:O	14:A:376:LEU:HD23	2.14	0.47
16:C:328:ILE:HD12	35:C:501:ATP:N1	2.28	0.47
17:D:167:ILE:CD1	17:D:214:MET:HE3	2.44	0.47
19:F:324:THR:O	19:F:326:VAL:N	2.46	0.47
22:I:52:ILE:HG23	22:I:52:ILE:O	2.13	0.47
27:N:174:ASP:OD2	27:n:200:ARG:NH2	2.47	0.47
28:O:96:ASP:OD1	28:O:100:GLN:NE2	2.39	0.47
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.46	0.47
29:p:142:CYS:SG	29:p:146:MET:HE1	2.54	0.47
30:q:146:TYR:O	30:q:147:TYR:C	2.57	0.47
31:r:74:ALA:HB2	31:r:235:LEU:HD13	1.97	0.47
1:U:177:LEU:HD21	1:U:204:ILE:HG21	1.95	0.47
5:Y:80:GLU:O	5:Y:84:LEU:HD23	2.14	0.47
10:d:254:GLU:OE2	10:d:257:THR:OG1	2.32	0.47
12:f:237:VAL:CG1	12:f:249:LEU:HD22	2.44	0.47
12:f:666:ILE:HG13	15:B:50:PRO:HG2	1.95	0.47
12:f:748:LEU:O	12:f:752:HIS:ND1	2.43	0.47
14:A:95:VAL:O	14:A:115:VAL:CA	2.52	0.47
16:C:34:ILE:O	16:C:37:ASP:OD1	2.32	0.47
17:D:202:VAL:HG22	17:D:308:ILE:HD13	1.94	0.47
18:E:303:LEU:HD21	18:E:338:PHE:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:311:ASP:O	18:E:315:ILE:HD12	2.14	0.47
19:F:249:LEU:HD21	19:F:271:ALA:HB1	1.94	0.47
21:H:65:VAL:HG12	21:H:218:PHE:HZ	1.79	0.47
24:K:51:GLU:OE1	24:K:206:MET:HG2	2.14	0.47
12:f:679:LEU:HD22	12:f:713:PHE:CZ	2.48	0.47
15:B:363:ARG:NH1	15:B:367:ILE:HG13	2.30	0.47
17:D:345:PHE:CE1	17:D:375:ILE:HG23	2.49	0.47
18:E:151:LEU:O	18:E:154:THR:C	2.58	0.47
20:G:87:SER:O	20:G:91:VAL:HG23	2.14	0.47
28:O:141:LEU:N	28:O:170:MET:HE3	2.29	0.47
27:n:192:ASN:O	27:n:196:LEU:HD13	2.14	0.47
33:t:205:LEU:HD23	33:t:206:SER:O	2.14	0.47
2:V:396:ILE:O	2:V:400:HIS:ND1	2.45	0.47
4:X:234:GLU:OE1	17:D:338:ARG:NH2	2.47	0.47
5:Y:18:ARG:O	5:Y:22:LEU:HD23	2.13	0.47
6:Z:133:LEU:HD13	6:Z:162:ILE:HG12	1.96	0.47
7:a:77:VAL:HG21	7:a:110:ALA:HB1	1.96	0.47
12:f:192:VAL:CG2	12:f:193:PRO:HD3	2.44	0.47
12:f:482:ILE:HG22	12:f:521:ALA:HB2	1.95	0.47
13:x:231:VAL:HG13	13:x:231:VAL:O	2.14	0.47
14:A:93:LEU:HD12	14:A:94:GLN:N	2.29	0.47
16:C:161:ILE:CD1	16:C:186:VAL:HG11	2.44	0.47
17:D:296:MET:HE1	17:D:309:MET:HE1	1.95	0.47
19:F:93:VAL:O	19:F:93:VAL:HG12	2.14	0.47
20:G:90:GLN:NE2	20:G:118:ILE:HG23	2.29	0.47
23:J:102:VAL:O	23:J:102:VAL:HG23	2.15	0.47
24:K:21:LEU:O	24:K:25:GLU:OE1	2.32	0.47
24:K:154:PHE:CD1	24:K:164:GLN:HA	2.49	0.47
25:L:19:ILE:O	25:L:19:ILE:HG23	2.14	0.47
26:M:121:HIS:O	26:M:124:THR:HG22	2.14	0.47
31:R:109:ALA:HB2	32:S:155:VAL:HG23	1.96	0.47
33:T:78:LEU:O	33:T:79:ALA:C	2.57	0.47
27:n:55:THR:HG22	27:n:60:ILE:HG22	1.95	0.47
27:n:198:MET:HE1	27:n:208:ILE:HG12	1.96	0.47
30:q:28:MET:HE2	31:r:172:TYR:CD2	2.50	0.47
2:V:166:TYR:CE1	2:V:170:LEU:HD11	2.50	0.47
2:V:265:ASP:O	2:V:269:LYS:HG3	2.15	0.47
3:W:88:MET:HE3	3:W:127:THR:HG23	1.95	0.47
3:W:125:ILE:HG23	3:W:145:LEU:HD21	1.95	0.47
6:Z:66:SER:O	6:Z:66:SER:OG	2.30	0.47
7:a:87:MET:HE1	7:a:93:ALA:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:176:ALA:O	7:a:180:LEU:HD23	2.14	0.47
12:f:339:ILE:HG22	12:f:339:ILE:O	2.14	0.47
12:f:658:ALA:HB2	12:f:693:ALA:CB	2.45	0.47
14:A:280:ILE:O	14:A:280:ILE:HG22	2.14	0.47
19:F:251:LEU:CD2	19:F:291:ILE:HD11	2.45	0.47
23:J:10:PHE:HE2	24:K:27:ALA:HB2	1.79	0.47
25:L:159:MET:HE3	26:M:59:TYR:HE1	1.80	0.47
27:N:226:ASP:OD1	27:N:227:GLN:N	2.47	0.47
29:P:6:TYR:CE1	29:P:31:GLN:NE2	2.82	0.47
28:o:210:LEU:H	28:o:210:LEU:HD12	1.79	0.47
30:q:35:MET:HG2	30:q:45:LEU:HD11	1.96	0.47
32:s:148:ALA:HA	32:s:160:ARG:NE	2.30	0.47
3:W:274:VAL:CG1	3:W:287:VAL:HG22	2.45	0.47
3:W:455:LEU:HD21	6:Z:103:LYS:N	2.30	0.47
10:d:272:ALA:O	10:d:273:GLY:C	2.57	0.47
12:f:553:THR:HG22	12:f:554:TYR:N	2.29	0.47
14:A:26:ASP:OD1	14:A:27:GLU:N	2.47	0.47
16:C:397:LYS:HD2	21:H:171:LYS:HD3	1.97	0.47
19:F:184:GLN:HG3	19:F:185:TYR:N	2.30	0.47
23:J:88:ARG:CZ	30:Q:69:MET:O	2.61	0.47
25:L:67:ASP:OD1	25:L:67:ASP:C	2.57	0.47
27:N:59:TYR:HB3	33:t:186:TYR:CE2	2.49	0.47
27:N:114:ALA:CB	27:N:154:MET:HE1	2.45	0.47
28:O:182:GLU:HA	28:O:182:GLU:OE2	2.15	0.47
27:n:222:VAL:HG23	27:n:222:VAL:O	2.14	0.47
31:r:226:ASP:O	31:r:228:TYR:N	2.48	0.47
31:r:246:VAL:O	31:r:247:SER:OG	2.26	0.47
32:s:173:LEU:HD23	32:s:206:VAL:HG12	1.97	0.47
33:t:175:VAL:HG12	33:t:177:TYR:CE2	2.49	0.47
33:t:183:ALA:N	33:t:192:GLN:OE1	2.47	0.47
2:V:86:VAL:HG23	2:V:87:SER:N	2.29	0.47
3:W:147:LYS:HD2	3:W:185:PHE:CE1	2.50	0.47
3:W:293:ASP:O	3:W:295:LYS:N	2.44	0.47
4:X:410:VAL:HG22	9:c:256:ASN:HA	1.96	0.47
5:Y:198:ALA:HB2	5:Y:226:VAL:HG12	1.95	0.47
5:Y:229:ILE:HD12	5:Y:295:TYR:CD1	2.50	0.47
6:Z:109:ASN:OD1	6:Z:119:SER:OG	2.07	0.47
12:f:609:VAL:HG23	15:B:74:MET:HE1	1.95	0.47
12:f:699:VAL:CG1	12:f:731:MET:HE2	2.44	0.47
14:A:93:LEU:HD22	14:A:141:GLY:HA2	1.95	0.47
14:A:378:PRO:O	14:A:379:ASN:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:153:ASN:OD1	15:B:154:HIS:N	2.48	0.47
16:C:32:GLN:OE1	16:C:32:GLN:HA	2.13	0.47
16:C:325:ARG:NH1	16:C:351:MET:O	2.48	0.47
17:D:284:GLU:OE1	17:D:287:ARG:NH2	2.48	0.47
17:D:363:TYR:OH	17:D:400:GLU:OE2	2.27	0.47
19:F:189:GLY:O	19:F:191:LEU:N	2.44	0.47
21:H:14:SER:OG	21:H:18:LYS:N	2.48	0.47
23:J:3:TYR:OH	24:K:9:ASP:OD2	2.31	0.47
25:L:36:VAL:HG23	25:L:36:VAL:O	2.15	0.47
25:L:122:ARG:HG2	26:M:129:VAL:HG12	1.97	0.47
25:L:173:GLU:OE1	26:M:58:LEU:HG	2.14	0.47
26:M:198:ILE:HG21	26:M:212:LEU:HD12	1.95	0.47
27:N:71:ILE:HD11	27:N:77:CYS:SG	2.55	0.47
27:N:226:ASP:O	27:N:230:LYS:NZ	2.43	0.47
28:O:86:CYS:SG	28:O:141:LEU:HB3	2.54	0.47
28:O:146:VAL:O	28:O:146:VAL:HG13	2.14	0.47
28:O:169:THR:HG21	28:O:177:ALA:HB1	1.97	0.47
29:P:17:LYS:N	29:P:158:MET:O	2.46	0.47
29:P:45:MET:HE1	29:P:68:LYS:N	2.29	0.47
29:P:50:TYR:CD1	29:P:190:ILE:HD11	2.50	0.47
30:q:30:ASP:OD1	30:q:30:ASP:O	2.33	0.47
1:U:167:ILE:HG21	1:U:204:ILE:HD13	1.96	0.47
2:V:264:TYR:HD2	2:V:295:ILE:HD13	1.80	0.47
3:W:298:GLU:OE1	3:W:298:GLU:N	2.48	0.47
4:X:96:PHE:HE2	4:X:109:LEU:HD13	1.76	0.47
5:Y:183:TYR:HE1	5:Y:213:LEU:HD11	1.77	0.47
7:a:210:VAL:HG12	7:a:213:PHE:CE1	2.50	0.47
7:a:360:VAL:HG22	9:c:308:VAL:HG22	1.94	0.47
12:f:606:VAL:HG11	15:B:70:ASP:OD2	2.15	0.47
17:D:189:GLU:OE2	17:D:193:GLN:NE2	2.48	0.47
19:F:339:ASP:O	19:F:342:LEU:N	2.38	0.47
22:I:110:LEU:HD23	22:I:110:LEU:C	2.40	0.47
23:J:71:MET:HE3	23:J:131:ALA:HB2	1.97	0.47
25:L:19:ILE:CG2	25:L:22:ILE:HD12	2.44	0.47
25:L:47:VAL:HG12	25:L:195:LEU:HD22	1.95	0.47
25:L:206:THR:N	25:L:209:ASN:OD1	2.44	0.47
28:O:58:GLY:O	28:O:202:ILE:HD11	2.15	0.47
29:p:61:GLN:HB2	30:q:85:ARG:NH2	2.29	0.47
33:t:51:VAL:HG13	33:t:51:VAL:O	2.15	0.47
33:t:142:TYR:HA	33:t:145:ARG:HG2	1.96	0.47
1:U:532:MET:HE1	1:U:555:VAL:HG21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:352:SER:C	2:V:353:LEU:HD12	2.40	0.47
3:W:171:VAL:HG11	3:W:185:PHE:CB	2.45	0.47
5:Y:208:PHE:CD2	5:Y:216:TYR:HD1	2.31	0.47
5:Y:259:TYR:HB2	5:Y:274:SER:HB3	1.96	0.47
6:Z:19:VAL:HG21	6:Z:124:ILE:HD12	1.96	0.47
10:d:153:GLN:O	10:d:157:LEU:HD13	2.14	0.47
12:f:187:LEU:O	12:f:190:GLU:N	2.47	0.47
12:f:679:LEU:HD23	12:f:679:LEU:O	2.15	0.47
15:B:77:GLU:O	15:B:78:PHE:C	2.55	0.47
17:D:351:LYS:HZ3	18:E:164:ILE:CG2	2.28	0.47
18:E:148:VAL:HG22	18:E:297:ARG:CZ	2.45	0.47
21:H:223:PRO:HA	21:H:226:VAL:HG12	1.96	0.47
27:N:209:ARG:HG2	27:N:222:VAL:HG12	1.96	0.47
29:P:204:MET:CE	31:r:255:HIS:ND1	2.78	0.47
30:Q:11:ASP:O	30:Q:11:ASP:OD1	2.33	0.47
30:Q:34:LYS:O	30:Q:45:LEU:HD23	2.15	0.47
32:S:216:TYR:CD2	28:o:67:MET:HE1	2.50	0.47
28:o:96:ASP:O	28:o:99:THR:OG1	2.23	0.47
1:U:583:MET:HE3	1:U:605:VAL:HG11	1.97	0.47
3:W:88:MET:HE1	3:W:131:VAL:HB	1.96	0.47
9:c:285:GLU:O	9:c:288:VAL:HG12	2.15	0.47
14:A:433:ASN:HB3	24:K:78:MET:HE1	1.96	0.47
15:B:245:ALA:HB1	15:B:279:PRO:O	2.15	0.47
15:B:251:VAL:HG22	16:C:278:ASN:ND2	2.29	0.47
16:C:259:LEU:HD23	16:C:259:LEU:H	1.80	0.47
18:E:89:LYS:C	18:E:90:SER:HG	2.17	0.47
19:F:272:PHE:CG	19:F:316:GLN:HG2	2.50	0.47
25:L:36:VAL:HG12	25:L:168:ALA:HB1	1.97	0.47
29:P:34:MET:HE2	29:P:183:MET:HE1	1.96	0.47
29:P:67:LEU:HD11	29:P:91:VAL:CG2	2.26	0.47
31:R:65:PHE:HB2	31:R:184:THR:HG22	1.97	0.47
31:R:85:ILE:HD11	29:p:176:ASP:O	2.15	0.47
33:T:253:ASN:O	33:T:256:ILE:HG22	2.15	0.47
30:q:138:LEU:H	30:q:138:LEU:HD12	1.80	0.47
33:t:65:VAL:HG12	33:t:237:VAL:CG1	2.45	0.47
2:V:98:LEU:HD21	2:V:209:LYS:CG	2.44	0.46
2:V:205:LEU:HD12	2:V:205:LEU:N	2.30	0.46
2:V:474:LEU:O	2:V:478:GLN:OE1	2.33	0.46
13:x:151:ARG:O	13:x:152:LYS:HB3	2.15	0.46
14:A:48:VAL:HG13	15:B:65:LEU:HD22	1.97	0.46
16:C:87:VAL:HG21	16:C:114:VAL:CG2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:253:LEU:O	17:D:256:GLU:HG3	2.15	0.46
2:V:254:LEU:HD22	2:V:270:LEU:HD13	1.98	0.46
3:W:363:ILE:HA	3:W:366:MET:HE2	1.97	0.46
19:F:182:THR:HA	19:F:242:ALA:HB1	1.96	0.46
27:N:207:VAL:HG11	33:t:257:ALA:HB2	1.96	0.46
28:O:167:TYR:OH	28:O:182:GLU:OE2	2.29	0.46
28:o:128:GLN:O	28:o:132:ARG:HG2	2.15	0.46
30:q:86:ARG:NH1	30:q:90:ASP:OD1	2.48	0.46
33:t:66:VAL:HG13	33:t:214:VAL:HG11	1.97	0.46
2:V:442:ILE:HG12	2:V:447:ILE:HD11	1.97	0.46
6:Z:54:PHE:CD1	6:Z:78:MET:HG2	2.50	0.46
7:a:114:CYS:O	7:a:118:ILE:HG13	2.16	0.46
7:a:331:VAL:HG12	7:a:333:MET:HE3	1.97	0.46
12:f:496:ASP:OD1	12:f:497:VAL:N	2.46	0.46
15:B:440:LEU:HD21	23:J:30:SER:H	1.79	0.46
17:D:164:TYR:HA	17:D:167:ILE:HG22	1.96	0.46
28:O:246:ARG:HD3	29:P:162:HIS:NE2	2.30	0.46
30:Q:84:THR:HG22	30:Q:118:MET:CE	2.40	0.46
29:p:67:LEU:HD12	29:p:90:MET:CE	2.43	0.46
31:r:226:ASP:O	31:r:227:ALA:C	2.58	0.46
32:s:128:ARG:NH1	32:s:155:VAL:HG11	2.31	0.46
1:U:486:MET:HE1	1:U:781:LEU:HD21	1.98	0.46
2:V:254:LEU:CD2	2:V:270:LEU:HD13	2.45	0.46
3:W:366:MET:O	3:W:370:TYR:HB2	2.15	0.46
5:Y:190:ALA:HB2	5:Y:287:LEU:HD11	1.97	0.46
6:Z:131:LEU:HD11	6:Z:200:GLY:CA	2.43	0.46
7:a:252:LYS:HA	7:a:255:TRP:NE1	2.30	0.46
12:f:399:LEU:HD12	12:f:410:ALA:HB3	1.98	0.46
12:f:583:VAL:HG12	12:f:584:SER:N	2.31	0.46
12:f:822:VAL:O	12:f:825:MET:HB2	2.16	0.46
13:x:218:LEU:HD13	13:x:231:VAL:HG21	1.97	0.46
14:A:93:LEU:HD11	15:B:132:TYR:HB2	1.97	0.46
16:C:161:ILE:HG12	16:C:199:LEU:HD21	1.98	0.46
18:E:92:LEU:CD1	18:E:107:ILE:HG21	2.45	0.46
24:K:35:SER:HB2	24:K:51:GLU:HG3	1.97	0.46
24:K:167:ALA:HB2	24:K:185:TYR:CD2	2.50	0.46
30:Q:30:ASP:OD1	30:Q:177:THR:OG1	2.26	0.46
30:q:60:ILE:HD12	30:q:84:THR:HG22	1.98	0.46
31:r:62:THR:OG1	31:r:187:VAL:HG23	2.15	0.46
2:V:170:LEU:HA	2:V:173:ILE:HD12	1.98	0.46
2:V:198:GLN:OE1	2:V:200:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:204:PRO:HB2	4:X:242:ILE:HD11	1.96	0.46
4:X:338:VAL:HG13	4:X:353:LEU:HD23	1.97	0.46
10:d:127:ASN:O	10:d:129:LEU:N	2.48	0.46
15:B:165:ASP:O	16:C:78:ARG:NH1	2.48	0.46
20:G:16:PHE:HB2	21:H:21:GLN:OE1	2.15	0.46
23:J:95:ARG:HB3	30:Q:62:LYS:HE2	1.97	0.46
26:M:197:ILE:O	26:M:200:ILE:HG22	2.15	0.46
28:O:137:ILE:O	28:O:139:ALA:N	2.47	0.46
28:O:262:LEU:HD12	28:O:263:GLU:O	2.16	0.46
32:S:198:ARG:O	32:S:202:LEU:HG	2.16	0.46
28:o:184:LYS:HG3	28:o:184:LYS:O	2.15	0.46
31:r:78:ARG:O	31:r:80:THR:HG23	2.14	0.46
31:r:171:TYR:HB2	31:r:179:ARG:NH2	2.30	0.46
31:r:219:ILE:HG22	31:r:233:VAL:HG22	1.95	0.46
2:V:309:MET:SD	2:V:331:LEU:HD23	2.55	0.46
3:W:176:SER:CB	3:W:181:GLU:OE2	2.63	0.46
3:W:243:ILE:HG21	3:W:273:TYR:CE1	2.50	0.46
5:Y:217:LYS:O	5:Y:220:VAL:HG12	2.16	0.46
5:Y:376:LEU:O	5:Y:380:VAL:HG12	2.15	0.46
9:c:49:VAL:CG2	18:E:103:THR:HG21	2.38	0.46
9:c:124:GLY:H	9:c:127:ILE:CD1	2.29	0.46
14:A:45:ILE:HA	14:A:48:VAL:HG12	1.98	0.46
14:A:405:THR:OG1	14:A:406:GLU:N	2.49	0.46
17:D:116:LEU:HB3	17:D:119:ILE:HD11	1.96	0.46
18:E:209:GLY:N	18:E:259:GLU:OE1	2.49	0.46
19:F:83:ASN:O	19:F:83:ASN:OD1	2.34	0.46
25:L:230:SER:OG	25:L:234:GLU:OE2	2.33	0.46
28:O:156:ILE:N	28:O:170:MET:HE1	2.30	0.46
27:n:62:ASN:OD1	28:o:165:LEU:HD21	2.15	0.46
1:U:105:ILE:HG21	16:C:23:TYR:CE2	2.51	0.46
3:W:31:CYS:HB3	3:W:43:VAL:HG13	1.98	0.46
4:X:339:ILE:CD1	4:X:345:VAL:HG21	2.45	0.46
5:Y:197:ALA:HB3	5:Y:226:VAL:HG11	1.97	0.46
9:c:292:MET:CE	10:d:346:LEU:HD12	2.46	0.46
10:d:296:PRO:HA	10:d:299:MET:HB2	1.98	0.46
12:f:462:ALA:O	12:f:466:LEU:HD23	2.16	0.46
12:f:783:SER:OG	12:f:787:LEU:HD12	2.16	0.46
16:C:190:GLY:O	16:C:296:ASN:OD1	2.34	0.46
16:C:273:MET:HE1	16:C:302:ASP:OD2	2.15	0.46
17:D:394:VAL:O	17:D:395:LEU:HD12	2.15	0.46
19:F:362:ARG:HD2	19:F:388:THR:OG1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:138:MET:HE3	20:G:140:LEU:CG	2.46	0.46
21:H:74:LEU:CD2	21:H:83:TYR:HE1	2.28	0.46
26:M:34:SER:OG	26:M:80:GLY:N	2.48	0.46
26:M:82:LEU:O	26:M:86:ARG:HG3	2.16	0.46
1:U:545:LEU:HB3	1:U:577:ILE:HG21	1.97	0.46
2:V:290:TYR:CD1	2:V:328:VAL:HG22	2.51	0.46
2:V:396:ILE:C	2:V:398:LEU:N	2.71	0.46
12:f:379:GLY:C	12:f:416:MET:HE3	2.40	0.46
12:f:491:GLY:HA2	12:f:527:VAL:HG21	1.97	0.46
12:f:726:ILE:HD11	12:f:761:MET:HB3	1.97	0.46
14:A:49:GLU:HG2	15:B:65:LEU:HD11	1.98	0.46
15:B:105:THR:OG1	15:B:106:PRO:HD3	2.15	0.46
15:B:112:LEU:HD11	15:B:115:ILE:HG13	1.98	0.46
16:C:164:VAL:HG11	16:C:186:VAL:HG23	1.97	0.46
16:C:252:ASP:OD1	16:C:253:SER:N	2.49	0.46
17:D:69:LYS:O	17:D:73:LEU:HD23	2.16	0.46
21:H:111:VAL:HG22	21:H:136:ILE:CD1	2.46	0.46
21:H:154:ALA:CB	22:I:80:THR:HG21	2.41	0.46
23:J:217:LEU:HD23	23:J:217:LEU:C	2.41	0.46
27:N:170:TYR:CZ	27:n:200:ARG:NH1	2.84	0.46
29:P:21:ALA:HB2	29:P:163:LEU:CD2	2.41	0.46
1:U:668:ALA:O	1:U:672:LEU:HD13	2.16	0.46
3:W:202:THR:HG22	3:W:233:LEU:HD22	1.97	0.46
4:X:181:SER:HB2	5:Y:247:LEU:CD2	2.46	0.46
6:Z:19:VAL:CG1	6:Z:97:THR:HG22	2.46	0.46
6:Z:67:VAL:HG23	6:Z:67:VAL:O	2.15	0.46
7:a:216:LEU:HD21	7:a:222:LEU:HD13	1.98	0.46
12:f:82:ILE:HG22	12:f:82:ILE:O	2.16	0.46
12:f:125:ILE:HD12	12:f:125:ILE:H	1.81	0.46
12:f:348:ILE:HD12	12:f:348:ILE:H	1.80	0.46
17:D:363:TYR:CZ	17:D:400:GLU:OE2	2.68	0.46
18:E:346:VAL:N	18:E:373:LYS:HE2	2.31	0.46
19:F:49:ASP:OD1	19:F:50:SER:N	2.49	0.46
28:O:245:TYR:OH	29:P:152:SER:O	2.32	0.46
29:P:45:MET:CE	29:P:67:LEU:HD22	2.46	0.46
29:P:107:PRO:HB2	29:P:124:LEU:HD13	1.98	0.46
30:Q:96:THR:HG23	30:Q:96:THR:O	2.16	0.46
30:Q:153:ARG:O	30:Q:157:VAL:HG23	2.16	0.46
32:s:222:ARG:NE	32:s:235:THR:OG1	2.48	0.46
2:V:108:LEU:HB2	2:V:174:PHE:CZ	2.51	0.46
3:W:107:GLN:NE2	3:W:111:TYR:CZ	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:192:VAL:HG11	12:f:217:LEU:HD22	1.98	0.46
12:f:776:LEU:HD23	12:f:827:PRO:CA	2.44	0.46
13:x:154:THR:HG22	13:x:154:THR:O	2.16	0.46
17:D:272:THR:O	17:D:318:ASP:HB2	2.16	0.46
25:L:105:VAL:HG12	25:L:105:VAL:O	2.15	0.46
26:M:174:LYS:O	26:M:177:ILE:N	2.49	0.46
31:R:180:ILE:HG22	31:R:181:SER:O	2.16	0.46
32:S:211:ALA:CB	32:S:238:LEU:HD11	2.46	0.46
1:U:506:ALA:HB1	1:U:543:LYS:HB3	1.98	0.45
3:W:412:ILE:O	3:W:413:ILE:C	2.57	0.45
8:b:90:ILE:CG2	8:b:127:LEU:HD11	2.46	0.45
10:d:311:GLY:N	10:d:312:PRO:CD	2.79	0.45
