



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:38 PM UTC

PDB ID : 7QXN / pdb_00007qxn
EMDB ID : EMD-14201
Title : Proteasome-ZFAND5 Complex Z+A state
Authors : Zhu, Y.; Lu, Y.
Deposited on : 2022-01-26
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

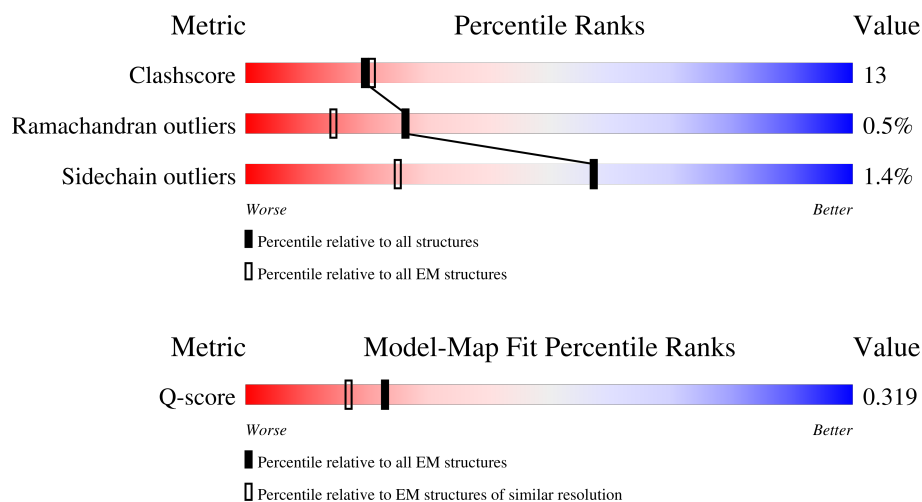
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



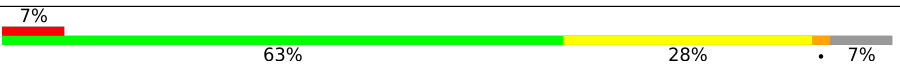
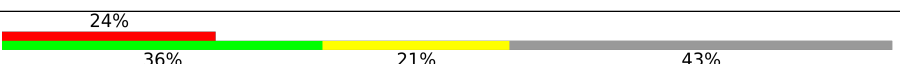
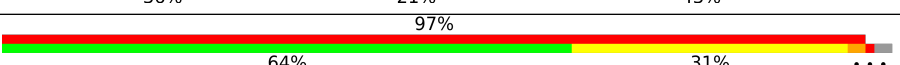
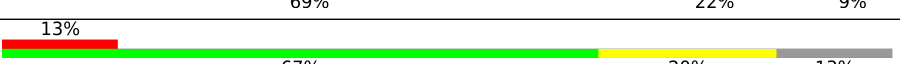
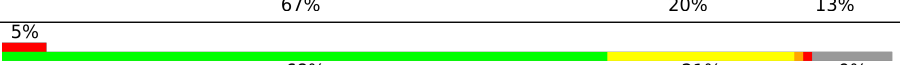
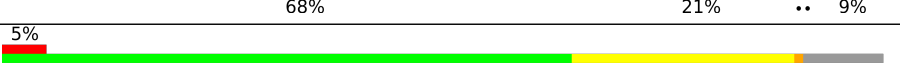
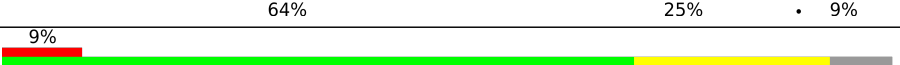
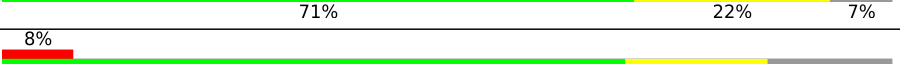
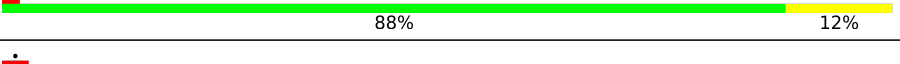
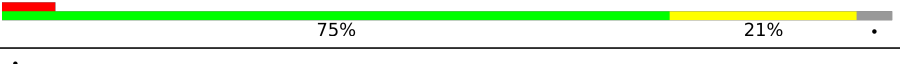
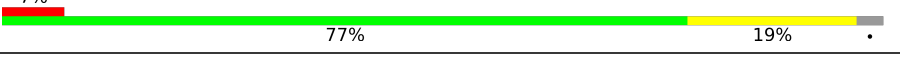
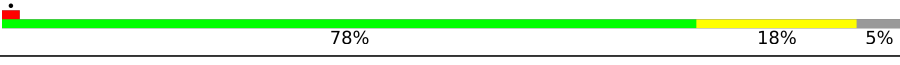
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	23% 59% 26% • 15%
2	V	533	35% 62% 31% • 5%
3	W	456	21% 66% 30% •
4	X	422	37% 73% 17% 10%

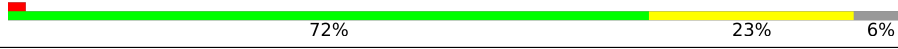
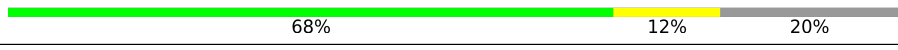
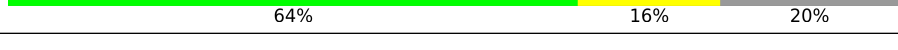
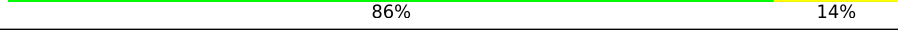
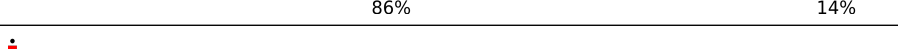
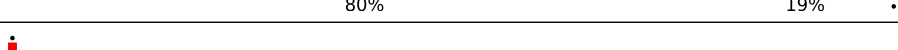
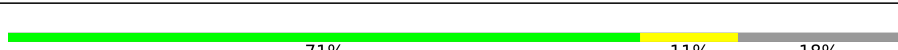
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103713 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	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	508	Total	C	N	O	S	0	0
			3994	2530	712	738	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3693	2332	635	701	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	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
			1458	910	261	279	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6857	4306	1174	1331	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
22	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

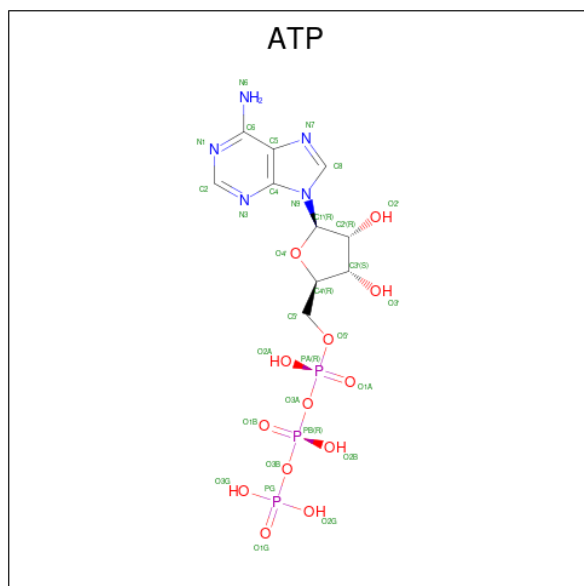
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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

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

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

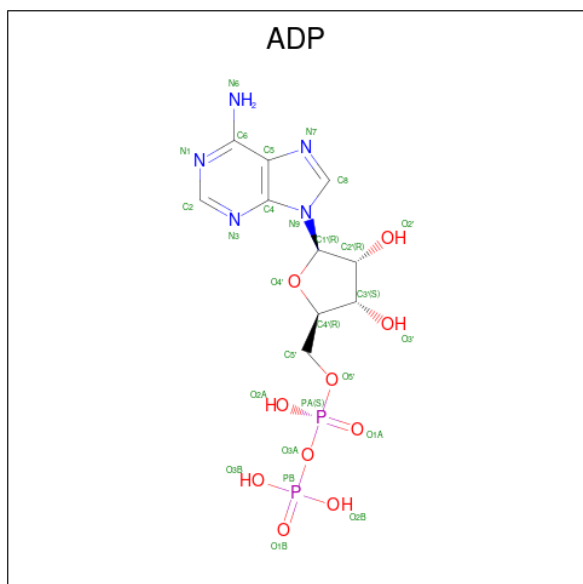
Continued from previous page...

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

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

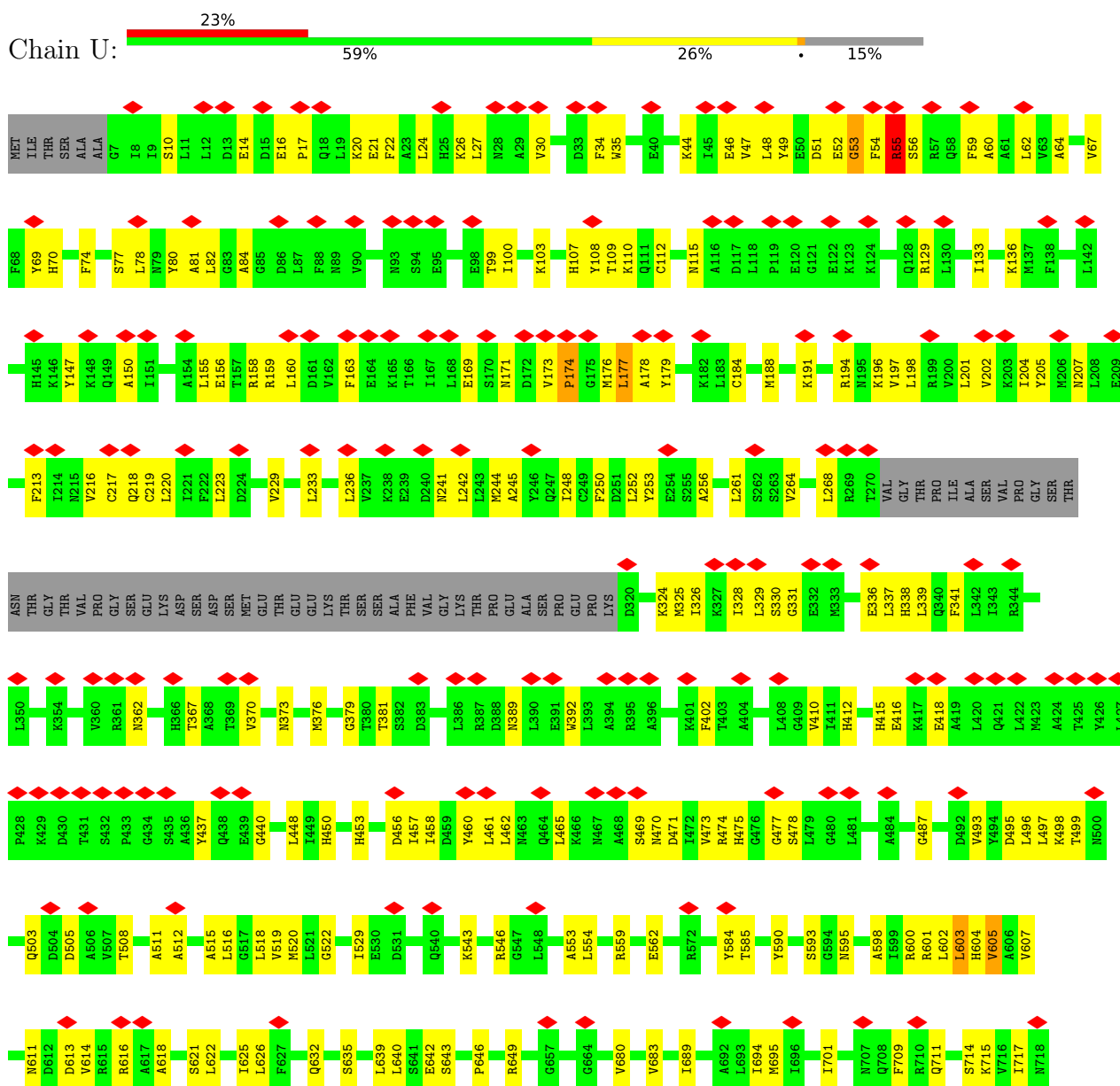
Continued from previous page...

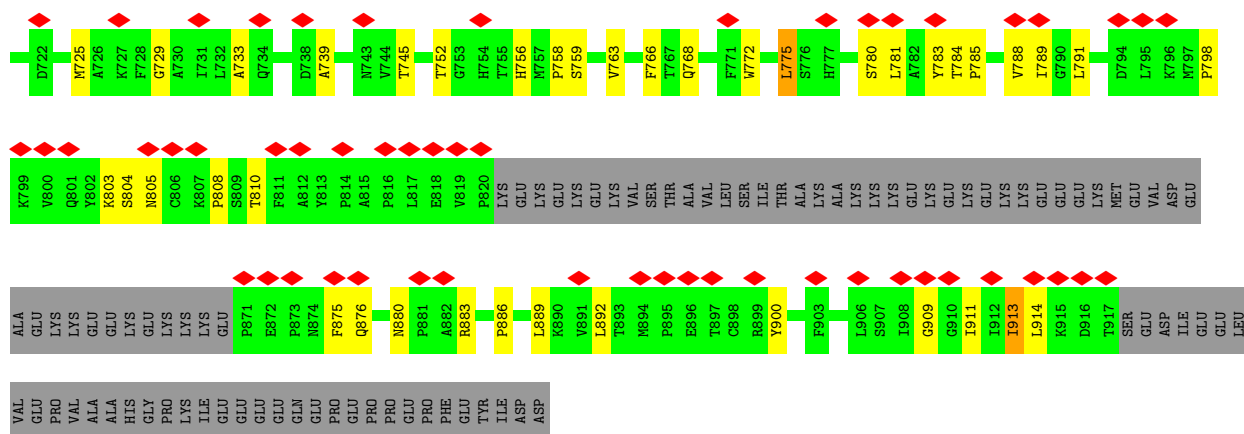
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	F	1	27	10	5	10	2	0

3 Residue-property plots

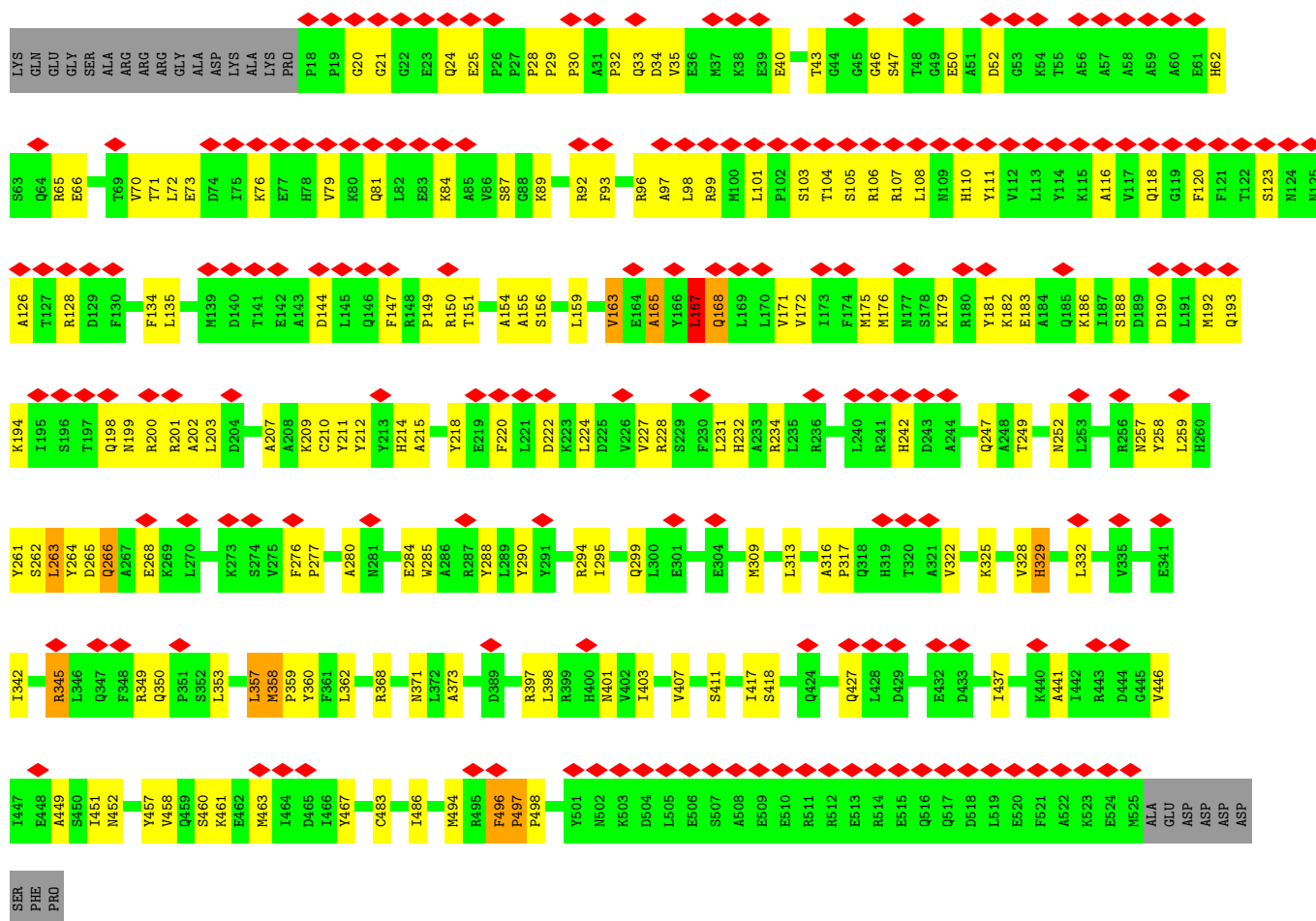
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



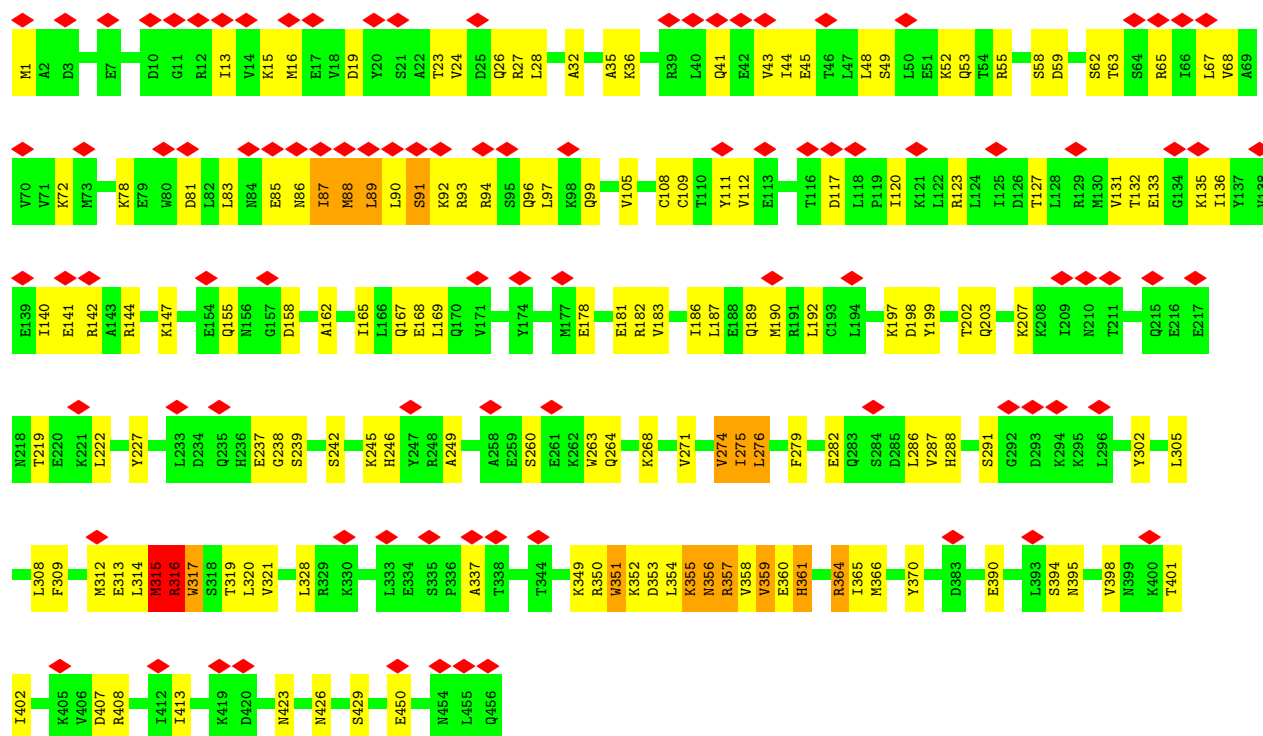


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

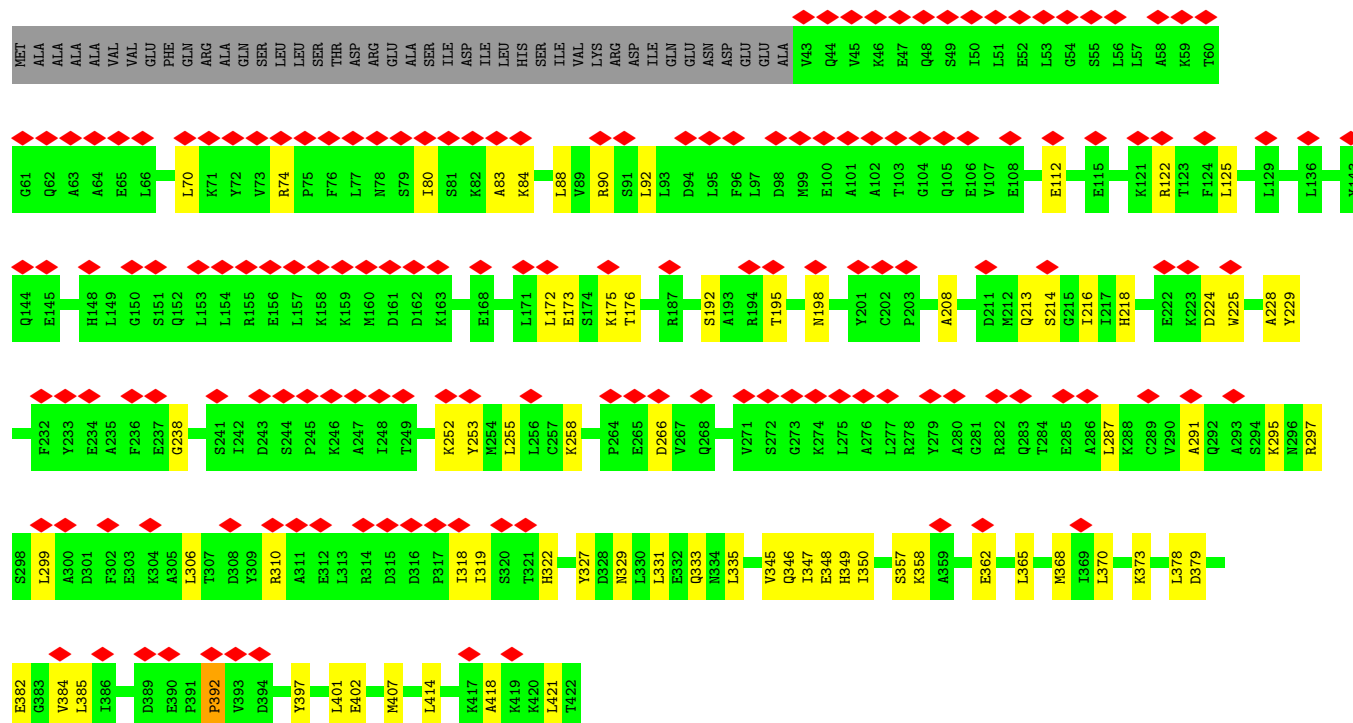
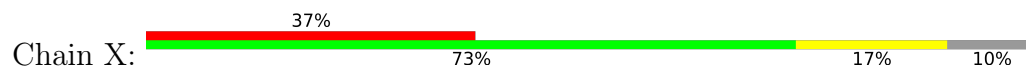


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12



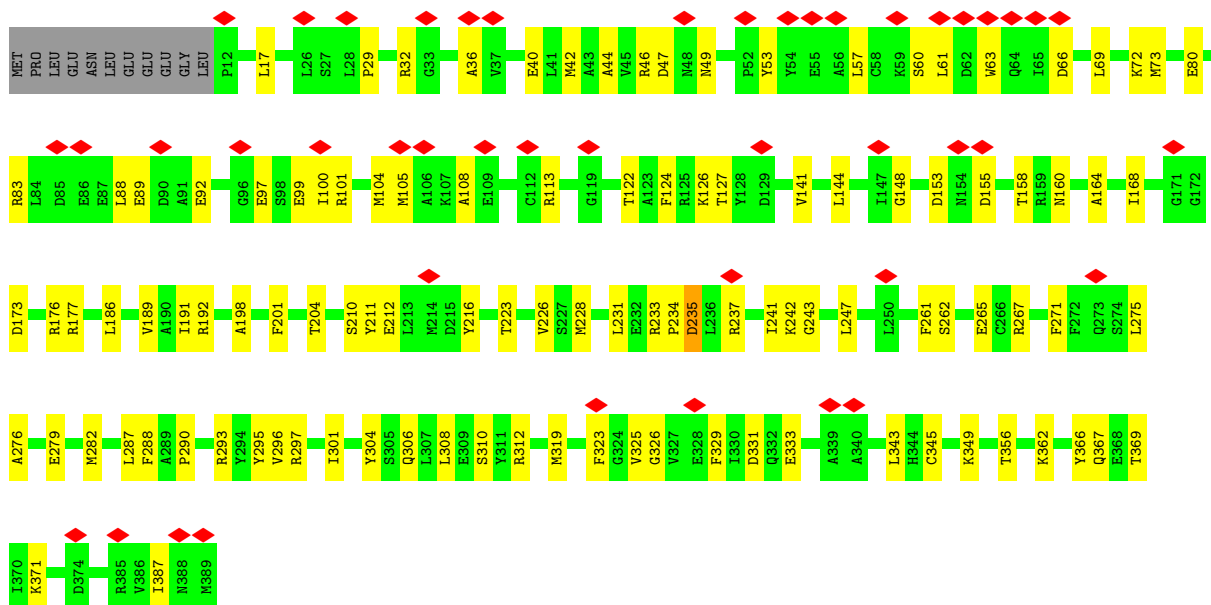


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

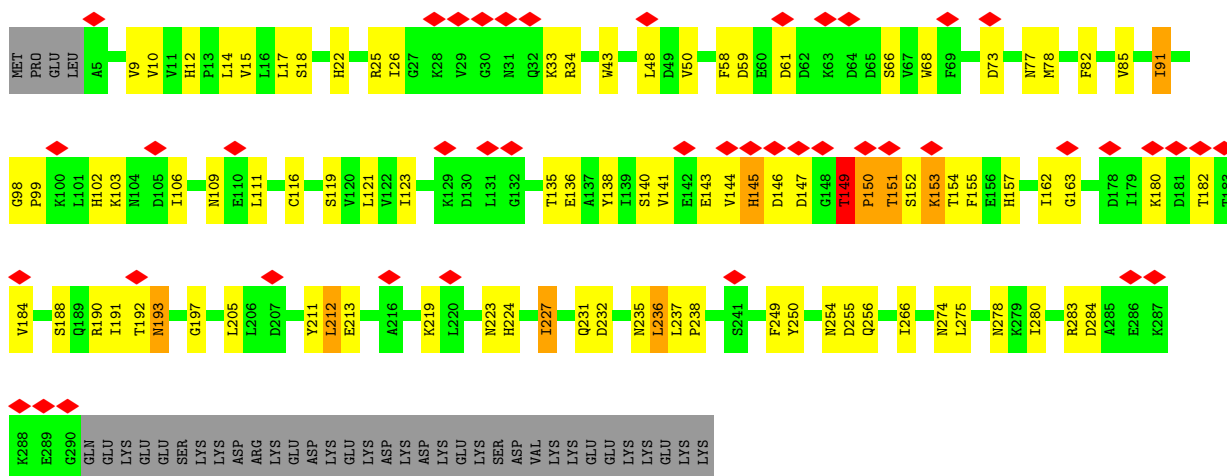


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

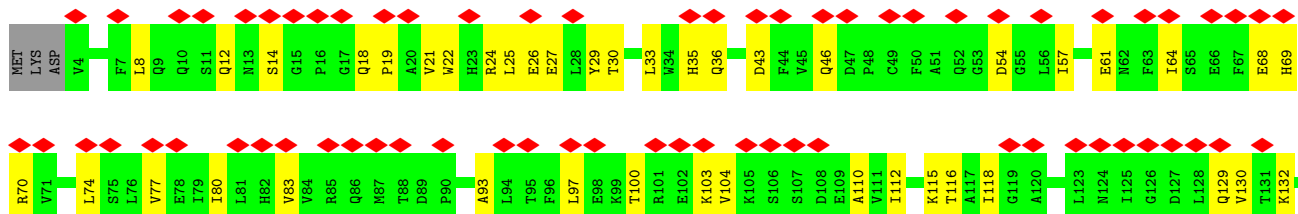




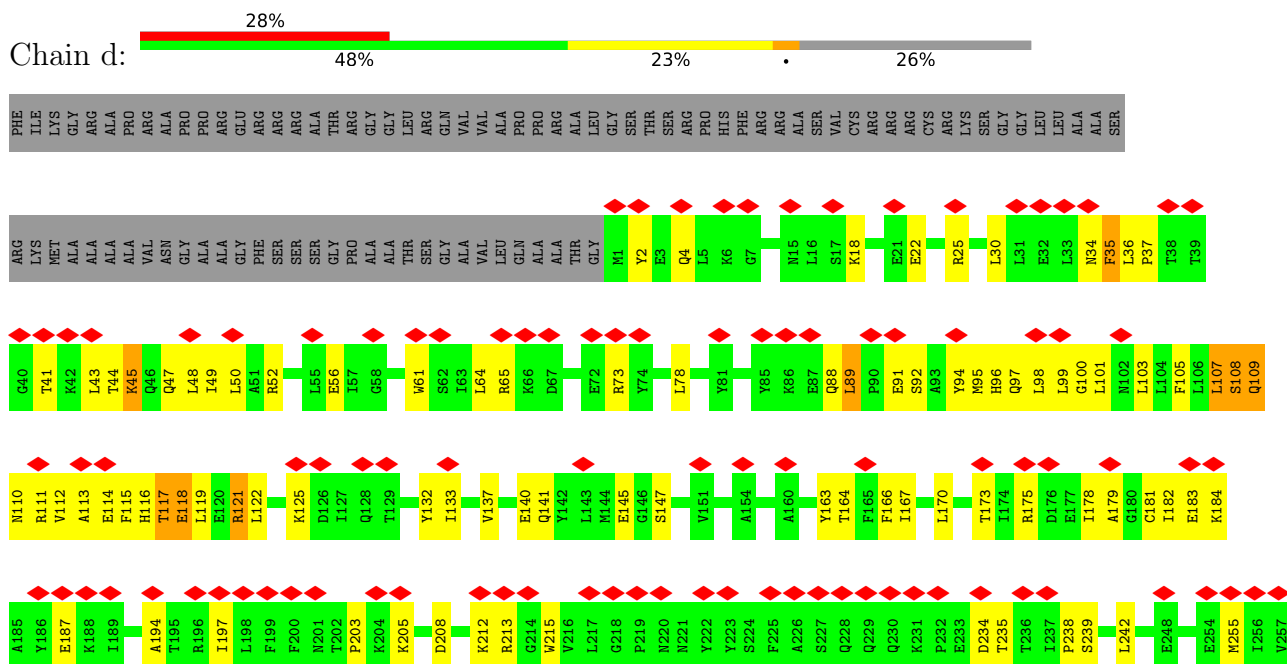
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



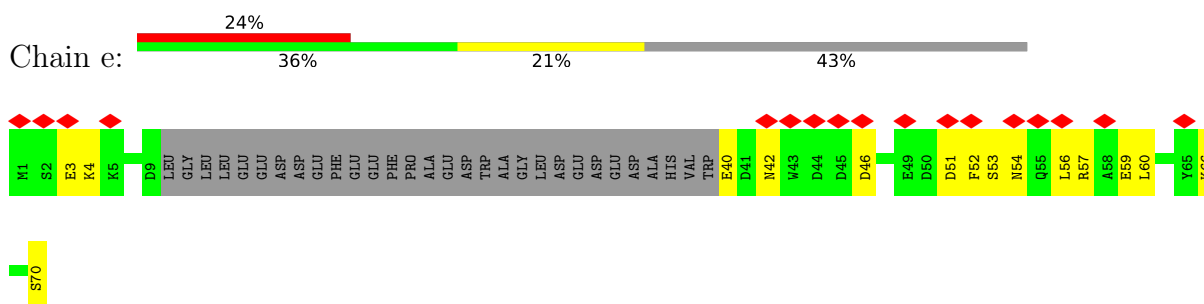
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



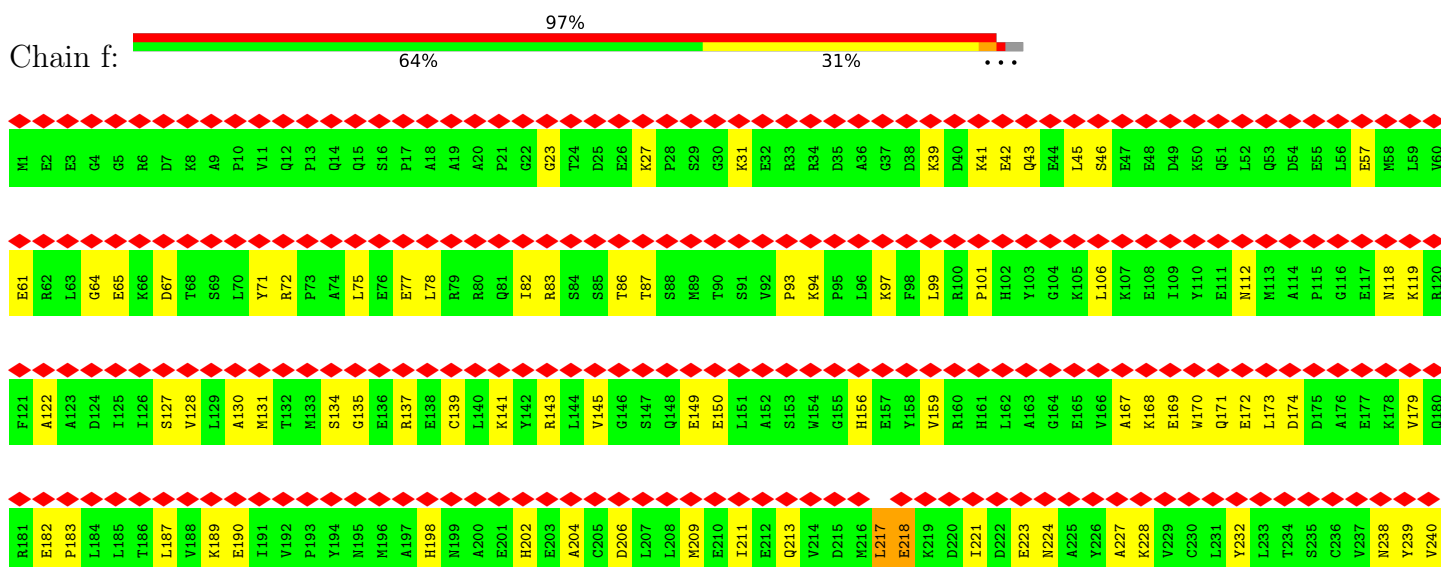
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 11: 26S proteasome complex subunit SEM1