12:f:272:LEU:O	12:f:274:ASP:N	2.50	0.45
16:C:381:GLU:O	16:C:385:MET:HG3	2.17	0.45
17:D:404:LYS:HA	17:D:407:ILE:HG22	1.98	0.45
18:E:151:LEU:HA	18:E:154:THR:CG2	2.46	0.45
18:E:194:ASN:O	18:E:195:PHE:CD2	2.69	0.45
19:F:88:TYR:HE1	19:F:161:LEU:HD13	1.81	0.45
21:H:53:LYS:O	21:H:54:SER:OG	2.32	0.45
21:H:55:ILE:HG22	21:H:55:ILE:O	2.15	0.45
21:H:69:THR:HG22	21:H:70:LYS:N	2.31	0.45
26:M:41:ARG:HB3	26:M:162:TRP:O	2.16	0.45
30:Q:38:MET:HE2	30:Q:44:LEU:CB	2.45	0.45
31:R:123:ARG:NH2	31:R:127:LEU:HD21	2.31	0.45
32:S:44:ALA:HB2	32:S:149:VAL:HG22	1.98	0.45
32:S:153:ASP:HB2	32:S:154:PRO:HD2	1.98	0.45
33:T:224:ARG:HA	27:n:60:ILE:HD11	1.98	0.45
30:q:21:ALA:O	30:q:28:MET:N	2.49	0.45
3:W:28:LEU:HD11	3:W:69:ALA:CB	2.46	0.45
4:X:267:VAL:HG13	4:X:268:GLN:N	2.31	0.45
4:X:394:ASP:OD2	5:Y:362:LYS:NZ	2.48	0.45
4:X:414:LEU:HD23	4:X:414:LEU:C	2.40	0.45
10:d:153:GLN:O	10:d:156:ILE:HG22	2.16	0.45
12:f:208:LEU:HD11	12:f:217:LEU:HD23	1.98	0.45
12:f:237:VAL:HA	12:f:240:VAL:HG23	1.97	0.45
13:x:281:VAL:O	13:x:281:VAL:HG12	2.15	0.45
16:C:34:ILE:HG21	17:D:51:LEU:HD11	1.98	0.45
16:C:281:ASP:OD1	16:C:282:GLY:N	2.49	0.45
18:E:71:VAL:HG11	18:E:100:LEU:HD11	1.96	0.45
18:E:306:GLU:O	18:E:309:ARG:NH2	2.49	0.45
25:L:74:ILE:HG22	25:L:132:LEU:CD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:162:TRP:HB3	26:M:182:MET:HE3	1.98	0.45
26:M:176:GLU:CG	26:M:197:ILE:HD13	2.46	0.45
30:Q:14:LEU:HD12	30:Q:182:ILE:HG13	1.97	0.45
27:n:38:MET:SD	27:n:38:MET:C	2.99	0.45
27:n:61:ALA:O	27:n:62:ASN:C	2.57	0.45
28:o:46:ILE:O	28:o:46:ILE:HG13	2.15	0.45
31:r:65:PHE:CE1	31:r:183:ALA:HB1	2.51	0.45
1:U:213:PHE:HB3	1:U:248:ILE:HD11	1.98	0.45
8:b:114:GLY:HA2	8:b:143:PHE:O	2.15	0.45
10:d:119:LEU:O	10:d:123:LEU:HD23	2.16	0.45
10:d:260:ILE:O	10:d:264:LEU:HG	2.17	0.45
14:A:90:GLU:O	14:A:92:PRO:HD3	2.16	0.45
14:A:281:GLY:HA3	14:A:299:MET:HG3	1.97	0.45
14:A:355:PHE:CE2	14:A:385:ILE:HD12	2.51	0.45
17:D:313:ARG:HH12	17:D:316:THR:HG23	1.81	0.45
17:D:415:GLU:HG3	20:G:159:TYR:CD2	2.51	0.45
18:E:373:LYS:HD2	18:E:373:LYS:C	2.41	0.45
19:F:223:VAL:HG13	19:F:352:ILE:HG12	1.98	0.45
31:R:85:ILE:O	31:R:85:ILE:HG13	2.16	0.45
33:T:195:LEU:HD23	33:T:213:LEU:HD21	1.97	0.45
29:p:28:PHE:HB2	29:p:39:PHE:CE2	2.52	0.45
33:t:205:LEU:HD23	33:t:206:SER:N	2.31	0.45
2:V:397:ARG:HA	2:V:400:HIS:ND1	2.31	0.45
3:W:118:LEU:HD13	3:W:152:ILE:HG23	1.99	0.45
6:Z:144:VAL:O	6:Z:144:VAL:HG13	2.14	0.45
6:Z:235:ASN:HD21	7:a:336:VAL:H	1.65	0.45
8:b:9:CYS:HB3	8:b:54:LEU:HD11	1.97	0.45
9:c:70:ILE:HD12	9:c:106:GLU:OE1	2.16	0.45
9:c:125:VAL:HG21	13:x:289:HIS:HA	1.99	0.45
12:f:744:MET:O	12:f:748:LEU:HD13	2.16	0.45
14:A:351:ARG:NE	14:A:377:CYS:O	2.50	0.45
15:B:278:ALA:HB3	15:B:280:SER:HB2	1.99	0.45
17:D:254:ALA:HB2	17:D:262:ILE:CG1	2.47	0.45
18:E:268:ASP:OD1	18:E:268:ASP:O	2.34	0.45
24:K:209:LYS:O	24:K:210:LEU:C	2.58	0.45
25:L:10:VAL:O	25:L:19:ILE:HD11	2.16	0.45
25:L:107:ARG:NH2	33:T:119:GLU:OE1	2.49	0.45
25:L:192:LEU:O	25:L:196:ARG:HG3	2.17	0.45
27:N:224:LEU:HD23	33:t:254:TRP:O	2.16	0.45
29:P:49:LEU:HD21	29:P:87:LEU:HD22	1.98	0.45
29:P:159:ASP:C	29:P:159:ASP:OD1	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:117:TYR:CZ	30:Q:132:HIS:CE1	3.05	0.45
29:p:4:MET:HE3	29:p:55:GLY:HA3	1.97	0.45
32:s:140:GLY:O	32:s:147:GLY:O	2.35	0.45
1:U:507:VAL:HG23	1:U:508:THR:N	2.32	0.45
6:Z:217:THR:HG21	6:Z:219:LYS:HZ3	1.80	0.45
7:a:206:LEU:HD11	7:a:261:LEU:CD2	2.43	0.45
8:b:113:VAL:HG11	8:b:153:LEU:HD21	1.99	0.45
8:b:113:VAL:HG21	8:b:140:ILE:HG23	1.99	0.45
10:d:308:TRP:O	10:d:321:GLN:NE2	2.50	0.45
12:f:266:LEU:HD23	12:f:267:ARG:N	2.31	0.45
12:f:475:ASN:O	12:f:477:MET:N	2.49	0.45
12:f:679:LEU:HD13	12:f:713:PHE:CD2	2.51	0.45
15:B:304:GLU:O	15:B:308:THR:HG23	2.17	0.45
23:J:3:TYR:CD2	23:J:12:PRO:HD3	2.52	0.45
24:K:37:ALA:CB	24:K:50:VAL:HG12	2.46	0.45
31:R:212:TYR:HH	31:R:237:HIS:CG	2.31	0.45
33:T:156:VAL:HA	33:T:168:GLY:O	2.17	0.45
29:p:67:LEU:HD13	29:p:91:VAL:HG22	1.99	0.45
31:r:60:THR:O	31:r:60:THR:HG23	2.17	0.45
1:U:797:MET:CE	1:U:881:PRO:HG3	2.47	0.45
2:V:224:LEU:O	2:V:257:ASN:ND2	2.50	0.45
7:a:81:LEU:HD11	7:a:117:ALA:CB	2.46	0.45
10:d:192:LEU:HD21	10:d:215:LEU:HD21	1.99	0.45
12:f:560:LEU:HD11	12:f:798:THR:HA	1.99	0.45
14:A:128:GLN:OE1	14:A:130:ALA:C	2.59	0.45
14:A:143:ASP:HB2	14:A:146:LYS:O	2.17	0.45
15:B:202:GLU:C	15:B:204:PRO:HD2	2.42	0.45
16:C:189:TYR:HE1	16:C:298:ILE:CD1	2.30	0.45
16:C:373:GLU:O	16:C:374:ARG:C	2.59	0.45
17:D:160:PRO:HG2	17:D:220:ALA:HB1	1.99	0.45
19:F:144:LYS:O	19:F:145:LEU:C	2.59	0.45
19:F:272:PHE:HE2	19:F:313:LEU:HD12	1.80	0.45
22:I:17:ARG:NH2	22:I:22:GLU:OE1	2.50	0.45
23:J:10:PHE:CE2	24:K:27:ALA:HB2	2.52	0.45
28:O:175:LEU:HD13	33:t:189:TYR:CD2	2.51	0.45
28:O:209:ASP:C	28:O:209:ASP:OD1	2.59	0.45
32:S:176:LEU:HD21	28:o:245:TYR:HE2	1.82	0.45
33:T:61:PHE:CD1	33:T:62:GLU:N	2.85	0.45
27:n:93:VAL:HG21	27:n:117:PHE:CE1	2.52	0.45
30:q:13:VAL:CG1	30:q:115:LEU:HD21	2.47	0.45
33:t:152:TRP:O	33:t:153:ASN:OD1	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:169:LEU:O	2:V:172:VAL:HG12	2.16	0.45
2:V:173:ILE:HG12	2:V:213:TYR:CE2	2.52	0.45
3:W:200:ILE:H	3:W:200:ILE:HD12	1.82	0.45
3:W:270:VAL:O	3:W:274:VAL:HG23	2.16	0.45
6:Z:211:TYR:CE2	6:Z:226:ILE:HG21	2.52	0.45
10:d:309:VAL:O	10:d:309:VAL:CG1	2.64	0.45
22:I:18:LEU:HD11	23:J:125:ARG:HD2	1.99	0.45
23:J:96:LEU:CD1	30:Q:62:LYS:HG3	2.47	0.45
28:O:55:ILE:HD12	28:O:57:LEU:CD1	2.47	0.45
29:P:12:MET:HE3	29:P:150:CYS:SG	2.56	0.45
31:R:66:LYS:HG2	31:R:71:VAL:HG22	1.99	0.45
32:S:119:MET:O	32:S:123:ILE:HG12	2.16	0.45
30:q:23:SER:O	30:q:24:ASN:HB3	2.17	0.45
31:r:173:VAL:HG13	31:r:179:ARG:HD3	1.98	0.45
33:t:46:THR:O	33:t:46:THR:HG22	2.15	0.45
33:t:152:TRP:NE1	33:t:172:MET:HE1	2.31	0.45
3:W:171:VAL:HG11	3:W:185:PHE:HB2	1.97	0.45
3:W:283:GLN:O	3:W:287:VAL:HG23	2.17	0.45
3:W:438:LEU:HD23	6:Z:233:VAL:HG23	1.99	0.45
5:Y:112:CYS:HB2	5:Y:147:ILE:HD11	1.99	0.45
5:Y:364:TRP:CZ2	5:Y:368:GLU:HG3	2.52	0.45
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.98	0.45
12:f:58:MET:C	12:f:58:MET:SD	3.00	0.45
12:f:541:THR:CG2	12:f:558:LEU:HD21	2.47	0.45
12:f:606:VAL:HG23	12:f:607:LEU:HD22	1.99	0.45
15:B:165:ASP:HB3	16:C:78:ARG:HH22	1.81	0.45
19:F:172:VAL:HG13	19:F:267:LEU:HD11	1.98	0.45
19:F:310:MET:CE	19:F:342:LEU:HD22	2.46	0.45
20:G:60:LEU:HD23	26:M:163:GLY:O	2.17	0.45
21:H:29:VAL:HG11	21:H:133:SER:OG	2.17	0.45
31:R:62:THR:HG23	31:R:75:ALA:HB2	1.98	0.45
31:R:195:TYR:OH	30:q:170:ARG:NH2	2.50	0.45
2:V:313:LEU:HD21	2:V:329:HIS:NE2	2.32	0.45
3:W:251:TYR:CZ	3:W:267:LEU:HD21	2.51	0.45
3:W:292:GLY:O	3:W:296:LEU:HB3	2.17	0.45
3:W:375:MET:HG3	3:W:413:ILE:HD11	1.98	0.45
6:Z:235:ASN:HD21	7:a:335:TRP:HA	1.81	0.45
16:C:298:ILE:HA	16:C:301:LEU:HD23	1.98	0.45
20:G:123:GLN:OE1	21:H:85:VAL:HG21	2.17	0.45
25:L:72:ILE:HD12	25:L:88:MET:SD	2.57	0.45
28:O:55:ILE:HD13	28:O:144:GLY:C	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:25:ILE:HG23	30:q:26:VAL:HG13	1.98	0.45
33:t:151:LEU:N	33:t:151:LEU:HD12	2.32	0.45
1:U:383:ASP:OD2	1:U:426:TYR:OH	2.15	0.45
1:U:536:ALA:O	1:U:545:LEU:HD21	2.17	0.45
3:W:117:ASP:O	3:W:120:ILE:N	2.44	0.45
4:X:104:GLY:N	4:X:106:GLU:OE2	2.47	0.45
6:Z:69:PHE:CG	6:Z:69:PHE:O	2.68	0.45
7:a:55:GLY:O	7:a:59:LEU:HD13	2.17	0.45
7:a:92:VAL:O	7:a:92:VAL:HG12	2.17	0.45
12:f:151:LEU:HA	12:f:154:TRP:HD1	1.81	0.45
12:f:435:SER:HB3	12:f:440:ILE:HG21	1.97	0.45
13:x:288:SER:O	13:x:289:HIS:HB2	2.16	0.45
15:B:229:GLY:O	15:B:391:SER:HB2	2.17	0.45
17:D:202:VAL:HG22	17:D:308:ILE:CD1	2.46	0.45
18:E:177:GLY:O	18:E:178:THR:C	2.60	0.45
22:I:147:LEU:HD23	22:I:147:LEU:C	2.42	0.45
24:K:133:MET:HA	24:K:133:MET:CE	2.41	0.45
30:Q:12:TYR:OH	30:Q:152:SER:O	2.33	0.45
30:Q:184:ASP:C	30:Q:184:ASP:OD1	2.58	0.45
30:q:7:ILE:HG21	30:q:143:LEU:HD11	1.99	0.45
31:r:171:TYR:HB3	31:r:179:ARG:CZ	2.46	0.45
32:s:112:THR:HG23	32:s:115:ALA:H	1.81	0.45
33:t:80:ARG:HG2	33:t:81:PHE:CD2	2.51	0.45
3:W:167:GLN:O	3:W:167:GLN:CD	2.61	0.44
3:W:196:VAL:O	3:W:196:VAL:HG22	2.17	0.44
12:f:196:MET:CE	12:f:217:LEU:HD21	2.47	0.44
12:f:237:VAL:O	12:f:245:ASN:OD1	2.34	0.44
12:f:675:PHE:CE2	12:f:693:ALA:HB1	2.52	0.44
14:A:70:THR:O	14:A:70:THR:CG2	2.64	0.44
15:B:107:MET:HB2	16:C:96:VAL:CG2	2.46	0.44
17:D:167:ILE:HD12	17:D:214:MET:HE3	1.98	0.44
18:E:331:ILE:CG2	18:E:374:VAL:HG11	2.46	0.44
20:G:13:ILE:HG23	20:G:14:THR:HG23	1.98	0.44
22:I:52:ILE:HG22	22:I:210:LYS:NZ	2.32	0.44
23:J:65:LEU:HD13	23:J:87:ALA:HB1	1.99	0.44
26:M:191:VAL:HG21	26:M:216:TRP:CE3	2.52	0.44
26:M:215:SER:CA	26:M:228:VAL:HG23	2.47	0.44
1:U:583:MET:CE	1:U:605:VAL:HG11	2.47	0.44
5:Y:162:GLU:HA	5:Y:165:LYS:NZ	2.32	0.44
7:a:73:PRO:HB3	7:a:104:VAL:HG13	1.99	0.44
7:a:134:THR:O	7:a:137:ASP:OD1	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:244:ASN:O	7:a:245:VAL:C	2.60	0.44
9:c:73:PHE:HE1	9:c:95:MET:CG	2.30	0.44
10:d:299:MET:HE1	10:d:316:TYR:CZ	2.51	0.44
12:f:491:GLY:HA2	12:f:527:VAL:HG11	2.00	0.44
16:C:379:THR:HG22	16:C:380:GLN:H	1.83	0.44
24:K:110:GLU:N	24:K:154:PHE:HE2	2.15	0.44
27:N:39:ALA:CB	27:N:48:LEU:HD23	2.46	0.44
28:O:238:LYS:HG3	28:O:239:GLY:N	2.33	0.44
28:O:262:LEU:HD13	29:P:48:ARG:HH12	1.79	0.44
30:Q:3:TYR:CE1	30:Q:136:ALA:N	2.86	0.44
32:S:175:PRO:HB2	29:p:149:MET:HE3	1.99	0.44
33:t:96:LEU:HG	33:t:155:MET:HE2	1.99	0.44
1:U:243:LEU:HD21	1:U:793:LYS:HG3	1.98	0.44
1:U:364:VAL:HG23	9:c:177:THR:HG21	1.98	0.44
3:W:111:TYR:O	3:W:112:VAL:C	2.58	0.44
4:X:162:ASP:CG	4:X:165:LEU:HB2	2.42	0.44
7:a:228:THR:HG22	7:a:229:ASP:N	2.32	0.44
10:d:117:GLY:O	10:d:121:LEU:HG	2.17	0.44
10:d:165:GLU:OE2	10:d:204:ARG:NH2	2.48	0.44
12:f:89:MET:C	12:f:90:THR:HG1	2.16	0.44
12:f:706:ILE:O	12:f:710:LEU:HD23	2.18	0.44
13:x:280:ARG:NH2	13:x:284:LYS:O	2.51	0.44
16:C:88:LYS:HA	16:C:94:LYS:HA	2.00	0.44
17:D:344:ILE:CD1	37:D:501:ADP:N6	2.81	0.44
18:E:181:THR:HG22	37:E:401:ADP:O1A	2.18	0.44
24:K:66:LYS:NZ	24:K:78:MET:O	2.44	0.44
26:M:109:LEU:HD23	26:M:109:LEU:C	2.42	0.44
26:M:216:TRP:CD1	26:M:220:LEU:HD21	2.53	0.44
29:P:36:THR:HG21	30:Q:125:ALA:HB1	2.00	0.44
27:n:167:SER:HA	27:n:170:TYR:HD2	1.83	0.44
30:q:5:ILE:HG13	30:q:131:ALA:HB2	2.00	0.44
1:U:504:ASP:OD1	1:U:535:TYR:OH	2.33	0.44
2:V:404:LYS:O	2:V:407:VAL:HG12	2.17	0.44
5:Y:145:LEU:HD23	5:Y:160:ASN:HB2	2.00	0.44
12:f:698:SER:O	12:f:732:VAL:HG12	2.17	0.44
15:B:223:ILE:C	15:B:224:LEU:HD12	2.43	0.44
17:D:173:GLN:HB3	17:D:333:PHE:CZ	2.52	0.44
17:D:241:GLY:N	17:D:284:GLU:OE2	2.50	0.44
19:F:206:MET:CE	19:F:246:ALA:HB2	2.48	0.44
19:F:317:LEU:HD22	19:F:347:ARG:HA	2.00	0.44
21:H:10:LEU:HD11	21:H:22:ILE:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J:66:ASP:HA	30:Q:69:MET:HE1	1.99	0.44
23:J:104:VAL:HG13	23:J:145:TYR:HE2	1.83	0.44
24:K:52:LYS:HB3	24:K:64:ILE:HD12	1.99	0.44
24:K:206:MET:HE1	24:K:210:LEU:HB2	2.00	0.44
27:N:71:ILE:HG22	27:N:97:LEU:HD23	1.99	0.44
27:N:137:TRP:CH2	27:N:215:GLU:OE1	2.71	0.44
27:N:170:TYR:CE2	27:n:200:ARG:HD2	2.52	0.44
27:N:170:TYR:O	27:n:200:ARG:NH2	2.50	0.44
31:R:223:THR:HG22	31:R:229:SER:O	2.17	0.44
33:T:141:MET:HE2	33:T:155:MET:CE	2.48	0.44
27:n:125:ARG:NH2	33:t:50:MET:HE3	2.32	0.44
28:o:142:VAL:HG13	28:o:168:VAL:CG2	2.47	0.44
30:q:4:LEU:HD11	30:q:47:VAL:HG13	1.99	0.44
1:U:160:LEU:O	1:U:163:PHE:HB3	2.18	0.44
2:V:231:LEU:HD12	2:V:250:LEU:HD23	2.00	0.44
3:W:27:ARG:O	3:W:30:GLU:HG3	2.17	0.44
3:W:299:ILE:HB	3:W:302:TYR:HB3	2.00	0.44
5:Y:155:ASP:OD1	5:Y:156:LEU:N	2.50	0.44
6:Z:11:VAL:HG12	6:Z:12:HIS:N	2.32	0.44
7:a:71:VAL:HG12	7:a:72:ASN:N	2.33	0.44
7:a:344:GLN:OE1	7:a:344:GLN:N	2.47	0.44
14:A:138:MET:HG2	14:A:138:MET:O	2.17	0.44
23:J:144:LEU:HD23	23:J:144:LEU:C	2.43	0.44
24:K:117:SER:O	24:K:121:LEU:HG	2.17	0.44
26:M:82:LEU:HD23	26:M:86:ARG:HH22	1.82	0.44
28:O:72:LYS:HE2	32:s:213:ARG:NH1	2.33	0.44
28:O:85:TYR:HB2	28:O:221:ILE:HD11	1.99	0.44
30:Q:60:ILE:HG13	30:Q:84:THR:HG23	2.00	0.44
28:o:102:ILE:O	28:o:102:ILE:HG22	2.17	0.44
28:o:137:ILE:HG23	28:o:137:ILE:O	2.17	0.44
31:r:202:TYR:OH	31:r:204:TYR:HA	2.18	0.44
1:U:198:LEU:CB	1:U:223:LEU:HD11	2.47	0.44
1:U:386:LEU:HD22	1:U:393:LEU:HD21	1.99	0.44
3:W:344:THR:N	3:W:347:GLY:HA3	2.32	0.44
3:W:395:ASN:O	3:W:399:ASN:ND2	2.50	0.44
4:X:339:ILE:HD11	4:X:345:VAL:HG21	2.00	0.44
4:X:393:VAL:HG23	4:X:393:VAL:O	2.17	0.44
5:Y:19:ILE:HD11	5:Y:44:ALA:HB1	1.99	0.44
5:Y:377:LEU:HA	5:Y:380:VAL:HG12	2.00	0.44
6:Z:263:ALA:CB	9:c:288:VAL:HG23	2.46	0.44
7:a:210:VAL:HG12	7:a:213:PHE:HE1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:437:GLU:OE1	12:f:437:GLU:N	2.51	0.44
12:f:562:LEU:HD23	12:f:595:VAL:CG2	2.48	0.44
12:f:654:VAL:HG12	12:f:693:ALA:HB2	1.99	0.44
13:x:146:PHE:CE1	13:x:167:ILE:HG23	2.52	0.44
15:B:249:ARG:O	15:B:250:VAL:CG2	2.64	0.44
15:B:438:LEU:HD22	15:B:439:TYR:CE2	2.52	0.44
16:C:164:VAL:CG2	16:C:313:ARG:HE	2.30	0.44
16:C:277:LEU:HD21	16:C:304:ALA:CB	2.47	0.44
19:F:275:ALA:CB	19:F:283:ILE:HD11	2.48	0.44
19:F:428:GLN:O	19:F:429:ALA:HB3	2.18	0.44
23:J:30:SER:HB2	23:J:46:GLU:HB3	1.99	0.44
24:K:91:LYS:CE	24:K:95:GLU:OE2	2.65	0.44
25:L:63:ILE:N	25:L:63:ILE:HD12	2.33	0.44
28:O:71:ASP:CB	29:P:131:MET:HE1	2.47	0.44
30:Q:4:LEU:HD13	30:Q:45:LEU:CB	2.47	0.44
27:n:86:THR:HG22	27:n:130:ALA:HB1	1.99	0.44
30:q:164:LEU:HD13	30:q:178:PHE:HB3	2.00	0.44
31:r:171:TYR:CE1	31:r:181:SER:HB2	2.53	0.44
32:s:221:LEU:HG	32:s:221:LEU:O	2.17	0.44
33:t:66:VAL:HG23	33:t:235:ALA:O	2.18	0.44
1:U:677:ASN:OD1	1:U:677:ASN:O	2.36	0.44
3:W:231:ILE:HD11	3:W:246:HIS:CB	2.47	0.44
3:W:373:ILE:HD12	7:a:326:GLU:HG2	1.99	0.44
4:X:53:LEU:O	4:X:57:LEU:HG	2.17	0.44
5:Y:304:TYR:OH	5:Y:333:GLU:CD	2.59	0.44
10:d:194:LEU:HD21	10:d:259:PHE:HE2	1.83	0.44
12:f:137:ARG:HH12	12:f:168:LYS:NZ	2.12	0.44
12:f:681:TYR:CD2	15:B:83:GLU:OE2	2.71	0.44
12:f:776:LEU:HD13	12:f:825:MET:HE2	1.99	0.44
14:A:380:SER:OG	14:A:385:ILE:HD11	2.18	0.44
16:C:298:ILE:O	16:C:299:ASP:C	2.61	0.44
25:L:52:ALA:HB2	25:L:59:HIS:NE2	2.33	0.44
25:L:215:VAL:HG22	25:L:216:GLY:N	2.32	0.44
30:Q:13:VAL:CG1	30:Q:183:ILE:HB	2.47	0.44
30:Q:101:ASN:C	30:Q:102:LEU:HD22	2.42	0.44
31:R:80:THR:HG23	31:R:80:THR:O	2.17	0.44
33:t:144:ARG:CZ	33:t:151:LEU:HD11	2.48	0.44
2:V:169:LEU:HA	2:V:172:VAL:HG12	2.00	0.44
3:W:275:ILE:HD12	3:W:309:PHE:CD2	2.53	0.44
3:W:420:ASP:OD1	3:W:421:PRO:HD2	2.17	0.44
4:X:16:LEU:C	4:X:16:LEU:HD23	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:44:GLN:O	4:X:47:GLU:HG2	2.17	0.44
4:X:137:TYR:HB3	4:X:146:ALA:HB2	2.00	0.44
7:a:108:ASP:HA	7:a:111:VAL:HG12	2.00	0.44
9:c:107:MET:HE1	13:x:271:GLN:O	2.18	0.44
10:d:155:SER:CB	10:d:163:SER:HG	2.28	0.44
12:f:739:ALA:HB3	15:B:208:PRO:HD2	1.99	0.44
12:f:808:ASN:OD1	12:f:809:ILE:N	2.51	0.44
15:B:99:VAL:HG13	15:B:138:PHE:CE1	2.52	0.44
16:C:140:VAL:HG21	17:D:299:PHE:CE1	2.53	0.44
16:C:184:LYS:NZ	16:C:286:THR:OG1	2.43	0.44
17:D:323:ARG:HB3	17:D:327:LEU:HD12	2.00	0.44
18:E:135:ILE:HD11	18:E:182:LEU:CD1	2.48	0.44
18:E:146:ARG:NE	18:E:150:GLU:OE2	2.42	0.44
19:F:293:THR:OG1	19:F:294:LYS:N	2.50	0.44
19:F:438:TYR:OH	24:K:19:GLY:O	2.32	0.44
23:J:35:VAL:CG2	23:J:191:VAL:HG22	2.48	0.44
23:J:85:ASN:OD1	30:Q:70:ARG:NE	2.51	0.44
25:L:200:PRO:O	25:L:201:ALA:HB3	2.17	0.44
30:Q:134:TYR:O	30:Q:137:PHE:N	2.51	0.44
1:U:636:VAL:HG23	17:D:53:PHE:HZ	1.83	0.44
1:U:803:LYS:HG3	1:U:877:LEU:HD22	2.00	0.44
3:W:317:TRP:HB2	3:W:358:VAL:HG11	2.00	0.44
4:X:151:SER:N	4:X:173:GLU:OE2	2.50	0.44
4:X:208:ALA:HB3	4:X:239:TYR:CE1	2.53	0.44
8:b:65:THR:CG2	8:b:71:ILE:HD11	2.48	0.44
8:b:184:ILE:HD12	8:b:184:ILE:H	1.83	0.44
10:d:319:ALA:O	10:d:320:SER:C	2.60	0.44
12:f:696:LEU:HD23	12:f:696:LEU:C	2.43	0.44
14:A:83:ASP:O	14:A:87:LEU:HG	2.18	0.44
14:A:115:VAL:HG23	14:A:119:ALA:H	1.82	0.44
14:A:321:THR:O	14:A:321:THR:HG23	2.18	0.44
18:E:155:ASN:OD1	18:E:157:GLU:N	2.51	0.44
19:F:184:GLN:HB3	19:F:187:ASP:HB2	1.99	0.44
20:G:84:THR:HB	26:M:157:VAL:HG12	1.99	0.44
20:G:107:TYR:CD1	20:G:107:TYR:C	2.96	0.44
25:L:29:VAL:HG21	25:L:149:PRO:CD	2.48	0.44
26:M:42:CYS:HB3	26:M:190:ILE:CD1	2.47	0.44
29:P:205:ASP:OD2	31:r:251:VAL:HB	2.18	0.44
32:S:56:ARG:NH2	32:S:241:ASP:O	2.46	0.44
29:p:149:MET:HE2	29:p:149:MET:H	1.83	0.44
31:r:60:THR:N	31:r:229:SER:OG	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:638:SER:HB3	1:U:671:LEU:HD11	2.00	0.43
1:U:790:GLY:HA3	1:U:914:LEU:HD11	1.98	0.43
3:W:132:THR:HG22	3:W:138:VAL:HG11	2.00	0.43
3:W:231:ILE:HD11	3:W:246:HIS:HB3	1.99	0.43
3:W:369:TYR:CG	7:a:312:MET:HE1	2.51	0.43
6:Z:283:ARG:CZ	6:Z:283:ARG:HB2	2.48	0.43
7:a:176:ALA:HB3	7:a:200:LEU:HD21	1.99	0.43
8:b:104:ASN:ND2	13:x:132:LYS:O	2.46	0.43
9:c:63:ASP:O	9:c:64:ASP:OD1	2.36	0.43
12:f:348:ILE:HG21	12:f:377:VAL:CG2	2.48	0.43
12:f:658:ALA:HB2	12:f:693:ALA:HB1	1.99	0.43
12:f:727:PHE:CZ	12:f:803:PHE:CE2	3.05	0.43
15:B:133:VAL:HB	15:B:157:HIS:O	2.18	0.43
15:B:223:ILE:CD1	15:B:347:ILE:HD13	2.48	0.43
16:C:151:ILE:HG22	16:C:152:GLY:N	2.33	0.43
16:C:376:VAL:O	16:C:376:VAL:HG12	2.17	0.43
18:E:60:VAL:C	18:E:61:LEU:HD12	2.43	0.43
18:E:138:LEU:N	18:E:138:LEU:HD12	2.32	0.43
18:E:276:ILE:O	18:E:277:MET:C	2.61	0.43
21:H:168:VAL:HG23	21:H:169:ASN:N	2.33	0.43
28:O:127:LYS:HD2	28:O:162:THR:HG21	2.00	0.43
28:O:245:TYR:CE2	29:P:152:SER:O	2.70	0.43
28:O:258:LYS:HG3	28:O:258:LYS:O	2.18	0.43
32:s:204:LYS:O	32:s:208:ILE:HG13	2.17	0.43
2:V:172:VAL:HA	2:V:175:MET:HE2	2.00	0.43
2:V:252:ASN:HD21	2:V:287:ARG:CB	2.31	0.43
7:a:35:HIS:O	7:a:36:GLN:HB2	2.18	0.43
7:a:112:ILE:HG23	7:a:138:VAL:CG2	2.48	0.43
10:d:193:GLY:HA2	10:d:196:LEU:HD12	2.00	0.43
14:A:239:ARG:NH1	15:B:320:ASP:OD2	2.43	0.43
14:A:282:GLY:O	14:A:328:ASP:N	2.51	0.43
15:B:316:LEU:HD21	15:B:327:VAL:HG21	2.00	0.43
15:B:404:LEU:O	15:B:408:ARG:HG3	2.18	0.43
18:E:196:LEU:HD21	18:E:225:HIS:HB2	1.99	0.43
24:K:36:THR:HG22	24:K:51:GLU:CG	2.47	0.43
28:O:102:ILE:HG13	28:O:126:LEU:CD2	2.47	0.43
28:O:190:GLU:OE1	28:O:192:GLU:N	2.48	0.43
29:P:193:ASP:N	29:P:193:ASP:OD1	2.48	0.43
29:P:195:ILE:O	29:P:195:ILE:HG13	2.18	0.43
31:R:64:ALA:HA	31:R:72:ILE:O	2.19	0.43
31:r:184:THR:HB	31:r:198:MET:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:9:ILE:HD12	1:U:9:ILE:H	1.82	0.43
1:U:567:ILE:HD13	1:U:586:VAL:HG22	2.00	0.43
2:V:113:LEU:HD22	2:V:174:PHE:CG	2.53	0.43
3:W:47:LEU:HD13	3:W:70:VAL:HG22	2.00	0.43
9:c:54:MET:HE1	9:c:87:VAL:HG22	2.00	0.43
10:d:318:PHE:O	10:d:319:ALA:C	2.61	0.43
12:f:745:LEU:HD23	12:f:766:GLN:CG	2.48	0.43
14:A:190:VAL:HG23	14:A:191:VAL:HG23	2.00	0.43
14:A:247:GLN:OE1	15:B:265:LYS:NZ	2.36	0.43
14:A:394:MET:HE2	15:B:216:ILE:HD13	2.01	0.43
17:D:230:VAL:HG12	17:D:231:VAL:N	2.33	0.43
18:E:76:GLY:N	18:E:77:PRO:HD2	2.32	0.43
20:G:79:VAL:HG12	20:G:139:ILE:HB	2.00	0.43
22:I:184:MET:HE1	22:I:192:LEU:HD13	1.99	0.43
25:L:160:SER:O	25:L:161:ILE:HG23	2.18	0.43
25:L:204:ASP:OD1	25:L:204:ASP:N	2.50	0.43
26:M:224:ARG:NH1	26:M:226:GLU:OE2	2.51	0.43
28:O:209:ASP:OD1	28:O:210:LEU:O	2.36	0.43
29:P:40:GLN:HG2	29:P:43:PHE:CE1	2.53	0.43
29:P:158:MET:SD	29:P:163:LEU:HA	2.59	0.43
30:Q:165:GLU:HA	30:Q:196:PHE:HE2	1.83	0.43
31:r:77:SER:HB2	31:r:90:VAL:H	1.83	0.43
1:U:199:ARG:CZ	1:U:223:LEU:HD23	2.48	0.43
1:U:263:SER:O	1:U:267:ASN:ND2	2.51	0.43
4:X:379:ASP:OD1	5:Y:313:SER:HB3	2.18	0.43
6:Z:147:ASP:OD1	6:Z:149:THR:HG22	2.19	0.43
6:Z:172:VAL:HG21	9:c:220:LEU:HD23	1.99	0.43
6:Z:213:GLU:O	6:Z:217:THR:HG22	2.17	0.43
7:a:172:TYR:HD2	7:a:203:ALA:HB2	1.83	0.43
12:f:215:ASP:HA	12:f:218:GLU:OE2	2.18	0.43
17:D:181:VAL:HG13	17:D:182:GLU:N	2.32	0.43
17:D:363:TYR:CE2	17:D:399:PHE:HB3	2.54	0.43
18:E:40:TYR:OH	19:F:72:LYS:HB3	2.19	0.43
20:G:58:ASP:OD2	20:G:60:LEU:HB2	2.18	0.43
20:G:61:LEU:CD2	20:G:66:VAL:HG21	2.48	0.43
20:G:79:VAL:CG1	20:G:139:ILE:HB	2.48	0.43
22:I:44:LEU:C	22:I:44:LEU:HD12	2.43	0.43
26:M:9:ASP:OD1	26:M:10:LEU:N	2.51	0.43
28:O:133:TYR:O	28:O:135:GLY:N	2.51	0.43
28:O:165:LEU:HD23	28:O:167:TYR:O	2.18	0.43
29:P:111:GLY:C	29:P:112:LEU:HD22	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:n:166:SER:O	27:n:170:TYR:CD2	2.72	0.43
30:q:180:VAL:HG22	30:q:181:ARG:N	2.34	0.43
1:U:701:ILE:H	1:U:701:ILE:HD12	1.83	0.43
1:U:797:MET:HE1	1:U:881:PRO:HG3	1.99	0.43
3:W:393:LEU:O	3:W:397:VAL:HG23	2.18	0.43
4:X:76:PHE:CD1	4:X:76:PHE:C	2.96	0.43
4:X:344:ARG:HG2	4:X:384:VAL:HG11	1.99	0.43
12:f:210:GLU:O	12:f:212:GLU:N	2.52	0.43
12:f:658:ALA:HB1	12:f:696:LEU:HB3	2.00	0.43
14:A:128:GLN:NE2	14:A:133:ASP:OD1	2.51	0.43
14:A:296:GLN:O	14:A:300:LEU:HG	2.19	0.43
14:A:304:ASN:OD1	14:A:304:ASN:C	2.59	0.43
15:B:67:ARG:HA	15:B:70:ASP:OD2	2.19	0.43
16:C:187:LEU:HB2	16:C:311:ILE:HG21	2.00	0.43
17:D:176:GLU:OE1	17:D:331:ILE:HG23	2.18	0.43
19:F:249:LEU:HD23	19:F:283:ILE:HG23	2.00	0.43
19:F:367:GLN:HG3	19:F:381:TYR:HD2	1.83	0.43
20:G:134:LEU:O	20:G:134:LEU:HD12	2.18	0.43
23:J:120:GLN:NE2	24:K:133:MET:CE	2.81	0.43
26:M:105:TYR:CE2	27:N:112:THR:OG1	2.71	0.43
27:N:62:ASN:O	27:N:63:ARG:C	2.62	0.43
30:Q:181:ARG:HG2	30:Q:181:ARG:HH11	1.83	0.43
28:o:240:THR:O	28:o:241:ARG:C	2.62	0.43
32:s:92:LEU:HD12	32:s:92:LEU:O	2.18	0.43
32:s:128:ARG:HH11	32:s:155:VAL:HG11	1.84	0.43
32:s:221:LEU:O	32:s:223:ILE:HG13	2.19	0.43
1:U:94:SER:OG	1:U:97:VAL:HG23	2.18	0.43
1:U:322:THR:O	1:U:326:ILE:HG12	2.18	0.43
2:V:419:LEU:O	2:V:422:ILE:N	2.52	0.43
3:W:83:LEU:O	3:W:87:ILE:HG12	2.19	0.43
4:X:274:LYS:HG3	4:X:275:LEU:HD12	2.01	0.43
4:X:335:LEU:O	4:X:339:ILE:HG22	2.18	0.43
7:a:269:LEU:O	7:a:272:ILE:HG22	2.19	0.43
9:c:177:THR:O	9:c:177:THR:CG2	2.66	0.43
12:f:210:GLU:C	12:f:212:GLU:H	2.27	0.43
12:f:246:SER:HA	12:f:249:LEU:HD23	2.01	0.43
13:x:127:MET:N	13:x:128:PRO:HD2	2.33	0.43
13:x:146:PHE:HA	13:x:157:LEU:HD12	1.99	0.43
14:A:94:GLN:CB	15:B:130:GLU:HG2	2.48	0.43
15:B:360:THR:O	15:B:364:ILE:HG12	2.18	0.43
16:C:102:ASN:OD1	16:C:103:ILE:HD12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:243:GLY:O	17:D:247:VAL:HG23	2.18	0.43
17:D:274:ARG:HH12	17:D:290:LEU:HD21	1.84	0.43
20:G:222:VAL:O	20:G:222:VAL:HG12	2.18	0.43
22:I:238:LYS:O	22:I:242:GLU:OE1	2.36	0.43
23:J:73:PHE:CD1	23:J:80:ALA:HB2	2.53	0.43
26:M:121:HIS:HA	26:M:124:THR:HG22	2.00	0.43
27:N:196:LEU:HD11	27:n:175:ALA:HB2	1.99	0.43
29:P:58:THR:HG23	29:P:59:ASP:N	2.33	0.43
30:Q:167:LEU:HD21	30:Q:175:LEU:HD12	2.00	0.43
31:R:133:ILE:HG23	31:R:133:ILE:O	2.17	0.43
29:p:156:PRO:O	29:p:157:ASN:CB	2.66	0.43
30:q:161:ARG:O	30:q:165:GLU:HG3	2.18	0.43
1:U:339:LEU:HD11	1:U:343:ILE:HD11	2.00	0.43
1:U:656:LEU:HD13	1:U:672:LEU:HD12	2.01	0.43
2:V:105:SER:O	2:V:108:LEU:HD23	2.19	0.43
2:V:192:MET:HE3	2:V:214:HIS:CD2	2.53	0.43
8:b:6:THR:OG1	8:b:49:VAL:HG12	2.18	0.43
9:c:31:VAL:HG23	9:c:203:ILE:HG21	2.00	0.43
9:c:78:SER:O	9:c:80:THR:N	2.45	0.43
12:f:189:LYS:O	12:f:193:PRO:HD3	2.19	0.43
14:A:45:ILE:HD13	15:B:62:LEU:HA	2.00	0.43
14:A:89:SER:OG	14:A:90:GLU:N	2.51	0.43
14:A:378:PRO:O	14:A:379:ASN:OD1	2.37	0.43
16:C:98:ASP:O	16:C:99:VAL:C	2.61	0.43
16:C:128:PRO:O	16:C:129:ASN:C	2.61	0.43
16:C:252:ASP:HB3	16:C:301:LEU:HD21	2.00	0.43
17:D:233:SER:CB	18:E:260:LEU:HD13	2.49	0.43
18:E:150:GLU:HA	18:E:191:LEU:HD21	2.01	0.43
19:F:96:LEU:HD23	19:F:97:LEU:N	2.34	0.43
20:G:153:LYS:HE2	20:G:163:PHE:CZ	2.53	0.43
21:H:124:SER:HB2	21:H:127:VAL:HG22	2.00	0.43
29:P:84:PRO:HB3	29:P:120:PHE:CD1	2.54	0.43
33:T:169:TYR:O	33:T:169:TYR:CG	2.70	0.43
27:n:38:MET:SD	27:n:190:THR:HG23	2.59	0.43
32:s:200:MET:SD	32:s:225:ILE:HD11	2.58	0.43
5:Y:272:PHE:HB3	11:e:52:PHE:CZ	2.54	0.43
10:d:129:LEU:O	10:d:130:PRO:C	2.62	0.43
12:f:662:MET:HG3	12:f:662:MET:O	2.19	0.43
12:f:739:ALA:C	12:f:741:LEU:H	2.27	0.43
16:C:319:PRO:O	16:C:320:PRO:C	2.60	0.43
17:D:418:LYS:OXT	20:G:159:TYR:OH	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:210:PHE:CE1	20:G:215:ILE:HD11	2.53	0.43
24:K:154:PHE:HD1	24:K:164:GLN:HA	1.82	0.43
27:n:153:MET:SD	33:t:81:PHE:CE2	3.12	0.43
30:q:131:ALA:HB3	30:q:140:LEU:CD1	2.39	0.43
31:r:97:ASN:HB2	31:r:100:LEU:HG	2.00	0.43
31:r:173:VAL:HG13	31:r:179:ARG:NH1	2.33	0.43
32:s:96:ILE:HD11	32:s:120:LEU:HD13	2.01	0.43
32:s:176:LEU:O	32:s:176:LEU:HD23	2.19	0.43
33:t:211:ARG:HA	33:t:214:VAL:HG22	2.00	0.43
1:U:37:GLU:OE2	2:V:266:GLN:HG3	2.19	0.43
1:U:676:THR:HG21	1:U:712:LEU:CD2	2.49	0.43
5:Y:41:LEU:O	5:Y:45:VAL:HG23	2.19	0.43
7:a:230:ARG:HG2	7:a:230:ARG:O	2.19	0.43
7:a:255:TRP:HB2	7:a:261:LEU:HD13	2.01	0.43
7:a:311:VAL:HG12	7:a:315:LEU:HD13	2.00	0.43
12:f:167:ALA:O	12:f:171:GLN:OE1	2.36	0.43
12:f:192:VAL:HB	12:f:217:LEU:HD13	2.00	0.43
12:f:560:LEU:HD11	12:f:798:THR:HG22	2.00	0.43
14:A:102:ILE:HD11	19:F:165:PRO:CD	2.49	0.43
14:A:130:ALA:O	14:A:132:THR:N	2.46	0.43
15:B:113:GLU:O	15:B:122:ILE:HB	2.19	0.43
16:C:108:VAL:O	16:C:108:VAL:HG12	2.19	0.43
17:D:181:VAL:CG2	17:D:261:ILE:HD13	2.48	0.43
17:D:360:LEU:HD21	17:D:399:PHE:CE2	2.54	0.43
18:E:146:ARG:CG	18:E:150:GLU:OE2	2.67	0.43
24:K:9:ASP:O	24:K:23:GLN:NE2	2.51	0.43
31:R:61:THR:N	31:R:76:ASP:OD2	2.52	0.43
31:R:200:ARG:NH1	30:q:142:ILE:HG23	2.34	0.43
32:S:47:ASP:OD1	32:S:47:ASP:N	2.51	0.43
32:S:120:LEU:HD23	32:S:138:ILE:HD11	2.00	0.43
27:n:82:SER:O	27:n:86:THR:HG23	2.19	0.43
33:t:204:VAL:HG12	33:t:205:LEU:N	2.33	0.43
3:W:83:LEU:HG	3:W:84:ASN:N	2.33	0.43
7:a:138:VAL:HG13	7:a:155:PHE:CE1	2.53	0.43
14:A:206:ILE:HG21	19:F:404:GLY:HA3	1.99	0.43
15:B:109:VAL:HG22	16:C:94:LYS:O	2.18	0.43
18:E:93:LYS:O	18:E:94:PRO:C	2.61	0.43
18:E:326:ILE:HA	18:E:329:GLU:OE1	2.19	0.43
19:F:369:HIS:CE1	37:F:501:ADP:O2'	2.72	0.43
20:G:61:LEU:CG	20:G:66:VAL:HG21	2.49	0.43
26:M:82:LEU:HD23	26:M:86:ARG:NH1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:196:LEU:HD21	27:N:231:PHE:CD2	2.51	0.43
29:P:13:ALA:HB3	29:P:137:VAL:HG22	1.98	0.43
31:R:156:MET:O	31:R:175:SER:N	2.52	0.43
31:R:163:TRP:CG	31:R:240:GLU:HA	2.53	0.43
33:T:59:VAL:HG12	33:T:60:LYS:N	2.34	0.43
28:o:130:LEU:HD23	28:o:137:ILE:CG2	2.48	0.43
30:q:139:THR:HG22	30:q:163:CYS:SG	2.58	0.43
31:r:160:ILE:HG12	31:r:179:ARG:HH22	1.83	0.43
1:U:451:ALA:O	1:U:453:HIS:N	2.52	0.42
1:U:800:VAL:HG22	1:U:801:GLN:N	2.33	0.42
2:V:363:LEU:HD21	2:V:398:LEU:CD2	2.49	0.42
3:W:33:LYS:NZ	3:W:37:GLU:OE2	2.30	0.42
3:W:406:VAL:HG12	3:W:413:ILE:HG12	2.01	0.42
3:W:438:LEU:HD23	6:Z:233:VAL:CG2	2.48	0.42
4:X:97:LEU:HD12	4:X:132:ARG:NH1	2.33	0.42
4:X:127:GLN:HG2	4:X:157:LEU:HD21	2.01	0.42
4:X:339:ILE:HD13	4:X:350:ILE:HD11	1.99	0.42
9:c:261:GLU:O	9:c:265:MET:HG3	2.19	0.42
12:f:646:MET:O	12:f:650:GLN:OE1	2.37	0.42
12:f:685:THR:HG23	12:f:686:LEU:N	2.33	0.42
12:f:759:LEU:HA	12:f:762:VAL:HG12	2.01	0.42
15:B:123:VAL:HG11	15:B:152:LEU:HD21	2.00	0.42
18:E:138:LEU:O	18:E:142:ILE:HG12	2.19	0.42
25:L:123:TYR:O	25:L:123:TYR:CG	2.72	0.42
30:Q:13:VAL:HG23	30:Q:115:LEU:HB2	2.01	0.42
30:Q:132:HIS:C	30:Q:136:ALA:HB2	2.44	0.42
33:t:67:ILE:HB	33:t:95:MET:HE3	2.01	0.42
1:U:501:LEU:C	1:U:503:GLN:H	2.27	0.42
1:U:788:VAL:HG12	1:U:884:VAL:HG21	2.01	0.42
2:V:482:PHE:HZ	5:Y:381:GLN:CG	2.32	0.42
3:W:68:VAL:HG12	3:W:72:LYS:CD	2.48	0.42
3:W:152:ILE:O	3:W:156:ASN:OD1	2.37	0.42
3:W:392:PHE:HE1	3:W:396:LEU:HD11	1.85	0.42
4:X:181:SER:HB2	5:Y:247:LEU:HD22	2.01	0.42
8:b:104:ASN:OD1	13:x:133:ALA:HA	2.19	0.42
8:b:143:PHE:CD2	8:b:179:LEU:HD21	2.53	0.42
9:c:107:MET:HE2	13:x:273:THR:H	1.84	0.42
10:d:223:ASN:OD1	10:d:226:ILE:N	2.47	0.42
12:f:262:PHE:N	12:f:263:PRO:HD3	2.34	0.42
12:f:556:ARG:HH22	12:f:648:ALA:HB3	1.84	0.42
12:f:658:ALA:HB2	12:f:693:ALA:CA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:91:GLN:HG3	14:A:93:LEU:HD23	2.01	0.42
14:A:93:LEU:O	14:A:94:GLN:HB2	2.19	0.42
14:A:255:ARG:NH1	14:A:259:GLU:OE1	2.49	0.42
14:A:300:LEU:CD1	19:F:290:ALA:HB2	2.50	0.42
15:B:112:LEU:HD13	15:B:144:LEU:HD12	2.01	0.42
16:C:339:THR:O	16:C:342:ILE:HG12	2.19	0.42
17:D:85:ILE:HG23	18:E:68:LYS:CD	2.49	0.42
24:K:64:ILE:O	24:K:64:ILE:HG13	2.19	0.42
24:K:78:MET:HG2	24:K:79:SER:N	2.34	0.42
26:M:220:LEU:HD23	26:M:220:LEU:H	1.84	0.42
26:M:231:ASP:OD1	26:M:232:ILE:HG12	2.18	0.42
28:O:254:VAL:HG12	28:O:255:LEU:H	1.81	0.42
29:P:30:ILE:HD12	30:Q:119:ASP:OD2	2.19	0.42
30:Q:27:GLN:O	30:q:170:ARG:CZ	2.67	0.42
32:s:74:LEU:CD1	32:s:80:ILE:HD13	2.49	0.42
32:s:74:LEU:HD11	32:s:80:ILE:HD13	2.01	0.42
2:V:235:LEU:O	2:V:239:THR:HG22	2.19	0.42
5:Y:45:VAL:HA	5:Y:50:MET:HE2	2.01	0.42
5:Y:163:LYS:O	5:Y:167:LEU:HD13	2.19	0.42
10:d:131:THR:O	10:d:131:THR:HG22	2.20	0.42
10:d:208:PHE:CE2	10:d:212:LEU:HD11	2.54	0.42
12:f:284:SER:O	12:f:285:CYS:C	2.62	0.42
12:f:502:LEU:CG	12:f:537:THR:HG21	2.47	0.42
12:f:684:PRO:O	12:f:688:ARG:NE	2.52	0.42
14:A:73:ALA:N	15:B:138:PHE:O	2.52	0.42
15:B:57:GLN:OE1	15:B:61:LYS:NZ	2.49	0.42
16:C:42:LEU:HD23	16:C:42:LEU:C	2.44	0.42
19:F:336:ASP:C	19:F:337:ILE:HD12	2.44	0.42
21:H:203:MET:SD	21:H:208:ILE:HD12	2.60	0.42
21:H:222:THR:HB	21:H:223:PRO:CD	2.50	0.42
23:J:68:ASN:OD1	23:J:68:ASN:N	2.52	0.42
26:M:28:MET:HE3	26:M:155:SER:HB2	2.00	0.42
27:N:76:PHE:CZ	27:N:218:VAL:HG11	2.54	0.42
27:N:207:VAL:HG23	27:N:207:VAL:O	2.20	0.42
28:O:98:THR:HG23	28:O:129:MET:CE	2.49	0.42
31:R:192:VAL:CG1	30:q:137:PHE:HB2	2.50	0.42
32:s:120:LEU:O	32:s:124:LEU:HG	2.20	0.42
1:U:153:ILE:HD13	16:C:20:LEU:HD22	2.01	0.42
1:U:472:ILE:H	1:U:472:ILE:HD12	1.83	0.42