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

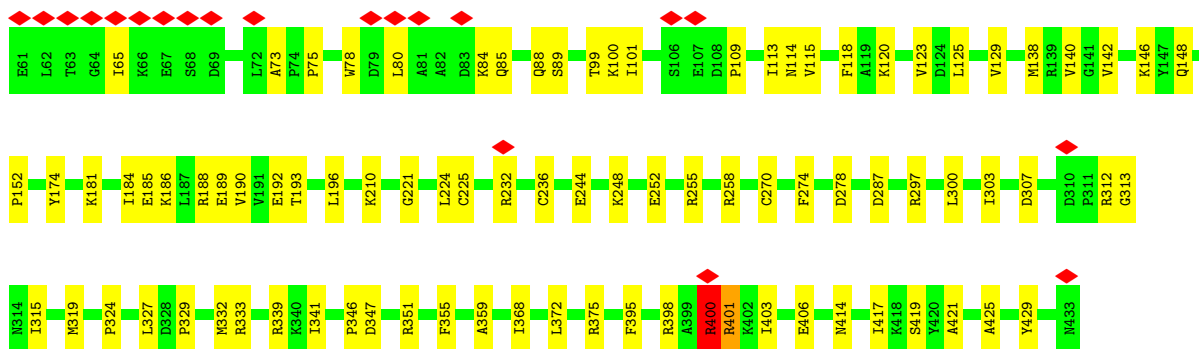


ARG	P841	Y781	V721	A661	A601	T541	S481	D421	S361	H301	P241
LYS	V842	H782	S722	M662	G602	I542	I482	V422	G362	G302	E242
ASN	S843	S783	Y723	G663	S603	M543	F483	G423	S363	P243	
ASN	V844	D784	N724	E664	G604	E544	G484	G424	Q364	F304	E244
TYR	R845	R785	S725	E665	M605	K545	L485	G425	V365	L305	N245
ASP	V846	G786	L726	I666	V606	S546	G486	L426	D366	E306	S246
LEU	G847	L787	F727	G667	L607	E547	L487	T427	S367	L307	A247
	Q848	W788	A728	A668	K608	T548	A488	Q428	A368	S308	L248
	A849	S789	M729	E669	V609	E549	Y489	I429	R369	E309	L249
	V850	Q790	G730	M670	Q610	L550	A490	D430	M370	D310	R250
	D851	V791	M731	A671	Q611	K551	G491	K431	N371	V311	C251
	S852	A792	V732	L672	L612	D552	S492	Y432	L372	E312	A252
	V853	V793	G733	R673	L613	T553	M493	L433	A373	E313	L253
	G854	A794	S734	T674	H614	Y554	R494	Y434	S374	Y314	G254
	Q855	G795	G735	F675	I615	A555	E495	S435	S375	E315	V255
	A856	L796	T736	G676	C616	R556	D496	S436	F376	D316	F256
	G857	T797	N737	H677	S617	W557	V497	E437	V377	L317	R257
	K858	W798	N738	L678	E618	L558	L498	D438	N378	T318	K258
	P859	V799	A739	L679	H619	P559	T499	Y439	G379	E319	F259
	K860	L800	R740	R680	F620	L560	L500	I440	F380	I320	S260
	T861	S801	L741	Y681	D621	G561	L501	K441	V381	M321	R261
	T862	S802	A742	G682	S622	L562	P503	S442	N382	S322	F262
	T863	F803	A743	E683	G623	G563	V504	G443	A383	N323	P263
	G864	L804	M744	P684	E624	L564	M505	L444	A384	V324	E264
	F865	D805	L745	T685	K625	N565	G506	L445	F385	Q325	A265
	Q866	V806	R746	L686	E626	H566	D507	L446	G386	L326	L266
	T867	R807	Q747	R687	E627	L567	S508	A447	Q387	N327	R267
	H868	N808	L748	R688	D628	G568	K509	C448	D388	S328	L268
	T869	I809	A749	A689	K629	K569	C449	C449	K389	N329	A269
	T870	L810	Q750	V690	D630	G570	S510	I450	L390	F330	L270
	P871	L811	Y751	P691	K631	E571	M512	V451	L391	L331	M271
	V872	G812	H752	L692	K632	A572	E513	M452	T392	A332	L272
	L873	K813	A753	A693	E633	I573	V514	S453	D393	L333	N273
	L874	S814	K754	L694	K634	E574	A515	G454	D394	A334	D274
	A875	H815	D755	A695	K635	A575	G516	V455	G395	R335	M275
	H876	Y816	P756	L696	D636	I576	G517	R456	N396	E276	E276
	G877	V817	N757	I697	K637	L577	V517	M457	K397	L337	L277
	E878	L818	N758	S698	D638	A578	T518	E458	V398	D338	V278
	R879	Y819	L759	V699	K639	A579	A519	C459	L399	I339	E279
	A880	G820	F760	S700	K640	L580	A521	D460	Y400	N340	D280
	E881	L821	M761	N701	E641	E581	A521	P461	K401	E341	I281
	L882	V822	V762	P702	A642	V582	G523	A462	N402	P342	F282
	A883	R763	L764	R703	P643	V583	M524	L463	K403	T343	T283
	T884	L824	G765	L704	A644	S584	I525	A464	D404	V344	S284
	E885	M825	A765	N705	D645	E585	I525	L465	H405	P345	C285
	E886	Q826	Q766	I706	M646	P586	A526	L466	G406	D346	K286
	F887	P827	G767	L707	G647	F587	V527	S467	M407	D347	D287
	L888	R828	L768	D708	A648	R588	G528	D468	L408	T348	V288
	P889	H829	T769	T709	H649	S589	S529	Y469	S409	Y349	V289
	VAL	L830	H770	L710	Q650	F590	C530	V470	A410	K350	V290
THR	V831	S711	L771	S711	G651	A591	N531	V471	A411	T351	Q291
PRO	T832	K712	G772	K712	V652	N592	G532	L471	K292	H352	K292
ILE	LEU	F833	K773	F713	A653	T593	D533	M472	A412	L353	Q293
GLU	GLY	D834	G774	S714	V654	L594	V534	S474	L414	E354	M294
PHE	E835	E835	T775	H715	L655	V595	T535	M475	G415	N355	A295
VAL	E836	E836	L776	D716	G656	D596	S536	M476	M416	N356	F296
ILE	L837	A717	T777	A717	V657	V597	T537	M477	I417	F357	M297
LEU	R838	D718	L778	D718	A658	C598	L539	R478	L418	F358	L298
	P839	P719	C779	P719	L659	A599	L479	L479	L419	G359	R300
		E720	P780	E720	T660	Y600	Q540	G480	V420	G360	

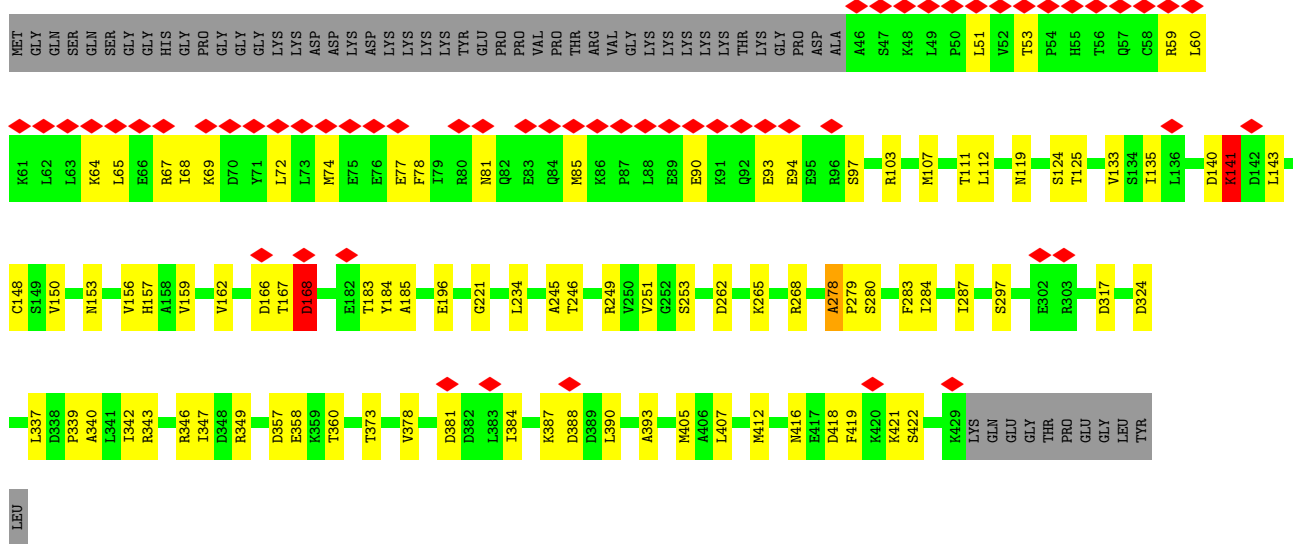
• Molecule 13: 26S protease regulatory subunit 7



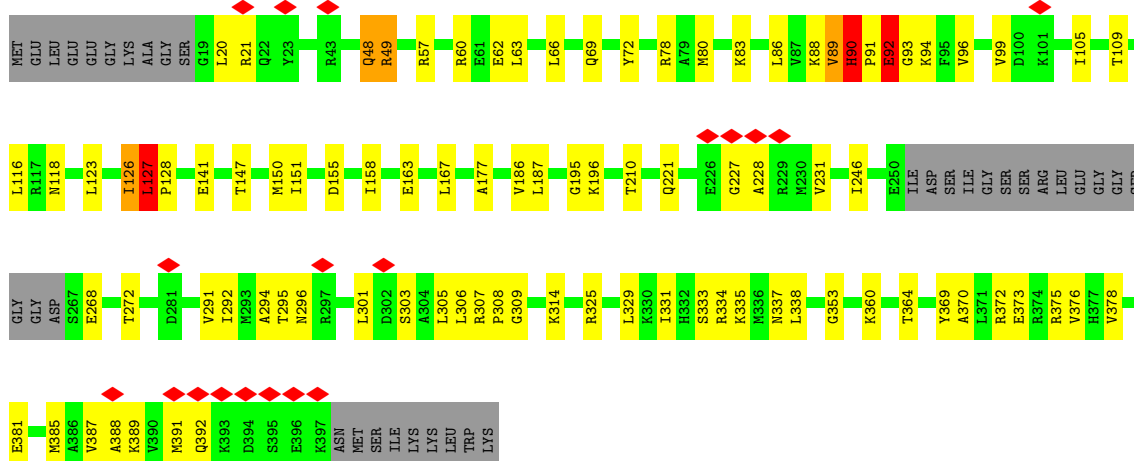
MET	PRO	ASP	TYR	LEU	GLY	ALA	ASP	GLN	ARG	LYS	THR	LYS	GLU	ASP	ASP	LYS	PRO	ARG	ALA	LEU	ASP	GLU	GLY	THR	TYR	GLN	SER	T40	Y41	S42	R43	Q44	I45	K46	Q47	V48	E49	D50	D51	I52	Q53	Q54	L55	L56	K57	K58	I59	N60
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



• Molecule 14: 26S protease regulatory subunit 4

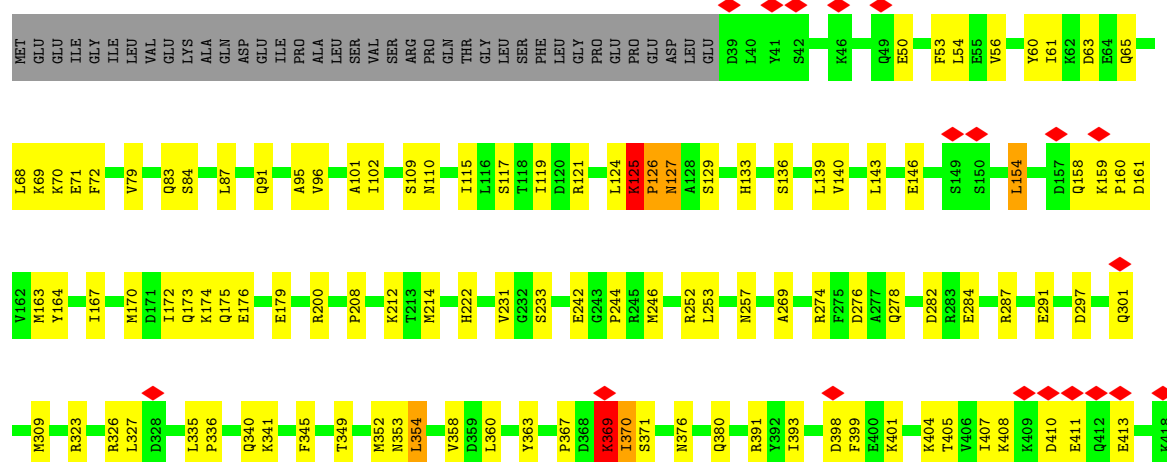


• Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8



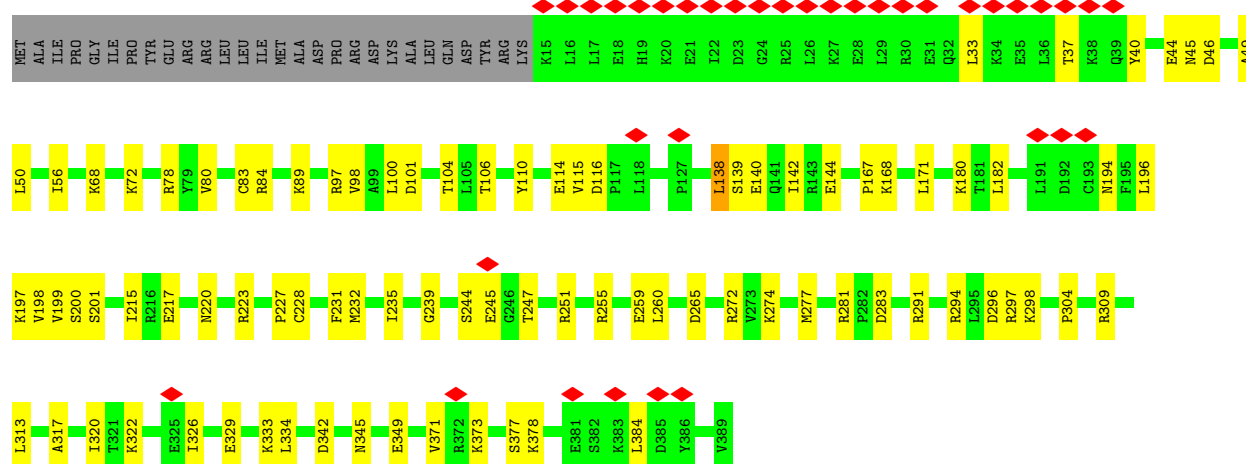
- Molecule 16: 26S protease regulatory subunit 6B

Chain D: 



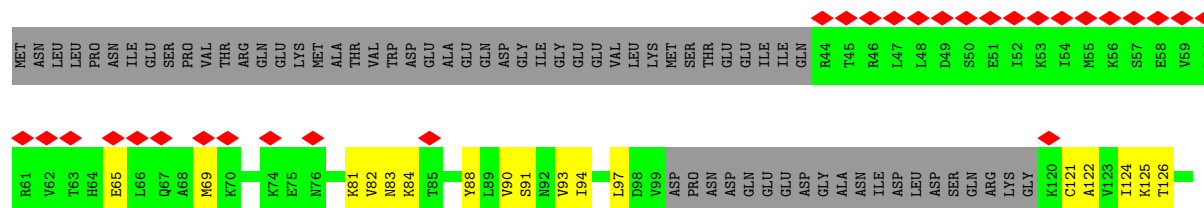
- Molecule 17: 26S proteasome regulatory subunit 10B

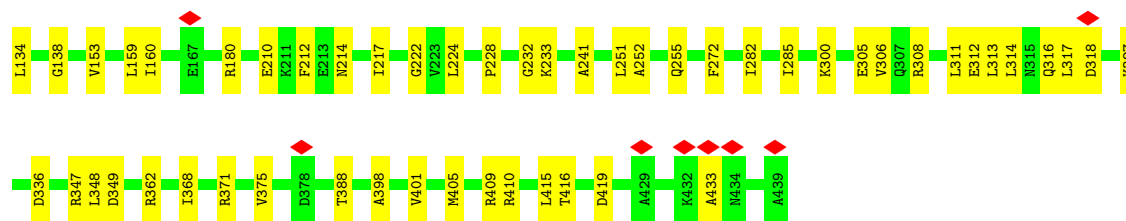
Chain E: 



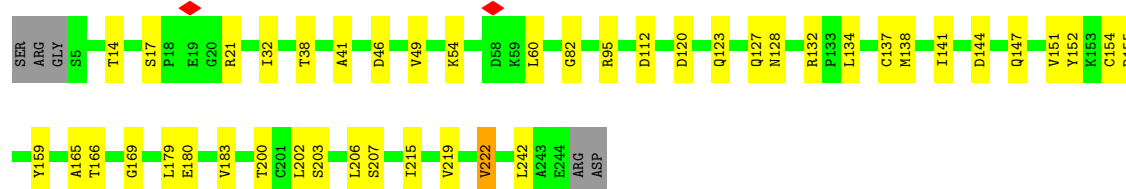
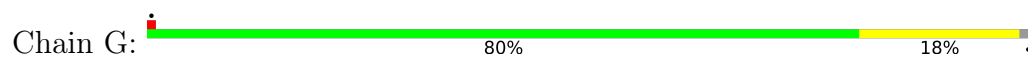
- Molecule 18: 26S protease regulatory subunit 6A

Chain F: 

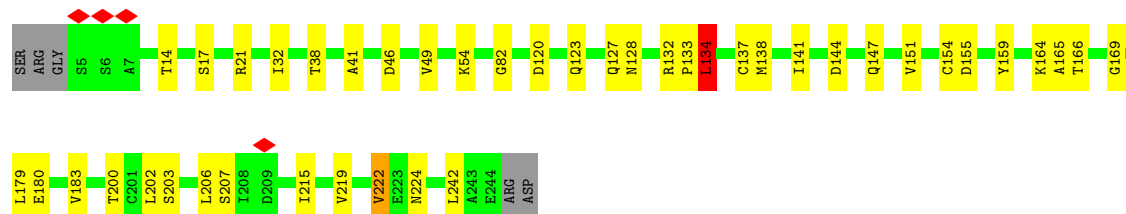
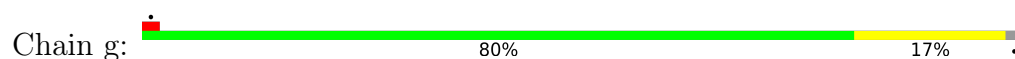




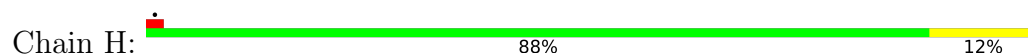
• Molecule 19: Proteasome subunit alpha type-6



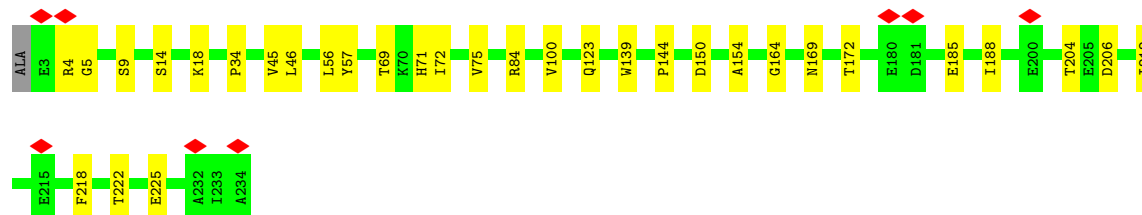
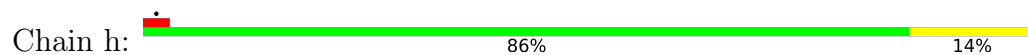
• Molecule 19: Proteasome subunit alpha type-6



• Molecule 20: Proteasome subunit alpha type-2

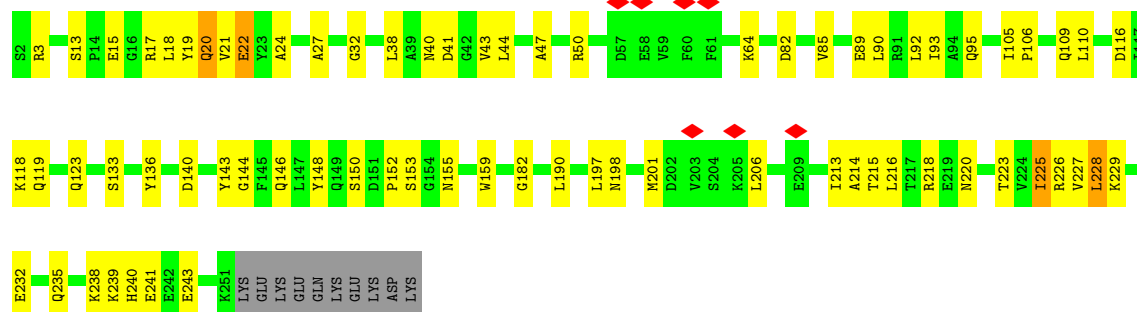


• Molecule 20: Proteasome subunit alpha type-2



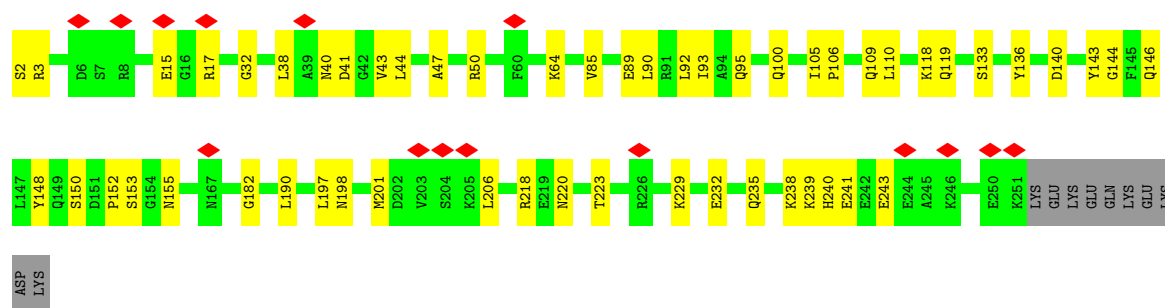
• Molecule 21: Proteasome subunit alpha type-4

Chain I:  68% 26%



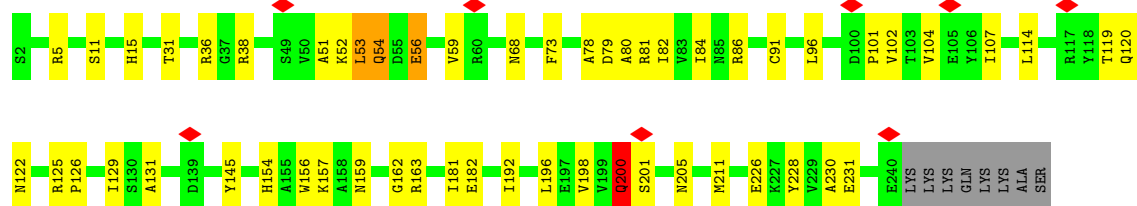
- Molecule 21: Proteasome subunit alpha type-4

Chain i:  6% 75% 21%



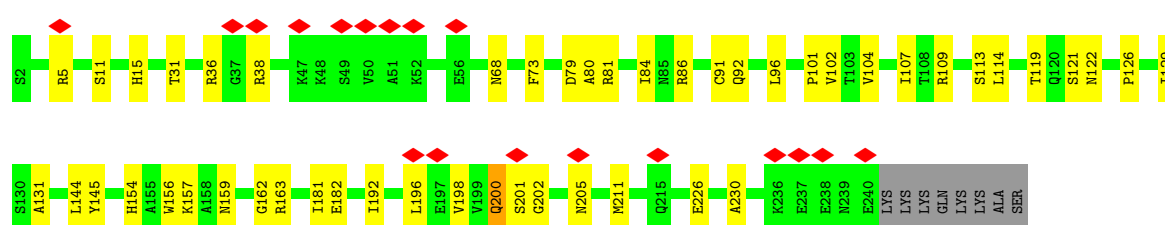
- Molecule 22: Proteasome subunit alpha type-7

Chain J:  74% 21%



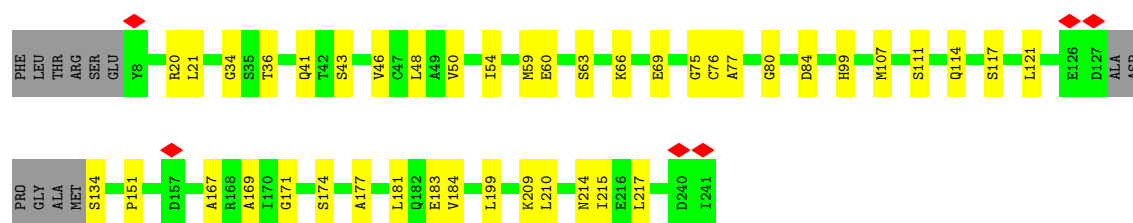
- Molecule 22: Proteasome subunit alpha type-7

Chain j:  7% 77% 19%



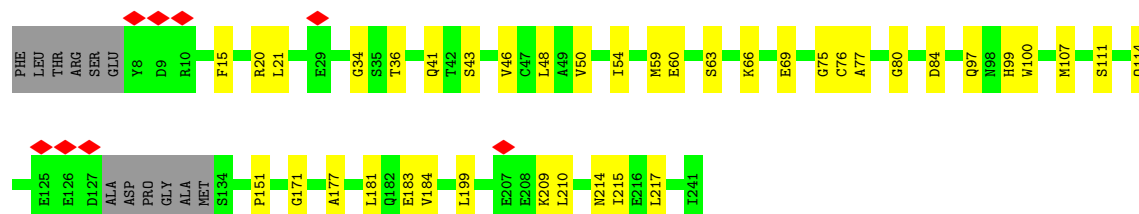
- Molecule 23: Proteasome subunit alpha type-5

Chain K: 



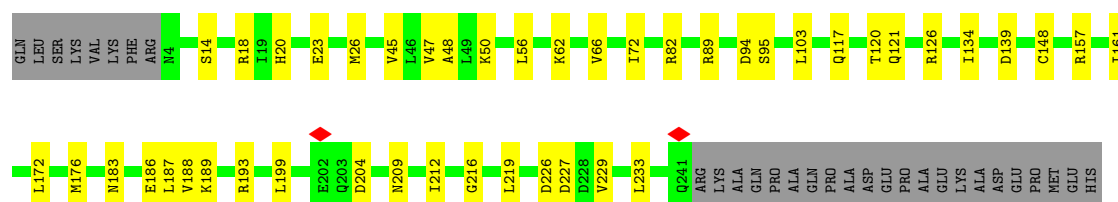
• Molecule 23: Proteasome subunit alpha type-5

Chain k: 



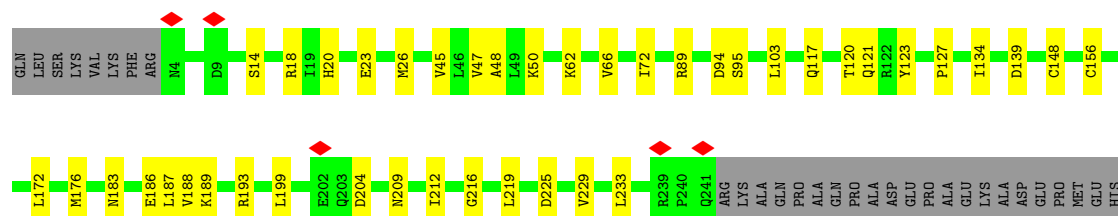
• Molecule 24: Isoform Long of Proteasome subunit alpha type-1

Chain L: 



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

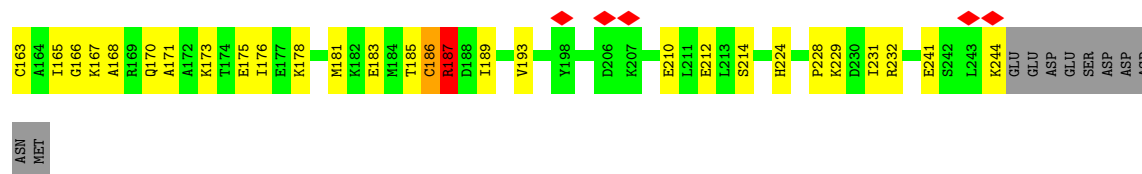
Chain l: 



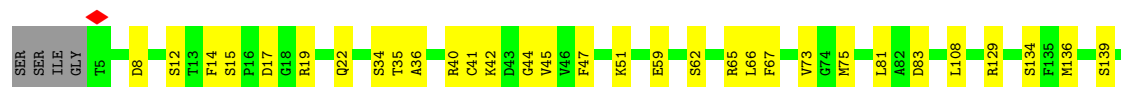
• Molecule 25: Proteasome subunit alpha type-3

Chain M: 

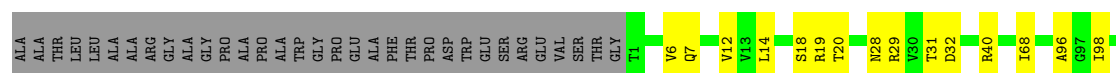




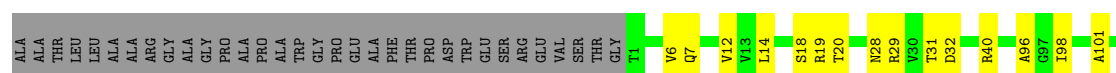
• Molecule 25: Proteasome subunit alpha type-3



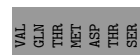
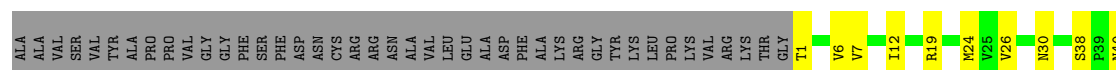
• Molecule 26: Proteasome subunit beta type-6



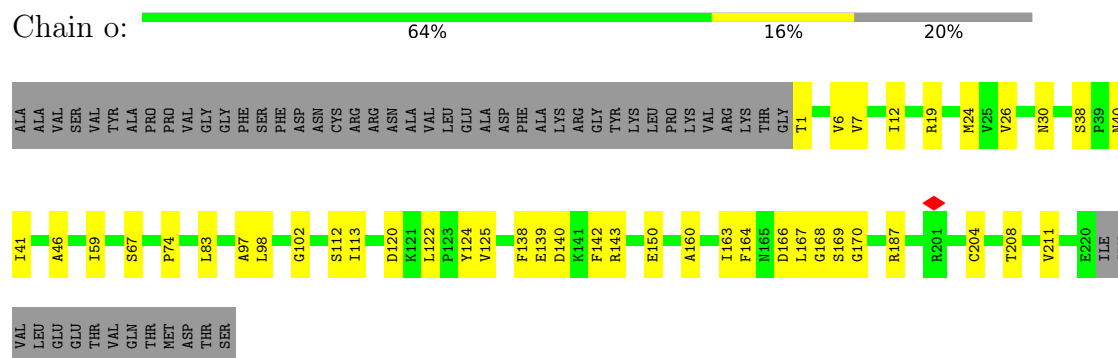
• Molecule 26: Proteasome subunit beta type-6



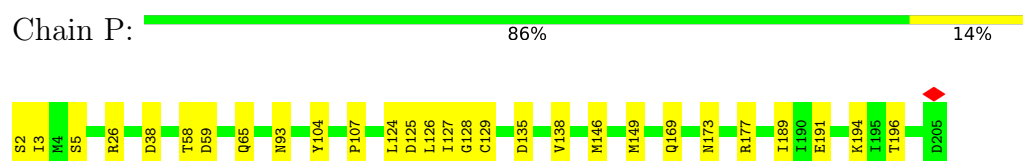
• Molecule 27: Proteasome subunit beta type-7



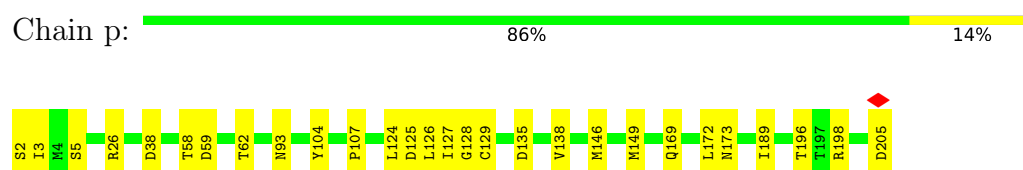
- Molecule 27: Proteasome subunit beta type-7



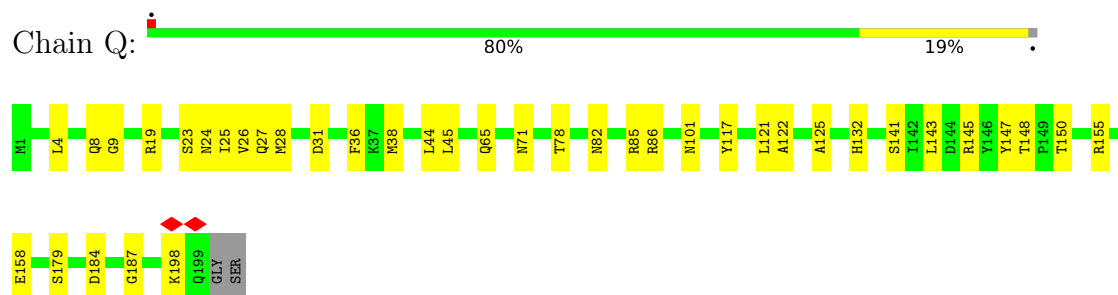
- Molecule 28: Proteasome subunit beta type-3