1:U:626:LEU:O	1:U:659:CYS:SG	2.76	0.42
2:V:85:ALA:O	2:V:89:LYS:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:496:PHE:CE2	16:C:47:ALA:CB	3.02	0.42
3:W:28:LEU:HD12	3:W:47:LEU:HD22	1.99	0.42
3:W:184:GLU:OE1	3:W:222:LEU:HD11	2.20	0.42
5:Y:316:LEU:HD11	5:Y:330:ILE:HG22	2.01	0.42
7:a:26:GLU:O	7:a:30:THR:HG23	2.18	0.42
7:a:101:ARG:HB3	7:a:101:ARG:NH1	2.35	0.42
9:c:73:PHE:HE1	9:c:95:MET:HG2	1.84	0.42
12:f:247:ALA:HA	12:f:250:ARG:NE	2.35	0.42
12:f:450:ILE:HB	12:f:487:LEU:HD13	2.00	0.42
14:A:186:LYS:HB3	14:A:339:ARG:HD3	2.02	0.42
15:B:105:THR:HB	16:C:98:ASP:OD2	2.20	0.42
15:B:209:GLU:N	15:B:209:GLU:OE1	2.52	0.42
16:C:403:LYS:HD2	21:H:156:PHE:CG	2.54	0.42
17:D:103:VAL:HG22	17:D:104:GLY:N	2.34	0.42
17:D:231:VAL:O	17:D:234:GLU:N	2.49	0.42
17:D:300:ASP:O	17:D:301:GLN:C	2.62	0.42
19:F:150:LEU:HD22	19:F:167:GLU:HB3	2.01	0.42
19:F:175:MET:CE	19:F:251:LEU:HA	2.50	0.42
25:L:18:ARG:NH2	25:L:23:GLU:OE2	2.53	0.42
30:Q:44:LEU:HD11	30:Q:102:LEU:HD12	2.01	0.42
32:s:76:ASP:O	32:s:231:ILE:HD11	2.19	0.42
32:s:184:LYS:O	32:s:186:MET:HE2	2.19	0.42
1:U:328:ILE:HD11	1:U:795:LEU:CD1	2.50	0.42
1:U:458:ILE:HG21	1:U:490:ARG:NH1	2.34	0.42
2:V:80:LYS:O	2:V:84:LYS:HG2	2.20	0.42
2:V:423:ALA:O	2:V:424:GLN:CB	2.68	0.42
8:b:179:LEU:HG	8:b:179:LEU:O	2.19	0.42
12:f:822:VAL:HG13	12:f:825:MET:SD	2.60	0.42
15:B:203:LEU:N	15:B:204:PRO:CD	2.83	0.42
16:C:63:LEU:HD21	17:D:79:VAL:HG22	2.01	0.42
17:D:181:VAL:HG13	17:D:182:GLU:HG3	2.01	0.42
18:E:135:ILE:HD13	18:E:186:ALA:CB	2.49	0.42
18:E:153:LEU:HD12	18:E:191:LEU:HD23	2.02	0.42
20:G:60:LEU:HD23	26:M:163:GLY:C	2.44	0.42
21:H:75:VAL:HG22	21:H:76:TYR:N	2.35	0.42
22:I:12:PHE:CE1	22:I:18:LEU:HD21	2.55	0.42
23:J:121:SER:HB3	23:J:124:ARG:HD2	2.01	0.42
25:L:101:ARG:HH11	25:L:101:ARG:HG3	1.84	0.42
27:N:57:GLY:O	27:N:58:SER:HB2	2.18	0.42
27:N:63:ARG:HH11	33:t:256:ILE:HD11	1.85	0.42
29:P:11:VAL:HG21	29:P:52:GLY:HA3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:63:VAL:HG12	29:P:103:TYR:CD2	2.54	0.42
30:Q:160:LEU:O	30:Q:164:LEU:HG	2.19	0.42
27:n:63:ARG:CZ	28:o:182:GLU:OE2	2.67	0.42
27:n:208:ILE:HG22	27:n:210:LEU:CD2	2.48	0.42
29:p:33:GLN:O	29:p:35:VAL:HG23	2.20	0.42
31:r:66:LYS:HG2	31:r:71:VAL:HG22	2.02	0.42
33:t:255:ASP:OD1	33:t:256:ILE:N	2.53	0.42
1:U:155:LEU:HD21	1:U:197:VAL:HG21	2.02	0.42
1:U:247:GLN:CG	1:U:904:LYS:HD3	2.49	0.42
2:V:470:ARG:HG2	2:V:473:GLN:HB3	2.01	0.42
3:W:69:ALA:HA	3:W:72:LYS:HD3	2.01	0.42
4:X:40:GLU:O	4:X:43:VAL:HG12	2.20	0.42
4:X:297:ARG:HG2	4:X:330:LEU:HD11	2.01	0.42
5:Y:174:TRP:O	5:Y:178:ASN:ND2	2.52	0.42
5:Y:229:ILE:HB	5:Y:295:TYR:CE1	2.54	0.42
7:a:94:LEU:HD13	7:a:122:LYS:NZ	2.34	0.42
13:x:251:ASN:OD1	13:x:252:GLN:N	2.53	0.42
14:A:153:LEU:HD21	15:B:132:TYR:CD1	2.55	0.42
16:C:379:THR:HG22	16:C:380:GLN:N	2.35	0.42
17:D:254:ALA:O	17:D:257:ASN:O	2.36	0.42
17:D:386:ALA:HB2	17:D:398:ASP:OD2	2.20	0.42
19:F:375:VAL:CG1	19:F:379:VAL:HG11	2.49	0.42
20:G:107:TYR:CD2	28:O:118:ARG:NH1	2.88	0.42
20:G:113:MET:CE	28:O:113:THR:HG22	2.50	0.42
22:I:45:LEU:CD2	22:I:75:SER:OG	2.68	0.42
23:J:211:MET:HE2	23:J:217:LEU:HD12	2.00	0.42
25:L:95:SER:O	25:L:99:PHE:O	2.38	0.42
29:P:136:PHE:HB3	29:P:150:CYS:SG	2.59	0.42
30:Q:47:VAL:O	30:Q:47:VAL:HG13	2.20	0.42
32:S:41:LEU:HD11	32:S:177:LEU:HD11	2.01	0.42
32:S:153:ASP:C	32:S:153:ASP:OD1	2.63	0.42
27:n:222:VAL:HB	27:n:224:LEU:HD11	2.01	0.42
30:q:14:LEU:HD12	30:q:181:ARG:O	2.19	0.42
31:r:65:PHE:CG	31:r:66:LYS:N	2.87	0.42
1:U:3:THR:HG23	10:d:177:ASP:OD1	2.19	0.42
1:U:491:GLN:O	1:U:495:ASP:OD1	2.38	0.42
5:Y:282:MET:SD	5:Y:288:PHE:CG	3.13	0.42
5:Y:319:MET:HE3	5:Y:330:ILE:CG2	2.50	0.42
5:Y:384:SER:CB	6:Z:272:LEU:HD21	2.50	0.42
7:a:29:TYR:O	7:a:32:LYS:N	2.49	0.42
7:a:179:PHE:O	7:a:183:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:32:TYR:HE2	9:c:66:THR:HG23	1.83	0.42
12:f:240:VAL:HB	12:f:245:ASN:OD1	2.20	0.42
12:f:690:VAL:O	12:f:694:LEU:HD23	2.20	0.42
15:B:364:ILE:HG22	15:B:395:ILE:HG21	2.01	0.42
16:C:150:MET:HE2	16:C:334:ARG:NH2	2.34	0.42
17:D:51:LEU:HD23	17:D:55:GLU:OE1	2.20	0.42
17:D:274:ARG:NH2	17:D:289:LEU:HD23	2.35	0.42
17:D:344:ILE:CD1	37:D:501:ADP:C6	3.03	0.42
23:J:134:VAL:HG12	23:J:144:LEU:CD1	2.50	0.42
26:M:24:VAL:HG22	26:M:124:THR:OG1	2.20	0.42
27:N:149:PRO:HD2	27:N:153:MET:HB3	2.01	0.42
28:O:74:CYS:SG	28:O:75:SER:N	2.93	0.42
29:P:33:GLN:NE2	30:Q:140:LEU:HD23	2.34	0.42
28:o:167:TYR:CD2	28:o:178:MET:HE1	2.55	0.42
30:q:139:THR:HA	30:q:163:CYS:SG	2.59	0.42
33:t:192:GLN:N	33:t:193:PRO:CD	2.83	0.42
1:U:233:LEU:O	1:U:237:VAL:HG23	2.19	0.42
2:V:313:LEU:HD11	2:V:329:HIS:CE1	2.55	0.42
2:V:395:ILE:O	2:V:395:ILE:CG2	2.67	0.42
3:W:165:ILE:H	3:W:165:ILE:HD12	1.85	0.42
3:W:406:VAL:HG23	4:X:342:PHE:CD1	2.55	0.42
4:X:154:LEU:HD12	4:X:155:ARG:N	2.35	0.42
9:c:57:MET:HE3	9:c:69:VAL:HG21	2.01	0.42
14:A:394:MET:CE	15:B:216:ILE:CD1	2.97	0.42
15:B:174:MET:CG	15:B:249:ARG:O	2.67	0.42
16:C:143:VAL:O	16:C:143:VAL:HG23	2.19	0.42
17:D:116:LEU:H	17:D:119:ILE:HD11	1.85	0.42
17:D:173:GLN:OE1	17:D:173:GLN:N	2.44	0.42
17:D:238:LYS:O	17:D:239:TYR:CB	2.68	0.42
18:E:197:LYS:HA	18:E:231:PHE:HB3	2.02	0.42
21:H:101:TYR:HE1	29:P:90:MET:HE2	1.85	0.42
22:I:45:LEU:HD11	22:I:137:ILE:HG23	2.01	0.42
22:I:52:ILE:O	22:I:53:HIS:C	2.63	0.42
24:K:70:ILE:HD13	24:K:93:ARG:HG3	2.01	0.42
25:L:48:ALA:HB3	25:L:63:ILE:HD11	2.01	0.42
28:O:148:VAL:HG23	28:O:149:THR:HG23	2.01	0.42
30:Q:101:ASN:HB3	30:Q:132:HIS:CE1	2.55	0.42
31:R:72:ILE:CG2	31:R:235:LEU:HD11	2.50	0.42
31:R:78:ARG:HD2	31:R:85:ILE:HB	2.02	0.42
33:T:108:LEU:O	33:T:112:LEU:HD23	2.19	0.42
29:p:121:ILE:HG22	29:p:137:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:549:ALA:HA	1:U:581:SER:HB2	2.02	0.42
3:W:436:MET:HA	3:W:439:VAL:HG22	2.02	0.42
9:c:283:HIS:O	9:c:286:GLU:HG2	2.20	0.42
12:f:125:ILE:HA	12:f:128:VAL:HG22	2.00	0.42
12:f:745:LEU:HD23	12:f:766:GLN:HG2	2.02	0.42
14:A:30:ILE:HD11	16:C:171:HIS:CG	2.55	0.42
14:A:86:THR:HG23	15:B:156:VAL:HG21	2.00	0.42
14:A:111:TYR:CD1	14:A:125:LEU:HD13	2.55	0.42
16:C:187:LEU:CB	16:C:311:ILE:HG21	2.49	0.42
19:F:72:LYS:HA	19:F:75:GLU:HG2	2.02	0.42
20:G:14:THR:HG21	20:G:129:ALA:HB2	2.02	0.42
21:H:6:TYR:CE2	21:H:15:PRO:HD3	2.54	0.42
23:J:74:ALA:HB3	23:J:161:ILE:HD12	2.01	0.42
24:K:99:HIS:HB2	24:K:107:MET:HE3	2.01	0.42
24:K:102:THR:HA	32:S:122:THR:HG21	2.01	0.42
25:L:206:THR:O	25:L:210:VAL:HG12	2.20	0.42
30:Q:145:ARG:CZ	31:r:217:ARG:HE	2.33	0.42
31:R:233:VAL:O	31:R:234:ASN:C	2.63	0.42
33:T:84:ILE:HG13	33:T:84:ILE:O	2.18	0.42
33:T:98:ALA:HB3	33:T:105:PHE:CD1	2.54	0.42
33:T:190:LEU:C	33:T:190:LEU:HD12	2.45	0.42
27:n:198:MET:HE1	27:n:208:ILE:CG1	2.50	0.42
29:p:88:MET:SD	29:p:89:SER:N	2.93	0.42
31:r:96:ILE:CD1	31:r:102:GLY:HA3	2.48	0.42
31:r:100:LEU:O	31:r:100:LEU:HD12	2.20	0.42
31:r:172:TYR:O	31:r:179:ARG:HA	2.20	0.42
32:s:39:THR:HG22	32:s:173:LEU:HD11	2.01	0.42
1:U:2:ILE:HD11	10:d:131:THR:HG23	2.01	0.42
1:U:368:ALA:HB2	1:U:728:PHE:CD2	2.55	0.42
2:V:416:ARG:O	2:V:416:ARG:HG2	2.20	0.42
3:W:298:GLU:O	3:W:299:ILE:C	2.61	0.42
4:X:335:LEU:HD21	4:X:361:VAL:HG23	2.02	0.42
8:b:16:MET:HG3	8:b:26:LEU:HD22	2.01	0.42
12:f:564:LEU:O	12:f:567:LEU:CD1	2.68	0.42
13:x:157:LEU:O	13:x:259:ARG:HA	2.20	0.42
14:A:138:MET:HE2	14:A:152:PRO:CB	2.46	0.42
16:C:322:GLU:C	16:C:324:ALA:H	2.27	0.42
20:G:214:GLU:O	20:G:215:ILE:HD13	2.20	0.42
23:J:188:ILE:HG22	23:J:192:ILE:CD1	2.50	0.42
24:K:40:ILE:HD12	24:K:40:ILE:N	2.35	0.42
25:L:121:GLN:O	26:M:129:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:137:TYR:CE2	25:L:217:LYS:HB2	2.55	0.42
28:O:207:PHE:O	32:s:66:ARG:NH2	2.47	0.42
29:P:111:GLY:O	29:P:112:LEU:HD22	2.20	0.42
30:Q:9:GLY:N	30:Q:12:TYR:O	2.53	0.42
30:Q:134:TYR:CG	30:q:25:ILE:HD11	2.55	0.42
30:Q:138:LEU:HD22	31:r:192:VAL:HG22	2.02	0.42
28:o:169:THR:O	28:o:174:SER:CB	2.68	0.42
33:t:80:ARG:HG2	33:t:81:PHE:CE2	2.55	0.42
33:t:204:VAL:HG12	33:t:205:LEU:H	1.85	0.42
1:U:155:LEU:CD2	1:U:197:VAL:HG21	2.49	0.41
1:U:621:SER:O	1:U:625:ILE:HG12	2.20	0.41
3:W:187:LEU:HD11	3:W:226:TYR:HA	2.01	0.41
3:W:287:VAL:HG13	3:W:306:LEU:HD11	2.02	0.41
4:X:8:GLU:HA	4:X:11:ARG:HG2	2.02	0.41
10:d:261:ASP:HA	10:d:264:LEU:HD12	2.01	0.41
12:f:606:VAL:HA	12:f:609:VAL:HG22	2.02	0.41
14:A:111:TYR:CE1	14:A:125:LEU:HD13	2.55	0.41
15:B:391:SER:OG	15:B:394:ASP:N	2.46	0.41
16:C:198:LEU:HD12	35:C:501:ATP:H2'	2.02	0.41
20:G:113:MET:HE1	28:O:112:SER:C	2.45	0.41
22:I:115:CYS:CB	23:J:81:ARG:HH12	2.33	0.41
23:J:139:ASP:HB3	31:R:165:LYS:HE3	2.02	0.41
25:L:207:THR:OG1	25:L:226:ASP:O	2.38	0.41
29:p:52:GLY:C	29:p:53:LEU:HD12	2.45	0.41
30:q:4:LEU:O	30:q:131:ALA:HB1	2.20	0.41
1:U:788:VAL:CG1	1:U:884:VAL:HG21	2.50	0.41
3:W:325:GLY:O	3:W:328:LEU:CD2	2.68	0.41
5:Y:14:ASN:OD1	5:Y:113:ARG:NH1	2.52	0.41
7:a:7:PHE:HZ	7:a:59:LEU:HD12	1.85	0.41
12:f:60:VAL:HG21	12:f:102:HIS:CD2	2.54	0.41
12:f:344:VAL:O	12:f:348:ILE:HD12	2.20	0.41
12:f:449:GLY:HA3	12:f:484:GLY:O	2.19	0.41
12:f:469:TYR:C	12:f:470:VAL:HG22	2.45	0.41
14:A:102:ILE:CG2	14:A:109:PRO:O	2.68	0.41
15:B:201:VAL:HB	15:B:202:GLU:OE2	2.19	0.41
16:C:119:ASP:OD1	16:C:119:ASP:N	2.49	0.41
17:D:299:PHE:O	17:D:299:PHE:CD1	2.73	0.41
18:E:36:LEU:HD21	19:F:70:LYS:HE2	2.02	0.41
19:F:153:VAL:CG1	19:F:158:TYR:HA	2.49	0.41
20:G:196:GLU:OE2	20:G:242:LEU:HB2	2.20	0.41
23:J:86:ARG:HD3	23:J:114:LEU:HD22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:21:VAL:O	26:M:21:VAL:HG23	2.20	0.41
29:P:144:GLU:O	32:s:172:MET:HG2	2.20	0.41
31:R:207:GLU:O	31:R:210:GLN:HG2	2.20	0.41
32:S:241:ASP:N	32:S:241:ASP:OD1	2.51	0.41
27:n:195:ALA:O	27:n:198:MET:HG2	2.20	0.41
28:o:91:THR:HG23	28:o:94:ASP:HB2	2.01	0.41
28:o:233:THR:HG22	28:o:234:VAL:N	2.35	0.41
29:p:135:ASP:OD1	29:p:136:PHE:N	2.48	0.41
29:p:184:GLY:HA2	29:p:202:ALA:HB3	2.03	0.41
31:r:144:ASN:O	31:r:148:GLN:NE2	2.52	0.41
31:r:255:HIS:C	31:r:255:HIS:CD2	2.97	0.41
32:s:92:LEU:HD21	32:s:120:LEU:HD11	2.01	0.41
33:t:78:LEU:HD12	33:t:79:ALA:N	2.35	0.41
1:U:138:PHE:O	1:U:141:CYS:HB2	2.20	0.41
2:V:353:LEU:O	2:V:354:LYS:C	2.63	0.41
2:V:453:HIS:CD2	10:d:286:GLU:HG2	2.55	0.41
3:W:70:VAL:HG11	3:W:90:LEU:HD11	2.03	0.41
7:a:131:THR:O	7:a:135:ILE:HG12	2.20	0.41
9:c:63:ASP:CG	9:c:64:ASP:H	2.28	0.41
10:d:146:ASP:O	10:d:150:ILE:HG12	2.21	0.41
12:f:208:LEU:HD22	12:f:214:VAL:HB	2.02	0.41
12:f:646:MET:HE2	12:f:646:MET:N	2.36	0.41
14:A:92:PRO:HD2	14:A:143:ASP:HA	2.02	0.41
14:A:236:CYS:SG	14:A:238:ILE:HD11	2.61	0.41
14:A:369:ARG:HE	14:A:372:LEU:HD13	1.86	0.41
14:A:391:GLU:OE1	15:B:349:ARG:NH1	2.53	0.41
35:B:501:ATP:O3A	16:C:307:ARG:NH1	2.53	0.41
16:C:145:ASP:OD1	16:C:145:ASP:N	2.48	0.41
16:C:161:ILE:HG13	16:C:165:ILE:HD13	2.02	0.41
16:C:238:ALA:HB2	16:C:246:ILE:HD11	2.01	0.41
17:D:225:ALA:HB2	17:D:259:PRO:HB2	2.02	0.41
17:D:415:GLU:HG3	20:G:159:TYR:HD2	1.84	0.41
19:F:240:CYS:O	19:F:244:THR:CB	2.68	0.41
20:G:109:ILE:O	20:G:109:ILE:HG23	2.20	0.41
20:G:234:GLU:OE1	20:G:234:GLU:N	2.49	0.41
21:H:65:VAL:HG11	21:H:211:GLY:HA3	2.03	0.41
21:H:188:ILE:HG21	21:H:229:TYR:CD2	2.55	0.41
22:I:52:ILE:HD13	22:I:209:GLU:HB2	2.02	0.41
23:J:104:VAL:CG2	23:J:133:ILE:HG22	2.49	0.41
26:M:21:VAL:HG23	26:M:24:VAL:HB	2.03	0.41
28:O:165:LEU:HD12	28:O:166:PRO:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:22:ILE:O	29:P:22:ILE:HG23	2.21	0.41
33:T:78:LEU:O	33:T:78:LEU:CD2	2.66	0.41
29:p:146:MET:HB3	29:p:174:ALA:HB2	2.02	0.41
30:q:12:TYR:OH	30:q:151:ILE:HG23	2.21	0.41
31:r:237:HIS:O	31:r:244:ILE:HG12	2.20	0.41
32:s:94:LYS:O	32:s:97:GLU:HG3	2.20	0.41
32:s:95:ILE:HG21	32:s:123:ILE:CD1	2.50	0.41
32:s:127:ARG:O	32:s:128:ARG:C	2.63	0.41
1:U:69:TYR:CE1	1:U:99:THR:HB	2.55	0.41
2:V:201:ARG:NE	16:C:33:LEU:HD11	2.35	0.41
3:W:64:SER:O	3:W:68:VAL:HG23	2.19	0.41
3:W:136:ILE:HA	3:W:139:GLU:OE2	2.20	0.41
3:W:372:ARG:HB2	7:a:325:ASP:OD1	2.21	0.41
6:Z:172:VAL:HG21	9:c:220:LEU:CD2	2.51	0.41
7:a:317:VAL:O	7:a:317:VAL:HG12	2.20	0.41
9:c:84:VAL:HB	13:x:280:ARG:HD3	2.01	0.41
9:c:237:HIS:ND1	9:c:298:GLN:OE1	2.54	0.41
10:d:129:LEU:HD23	10:d:174:TYR:CZ	2.55	0.41
13:x:273:THR:O	13:x:273:THR:CG2	2.64	0.41
13:x:274:ASN:OD1	13:x:274:ASN:C	2.63	0.41
15:B:112:LEU:HD11	15:B:115:ILE:HG12	2.02	0.41
15:B:423:LYS:O	15:B:427:LEU:HD23	2.19	0.41
16:C:266:ASP:HB2	16:C:269:VAL:HG12	2.02	0.41
17:D:407:ILE:HG23	17:D:408:LYS:N	2.34	0.41
18:E:363:VAL:O	18:E:363:VAL:HG22	2.20	0.41
21:H:76:TYR:CD1	21:H:76:TYR:C	2.98	0.41
33:T:217:CYS:O	33:T:220:VAL:HG12	2.20	0.41
31:r:74:ALA:HB1	31:r:219:ILE:HD11	2.02	0.41
32:s:75:THR:O	32:s:76:ASP:C	2.64	0.41
32:s:151:SER:HB2	32:s:164:LYS:HE3	2.03	0.41
32:s:181:VAL:HB	32:s:202:LEU:HD13	2.02	0.41
1:U:127:ASP:OD2	1:U:129:ARG:NH2	2.53	0.41
1:U:153:ILE:HG13	16:C:24:TYR:OH	2.21	0.41
1:U:246:TYR:CD2	1:U:795:LEU:HD21	2.55	0.41
2:V:92:ARG:O	2:V:93:PHE:HB2	2.20	0.41
2:V:416:ARG:O	5:Y:350:VAL:HG23	2.20	0.41
3:W:55:ARG:O	3:W:58:SER:N	2.52	0.41
3:W:136:ILE:O	3:W:136:ILE:HG22	2.19	0.41
5:Y:382:LYS:O	5:Y:386:VAL:HG23	2.20	0.41
7:a:56:LEU:CD2	7:a:83:VAL:HG22	2.49	0.41
8:b:6:THR:HG21	8:b:40:LYS:HE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:121:TRP:O	9:c:122:LEU:HD23	2.19	0.41
12:f:674:THR:HG22	15:B:75:GLU:HG3	1.99	0.41
14:A:95:VAL:HB	14:A:115:VAL:HA	2.03	0.41
14:A:148:GLN:OE1	14:A:148:GLN:N	2.52	0.41
14:A:387:SER:O	14:A:391:GLU:HG2	2.20	0.41
17:D:344:ILE:HD12	37:D:501:ADP:C6	2.55	0.41
18:E:41:GLU:OE2	18:E:45:ASN:ND2	2.53	0.41
20:G:195:VAL:HG11	20:G:238:HIS:ND1	2.35	0.41
23:J:30:SER:O	23:J:61:LYS:NZ	2.54	0.41
26:M:174:LYS:O	26:M:178:GLU:OE1	2.38	0.41
27:N:93:VAL:HG11	27:N:117:PHE:CE2	2.54	0.41
28:O:91:THR:HG23	28:O:94:ASP:HB2	2.02	0.41
30:Q:3:TYR:HE1	30:Q:136:ALA:CA	2.32	0.41
30:Q:51:GLY:CA	31:R:177:GLY:O	2.68	0.41
32:S:96:ILE:HD11	32:S:120:LEU:HD13	2.03	0.41
27:n:38:MET:CG	27:n:190:THR:HG23	2.50	0.41
28:o:241:ARG:NH1	29:p:154:TRP:O	2.53	0.41
32:s:80:ILE:HG22	32:s:138:ILE:HD12	2.02	0.41
1:U:377:HIS:O	1:U:378:CYS:C	2.64	0.41
2:V:168:GLN:HG3	2:V:191:LEU:HD22	2.03	0.41
3:W:206:SER:HB2	3:W:230:MET:HE3	2.01	0.41
5:Y:68:ASP:N	5:Y:68:ASP:OD1	2.53	0.41
7:a:128:LEU:HA	7:a:131:THR:OG1	2.19	0.41
9:c:49:VAL:HG22	18:E:103:THR:CG2	2.41	0.41
12:f:666:ILE:HG23	12:f:667:GLY:N	2.35	0.41
12:f:761:MET:HE3	12:f:764:LEU:HD23	2.01	0.41
14:A:135:GLU:HB2	14:A:138:MET:HB2	2.02	0.41
14:A:430:MET:O	14:A:430:MET:HG2	2.20	0.41
19:F:437:TYR:HB2	24:K:159:SER:OG	2.20	0.41
21:H:196:LYS:N	21:H:203:MET:HE1	2.35	0.41
22:I:46:ALA:CB	22:I:197:LEU:HD11	2.42	0.41
25:L:9:ASP:OD1	25:L:12:VAL:HG22	2.20	0.41
26:M:193:GLU:OE1	26:M:196:LYS:NZ	2.53	0.41
27:N:207:VAL:HG11	33:t:257:ALA:CB	2.51	0.41
28:O:62:ARG:HB3	28:O:213:GLY:HA2	2.03	0.41
30:Q:50:ALA:O	30:Q:52:ASP:N	2.51	0.41
33:T:57:LEU:CD1	33:T:221:LEU:HD11	2.50	0.41
33:T:161:ALA:O	33:T:162:ASP:OD1	2.38	0.41
1:U:485:ALA:O	1:U:486:MET:C	2.64	0.41
1:U:639:LEU:HD13	17:D:60:TYR:CE2	2.56	0.41
1:U:833:LEU:HD13	15:B:74:MET:HE3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:458:VAL:O	2:V:459:GLN:C	2.62	0.41
3:W:44:ILE:CD1	3:W:82:LEU:HD12	2.50	0.41
4:X:211:ASP:O	4:X:231:TYR:HB3	2.21	0.41
4:X:354:ILE:HG22	4:X:354:ILE:O	2.20	0.41
5:Y:376:LEU:CD2	6:Z:265:LEU:HD21	2.50	0.41
8:b:16:MET:SD	8:b:25:ARG:HB3	2.61	0.41
8:b:63:THR:O	8:b:64:LEU:C	2.64	0.41
9:c:62:VAL:HG21	9:c:68:ARG:HD2	2.03	0.41
12:f:93:PRO:O	12:f:96:LEU:O	2.39	0.41
16:C:214:VAL:CG2	16:C:234:LEU:HD21	2.46	0.41
17:D:349:THR:O	17:D:349:THR:HG22	2.21	0.41
18:E:154:THR:O	18:E:155:ASN:C	2.63	0.41
20:G:175:SER:HA	20:G:205:VAL:HG11	2.03	0.41
26:M:16:SER:C	26:M:18:ASP:H	2.28	0.41
27:N:60:ILE:HG23	28:O:178:MET:HE3	2.03	0.41
29:P:11:VAL:O	29:P:146:MET:HE1	2.20	0.41
29:P:133:THR:CG2	29:P:136:PHE:O	2.69	0.41
29:P:141:THR:O	29:P:142:CYS:SG	2.78	0.41
29:P:149:MET:HB3	29:P:170:ALA:HB1	2.01	0.41
30:Q:55:GLN:OE1	31:R:147:TYR:CD2	2.74	0.41
31:R:174:ASP:OD1	31:R:178:ASN:HB2	2.21	0.41
32:s:176:LEU:HD23	32:s:176:LEU:C	2.46	0.41
33:t:198:VAL:HG21	33:t:213:LEU:HD21	2.02	0.41
33:t:231:ARG:HE	33:t:247:PRO:HB2	1.85	0.41
1:U:216:VAL:O	1:U:220:LEU:HD23	2.21	0.41
1:U:628:ARG:NH2	1:U:755:THR:OG1	2.54	0.41
2:V:200:ARG:HB3	2:V:203:LEU:HB3	2.02	0.41
3:W:84:ASN:HB2	3:W:127:THR:HG21	2.02	0.41
3:W:275:ILE:HD12	3:W:309:PHE:CG	2.55	0.41
4:X:267:VAL:HG11	4:X:291:ALA:HB3	2.02	0.41
4:X:415:TYR:CE1	5:Y:383:LEU:HD12	2.54	0.41
5:Y:105:MET:O	5:Y:109:GLU:HG3	2.20	0.41
6:Z:72:HIS:HB2	6:Z:115:TYR:OH	2.20	0.41
7:a:18:GLN:HG2	7:a:44:PHE:CE1	2.55	0.41
9:c:87:VAL:HG21	13:x:278:PHE:CZ	2.55	0.41
9:c:285:GLU:HA	9:c:288:VAL:HG12	2.03	0.41
13:x:119:ILE:O	13:x:119:ILE:HG22	2.21	0.41
15:B:372:MET:O	15:B:374:LEU:HD12	2.20	0.41
16:C:72:TYR:O	16:C:115:ALA:HA	2.20	0.41
16:C:114:VAL:HG11	16:C:123:LEU:HD11	2.02	0.41
17:D:349:THR:HG23	17:D:354:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:89:LEU:HD21	19:F:126:THR:HB	2.02	0.41
19:F:391:PHE:O	19:F:395:GLN:HB2	2.20	0.41
26:M:40:ILE:HD12	26:M:194:VAL:HG22	2.03	0.41
30:Q:13:VAL:O	30:Q:15:VAL:HG13	2.21	0.41
31:R:195:TYR:CZ	30:q:170:ARG:NH1	2.88	0.41
31:R:197:VAL:HG12	30:q:145:ARG:HB2	2.02	0.41
30:q:136:ALA:O	30:q:139:THR:OG1	2.26	0.41
1:U:1:MET:HB2	10:d:132:THR:HG21	2.03	0.41
1:U:374:SER:OG	1:U:410:VAL:HB	2.20	0.41
1:U:406:ALA:O	1:U:410:VAL:HG23	2.21	0.41
2:V:236:ARG:NH2	2:V:239:THR:HG21	2.35	0.41
2:V:398:LEU:O	2:V:401:ASN:N	2.53	0.41
3:W:25:ASP:O	3:W:29:PRO:CD	2.69	0.41
3:W:394:SER:O	3:W:398:VAL:HG22	2.21	0.41
4:X:43:VAL:HA	4:X:46:LYS:HG2	2.03	0.41
4:X:96:PHE:HA	4:X:99:MET:CE	2.49	0.41
5:Y:49:ASN:HA	5:Y:73:MET:HE3	2.03	0.41
5:Y:348:ASP:OD1	5:Y:348:ASP:C	2.64	0.41
6:Z:146:ASP:O	6:Z:146:ASP:OD1	2.39	0.41
7:a:134:THR:O	7:a:138:VAL:HG12	2.20	0.41
8:b:6:THR:HG22	8:b:108:ARG:HB3	2.03	0.41
8:b:140:ILE:HG21	8:b:153:LEU:HD23	2.03	0.41
9:c:29:GLU:OE2	9:c:161:ARG:NH2	2.52	0.41
9:c:84:VAL:HG13	13:x:278:PHE:CZ	2.55	0.41
9:c:296:ILE:HG23	10:d:339:VAL:CG1	2.51	0.41
10:d:271:ILE:O	10:d:275:ILE:HG12	2.20	0.41
10:d:319:ALA:O	10:d:321:GLN:NE2	2.54	0.41
12:f:96:LEU:HD12	12:f:132:THR:OG1	2.21	0.41
12:f:150:GLU:O	12:f:151:LEU:HB2	2.20	0.41
12:f:420:TRP:CD1	12:f:420:TRP:N	2.89	0.41
12:f:528:GLY:CA	12:f:567:LEU:HD13	2.51	0.41
12:f:560:LEU:HD21	12:f:798:THR:HG22	2.02	0.41
12:f:680:ARG:HD3	12:f:681:TYR:CE1	2.55	0.41
12:f:727:PHE:HB2	12:f:761:MET:HE2	2.03	0.41
14:A:55:LEU:HB3	15:B:72:LEU:CD2	2.51	0.41
14:A:96:ALA:HB2	14:A:142:VAL:HG21	2.02	0.41
14:A:123:VAL:HG13	14:A:148:GLN:HA	2.03	0.41
14:A:220:THR:O	14:A:220:THR:CG2	2.69	0.41
14:A:244:GLU:O	14:A:245:LEU:HD12	2.21	0.41
14:A:278:ASP:O	14:A:278:ASP:OD1	2.39	0.41
15:B:52:VAL:O	15:B:52:VAL:HG23	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:141:LYS:O	15:B:142:ASP:HB2	2.21	0.41
15:B:378:VAL:HG11	15:B:419:PHE:CE2	2.56	0.41
16:C:21:ARG:HG2	16:C:25:LEU:HD12	2.01	0.41
16:C:82:LYS:O	16:C:83:LYS:HG2	2.21	0.41
17:D:201:GLY:HA2	17:D:307:VAL:O	2.20	0.41
17:D:214:MET:HE1	37:D:501:ADP:C2	2.55	0.41
17:D:254:ALA:HB1	17:D:305:VAL:CG1	2.51	0.41
17:D:305:VAL:C	17:D:306:LYS:HD3	2.46	0.41
17:D:323:ARG:NH1	17:D:327:LEU:HG	2.36	0.41
18:E:62:LYS:HB3	18:E:70:ILE:HD13	2.03	0.41
18:E:76:GLY:N	18:E:77:PRO:CD	2.83	0.41
18:E:87:LEU:HD23	18:E:88:ASP:O	2.21	0.41
19:F:93:VAL:O	19:F:94:ILE:C	2.63	0.41
19:F:222:GLY:HA3	19:F:348:LEU:HA	2.03	0.41
20:G:65:THR:HG21	26:M:160:GLY:HA3	2.03	0.41
21:H:222:THR:HB	21:H:223:PRO:HD2	2.03	0.41
22:I:119:GLN:HA	22:I:122:THR:HG22	2.03	0.41
23:J:42:VAL:CG2	23:J:210:VAL:HG12	2.50	0.41
23:J:111:ILE:HG22	23:J:115:LYS:HD2	2.02	0.41
23:J:155:ALA:H	24:K:63:SER:CB	2.31	0.41
24:K:13:ASN:OD1	24:K:13:ASN:C	2.63	0.41
24:K:46:VAL:HG12	24:K:220:VAL:HB	2.03	0.41
25:L:66:VAL:CG1	25:L:67:ASP:H	2.34	0.41
25:L:107:ARG:NH1	33:T:119:GLU:OE1	2.54	0.41
26:M:64:ASN:HB3	26:M:82:LEU:CD2	2.51	0.41
27:N:207:VAL:HG13	33:t:254:TRP:CE3	2.56	0.41
28:O:239:GLY:HA3	32:s:208:ILE:HG23	2.02	0.41
28:O:243:GLY:O	32:s:201:ARG:NH1	2.54	0.41
29:P:204:MET:HE1	31:r:255:HIS:ND1	2.36	0.41
31:R:160:ILE:O	31:R:160:ILE:HG23	2.20	0.41
33:T:98:ALA:HB2	33:T:155:MET:HG2	2.02	0.41
33:T:143:SER:O	33:T:147:LYS:HD3	2.21	0.41
27:n:196:LEU:O	27:n:200:ARG:HG2	2.21	0.41
28:o:142:VAL:HG13	28:o:168:VAL:HG21	2.03	0.41
31:r:75:ALA:N	31:r:219:ILE:HD11	2.36	0.41
32:s:150:TYR:HB3	32:s:152:PHE:HE1	1.86	0.41
33:t:66:VAL:CG1	33:t:214:VAL:HG11	2.51	0.41
2:V:113:LEU:HB2	2:V:174:PHE:CZ	2.56	0.41
2:V:201:ARG:HE	16:C:33:LEU:HD11	1.85	0.41
2:V:421:ASP:O	2:V:424:GLN:O	2.39	0.41
3:W:67:LEU:HD23	3:W:90:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:65:GLU:O	4:X:69:LEU:HD13	2.21	0.41
4:X:366:SER:O	4:X:370:LEU:HD13	2.20	0.41
5:Y:233:ARG:HB3	5:Y:234:PRO:HD3	2.02	0.41
5:Y:282:MET:CE	5:Y:295:TYR:CD2	3.04	0.41
6:Z:70:LEU:HD11	6:Z:112:MET:HE1	2.03	0.41
6:Z:206:LEU:HD21	7:a:357:CYS:SG	2.61	0.41
7:a:213:PHE:CD2	7:a:240:PHE:HB3	2.55	0.41
8:b:39:SER:CB	8:b:189:LEU:HD11	2.51	0.41
12:f:237:VAL:HG13	12:f:249:LEU:CD2	2.51	0.41
15:B:369:THR:OG1	15:B:374:LEU:HD11	2.21	0.41
17:D:246:MET:O	17:D:250:VAL:HG23	2.21	0.41
19:F:52:ILE:HG22	19:F:56:LYS:HE3	2.02	0.41
19:F:72:LYS:O	19:F:75:GLU:HG2	2.21	0.41
19:F:85:THR:O	19:F:88:TYR:CE1	2.74	0.41
23:J:92:GLN:OE1	30:Q:62:LYS:O	2.39	0.41
23:J:178:ASP:O	23:J:181:ILE:O	2.39	0.41
24:K:110:GLU:CA	24:K:154:PHE:HE2	2.33	0.41
24:K:155:HIS:O	24:K:162:PHE:HA	2.20	0.41
29:P:43:PHE:CE2	29:P:64:ALA:HB2	2.55	0.41
29:P:171:MET:CE	29:P:185:VAL:HG13	2.45	0.41
29:P:180:VAL:O	29:P:180:VAL:HG12	2.21	0.41
31:R:233:VAL:HG23	31:R:249:ASP:O	2.21	0.41
33:T:141:MET:HE2	33:T:155:MET:HE2	2.03	0.41
27:n:36:THR:HG21	27:n:197:ALA:HB1	1.97	0.41
31:r:113:PHE:O	31:r:117:LEU:HD23	2.21	0.41
32:s:92:LEU:HD11	32:s:120:LEU:CD1	2.51	0.41
32:s:204:LYS:HA	32:s:221:LEU:HD21	2.03	0.41
33:t:90:VAL:CG2	33:t:112:LEU:HD21	2.51	0.41
1:U:53:GLY:O	1:U:56:SER:OG	2.19	0.40
1:U:368:ALA:C	1:U:731:ILE:HG21	2.46	0.40
1:U:649:ARG:NH1	1:U:678:ASP:OD1	2.54	0.40
2:V:275:VAL:HG23	2:V:275:VAL:O	2.21	0.40
2:V:375:PHE:CE2	2:V:398:LEU:HD23	2.57	0.40
3:W:244:CYS:SG	3:W:274:VAL:HG22	2.61	0.40
3:W:373:ILE:O	3:W:373:ILE:HG23	2.21	0.40
7:a:172:TYR:CD2	7:a:203:ALA:HB2	2.56	0.40
10:d:291:LEU:HD13	10:d:293:PHE:CZ	2.56	0.40
12:f:118:ASN:O	12:f:119:LYS:HB3	2.20	0.40
12:f:646:MET:O	12:f:649:HIS:HB3	2.20	0.40
14:A:226:ALA:O	14:A:229:VAL:HG12	2.21	0.40
15:B:124:SER:HA	15:B:130:GLU:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:137:ILE:O	19:F:160:ILE:HB	2.21	0.40
20:G:134:LEU:HD13	20:G:136:CYS:SG	2.61	0.40
20:G:172:GLN:O	20:G:176:THR:HG23	2.20	0.40
23:J:158:ALA:N	24:K:58:LEU:HD12	2.36	0.40
26:M:174:LYS:O	26:M:175:THR:C	2.63	0.40
30:Q:185:LYS:O	30:Q:186:ASN:HB3	2.20	0.40
30:q:13:VAL:HG12	30:q:13:VAL:O	2.21	0.40
31:r:103:THR:O	31:r:158:THR:OG1	2.25	0.40
33:t:106:GLN:HA	33:t:109:LYS:HG2	2.03	0.40
33:t:245:GLU:HB3	33:t:248:LEU:HD11	2.02	0.40
2:V:166:TYR:HE1	2:V:170:LEU:HD11	1.85	0.40
4:X:154:LEU:HD12	4:X:154:LEU:C	2.46	0.40
6:Z:35:VAL:HG22	6:Z:97:THR:OG1	2.21	0.40
9:c:84:VAL:HG23	9:c:129:THR:HG22	2.03	0.40
12:f:181:ARG:O	12:f:185:LEU:N	2.48	0.40
13:x:194:VAL:HG13	13:x:246:ILE:HG23	2.04	0.40
14:A:93:LEU:HD13	14:A:153:LEU:HD13	2.03	0.40
14:A:390:THR:HA	15:B:216:ILE:HD11	2.03	0.40
15:B:112:LEU:HB2	15:B:150:VAL:HG11	2.03	0.40
15:B:177:GLU:HA	15:B:177:GLU:OE1	2.21	0.40
18:E:313:LEU:O	18:E:343:LEU:HD13	2.21	0.40
21:H:10:LEU:HG	21:H:10:LEU:O	2.22	0.40
22:I:194:ILE:HD11	22:I:213:ILE:HD11	2.03	0.40
24:K:167:ALA:HB2	24:K:185:TYR:CE2	2.55	0.40
28:O:126:LEU:HD13	28:O:156:ILE:HD12	2.02	0.40
29:P:40:GLN:HG2	29:P:43:PHE:HE1	1.86	0.40
29:P:153:LEU:HG	29:P:166:THR:HG23	2.04	0.40
32:S:40:ILE:HD13	32:S:83:SER:HB2	2.04	0.40
32:S:176:LEU:N	29:p:149:MET:HE1	2.37	0.40
33:T:51:VAL:O	33:T:51:VAL:CG2	2.68	0.40
1:U:627:PHE:CD1	1:U:627:PHE:C	2.99	0.40
3:W:112:VAL:HG21	3:W:128:LEU:HD12	2.04	0.40
3:W:181:GLU:O	3:W:185:PHE:CD2	2.75	0.40
3:W:181:GLU:OE1	3:W:185:PHE:CE2	2.75	0.40
4:X:15:LEU:HD13	4:X:22:ALA:HB3	2.02	0.40
4:X:287:LEU:HD11	4:X:319:ILE:HD11	2.04	0.40
9:c:118:PHE:O	9:c:118:PHE:CD2	2.75	0.40
9:c:293:THR:HG23	9:c:294:SER:N	2.37	0.40
9:c:299:CYS:O	9:c:303:MET:SD	2.80	0.40
12:f:345:PRO:HA	12:f:348:ILE:HD13	2.03	0.40
12:f:473:ASN:HA	12:f:478:ARG:HH12	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:533:ASP:O	12:f:537:THR:HG23	2.21	0.40
14:A:209:PRO:HD3	19:F:405:MET:HE3	2.03	0.40
17:D:223:THR:HG22	17:D:224:THR:N	2.36	0.40
18:E:67:GLU:HA	18:E:83:CYS:SG	2.61	0.40
19:F:161:LEU:O	19:F:162:GLU:C	2.62	0.40
19:F:388:THR:HB	19:F:391:PHE:HB2	2.04	0.40
22:I:48:GLU:OE1	22:I:50:ARG:HG2	2.21	0.40
25:L:16:GLN:HE21	25:L:18:ARG:HD3	1.86	0.40
29:P:24:ALA:C	29:P:171:MET:HE1	2.45	0.40
32:S:34:VAL:O	32:S:34:VAL:CG1	2.69	0.40
33:T:93:SER:O	33:T:94:THR:OG1	2.33	0.40
33:t:70:ASP:O	33:t:86:ARG:NH1	2.54	0.40
1:U:183:LEU:HD23	1:U:183:LEU:HA	1.97	0.40
1:U:680:VAL:CG2	1:U:683:VAL:HB	2.50	0.40
2:V:419:LEU:CD2	2:V:435:GLU:HG3	2.52	0.40
5:Y:220:VAL:HG11	5:Y:249:VAL:HG11	2.03	0.40
6:Z:62:ASP:OD1	6:Z:63:LYS:HD2	2.21	0.40
7:a:201:GLY:O	7:a:205:LEU:CD1	2.70	0.40
10:d:282:ILE:O	10:d:282:ILE:HG23	2.20	0.40
14:A:41:TYR:OH	15:B:58:CYS:HA	2.20	0.40
15:B:116:ILE:O	15:B:120:HIS:O	2.40	0.40
16:C:297:ARG:NH2	16:C:300:ILE:HD11	2.37	0.40
20:G:90:GLN:HE22	20:G:118:ILE:HG23	1.87	0.40
20:G:163:PHE:CE2	21:H:57:TYR:CE1	3.10	0.40
21:H:15:PRO:HA	22:I:23:TYR:CD1	2.56	0.40
25:L:12:VAL:HG23	25:L:12:VAL:O	2.22	0.40
25:L:159:MET:CG	25:L:160:SER:N	2.85	0.40
28:O:241:ARG:NH1	28:O:245:TYR:OH	2.54	0.40
32:s:137:ILE:O	32:s:137:ILE:HG23	2.21	0.40
3:W:55:ARG:HH11	3:W:55:ARG:HG2	1.85	0.40
3:W:190:MET:O	3:W:194:LEU:HD23	2.22	0.40
3:W:325:GLY:O	3:W:328:LEU:HD22	2.21	0.40
3:W:408:ARG:HH11	4:X:349:HIS:HB2	1.87	0.40
6:Z:275:LEU:C	6:Z:275:LEU:HD23	2.45	0.40
7:a:240:PHE:CE2	7:a:248:PHE:CE1	3.10	0.40
7:a:356:TRP:O	7:a:360:VAL:HG23	2.22	0.40
10:d:291:LEU:O	10:d:293:PHE:N	2.53	0.40
14:A:190:VAL:HG21	14:A:212:VAL:CG2	2.39	0.40
15:B:270:LEU:HD23	15:B:270:LEU:C	2.47	0.40
15:B:440:LEU:CD2	23:J:30:SER:H	2.33	0.40
16:C:108:VAL:HG22	16:C:126:ILE:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:376:VAL:HA	17:D:194:ILE:CD1	2.52	0.40
17:D:85:ILE:O	18:E:80:VAL:HG23	2.22	0.40
17:D:162:VAL:HG22	17:D:163:MET:N	2.36	0.40
17:D:289:LEU:HD21	17:D:318:ASP:HB2	2.04	0.40
20:G:54:LYS:NZ	20:G:63:SER:OG	2.41	0.40
20:G:60:LEU:N	20:G:60:LEU:HD12	2.36	0.40
20:G:125:TYR:CD1	20:G:131:MET:HG3	2.56	0.40
20:G:158:GLY:O	21:H:84:ARG:NH2	2.55	0.40
23:J:176:TYR:CD2	24:K:58:LEU:HD11	2.57	0.40
24:K:88:LEU:HD21	24:K:137:PHE:CD2	2.57	0.40
24:K:97:GLN:HG3	31:R:124:ILE:CD1	2.52	0.40
27:N:159:PHE:CZ	27:N:174:ASP:OD1	2.75	0.40
32:S:56:ARG:HE	32:S:219:ASP:CG	2.30	0.40
27:n:182:THR:HG22	27:n:185:GLU:HG2	2.02	0.40
31:r:71:VAL:HB	31:r:238:VAL:CG2	2.52	0.40
33:t:145:ARG:HG3	33:t:146:SER:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	849/953 (89%)	775 (91%)	74 (9%)	0	100	100
2	V	417/534 (78%)	364 (87%)	53 (13%)	0	100	100
3	W	420/456 (92%)	376 (90%)	44 (10%)	0	100	100
4	X	419/422 (99%)	388 (93%)	31 (7%)	0	100	100
5	Y	377/389 (97%)	357 (95%)	20 (5%)	0	100	100
6	Z	285/324 (88%)	271 (95%)	14 (5%)	0	100	100
7	a	373/376 (99%)	333 (89%)	40 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	b	189/377 (50%)	173 (92%)	16 (8%)	0	100	100
9	c	273/310 (88%)	243 (89%)	30 (11%)	0	100	100
10	d	252/350 (72%)	212 (84%)	40 (16%)	0	100	100
11	e	32/70 (46%)	23 (72%)	8 (25%)	1 (3%)	3	21
12	f	715/908 (79%)	611 (86%)	102 (14%)	2 (0%)	37	66
13	x	170/289 (59%)	154 (91%)	16 (9%)	0	100	100
14	A	401/433 (93%)	329 (82%)	71 (18%)	1 (0%)	44	71
15	B	384/440 (87%)	335 (87%)	49 (13%)	0	100	100
16	C	387/406 (95%)	347 (90%)	40 (10%)	0	100	100
17	D	369/418 (88%)	317 (86%)	51 (14%)	1 (0%)	37	66
18	E	280/389 (72%)	224 (80%)	55 (20%)	1 (0%)	30	61
19	F	362/439 (82%)	290 (80%)	72 (20%)	0	100	100
20	G	239/246 (97%)	213 (89%)	26 (11%)	0	100	100
21	H	231/234 (99%)	216 (94%)	15 (6%)	0	100	100
22	I	256/261 (98%)	243 (95%)	13 (5%)	0	100	100
23	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
24	K	228/241 (95%)	205 (90%)	23 (10%)	0	100	100
25	L	234/263 (89%)	200 (86%)	33 (14%)	1 (0%)	30	61
26	M	243/255 (95%)	225 (93%)	18 (7%)	0	100	100
27	N	196/239 (82%)	170 (87%)	26 (13%)	0	100	100
27	n	171/239 (72%)	162 (95%)	9 (5%)	0	100	100
28	O	219/277 (79%)	198 (90%)	21 (10%)	0	100	100
28	o	165/277 (60%)	152 (92%)	13 (8%)	0	100	100
29	P	202/205 (98%)	175 (87%)	27 (13%)	0	100	100
29	p	152/205 (74%)	127 (84%)	24 (16%)	1 (1%)	19	50
30	Q	195/201 (97%)	173 (89%)	22 (11%)	0	100	100
30	q	163/201 (81%)	149 (91%)	13 (8%)	1 (1%)	22	53
31	R	197/263 (75%)	180 (91%)	17 (9%)	0	100	100
31	r	181/263 (69%)	160 (88%)	21 (12%)	0	100	100
32	S	210/241 (87%)	195 (93%)	15 (7%)	0	100	100
32	s	202/241 (84%)	181 (90%)	21 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	T	211/264 (80%)	184 (87%)	27 (13%)	0	100	100
33	t	202/264 (76%)	178 (88%)	24 (12%)	0	100	100
All	All	11288/13411 (84%)	10031 (89%)	1248 (11%)	9 (0%)	50	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	f	211	ILE
17	D	239	TYR
11	e	43	TRP
30	q	24	ASN
18	E	273	VAL
12	f	404	ASP
25	L	67	ASP
29	p	157	ASN
14	A	102	ILE