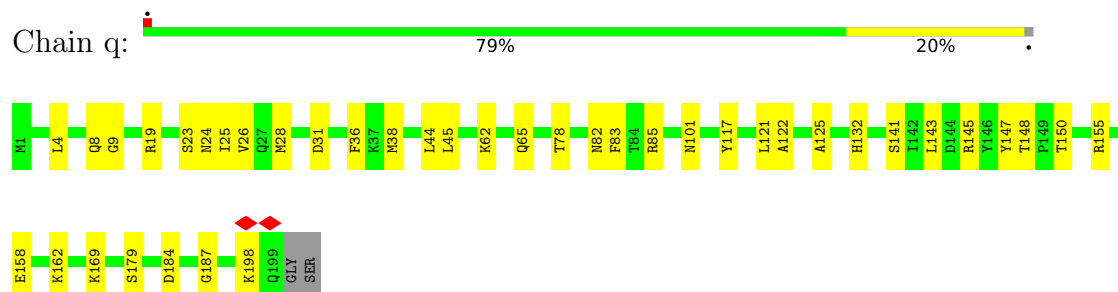
- Molecule 28: Proteasome subunit beta type-3



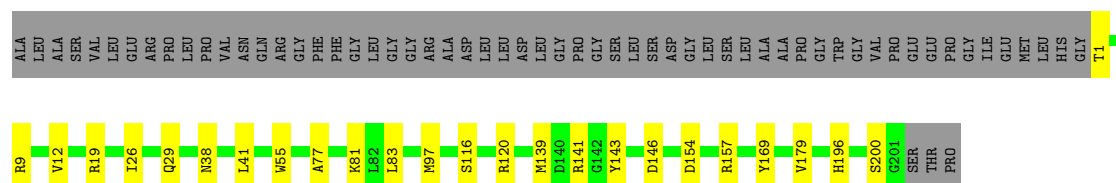
- Molecule 29: Proteasome subunit beta type-2



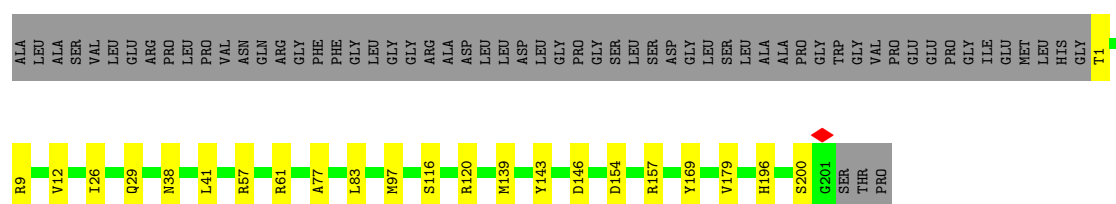
- Molecule 29: Proteasome subunit beta type-2



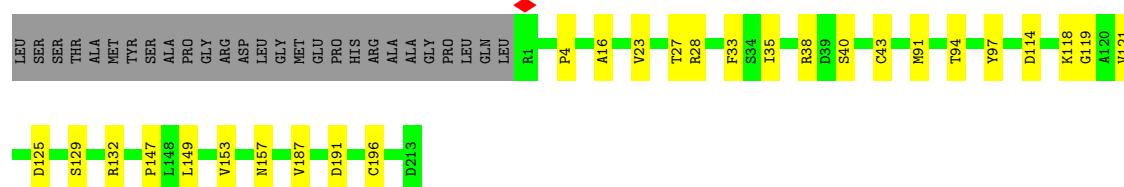
• Molecule 30: Proteasome subunit beta type-5

Chain R:  67% 10% 23%

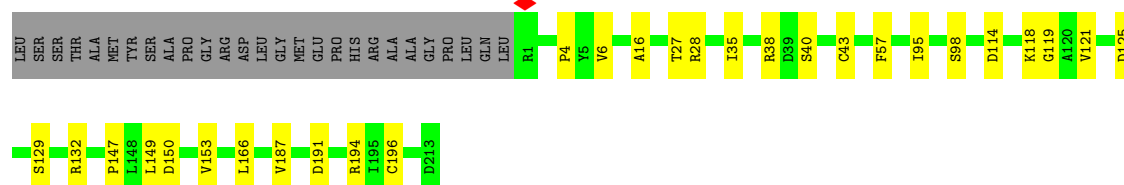
• Molecule 30: Proteasome subunit beta type-5

Chain r:  68% 9% 23%

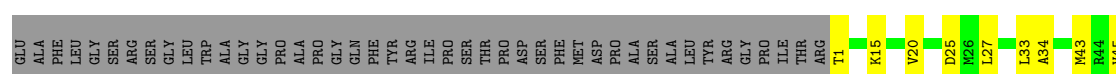
• Molecule 31: Proteasome subunit beta type-1

Chain S:  78% 11% 11%

• Molecule 31: Proteasome subunit beta type-1

Chain s:  77% 12% 11%

• Molecule 32: Proteasome subunit beta type-4

Chain T:  71% 11% 18%



● Molecule 32: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0394	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ATP, 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	0.26	0/6449	0.61	4/8729 (0.0%)
2	V	0.31	0/4072	0.72	3/5510 (0.1%)
3	W	0.30	0/3740	0.70	4/5027 (0.1%)
4	X	0.24	0/3053	0.56	0/4115
5	Y	0.30	0/3173	0.64	0/4273
6	Z	0.27	0/2324	0.64	1/3150 (0.0%)
7	a	0.27	0/3053	0.64	1/4133 (0.0%)
8	b	0.23	0/1478	0.65	0/2001
9	c	0.29	0/2302	0.65	0/3110
10	d	0.28	0/2162	0.71	0/2919
11	e	0.24	0/338	0.64	0/450
12	f	0.26	0/6970	0.74	8/9420 (0.1%)
13	A	0.29	0/3148	0.62	1/4250 (0.0%)
14	B	0.30	1/3061 (0.0%)	0.61	1/4129 (0.0%)
15	C	0.28	0/2902	0.60	2/3904 (0.1%)
16	D	0.31	0/3089	0.68	2/4168 (0.0%)
17	E	0.28	0/2904	0.59	2/3924 (0.1%)
18	F	0.28	0/2896	0.54	0/3912
19	G	0.26	0/1859	0.48	0/2523
19	g	0.25	0/1859	0.47	0/2523
20	H	0.26	0/1743	0.47	0/2372
20	h	0.26	0/1743	0.47	0/2372
21	I	0.28	0/1942	0.55	0/2628
21	i	0.27	0/1942	0.53	0/2628
22	J	0.27	0/1737	0.55	0/2369
22	j	0.26	0/1728	0.54	0/2358
23	K	0.27	0/1747	0.47	0/2364
23	k	0.27	0/1747	0.47	0/2364
24	L	0.27	0/1885	0.55	0/2552
24	l	0.27	0/1885	0.57	2/2552 (0.1%)
25	M	0.27	0/1891	0.54	2/2552 (0.1%)
25	m	0.27	0/1891	0.51	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.27	0/1454	0.44	0/1967
26	n	0.27	0/1454	0.44	0/1967
27	O	0.28	0/1670	0.46	0/2265
27	o	0.28	0/1670	0.46	0/2265
28	P	0.28	0/1620	0.46	0/2184
28	p	0.28	0/1620	0.46	0/2184
29	Q	0.30	0/1603	0.52	0/2174
29	q	0.30	0/1603	0.52	0/2174
30	R	0.30	0/1579	0.45	0/2134
30	r	0.30	0/1579	0.44	0/2134
31	S	0.29	0/1671	0.46	0/2253
31	s	0.29	0/1674	0.46	0/2257
32	T	0.29	0/1700	0.49	0/2305
32	t	0.29	0/1700	0.49	0/2305
All	All	0.28	1/105310 (0.0%)	0.58	33/142401 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	53	THR	C-N	5.05	1.40	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	106	ILE	N-CA-C	-10.48	103.75	113.71
13	A	65	ILE	N-CA-C	-8.82	104.73	113.20
3	W	356	ASN	O-C-N	7.94	130.60	122.03
3	W	351	TRP	N-CA-C	-7.58	102.99	111.71
12	f	713	PHE	N-CA-C	-7.56	102.98	111.07
12	f	763	ARG	N-CA-C	7.34	121.89	113.15
1	U	178	ALA	N-CA-C	-6.86	103.80	112.93
16	D	125	LYS	N-CA-C	6.74	124.70	109.81
12	f	808	ASN	N-CA-C	6.68	119.37	108.08
1	U	55	ARG	N-CA-C	-6.19	97.62	110.80
25	M	187	ARG	N-CA-C	-6.14	97.72	110.80
1	U	53	GLY	N-CA-C	-6.11	98.71	113.18
12	f	679	LEU	N-CA-C	5.96	118.93	109.81
15	C	92	GLU	CA-C-N	5.77	128.92	122.69
15	C	92	GLU	C-N-CA	5.77	128.92	122.69
7	a	221	VAL	N-CA-C	-5.71	107.70	113.47
12	f	755	ASP	N-CA-C	-5.69	104.87	112.55
25	M	185	THR	N-CA-C	-5.58	100.71	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	116	ASP	CA-C-N	5.48	124.94	119.24
17	E	116	ASP	C-N-CA	5.48	124.94	119.24
12	f	808	ASN	CB-CA-C	-5.42	110.35	116.63
2	V	165	ALA	CA-C-N	5.41	131.86	121.54
2	V	165	ALA	C-N-CA	5.41	131.86	121.54
2	V	28	PRO	N-CA-C	5.29	117.15	110.70
14	B	168	ASP	N-CA-C	5.24	121.38	109.81
16	D	127	ASN	N-CA-C	-5.20	102.63	110.06
24	l	225	ASP	CA-C-N	5.20	131.46	121.54
24	l	225	ASP	C-N-CA	5.20	131.46	121.54
1	U	54	PHE	N-CA-C	5.14	117.14	109.59
3	W	140	ILE	CA-C-N	5.12	131.62	122.09
3	W	140	ILE	C-N-CA	5.12	131.62	122.09
12	f	755	ASP	CA-C-N	5.01	126.10	119.84
12	f	755	ASP	C-N-CA	5.01	126.10	119.84

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	6334	0	6366	194	0
2	V	3994	0	3960	177	0
3	W	3693	0	3813	203	0
4	X	3009	0	3113	48	0
5	Y	3115	0	3120	85	0
6	Z	2281	0	2312	94	0
7	a	2995	0	3012	154	0
8	b	1458	0	1505	79	0
9	c	2260	0	2276	81	0
10	d	2116	0	2146	130	0
11	e	334	0	294	16	0
12	f	6857	0	6850	310	0
13	A	3096	0	3140	80	0
14	B	3018	0	3082	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	2864	0	2971	98	0
16	D	3039	0	3075	113	0
17	E	2860	0	2827	59	0
18	F	2858	0	2853	46	0
19	G	1826	0	1796	34	0
19	g	1826	0	1796	32	0
20	H	1708	0	1594	18	0
20	h	1708	0	1594	19	0
21	I	1912	0	1851	62	0
21	i	1912	0	1851	33	0
22	J	1713	0	1537	47	0
22	j	1704	0	1517	29	0
23	K	1722	0	1673	26	0
23	k	1722	0	1673	23	0
24	L	1850	0	1822	29	0
24	l	1850	0	1822	27	0
25	M	1856	0	1816	53	0
25	m	1856	0	1816	38	0
26	N	1430	0	1398	19	0
26	n	1430	0	1398	17	0
27	O	1643	0	1644	26	0
27	o	1643	0	1644	29	0
28	P	1591	0	1609	20	0
28	p	1591	0	1609	20	0
29	Q	1570	0	1547	27	0
29	q	1570	0	1547	29	0
30	R	1548	0	1499	17	0
30	r	1548	0	1499	14	0
31	S	1641	0	1618	23	0
31	s	1644	0	1627	19	0
32	T	1667	0	1628	21	0
32	t	1667	0	1628	18	0
33	c	1	0	0	0	0
34	A	31	0	12	1	0
34	B	31	0	12	1	0
34	D	31	0	12	1	0
34	E	31	0	12	3	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	27	0	12	1	0
36	F	27	0	12	1	0
All	All	103713	0	102840	2588	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 13.