5.3.2 Protein sidechains [i](#)

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	U	730/816 (90%)	730 (100%)	0	100	100
2	V	371/460 (81%)	371 (100%)	0	100	100
3	W	391/416 (94%)	391 (100%)	0	100	100
4	X	361/362 (100%)	361 (100%)	0	100	100
5	Y	335/344 (97%)	335 (100%)	0	100	100
6	Z	258/295 (88%)	258 (100%)	0	100	100
7	a	335/336 (100%)	335 (100%)	0	100	100
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	244/268 (91%)	244 (100%)	0	100	100
10	d	227/294 (77%)	226 (100%)	1 (0%)	89	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	e	34/63 (54%)	34 (100%)	0	100	100
12	f	611/763 (80%)	611 (100%)	0	100	100
13	x	156/253 (62%)	156 (100%)	0	100	100
14	A	348/372 (94%)	348 (100%)	0	100	100
15	B	344/385 (89%)	344 (100%)	0	100	100
16	C	340/352 (97%)	340 (100%)	0	100	100
17	D	327/366 (89%)	327 (100%)	0	100	100
18	E	261/341 (76%)	261 (100%)	0	100	100
19	F	315/379 (83%)	315 (100%)	0	100	100
20	G	206/210 (98%)	206 (100%)	0	100	100
21	H	190/191 (100%)	189 (100%)	1 (0%)	86	91
22	I	218/221 (99%)	218 (100%)	0	100	100
23	J	203/211 (96%)	203 (100%)	0	100	100
24	K	195/203 (96%)	194 (100%)	1 (0%)	86	91
25	L	202/224 (90%)	202 (100%)	0	100	100
26	M	202/212 (95%)	202 (100%)	0	100	100
27	N	154/181 (85%)	154 (100%)	0	100	100
27	n	138/181 (76%)	138 (100%)	0	100	100
28	O	182/228 (80%)	182 (100%)	0	100	100
28	o	138/228 (60%)	138 (100%)	0	100	100
29	P	173/174 (99%)	173 (100%)	0	100	100
29	p	136/174 (78%)	136 (100%)	0	100	100
30	Q	168/171 (98%)	168 (100%)	0	100	100
30	q	148/171 (86%)	148 (100%)	0	100	100
31	R	155/202 (77%)	155 (100%)	0	100	100
31	r	142/202 (70%)	142 (100%)	0	100	100
32	S	177/199 (89%)	177 (100%)	0	100	100
32	s	172/199 (86%)	172 (100%)	0	100	100
33	T	176/215 (82%)	176 (100%)	0	100	100
33	t	171/215 (80%)	171 (100%)	0	100	100
All	All	9801/11389 (86%)	9798 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	d	153	GLN
21	H	102	GLN
24	K	214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	247	GLN
1	U	345	ASN
1	U	880	ASN
2	V	252	ASN
2	V	311	ASN
2	V	319	HIS
2	V	347	GLN
3	W	236	HIS
4	X	198	ASN
5	Y	251	HIS
5	Y	365	GLN
6	Z	12	HIS
6	Z	224	HIS
6	Z	235	ASN
7	a	18	GLN
7	a	40	GLN
7	a	46	GLN
7	a	241	ASN
8	b	99	HIS
9	c	295	ASN
10	d	189	HIS
12	f	156	HIS
12	f	291	GLN
12	f	327	ASN
12	f	396	ASN
12	f	770	HIS
13	x	239	GLN
14	A	60	ASN
15	B	315	GLN
16	C	22	GLN
16	C	90	HIS
16	C	106	ASN
16	C	182	GLN
17	D	74	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	99	ASN
17	D	193	GLN
19	F	83	ASN
19	F	428	GLN
20	G	68	HIS
20	G	90	GLN
22	I	30	HIS
22	I	40	ASN
22	I	146	GLN
22	I	198	ASN
23	J	15	HIS
23	J	120	GLN
24	K	155	HIS
24	K	221	GLN
24	K	224	GLN
25	L	16	GLN
25	L	203	GLN
29	P	65	GLN
30	Q	63	ASN
30	Q	132	HIS
30	Q	186	ASN
32	S	36	ASN
32	S	187	GLN
32	S	188	ASN
33	T	126	HIS
27	n	41	GLN
29	p	33	GLN
30	q	87	ASN
31	r	221	GLN
32	s	64	HIS
32	s	191	HIS
33	t	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
35	ATP	B	501	36	28,33,33	0.71	0	34,52,52	1.20	5 (14%)
35	ATP	C	501	36	28,33,33	0.86	1 (3%)	34,52,52	0.94	2 (5%)
35	ATP	A	501	36	28,33,33	1.04	2 (7%)	34,52,52	0.95	3 (8%)
37	ADP	E	401	36	24,29,29	0.88	0	29,45,45	1.26	2 (6%)
37	ADP	D	501	36	24,29,29	0.82	0	29,45,45	1.30	2 (6%)
37	ADP	F	501	-	24,29,29	0.80	1 (4%)	29,45,45	0.94	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	B	501	36	-	4/18/38/38	0/3/3/3
35	ATP	C	501	36	-	5/18/38/38	0/3/3/3
35	ATP	A	501	36	-	6/18/38/38	0/3/3/3
37	ADP	E	401	36	-	3/12/32/32	0/3/3/3
37	ADP	D	501	36	-	2/12/32/32	0/3/3/3
37	ADP	F	501	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	ATP	PA-O3A	-2.96	1.56	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	ATP	PB-O3B	-2.79	1.56	1.59
35	C	501	ATP	PA-O3A	-2.10	1.57	1.59
37	F	501	ADP	C8-N7	-2.02	1.31	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	501	ADP	N3-C2-N1	-4.44	122.65	128.67
37	E	401	ADP	N3-C2-N1	-4.18	123.00	128.67
35	B	501	ATP	C4'-O4'-C1'	-3.85	106.40	109.92
37	E	401	ADP	C4-C5-N7	-2.58	106.61	109.34
35	B	501	ATP	O4'-C1'-N9	-2.37	105.60	108.75
37	F	501	ADP	C4'-O4'-C1'	-2.34	107.79	109.92
35	A	501	ATP	C5-C6-N6	2.33	123.86	120.31
35	C	501	ATP	C5-C6-N6	2.32	123.84	120.31
35	B	501	ATP	C5-C6-N6	2.25	123.73	120.31
37	D	501	ADP	C4-C5-N7	-2.19	107.03	109.34
37	F	501	ADP	C5-C6-N6	2.13	123.56	120.31
35	B	501	ATP	O2'-C2'-C3'	-2.11	105.06	111.82
35	B	501	ATP	O3'-C3'-C2'	-2.09	105.10	111.82
35	C	501	ATP	O3'-C3'-C2'	-2.07	105.17	111.82
35	A	501	ATP	O3'-C3'-C2'	-2.06	105.21	111.82
35	A	501	ATP	O2'-C2'-C3'	-2.02	105.35	111.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3B-PG-O2G
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O1A
37	D	501	ADP	PA-O3A-PB-O2B
37	E	401	ADP	O4'-C4'-C5'-O5'
37	E	401	ADP	PB-O3A-PA-O1A
35	C	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	PB-O3B-PG-O1G
35	C	501	ATP	C3'-C4'-C5'-O5'
37	D	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	C5'-O5'-PA-O1A
35	B	501	ATP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

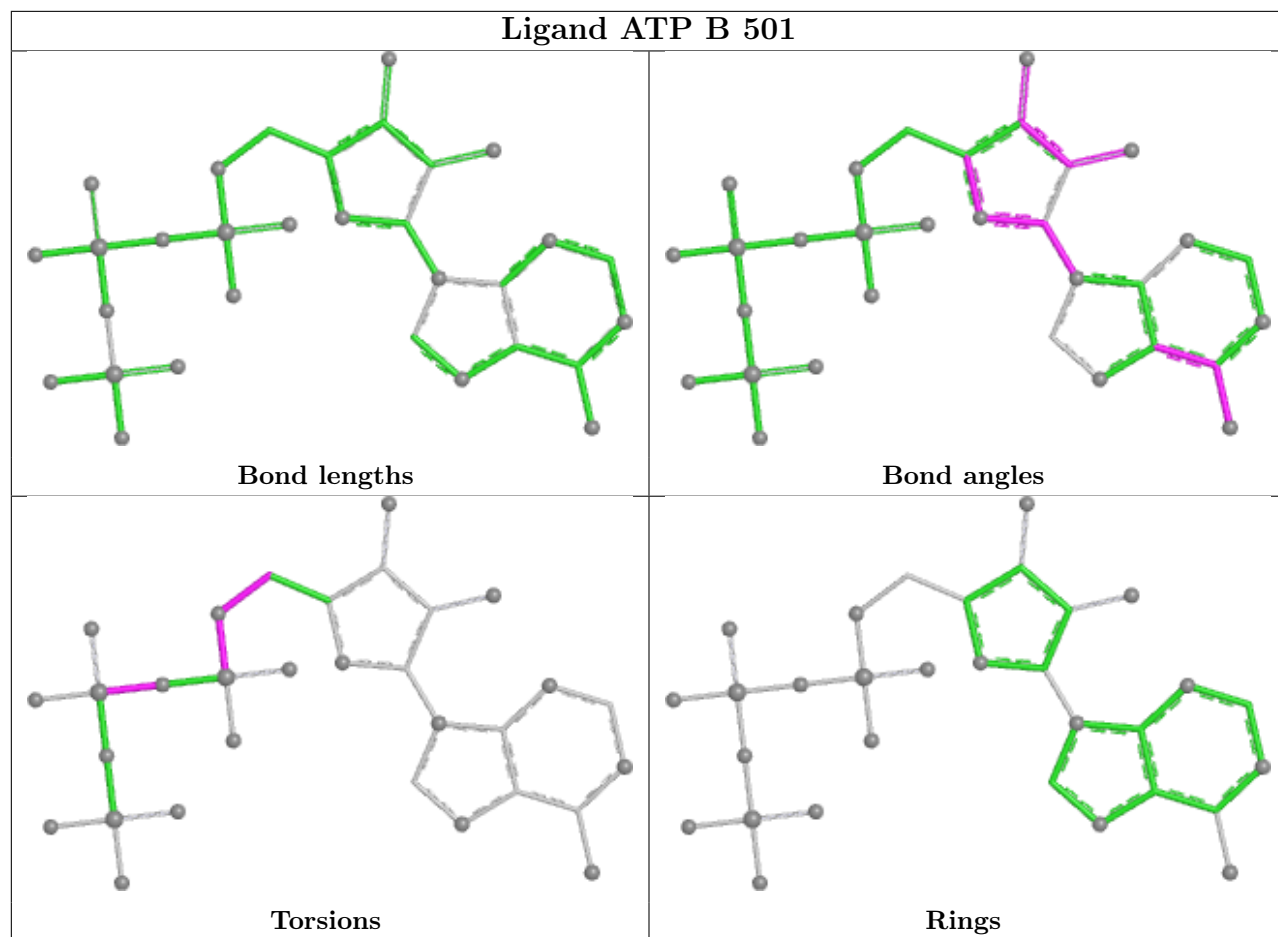
Mol	Chain	Res	Type	Atoms
35	B	501	ATP	PA-O3A-PB-O2B
35	C	501	ATP	PG-O3B-PB-O2B
37	E	401	ADP	PB-O3A-PA-O2A
37	F	501	ADP	C4'-C5'-O5'-PA
35	B	501	ATP	PA-O3A-PB-O1B
35	A	501	ATP	PA-O3A-PB-O1B
35	A	501	ATP	PA-O3A-PB-O2B
35	C	501	ATP	PA-O3A-PB-O2B

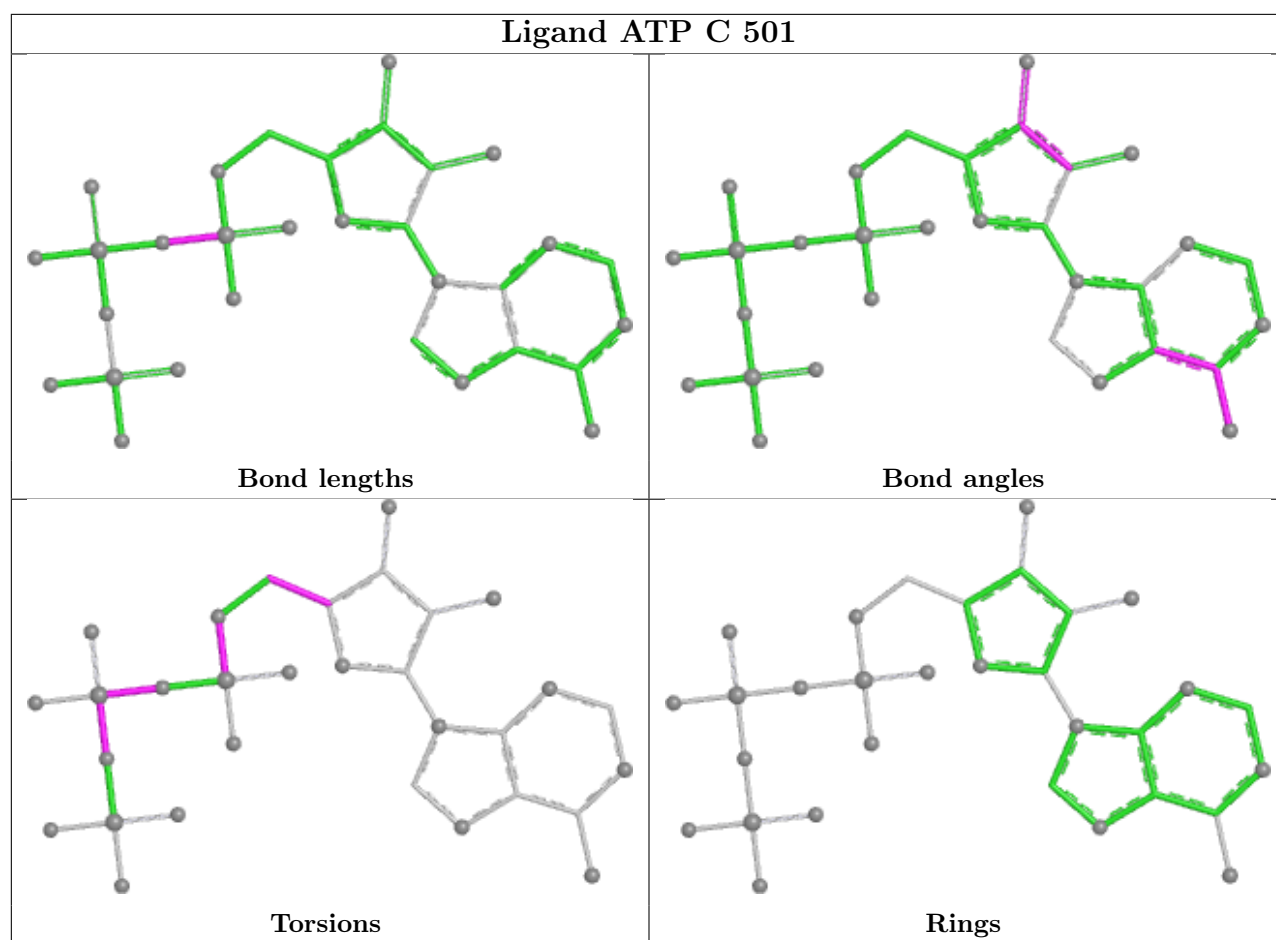
There are no ring outliers.

6 monomers are involved in 17 short contacts:

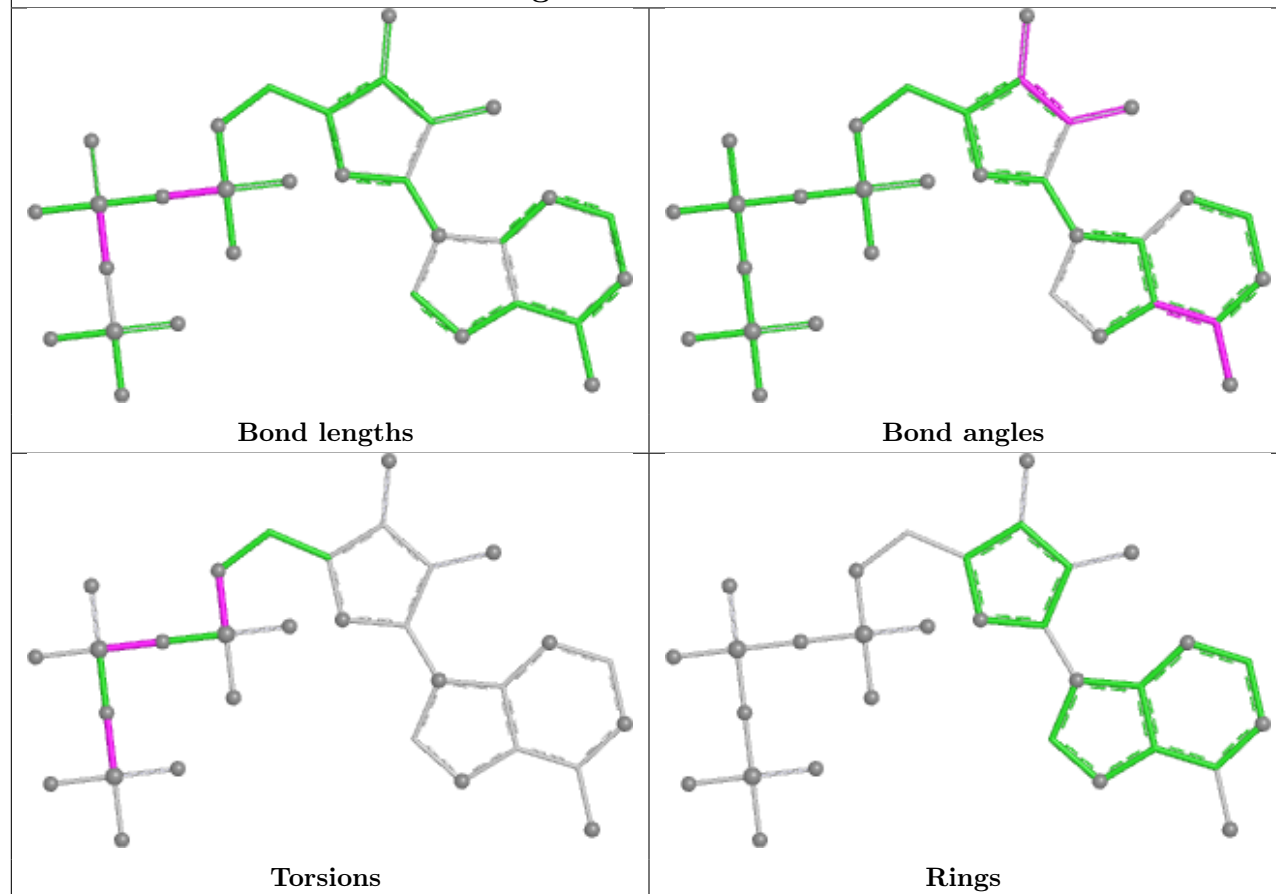
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	1	0
35	C	501	ATP	3	0
35	A	501	ATP	3	0
37	E	401	ADP	2	0
37	D	501	ADP	6	0
37	F	501	ADP	2	0

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.