All (2588) 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)
13:A:49:GLU:HA	14:B:65:LEU:CD1	1.31	1.59
13:A:49:GLU:CA	14:B:65:LEU:HD13	1.29	1.57
3:W:89:LEU:CD1	3:W:93:ARG:HG2	1.41	1.48
15:C:127:LEU:HD21	16:D:96:VAL:CG2	1.44	1.46
25:M:41:CYS:SG	25:M:186:CYS:HB3	1.53	1.46
25:M:41:CYS:SG	25:M:189:ILE:HG13	1.52	1.45
2:V:263:LEU:HD12	2:V:264:TYR:N	1.32	1.44
15:C:127:LEU:CD2	15:C:128:PRO:HD3	1.43	1.43
6:Z:149:THR:HB	6:Z:150:PRO:CD	1.43	1.41
10:d:36:LEU:CD1	10:d:37:PRO:HD2	1.51	1.41
15:C:127:LEU:HD22	15:C:128:PRO:CD	1.53	1.38
7:a:145:LEU:HB2	7:a:146:PRO:CD	1.45	1.38
12:f:838:ARG:HB3	12:f:839:PRO:CD	1.50	1.37
12:f:673:ARG:NE	12:f:712:LYS:HG2	1.39	1.37
15:C:90:HIS:CD2	15:C:91:PRO:HD2	1.59	1.37
10:d:36:LEU:HD12	10:d:37:PRO:CD	1.55	1.36
15:C:90:HIS:CE1	16:D:110:ASN:H	1.45	1.34
3:W:317:TRP:HZ2	3:W:351:TRP:CE3	1.46	1.31
1:U:22:PHE:CE1	10:d:30:LEU:HD11	1.65	1.30
8:b:22:LEU:CB	8:b:23:PRO:HD3	1.61	1.28
12:f:681:TYR:CD2	12:f:858:LYS:HG3	1.67	1.27
15:C:127:LEU:CD2	16:D:96:VAL:HG22	1.63	1.27
16:D:341:LYS:HE3	16:D:370:ILE:CG2	1.64	1.27
14:B:278:ALA:HB1	14:B:279:PRO:CD	1.65	1.26
12:f:755:ASP:CG	12:f:756:PRO:HD3	1.60	1.25
7:a:183:VAL:O	7:a:186:LYS:NZ	1.72	1.23
10:d:36:LEU:CG	10:d:37:PRO:HD2	1.67	1.22
10:d:45:LYS:CG	10:d:49:ILE:HG22	1.71	1.21
3:W:315:MET:HE1	3:W:320:LEU:CD1	1.71	1.20
15:C:127:LEU:CD1	15:C:128:PRO:HD2	1.73	1.19
3:W:315:MET:CE	3:W:320:LEU:CG	2.21	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:188:LEU:CD1	7:a:193:GLN:HE21	1.54	1.18
16:D:341:LYS:CE	16:D:370:ILE:HG21	1.72	1.18
13:A:49:GLU:CA	14:B:65:LEU:CD1	2.00	1.16
2:V:497:PRO:CD	2:V:498:PRO:HD3	1.75	1.16
3:W:317:TRP:CZ2	3:W:351:TRP:CZ3	2.32	1.16
3:W:357:ARG:H	3:W:357:ARG:HD2	1.07	1.15
3:W:315:MET:HE1	3:W:320:LEU:CG	1.77	1.15
12:f:673:ARG:CZ	12:f:712:LYS:HG2	1.76	1.15
19:G:46:ASP:O	19:G:222:VAL:HG23	1.48	1.14
25:M:41:CYS:SG	25:M:189:ILE:CG1	2.36	1.14
3:W:83:LEU:HD12	3:W:90:LEU:HD21	1.26	1.14
6:Z:146:ASP:HA	7:a:178:ARG:NH2	1.63	1.13
6:Z:149:THR:HB	6:Z:150:PRO:HD3	1.21	1.13
12:f:712:LYS:HE3	12:f:782:HIS:CD2	1.84	1.13
10:d:52:ARG:HH11	10:d:89:LEU:CD2	1.61	1.13
3:W:317:TRP:HZ2	3:W:351:TRP:CZ3	1.65	1.13
6:Z:149:THR:HB	6:Z:150:PRO:HD2	1.29	1.12
10:d:52:ARG:HH11	10:d:89:LEU:HD21	1.12	1.13
7:a:188:LEU:HD21	7:a:193:GLN:NE2	1.63	1.12
10:d:122:LEU:HD13	10:d:125:LYS:HB2	1.19	1.12
3:W:89:LEU:CD1	3:W:93:ARG:CG	2.28	1.11
7:a:188:LEU:HD11	7:a:193:GLN:HE21	1.14	1.11
1:U:22:PHE:CD1	10:d:30:LEU:HD11	1.84	1.11
15:C:90:HIS:CD2	15:C:91:PRO:CD	2.34	1.11
25:M:41:CYS:SG	25:M:189:ILE:HG21	1.91	1.10
3:W:87:ILE:HB	3:W:91:SER:HA	1.19	1.10
12:f:759:LEU:HG	12:f:806:VAL:HG11	1.34	1.10
7:a:145:LEU:HB2	7:a:146:PRO:HD2	1.27	1.09
12:f:761:MET:HE2	12:f:766:GLN:HA	1.33	1.09
25:M:41:CYS:SG	25:M:186:CYS:CB	2.39	1.09
15:C:90:HIS:CE1	16:D:110:ASN:N	2.21	1.09
3:W:317:TRP:CZ2	3:W:351:TRP:CE3	2.39	1.09
3:W:89:LEU:HD13	3:W:93:ARG:HG2	1.31	1.09
3:W:315:MET:CE	3:W:320:LEU:HG	1.81	1.08
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.34	1.08
15:C:90:HIS:HE1	16:D:110:ASN:N	1.52	1.08
8:b:22:LEU:CB	8:b:23:PRO:CD	2.31	1.08
19:g:134:LEU:H	19:g:134:LEU:HD12	1.16	1.08
2:V:263:LEU:CD1	2:V:264:TYR:H	1.67	1.07
2:V:497:PRO:CG	2:V:498:PRO:HD3	1.83	1.07
3:W:315:MET:HE2	3:W:320:LEU:CB	1.84	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:838:ARG:CB	12:f:839:PRO:HD3	1.83	1.06
6:Z:149:THR:CB	6:Z:150:PRO:CD	2.33	1.06
10:d:36:LEU:HD12	10:d:37:PRO:HD3	1.34	1.06
3:W:89:LEU:HD13	3:W:93:ARG:CG	1.85	1.05
3:W:89:LEU:HD11	3:W:93:ARG:HG2	1.11	1.05
7:a:145:LEU:HB2	7:a:146:PRO:HD3	1.29	1.05
10:d:122:LEU:CD1	10:d:125:LYS:HB2	1.86	1.05
14:B:278:ALA:HB1	14:B:279:PRO:HD2	1.09	1.05
8:b:22:LEU:HB3	8:b:23:PRO:CD	1.87	1.05
16:D:91:GLN:NE2	16:D:127:ASN:HB3	1.71	1.05
10:d:122:LEU:HD13	10:d:125:LYS:CB	1.87	1.04
3:W:356:ASN:O	3:W:360:GLU:HB2	1.57	1.04
19:g:46:ASP:O	19:g:222:VAL:HG23	1.56	1.04
7:a:145:LEU:CB	7:a:146:PRO:CD	2.36	1.04
14:B:278:ALA:CB	14:B:279:PRO:HD2	1.86	1.04
15:C:127:LEU:HD13	15:C:128:PRO:CD	1.87	1.03
2:V:263:LEU:CD1	2:V:264:TYR:N	2.20	1.03
3:W:89:LEU:HD13	3:W:93:ARG:CB	1.88	1.03
8:b:22:LEU:HB3	8:b:23:PRO:HD3	1.04	1.03
7:a:188:LEU:CD2	7:a:193:GLN:NE2	2.22	1.02
13:A:49:GLU:CB	14:B:65:LEU:HD11	1.88	1.02
2:V:496:PHE:H	2:V:497:PRO:CD	1.72	1.02
31:S:23:VAL:HB	31:S:196:CYS:SG	1.98	1.01
15:C:127:LEU:CD2	16:D:96:VAL:CG2	2.30	1.01
16:D:341:LYS:HE3	16:D:370:ILE:HG21	1.02	1.01
12:f:673:ARG:NH2	12:f:712:LYS:HB3	1.75	1.00
13:A:49:GLU:CB	14:B:65:LEU:CD1	2.40	1.00
12:f:760:PHE:O	12:f:762:VAL:HG22	1.62	1.00
10:d:238:PRO:O	10:d:242:LEU:HB2	1.62	0.99
6:Z:146:ASP:HA	7:a:178:ARG:HH22	1.17	0.99
10:d:45:LYS:HG2	10:d:49:ILE:HG22	1.03	0.99
16:D:341:LYS:CE	16:D:370:ILE:CG2	2.35	0.99
12:f:673:ARG:NE	12:f:712:LYS:CG	2.25	0.99
21:I:17:ARG:HD2	21:I:22:GLU:OE2	1.62	0.99
12:f:680:ARG:HE	12:f:715:HIS:CE1	1.80	0.99
10:d:36:LEU:HG	10:d:37:PRO:HD2	1.43	0.99
2:V:165:ALA:HB3	2:V:167:LEU:HD22	1.41	0.98
2:V:497:PRO:CD	2:V:498:PRO:CD	2.40	0.98
2:V:497:PRO:HD2	2:V:498:PRO:HD3	1.42	0.98
3:W:315:MET:HE1	3:W:320:LEU:HD12	1.42	0.98
10:d:36:LEU:HD12	10:d:37:PRO:HD2	1.20	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:315:MET:SD	3:W:320:LEU:HD12	2.04	0.98
10:d:36:LEU:CD1	10:d:37:PRO:CD	2.26	0.98
1:U:22:PHE:CE1	10:d:30:LEU:CD1	2.46	0.98
12:f:755:ASP:CB	12:f:756:PRO:HD3	1.93	0.98
2:V:497:PRO:HD2	2:V:498:PRO:CD	1.93	0.98
3:W:315:MET:CE	3:W:320:LEU:CD1	2.42	0.97
3:W:315:MET:CE	3:W:320:LEU:HD12	1.92	0.97
3:W:317:TRP:CZ2	3:W:351:TRP:HZ3	1.77	0.97
3:W:83:LEU:CD2	3:W:89:LEU:HD23	1.95	0.96
10:d:45:LYS:HG2	10:d:49:ILE:CG2	1.96	0.96
3:W:315:MET:HE2	3:W:320:LEU:CA	1.96	0.96
7:a:188:LEU:HD12	7:a:189:PRO:HD2	1.47	0.96
12:f:680:ARG:NE	12:f:715:HIS:CE1	2.33	0.96
3:W:316:ARG:HG3	3:W:316:ARG:HH21	1.31	0.95
14:B:246:THR:OG1	14:B:280:SER:HB3	1.66	0.95
14:B:358:GLU:OE2	22:J:200:GLN:HG3	1.64	0.95
1:U:457:ILE:O	1:U:461:LEU:HB2	1.66	0.95
2:V:497:PRO:HG2	2:V:498:PRO:HD3	1.45	0.95
3:W:83:LEU:CD1	3:W:90:LEU:HD21	1.96	0.94
16:D:91:GLN:HE21	16:D:127:ASN:HB3	1.32	0.94
1:U:601:ARG:O	1:U:605:VAL:HG12	1.68	0.94
15:C:90:HIS:HE1	16:D:110:ASN:H	0.97	0.93
12:f:41:LYS:O	12:f:45:LEU:HB2	1.68	0.93
7:a:188:LEU:HD21	7:a:193:GLN:CD	1.94	0.93
3:W:315:MET:HE2	3:W:320:LEU:HA	1.48	0.93
12:f:838:ARG:CB	12:f:839:PRO:CD	2.41	0.93
3:W:315:MET:HE1	3:W:320:LEU:HG	1.42	0.92
12:f:673:ARG:CZ	12:f:712:LYS:CG	2.46	0.92
12:f:681:TYR:HD2	12:f:858:LYS:HG3	1.24	0.92
12:f:395:GLY:O	12:f:399:LEU:HB2	1.68	0.92
25:M:41:CYS:HG	25:M:186:CYS:HB3	1.14	0.92
3:W:317:TRP:HZ2	3:W:351:TRP:HE3	1.12	0.91
15:C:127:LEU:HD13	15:C:128:PRO:HD2	0.94	0.91
3:W:89:LEU:HD11	3:W:93:ARG:CG	1.96	0.91
15:C:387:VAL:O	15:C:391:MET:HB2	1.71	0.91
10:d:45:LYS:CG	10:d:49:ILE:CG2	2.49	0.91
14:B:278:ALA:CB	14:B:279:PRO:CD	2.41	0.91
15:C:127:LEU:HD21	16:D:96:VAL:HG22	0.92	0.90
3:W:315:MET:HE2	3:W:320:LEU:CG	1.95	0.90
8:b:21:PHE:CE2	8:b:144:GLY:HA2	2.06	0.90
7:a:188:LEU:HD11	7:a:193:GLN:NE2	1.86	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:263:LEU:HD12	2:V:264:TYR:CA	2.01	0.89
16:D:354:LEU:CD2	16:D:358:VAL:HB	2.03	0.89
12:f:759:LEU:HD11	12:f:806:VAL:HB	1.53	0.89
1:U:22:PHE:CE2	1:U:26:LYS:CE	2.56	0.89
2:V:496:PHE:H	2:V:497:PRO:HD3	1.37	0.89
21:I:216:LEU:HB2	21:I:225:ILE:HG13	1.54	0.89
2:V:496:PHE:N	2:V:497:PRO:CD	2.35	0.89
3:W:83:LEU:HD12	3:W:90:LEU:CD2	2.02	0.89
12:f:673:ARG:HE	12:f:712:LYS:HG2	1.38	0.89
15:C:90:HIS:HD2	15:C:91:PRO:HD2	1.07	0.89
1:U:176:MET:HE1	1:U:179:TYR:OH	1.72	0.88
7:a:189:PRO:HB2	7:a:192:GLU:HB2	1.55	0.88
12:f:838:ARG:HB3	12:f:839:PRO:HD3	0.91	0.88
15:C:388:ALA:O	15:C:392:GLN:HB2	1.73	0.88
1:U:176:MET:SD	1:U:179:TYR:CE2	2.66	0.88
8:b:22:LEU:HB2	8:b:23:PRO:HD3	1.56	0.88
3:W:279:PHE:CD1	3:W:364:ARG:NH2	2.42	0.88
1:U:176:MET:SD	1:U:179:TYR:HE2	1.97	0.88
3:W:315:MET:CE	3:W:320:LEU:CB	2.48	0.88
7:a:142:LEU:CD2	7:a:151:VAL:HG21	2.04	0.87
7:a:142:LEU:HD21	7:a:151:VAL:HG21	1.57	0.87
2:V:345:ARG:NH1	2:V:345:ARG:O	2.08	0.87
12:f:281:ILE:H	12:f:281:ILE:HD13	1.37	0.87
2:V:165:ALA:HB3	2:V:167:LEU:CD2	2.05	0.87
3:W:83:LEU:HD23	3:W:89:LEU:HD23	1.56	0.86
16:D:125:LYS:O	16:D:125:LYS:NZ	2.08	0.86
16:D:369:LYS:H	16:D:369:LYS:HD2	1.38	0.86
12:f:755:ASP:CG	12:f:756:PRO:CD	2.48	0.86
25:M:41:CYS:SG	25:M:189:ILE:CG2	2.63	0.85
3:W:364:ARG:HG2	3:W:364:ARG:HH11	1.39	0.85
3:W:357:ARG:HD2	3:W:357:ARG:N	1.91	0.85
2:V:263:LEU:HD12	2:V:264:TYR:CB	2.07	0.85
2:V:165:ALA:CB	2:V:167:LEU:HD22	2.06	0.85
3:W:83:LEU:HD23	3:W:89:LEU:HA	1.57	0.85
9:c:191:ALA:O	9:c:196:LEU:HB2	1.77	0.85
10:d:52:ARG:HH22	10:d:88:GLN:NE2	1.74	0.84
6:Z:146:ASP:CA	7:a:178:ARG:HH22	1.90	0.84
15:C:90:HIS:CG	15:C:91:PRO:CD	2.60	0.84
3:W:315:MET:HE2	3:W:320:LEU:HG	1.56	0.84
10:d:52:ARG:NH1	10:d:89:LEU:CD2	2.40	0.84
3:W:352:LYS:HA	3:W:355:LYS:HB3	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:263:LEU:HD12	2:V:264:TYR:H	1.03	0.84
1:U:22:PHE:CZ	10:d:30:LEU:HD11	2.12	0.84
10:d:114:GLU:HA	10:d:117:THR:CG2	2.08	0.84
22:J:56:GLU:N	22:J:56:GLU:OE1	2.11	0.84
13:A:270:CYS:SG	13:A:315:ILE:HG12	2.18	0.84
6:Z:250:TYR:O	6:Z:254:ASN:HB2	1.77	0.84
12:f:761:MET:HE2	12:f:766:GLN:CA	2.08	0.84
16:D:353:ASN:HD22	16:D:393:ILE:HG12	1.40	0.84
7:a:189:PRO:HB2	7:a:192:GLU:CB	2.08	0.83
12:f:673:ARG:NH2	12:f:712:LYS:CB	2.40	0.83
6:Z:149:THR:CB	6:Z:150:PRO:HD3	1.99	0.83
7:a:186:LYS:HZ2	7:a:186:LYS:H	1.22	0.83
13:A:49:GLU:N	14:B:65:LEU:HD13	1.92	0.83
16:D:376:ASN:O	16:D:380:GLN:HB2	1.78	0.83
1:U:56:SER:O	1:U:60:ALA:HB2	1.78	0.83
2:V:345:ARG:NE	2:V:345:ARG:HA	1.91	0.83
5:Y:319:MET:O	5:Y:323:PHE:HB3	1.77	0.83
6:Z:212:LEU:HD11	7:a:350:LYS:HB2	1.61	0.83
12:f:486:GLY:O	12:f:490:ALA:HB2	1.78	0.82
15:C:127:LEU:CG	15:C:128:PRO:CD	2.57	0.82
12:f:673:ARG:NH2	12:f:712:LYS:CG	2.41	0.82
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.43	0.82
12:f:759:LEU:CG	12:f:806:VAL:HG11	2.09	0.82
8:b:22:LEU:CD2	8:b:177:PRO:O	2.28	0.82
16:D:369:LYS:HD2	16:D:369:LYS:N	1.93	0.82
5:Y:304:TYR:O	5:Y:308:LEU:HB2	1.78	0.81
12:f:145:VAL:O	12:f:149:GLU:HB3	1.80	0.81
3:W:87:ILE:HB	3:W:91:SER:CA	2.09	0.81
7:a:145:LEU:CB	7:a:146:PRO:HD3	2.03	0.81
1:U:458:ILE:O	1:U:462:LEU:HB2	1.80	0.81
9:c:280:PRO:O	9:c:284:LEU:HB2	1.81	0.81
7:a:93:ALA:O	7:a:97:LEU:HB2	1.80	0.81
13:A:400:ARG:HG2	13:A:400:ARG:HH11	1.46	0.81
1:U:22:PHE:HZ	10:d:34:ASN:OD1	1.62	0.80
9:c:92:GLN:O	9:c:96:LEU:HB2	1.80	0.80
1:U:184:CYS:O	1:U:188:MET:HB2	1.80	0.80
24:L:172:LEU:O	24:L:176:MET:HB3	1.81	0.80
12:f:763:ARG:HG2	12:f:763:ARG:HH11	1.45	0.80
24:l:172:LEU:O	24:l:176:MET:HB3	1.81	0.80
2:V:46:GLY:O	2:V:50:GLU:HB2	1.80	0.80
6:Z:153:LYS:HB2	6:Z:153:LYS:NZ	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:127:LEU:CD1	15:C:128:PRO:CD	2.55	0.80
19:g:134:LEU:H	19:g:134:LEU:CD1	1.95	0.80
3:W:350:ARG:HA	3:W:353:ASP:CB	2.12	0.79
3:W:355:LYS:HE3	3:W:356:ASN:HA	1.64	0.79
10:d:52:ARG:HH22	10:d:88:GLN:HE21	1.24	0.79
15:C:90:HIS:CG	15:C:91:PRO:HD3	2.17	0.79
10:d:107:LEU:CD1	10:d:140:GLU:HB2	2.13	0.79
16:D:133:HIS:HD2	16:D:136:SER:H	1.31	0.79
7:a:184:ASP:C	7:a:186:LYS:HZ3	1.90	0.79
1:U:176:MET:CE	1:U:179:TYR:OH	2.31	0.78
13:A:49:GLU:HA	14:B:65:LEU:HD11	1.62	0.78
1:U:176:MET:SD	1:U:179:TYR:OH	2.40	0.78
10:d:121:ARG:CB	10:d:121:ARG:HH11	1.96	0.78
7:a:148:VAL:HG23	7:a:151:VAL:HB	1.66	0.78
16:D:253:LEU:O	16:D:257:ASN:HB2	1.84	0.78
6:Z:232:ASP:O	6:Z:236:LEU:HB2	1.83	0.78
22:J:54:GLN:HA	22:J:54:GLN:HE21	1.49	0.78
1:U:22:PHE:CE2	1:U:26:LYS:HE2	2.19	0.78
2:V:257:ASN:OD1	2:V:261:TYR:CD2	2.37	0.78
13:A:49:GLU:HB2	14:B:65:LEU:HD11	1.66	0.78
25:M:41:CYS:SG	25:M:189:ILE:CB	2.72	0.77
3:W:274:VAL:HG13	3:W:286:LEU:CD2	2.15	0.77
10:d:52:ARG:NH1	10:d:89:LEU:HD21	1.96	0.77
12:f:213:GLN:O	12:f:217:LEU:HB2	1.83	0.77
15:C:48:GLN:HA	15:C:48:GLN:NE2	1.99	0.77
2:V:357:LEU:HD12	2:V:357:LEU:O	1.85	0.77
3:W:35:ALA:O	3:W:87:ILE:CD1	2.33	0.77
7:a:186:LYS:NZ	7:a:186:LYS:H	1.82	0.77
13:A:417:ILE:O	13:A:421:ALA:HB2	1.85	0.77
15:C:127:LEU:CD2	15:C:128:PRO:CD	2.31	0.77
3:W:83:LEU:HD21	3:W:89:LEU:HD23	1.67	0.77
12:f:67:ASP:O	12:f:71:TYR:HB2	1.84	0.77
3:W:276:LEU:HD22	3:W:353:ASP:O	1.85	0.77
8:b:22:LEU:HB2	8:b:23:PRO:CD	2.10	0.76
12:f:681:TYR:CD2	12:f:763:ARG:NH1	2.53	0.76
7:a:186:LYS:HA	7:a:186:LYS:HE3	1.67	0.76
2:V:116:ALA:O	2:V:120:PHE:HB2	1.86	0.76
3:W:83:LEU:CD1	3:W:90:LEU:CD2	2.61	0.76
12:f:755:ASP:OD1	12:f:755:ASP:N	2.14	0.76
25:m:41:CYS:SG	25:m:186:CYS:HB3	2.25	0.76
9:c:192:LEU:HA	9:c:196:LEU:HD23	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:105:VAL:O	3:W:109:CYS:HB2	1.86	0.76
28:P:2:SER:N	28:P:5:SER:HG	1.82	0.76
10:d:48:LEU:HB3	10:d:88:GLN:NE2	2.02	0.75
12:f:764:LEU:N	12:f:764:LEU:HD23	2.00	0.75
16:D:354:LEU:HD21	16:D:358:VAL:HB	1.68	0.75
2:V:263:LEU:CD1	2:V:264:TYR:HB3	2.16	0.75
15:C:127:LEU:HD21	16:D:96:VAL:HG21	1.66	0.75
28:p:2:SER:N	28:p:5:SER:HG	1.84	0.75
6:Z:144:VAL:HG22	6:Z:150:PRO:HA	1.68	0.75
6:Z:146:ASP:HA	7:a:178:ARG:CZ	2.16	0.75
13:A:49:GLU:HB2	14:B:65:LEU:CD1	2.14	0.75
16:D:50:GLU:O	16:D:54:LEU:HB2	1.86	0.75
1:U:177:LEU:HD13	1:U:177:LEU:C	2.12	0.75
2:V:345:ARG:HA	2:V:345:ARG:CZ	2.16	0.75
2:V:358:MET:HB3	2:V:359:PRO:HD3	1.69	0.75
3:W:356:ASN:O	3:W:360:GLU:CB	2.35	0.75
12:f:761:MET:HG3	12:f:766:GLN:HG2	1.67	0.75
15:C:127:LEU:CG	15:C:128:PRO:HD3	2.17	0.75
10:d:114:GLU:HA	10:d:117:THR:HG22	1.68	0.74
1:U:55:ARG:HB2	1:U:55:ARG:NH2	2.01	0.74
2:V:266:GLN:HG3	2:V:295:ILE:HD12	1.68	0.74
8:b:52:ILE:HD12	8:b:59:GLU:O	1.87	0.74
12:f:759:LEU:CD1	12:f:806:VAL:CG1	2.65	0.74
19:g:46:ASP:O	19:g:222:VAL:CG2	2.35	0.74
1:U:22:PHE:CZ	10:d:30:LEU:CD1	2.68	0.74
7:a:188:LEU:CD1	7:a:189:PRO:HD2	2.17	0.74
12:f:213:GLN:O	12:f:217:LEU:CB	2.35	0.74
6:Z:25:ARG:HH11	9:c:104:ARG:H	1.32	0.74
9:c:157:ILE:HG21	9:c:205:ILE:CD1	2.17	0.74
1:U:55:ARG:HB2	1:U:55:ARG:CZ	2.17	0.74
12:f:712:LYS:O	12:f:715:HIS:CB	2.36	0.73
16:D:335:LEU:HD21	16:D:370:ILE:O	1.88	0.73
7:a:188:LEU:CD1	7:a:193:GLN:NE2	2.40	0.73
12:f:763:ARG:HG2	12:f:763:ARG:NH1	1.99	0.73
22:J:53:LEU:O	22:J:53:LEU:HD22	1.89	0.73
1:U:74:PHE:O	1:U:78:LEU:HB2	1.88	0.73
13:A:400:ARG:HG2	13:A:400:ARG:NH1	2.01	0.73
3:W:315:MET:SD	3:W:320:LEU:HB2	2.28	0.73
15:C:90:HIS:CD2	15:C:90:HIS:H	2.06	0.73
1:U:22:PHE:CE2	1:U:26:LYS:HE3	2.23	0.72
12:f:217:LEU:HD13	12:f:217:LEU:C	2.14	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:21:GLY:O	2:V:25:GLU:HB2	1.89	0.72
9:c:85:GLU:OE1	9:c:85:GLU:HA	1.88	0.72
6:Z:146:ASP:OD1	7:a:177:LEU:HD13	1.89	0.72
8:b:51:LEU:C	8:b:51:LEU:HD12	2.14	0.72
8:b:52:ILE:CD1	8:b:60:VAL:HA	2.20	0.72
12:f:679:LEU:HD21	12:f:686:LEU:HD11	1.70	0.72
5:Y:101:ARG:O	5:Y:105:MET:HB3	1.89	0.72
12:f:673:ARG:HE	12:f:712:LYS:CG	1.94	0.72
12:f:691:PRO:HD3	12:f:713:PHE:CE2	2.24	0.72
31:s:43:CYS:SG	31:s:194:ARG:HG2	2.30	0.71
3:W:282:GLU:O	3:W:286:LEU:HB2	1.90	0.71
25:M:41:CYS:HG	25:M:186:CYS:CB	1.92	0.71
3:W:89:LEU:HD13	3:W:93:ARG:HB2	1.73	0.71
15:C:126:ILE:HD12	15:C:126:ILE:N	2.04	0.71
2:V:494:MET:HE1	6:Z:274:ASN:HB2	1.72	0.71
3:W:35:ALA:O	3:W:87:ILE:HD12	1.91	0.71
10:d:121:ARG:HH11	10:d:121:ARG:CA	2.04	0.71
14:B:278:ALA:HB1	14:B:279:PRO:HD3	1.71	0.71
21:i:143:TYR:HB2	21:i:146:GLN:HE21	1.56	0.71
3:W:316:ARG:HD2	3:W:319:THR:OG1	1.90	0.70
10:d:45:LYS:NZ	10:d:45:LYS:HB3	2.05	0.70
12:f:283:THR:O	12:f:287:ASP:HB2	1.91	0.70
13:A:49:GLU:CG	14:B:65:LEU:HD11	2.20	0.70
23:k:177:ALA:O	23:k:181:LEU:HB2	1.91	0.70
3:W:314:LEU:HD23	3:W:358:VAL:HG12	1.72	0.70
15:C:127:LEU:CG	15:C:128:PRO:HD2	2.19	0.70
16:D:341:LYS:CE	16:D:370:ILE:HG22	2.21	0.70
23:K:177:ALA:O	23:K:181:LEU:HB2	1.91	0.70
10:d:94:TYR:O	10:d:98:LEU:HB2	1.90	0.70
3:W:87:ILE:HD13	3:W:91:SER:HB2	1.73	0.70
3:W:316:ARG:HG3	3:W:316:ARG:NH2	1.99	0.70
10:d:107:LEU:HD23	10:d:107:LEU:C	2.17	0.70
21:I:143:TYR:HB2	21:I:146:GLN:HE21	1.56	0.70
12:f:681:TYR:O	12:f:687:ARG:NH1	2.25	0.70
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.25	0.70
2:V:496:PHE:N	2:V:497:PRO:HD2	2.05	0.70
7:a:184:ASP:C	7:a:186:LYS:NZ	2.49	0.70
16:D:91:GLN:HE21	16:D:127:ASN:CB	2.02	0.70
3:W:364:ARG:HG2	3:W:364:ARG:NH1	1.98	0.70
3:W:83:LEU:HG	3:W:90:LEU:CD2	2.23	0.69
12:f:761:MET:CE	12:f:766:GLN:HA	2.19	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:263:LEU:CG	2:V:264:TYR:H	2.05	0.69
22:J:53:LEU:HD13	22:J:54:GLN:HG2	1.74	0.69
1:U:177:LEU:O	1:U:177:LEU:HD22	1.93	0.69
21:i:2:SER:N	24:l:123:TYR:HH	1.90	0.69
3:W:15:LYS:O	3:W:19:ASP:HB3	1.93	0.69
7:a:188:LEU:HD12	7:a:189:PRO:CD	2.21	0.69
19:G:46:ASP:O	19:G:222:VAL:CG2	2.36	0.69
7:a:186:LYS:HZ2	7:a:186:LYS:N	1.90	0.69
12:f:281:ILE:HD13	12:f:281:ILE:N	2.07	0.69
12:f:646:MET:CE	14:B:64:LYS:HG2	2.23	0.69
12:f:691:PRO:HG3	12:f:713:PHE:HE2	1.57	0.69
14:B:245:ALA:HB1	14:B:279:PRO:O	1.92	0.69
4:X:175:LYS:HG2	4:X:213:GLN:HE22	1.57	0.69
2:V:284:GLU:O	2:V:288:TYR:HB2	1.93	0.69
2:V:497:PRO:HD2	2:V:498:PRO:HD2	1.72	0.69
3:W:83:LEU:HG	3:W:90:LEU:HG	1.75	0.69
3:W:90:LEU:HD12	3:W:97:LEU:HD12	1.73	0.69
10:d:208:ASP:O	10:d:212:LYS:HB2	1.92	0.69
19:g:202:LEU:O	19:g:206:LEU:HB2	1.93	0.69
21:I:215:THR:O	21:I:225:ILE:HG12	1.91	0.69
2:V:266:GLN:HG2	2:V:299:GLN:OE1	1.93	0.68
12:f:755:ASP:OD1	12:f:756:PRO:HD3	1.93	0.68
12:f:130:ALA:O	12:f:134:SER:N	2.22	0.68
3:W:41:GLN:HG3	3:W:94:ARG:HH12	1.59	0.68
12:f:681:TYR:CE2	12:f:858:LYS:HG3	2.25	0.68
19:G:202:LEU:O	19:G:206:LEU:HB2	1.93	0.68
25:M:47:PHE:HB2	25:M:214:SER:HB3	1.74	0.68
2:V:497:PRO:N	2:V:498:PRO:CD	2.53	0.68
12:f:168:LYS:O	12:f:172:GLU:HB2	1.94	0.68
12:f:755:ASP:OD1	12:f:756:PRO:CD	2.41	0.68
10:d:45:LYS:CD	10:d:49:ILE:CG2	2.71	0.68
1:U:174:PRO:HD2	1:U:176:MET:HG2	1.75	0.68
5:Y:42:MET:SD	5:Y:46:ARG:NH2	2.67	0.68
10:d:45:LYS:CD	10:d:49:ILE:HG22	2.23	0.68
10:d:45:LYS:HD3	10:d:49:ILE:CG2	2.23	0.68
6:Z:146:ASP:CA	7:a:178:ARG:NH2	2.49	0.68
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.75	0.68
25:m:47:PHE:HB2	25:m:214:SER:HB3	1.74	0.68
7:a:188:LEU:CG	7:a:193:GLN:HE21	2.07	0.67
1:U:17:PRO:HB2	1:U:55:ARG:HH12	1.58	0.67
2:V:101:LEU:O	2:V:105:SER:HB3	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:229:VAL:O	1:U:233:LEU:HB2	1.95	0.67
2:V:257:ASN:OD1	2:V:261:TYR:CE2	2.47	0.67
14:B:166:ASP:OD1	15:C:78:ARG:NH2	2.24	0.67
12:f:712:LYS:HE3	12:f:782:HIS:HD2	1.57	0.67
12:f:774:GLY:C	12:f:776:LEU:H	2.02	0.67
1:U:601:ARG:HA	1:U:604:HIS:HB3	1.76	0.67
1:U:701:ILE:HG21	1:U:810:THR:HA	1.77	0.67
3:W:312:MET:HE2	7:a:312:MET:HB3	1.76	0.67
4:X:90:ARG:HH21	4:X:125:LEU:HA	1.60	0.67
6:Z:153:LYS:HB2	6:Z:153:LYS:HZ1	1.57	0.67
9:c:157:ILE:HG21	9:c:205:ILE:HD13	1.76	0.67
13:A:236:CYS:SG	13:A:270:CYS:HB3	2.35	0.67
3:W:355:LYS:O	3:W:359:VAL:HB	1.94	0.67
1:U:603:LEU:HD21	16:D:60:TYR:HD1	1.58	0.67
3:W:357:ARG:H	3:W:357:ARG:CD	1.95	0.67
4:X:392:PRO:HB2	5:Y:362:LYS:HE3	1.77	0.67
8:b:21:PHE:CE2	8:b:144:GLY:CA	2.77	0.67
12:f:755:ASP:CB	12:f:756:PRO:CD	2.72	0.67
1:U:219:CYS:O	1:U:223:LEU:HB2	1.94	0.66
7:a:188:LEU:HD11	7:a:193:GLN:HG2	1.77	0.66
2:V:167:LEU:N	2:V:167:LEU:HD23	2.10	0.66
2:V:263:LEU:HD12	2:V:264:TYR:HB3	1.77	0.66
3:W:63:THR:HA	3:W:68:VAL:HG22	1.76	0.66
10:d:36:LEU:CG	10:d:37:PRO:CD	2.62	0.66
12:f:217:LEU:HD22	12:f:239:TYR:CE1	2.30	0.66
12:f:761:MET:CG	12:f:766:GLN:HG2	2.25	0.66
1:U:325:MET:O	1:U:329:LEU:HB2	1.96	0.66
18:F:252:ALA:HB3	18:F:255:GLN:HB2	1.77	0.66
3:W:309:PHE:HE2	3:W:357:ARG:HB3	1.59	0.66
6:Z:109:ASN:ND2	6:Z:140:SER:OG	2.29	0.66
12:f:712:LYS:O	12:f:715:HIS:HB2	1.96	0.66
14:B:74:MET:O	14:B:78:PHE:HB2	1.95	0.66
3:W:89:LEU:HD11	3:W:133:GLU:OE2	1.96	0.66
15:C:90:HIS:CD2	15:C:91:PRO:HD3	2.29	0.66
28:p:62:THR:OG1	29:q:85:ARG:NH2	2.29	0.66
2:V:62:HIS:HA	2:V:65:ARG:HB3	1.76	0.66
3:W:321:VAL:CG2	3:W:351:TRP:HH2	2.09	0.66
10:d:45:LYS:HD2	10:d:45:LYS:C	2.21	0.66
3:W:203:GLN:O	3:W:207:LYS:HB2	1.95	0.66
12:f:774:GLY:C	12:f:776:LEU:N	2.51	0.66
16:D:172:ILE:O	16:D:176:GLU:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:312:GLU:O	18:F:316:GLN:HB3	1.96	0.66
9:c:122:LEU:HB2	9:c:200:TYR:CE1	2.31	0.66
10:d:122:LEU:HB2	10:d:125:LYS:HB2	1.77	0.66
7:a:231:GLN:O	7:a:235:ASP:HB2	1.96	0.65
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.79	0.65
1:U:173:VAL:HG13	1:U:176:MET:O	1.96	0.65
10:d:52:ARG:NH1	10:d:89:LEU:HD23	2.09	0.65
12:f:331:LEU:HD13	12:f:808:ASN:ND2	2.12	0.65
2:V:84:LYS:HG2	2:V:123:SER:HB2	1.79	0.65
2:V:263:LEU:CD1	2:V:264:TYR:CB	2.73	0.65
10:d:107:LEU:HD12	10:d:140:GLU:HB2	1.79	0.65
12:f:567:LEU:HD11	12:f:775:THR:OG1	1.96	0.65
3:W:356:ASN:O	3:W:360:GLU:N	2.29	0.65
5:Y:233:ARG:N	5:Y:234:PRO:HD2	2.11	0.65
3:W:321:VAL:HG21	3:W:351:TRP:HH2	1.62	0.65
5:Y:122:THR:O	5:Y:126:LYS:HB2	1.95	0.65
12:f:712:LYS:HE3	12:f:782:HIS:NE2	2.12	0.65
7:a:21:VAL:O	7:a:25:LEU:HB2	1.97	0.65
2:V:79:VAL:HG13	2:V:81:GLN:H	1.62	0.65
7:a:321:LYS:HB2	7:a:335:TRP:HB3	1.78	0.65
21:I:85:VAL:O	21:I:89:GLU:HB2	1.97	0.65
3:W:87:ILE:CD1	3:W:91:SER:HB2	2.26	0.65
7:a:341:LEU:HB2	7:a:345:GLN:HE21	1.61	0.65
3:W:317:TRP:HH2	3:W:354:LEU:CD1	2.09	0.65
16:D:87:LEU:HB3	17:E:80:VAL:HB	1.78	0.65
2:V:144:ASP:H	2:V:150:ARG:HH22	1.45	0.64
3:W:317:TRP:CZ2	3:W:351:TRP:HE3	1.93	0.64
15:C:90:HIS:CB	15:C:91:PRO:CD	2.75	0.64
21:i:85:VAL:O	21:i:89:GLU:HB2	1.97	0.64
12:f:442:SER:O	12:f:446:LEU:HB2	1.97	0.64
17:E:83:CYS:HB2	17:E:89:LYS:HE2	1.79	0.64
8:b:21:PHE:HE2	8:b:144:GLY:CA	2.10	0.64
19:g:133:PRO:HG2	25:m:14:PHE:HE2	1.61	0.64
3:W:169:LEU:O	3:W:182:ARG:NH1	2.30	0.64
5:Y:40:GLU:O	5:Y:44:ALA:HB2	1.97	0.64
8:b:22:LEU:HD21	8:b:177:PRO:O	1.96	0.64
8:b:51:LEU:HD12	8:b:51:LEU:O	1.98	0.64
10:d:103:LEU:HD13	10:d:118:GLU:OE1	1.97	0.64
11:e:42:ASN:O	11:e:46:ASP:HB2	1.97	0.64
23:k:100:TRP:O	30:r:57:ARG:NH2	2.30	0.64
24:l:14:SER:HB3	24:l:18:ARG:H	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.80	0.64
12:f:276:GLU:O	12:f:286:LYS:NZ	2.31	0.64
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.79	0.64
10:d:45:LYS:HB3	10:d:45:LYS:HZ3	1.60	0.64
11:e:56:LEU:HG	11:e:59:GLU:OE1	1.97	0.64
22:J:52:LYS:HD2	22:J:52:LYS:N	2.13	0.64
14:B:279:PRO:HA	14:B:324:ASP:O	1.98	0.64
21:I:24:ALA:O	21:I:27:ALA:N	2.30	0.64
1:U:26:LYS:HD3	10:d:34:ASN:HD21	1.63	0.64
3:W:162:ALA:HB1	3:W:192:LEU:HB3	1.79	0.64
7:a:159:SER:O	7:a:163:TYR:HB2	1.98	0.64
7:a:227:ASN:O	7:a:231:GLN:NE2	2.31	0.64
10:d:30:LEU:HD13	10:d:35:PHE:CE1	2.33	0.64
12:f:773:LYS:HA	12:f:773:LYS:CE	2.28	0.64
24:L:14:SER:HB3	24:L:18:ARG:H	1.61	0.64
2:V:461:LYS:HE3	2:V:463:MET:HB2	1.79	0.64
2:V:496:PHE:H	2:V:497:PRO:HD2	1.56	0.64
6:Z:212:LEU:HD23	6:Z:212:LEU:O	1.98	0.64
9:c:163:ILE:HG22	9:c:199:HIS:C	2.23	0.64
14:B:418:ASP:O	14:B:422:SER:HB2	1.97	0.64
16:D:163:MET:HA	16:D:222:HIS:HE1	1.63	0.64
13:A:355:PHE:O	13:A:359:ALA:HB3	1.97	0.63
29:q:19:ARG:HH21	29:q:31:ASP:HB2	1.63	0.63
2:V:397:ARG:NH1	10:d:116:HIS:ND1	2.47	0.63
5:Y:234:PRO:O	5:Y:237:ARG:HG3	1.99	0.63
8:b:34:ASN:O	8:b:38:HIS:ND1	2.30	0.63
12:f:759:LEU:HD12	12:f:806:VAL:HG12	1.80	0.63
13:A:49:GLU:HG3	14:B:65:LEU:HD11	1.81	0.63
15:C:90:HIS:CG	15:C:91:PRO:HD2	2.24	0.63
16:D:91:GLN:NE2	16:D:127:ASN:CB	2.57	0.63
29:Q:19:ARG:HH21	29:Q:31:ASP:HB2	1.63	0.63
1:U:176:MET:SD	1:U:179:TYR:CZ	2.91	0.63
3:W:92:LYS:HB3	3:W:94:ARG:HG2	1.80	0.63
12:f:772:GLY:O	12:f:807:ARG:NH2	2.31	0.63
18:F:232:GLY:HA2	36:F:501:ADP:H5'2	1.81	0.63
23:K:167:ALA:H	24:L:56:LEU:HD13	1.63	0.63
12:f:283:THR:O	12:f:287:ASP:CB	2.45	0.63
2:V:201:ARG:HE	2:V:242:HIS:HB3	1.62	0.63
3:W:349:LYS:O	3:W:353:ASP:N	2.32	0.63
7:a:14:SER:HB2	7:a:18:GLN:HG2	1.80	0.63
12:f:838:ARG:HB3	12:f:839:PRO:HD2	1.70	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:244:PRO:HB3	16:D:291:GLU:HG3	1.81	0.63
25:M:41:CYS:HB2	25:M:186:CYS:SG	2.39	0.63
3:W:65:ARG:HG3	3:W:67:LEU:H	1.64	0.62
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.80	0.62
15:C:127:LEU:CB	15:C:128:PRO:CD	2.77	0.62
27:o:163:ILE:HG12	27:o:170:GLY:HA2	1.81	0.62
1:U:456:ASP:O	1:U:460:TYR:HB3	1.99	0.62
22:J:56:GLU:HB2	22:J:59:VAL:HG12	1.81	0.62
21:i:3:ARG:HB2	22:j:5:ARG:HH12	1.64	0.62
2:V:218:TYR:HA	2:V:222:ASP:HB2	1.82	0.62
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.82	0.62
10:d:49:ILE:HD13	10:d:89:LEU:CD2	2.29	0.62
16:D:341:LYS:HE2	16:D:370:ILE:HG21	1.77	0.62
16:D:345:PHE:HB3	16:D:360:LEU:HD23	1.80	0.62
21:I:213:ILE:O	21:I:227:VAL:HG13	2.00	0.62
2:V:258:TYR:O	2:V:262:SER:CA	2.47	0.62
6:Z:73:ASP:OD1	6:Z:77:ASN:ND2	2.33	0.62
1:U:10:SER:HB2	10:d:73:ARG:HA	1.81	0.62
7:a:186:LYS:HA	7:a:186:LYS:CE	2.29	0.62
11:e:56:LEU:HB3	11:e:59:GLU:HB2	1.82	0.62
10:d:48:LEU:O	10:d:52:ARG:HB2	1.99	0.62
2:V:150:ARG:O	2:V:154:ALA:HB3	1.99	0.62
2:V:258:TYR:O	2:V:262:SER:HB3	2.00	0.62
6:Z:211:TYR:C	6:Z:213:GLU:H	2.08	0.62
10:d:95:MET:O	10:d:99:LEU:HB2	1.99	0.62
17:E:101:ASP:HB3	17:E:106:THR:H	1.65	0.62
27:O:163:ILE:HG12	27:O:170:GLY:HA2	1.82	0.62
1:U:512:ALA:O	1:U:516:LEU:HB2	1.99	0.62
4:X:84:LYS:O	4:X:88:LEU:HB2	2.00	0.62
9:c:64:ASP:OD1	9:c:139:ARG:NH2	2.33	0.62
12:f:772:GLY:O	12:f:807:ARG:NH1	2.32	0.62
29:Q:27:GLN:NE2	29:q:169:LYS:O	2.31	0.62
2:V:151:THR:O	2:V:155:ALA:HB2	2.00	0.62
2:V:322:VAL:HB	2:V:325:LYS:HB3	1.82	0.62
5:Y:29:PRO:HB2	5:Y:32:ARG:HB3	1.81	0.62
12:f:281:ILE:H	12:f:281:ILE:CD1	2.00	0.62
12:f:744:MET:O	12:f:748:LEU:HB2	1.99	0.62
17:E:342:ASP:OD2	17:E:378:LYS:NZ	2.33	0.62
21:I:216:LEU:CB	21:I:225:ILE:HG13	2.29	0.62
13:A:400:ARG:HH11	13:A:400:ARG:CG	2.12	0.61
1:U:17:PRO:HB2	1:U:55:ARG:NH1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:114:GLU:HA	10:d:117:THR:HG21	1.81	0.61
12:f:681:TYR:HD2	12:f:763:ARG:HH12	1.46	0.61
12:f:712:LYS:CE	12:f:782:HIS:CD2	2.73	0.61
12:f:764:LEU:HD23	12:f:764:LEU:H	1.62	0.61
19:g:132:ARG:HB2	25:m:12:SER:HA	1.80	0.61
26:n:120:MET:H	32:t:61:GLN:HE22	1.49	0.61
1:U:47:VAL:O	1:U:51:ASP:HB2	1.99	0.61
13:A:236:CYS:SG	13:A:270:CYS:CB	2.88	0.61
13:A:401:ARG:CZ	13:A:401:ARG:HB2	2.28	0.61
21:I:18:LEU:HD11	21:I:21:VAL:HG22	1.82	0.61
30:r:196:HIS:O	30:r:200:SER:HB3	2.00	0.61
1:U:22:PHE:CZ	1:U:26:LYS:HE3	2.35	0.61
4:X:299:LEU:HD21	4:X:331:LEU:HA	1.82	0.61
8:b:100:ARG:HH12	8:b:105:HIS:HB2	1.65	0.61
9:c:157:ILE:CG2	9:c:205:ILE:HD13	2.30	0.61
16:D:91:GLN:HE22	16:D:127:ASN:HB3	1.65	0.61
25:m:108:LEU:HD21	25:m:139:SER:HB3	1.81	0.61
3:W:88:MET:SD	3:W:88:MET:N	2.64	0.61
9:c:157:ILE:HG23	9:c:157:ILE:O	2.00	0.61
19:G:134:LEU:CD1	19:G:134:LEU:H	2.14	0.61
1:U:77:SER:O	1:U:81:ALA:HB2	2.00	0.61
3:W:49:SER:O	3:W:53:GLN:HB2	2.00	0.61
7:a:64:ILE:O	7:a:68:GLU:HB2	2.01	0.61
9:c:122:LEU:HB2	9:c:200:TYR:CZ	2.36	0.61
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.82	0.61
2:V:258:TYR:O	2:V:262:SER:CB	2.49	0.61
2:V:258:TYR:O	2:V:262:SER:N	2.33	0.61
7:a:188:LEU:CD2	7:a:193:GLN:HE21	1.96	0.61
12:f:39:LYS:O	12:f:43:GLN:HB2	2.01	0.61
14:B:279:PRO:HB3	14:B:324:ASP:OD2	2.01	0.61
30:R:196:HIS:O	30:R:200:SER:HB3	2.00	0.61
7:a:183:VAL:O	7:a:183:VAL:HG22	2.00	0.61
12:f:373:ALA:HB2	12:f:744:MET:HA	1.83	0.61
16:D:336:PRO:O	16:D:341:LYS:NZ	2.34	0.61
3:W:302:TYR:HA	3:W:305:LEU:HB2	1.82	0.61
5:Y:160:ASN:O	5:Y:164:ALA:HB2	2.01	0.61
7:a:148:VAL:O	7:a:148:VAL:HG22	2.00	0.61
12:f:613:LEU:HB2	14:B:74:MET:HE3	1.82	0.61
12:f:673:ARG:HH22	12:f:709:THR:HA	1.65	0.61
14:B:60:LEU:O	14:B:64:LYS:HG3	2.01	0.61
5:Y:36:ALA:O	5:Y:40:GLU:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:157:ILE:CG2	9:c:205:ILE:CD1	2.79	0.61
16:D:335:LEU:HD11	16:D:370:ILE:O	2.01	0.61
2:V:190:ASP:OD1	2:V:234:ARG:NH1	2.33	0.60
4:X:414:LEU:O	4:X:418:ALA:HB3	2.01	0.60
12:f:228:LYS:H	14:B:59:ARG:HH22	1.49	0.60
16:D:369:LYS:H	16:D:369:LYS:CD	2.11	0.60
18:F:83:ASN:ND2	18:F:88:TYR:OH	2.34	0.60
2:V:418:SER:HA	2:V:457:TYR:HA	1.81	0.60
3:W:315:MET:CE	3:W:320:LEU:HB2	2.31	0.60
8:b:142:ASN:HD22	8:b:172:THR:HA	1.66	0.60
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.82	0.60
1:U:376:MET:HA	1:U:739:ALA:HA	1.83	0.60
5:Y:191:ILE:HD11	11:e:40:GLU:HB3	1.82	0.60
10:d:122:LEU:HD12	10:d:122:LEU:O	2.01	0.60
13:A:339:ARG:NH2	18:F:405:MET:SD	2.74	0.60
20:H:69:THR:HG23	20:H:71:HIS:H	1.66	0.60
3:W:364:ARG:HH11	3:W:364:ARG:CG	2.14	0.60
8:b:2:VAL:O	8:b:44:ASN:ND2	2.33	0.60
2:V:194:LYS:HE2	2:V:200:ARG:HH21	1.65	0.60
3:W:83:LEU:HG	3:W:90:LEU:HD23	1.82	0.60
7:a:185:ILE:HG22	7:a:185:ILE:O	2.02	0.60
10:d:89:LEU:HD13	10:d:92:SER:HB3	1.82	0.60
25:M:108:LEU:HD21	25:M:139:SER:HB3	1.81	0.60
2:V:194:LYS:HG3	2:V:200:ARG:HE	1.67	0.60
3:W:83:LEU:HG	3:W:90:LEU:CG	2.31	0.60
6:Z:238:PRO:HG2	9:c:309:PHE:HB3	1.83	0.60
7:a:367:VAL:O	7:a:371:ALA:HB3	2.00	0.60
14:B:103:ARG:NH2	14:B:107:MET:SD	2.73	0.60
20:H:119:GLN:NE2	21:I:82:ASP:OD1	2.32	0.60
3:W:314:LEU:CD2	3:W:358:VAL:HG12	2.31	0.60
5:Y:101:ARG:NH2	5:Y:126:LYS:O	2.34	0.60
12:f:183:PRO:O	12:f:187:LEU:HB3	2.01	0.60
12:f:786:GLN:OE1	12:f:786:GLN:HA	2.00	0.60
3:W:28:LEU:O	3:W:32:ALA:HB2	2.02	0.60
8:b:21:PHE:HE2	8:b:144:GLY:N	2.00	0.60
23:k:76:CYS:SG	23:k:77:ALA:N	2.75	0.60
13:A:210:LYS:NZ	13:A:313:GLY:O	2.35	0.60
31:S:35:ILE:HB	32:T:151:ARG:HH12	1.66	0.60
2:V:97:ALA:H	2:V:107:ARG:HE	1.50	0.60
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.35	0.59
6:Z:135:THR:HG21	6:Z:162:ILE:HD11	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:255:TRP:O	7:a:258:GLN:NE2	2.35	0.59
7:a:342:ASP:OD1	7:a:345:GLN:NE2	2.35	0.59
8:b:18:ASN:ND2	8:b:20:ASP:OD2	2.33	0.59
12:f:759:LEU:HD12	12:f:806:VAL:CG1	2.32	0.59
5:Y:49:ASN:HD21	5:Y:113:ARG:HH11	1.51	0.59
5:Y:233:ARG:NH2	5:Y:306:GLN:NE2	2.49	0.59
9:c:192:LEU:CA	9:c:196:LEU:HD23	2.31	0.59
16:D:68:LEU:O	16:D:72:PHE:HB2	2.02	0.59
27:O:138:PHE:O	27:O:142:PHE:HB2	2.02	0.59
27:o:138:PHE:O	27:o:142:PHE:HB2	2.02	0.59
6:Z:256:GLN:NE2	9:c:295:ASN:O	2.34	0.59
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.84	0.59
14:B:153:ASN:HD22	14:B:156:VAL:HG22	1.67	0.59
15:C:83:LYS:HD2	15:C:105:ILE:HD11	1.85	0.59
16:D:117:SER:HA	16:D:121:ARG:HH22	1.65	0.59
2:V:357:LEU:CD1	2:V:360:TYR:HB3	2.33	0.59
9:c:115:HIS:HB3	9:c:118:PHE:HB2	1.84	0.59
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.84	0.59
14:B:51:LEU:CD1	14:B:64:LYS:NZ	2.65	0.59
14:B:112:LEU:HD12	14:B:148:CYS:HB3	1.85	0.59
17:E:97:ARG:HH12	17:E:114:GLU:HB3	1.65	0.59
23:K:76:CYS:SG	23:K:77:ALA:N	2.75	0.59
31:S:4:PRO:O	32:T:100:ARG:NH2	2.35	0.59
2:V:128:ARG:HE	2:V:167:LEU:HD12	1.67	0.59
2:V:210:CYS:O	2:V:214:HIS:HB2	2.02	0.59
12:f:712:LYS:O	12:f:715:HIS:HB3	2.02	0.59
2:V:163:VAL:HG22	2:V:175:MET:HG2	1.84	0.59
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.59
14:B:196:GLU:OE2	14:B:349:ARG:NH1	2.33	0.59
24:L:117:GLN:NE2	25:M:83:ASP:OD1	2.36	0.59
7:a:148:VAL:CG2	7:a:151:VAL:HB	2.32	0.59
8:b:22:LEU:HD21	8:b:178:SER:HA	1.85	0.59
15:C:90:HIS:NE2	16:D:109:SER:HB2	2.18	0.59
16:D:129:SER:OG	16:D:252:ARG:NH1	2.35	0.59
20:h:69:THR:HG23	20:h:71:HIS:H	1.66	0.59
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.84	0.59
3:W:135:LYS:HZ3	3:W:144:ARG:HH21	1.51	0.59
7:a:186:LYS:N	7:a:186:LYS:HD2	2.18	0.59
15:C:63:LEU:HD12	16:D:79:VAL:HA	1.85	0.59
27:O:7:VAL:HG22	27:O:12:ILE:HG12	1.84	0.59
2:V:62:HIS:O	2:V:66:GLU:HB2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:118:GLU:O	10:d:121:ARG:HB2	2.03	0.59
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.74	0.59
1:U:643:SER:O	1:U:649:ARG:NH1	2.35	0.58
5:Y:329:PHE:HE1	11:e:56:LEU:HD21	1.68	0.58
10:d:18:LYS:O	10:d:22:GLU:HB2	2.03	0.58
12:f:838:ARG:HH11	12:f:838:ARG:CG	2.15	0.58
7:a:142:LEU:HD21	7:a:151:VAL:HG11	1.84	0.58
10:d:2:TYR:O	10:d:25:ARG:NH2	2.36	0.58
12:f:128:VAL:O	12:f:128:VAL:HG12	2.03	0.58
1:U:218:GLN:NE2	1:U:752:THR:O	2.36	0.58
1:U:522:GLY:O	1:U:559:ARG:NH2	2.36	0.58
4:X:327:TYR:O	4:X:331:LEU:HB2	2.03	0.58
12:f:646:MET:HE1	14:B:64:LYS:HG2	1.85	0.58
12:f:759:LEU:HD11	12:f:806:VAL:CB	2.29	0.58
18:F:313:LEU:O	18:F:317:LEU:HB2	2.02	0.58
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.84	0.58
15:C:151:ILE:HG21	15:C:158:ILE:HD11	1.86	0.58
21:i:218:ARG:NH1	21:i:223:THR:OG1	2.36	0.58
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.84	0.58
2:V:494:MET:HE1	6:Z:274:ASN:CB	2.33	0.58
9:c:52:GLU:H	9:c:82:VAL:HG13	1.67	0.58
16:D:115:ILE:HA	16:D:139:LEU:HB2	1.86	0.58
18:F:210:GLU:O	18:F:214:ASN:HB2	2.03	0.58
19:G:134:LEU:N	19:G:134:LEU:HD12	2.19	0.58
29:Q:78:THR:O	29:Q:82:ASN:HB2	2.03	0.58
1:U:155:LEU:O	1:U:158:ARG:NH1	2.35	0.58
1:U:242:LEU:HA	1:U:245:ALA:HB3	1.85	0.58
1:U:362:ASN:HB2	9:c:173:GLU:HB2	1.86	0.58
4:X:397:TYR:O	4:X:401:LEU:HB2	2.03	0.58
5:Y:192:ARG:NH2	5:Y:290:PRO:O	2.36	0.58
16:D:164:TYR:O	16:D:174:LYS:NZ	2.36	0.58
27:o:7:VAL:HG22	27:o:12:ILE:HG12	1.84	0.58
3:W:89:LEU:HD22	3:W:89:LEU:C	2.28	0.58
12:f:759:LEU:CD1	12:f:806:VAL:HG11	2.33	0.58
14:B:51:LEU:HD12	14:B:64:LYS:NZ	2.19	0.58
15:C:196:LYS:NZ	15:C:295:THR:O	2.36	0.58
2:V:497:PRO:CG	2:V:498:PRO:CD	2.73	0.58
12:f:691:PRO:HG3	12:f:713:PHE:CE2	2.38	0.58
13:A:248:LYS:NZ	16:D:278:GLN:OE1	2.35	0.58
19:g:134:LEU:HD12	19:g:134:LEU:N	2.01	0.58
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:1:MET:HG3	3:W:43:VAL:HG11	1.86	0.58
8:b:124:LEU:O	8:b:128:ALA:HB2	2.04	0.58
9:c:38:LEU:HD11	9:c:155:VAL:HG11	1.85	0.58
12:f:369:ARG:HA	12:f:372:LEU:HD13	1.85	0.58
12:f:838:ARG:HG3	12:f:838:ARG:NH1	2.18	0.58
13:A:192:GLU:HB2	13:A:196:LEU:HD13	1.86	0.58
14:B:81:ASN:O	14:B:85:MET:HB3	2.04	0.58
27:O:164:PHE:O	31:s:38:ARG:NH2	2.37	0.58
28:P:58:THR:O	29:Q:85:ARG:NH2	2.36	0.58
4:X:379:ASP:HB3	4:X:384:VAL:H	1.69	0.57
7:a:54:ASP:HB2	7:a:83:VAL:HG22	1.85	0.57
12:f:691:PRO:CG	12:f:713:PHE:HE2	2.16	0.57
18:F:228:PRO:O	18:F:233:LYS:NZ	2.37	0.57
19:G:137:CYS:SG	19:G:138:MET:N	2.77	0.57
22:J:38:ARG:NH1	22:J:181:ILE:O	2.37	0.57
23:K:36:THR:HA	23:K:171:GLY:HA3	1.86	0.57
2:V:168:GLN:HG2	2:V:220:PHE:CE2	2.39	0.57
3:W:407:ASP:H	3:W:413:ILE:HG22	1.69	0.57
6:Z:123:ILE:HB	6:Z:136:GLU:HB3	1.86	0.57
12:f:773:LYS:N	12:f:773:LYS:HE3	2.19	0.57
12:f:838:ARG:HH11	12:f:838:ARG:C	2.12	0.57
21:I:20:GLN:HA	21:I:20:GLN:OE1	1.98	0.57
20:h:100:VAL:HG13	28:p:93:ASN:HD22	1.69	0.57
12:f:691:PRO:CD	12:f:713:PHE:HE2	2.18	0.57
22:j:38:ARG:NH1	22:j:181:ILE:O	2.37	0.57
2:V:259:LEU:HA	2:V:262:SER:HB3	1.85	0.57
3:W:227:TYR:O	3:W:246:HIS:NE2	2.32	0.57
5:Y:104:MET:O	5:Y:108:ALA:HB3	2.03	0.57
9:c:141:VAL:HG22	9:c:161:ARG:HH11	1.68	0.57
12:f:673:ARG:CD	12:f:712:LYS:HE2	2.34	0.57
13:A:85:GLN:HA	13:A:88:GLN:HB3	1.85	0.57
17:E:265:ASP:OD2	17:E:291:ARG:NH1	2.38	0.57
18:F:311:LEU:HD23	18:F:314:LEU:HD12	1.85	0.57
3:W:356:ASN:C	3:W:360:GLU:HB2	2.28	0.57
10:d:36:LEU:HG	10:d:37:PRO:CD	2.28	0.57
12:f:575:ALA:O	12:f:579:ALA:HB3	2.05	0.57
14:B:251:VAL:HG12	14:B:253:SER:H	1.68	0.57
18:F:93:VAL:HA	18:F:124:ILE:HG22	1.86	0.57
21:i:118:LYS:HD3	21:i:152:PRO:HA	1.86	0.57
3:W:309:PHE:CE2	3:W:357:ARG:HB3	2.39	0.57
8:b:52:ILE:HD13	8:b:60:VAL:HA	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.87	0.57
18:F:222:GLY:O	18:F:349:ASP:N	2.36	0.57
31:S:43:CYS:SG	31:S:196:CYS:HB3	2.45	0.57
2:V:371:ASN:OD1	2:V:427:GLN:NE2	2.37	0.57
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.85	0.57
10:d:178:ILE:O	10:d:182:ILE:HB	2.04	0.57
12:f:780:PRO:O	12:f:784:ASP:HB2	2.05	0.57
17:E:304:PRO:O	17:E:309:ARG:NH1	2.38	0.57
25:m:214:SER:HG	25:m:224:HIS:HE2	1.49	0.57
1:U:900:TYR:HB3	1:U:914:LEU:HG	1.86	0.57
28:P:2:SER:N	28:P:5:SER:OG	2.38	0.57
29:q:78:THR:O	29:q:82:ASN:HB2	2.03	0.57
2:V:210:CYS:O	2:V:214:HIS:CB	2.53	0.57
7:a:189:PRO:HB2	7:a:192:GLU:HB3	1.85	0.57
16:D:96:VAL:HG23	16:D:102:ILE:HD11	1.86	0.57
34:E:401:ATP:O3G	18:F:347:ARG:NH2	2.38	0.57
30:R:139:MET:O	30:R:143:TYR:HB2	2.05	0.57
28:p:2:SER:N	28:p:5:SER:OG	2.38	0.57
1:U:169:GLU:HG3	1:U:171:ASN:H	1.70	0.57
3:W:142:ARG:HH21	3:W:181:GLU:HB3	1.69	0.57
5:Y:233:ARG:NH2	5:Y:306:GLN:HE21	2.03	0.57
10:d:114:GLU:CA	10:d:117:THR:HG22	2.35	0.57
31:S:38:ARG:NH2	27:o:164:PHE:O	2.38	0.57
29:q:8:GLN:NE2	29:q:9:GLY:O	2.38	0.57
30:r:139:MET:O	30:r:143:TYR:HB2	2.05	0.57
1:U:603:LEU:HD21	16:D:60:TYR:CD1	2.38	0.56
3:W:144:ARG:HA	3:W:147:LYS:HE3	1.87	0.56
7:a:183:VAL:HG22	7:a:186:LYS:NZ	2.20	0.56
7:a:183:VAL:C	7:a:186:LYS:NZ	2.60	0.56
10:d:45:LYS:HD3	10:d:49:ILE:HG21	1.85	0.56
10:d:47:GLN:HG2	10:d:48:LEU:HG	1.87	0.56
16:D:208:PRO:HB2	17:E:291:ARG:HD3	1.85	0.56
23:k:36:THR:HA	23:k:171:GLY:HA3	1.86	0.56
26:n:32:ASP:OD1	26:n:186:ARG:NH2	2.38	0.56
5:Y:168:ILE:HG23	5:Y:173:ASP:HB2	1.88	0.56
24:L:26:MET:HE1	24:L:148:CYS:HB2	1.87	0.56
24:l:26:MET:HE1	24:l:148:CYS:HB2	1.87	0.56
1:U:46:GLU:HA	1:U:49:TYR:HB3	1.88	0.56
6:Z:10:VAL:HG13	6:Z:163:GLY:HA3	1.86	0.56
6:Z:17:LEU:HD22	9:c:36:LEU:HB3	1.86	0.56
8:b:21:PHE:HE2	8:b:144:GLY:H	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:33:ILE:HG23	9:c:69:VAL:HG13	1.87	0.56
10:d:103:LEU:CD1	10:d:118:GLU:OE1	2.53	0.56
10:d:107:LEU:HD11	10:d:140:GLU:HB2	1.87	0.56
11:e:54:ASN:OD1	11:e:57:ARG:NH2	2.39	0.56
12:f:150:GLU:O	12:f:156:HIS:ND1	2.39	0.56
12:f:673:ARG:HH21	12:f:712:LYS:CG	2.15	0.56
12:f:755:ASP:HB2	12:f:756:PRO:HD3	1.87	0.56
12:f:813:LYS:HD3	12:f:815:HIS:HE1	1.70	0.56
13:A:56:LEU:HD12	14:B:72:LEU:HD21	1.88	0.56
14:B:221:GLY:HA3	14:B:347:ILE:HA	1.87	0.56
18:F:138:GLY:HA3	18:F:159:LEU:HD11	1.87	0.56
21:I:118:LYS:HD3	21:I:152:PRO:HA	1.86	0.56
32:T:49:THR:HB	32:T:85:PRO:HG3	1.87	0.56
23:k:183:GLU:HG3	23:k:184:VAL:HG13	1.87	0.56
1:U:416:GLU:OE1	1:U:450:HIS:NE2	2.38	0.56
2:V:200:ARG:HD2	2:V:242:HIS:HB2	1.87	0.56
7:a:93:ALA:O	7:a:97:LEU:CB	2.53	0.56
7:a:148:VAL:HG22	7:a:152:HIS:H	1.70	0.56
10:d:35:PHE:N	10:d:35:PHE:CD1	2.73	0.56
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.86	0.56
13:A:51:ASP:O	13:A:55:LEU:HB2	2.05	0.56
16:D:212:LYS:NZ	34:D:501:ATP:O1G	2.38	0.56
31:S:147:PRO:HB2	28:p:149:MET:HE3	1.86	0.56
1:U:729:GLY:O	1:U:733:ALA:HB2	2.05	0.56
10:d:97:GLN:HE21	10:d:132:TYR:HD2	1.53	0.56
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.87	0.56
23:K:183:GLU:HG3	23:K:184:VAL:HG13	1.87	0.56
25:M:41:CYS:HG	25:M:189:ILE:HG21	1.68	0.56
3:W:274:VAL:HG13	3:W:286:LEU:HD21	1.87	0.56
13:A:101:ILE:HD12	13:A:138:MET:HB3	1.88	0.56
15:C:141:GLU:O	16:D:323:ARG:NH1	2.38	0.56
27:o:1:THR:N	27:o:168:GLY:O	2.38	0.56
3:W:349:LYS:O	3:W:353:ASP:CB	2.54	0.56
30:R:196:HIS:O	30:R:200:SER:CB	2.54	0.56
27:o:41:ILE:HG12	27:o:102:GLY:HA3	1.88	0.56
31:s:27:THR:HB	31:s:40:SER:H	1.70	0.56
1:U:593:SER:OG	1:U:595:ASN:ND2	2.39	0.56
2:V:98:LEU:HA	2:V:104:THR:HG22	1.87	0.56
12:f:713:PHE:O	12:f:713:PHE:HD1	1.88	0.56
17:E:194:ASN:HB3	17:E:228:CYS:HA	1.86	0.56
32:t:180:ASP:HB3	32:t:183:SER:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.88	0.56
13:A:252:GLU:OE2	13:A:255:ARG:NH1	2.39	0.56
18:F:97:LEU:HB2	18:F:121:CYS:HB2	1.88	0.56
26:N:32:ASP:OD1	26:N:186:ARG:NH2	2.38	0.56
29:Q:8:GLN:NE2	29:Q:9:GLY:O	2.38	0.56
27:o:30:ASN:OD1	27:o:187:ARG:NH2	2.38	0.56
30:r:196:HIS:O	30:r:200:SER:CB	2.54	0.56
1:U:59:PHE:HA	1:U:62:LEU:HD13	1.88	0.56
1:U:177:LEU:HD11	1:U:205:TYR:HE1	1.70	0.56
7:a:19:PRO:HA	7:a:22:TRP:HD1	1.71	0.56
12:f:335:ARG:HB3	12:f:853:VAL:HG21	1.87	0.56
21:I:119:GLN:NE2	22:J:79:ASP:OD1	2.39	0.56
27:O:1:THR:N	27:O:168:GLY:O	2.38	0.56
32:t:27:LEU:HD11	32:t:34:ALA:HB1	1.88	0.56
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.88	0.55
2:V:247:GLN:NE2	2:V:276:PHE:O	2.39	0.55
5:Y:367:GLN:HE21	5:Y:371:LYS:HE2	1.71	0.55
10:d:121:ARG:HH11	10:d:121:ARG:CG	2.18	0.55
12:f:135:GLY:O	12:f:139:CYS:HB2	2.06	0.55
12:f:213:GLN:NE2	12:f:246:SER:OG	2.39	0.55
32:t:49:THR:HB	32:t:85:PRO:HG3	1.87	0.55
1:U:496:LEU:HA	1:U:499:THR:HG22	1.89	0.55
3:W:83:LEU:CG	3:W:90:LEU:CD2	2.84	0.55
6:Z:149:THR:CB	6:Z:150:PRO:HD2	2.18	0.55
7:a:324:ILE:HA	7:a:331:VAL:HG12	1.88	0.55
9:c:89:PRO:O	9:c:93:ALA:HB2	2.05	0.55
10:d:49:ILE:HD13	10:d:89:LEU:HD23	1.87	0.55
29:Q:155:ARG:HA	29:Q:158:GLU:HG2	1.88	0.55
32:T:180:ASP:HB3	32:T:183:SER:HB3	1.88	0.55
24:l:66:VAL:HA	24:l:89:ARG:HE	1.72	0.55
25:m:175:GLU:HA	25:m:178:LYS:HD3	1.88	0.55
25:m:241:GLU:O	25:m:244:LYS:NZ	2.35	0.55
31:s:153:VAL:HG13	31:s:166:LEU:HD11	1.89	0.55
1:U:14:GLU:HG3	1:U:16:GLU:H	1.71	0.55
10:d:61:TRP:HA	10:d:64:LEU:HD13	1.88	0.55
12:f:291:GLN:HE22	12:f:324:VAL:HG11	1.72	0.55
15:C:127:LEU:CD2	16:D:96:VAL:HG21	2.29	0.55
21:I:225:ILE:O	21:I:225:ILE:HD13	2.06	0.55
27:O:30:ASN:OD1	27:O:187:ARG:NH2	2.38	0.55
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.89	0.55
10:d:30:LEU:HD13	10:d:35:PHE:CZ	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:167:PRO:O	17:E:274:LYS:NZ	2.34	0.55
19:G:120:ASP:OD1	20:H:84:ARG:NH1	2.40	0.55
26:n:18:SER:HB2	26:n:31:THR:H	1.71	0.55
1:U:22:PHE:CZ	10:d:34:ASN:OD1	2.53	0.55
1:U:44:LYS:HD3	1:U:47:VAL:HG21	1.89	0.55
2:V:228:ARG:O	2:V:232:HIS:ND1	2.39	0.55
6:Z:223:ASN:HB3	6:Z:227:ILE:HG12	1.89	0.55
7:a:183:VAL:HG21	7:a:186:LYS:O	2.07	0.55
8:b:101:GLN:OE1	9:c:101:GLN:NE2	2.39	0.55
9:c:254:ASN:OD1	9:c:278:GLN:NE2	2.40	0.55
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.88	0.55
14:B:111:THR:HB	14:B:124:SER:HB2	1.86	0.55
16:D:341:LYS:HE2	16:D:370:ILE:CG2	2.32	0.55
17:E:345:ASN:O	17:E:349:GLU:HB2	2.06	0.55
24:L:157:ARG:NH2	25:M:56:LYS:O	2.39	0.55
26:N:18:SER:HB2	26:N:31:THR:H	1.71	0.55
5:Y:47:ASP:OD2	5:Y:113:ARG:NH2	2.40	0.55
10:d:113:ALA:O	10:d:117:THR:HG22	2.06	0.55
16:D:353:ASN:ND2	16:D:393:ILE:HG12	2.17	0.55
16:D:391:ARG:NH2	16:D:398:ASP:OD2	2.39	0.55
21:I:133:SER:HB2	21:I:152:PRO:HD3	1.89	0.55
19:g:164:LYS:NZ	20:h:57:TYR:O	2.40	0.55
23:k:99:HIS:HB2	23:k:107:MET:HE3	1.89	0.55
29:q:155:ARG:HA	29:q:158:GLU:HG2	1.88	0.55
5:Y:101:ARG:HE	5:Y:127:THR:HA	1.71	0.55
15:C:60:ARG:NH2	16:D:71:GLU:OE2	2.39	0.55
24:L:66:VAL:HA	24:L:89:ARG:HE	1.72	0.55
27:O:41:ILE:HG12	27:O:102:GLY:HA3	1.88	0.55
21:i:40:ASN:ND2	21:i:182:GLY:O	2.40	0.55
29:q:143:LEU:O	29:q:147:TYR:HB2	2.07	0.55
7:a:183:VAL:HG22	7:a:186:LYS:HZ2	1.72	0.55
12:f:330:PHE:HA	12:f:333:LEU:HB2	1.88	0.55
14:B:51:LEU:CD1	14:B:64:LYS:HZ1	2.18	0.55
28:p:58:THR:OG1	29:q:121:LEU:O	2.20	0.55
2:V:266:GLN:H	2:V:266:GLN:CD	2.14	0.55
8:b:21:PHE:HD1	8:b:177:PRO:HB3	1.72	0.55
16:D:363:TYR:HE2	16:D:399:PHE:HB3	1.72	0.55
25:M:175:GLU:HA	25:M:178:LYS:HD3	1.89	0.55
2:V:259:LEU:HD11	2:V:294:ARG:HD2	1.88	0.55
5:Y:141:VAL:HG13	5:Y:160:ASN:HB2	1.89	0.55
8:b:38:HIS:O	8:b:42:ARG:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:31:VAL:HB	9:c:205:ILE:HG22	1.89	0.55
12:f:739:ALA:HB1	12:f:743:ALA:HB2	1.89	0.55
13:A:49:GLU:N	14:B:65:LEU:CD1	2.62	0.55
17:E:180:LYS:NZ	34:E:401:ATP:O2G	2.40	0.55
29:Q:143:LEU:O	29:Q:147:TYR:HB2	2.07	0.55
31:S:27:THR:HB	31:S:40:SER:H	1.70	0.55
21:i:133:SER:HB2	21:i:152:PRO:HD3	1.89	0.55
22:j:68:ASN:HA	22:j:211:MET:HE1	1.89	0.55
1:U:62:LEU:HD12	1:U:84:ALA:HB1	1.89	0.54
2:V:277:PRO:HD2	2:V:285:TRP:HZ3	1.72	0.54
1:U:640:LEU:HD23	15:C:49:ARG:HH12	1.72	0.54
2:V:325:LYS:HA	2:V:328:VAL:HG12	1.88	0.54
12:f:773:LYS:CE	12:f:773:LYS:CA	2.86	0.54
13:A:189:GLU:OE2	18:F:409:ARG:NH2	2.40	0.54
15:C:90:HIS:CB	15:C:91:PRO:HD3	2.37	0.54
16:D:376:ASN:O	16:D:380:GLN:CB	2.53	0.54
18:F:153:VAL:HG22	18:F:160:ILE:HG22	1.89	0.54
32:T:27:LEU:HD11	32:T:34:ALA:HB1	1.88	0.54
1:U:112:CYS:HA	1:U:115:ASN:HB2	1.89	0.54
3:W:245:LYS:O	3:W:249:ALA:HB2	2.07	0.54
11:e:53:SER:O	11:e:57:ARG:NH2	2.37	0.54
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.88	0.54
12:f:335:ARG:NH2	12:f:338:ASP:OD2	2.40	0.54
12:f:673:ARG:CZ	12:f:712:LYS:CB	2.84	0.54
19:G:41:ALA:HB3	19:G:166:THR:HB	1.90	0.54
23:K:99:HIS:HB2	23:K:107:MET:HE3	1.89	0.54
31:S:28:ARG:NH2	31:S:191:ASP:OD1	2.41	0.54
19:g:41:ALA:HB3	19:g:166:THR:HB	1.90	0.54
12:f:469:TYR:O	12:f:472:HIS:ND1	2.35	0.54
21:I:15:GLU:OE2	21:I:17:ARG:NE	2.41	0.54
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.40	0.54
1:U:163:PHE:HE2	1:U:201:LEU:HD11	1.72	0.54
2:V:89:LYS:HD2	2:V:93:PHE:HE2	1.72	0.54
7:a:70:ARG:HG2	8:b:17:ARG:HB3	1.88	0.54
10:d:181:CYS:HB2	10:d:184:LYS:HE2	1.89	0.54
12:f:704:LEU:O	12:f:708:ASP:HB2	2.07	0.54
18:F:318:ASP:HB3	18:F:347:ARG:HG2	1.88	0.54
23:K:50:VAL:HG11	23:K:66:LYS:HB2	1.90	0.54
23:k:50:VAL:HG11	23:k:66:LYS:HB2	1.90	0.54
1:U:607:VAL:HG11	16:D:63:ASP:HB3	1.89	0.54