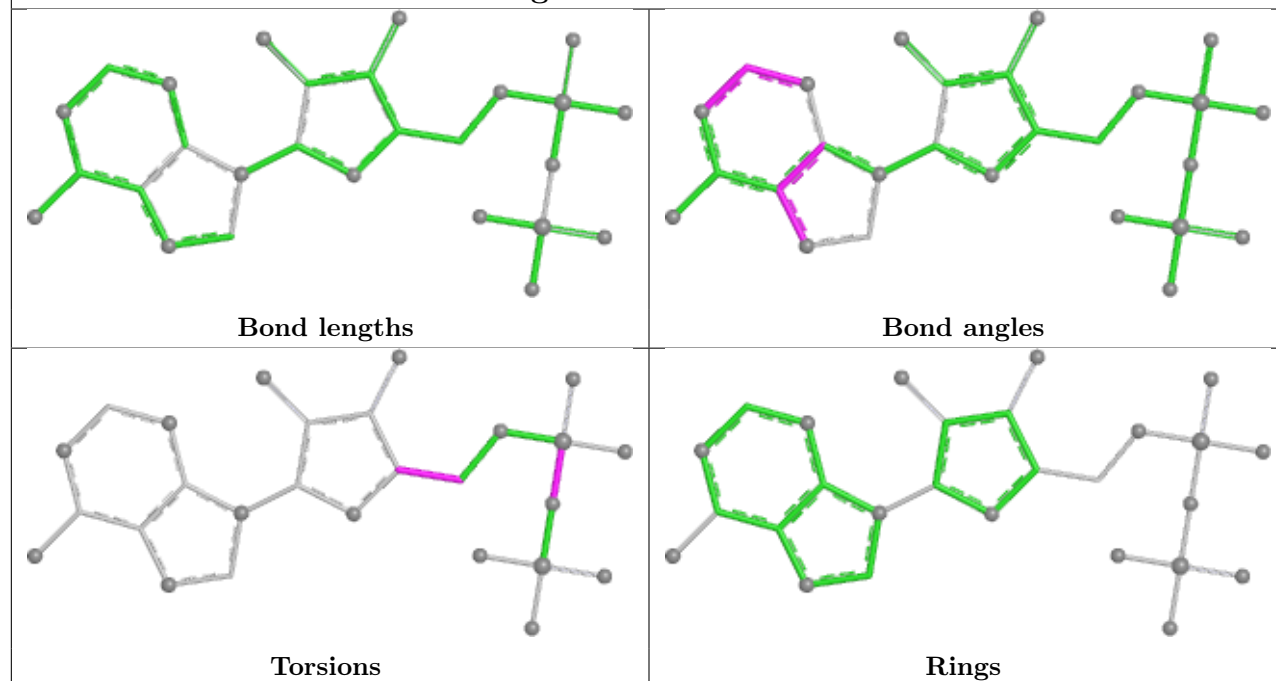


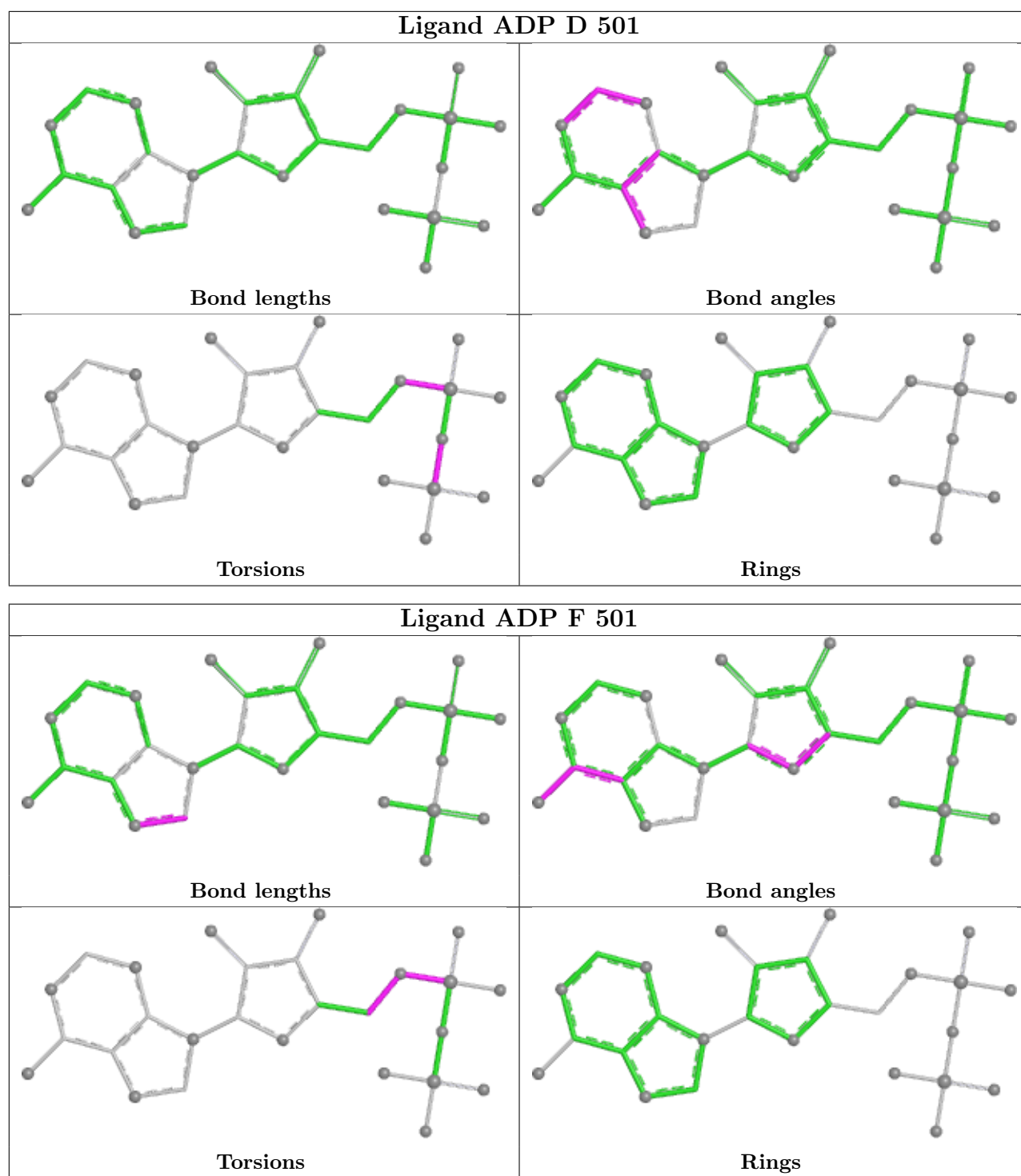


Ligand ATP A 501



Ligand ADP E 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

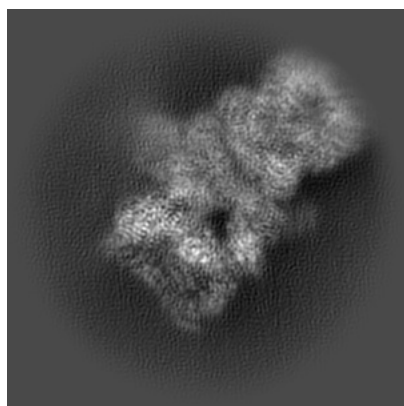
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44952. These allow visual inspection of the internal detail of the map and identification of artifacts.

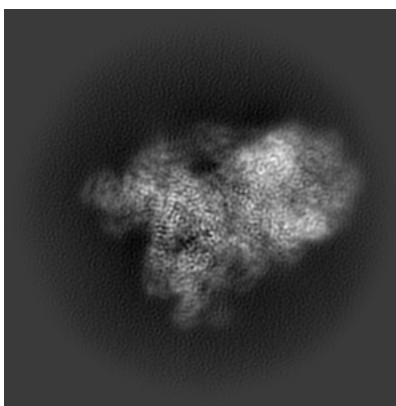
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

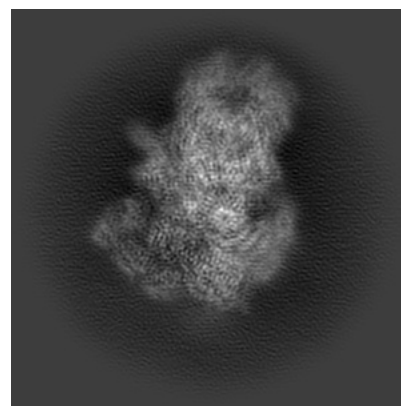
6.1.1 Primary map



X

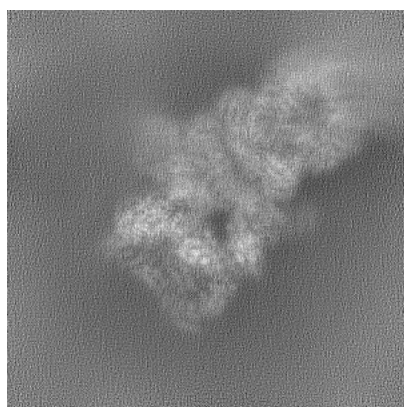


Y

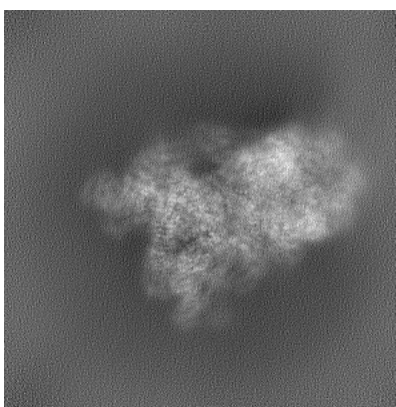


Z

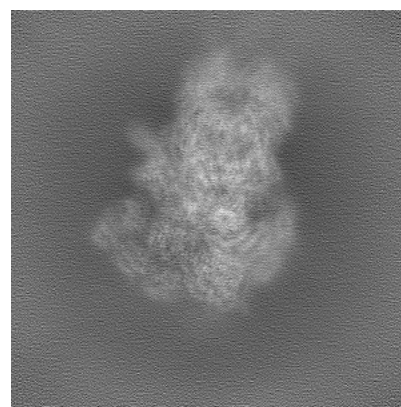
6.1.2 Raw map



X



Y

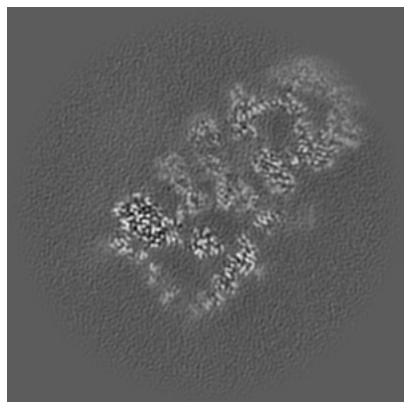


Z

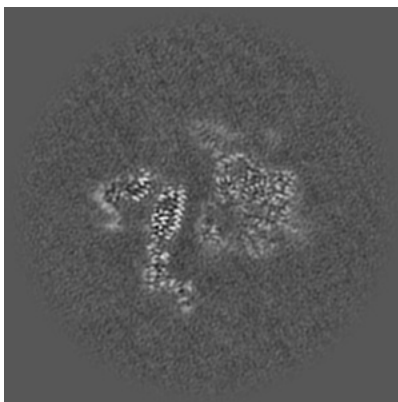
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

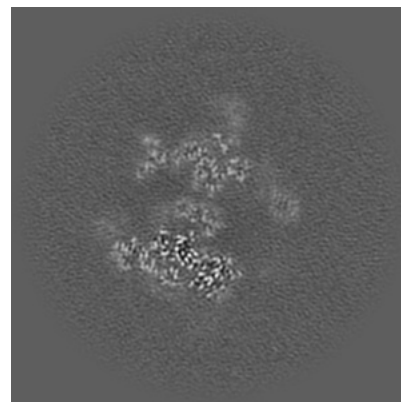
6.2.1 Primary map



X Index: 220

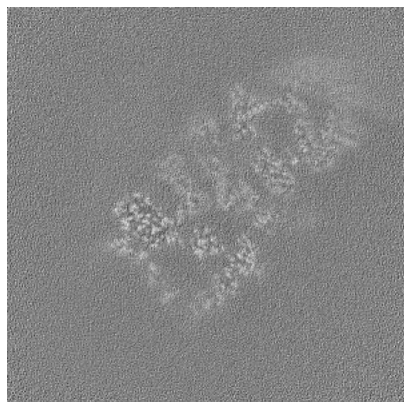


Y Index: 220

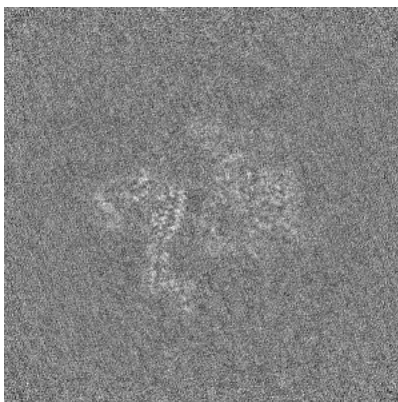


Z Index: 220

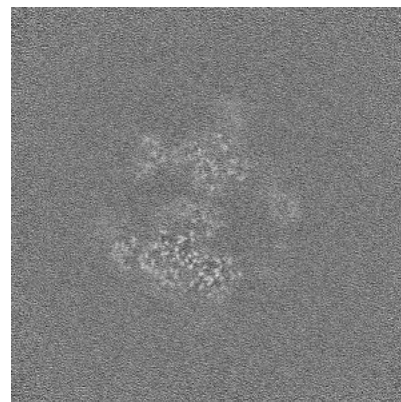
6.2.2 Raw map



X Index: 220



Y Index: 220

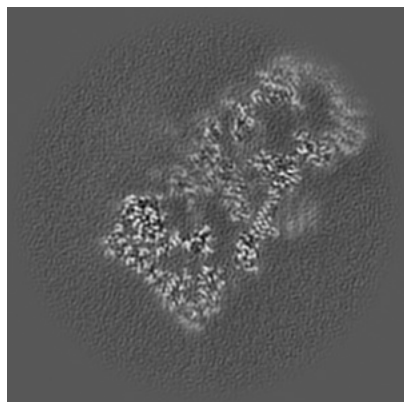


Z Index: 220

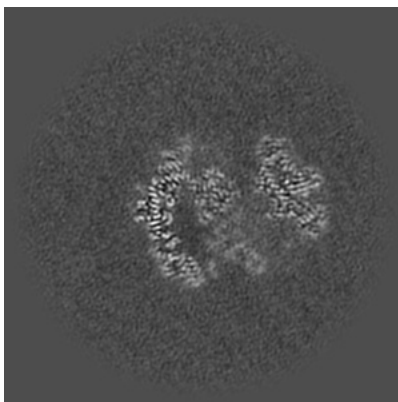
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

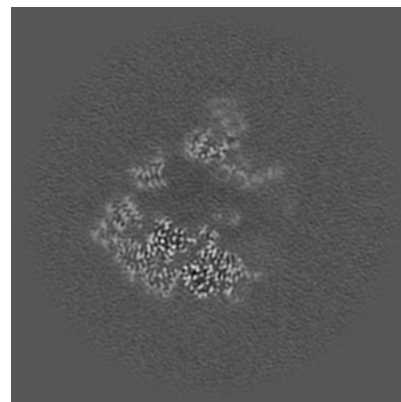
6.3.1 Primary map



X Index: 232

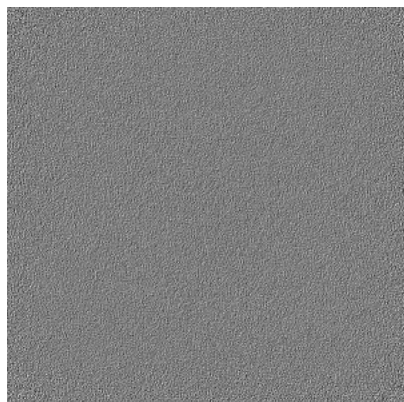


Y Index: 256

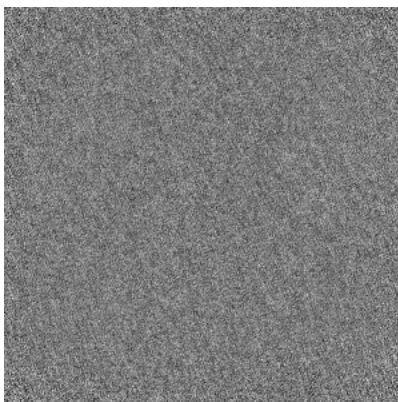


Z Index: 203

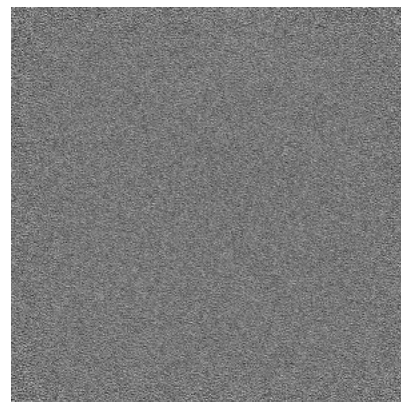
6.3.2 Raw map



X Index: 0



Y Index: 0

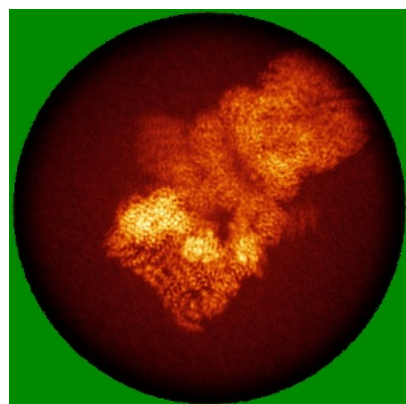


Z Index: 0

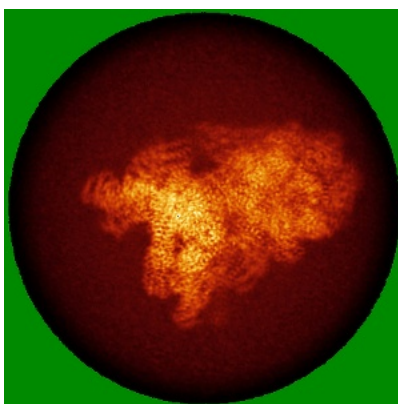
The images above show the largest variance slices of the map in three orthogonal directions.

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

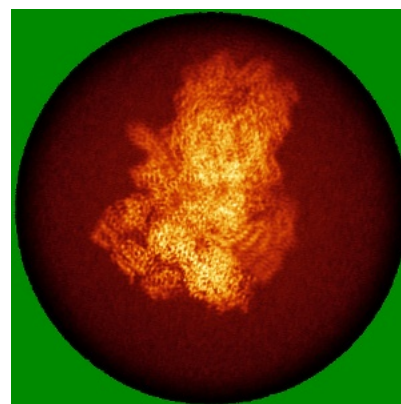
6.4.1 Primary map



X

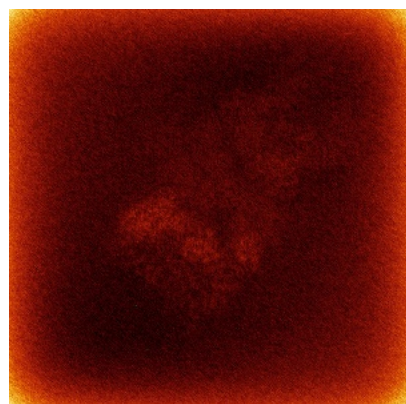


Y

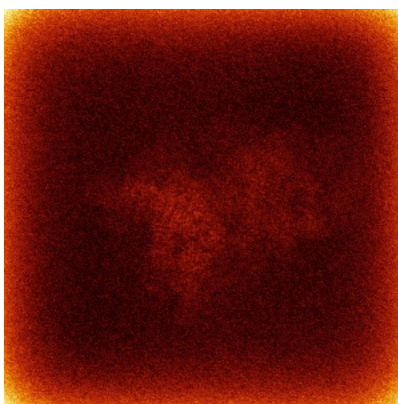


Z

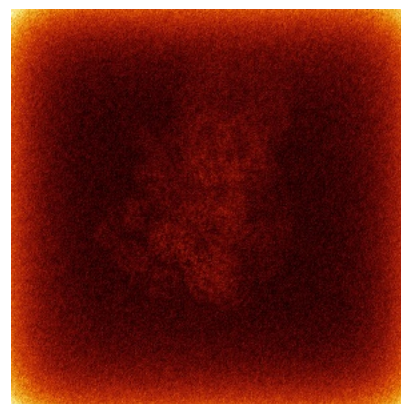
6.4.2 Raw map



X



Y

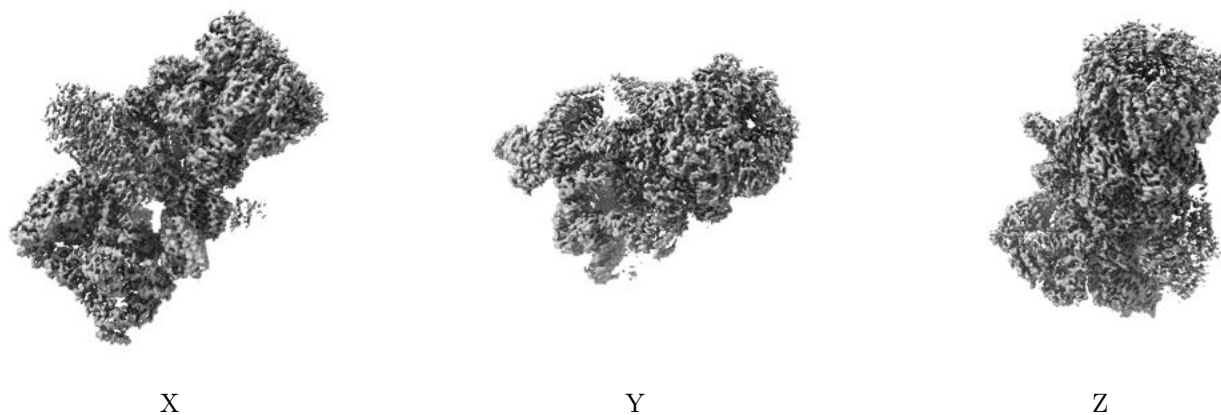


Z

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

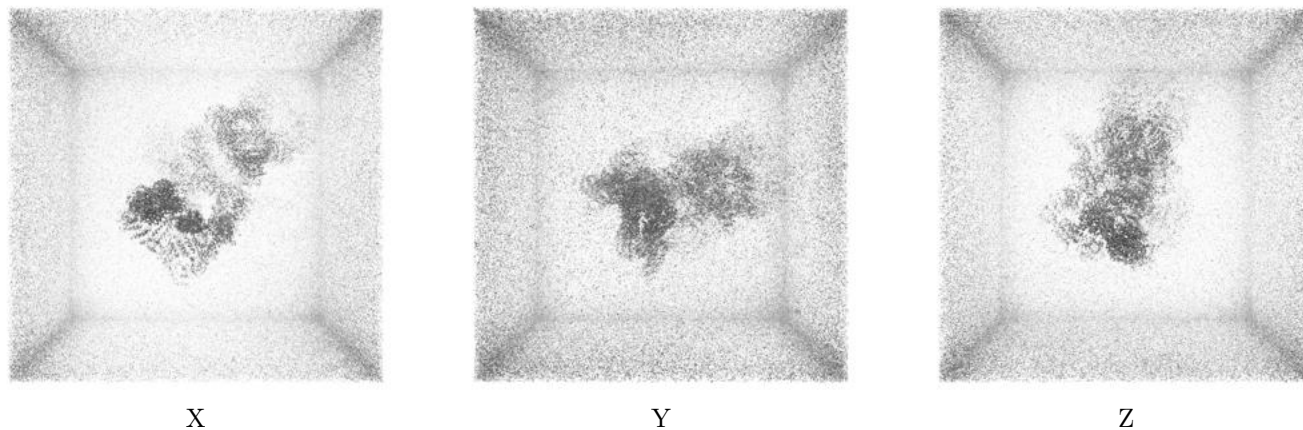
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