3:W:317:TRP:HH2	3:W:354:LEU:HD12	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:559:PRO:HB2	12:f:594:LEU:HG	1.89	0.54
12:f:681:TYR:CD2	12:f:858:LYS:CG	2.63	0.54
12:f:763:ARG:HH11	12:f:763:ARG:CG	2.14	0.54
12:f:766:GLN:OE1	12:f:807:ARG:HD2	2.07	0.54
16:D:50:GLU:HA	16:D:53:PHE:HB3	1.88	0.54
31:S:157:ASN:ND2	28:p:172:LEU:O	2.41	0.54
1:U:798:PRO:O	1:U:880:ASN:ND2	2.39	0.54
2:V:494:MET:O	2:V:494:MET:HG2	2.07	0.54
6:Z:146:ASP:CG	7:a:177:LEU:HD13	2.33	0.54
8:b:121:GLU:HA	8:b:124:LEU:HG	1.90	0.54
10:d:48:LEU:HB3	10:d:88:GLN:HE22	1.70	0.54
12:f:759:LEU:HG	12:f:759:LEU:O	2.07	0.54
16:D:349:THR:HA	16:D:352:MET:HE3	1.88	0.54
23:k:209:LYS:O	23:k:214:ASN:ND2	2.40	0.54
3:W:24:VAL:HG22	3:W:27:ARG:HH12	1.73	0.54
7:a:197:ALA:HB2	7:a:222:LEU:HD22	1.88	0.54
8:b:15:TYR:O	8:b:25:ARG:NH1	2.41	0.54
32:T:27:LEU:HD22	32:T:184:TYR:HB2	1.90	0.54
19:g:144:ASP:HB3	19:g:147:GLN:HB2	1.89	0.54
1:U:219:CYS:SG	1:U:220:LEU:N	2.81	0.54
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.72	0.54
8:b:72:LEU:O	8:b:76:HIS:ND1	2.33	0.54
12:f:42:GLU:O	12:f:46:SER:HB3	2.08	0.54
18:F:282:ILE:HG22	18:F:327:LYS:HB2	1.89	0.54
28:P:126:LEU:HD12	28:P:127:ILE:HG23	1.89	0.54
19:g:38:THR:HA	19:g:169:GLY:HA3	1.90	0.54
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.73	0.54
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.90	0.54
8:b:151:GLU:OE1	8:b:152:LYS:NZ	2.36	0.54
13:A:190:VAL:HG21	13:A:339:ARG:HG3	1.89	0.54
16:D:297:ASP:OD2	16:D:326:ARG:NH2	2.41	0.54
21:I:116:ASP:OD1	22:J:81:ARG:NH1	2.37	0.54
23:K:209:LYS:O	23:K:214:ASN:ND2	2.40	0.54
1:U:261:LEU:HA	1:U:264:VAL:HG12	1.89	0.53
8:b:154:THR:O	8:b:158:ASN:HB2	2.08	0.53
10:d:109:GLN:OE1	10:d:111:ARG:NH1	2.41	0.53
20:H:222:THR:OG1	20:H:225:GLU:OE1	2.26	0.53
1:U:584:TYR:OH	1:U:768:GLN:NE2	2.41	0.53
1:U:780:SER:HA	1:U:783:TYR:HD2	1.73	0.53
2:V:33:GLN:NE2	2:V:118:GLN:OE1	2.41	0.53
3:W:55:ARG:HH22	3:W:78:LYS:HE3	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:287:VAL:O	3:W:291:SER:HB2	2.08	0.53
8:b:52:ILE:CD1	8:b:59:GLU:O	2.55	0.53
30:R:1:THR:N	30:R:169:TYR:O	2.42	0.53
30:R:19:ARG:NH2	28:p:205:ASP:OD2	2.41	0.53
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.90	0.53
7:a:186:LYS:CE	7:a:186:LYS:CA	2.85	0.53
12:f:250:ARG:NH1	12:f:281:ILE:HG13	2.24	0.53
12:f:668:ALA:O	12:f:705:ASN:ND2	2.41	0.53
12:f:713:PHE:CD1	12:f:713:PHE:C	2.86	0.53
21:I:40:ASN:ND2	21:I:182:GLY:O	2.40	0.53
22:J:68:ASN:HA	22:J:211:MET:HE1	1.89	0.53
28:p:126:LEU:HD12	28:p:127:ILE:HG23	1.89	0.53
3:W:135:LYS:HG2	3:W:136:ILE:HD12	1.90	0.53
15:C:89:VAL:HG12	15:C:90:HIS:CD2	2.44	0.53
19:G:32:ILE:HA	19:G:82:GLY:HA2	1.91	0.53
28:P:65:GLN:OE1	29:Q:86:ARG:NH2	2.41	0.53
28:P:124:LEU:HD23	28:P:128:GLY:HA2	1.89	0.53
19:g:32:ILE:HA	19:g:82:GLY:HA2	1.91	0.53
28:p:124:LEU:HD23	28:p:128:GLY:HA2	1.89	0.53
7:a:129:GLN:HG3	7:a:130:VAL:HG23	1.90	0.53
12:f:684:PRO:HA	12:f:687:ARG:HB3	1.91	0.53
14:B:166:ASP:OD2	15:C:78:ARG:NE	2.41	0.53
22:J:86:ARG:HE	22:J:114:LEU:HD11	1.74	0.53
23:K:41:GLN:HA	23:K:46:VAL:HG22	1.91	0.53
28:p:2:SER:OG	28:p:3:ILE:N	2.41	0.53
1:U:30:VAL:HG23	1:U:34:PHE:HE1	1.72	0.53
5:Y:104:MET:O	5:Y:108:ALA:CB	2.57	0.53
6:Z:146:ASP:CG	7:a:178:ARG:HH22	2.16	0.53
26:N:127:ILE:HG12	26:N:132:SER:HB2	1.90	0.53
30:r:1:THR:N	30:r:169:TYR:O	2.42	0.53
31:s:28:ARG:NH2	31:s:191:ASP:OD1	2.41	0.53
32:t:27:LEU:HD22	32:t:184:TYR:HB2	1.90	0.53
4:X:253:TYR:HE1	4:X:318:ILE:HD11	1.73	0.53
5:Y:69:LEU:HA	5:Y:72:LYS:HE3	1.90	0.53
8:b:22:LEU:HD22	8:b:22:LEU:N	2.23	0.53
16:D:233:SER:OG	17:E:259:GLU:OE1	2.26	0.53
19:G:144:ASP:HB3	19:G:147:GLN:HB2	1.89	0.53
3:W:288:HIS:HA	3:W:291:SER:HB3	1.91	0.53
10:d:91:GLU:OE1	10:d:96:HIS:NE2	2.42	0.53
12:f:674:THR:O	12:f:678:LEU:HB3	2.09	0.53
16:D:354:LEU:HD23	16:D:358:VAL:HB	1.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:38:THR:HA	19:G:169:GLY:HA3	1.90	0.53
21:i:15:GLU:OE2	21:i:17:ARG:NE	2.41	0.53
26:n:127:ILE:HG12	26:n:132:SER:HB2	1.90	0.53
31:s:43:CYS:HB2	31:s:196:CYS:SG	2.49	0.53
2:V:467:TYR:O	6:Z:254:ASN:ND2	2.42	0.53
4:X:70:LEU:HD11	4:X:92:LEU:HB3	1.91	0.53
8:b:26:LEU:HD11	8:b:80:PRO:HG3	1.91	0.53
10:d:208:ASP:O	10:d:212:LYS:CB	2.57	0.53
12:f:67:ASP:O	12:f:71:TYR:CB	2.56	0.53
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.90	0.53
14:B:65:LEU:O	14:B:69:LYS:N	2.36	0.53
18:F:313:LEU:O	18:F:317:LEU:CB	2.56	0.53
21:I:223:THR:O	21:I:223:THR:HG22	2.08	0.53
31:S:23:VAL:O	31:S:196:CYS:SG	2.59	0.53
22:j:86:ARG:HE	22:j:114:LEU:HD11	1.74	0.53
7:a:264:ASN:HB3	7:a:267:GLN:HE21	1.74	0.53
19:G:17:SER:OG	19:G:21:ARG:N	2.39	0.53
23:K:48:LEU:HD21	23:K:77:ALA:HB2	1.91	0.53
28:P:149:MET:HE3	31:s:147:PRO:HB2	1.91	0.53
1:U:598:ALA:O	1:U:602:LEU:CB	2.57	0.52
6:Z:193:ASN:OD1	9:c:228:GLY:N	2.37	0.52
15:C:221:GLN:HE22	15:C:228:ALA:HB3	1.73	0.52
22:j:200:GLN:OE1	22:j:202:GLY:N	2.42	0.52
23:k:41:GLN:HA	23:k:46:VAL:HG22	1.91	0.52
25:m:189:ILE:O	25:m:193:VAL:HB	2.10	0.52
2:V:452:ASN:ND2	10:d:187:GLU:OE2	2.41	0.52
8:b:16:MET:HA	8:b:25:ARG:HH11	1.74	0.52
10:d:34:ASN:C	10:d:36:LEU:H	2.16	0.52
12:f:57:GLU:HG2	12:f:93:PRO:HB3	1.91	0.52
12:f:465:LEU:O	12:f:481:SER:OG	2.26	0.52
12:f:673:ARG:HH21	12:f:712:LYS:HG3	1.73	0.52
13:A:274:PHE:HB2	13:A:319:MET:HA	1.92	0.52
15:C:99:VAL:HA	15:C:123:LEU:HB3	1.92	0.52
17:E:313:LEU:O	17:E:317:ALA:HB2	2.08	0.52
18:F:433:ALA:HB3	23:K:20:ARG:HH22	1.74	0.52
19:G:17:SER:HG	19:G:21:ARG:H	1.56	0.52
25:M:8:ASP:O	25:M:22:GLN:NE2	2.42	0.52
31:S:23:VAL:CB	31:S:196:CYS:SG	2.87	0.52
25:m:15:SER:OG	25:m:19:ARG:N	2.41	0.52
29:q:38:MET:O	29:q:65:GLN:NE2	2.42	0.52
3:W:78:LYS:HA	3:W:81:ASP:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:83:LEU:HA	3:W:90:LEU:H	1.74	0.52
5:Y:329:PHE:O	5:Y:333:GLU:HB2	2.10	0.52
7:a:186:LYS:H	7:a:186:LYS:HD2	1.74	0.52
10:d:49:ILE:CD1	10:d:89:LEU:CD2	2.87	0.52
16:D:309:MET:HE1	16:D:327:LEU:HD21	1.91	0.52
17:E:98:VAL:HG12	17:E:110:TYR:HA	1.92	0.52
19:G:155:ASP:OD1	19:G:159:TYR:N	2.41	0.52
22:J:31:THR:HA	22:J:162:GLY:HA3	1.92	0.52
25:M:66:LEU:HD21	25:M:214:SER:HB2	1.91	0.52
25:M:189:ILE:O	25:M:193:VAL:HB	2.10	0.52
1:U:55:ARG:CZ	1:U:55:ARG:CB	2.85	0.52
1:U:646:PRO:HA	1:U:649:ARG:HB2	1.90	0.52
1:U:772:TRP:HB3	1:U:775:LEU:HB2	1.90	0.52
5:Y:312:ARG:HA	5:Y:356:THR:HG22	1.92	0.52
6:Z:146:ASP:CB	7:a:178:ARG:HH22	2.21	0.52
7:a:292:THR:HG23	7:a:295:GLU:H	1.75	0.52
9:c:25:VAL:O	9:c:176:GLN:NE2	2.42	0.52
12:f:213:GLN:O	12:f:217:LEU:HB3	2.10	0.52
15:C:163:GLU:HA	15:C:167:LEU:HD13	1.92	0.52
15:C:370:ALA:HB1	15:C:375:ARG:HB2	1.92	0.52
18:F:272:PHE:HD2	18:F:316:GLN:HG3	1.74	0.52
24:L:72:ILE:HG22	24:L:134:ILE:HG12	1.92	0.52
24:L:139:ASP:H	32:T:81:HIS:HE1	1.58	0.52
1:U:373:ASN:HA	1:U:376:MET:HG2	1.91	0.52
1:U:389:ASN:HD21	1:U:392:TRP:HE3	1.57	0.52
1:U:503:GLN:HB2	1:U:508:THR:HG21	1.91	0.52
2:V:497:PRO:CD	2:V:498:PRO:HD2	2.29	0.52
5:Y:57:LEU:HD11	5:Y:63:TRP:HB2	1.91	0.52
10:d:212:LYS:HD2	10:d:213:ARG:HG2	1.91	0.52
12:f:673:ARG:HD3	12:f:712:LYS:HE2	1.91	0.52
29:Q:36:PHE:HB2	29:Q:44:LEU:HB3	1.91	0.52
29:q:36:PHE:HB2	29:q:44:LEU:HB3	1.91	0.52
3:W:87:ILE:CB	3:W:91:SER:HA	2.14	0.52
12:f:755:ASP:OD1	12:f:756:PRO:HD2	2.08	0.52
16:D:284:GLU:OE1	16:D:287:ARG:NH1	2.43	0.52
17:E:329:GLU:O	17:E:333:LYS:HB2	2.09	0.52
19:G:134:LEU:CD1	19:G:134:LEU:N	2.73	0.52
21:I:17:ARG:CD	21:I:22:GLU:OE2	2.48	0.52
25:M:186:CYS:CB	25:M:189:ILE:HB	2.40	0.52
19:g:138:MET:HB3	19:g:154:CYS:HB3	1.91	0.52
1:U:176:MET:CE	1:U:179:TYR:HH	2.19	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:262:SER:OG	5:Y:267:ARG:O	2.27	0.52
10:d:121:ARG:CA	10:d:121:ARG:NH1	2.73	0.52
12:f:712:LYS:NZ	12:f:781:TYR:CE2	2.78	0.52
13:A:80:LEU:O	13:A:85:GLN:NE2	2.43	0.52
14:B:337:LEU:HD11	14:B:342:ILE:HD11	1.92	0.52
24:l:72:ILE:HG22	24:l:134:ILE:HG12	1.92	0.52
25:m:66:LEU:HD21	25:m:214:SER:HB2	1.91	0.52
1:U:642:GLU:OE1	15:C:57:ARG:NH2	2.42	0.52
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.91	0.52
16:D:407:ILE:HG13	16:D:408:LYS:H	1.75	0.52
20:h:222:THR:OG1	20:h:225:GLU:OE1	2.26	0.52
23:k:48:LEU:HD21	23:k:77:ALA:HB2	1.91	0.52
2:V:313:LEU:HD21	2:V:329:HIS:HE1	1.74	0.52
3:W:112:VAL:HA	3:W:120:ILE:HD11	1.91	0.52
6:Z:25:ARG:HH12	9:c:99:LEU:HD13	1.74	0.52
8:b:100:ARG:NH1	8:b:102:GLY:O	2.43	0.52
12:f:282:PHE:HE2	12:f:284:SER:HB2	1.73	0.52
13:A:189:GLU:O	13:A:193:THR:OG1	2.28	0.52
16:D:200:ARG:HH22	16:D:301:GLN:H	1.56	0.52
22:J:54:GLN:HE21	22:J:54:GLN:CA	2.14	0.52
5:Y:88:LEU:HA	5:Y:100:ILE:HG12	1.92	0.52
8:b:22:LEU:CD2	8:b:22:LEU:N	2.73	0.52
10:d:183:GLU:HA	10:d:215:TRP:HE1	1.75	0.52
12:f:814:SER:HA	12:f:882:LEU:HD12	1.90	0.52
17:E:199:VAL:HG23	17:E:201:SER:H	1.74	0.52
25:M:241:GLU:O	25:M:244:LYS:NZ	2.35	0.52
5:Y:293:ARG:HH12	11:e:57:ARG:HA	1.74	0.51
7:a:43:ASP:HA	7:a:46:GLN:HG2	1.92	0.51
12:f:167:ALA:HA	12:f:170:TRP:HD1	1.75	0.51
22:J:11:SER:OG	22:J:15:HIS:N	2.43	0.51
29:Q:38:MET:O	29:Q:65:GLN:NE2	2.42	0.51
7:a:132:LYS:O	7:a:136:GLU:HB2	2.09	0.51
9:c:84:VAL:HG21	9:c:126:ASP:OD1	2.10	0.51
12:f:294:MET:HB2	12:f:320:ILE:HG22	1.92	0.51
12:f:625:LYS:HB2	12:f:628:ASP:HB3	1.91	0.51
24:L:48:ALA:HB1	24:L:62:LYS:HE3	1.93	0.51
25:M:35:THR:HA	25:M:166:GLY:HA3	1.92	0.51
2:V:106:ARG:O	2:V:110:HIS:ND1	2.44	0.51
3:W:260:SER:O	3:W:264:GLN:N	2.43	0.51
3:W:268:LYS:NZ	3:W:302:TYR:OH	2.40	0.51
7:a:21:VAL:HA	7:a:24:ARG:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:186:LYS:N	7:a:186:LYS:CD	2.73	0.51
10:d:235:THR:O	10:d:239:SER:N	2.44	0.51
14:B:405:MET:HE2	14:B:421:LYS:HD2	1.92	0.51
22:j:11:SER:OG	22:j:15:HIS:N	2.43	0.51
22:j:31:THR:HA	22:j:162:GLY:HA3	1.92	0.51
23:k:97:GLN:HB3	30:r:61:ARG:HG3	1.91	0.51
24:l:117:GLN:O	24:l:120:THR:OG1	2.27	0.51
25:m:35:THR:HA	25:m:166:GLY:HA3	1.92	0.51
26:n:19:ARG:NH1	26:n:168:GLY:O	2.43	0.51
22:j:73:PHE:HA	22:j:131:ALA:HA	1.92	0.51
29:q:141:SER:O	29:q:145:ARG:HB2	2.10	0.51
2:V:128:ARG:HH21	2:V:167:LEU:HB2	1.74	0.51
5:Y:104:MET:HB2	5:Y:108:ALA:HB2	1.93	0.51
29:Q:141:SER:O	29:Q:145:ARG:HB2	2.10	0.51
24:l:48:ALA:HB1	24:l:62:LYS:HE3	1.93	0.51
29:q:184:ASP:OD1	29:q:187:GLY:N	2.42	0.51
12:f:243:PRO:HA	12:f:247:ALA:HB3	1.92	0.51
13:A:221:GLY:O	13:A:225:CYS:HB2	2.10	0.51
15:C:187:LEU:HB3	15:C:314:LYS:HG2	1.91	0.51
21:I:3:ARG:HB2	22:J:5:ARG:HH12	1.75	0.51
24:L:117:GLN:O	24:L:120:THR:OG1	2.27	0.51
26:N:29:ARG:NH1	27:O:139:GLU:OE2	2.44	0.51
27:O:112:SER:OG	27:O:120:ASP:OD1	2.28	0.51
1:U:213:PHE:HE2	1:U:244:MET:HB2	1.75	0.51
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.92	0.51
2:V:71:THR:HG21	11:e:3:GLU:HB2	1.92	0.51
2:V:126:ALA:HB2	2:V:134:PHE:HE2	1.76	0.51
3:W:165:ILE:HD13	3:W:189:GLN:HB3	1.92	0.51
4:X:297:ARG:HH21	4:X:333:GLN:HE21	1.56	0.51
6:Z:66:SER:OG	6:Z:103:LYS:NZ	2.44	0.51
10:d:118:GLU:O	10:d:118:GLU:HG2	2.09	0.51
13:A:52:ILE:HA	13:A:55:LEU:HB3	1.92	0.51
14:B:150:VAL:HG12	14:B:162:VAL:HG23	1.92	0.51
14:B:183:THR:OG1	14:B:184:TYR:N	2.43	0.51
15:C:196:LYS:HD3	15:C:294:ALA:HB1	1.92	0.51
16:D:83:GLN:HG2	16:D:140:VAL:HG13	1.93	0.51
19:G:138:MET:HB3	19:G:154:CYS:HB3	1.91	0.51
24:L:183:ASN:O	24:L:187:LEU:HB2	2.11	0.51
29:Q:184:ASP:OD1	29:Q:187:GLY:N	2.42	0.51
19:g:17:SER:HG	19:g:21:ARG:H	1.57	0.51
2:V:150:ARG:O	2:V:154:ALA:CB	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:451:ILE:HG23	2:V:458:VAL:HG22	1.93	0.51
5:Y:40:GLU:O	5:Y:44:ALA:CB	2.58	0.51
8:b:124:LEU:HD13	8:b:156:PHE:HB2	1.93	0.51
9:c:51:MET:HA	9:c:82:VAL:HG22	1.92	0.51
12:f:760:PHE:O	12:f:762:VAL:N	2.44	0.51
15:C:373:GLU:HG3	15:C:375:ARG:HG3	1.93	0.51
24:l:117:GLN:NE2	25:m:83:ASP:OD1	2.43	0.51
25:m:8:ASP:O	25:m:22:GLN:NE2	2.42	0.51
27:o:112:SER:OG	27:o:120:ASP:OD1	2.28	0.51
31:s:149:LEU:O	31:s:153:VAL:HB	2.11	0.51
2:V:72:LEU:O	2:V:76:LYS:HB2	2.10	0.51
2:V:322:VAL:HG12	11:e:4:LYS:HE3	1.93	0.51
5:Y:243:GLY:O	5:Y:247:LEU:HB2	2.10	0.51
6:Z:9:VAL:HA	6:Z:48:LEU:HB3	1.92	0.51
12:f:198:HIS:O	12:f:202:HIS:HB2	2.10	0.51
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.92	0.51
14:B:262:ASP:OD1	14:B:265:LYS:NZ	2.44	0.51
15:C:49:ARG:HD2	15:C:49:ARG:C	2.36	0.51
15:C:301:LEU:HD13	15:C:305:LEU:HD23	1.93	0.51
22:J:73:PHE:HA	22:J:131:ALA:HA	1.91	0.51
20:h:34:PRO:HA	20:h:164:GLY:HA3	1.93	0.51
3:W:93:ARG:NE	3:W:133:GLU:OE2	2.44	0.51
17:E:144:GLU:OE2	17:E:297:ARG:NH1	2.44	0.51
30:r:26:ILE:HG21	30:r:29:GLN:HE21	1.76	0.51
1:U:714:SER:HA	1:U:717:ILE:HG22	1.92	0.50
2:V:407:VAL:O	2:V:411:SER:OG	2.29	0.50
7:a:132:LYS:O	7:a:136:GLU:CB	2.59	0.50
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.92	0.50
12:f:78:LEU:HA	12:f:82:ILE:HD11	1.93	0.50
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.93	0.50
12:f:838:ARG:HH11	12:f:838:ARG:HG3	1.74	0.50
17:E:72:LYS:HB2	17:E:78:ARG:HG2	1.92	0.50
19:g:17:SER:OG	19:g:21:ARG:N	2.39	0.50
24:l:183:ASN:O	24:l:187:LEU:HB2	2.11	0.50
27:o:204:CYS:HB2	27:o:208:THR:HG21	1.92	0.50
29:q:23:SER:HB2	29:q:28:MET:HG2	1.93	0.50
1:U:160:LEU:HD21	1:U:196:LYS:HB3	1.92	0.50
1:U:245:ALA:O	1:U:324:LYS:NZ	2.42	0.50
3:W:93:ARG:NH2	3:W:133:GLU:O	2.45	0.50
7:a:12:GLN:HE21	7:a:19:PRO:HB3	1.74	0.50
10:d:48:LEU:O	10:d:52:ARG:CB	2.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Q:23:SER:HB2	29:Q:28:MET:HG2	1.93	0.50
31:s:35:ILE:HB	32:t:151:ARG:HH12	1.74	0.50
1:U:198:LEU:HD23	1:U:223:LEU:HD13	1.93	0.50
1:U:252:LEU:O	1:U:256:ALA:CB	2.59	0.50
6:Z:250:TYR:O	6:Z:254:ASN:CB	2.56	0.50
7:a:100:THR:HA	7:a:103:LYS:HG2	1.94	0.50
16:D:242:GLU:O	16:D:246:MET:HB2	2.11	0.50
17:E:182:LEU:HD22	34:E:401:ATP:H2'	1.92	0.50
23:K:20:ARG:HG2	23:K:21:LEU:H	1.76	0.50
26:N:19:ARG:NH1	26:N:168:GLY:O	2.43	0.50
19:g:137:CYS:SG	19:g:138:MET:N	2.77	0.50
1:U:51:ASP:C	1:U:53:GLY:H	2.19	0.50
1:U:64:ALA:HA	1:U:67:VAL:HG12	1.92	0.50
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.94	0.50
2:V:32:PRO:HA	2:V:35:VAL:HG22	1.94	0.50
9:c:157:ILE:HG21	9:c:205:ILE:HD11	1.91	0.50
12:f:378:ASN:O	12:f:382:ASN:ND2	2.41	0.50
20:H:34:PRO:HA	20:H:164:GLY:HA3	1.93	0.50
19:g:200:THR:HG23	19:g:242:LEU:HD11	1.94	0.50
1:U:74:PHE:O	1:U:78:LEU:CB	2.59	0.50
4:X:173:GLU:HA	4:X:176:THR:HG22	1.92	0.50
7:a:186:LYS:H	7:a:186:LYS:CE	2.25	0.50
12:f:183:PRO:O	12:f:187:LEU:CB	2.60	0.50
16:D:84:SER:O	17:E:68:LYS:NZ	2.45	0.50
19:G:202:LEU:HB2	19:G:206:LEU:HD13	1.92	0.50
27:O:204:CYS:HB2	27:O:208:THR:HG21	1.92	0.50
19:g:202:LEU:HB2	19:g:206:LEU:HD13	1.92	0.50
5:Y:122:THR:O	5:Y:126:LYS:CB	2.59	0.50
6:Z:283:ARG:NH1	6:Z:284:ASP:OD1	2.45	0.50
12:f:64:GLY:HA2	12:f:67:ASP:HB3	1.93	0.50
12:f:439:TYR:OH	12:f:475:ASN:ND2	2.43	0.50
12:f:691:PRO:CD	12:f:713:PHE:CE2	2.93	0.50
12:f:773:LYS:HE3	12:f:773:LYS:H	1.73	0.50
13:A:55:LEU:HD12	13:A:58:LYS:HB2	1.92	0.50
13:A:99:THR:HG22	13:A:115:VAL:HG12	1.93	0.50
14:B:387:LYS:HB3	14:B:390:LEU:HD23	1.94	0.50
15:C:72:TYR:N	15:C:116:LEU:O	2.45	0.50
15:C:381:GLU:O	15:C:385:MET:HB2	2.12	0.50
19:G:200:THR:HG23	19:G:242:LEU:HD11	1.94	0.50
19:g:141:ILE:HG22	19:g:151:VAL:HG22	1.94	0.50
1:U:336:GLU:HA	1:U:339:LEU:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:197:LYS:HD2	3:W:199:TYR:CZ	2.46	0.50
3:W:198:ASP:O	3:W:202:THR:OG1	2.26	0.50
3:W:274:VAL:CG1	3:W:286:LEU:CD2	2.90	0.50
6:Z:15:VAL:HA	6:Z:18:SER:HB3	1.94	0.50
7:a:182:CYS:SG	7:a:183:VAL:N	2.84	0.50
18:F:180:ARG:NH1	18:F:241:ALA:O	2.45	0.50
20:H:4:ARG:NH1	20:H:5:GLY:O	2.44	0.50
25:M:51:LYS:NZ	25:M:62:SER:O	2.33	0.50
25:M:168:ALA:HB1	25:M:171:ALA:HB3	1.94	0.50
1:U:268:LEU:HD22	1:U:329:LEU:HD11	1.93	0.50
1:U:338:HIS:CE1	1:U:785:PRO:HB3	2.47	0.50
1:U:410:VAL:HG23	1:U:448:LEU:HD13	1.94	0.50
1:U:600:ARG:HE	16:D:56:VAL:HG22	1.77	0.50
1:U:603:LEU:HD23	1:U:603:LEU:C	2.37	0.50
1:U:614:VAL:O	1:U:618:ALA:HB2	2.12	0.50
2:V:325:LYS:O	2:V:329:HIS:HB2	2.12	0.50
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.29	0.50
2:V:497:PRO:N	2:V:498:PRO:HD2	2.27	0.50
3:W:239:SER:HB3	3:W:242:SER:HB3	1.93	0.50
3:W:279:PHE:CG	3:W:364:ARG:NH2	2.80	0.50
3:W:355:LYS:O	3:W:355:LYS:HD2	2.11	0.50
4:X:252:LYS:HA	4:X:287:LEU:HD11	1.94	0.50
6:Z:180:LYS:O	16:D:70:LYS:NZ	2.40	0.50
9:c:92:GLN:O	9:c:96:LEU:CB	2.56	0.50
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.94	0.50
12:f:680:ARG:NE	12:f:715:HIS:HE1	2.05	0.50
15:C:372:ARG:HH22	16:D:175:GLN:HE22	1.60	0.50
19:G:141:ILE:HG22	19:G:151:VAL:HG22	1.94	0.50
20:h:4:ARG:NH1	20:h:5:GLY:O	2.44	0.50
23:k:20:ARG:HG2	23:k:21:LEU:H	1.76	0.50
25:m:136:MET:HE3	25:m:163:CYS:HB3	1.94	0.50
1:U:440:GLY:HA2	1:U:473:VAL:HG22	1.93	0.50
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.45	0.50
3:W:68:VAL:HG12	3:W:72:LYS:HE3	1.94	0.50
4:X:421:LEU:HD21	6:Z:280:ILE:HD13	1.94	0.50
7:a:148:VAL:HG22	7:a:152:HIS:HB3	1.94	0.50
13:A:395:PHE:HA	13:A:398:ARG:HG2	1.93	0.50
21:I:109:GLN:OE1	29:Q:71:ASN:ND2	2.42	0.50
26:N:136:TYR:HE2	32:T:33:LEU:HD21	1.77	0.50
25:m:168:ALA:HB1	25:m:171:ALA:HB3	1.94	0.50
25:m:181:MET:N	25:m:181:MET:SD	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:22:PHE:CZ	1:U:26:LYS:CE	2.94	0.49
2:V:172:VAL:O	2:V:176:MET:HB2	2.11	0.49
3:W:89:LEU:HD11	3:W:93:ARG:CD	2.42	0.49
4:X:225:TRP:O	4:X:229:TYR:HB2	2.12	0.49
23:K:43:SER:HA	23:K:151:PRO:HG3	1.93	0.49
25:M:136:MET:HE3	25:M:163:CYS:HB3	1.94	0.49
23:k:43:SER:HA	23:k:151:PRO:HG3	1.93	0.49
2:V:96:ARG:HB3	2:V:98:LEU:HG	1.94	0.49
2:V:328:VAL:O	2:V:332:LEU:HB2	2.11	0.49
3:W:108:CYS:SG	3:W:123:ARG:NE	2.74	0.49
5:Y:53:TYR:O	5:Y:57:LEU:HB2	2.11	0.49
7:a:172:TYR:O	7:a:176:ALA:CB	2.59	0.49
10:d:121:ARG:NH1	10:d:121:ARG:N	2.60	0.49
12:f:217:LEU:HD22	12:f:239:TYR:HE1	1.76	0.49
12:f:403:LYS:O	12:f:406:GLY:N	2.43	0.49
15:C:231:VAL:HG21	15:C:272:THR:HG23	1.94	0.49
18:F:312:GLU:O	18:F:316:GLN:CB	2.60	0.49
30:R:26:ILE:HG21	30:R:29:GLN:HE21	1.76	0.49
19:g:155:ASP:OD1	19:g:159:TYR:N	2.41	0.49
29:q:19:ARG:HH11	29:q:179:SER:HB3	1.77	0.49
2:V:70:VAL:HG21	2:V:209:LYS:HD3	1.94	0.49
6:Z:68:TRP:HE1	6:Z:111:LEU:HD22	1.78	0.49
8:b:6:THR:HB	8:b:49:VAL:HG22	1.94	0.49
12:f:217:LEU:C	12:f:217:LEU:CD1	2.85	0.49
20:H:139:TRP:HA	20:H:144:PRO:HA	1.94	0.49
22:J:54:GLN:HA	22:J:54:GLN:NE2	2.22	0.49
27:O:112:SER:HB3	27:O:125:VAL:HG11	1.94	0.49
29:Q:19:ARG:HH11	29:Q:179:SER:HB3	1.77	0.49
24:l:189:LYS:HZ3	24:l:193:ARG:HH22	1.60	0.49
6:Z:73:ASP:H	8:b:63:THR:HG21	1.78	0.49
9:c:269:GLN:HA	9:c:272:ILE:HG22	1.94	0.49
1:U:758:PRO:HB2	1:U:781:LEU:HB3	1.94	0.49
2:V:163:VAL:HA	2:V:175:MET:HE2	1.94	0.49
2:V:266:GLN:N	2:V:266:GLN:NE2	2.60	0.49
6:Z:146:ASP:OD2	7:a:177:LEU:CD1	2.60	0.49
7:a:160:SER:O	7:a:164:GLN:HB2	2.12	0.49
8:b:21:PHE:HE2	8:b:144:GLY:HA2	1.62	0.49
8:b:24:THR:HG22	8:b:26:LEU:H	1.77	0.49
9:c:78:SER:OG	9:c:85:GLU:HG3	2.12	0.49
12:f:137:ARG:HA	12:f:141:LYS:HD3	1.95	0.49
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:823:ALA:HB1	12:f:825:MET:HG3	1.94	0.49
16:D:411:GLU:HG2	16:D:413:GLU:H	1.78	0.49
21:I:18:LEU:HD11	21:I:21:VAL:HG13	1.94	0.49
24:L:189:LYS:HZ2	24:L:193:ARG:HH22	1.59	0.49
19:g:165:ALA:HB3	20:h:56:LEU:HD22	1.94	0.49
20:h:139:TRP:HA	20:h:144:PRO:HA	1.95	0.49
22:j:31:THR:OG1	22:j:163:ARG:O	2.30	0.49
26:n:138:TYR:O	26:n:142:THR:OG1	2.28	0.49
2:V:135:LEU:HB3	2:V:181:TYR:HE2	1.76	0.49
2:V:284:GLU:O	2:V:288:TYR:CB	2.60	0.49
3:W:315:MET:SD	3:W:320:LEU:CD1	2.91	0.49
5:Y:271:PHE:O	5:Y:275:LEU:HB2	2.12	0.49
12:f:42:GLU:O	12:f:46:SER:CB	2.60	0.49
12:f:169:GLU:HA	12:f:172:GLU:HB3	1.94	0.49
12:f:227:ALA:HB3	12:f:232:TYR:HB2	1.94	0.49
12:f:524:MET:HA	12:f:776:LEU:HD23	1.94	0.49
13:A:49:GLU:HA	14:B:65:LEU:HD13	0.55	0.49
13:A:113:ILE:HD11	13:A:142:VAL:HG21	1.95	0.49
19:G:200:THR:HA	19:G:203:SER:HB2	1.95	0.49
21:i:198:ASN:HA	21:i:206:LEU:HD21	1.95	0.49
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.93	0.49
3:W:28:LEU:O	3:W:32:ALA:CB	2.61	0.49
3:W:89:LEU:C	3:W:89:LEU:CD2	2.86	0.49
10:d:175:ARG:O	10:d:179:ALA:CB	2.60	0.49
12:f:756:PRO:HG2	12:f:758:ASN:O	2.12	0.49
12:f:772:GLY:O	12:f:807:ARG:CZ	2.61	0.49
19:G:132:ARG:NH2	19:G:132:ARG:HG2	2.27	0.49
19:G:165:ALA:HB1	19:G:179:LEU:HD13	1.95	0.49
26:n:40:ARG:NH2	26:n:182:SER:O	2.46	0.49
28:p:125:ASP:OD1	28:p:129:CYS:N	2.40	0.49
1:U:82:LEU:O	1:U:129:ARG:NH2	2.36	0.49
1:U:219:CYS:O	1:U:223:LEU:CB	2.60	0.49
1:U:241:ASN:HD22	1:U:244:MET:HE3	1.76	0.49
6:Z:85:VAL:HA	9:c:76:PRO:HB3	1.95	0.49
6:Z:138:TYR:HA	6:Z:157:HIS:HA	1.95	0.49
12:f:137:ARG:HH21	12:f:159:VAL:HG22	1.77	0.49
12:f:438:ASP:HA	12:f:477:MET:HE2	1.94	0.49
21:I:214:ALA:CB	21:I:227:VAL:HG22	2.43	0.49
22:J:31:THR:OG1	22:J:163:ARG:O	2.30	0.49
23:K:199:LEU:HD11	23:K:217:LEU:HD11	1.95	0.49
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:177:LEU:HD13	1:U:177:LEU:O	2.13	0.49
2:V:193:GLN:O	2:V:199:ASN:ND2	2.45	0.49
3:W:321:VAL:HG21	3:W:351:TRP:CH2	2.43	0.49
3:W:390:GLU:HG3	3:W:408:ARG:HH21	1.78	0.49
5:Y:282:MET:HG3	5:Y:288:PHE:HB3	1.94	0.49
12:f:437:GLU:HG3	12:f:440:ILE:HD12	1.95	0.49
12:f:567:LEU:CD1	12:f:775:THR:OG1	2.60	0.49
12:f:733:GLY:O	12:f:746:ARG:NH1	2.38	0.49
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.93	0.49
26:n:144:ARG:H	26:n:147:MET:HE3	1.78	0.49
1:U:381:THR:HG22	1:U:412:HIS:HA	1.93	0.49
2:V:183:GLU:HA	2:V:186:LYS:HB3	1.95	0.49
4:X:214:SER:O	4:X:218:HIS:ND1	2.42	0.49
17:E:215:ILE:HD13	17:E:260:LEU:HB2	1.95	0.49
17:E:313:LEU:O	17:E:317:ALA:CB	2.61	0.49
21:I:41:ASP:OD1	21:I:41:ASP:N	2.46	0.49
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.94	0.49
1:U:495:ASP:OD1	1:U:498:LYS:NZ	2.41	0.48
5:Y:17:LEU:HD22	5:Y:212:GLU:HB2	1.95	0.48
8:b:139:ASP:OD1	8:b:169:HIS:N	2.45	0.48
10:d:121:ARG:HH11	10:d:121:ARG:N	2.11	0.48
15:C:126:ILE:N	15:C:126:ILE:CD1	2.73	0.48
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.95	0.48
30:R:141:ARG:NH2	29:q:162:LYS:O	2.46	0.48
19:g:200:THR:HA	19:g:203:SER:HB2	1.95	0.48
1:U:220:LEU:HA	1:U:223:LEU:HB3	1.94	0.48
2:V:198:GLN:O	2:V:202:ALA:HB3	2.13	0.48
6:Z:78:MET:HB2	9:c:98:MET:HE2	1.93	0.48
7:a:221:VAL:HG23	7:a:222:LEU:HG	1.93	0.48
7:a:294:GLU:OE2	7:a:298:LYS:NZ	2.47	0.48
8:b:25:ARG:NH2	8:b:145:GLU:OE1	2.43	0.48