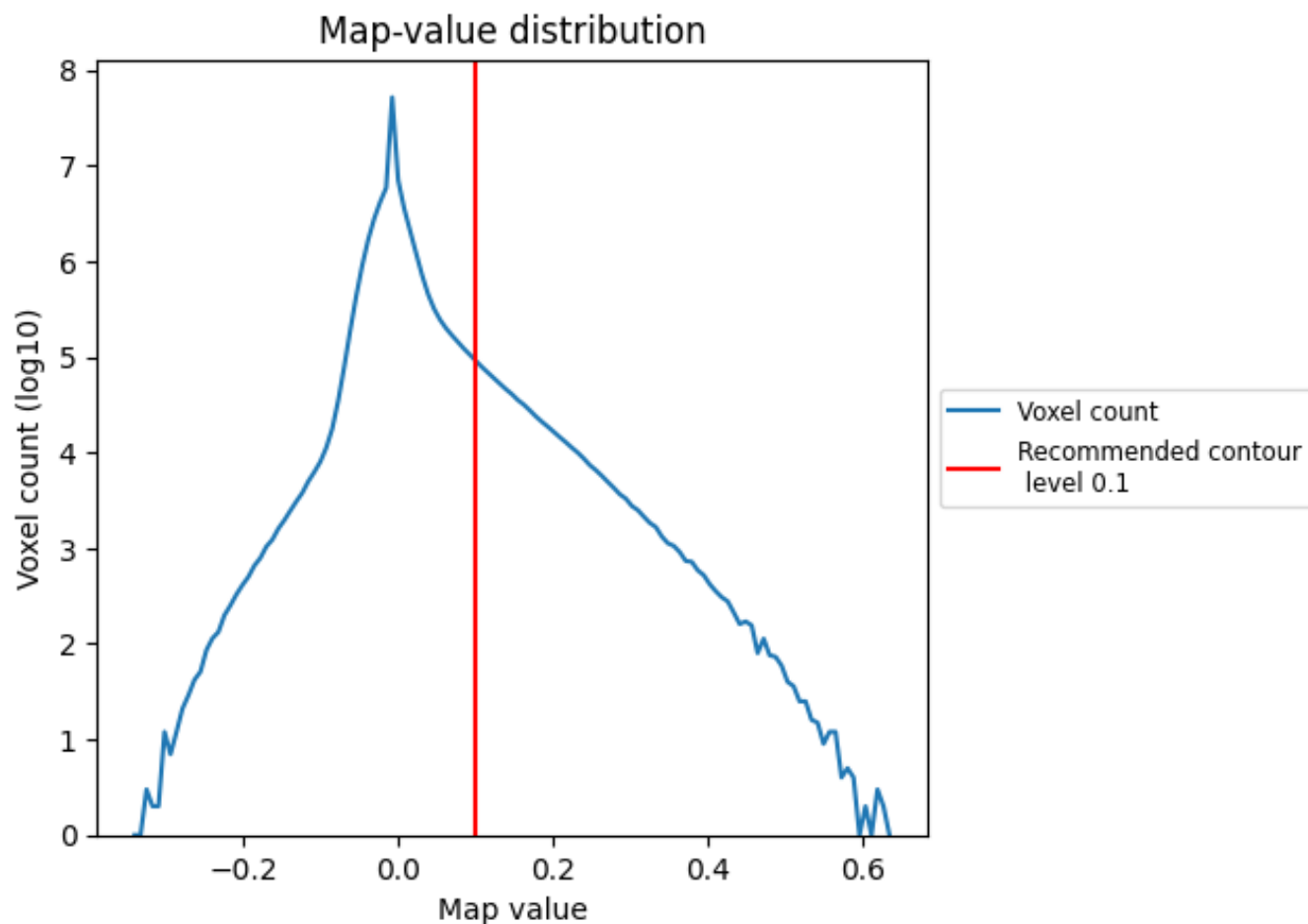
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

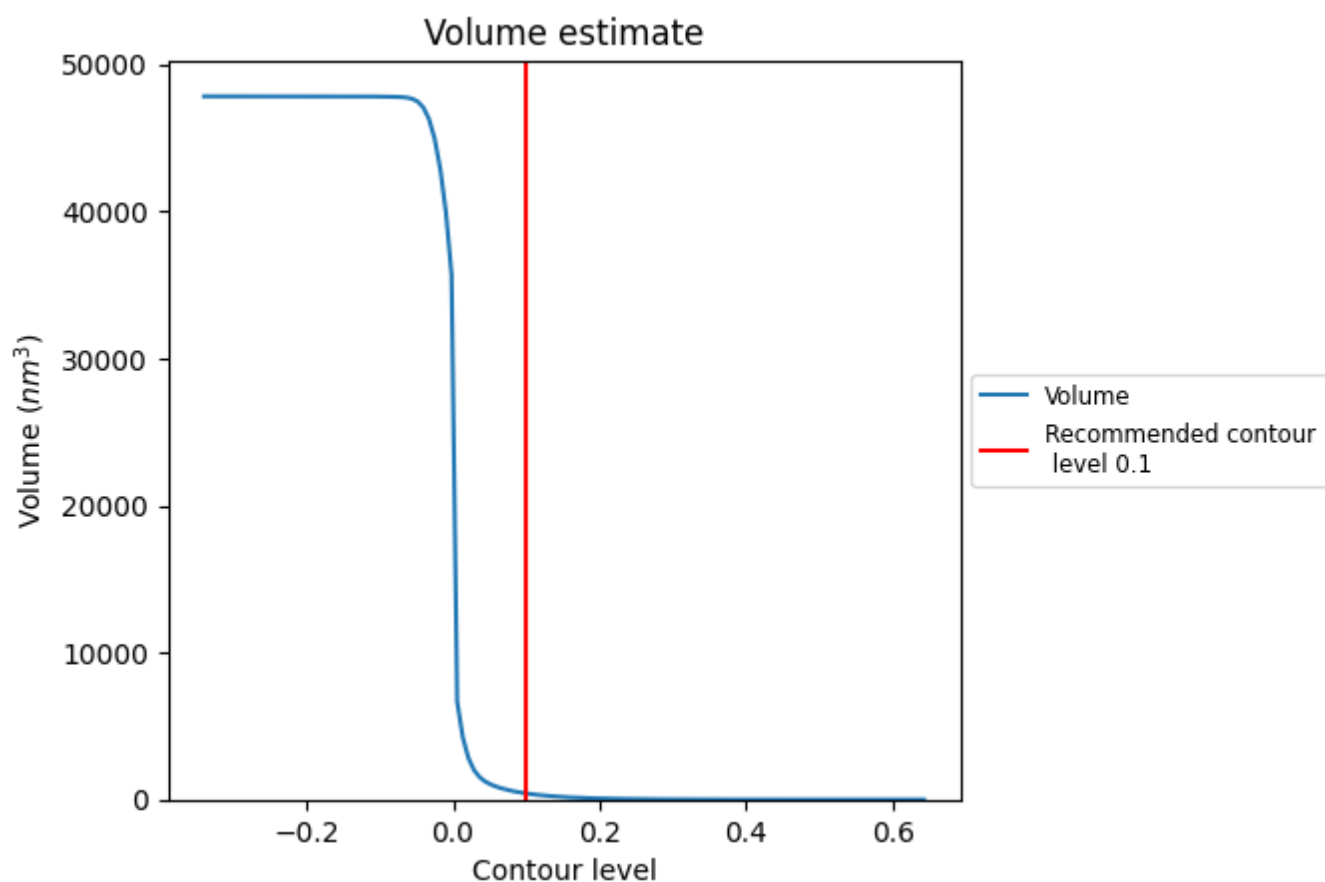
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

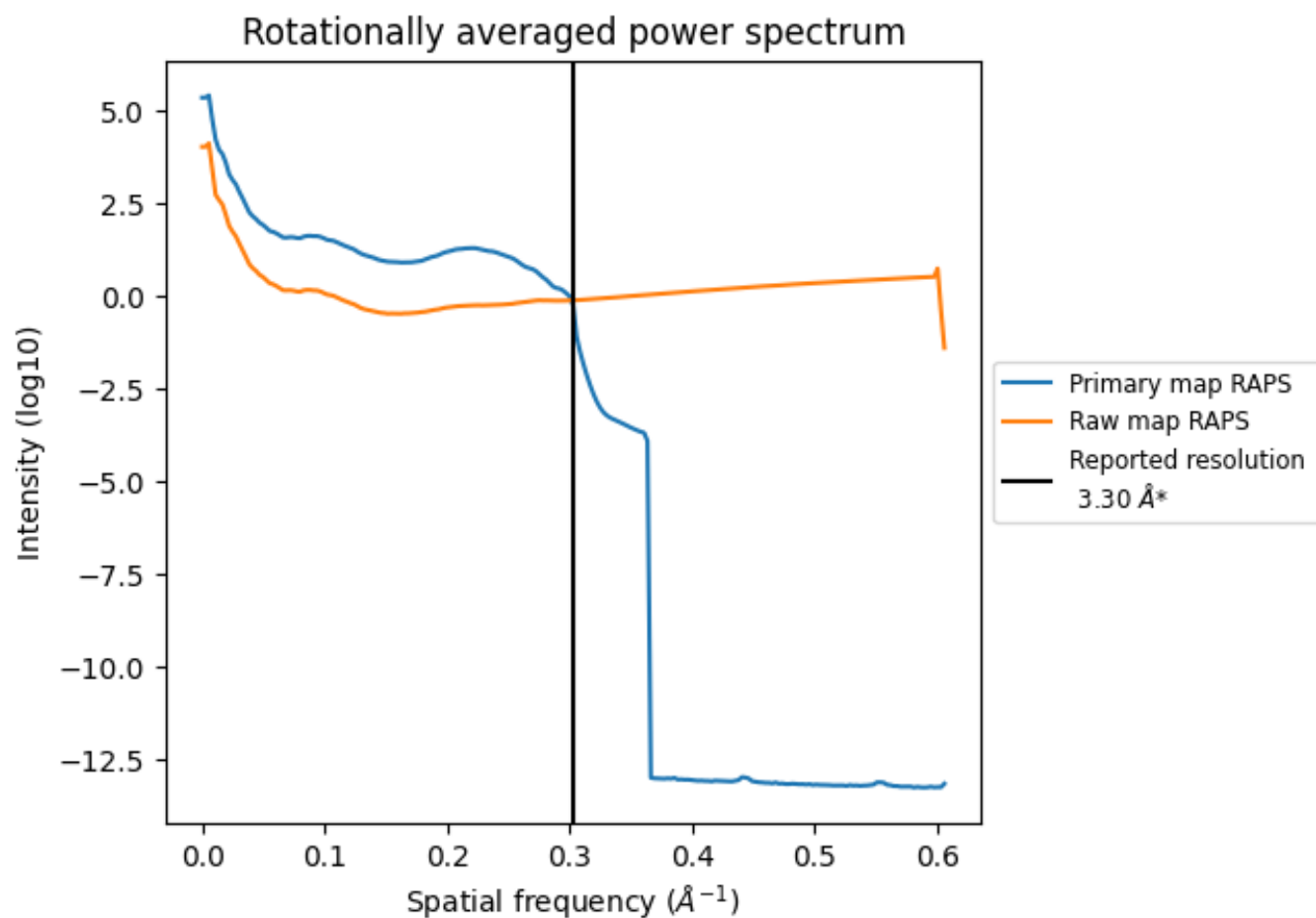
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 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 ⓘ

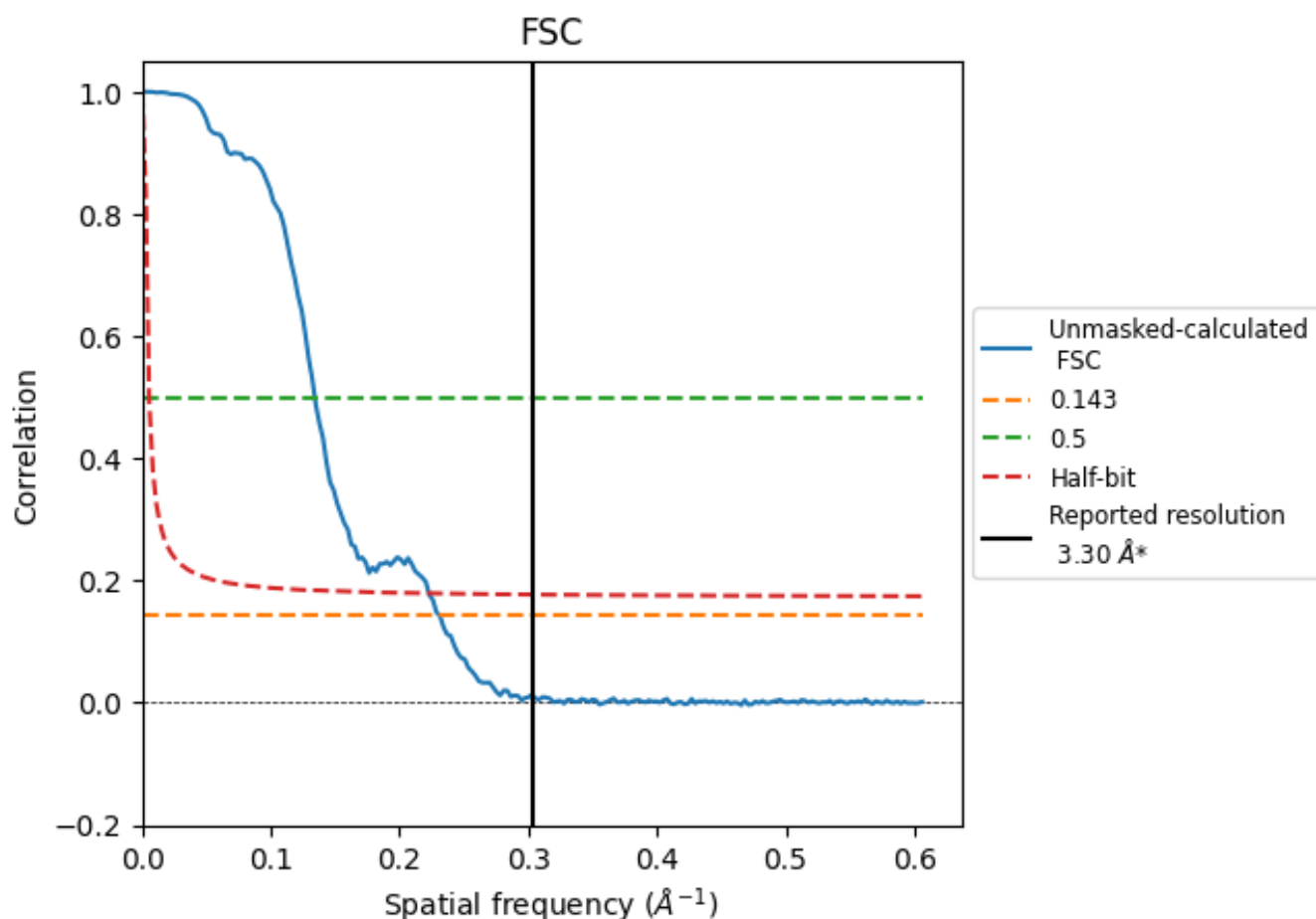


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

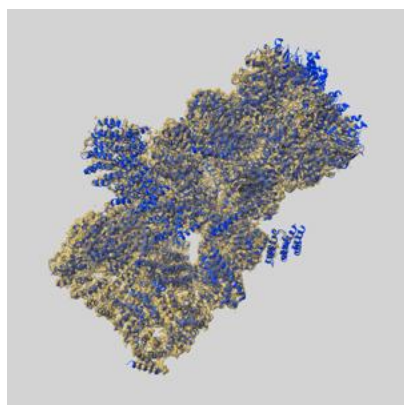
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	7.46	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.3 by more than 10 %

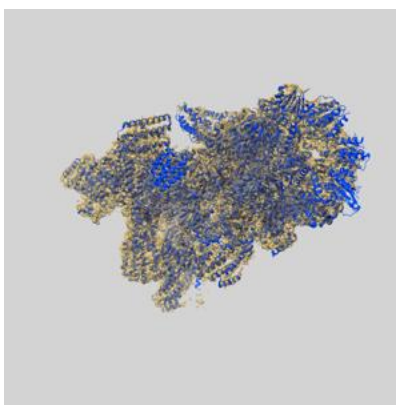
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44952 and PDB model 9BW4. Per-residue inclusion information can be found in section [3](#) on page [12](#).

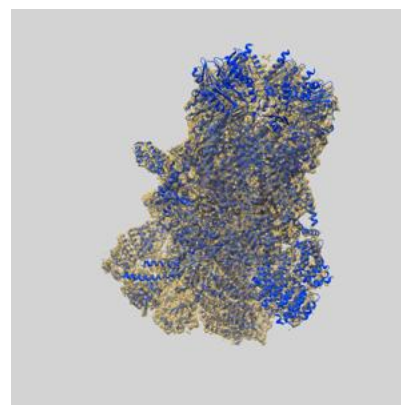
9.1 Map-model overlay [i](#)



X



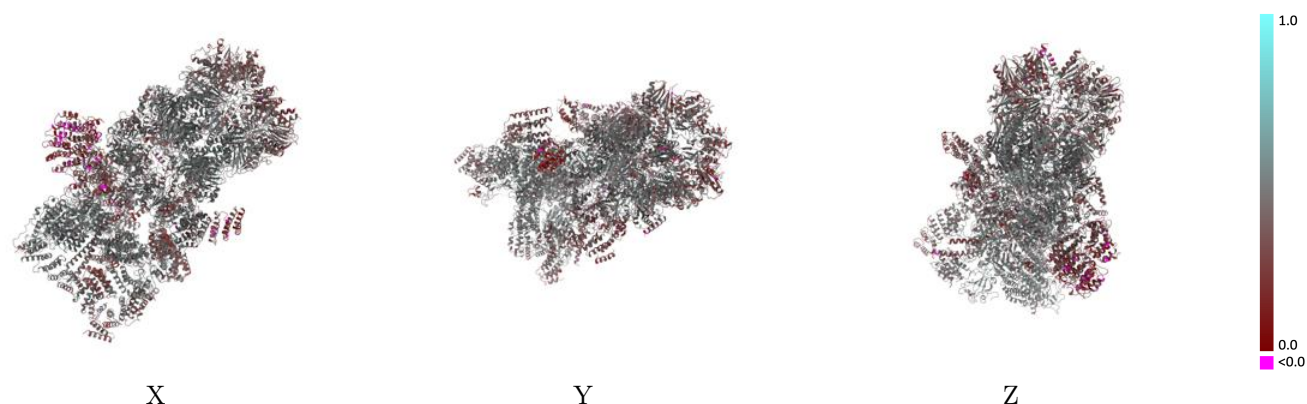
Y



Z

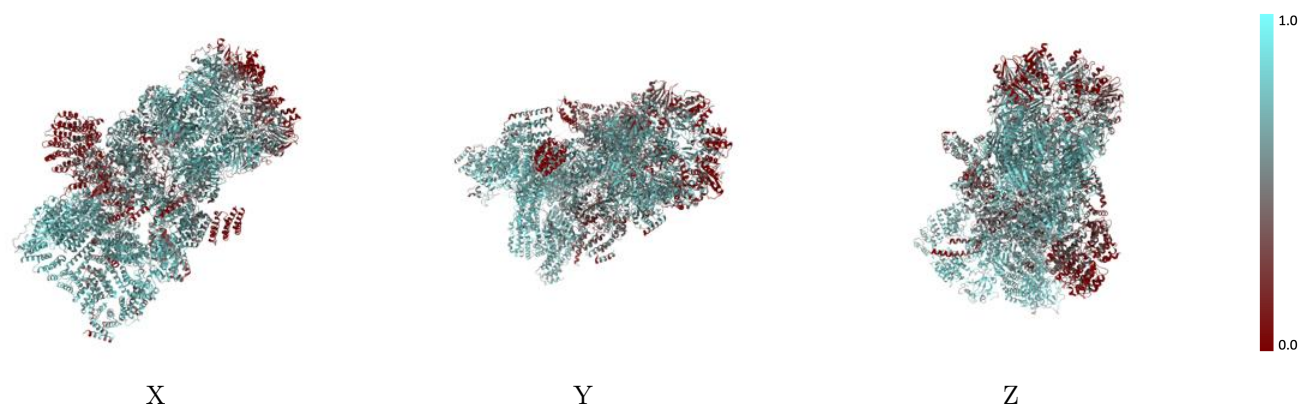
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



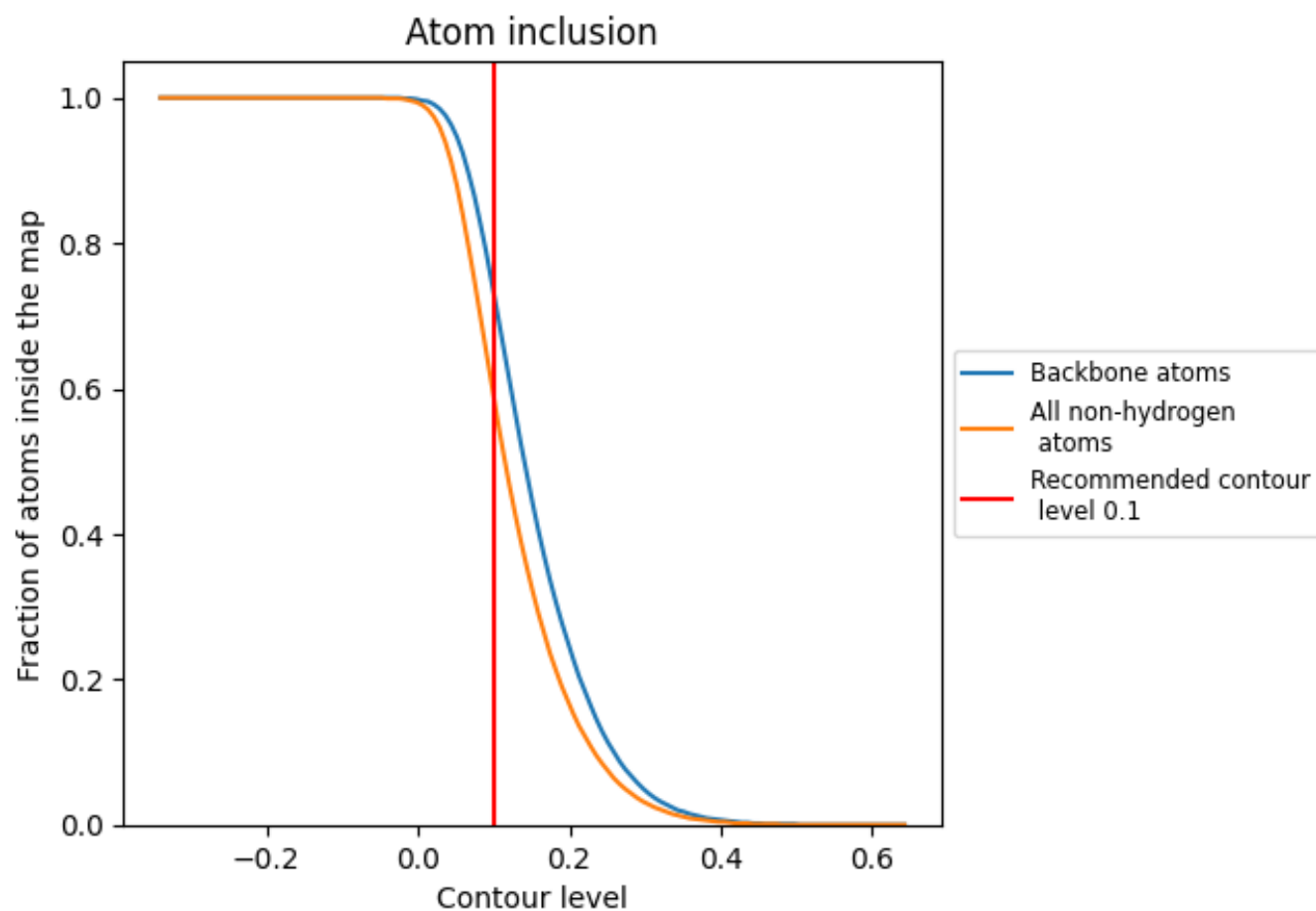
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.4290
A	 0.5130	 0.4200
B	 0.5430	 0.4470
C	 0.6400	 0.4670
D	 0.6060	 0.4520
E	 0.4040	 0.3570
F	 0.4630	 0.4150
G	 0.6670	 0.4630
H	 0.7210	 0.5060
I	 0.6300	 0.4600
J	 0.6450	 0.4600
K	 0.6790	 0.4660
L	 0.7270	 0.4890
M	 0.6620	 0.4510
N	 0.6380	 0.4560
O	 0.6570	 0.4670
P	 0.6940	 0.4850
Q	 0.6460	 0.4490
R	 0.7010	 0.4520
S	 0.6720	 0.4510
T	 0.6810	 0.4590
U	 0.7520	 0.4760
V	 0.6870	 0.4250
W	 0.6170	 0.4120
X	 0.5200	 0.3950
Y	 0.7030	 0.4430
Z	 0.7690	 0.5030
a	 0.7140	 0.4270
b	 0.7540	 0.4510
c	 0.7740	 0.4980
d	 0.6320	 0.3910
e	 0.6810	 0.4530
f	 0.2170	 0.2630
n	 0.3040	 0.3700
o	 0.2210	 0.3400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	 0.2800	 0.3700
q	 0.3150	 0.3850
r	 0.3980	 0.3970
s	 0.4530	 0.4100
t	 0.4620	 0.3980
x	 0.7180	 0.4650