12:f:137:ARG:O	12:f:141:LYS:HB2	2.13	0.48
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.95	0.48
13:A:287:ASP:N	13:A:287:ASP:OD1	2.46	0.48
20:H:71:HIS:HA	20:H:218:PHE:H	1.78	0.48
21:I:218:ARG:NH2	21:I:220:ASN:O	2.46	0.48
25:M:15:SER:OG	25:M:19:ARG:N	2.41	0.48
31:S:149:LEU:O	31:S:153:VAL:HB	2.11	0.48
32:T:136:SER:HB2	32:T:150:LEU:HD13	1.95	0.48
23:k:199:LEU:HD11	23:k:217:LEU:HD11	1.95	0.48
24:l:189:LYS:HG3	24:l:193:ARG:HH12	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:21:GLU:HA	1:U:24:LEU:HG	1.95	0.48
1:U:21:GLU:HG2	1:U:55:ARG:O	2.13	0.48
1:U:252:LEU:O	1:U:256:ALA:HB3	2.12	0.48
1:U:402:PHE:HB2	1:U:437:TYR:HB3	1.95	0.48
5:Y:168:ILE:HG21	5:Y:177:ARG:HB2	1.94	0.48
5:Y:173:ASP:H	15:C:335:LYS:HA	1.79	0.48
9:c:154:LYS:HD2	9:c:156:VAL:HG22	1.94	0.48
21:I:13:SER:CB	21:I:19:TYR:CE2	2.96	0.48
21:i:197:LEU:O	21:i:201:MET:CB	2.61	0.48
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.79	0.48
6:Z:43:TRP:HB3	6:Z:48:LEU:HD22	1.95	0.48
7:a:245:VAL:O	7:a:249:GLN:HB2	2.13	0.48
10:d:137:VAL:O	10:d:141:GLN:HB2	2.13	0.48
12:f:709:THR:O	12:f:713:PHE:HB2	2.14	0.48
14:B:74:MET:O	14:B:78:PHE:CB	2.60	0.48
14:B:249:ARG:HG3	14:B:283:PHE:HD2	1.78	0.48
21:I:213:ILE:HB	21:I:228:LEU:HD11	1.95	0.48
20:h:71:HIS:HA	20:h:218:PHE:H	1.78	0.48
20:h:150:ASP:OD1	20:h:154:ALA:N	2.46	0.48
21:i:218:ARG:NH2	21:i:220:ASN:O	2.46	0.48
1:U:469:SER:OG	1:U:470:ASN:N	2.47	0.48
2:V:40:GLU:HA	2:V:43:THR:HB	1.96	0.48
3:W:52:LYS:HD3	3:W:55:ARG:HD3	1.94	0.48
12:f:232:TYR:HE2	12:f:263:PRO:HG2	1.78	0.48
12:f:773:LYS:HE3	12:f:773:LYS:CA	2.43	0.48
12:f:773:LYS:C	12:f:775:THR:H	2.20	0.48
14:B:93:GLU:O	14:B:97:SER:CB	2.62	0.48
26:N:40:ARG:NH2	26:N:182:SER:O	2.46	0.48
27:O:143:ARG:NH2	27:O:150:GLU:OE1	2.47	0.48
29:q:85:ARG:HG2	29:q:122:ALA:HB1	1.95	0.48
29:q:148:THR:HG22	29:q:150:THR:H	1.78	0.48
31:s:4:PRO:O	32:t:100:ARG:NH2	2.46	0.48
1:U:133:ILE:HA	1:U:136:LYS:HB3	1.96	0.48
10:d:116:HIS:HA	10:d:119:LEU:HD23	1.95	0.48
21:I:85:VAL:O	21:I:89:GLU:CB	2.62	0.48
21:I:198:ASN:HA	21:I:206:LEU:HD21	1.95	0.48
25:M:41:CYS:SG	25:M:186:CYS:SG	3.11	0.48
28:P:125:ASP:OD1	28:P:129:CYS:N	2.40	0.48
1:U:337:LEU:HD21	1:U:789:ILE:HG21	1.96	0.48
2:V:441:ALA:O	2:V:446:VAL:N	2.46	0.48
2:V:494:MET:HE2	6:Z:275:LEU:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:317:TRP:CZ3	3:W:354:LEU:HB3	2.49	0.48
5:Y:173:ASP:HA	15:C:334:ARG:HG3	1.94	0.48
10:d:45:LYS:HG2	10:d:45:LYS:O	2.13	0.48
10:d:121:ARG:CG	10:d:121:ARG:NH1	2.76	0.48
12:f:606:VAL:HG21	14:B:67:ARG:HG2	1.94	0.48
15:C:78:ARG:HH12	15:C:80:MET:HE3	1.77	0.48
26:N:144:ARG:H	26:N:147:MET:HE3	1.78	0.48
28:P:2:SER:OG	28:P:3:ILE:N	2.41	0.48
29:Q:4:LEU:HD22	29:Q:45:LEU:HB3	1.95	0.48
1:U:241:ASN:HB3	1:U:244:MET:HG2	1.95	0.48
4:X:335:LEU:HD21	4:X:365:LEU:HD21	1.95	0.48
9:c:157:ILE:CG2	9:c:205:ILE:HD11	2.44	0.48
13:A:125:LEU:HD23	13:A:129:VAL:HG23	1.95	0.48
14:B:412:MET:HE1	15:C:177:ALA:HB1	1.96	0.48
18:F:97:LEU:N	18:F:121:CYS:O	2.45	0.48
19:G:203:SER:O	19:G:207:SER:HA	2.14	0.48
21:I:15:GLU:HG3	21:I:17:ARG:HG2	1.96	0.48
21:I:90:LEU:HA	21:I:93:ILE:HD12	1.96	0.48
27:o:46:ALA:HB3	27:o:97:ALA:HB3	1.95	0.48
2:V:156:SER:HA	2:V:159:LEU:HB2	1.96	0.48
3:W:187:LEU:HA	3:W:190:MET:HE3	1.95	0.48
5:Y:60:SER:OG	5:Y:61:LEU:N	2.46	0.48
6:Z:26:ILE:HD13	6:Z:33:LYS:HD3	1.95	0.48
8:b:18:ASN:OD1	8:b:20:ASP:OD1	2.31	0.48
10:d:108:SER:C	10:d:110:ASN:H	2.22	0.48
12:f:754:LYS:O	12:f:754:LYS:HG2	2.13	0.48
14:B:279:PRO:CB	14:B:324:ASP:OD2	2.61	0.48
16:D:91:GLN:HE21	16:D:127:ASN:CA	2.26	0.48
27:O:24:MET:HE3	31:s:187:VAL:HG21	1.94	0.48
19:g:49:VAL:HG22	19:g:219:VAL:HG23	1.96	0.48
21:i:15:GLU:HG3	21:i:17:ARG:HG2	1.96	0.48
21:i:41:ASP:OD1	21:i:41:ASP:N	2.46	0.48
25:m:51:LYS:NZ	25:m:62:SER:O	2.32	0.48
27:o:143:ARG:NH2	27:o:150:GLU:OE1	2.47	0.48
32:t:43:MET:HE3	32:t:45:VAL:HG22	1.96	0.48
32:t:136:SER:HB2	32:t:150:LEU:HD13	1.95	0.48
1:U:147:TYR:HA	1:U:150:ALA:HB3	1.96	0.48
5:Y:234:PRO:HA	5:Y:237:ARG:CG	2.43	0.48
7:a:145:LEU:HD13	7:a:146:PRO:HD2	1.96	0.48
7:a:184:ASP:O	7:a:186:LYS:NZ	2.45	0.48
12:f:291:GLN:HE21	12:f:879:ARG:NH2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:770:HIS:C	12:f:770:HIS:ND1	2.72	0.48
13:A:140:VAL:HG12	13:A:152:PRO:HA	1.96	0.48
19:G:49:VAL:HG22	19:G:219:VAL:HG23	1.96	0.48
28:P:26:ARG:HH21	28:P:38:ASP:HA	1.79	0.48
29:Q:148:THR:HG22	29:Q:150:THR:H	1.78	0.48
22:j:119:THR:HG22	22:j:126:PRO:HB3	1.96	0.48
24:l:139:ASP:H	32:t:81:HIS:HE1	1.62	0.48
29:q:4:LEU:HD22	29:q:45:LEU:HB3	1.95	0.48
1:U:791:LEU:O	1:U:914:LEU:N	2.45	0.47
2:V:159:LEU:HG	2:V:182:LYS:HD3	1.96	0.47
2:V:227:VAL:O	2:V:231:LEU:HB2	2.14	0.47
8:b:21:PHE:CZ	8:b:144:GLY:HA2	2.49	0.47
8:b:51:LEU:N	8:b:62:THR:OG1	2.39	0.47
9:c:140:ALA:O	9:c:161:ARG:NE	2.47	0.47
10:d:101:LEU:HD12	10:d:163:TYR:HE1	1.78	0.47
12:f:513:GLU:HA	12:f:557:TRP:HZ3	1.79	0.47
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.95	0.47
15:C:155:ASP:HA	15:C:158:ILE:HD12	1.96	0.47
15:C:186:VAL:HB	15:C:292:ILE:HG12	1.96	0.47
16:D:125:LYS:HD2	16:D:125:LYS:HA	1.61	0.47
16:D:269:ALA:O	17:E:255:ARG:NE	2.44	0.47
17:E:198:VAL:HG12	17:E:200:SER:H	1.79	0.47
17:E:247:THR:O	17:E:251:ARG:NH2	2.47	0.47
21:I:197:LEU:O	21:I:201:MET:CB	2.61	0.47
24:L:216:GLY:HA3	24:L:219:LEU:HB3	1.95	0.47
21:i:90:LEU:HA	21:i:93:ILE:HD12	1.96	0.47
1:U:632:GLN:O	1:U:635:SER:OG	2.28	0.47
1:U:639:LEU:HD21	16:D:61:ILE:HD11	1.95	0.47
2:V:179:LYS:HA	2:V:182:LYS:HE3	1.95	0.47
7:a:186:LYS:H	7:a:186:LYS:CD	2.27	0.47
12:f:265:ALA:HB3	12:f:268:LEU:HB2	1.96	0.47
12:f:305:LEU:HB2	12:f:317:LEU:HD22	1.95	0.47
15:C:337:ASN:ND2	15:C:376:VAL:O	2.47	0.47
20:H:150:ASP:OD1	20:H:154:ALA:N	2.46	0.47
29:Q:85:ARG:HG2	29:Q:122:ALA:HB1	1.95	0.47
31:S:38:ARG:HH12	32:T:151:ARG:HD3	1.79	0.47
26:n:28:ASN:HD21	27:o:122:LEU:HD21	1.80	0.47
1:U:22:PHE:CG	10:d:30:LEU:HD11	2.43	0.47
1:U:328:ILE:HG13	1:U:329:LEU:HG	1.95	0.47
3:W:58:SER:O	3:W:62:SER:OG	2.27	0.47
3:W:117:ASP:HA	3:W:120:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:155:GLN:NE2	3:W:158:ASP:OD1	2.47	0.47
9:c:57:MET:HE2	9:c:69:VAL:HG21	1.97	0.47
13:A:297:ARG:HH22	18:F:306:VAL:HG21	1.78	0.47
16:D:115:ILE:HG22	16:D:139:LEU:HD12	1.96	0.47
24:L:189:LYS:HG3	24:L:193:ARG:HH12	1.78	0.47
21:i:85:VAL:O	21:i:89:GLU:CB	2.62	0.47
22:j:104:VAL:HA	22:j:107:ILE:HG22	1.96	0.47
27:o:112:SER:HB3	27:o:125:VAL:HG11	1.94	0.47
2:V:194:LYS:HA	2:V:199:ASN:HB2	1.96	0.47
9:c:57:MET:HG2	9:c:72:VAL:HG22	1.95	0.47
10:d:49:ILE:HG23	10:d:50:LEU:HD12	1.96	0.47
12:f:650:GLN:HG3	14:B:68:ILE:HG12	1.96	0.47
13:A:372:LEU:HD23	13:A:375:ARG:HH21	1.78	0.47
18:F:368:ILE:HG23	18:F:371:ARG:HH22	1.80	0.47
20:H:185:GLU:HA	20:H:188:ILE:HD12	1.97	0.47
21:I:159:TRP:CZ3	22:J:54:GLN:HG3	2.49	0.47
22:J:56:GLU:O	22:J:59:VAL:HG12	2.14	0.47
32:T:43:MET:HE3	32:T:45:VAL:HG22	1.96	0.47
28:p:138:VAL:HG11	28:p:146:MET:HB3	1.96	0.47
31:s:43:CYS:CB	31:s:196:CYS:SG	3.03	0.47
1:U:109:THR:OG1	1:U:156:GLU:O	2.26	0.47
1:U:204:ILE:HD12	1:U:207:ASN:HB2	1.96	0.47
2:V:350:GLN:H	2:V:353:LEU:HB3	1.80	0.47
3:W:36:LYS:O	3:W:87:ILE:HD11	2.14	0.47
3:W:260:SER:HA	3:W:263:TRP:HB3	1.95	0.47
3:W:287:VAL:O	3:W:291:SER:CB	2.63	0.47
6:Z:184:VAL:HG13	6:Z:188:SER:HB3	1.96	0.47
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.96	0.47
10:d:145:GLU:HG2	10:d:147:SER:H	1.79	0.47
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.96	0.47
13:A:312:ARG:HB2	13:A:315:ILE:HD12	1.96	0.47
18:F:122:ALA:HB3	18:F:134:LEU:HD11	1.96	0.47
25:M:186:CYS:HA	25:M:189:ILE:CG1	2.45	0.47
25:M:187:ARG:HD2	25:M:187:ARG:HA	1.48	0.47
29:Q:38:MET:HE1	29:Q:44:LEU:HB2	1.96	0.47
31:S:119:GLY:O	31:S:132:ARG:NH2	2.45	0.47
28:p:26:ARG:HH21	28:p:38:ASP:HA	1.79	0.47
3:W:282:GLU:O	3:W:286:LEU:CB	2.61	0.47
6:Z:205:LEU:HD11	7:a:357:CYS:HA	1.97	0.47
7:a:194:GLN:HB3	7:a:225:LEU:HG	1.97	0.47
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:119:THR:HG22	22:J:126:PRO:HB3	1.96	0.47
1:U:80:TYR:O	1:U:84:ALA:HB2	2.14	0.47
1:U:204:ILE:HA	1:U:207:ASN:HB2	1.96	0.47
2:V:73:GLU:N	2:V:73:GLU:OE1	2.48	0.47
3:W:357:ARG:O	3:W:361:HIS:N	2.47	0.47
5:Y:233:ARG:O	5:Y:237:ARG:CG	2.63	0.47
5:Y:235:ASP:OD1	5:Y:235:ASP:N	2.47	0.47
5:Y:387:ILE:HD13	6:Z:275:LEU:HD12	1.97	0.47
6:Z:58:PHE:HE1	6:Z:68:TRP:HB2	1.80	0.47
7:a:188:LEU:HD11	7:a:193:GLN:CG	2.45	0.47
9:c:213:GLU:HA	9:c:216:MET:HG2	1.95	0.47
12:f:575:ALA:O	12:f:579:ALA:CB	2.62	0.47
13:A:224:LEU:HG	34:A:501:ATP:H2'	1.97	0.47
13:A:244:GLU:HG2	14:B:268:ARG:HD3	1.96	0.47
17:E:46:ASP:HA	17:E:49:ALA:HB3	1.96	0.47
17:E:220:ASN:OD1	17:E:223:ARG:NH2	2.48	0.47
21:I:213:ILE:CG2	21:I:228:LEU:HD11	2.45	0.47
22:J:91:CYS:HB2	22:J:102:VAL:HG21	1.97	0.47
23:K:117:SER:HB2	24:L:82:ARG:HH12	1.78	0.47
25:M:186:CYS:HA	25:M:189:ILE:HB	1.96	0.47
28:P:138:VAL:HG11	28:P:146:MET:HB3	1.96	0.47
20:h:14:SER:OG	20:h:18:LYS:N	2.46	0.47
23:k:54:ILE:HA	23:k:59:MET:HE1	1.97	0.47
24:l:216:GLY:HA3	24:l:219:LEU:HB3	1.95	0.47
29:q:38:MET:HE1	29:q:44:LEU:HB2	1.96	0.47
1:U:174:PRO:HD2	1:U:176:MET:CG	2.43	0.47
2:V:198:GLN:O	2:V:202:ALA:CB	2.62	0.47
12:f:171:GLN:HE22	12:f:182:GLU:HB2	1.80	0.47
12:f:759:LEU:CD1	12:f:806:VAL:HB	2.35	0.47
12:f:761:MET:CE	12:f:766:GLN:HG2	2.45	0.47
18:F:410:ARG:NH2	18:F:419:ASP:OD2	2.48	0.47
26:N:7:GLN:HA	26:N:12:VAL:HA	1.97	0.47
19:g:203:SER:O	19:g:207:SER:HA	2.14	0.47
31:s:125:ASP:OD1	31:s:129:SER:N	2.48	0.47
1:U:177:LEU:C	1:U:177:LEU:CD1	2.85	0.47
2:V:92:ARG:O	2:V:96:ARG:NH1	2.48	0.47
2:V:494:MET:HE2	6:Z:274:ASN:C	2.39	0.47
5:Y:276:ALA:HB1	11:e:60:LEU:HD12	1.97	0.47
13:A:55:LEU:HA	13:A:58:LYS:HB2	1.96	0.47
14:B:317:ASP:HB2	14:B:346:ARG:HG2	1.97	0.47
22:J:36:ARG:HE	22:J:157:LYS:HA	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:98:LEU:HB2	27:O:113:ILE:HB	1.96	0.47
20:h:45:VAL:HG22	20:h:212:ILE:HG22	1.97	0.47
22:j:36:ARG:HE	22:j:157:LYS:HA	1.80	0.47
1:U:458:ILE:O	1:U:462:LEU:CB	2.59	0.47
2:V:30:PRO:O	2:V:34:ASP:N	2.47	0.47
3:W:13:ILE:HA	3:W:16:MET:HG2	1.97	0.47
6:Z:227:ILE:O	6:Z:231:GLN:HB2	2.15	0.47
12:f:372:LEU:HD11	12:f:403:LYS:HE3	1.95	0.47
12:f:681:TYR:CG	12:f:858:LYS:HE2	2.50	0.47
14:B:373:THR:OG1	14:B:412:MET:O	2.33	0.47
16:D:401:LYS:O	16:D:405:THR:OG1	2.29	0.47
18:F:305:GLU:HA	18:F:308:ARG:HH11	1.79	0.47
21:I:106:PRO:HD2	21:I:109:GLN:HE21	1.80	0.47
22:J:104:VAL:HA	22:J:107:ILE:HG22	1.96	0.47
27:O:46:ALA:HB3	27:O:97:ALA:HB3	1.95	0.47
20:h:185:GLU:HA	20:h:188:ILE:HD12	1.97	0.47
2:V:101:LEU:O	2:V:105:SER:CB	2.63	0.46
2:V:266:GLN:CD	2:V:266:GLN:N	2.72	0.46
6:Z:212:LEU:HD21	7:a:350:LYS:HD2	1.96	0.46
7:a:35:His:NE2	8:b:14:GLU:O	2.48	0.46
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.96	0.46
12:f:713:PHE:HD1	12:f:713:PHE:C	2.24	0.46
16:D:159:LYS:HA	16:D:160:PRO:HD3	1.80	0.46
25:M:170:GLN:HA	25:M:173:LYS:HG2	1.97	0.46
3:W:315:MET:SD	3:W:315:MET:N	2.88	0.46
5:Y:80:GLU:HA	5:Y:83:ARG:HG2	1.96	0.46
6:Z:146:ASP:HA	7:a:178:ARG:NH1	2.30	0.46
11:e:54:ASN:HA	11:e:57:ARG:HE	1.80	0.46
12:f:691:PRO:HD3	12:f:713:PHE:CZ	2.49	0.46
16:D:335:LEU:HD11	16:D:371:SER:HA	1.97	0.46
17:E:373:LYS:O	17:E:377:SER:HB3	2.14	0.46
18:F:410:ARG:NH2	18:F:416:THR:OG1	2.41	0.46
26:n:7:GLN:HA	26:n:12:VAL:HA	1.97	0.46
3:W:23:THR:HA	3:W:26:GLN:HB2	1.97	0.46
3:W:83:LEU:CG	3:W:90:LEU:HD23	2.44	0.46
3:W:274:VAL:CG1	3:W:286:LEU:HG	2.45	0.46
5:Y:66:ASP:HA	5:Y:69:LEU:HD13	1.96	0.46
7:a:74:LEU:CD1	7:a:150:SER:OG	2.64	0.46
7:a:170:ALA:HA	7:a:173:TYR:HB3	1.98	0.46
17:E:244:SER:H	18:F:300:LYS:HA	1.80	0.46
25:M:229:LYS:HG2	25:M:232:ARG:HH11	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:125:ASP:OD1	31:S:129:SER:N	2.48	0.46
25:m:34:SER:HA	25:m:167:LYS:HE3	1.98	0.46
1:U:598:ALA:O	1:U:602:LEU:HB3	2.14	0.46
3:W:93:ARG:H	3:W:96:GLN:HE21	1.63	0.46
8:b:26:LEU:O	8:b:30:GLN:HB2	2.15	0.46
10:d:170:LEU:HA	10:d:173:THR:HG22	1.97	0.46
13:A:73:ALA:HA	14:B:140:ASP:HB3	1.97	0.46
21:I:214:ALA:HB2	21:I:227:VAL:HG22	1.96	0.46
25:m:229:LYS:HG2	25:m:232:ARG:HH11	1.80	0.46
32:t:45:VAL:HB	32:t:49:THR:HG23	1.97	0.46
1:U:367:THR:HA	1:U:370:VAL:HG22	1.98	0.46
2:V:249:THR:HG22	2:V:284:GLU:HG3	1.97	0.46
3:W:355:LYS:C	3:W:355:LYS:CD	2.89	0.46
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.80	0.46
8:b:9:CYS:HB3	8:b:111:ALA:HA	1.98	0.46
8:b:21:PHE:CD1	8:b:177:PRO:HB3	2.50	0.46
12:f:139:CYS:O	12:f:143:ARG:NH1	2.48	0.46
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.97	0.46
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.97	0.46
12:f:773:LYS:HA	12:f:773:LYS:HD3	1.71	0.46
13:A:329:PRO:HA	13:A:332:MET:HB2	1.98	0.46
17:E:171:LEU:HD21	17:E:298:LYS:HG2	1.96	0.46
29:Q:198:LYS:HA	29:q:198:LYS:HA	1.97	0.46
22:j:38:ARG:HH12	22:j:182:GLU:HA	1.81	0.46
27:o:98:LEU:HB2	27:o:113:ILE:HB	1.96	0.46
4:X:198:ASN:HD21	15:C:389:LYS:HB2	1.79	0.46
5:Y:198:ALA:HA	5:Y:201:PHE:HB2	1.97	0.46
6:Z:12:HIS:ND1	6:Z:50:VAL:O	2.34	0.46
7:a:172:TYR:O	7:a:176:ALA:HB2	2.15	0.46
12:f:39:LYS:O	12:f:43:GLN:CB	2.64	0.46
12:f:61:GLU:HB2	12:f:65:GLU:HB2	1.96	0.46
12:f:189:LYS:HG2	12:f:190:GLU:HG2	1.98	0.46
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.98	0.46
12:f:571:GLU:HG3	12:f:573:ILE:H	1.81	0.46
16:D:119:ILE:O	16:D:121:ARG:NH1	2.45	0.46
21:I:38:LEU:HB3	21:I:43:VAL:HG23	1.97	0.46
21:I:47:ALA:HB1	21:I:64:LYS:HE3	1.98	0.46
23:K:34:GLY:HA3	23:K:80:GLY:H	1.81	0.46
23:K:54:ILE:HA	23:K:59:MET:HE1	1.97	0.46
23:K:69:GLU:HA	23:K:75:GLY:HA2	1.97	0.46
25:M:17:ASP:OD2	25:M:19:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:6:VAL:HG23	27:O:124:TYR:HB3	1.98	0.46
27:O:138:PHE:O	27:O:142:PHE:CB	2.64	0.46
23:k:84:ASP:OD1	23:k:84:ASP:N	2.47	0.46
2:V:358:MET:CB	2:V:359:PRO:HD3	2.43	0.46
5:Y:241:ILE:HG23	5:Y:242:LYS:HG2	1.98	0.46
6:Z:59:ASP:HB2	8:b:99:HIS:CE1	2.51	0.46
7:a:27:GLU:O	7:a:30:THR:OG1	2.32	0.46
9:c:39:LEU:HD23	9:c:42:LEU:HD21	1.98	0.46
12:f:240:VAL:O	12:f:257:ARG:NH2	2.40	0.46
12:f:723:TYR:O	12:f:727:PHE:HB3	2.15	0.46
15:C:360:LYS:O	15:C:364:THR:OG1	2.31	0.46
16:D:167:ILE:HD11	16:D:214:MET:HG2	1.98	0.46
16:D:276:ASP:N	16:D:282:ASP:OD2	2.48	0.46
22:J:38:ARG:HH12	22:J:182:GLU:HA	1.81	0.46
24:l:20:HIS:HA	24:l:23:GLU:HB2	1.97	0.46
2:V:252:ASN:HD21	2:V:288:TYR:HB2	1.80	0.46
3:W:274:VAL:HG13	3:W:286:LEU:HD23	1.95	0.46
5:Y:326:GLY:HA3	11:e:66:LYS:HD2	1.97	0.46
12:f:830:LEU:N	12:f:859:PRO:O	2.49	0.46
12:f:838:ARG:NH1	12:f:838:ARG:C	2.73	0.46
20:H:9:SER:OG	20:H:123:GLN:O	2.31	0.46
21:I:92:LEU:HA	21:I:95:GLN:HB2	1.98	0.46
32:t:1:THR:N	32:t:105:PRO:O	2.42	0.46
1:U:379:GLY:N	1:U:410:VAL:O	2.45	0.46
2:V:147:PHE:O	2:V:150:ARG:N	2.43	0.46
6:Z:82:PHE:HA	6:Z:85:VAL:HG12	1.98	0.46
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.98	0.46
10:d:122:LEU:HD13	10:d:125:LYS:HB3	1.92	0.46
12:f:168:LYS:O	12:f:172:GLU:CB	2.63	0.46
12:f:838:ARG:HD2	12:f:838:ARG:HA	1.56	0.46
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.49	0.46
19:G:54:LYS:NZ	19:G:215:ILE:O	2.49	0.46
20:H:45:VAL:HG22	20:H:212:ILE:HG22	1.97	0.46
24:L:199:LEU:HD13	24:L:204:ASP:HA	1.98	0.46
32:T:45:VAL:HB	32:T:49:THR:HG23	1.97	0.46
22:j:91:CYS:HB2	22:j:102:VAL:HG21	1.97	0.46
31:s:114:ASP:OD1	31:s:118:LYS:N	2.40	0.46
1:U:590:TYR:HD1	1:U:595:ASN:HD22	1.63	0.46
2:V:483:CYS:HA	2:V:486:ILE:HG22	1.98	0.46
3:W:141:GLU:HG3	3:W:142:ARG:HD2	1.98	0.46
4:X:331:LEU:O	4:X:335:LEU:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:148:GLY:O	5:Y:153:ASP:N	2.49	0.46
5:Y:228:MET:SD	5:Y:295:TYR:OH	2.74	0.46
8:b:21:PHE:HB2	8:b:25:ARG:HG2	1.98	0.46
12:f:556:ARG:CD	12:f:786:GLN:HB2	2.25	0.46
12:f:764:LEU:HD13	12:f:775:THR:HG22	1.98	0.46
16:D:401:LYS:HA	16:D:404:LYS:HE2	1.98	0.46
21:I:133:SER:OG	21:I:150:SER:O	2.30	0.46
25:M:34:SER:HA	25:M:167:LYS:HE3	1.98	0.46
25:m:17:ASP:OD2	25:m:19:ARG:NH2	2.48	0.46
6:Z:22:HIS:HA	6:Z:25:ARG:HG2	1.98	0.45
9:c:146:ASP:OD2	9:c:149:GLN:NE2	2.49	0.45
12:f:682:GLY:HA3	12:f:687:ARG:NH1	2.23	0.45
16:D:336:PRO:HB3	16:D:340:GLN:HB2	1.98	0.45
24:L:121:GLN:HG3	25:M:129:ARG:HG2	1.98	0.45
26:N:28:ASN:HD21	27:O:122:LEU:HD21	1.78	0.45
30:R:77:ALA:O	30:R:120:ARG:NH2	2.49	0.45
23:k:60:GLU:OE1	23:k:63:SER:N	2.49	0.45
2:V:52:ASP:HB2	2:V:149:PRO:HG2	1.98	0.45
2:V:211:TYR:O	2:V:215:ALA:HB2	2.16	0.45
3:W:123:ARG:HH12	3:W:127:THR:HB	1.81	0.45
5:Y:57:LEU:HA	5:Y:60:SER:HB3	1.97	0.45
5:Y:173:ASP:HB3	5:Y:176:ARG:HB2	1.98	0.45
7:a:255:TRP:HB3	7:a:261:LEU:HD11	1.99	0.45
8:b:141:ILE:HG21	8:b:184:ILE:HG22	1.99	0.45
12:f:485:LEU:O	12:f:489:TYR:HB2	2.17	0.45
13:A:100:LYS:O	13:A:114:ASN:N	2.49	0.45
25:M:181:MET:N	25:M:181:MET:SD	2.84	0.45
31:S:33:PHE:HA	27:o:167:LEU:HD12	1.98	0.45
20:h:9:SER:OG	20:h:123:GLN:O	2.31	0.45
23:k:69:GLU:HA	23:k:75:GLY:HA2	1.97	0.45
24:l:186:GLU:HA	24:l:189:LYS:HG2	1.98	0.45
1:U:543:LYS:HG2	1:U:546:ARG:HH12	1.81	0.45
2:V:451:ILE:HG13	2:V:458:VAL:HG13	1.97	0.45
3:W:426:ASN:O	3:W:429:SER:OG	2.30	0.45
5:Y:231:LEU:HB2	5:Y:235:ASP:OD2	2.16	0.45
5:Y:325:VAL:HB	11:e:70:SER:HB2	1.98	0.45
8:b:56:ASN:N	8:b:83:LYS:O	2.49	0.45
10:d:175:ARG:O	10:d:179:ALA:HB2	2.17	0.45
12:f:217:LEU:HD13	12:f:217:LEU:O	2.16	0.45
15:C:195:GLY:N	36:C:501:ADP:O1A	2.49	0.45
1:U:229:VAL:O	1:U:233:LEU:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:35:ALA:HA	3:W:44:ILE:HD11	1.99	0.45
3:W:132:THR:HA	16:D:393:ILE:HD12	1.99	0.45
6:Z:193:ASN:HD22	6:Z:197:GLY:HA3	1.82	0.45
9:c:49:VAL:HG13	9:c:50:PRO:HD3	1.99	0.45
24:L:20:HIS:HA	24:L:23:GLU:HB2	1.97	0.45
32:T:89:HIS:NE2	32:T:124:TYR:O	2.47	0.45
25:m:170:GLN:HA	25:m:173:LYS:HG2	1.97	0.45
31:s:119:GLY:O	31:s:132:ARG:NH2	2.45	0.45
1:U:250:PHE:HE1	1:U:328:ILE:HA	1.82	0.45
6:Z:116:CYS:O	6:Z:119:SER:OG	2.31	0.45
9:c:55:GLY:HA3	9:c:74:ALA:HA	1.97	0.45
12:f:505:MET:HE3	12:f:537:THR:HG22	1.98	0.45
15:C:221:GLN:NE2	15:C:227:GLY:O	2.49	0.45
22:J:54:GLN:CA	22:J:54:GLN:NE2	2.79	0.45
22:J:56:GLU:HB2	22:J:59:VAL:CG1	2.47	0.45
20:h:46:LEU:HD13	20:h:75:VAL:HG22	1.99	0.45
24:l:156:CYS:HA	25:m:59:GLU:H	1.80	0.45
1:U:493:VAL:O	1:U:497:LEU:HB2	2.16	0.45
2:V:211:TYR:HA	2:V:214:HIS:HB3	1.99	0.45
5:Y:231:LEU:HD13	5:Y:235:ASP:HB2	1.98	0.45
6:Z:61:ASP:OD2	8:b:91:ARG:NH1	2.50	0.45
9:c:161:ARG:HB3	9:c:201:TYR:CZ	2.52	0.45
12:f:127:SER:HA	12:f:131:MET:HB2	1.99	0.45
12:f:773:LYS:HB3	12:f:774:GLY:H	1.57	0.45
16:D:146:GLU:O	16:D:252:ARG:NH2	2.39	0.45
17:E:50:LEU:HD13	18:F:82:VAL:HG11	1.99	0.45
17:E:227:PRO:HA	17:E:272:ARG:HB3	1.99	0.45
18:F:65:GLU:O	18:F:69:MET:CB	2.64	0.45
31:S:35:ILE:O	32:T:151:ARG:NH2	2.41	0.45
31:S:91:MET:O	31:S:94:THR:OG1	2.32	0.45
27:o:6:VAL:HG23	27:o:124:TYR:HB3	1.98	0.45
27:o:138:PHE:O	27:o:142:PHE:CB	2.64	0.45
29:q:19:ARG:HB3	29:q:31:ASP:HA	1.98	0.45
1:U:24:LEU:HA	1:U:27:LEU:HB2	1.98	0.45
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.39	0.45
2:V:373:ALA:H	2:V:427:GLN:NE2	2.14	0.45
3:W:237:GLU:HG2	3:W:238:GLY:H	1.81	0.45
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.65	0.45
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.97	0.45
9:c:303:MET:HE2	10:d:239:SER:HA	1.98	0.45
10:d:108:SER:C	10:d:110:ASN:N	2.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R:83:LEU:HD11	30:R:97:MET:HE1	1.99	0.45
30:r:77:ALA:O	30:r:120:ARG:NH2	2.49	0.45
1:U:519:VAL:HG23	1:U:520:MET:HG2	1.98	0.45
2:V:290:TYR:HE1	2:V:309:MET:HE1	1.82	0.45
2:V:407:VAL:O	2:V:411:SER:CB	2.65	0.45
7:a:144:ASN:ND2	7:a:144:ASN:C	2.73	0.45
7:a:156:TYR:O	7:a:159:SER:OG	2.35	0.45
14:B:93:GLU:O	14:B:97:SER:HB3	2.17	0.45
19:G:14:THR:OG1	19:G:128:ASN:O	2.33	0.45
27:O:120:ASP:OD1	27:O:120:ASP:N	2.50	0.45
20:h:204:THR:OG1	20:h:206:ASP:OD1	2.30	0.45
21:i:106:PRO:HD2	21:i:109:GLN:HE21	1.80	0.45
27:o:166:ASP:HB3	27:o:169:SER:HB2	1.98	0.45
29:q:141:SER:O	29:q:145:ARG:CB	2.65	0.45
3:W:245:LYS:O	3:W:249:ALA:CB	2.65	0.45
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.99	0.45
6:Z:249:PHE:HZ	9:c:303:MET:HG2	1.82	0.45
9:c:192:LEU:HA	9:c:196:LEU:CD2	2.43	0.45
12:f:744:MET:O	12:f:748:LEU:CB	2.63	0.45
13:A:368:ILE:HG22	13:A:406:GLU:HB2	1.99	0.45
13:A:401:ARG:CZ	13:A:401:ARG:CB	2.95	0.45
14:B:418:ASP:O	14:B:422:SER:CB	2.63	0.45
15:C:49:ARG:C	15:C:49:ARG:CD	2.90	0.45
16:D:410:ASP:OD1	16:D:410:ASP:N	2.50	0.45
27:O:19:ARG:HH21	27:O:26:VAL:HG22	1.82	0.45
31:S:114:ASP:OD1	31:S:118:LYS:N	2.40	0.45
21:i:38:LEU:HB3	21:i:43:VAL:HG23	1.98	0.45
21:i:136:TYR:HB2	21:i:148:TYR:HB2	1.99	0.45
32:t:89:HIS:NE2	32:t:124:TYR:O	2.47	0.45
1:U:56:SER:O	1:U:60:ALA:CB	2.59	0.45
2:V:108:LEU:HA	2:V:111:TYR:HD2	1.82	0.45
5:Y:297:ARG:HH22	11:e:51:ASP:HB3	1.81	0.45
6:Z:98:GLY:HA3	6:Z:123:ILE:HG23	1.99	0.45
7:a:143:ASN:ND2	7:a:145:LEU:HD11	2.32	0.45
12:f:23:GLY:HA2	12:f:27:LYS:HD3	1.99	0.45
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.98	0.45
15:C:147:THR:HG22	15:C:150:MET:HE3	1.99	0.45
15:C:246:ILE:HB	15:C:291:VAL:HG12	1.99	0.45
17:E:45:ASN:O	17:E:49:ALA:HB2	2.17	0.45
19:G:60:LEU:O	25:M:161:TRP:N	2.46	0.45
20:H:46:LEU:HD13	20:H:75:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:225:ILE:O	21:I:225:ILE:HG23	2.17	0.45
21:I:229:LYS:N	21:I:232:GLU:OE2	2.50	0.45
22:J:120:GLN:O	23:K:134:SER:OG	2.32	0.45
30:R:38:ASN:HD22	30:R:41:LEU:HD12	1.82	0.45
19:g:123:GLN:OE1	19:g:127:GLN:NE2	2.43	0.45
20:h:169:ASN:O	20:h:172:THR:OG1	2.33	0.45
21:i:92:LEU:HA	21:i:95:GLN:HB2	1.98	0.45
24:l:18:ARG:NH1	24:l:23:GLU:OE2	2.49	0.45
24:l:199:LEU:HD13	24:l:204:ASP:HA	1.98	0.45
27:o:160:ALA:HA	27:o:163:ILE:HD12	1.99	0.45
5:Y:160:ASN:O	5:Y:164:ALA:CB	2.64	0.44
6:Z:211:TYR:C	6:Z:213:GLU:N	2.70	0.44
7:a:188:LEU:HB2	7:a:189:PRO:CD	2.47	0.44
10:d:118:GLU:CD	10:d:118:GLU:C	2.85	0.44
12:f:788:MET:HB3	12:f:789:SER:H	1.56	0.44
13:A:300:LEU:HD23	13:A:303:ILE:HD12	1.97	0.44
14:B:133:VAL:HG11	14:B:157:HIS:HB2	1.98	0.44
17:E:334:LEU:HB3	17:E:371:VAL:HG11	1.99	0.44
18:F:398:ALA:HA	18:F:401:VAL:HG12	1.98	0.44
21:I:32:GLY:H	21:I:50:ARG:HH21	1.66	0.44
23:K:60:GLU:OE1	23:K:63:SER:N	2.49	0.44
25:M:65:ARG:HG2	25:M:81:LEU:HD11	1.98	0.44
28:P:177:ARG:NH2	31:s:150:ASP:OD2	2.41	0.44
29:Q:19:ARG:HB3	29:Q:31:ASP:HA	1.98	0.44
31:S:43:CYS:SG	31:S:196:CYS:CB	3.06	0.44
31:S:187:VAL:HG21	27:o:24:MET:HE3	2.00	0.44
19:g:120:ASP:OD1	20:h:84:ARG:NH1	2.50	0.44
21:i:47:ALA:HB1	21:i:64:LYS:HE3	1.98	0.44
22:j:68:ASN:HD21	22:j:101:PRO:HB2	1.83	0.44
23:k:34:GLY:HA3	23:k:80:GLY:H	1.81	0.44
30:r:83:LEU:HD11	30:r:97:MET:HE1	1.99	0.44
1:U:20:LYS:HB3	1:U:48:LEU:HD22	2.00	0.44
1:U:598:ALA:O	1:U:602:LEU:HB2	2.17	0.44
5:Y:124:PHE:HA	5:Y:127:THR:HG22	1.98	0.44
5:Y:331:ASP:OD1	5:Y:349:LYS:NZ	2.49	0.44
6:Z:34:ARG:HE	6:Z:102:HIS:CD2	2.35	0.44
6:Z:180:LYS:HG2	6:Z:182:THR:HG23	1.99	0.44
9:c:192:LEU:N	9:c:196:LEU:HD22	2.32	0.44
10:d:56:GLU:HA	10:d:78:LEU:HD11	1.99	0.44
12:f:826:GLN:HE22	12:f:828:ARG:HD3	1.81	0.44
14:B:90:GLU:H	14:B:94:GLU:HB3	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:154:LEU:N	16:D:158:GLN:HG3	2.31	0.44
21:I:228:LEU:H	21:I:228:LEU:HG	1.46	0.44
27:O:166:ASP:HB3	27:O:169:SER:HB2	1.98	0.44
22:j:200:GLN:HB3	22:j:201:SER:H	1.64	0.44
25:m:40:ARG:HA	25:m:45:VAL:HA	1.99	0.44
1:U:188:MET:HE3	1:U:194:ARG:HG3	1.98	0.44
4:X:362:GLU:HG3	4:X:378:LEU:HD21	1.98	0.44
7:a:145:LEU:CD1	7:a:146:PRO:HD2	2.47	0.44
9:c:120:CYS:HA	9:c:144:VAL:HG11	1.98	0.44
12:f:75:LEU:HD13	12:f:77:GLU:HG3	1.99	0.44
12:f:485:LEU:HD22	12:f:501:LEU:HD11	1.98	0.44
14:B:343:ARG:HE	14:B:346:ARG:NH1	2.15	0.44
15:C:90:HIS:CD2	15:C:90:HIS:N	2.76	0.44
24:L:186:GLU:HA	24:L:189:LYS:HG2	1.98	0.44
27:O:59:ILE:HG13	27:O:83:LEU:HD21	1.98	0.44
25:m:228:PRO:HD2	25:m:231:ILE:HD12	1.98	0.44
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.98	0.44
4:X:208:ALA:HB2	4:X:238:GLY:HA3	1.99	0.44
4:X:357:SER:OG	4:X:358:LYS:N	2.51	0.44
4:X:407:MET:HE2	6:Z:266:ILE:HG23	1.99	0.44
7:a:18:GLN:HG3	7:a:22:TRP:HE1	1.83	0.44
8:b:16:MET:HE3	8:b:25:ARG:HB3	1.98	0.44
10:d:164:THR:HA	10:d:167:ILE:HG12	1.98	0.44
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.83	0.44
13:A:324:PRO:HA	13:A:327:LEU:HD13	2.00	0.44
13:A:400:ARG:HD3	13:A:400:ARG:HA	1.25	0.44
19:G:132:ARG:HG2	19:G:132:ARG:HH21	1.82	0.44
24:L:229:VAL:O	24:L:233:LEU:N	2.48	0.44
25:M:40:ARG:HA	25:M:45:VAL:HA	1.99	0.44
27:O:160:ALA:HA	27:O:163:ILE:HD12	1.99	0.44
21:i:32:GLY:H	21:i:50:ARG:HH21	1.66	0.44
21:i:229:LYS:N	21:i:232:GLU:OE2	2.50	0.44
25:m:65:ARG:HG2	25:m:81:LEU:HD11	1.99	0.44
1:U:886:PRO:HA	1:U:889:LEU:HG	2.00	0.44
2:V:373:ALA:H	2:V:427:GLN:HE21	1.66	0.44
7:a:212:ASN:HD21	7:a:215:GLU:HB3	1.82	0.44
9:c:267:PRO:HA	9:c:270:LEU:HB2	2.00	0.44
12:f:640:LYS:HG2	12:f:678:LEU:HD13	2.00	0.44
12:f:838:ARG:HH11	12:f:838:ARG:CA	2.31	0.44
18:F:81:LYS:HA	18:F:84:LYS:HE2	1.99	0.44
21:I:238:LYS:HA	21:I:241:GLU:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:15:PHE:HE2	24:l:127:PRO:HD2	1.82	0.44
24:l:121:GLN:HG3	25:m:129:ARG:HE	1.83	0.44
25:m:73:VAL:HA	25:m:139:SER:HB2	1.99	0.44
3:W:450:GLU:OE2	6:Z:219:LYS:NZ	2.49	0.44
4:X:258:LYS:HD3	4:X:266:ASP:HB2	2.00	0.44
9:c:280:PRO:O	9:c:284:LEU:CB	2.59	0.44
10:d:234:ASP:OD1	10:d:234:ASP:N	2.50	0.44
12:f:218:GLU:CD	12:f:218:GLU:C	2.85	0.44
12:f:568:GLY:H	12:f:599:ALA:HA	1.82	0.44
13:A:174:TYR:HE2	13:A:232:ARG:HB2	1.83	0.44
15:C:62:GLU:O	15:C:66:LEU:N	2.42	0.44
18:F:212:PHE:HD1	18:F:217:ILE:HD11	1.83	0.44
25:M:173:LYS:HA	25:M:176:ILE:HD12	2.00	0.44
2:V:265:ASP:O	2:V:268:GLU:HB3	2.17	0.44
3:W:423:ASN:HA	3:W:426:ASN:HB3	2.00	0.44
10:d:61:TRP:HZ3	10:d:65:ARG:HH21	1.66	0.44
10:d:100:GLY:HA3	10:d:133:ILE:HD12	1.99	0.44
12:f:541:THR:O	12:f:545:LYS:HB3	2.17	0.44
17:E:168:LYS:N	17:E:296:ASP:OD2	2.48	0.44
21:I:136:TYR:HB2	21:I:148:TYR:HB2	1.99	0.44
2:V:43:THR:O	2:V:47:SER:OG	2.27	0.44
5:Y:261:PHE:O	5:Y:265:GLU:HB2	2.17	0.44
6:Z:153:LYS:NZ	6:Z:153:LYS:CB	2.73	0.44
7:a:152:HIS:HE1	7:a:179:PHE:O	2.01	0.44
8:b:49:VAL:N	8:b:65:THR:O	2.47	0.44
9:c:91:PHE:O	9:c:95:MET:HB3	2.18	0.44
10:d:194:ALA:HA	10:d:197:ILE:HG12	2.00	0.44
13:A:75:PRO:O	13:A:78:TRP:NE1	2.51	0.44
16:D:65:GLN:OE1	16:D:69:LYS:NZ	2.51	0.44
16:D:363:TYR:CE2	16:D:399:PHE:HB3	2.52	0.44
19:G:134:LEU:H	19:G:134:LEU:HD12	1.77	0.44
21:I:235:GLN:O	21:I:239:LYS:HB2	2.18	0.44
25:M:228:PRO:HD2	25:M:231:ILE:HD12	1.98	0.44
26:N:120:MET:H	32:T:61:GLN:HE22	1.64	0.44
21:i:153:SER:OG	21:i:155:ASN:OD1	2.35	0.44
21:i:238:LYS:HA	21:i:241:GLU:HB2	2.00	0.44
1:U:791:LEU:HD22	1:U:911:ILE:HD11	1.99	0.44
2:V:84:LYS:HA	2:V:87:SER:HB2	2.00	0.44
6:Z:146:ASP:OD2	7:a:177:LEU:HD12	2.17	0.44
12:f:609:VAL:HA	12:f:612:LEU:HB3	1.99	0.44
13:A:115:VAL:HG21	13:A:118:PHE:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:181:LYS:HA	13:A:184:ILE:HD12	1.99	0.44
24:L:18:ARG:NH1	24:L:23:GLU:OE2	2.50	0.44
27:O:67:SER:HB3	27:O:74:PRO:HG3	2.00	0.44
27:o:59:ILE:HG13	27:o:83:LEU:HD21	1.98	0.44
30:r:38:ASN:HD22	30:r:41:LEU:HD12	1.82	0.44
1:U:475:HIS:HD2	1:U:511:ALA:HB2	1.83	0.43
3:W:144:ARG:HG3	3:W:147:LYS:HZ2	1.82	0.43
7:a:104:VAL:HG12	7:a:110:ALA:HB2	2.00	0.43
7:a:290:GLN:O	7:a:330:ARG:NH2	2.50	0.43
7:a:321:LYS:O	7:a:334:THR:OG1	2.35	0.43
8:b:109:ILE:HB	8:b:138:VAL:HG22	2.00	0.43
13:A:84:LYS:O	13:A:88:GLN:CB	2.66	0.43
14:B:183:THR:HG23	14:B:185:ALA:H	1.83	0.43
14:B:284:ILE:HG21	14:B:287:ILE:HD12	1.99	0.43
17:E:40:TYR:O	17:E:44:GLU:CB	2.66	0.43
21:I:153:SER:OG	21:I:155:ASN:OD1	2.35	0.43
23:K:121:LEU:HD21	24:L:126:ARG:HH12	1.83	0.43
25:M:214:SER:HG	25:M:224:HIS:HE2	1.56	0.43
27:O:38:SER:OG	27:O:40:ASN:OD1	2.26	0.43
30:R:12:VAL:HB	30:R:179:VAL:HB	2.00	0.43
27:o:19:ARG:HH21	27:o:26:VAL:HG22	1.82	0.43
27:o:211:VAL:HG11	28:p:198:ARG:HD3	2.00	0.43
1:U:415:HIS:CD2	1:U:418:GLU:H	2.36	0.43
3:W:312:MET:HE3	3:W:365:ILE:HD12	2.00	0.43
3:W:321:VAL:HG23	3:W:351:TRP:HH2	1.83	0.43
7:a:189:PRO:CB	7:a:192:GLU:HB2	2.37	0.43
7:a:360:VAL:O	7:a:364:GLU:HB2	2.18	0.43
9:c:174:PRO:HB2	9:c:175:ARG:HG3	2.00	0.43
10:d:122:LEU:CD1	10:d:125:LYS:C	2.91	0.43
12:f:243:PRO:HD2	12:f:257:ARG:HH22	1.84	0.43
12:f:282:PHE:CD1	12:f:282:PHE:N	2.86	0.43
12:f:282:PHE:CE2	12:f:284:SER:HB2	2.52	0.43
12:f:331:LEU:HD13	12:f:808:ASN:HD22	1.83	0.43
13:A:52:ILE:HD12	13:A:55:LEU:HB3	2.00	0.43
17:E:309:ARG:O	17:E:313:LEU:HB2	2.18	0.43
22:J:192:ILE:O	22:J:196:LEU:CB	2.67	0.43
32:T:25:ASP:HA	32:T:187:PHE:HA	2.00	0.43
19:g:14:THR:OG1	19:g:128:ASN:O	2.33	0.43
19:g:54:LYS:NZ	19:g:215:ILE:O	2.49	0.43
21:i:133:SER:OG	21:i:150:SER:O	2.30	0.43
27:o:120:ASP:OD1	27:o:120:ASP:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:101:ASN:HB3	29:q:132:HIS:CD2	2.53	0.43
32:t:89:HIS:CE1	32:t:131:ALA:HB1	2.53	0.43
2:V:203:LEU:O	2:V:207:ALA:HB2	2.17	0.43
7:a:145:LEU:HD12	7:a:147:GLY:H	1.83	0.43
7:a:215:GLU:O	7:a:219:HIS:HB2	2.19	0.43
8:b:125:VAL:HA	8:b:128:ALA:HB3	2.00	0.43
13:A:113:ILE:HD12	13:A:123:VAL:HG21	2.00	0.43
14:B:119:ASN:HB2	14:B:135:ILE:HB	2.00	0.43
17:E:317:ALA:HA	17:E:320:ILE:HD12	2.00	0.43
22:j:192:ILE:O	22:j:196:LEU:CB	2.67	0.43
25:m:173:LYS:HA	25:m:176:ILE:HD12	2.00	0.43
2:V:342:ILE:HG12	2:V:368:ARG:HD2	2.00	0.43
3:W:183:VAL:HA	3:W:186:ILE:HG22	1.99	0.43
3:W:317:TRP:HH2	3:W:354:LEU:HD13	1.82	0.43
7:a:270:ARG:HH11	7:a:310:LEU:HA	1.83	0.43
12:f:764:LEU:N	12:f:764:LEU:CD2	2.73	0.43
13:A:85:GLN:O	13:A:89:SER:OG	2.26	0.43
22:J:200:GLN:HB3	22:J:201:SER:H	1.61	0.43
23:K:177:ALA:O	23:K:181:LEU:CB	2.62	0.43
25:m:15:SER:N	25:m:19:ARG:O	2.47	0.43
26:n:29:ARG:NH1	27:o:139:GLU:OE2	2.51	0.43
30:r:12:VAL:HB	30:r:179:VAL:HB	2.00	0.43
1:U:756:HIS:HD2	1:U:759:SER:HB2	1.82	0.43
2:V:89:LYS:HD3	2:V:92:ARG:NH1	2.34	0.43
2:V:188:SER:O	2:V:192:MET:HB2	2.19	0.43
2:V:417:ILE:O	2:V:458:VAL:N	2.47	0.43
3:W:48:LEU:O	3:W:52:LYS:HB2	2.18	0.43
7:a:188:LEU:HD22	7:a:193:GLN:NE2	2.25	0.43
8:b:124:LEU:O	8:b:128:ALA:CB	2.67	0.43
9:c:118:PHE:HB3	9:c:121:TRP:CH2	2.54	0.43
12:f:667:GLY:HA2	12:f:671:ALA:HB3	1.99	0.43
15:C:325:ARG:HD3	15:C:353:GLY:HA2	2.00	0.43
16:D:125:LYS:HZ2	16:D:125:LYS:C	2.13	0.43
16:D:125:LYS:N	16:D:126:PRO:HD3	2.33	0.43
24:L:183:ASN:O	24:L:187:LEU:CB	2.66	0.43
25:M:186:CYS:HB3	25:M:189:ILE:HB	2.00	0.43
29:Q:141:SER:O	29:Q:145:ARG:CB	2.65	0.43
32:T:89:HIS:CE1	32:T:131:ALA:HB1	2.53	0.43
21:i:44:LEU:HD22	21:i:190:LEU:HD23	2.01	0.43
32:t:25:ASP:HA	32:t:187:PHE:HA	2.00	0.43
1:U:505:ASP:HB3	1:U:508:THR:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:257:ASN:ND2	2:V:261:TYR:HE2	2.17	0.43
3:W:271:VAL:O	3:W:275:ILE:HG13	2.18	0.43
3:W:274:VAL:CG1	3:W:286:LEU:HD23	2.47	0.43
6:Z:145:HIS:O	7:a:178:ARG:CZ	2.67	0.43
7:a:188:LEU:CB	7:a:189:PRO:CD	2.96	0.43
9:c:161:ARG:O	9:c:200:TYR:CB	2.67	0.43
10:d:48:LEU:CB	10:d:88:GLN:HE22	2.29	0.43
12:f:545:LYS:HE3	12:f:588:ARG:HA	1.99	0.43
17:E:232:MET:HB3	17:E:277:MET:HG2	1.99	0.43
17:E:244:SER:HB2	18:F:300:LYS:HG3	2.00	0.43
21:I:119:GLN:HG3	22:J:78:ALA:HB1	2.01	0.43
23:k:177:ALA:O	23:k:181:LEU:CB	2.62	0.43
27:o:67:SER:HB3	27:o:74:PRO:HG3	2.00	0.43
2:V:224:LEU:HG	2:V:257:ASN:HD22	1.83	0.43
3:W:35:ALA:O	3:W:87:ILE:HD11	2.15	0.43
3:W:89:LEU:HD13	3:W:93:ARG:HB3	1.87	0.43
10:d:101:LEU:HG	10:d:166:PHE:HE2	1.83	0.43
12:f:608:LYS:HA	12:f:611:GLN:HG2	2.00	0.43
12:f:696:LEU:HD11	14:B:141:LYS:NZ	2.32	0.43
15:C:88:LYS:HB3	15:C:94:LYS:HG2	2.01	0.43
16:D:253:LEU:O	16:D:257:ASN:CB	2.62	0.43
21:I:213:ILE:O	21:I:227:VAL:CG1	2.66	0.43
28:P:58:THR:OG1	29:Q:121:LEU:O	2.32	0.43
29:Q:101:ASN:HB3	29:Q:132:HIS:CD2	2.53	0.43
32:T:1:THR:N	32:T:105:PRO:O	2.42	0.43
21:i:235:GLN:O	21:i:239:LYS:HB2	2.18	0.43
22:j:80:ALA:HA	22:j:129:ILE:HD13	2.01	0.43
1:U:100:ILE:HA	1:U:103:LYS:HE2	2.01	0.43
1:U:236:LEU:HD22	1:U:244:MET:HG3	2.00	0.43
1:U:474:ARG:O	1:U:478:SER:CB	2.67	0.43
1:U:711:GLN:O	1:U:715:LYS:HB2	2.19	0.43
7:a:100:THR:HG22	7:a:103:LYS:HE2	2.01	0.43
7:a:206:LEU:HD11	7:a:260:ASP:HB3	2.00	0.43
12:f:291:GLN:HB3	12:f:879:ARG:HH21	1.84	0.43
12:f:811:LEU:HD21	12:f:862:ILE:HD13	2.00	0.43
13:A:347:ASP:OD1	13:A:347:ASP:N	2.52	0.43
14:B:265:LYS:HA	14:B:268:ARG:HE	1.84	0.43
15:C:80:MET:HE1	15:C:86:LEU:HB2	2.00	0.43
15:C:329:LEU:O	15:C:333:SER:CB	2.67	0.43
22:J:68:ASN:HD21	22:J:101:PRO:HB2	1.83	0.43
22:J:80:ALA:HA	22:J:129:ILE:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:P:191:GLU:OE2	28:P:194:LYS:NZ	2.36	0.43
24:l:183:ASN:O	24:l:187:LEU:CB	2.66	0.43
30:r:154:ASP:OD1	30:r:157:ARG:NH1	2.52	0.43
2:V:357:LEU:HD13	2:V:360:TYR:HB3	2.00	0.43
2:V:398:LEU:HD13	2:V:401:ASN:HD22	1.84	0.43
3:W:89:LEU:HD22	3:W:89:LEU:O	2.19	0.43
3:W:317:TRP:HE3	3:W:358:VAL:HG21	1.84	0.43
3:W:352:LYS:C	3:W:354:LEU:H	2.26	0.43
5:Y:155:ASP:O	5:Y:158:THR:OG1	2.34	0.43
7:a:112:ILE:O	7:a:116:THR:OG1	2.35	0.43
7:a:188:LEU:HD21	7:a:193:GLN:CG	2.47	0.43
8:b:95:LEU:O	8:b:99:HIS:ND1	2.43	0.43
9:c:91:PHE:O	9:c:95:MET:CB	2.66	0.43
10:d:112:VAL:O	10:d:116:HIS:HD2	2.02	0.43
14:B:107:MET:HB2	15:C:96:VAL:HB	1.99	0.43
18:F:251:LEU:HD12	18:F:285:ILE:HG12	2.01	0.43
20:H:100:VAL:HG13	28:P:93:ASN:HD22	1.84	0.43
25:M:42:LYS:HD2	25:M:183:GLU:HA	2.01	0.43
25:M:73:VAL:HA	25:M:139:SER:HB2	1.99	0.43
22:j:92:GLN:HG3	29:q:62:LYS:HB3	2.00	0.43
1:U:515:ALA:HA	1:U:518:LEU:HB2	2.00	0.43
5:Y:72:LYS:HG3	5:Y:73:MET:HG3	2.00	0.43
12:f:173:LEU:HD23	12:f:174:ASP:HB2	2.00	0.43
12:f:198:HIS:CD2	12:f:238:ASN:HB3	2.53	0.43
14:B:393:ALA:HB1	15:C:309:GLY:HA3	2.01	0.43
15:C:86:LEU:HD11	15:C:94:LYS:HD3	2.01	0.43
15:C:295:THR:OG1	15:C:296:ASN:N	2.52	0.43
19:G:123:GLN:OE1	19:G:127:GLN:NE2	2.43	0.43
21:I:123:GLN:HG3	22:J:125:ARG:HE	1.84	0.43
21:I:240:HIS:ND1	21:I:243:GLU:OE2	2.52	0.43
22:J:104:VAL:HG13	22:J:145:TYR:HE2	1.84	0.43
21:i:105:ILE:HD13	21:i:110:LEU:HD13	2.01	0.43
21:i:240:HIS:ND1	21:i:243:GLU:OE2	2.52	0.43
25:m:66:LEU:HD13	25:m:212:GLU:HG2	2.01	0.43
25:m:134:SER:HB2	25:m:153:PRO:HD3	2.01	0.43
4:X:370:LEU:HD21	5:Y:310:SER:HB2	2.01	0.42
5:Y:204:THR:O	5:Y:216:TYR:OH	2.32	0.42
8:b:62:THR:HG21	8:b:71:ILE:HG13	1.99	0.42
9:c:238:CYS:HA	9:c:241:ASN:HD22	1.83	0.42
12:f:380:PHE:O	12:f:755:ASP:HB2	2.19	0.42
13:A:429:TYR:HE2	14:B:340:ALA:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:345:PHE:O	16:D:349:THR:OG1	2.26	0.42
25:M:15:SER:N	25:M:19:ARG:O	2.47	0.42
28:p:169:GLN:O	28:p:173:ASN:ND2	2.52	0.42
1:U:804:SER:OG	1:U:805:ASN:N	2.50	0.42
5:Y:97:GLU:N	5:Y:99:GLU:OE2	2.43	0.42
7:a:135:ILE:HD11	7:a:159:SER:HB3	2.00	0.42
12:f:614:HIS:HE1	14:B:77:GLU:HB2	1.84	0.42
12:f:788:MET:O	12:f:790:GLN:N	2.52	0.42
15:C:20:LEU:HD12	15:C:21:ARG:HE	1.84	0.42
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.83	0.42
17:E:235:ILE:O	17:E:239:GLY:N	2.43	0.42
21:I:105:ILE:HD13	21:I:110:LEU:HD13	2.01	0.42
25:M:51:LYS:O	25:M:210:GLU:N	2.52	0.42
25:M:134:SER:HB2	25:M:153:PRO:HD3	2.01	0.42
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.85	0.42
2:V:171:VAL:HG12	2:V:175:MET:HG3	2.02	0.42
2:V:257:ASN:CG	2:V:261:TYR:CE2	2.97	0.42
5:Y:210:SER:OG	5:Y:211:TYR:N	2.52	0.42
7:a:142:LEU:HD21	7:a:151:VAL:CG2	2.36	0.42
7:a:374:ILE:HG23	10:d:255:MET:HE3	2.01	0.42
12:f:171:GLN:HE21	12:f:179:VAL:HA	1.84	0.42
12:f:405:HIS:O	12:f:409:SER:OG	2.31	0.42
17:E:196:LEU:O	17:E:231:PHE:N	2.37	0.42
17:E:329:GLU:O	17:E:333:LYS:CB	2.67	0.42
25:M:51:LYS:HB3	25:M:210:GLU:HB3	2.00	0.42
28:P:169:GLN:O	28:P:173:ASN:ND2	2.52	0.42
24:l:50:LYS:N	24:l:209:ASN:O	2.45	0.42
25:m:51:LYS:HB3	25:m:210:GLU:HB3	2.00	0.42
30:r:97:MET:O	30:r:116:SER:N	2.52	0.42
1:U:680:VAL:HB	1:U:683:VAL:HG12	2.01	0.42
2:V:497:PRO:HG3	6:Z:278:ASN:HB3	2.01	0.42
5:Y:345:CYS:HA	5:Y:356:THR:HA	2.02	0.42
6:Z:34:ARG:HE	6:Z:102:HIS:CG	2.37	0.42
12:f:297:MET:HA	12:f:772:GLY:HA2	2.00	0.42
12:f:681:TYR:HD2	12:f:858:LYS:CG	2.11	0.42
13:A:346:PRO:O	13:A:351:ARG:NH1	2.52	0.42
14:B:419:PHE:HA	14:B:422:SER:HB3	2.01	0.42
15:C:90:HIS:HE1	16:D:110:ASN:CA	2.27	0.42
19:G:180:GLU:HA	19:G:183:VAL:HG12	2.01	0.42
21:I:216:LEU:HG	21:I:225:ILE:HB	2.00	0.42
22:J:51:ALA:HB3	22:J:54:GLN:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:P:135:ASP:OD1	28:P:135:ASP:N	2.45	0.42
30:R:154:ASP:OD1	30:R:157:ARG:NH1	2.52	0.42
1:U:640:LEU:HD21	16:D:60:TYR:HE2	1.84	0.42
3:W:45:GLU:O	3:W:99:GLN:NE2	2.51	0.42
3:W:312:MET:HG3	3:W:313:GLU:H	1.84	0.42
4:X:122:ARG:HH21	20:H:185:GLU:HG3	1.84	0.42
9:c:42:LEU:O	9:c:46:ARG:CB	2.66	0.42
13:A:146:LYS:HD2	13:A:148:GLN:HG2	2.01	0.42
13:A:258:ARG:HH22	18:F:255:GLN:HA	1.84	0.42
14:B:388:ASP:OD1	14:B:388:ASP:N	2.53	0.42
17:E:139:SER:HA	17:E:142:ILE:HD12	2.02	0.42
21:I:44:LEU:HD22	21:I:190:LEU:HD23	2.01	0.42
30:R:97:MET:O	30:R:116:SER:N	2.52	0.42
21:i:140:ASP:OD1	21:i:144:GLY:N	2.53	0.42
22:j:201:SER:HA	22:j:205:ASN:HB2	2.02	0.42
25:m:42:LYS:HD2	25:m:183:GLU:HA	2.01	0.42
26:n:6:VAL:HG22	26:n:125:PHE:HB2	2.02	0.42
1:U:456:ASP:O	1:U:460:TYR:CB	2.65	0.42
1:U:553:ALA:HA	1:U:585:THR:HG23	2.01	0.42
2:V:20:GLY:O	2:V:24:GLN:HB2	2.19	0.42
8:b:180:ALA:HA	8:b:183:LEU:HD13	2.02	0.42
12:f:72:ARG:HH21	12:f:112:ASN:HB3	1.83	0.42
13:A:185:GLU:OE1	13:A:188:ARG:NH2	2.52	0.42
13:A:186:LYS:HE3	13:A:341:ILE:HG13	2.01	0.42
15:C:150:MET:HA	15:C:331:ILE:HG21	2.02	0.42
25:m:51:LYS:O	25:m:210:GLU:N	2.52	0.42
28:p:59:ASP:OD2	28:p:104:TYR:N	2.41	0.42
1:U:622:LEU:O	1:U:626:LEU:HB2	2.19	0.42
1:U:803:LYS:HB2	1:U:875:PHE:HA	2.01	0.42
2:V:345:ARG:NE	2:V:345:ARG:CA	2.73	0.42
5:Y:366:TYR:O	5:Y:369:THR:OG1	2.30	0.42
7:a:188:LEU:CD1	7:a:192:GLU:OE1	2.67	0.42
8:b:90:ILE:HB	8:b:127:LEU:HD13	2.01	0.42
10:d:122:LEU:CD1	10:d:125:LYS:CB	2.68	0.42
12:f:479:LEU:HA	12:f:514:VAL:HG13	2.01	0.42
12:f:569:LYS:HD3	12:f:574:GLU:HG3	2.02	0.42
12:f:665:GLU:O	12:f:669:GLU:HB2	2.20	0.42
13:A:120:LYS:HB2	18:F:90:VAL:HG21	2.02	0.42
17:E:304:PRO:HB2	17:E:309:ARG:HG3	2.00	0.42
26:N:141:ALA:HB2	26:n:162:LEU:HD11	2.01	0.42
21:i:119:GLN:NE2	22:j:79:ASP:OD1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:96:LEU:HB2	29:q:62:LYS:HG3	2.02	0.42
22:j:121:SER:OG	22:j:122:ASN:N	2.53	0.42
24:l:47:VAL:HG13	24:l:212:ILE:HG13	2.02	0.42
1:U:325:MET:HB2	1:U:329:LEU:HD12	2.01	0.42
2:V:209:LYS:HA	2:V:212:TYR:HD2	1.85	0.42
4:X:224:ASP:O	4:X:228:ALA:CB	2.68	0.42
6:Z:136:GLU:OE2	6:Z:157:HIS:ND1	2.52	0.42
7:a:21:VAL:O	7:a:25:LEU:CB	2.66	0.42
7:a:143:ASN:OD1	7:a:143:ASN:N	2.33	0.42
10:d:48:LEU:CB	10:d:88:GLN:NE2	2.80	0.42
12:f:83:ARG:O	12:f:87:THR:OG1	2.33	0.42
12:f:614:HIS:CE1	14:B:77:GLU:HB2	2.54	0.42
14:B:297:SER:OG	15:C:268:GLU:OE2	2.31	0.42
14:B:378:VAL:HG12	14:B:416:ASN:HA	2.02	0.42
22:J:121:SER:OG	22:J:122:ASN:N	2.53	0.42
22:J:226:GLU:O	22:J:230:ALA:HB2	2.19	0.42
23:K:84:ASP:OD1	23:K:84:ASP:N	2.47	0.42
22:j:104:VAL:HG13	22:j:145:TYR:HE2	1.84	0.42
25:m:67:PHE:HB2	25:m:75:MET:HB3	2.02	0.42
1:U:729:GLY:O	1:U:733:ALA:CB	2.67	0.42
3:W:305:LEU:HD13	3:W:308:LEU:HD12	2.02	0.42
3:W:366:MET:O	3:W:370:TYR:HB2	2.20	0.42
4:X:329:ASN:O	4:X:333:GLN:HB2	2.20	0.42
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.63	0.42
7:a:61:GLU:HA	7:a:64:ILE:HB	2.02	0.42
8:b:36:VAL:HG12	8:b:188:ILE:HD12	2.01	0.42
9:c:89:PRO:O	9:c:93:ALA:CB	2.68	0.42
12:f:31:LYS:HE2	12:f:31:LYS:HB3	1.87	0.42
16:D:115:ILE:H	16:D:115:ILE:HG13	1.71	0.42
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.45	0.42
18:F:375:VAL:HG22	18:F:415:LEU:HD12	2.02	0.42
22:J:82:ILE:H	22:J:82:ILE:HG13	1.72	0.42
26:N:6:VAL:HG22	26:N:125:PHE:HB2	2.02	0.42
32:T:15:LYS:HG2	32:T:20:VAL:HG22	2.02	0.42
24:l:94:ASP:OD1	24:l:95:SER:N	2.53	0.42
26:n:96:ALA:HB1	26:n:98:ILE:HG12	2.02	0.42
4:X:306:LEU:O	4:X:310:ARG:HB2	2.20	0.42
4:X:345:VAL:HG12	4:X:385:LEU:HB2	2.02	0.42
7:a:188:LEU:HB2	7:a:189:PRO:HD2	2.02	0.42
8:b:37:CYS:O	8:b:41:THR:CB	2.68	0.42
8:b:52:ILE:HD12	8:b:52:ILE:HA	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:237:HIS:CE1	9:c:241:ASN:HD21	2.38	0.42
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.85	0.42
12:f:719:PRO:HB3	12:f:754:LYS:HB2	2.02	0.42
12:f:774:GLY:O	12:f:776:LEU:N	2.52	0.42
14:B:141:LYS:HB2	14:B:141:LYS:HE3	1.52	0.42
14:B:234:LEU:N	34:B:501:ATP:O1A	2.51	0.42
15:C:127:LEU:HD23	15:C:127:LEU:HA	1.76	0.42
21:I:140:ASP:OD1	21:I:144:GLY:N	2.53	0.42
24:L:47:VAL:HG13	24:L:212:ILE:HG13	2.02	0.42
28:P:107:PRO:HG2	28:P:124:LEU:HB2	2.01	0.42
19:g:180:GLU:HA	19:g:183:VAL:HG12	2.01	0.42
27:o:19:ARG:NH1	27:o:167:LEU:O	2.53	0.42
1:U:804:SER:HA	1:U:892:LEU:HA	2.01	0.41
1:U:808:PRO:HB3	1:U:876:GLN:HE22	1.85	0.41
1:U:913:ILE:H	1:U:913:ILE:HG13	1.58	0.41
2:V:449:ALA:HB3	2:V:460:SER:HA	2.01	0.41
3:W:317:TRP:CE2	3:W:351:TRP:CZ3	3.01	0.41
3:W:356:ASN:HB2	3:W:357:ARG:NH1	2.36	0.41
9:c:237:HIS:CE1	9:c:298:GLN:HE21	2.37	0.41
12:f:371:ASN:HA	12:f:374:SER:HB2	2.01	0.41
13:A:278:ASP:N	13:A:278:ASP:OD1	2.51	0.41
17:E:140:GLU:O	17:E:144:GLU:HB2	2.20	0.41
22:J:56:GLU:C	22:J:56:GLU:CD	2.87	0.41
24:L:45:VAL:HG11	24:L:188:VAL:HG22	2.01	0.41
24:L:50:LYS:N	24:L:209:ASN:O	2.45	0.41
26:N:96:ALA:HB1	26:N:98:ILE:HG12	2.02	0.41
29:Q:117:TYR:HB3	29:Q:125:ALA:HB3	2.02	0.41
19:g:123:GLN:O	19:g:127:GLN:HB2	2.20	0.41
23:k:210:LEU:HD11	23:k:215:ILE:HG12	2.02	0.41
27:o:38:SER:OG	27:o:40:ASN:OD1	2.26	0.41
1:U:487:GLY:N	1:U:518:LEU:O	2.43	0.41
1:U:695:MET:HE3	1:U:695:MET:HB2	1.88	0.41
2:V:194:LYS:H	2:V:194:LYS:HD2	1.85	0.41
3:W:309:PHE:O	3:W:361:HIS:CE1	2.73	0.41
4:X:348:GLU:HG3	4:X:358:LYS:HD3	2.00	0.41
4:X:382:GLU:HG2	4:X:384:VAL:HG23	2.02	0.41
6:Z:231:GLN:HE22	7:a:339:ARG:H	1.67	0.41
6:Z:237:LEU:HD21	9:c:310:LYS:HD3	2.01	0.41
7:a:26:GLU:HA	7:a:29:TYR:HE1	1.84	0.41
7:a:141:MET:N	7:a:141:MET:SD	2.93	0.41
12:f:548:THR:HG21	12:f:554:TYR:HE2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:163:MET:SD	16:D:163:MET:N	2.94	0.41
16:D:172:ILE:O	16:D:176:GLU:CB	2.66	0.41
17:E:33:LEU:O	17:E:37:THR:CB	2.68	0.41
20:H:169:ASN:O	20:H:172:THR:OG1	2.33	0.41
22:J:201:SER:HA	22:J:205:ASN:HB2	2.02	0.41
25:M:66:LEU:HD13	25:M:212:GLU:HG2	2.01	0.41
22:j:226:GLU:O	22:j:230:ALA:HB2	2.19	0.41
1:U:253:TYR:CZ	1:U:331:GLY:HA3	2.55	0.41
1:U:450:HIS:HB3	1:U:453:HIS:HB2	2.01	0.41
1:U:745:THR:O	1:U:784:THR:N	2.43	0.41
3:W:81:ASP:O	3:W:85:GLU:HG3	2.20	0.41
5:Y:279:GLU:HB2	5:Y:296:VAL:HG21	2.03	0.41
10:d:105:PHE:HB2	10:d:166:PHE:CZ	2.56	0.41
12:f:223:GLU:HA	14:B:60:LEU:HD21	2.03	0.41
12:f:673:ARG:HE	12:f:712:LYS:HG3	1.81	0.41
15:C:90:HIS:HB2	15:C:91:PRO:HD3	2.00	0.41
16:D:274:ARG:H	17:E:245:GLU:CD	2.29	0.41
17:E:101:ASP:OD2	17:E:104:THR:N	2.52	0.41
18:F:336:ASP:N	18:F:336:ASP:OD1	2.52	0.41
21:I:159:TRP:HZ3	22:J:54:GLN:HG3	1.84	0.41
23:K:169:ALA:O	23:K:174:SER:OG	2.30	0.41
26:N:20:THR:HB	26:N:28:ASN:HB3	2.01	0.41
26:N:138:TYR:O	26:N:142:THR:OG1	2.28	0.41
31:s:95:ILE:O	31:s:98:SER:OG	2.32	0.41
1:U:69:TYR:CZ	1:U:99:THR:HB	2.55	0.41
1:U:474:ARG:O	1:U:478:SER:OG	2.36	0.41
3:W:108:CYS:HA	3:W:111:TYR:HB2	2.02	0.41
4:X:291:ALA:O	4:X:295:LYS:HB2	2.21	0.41
5:Y:293:ARG:HH21	11:e:52:PHE:HB3	1.84	0.41
6:Z:138:TYR:HB3	6:Z:155:PHE:HB3	2.02	0.41
9:c:192:LEU:CA	9:c:196:LEU:CD2	2.98	0.41
12:f:516:GLY:HA3	12:f:557:TRP:HE3	1.85	0.41
13:A:414:ASN:O	13:A:419:SER:N	2.52	0.41
21:I:18:LEU:CD1	21:I:21:VAL:HG22	2.50	0.41
22:J:228:TYR:HA	22:J:231:GLU:HG2	2.02	0.41
26:N:138:TYR:O	26:N:142:THR:CB	2.69	0.41
24:l:45:VAL:HG11	24:l:188:VAL:HG22	2.01	0.41
28:p:135:ASP:OD1	28:p:135:ASP:N	2.45	0.41
1:U:35:TRP:CZ2	1:U:70:HIS:HB3	2.56	0.41
3:W:276:LEU:N	3:W:276:LEU:HD23	2.35	0.41
5:Y:223:THR:HA	5:Y:226:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:190:ARG:HH12	9:c:297:VAL:HA	1.85	0.41
12:f:616:CYS:SG	12:f:632:LYS:NZ	2.77	0.41
12:f:808:ASN:HB3	12:f:809:ILE:H	1.46	0.41
17:E:197:LYS:HA	17:E:231:PHE:HB3	2.03	0.41
19:G:95:ARG:NH2	26:N:68:ILE:O	2.53	0.41
23:K:210:LEU:HD11	23:K:215:ILE:HG12	2.02	0.41
24:L:204:ASP:OD1	24:L:204:ASP:N	2.53	0.41
29:Q:25:ILE:HG13	29:Q:26:VAL:HG13	2.03	0.41
32:T:171:ARG:NH2	27:o:140:ASP:OD2	2.54	0.41
22:j:154:HIS:HD2	22:j:156:TRP:NE1	2.19	0.41
32:t:9:THR:O	32:t:41:ARG:NH2	2.53	0.41
32:t:15:LYS:HG2	32:t:20:VAL:HG22	2.02	0.41
4:X:224:ASP:O	4:X:228:ALA:HB3	2.21	0.41
6:Z:193:ASN:ND2	6:Z:197:GLY:HA3	2.35	0.41
10:d:107:LEU:HB2	10:d:115:PHE:CE1	2.56	0.41
12:f:82:ILE:O	12:f:86:THR:OG1	2.32	0.41
15:C:307:ARG:HA	15:C:308:PRO:HD3	1.93	0.41
15:C:338:LEU:HD13	15:C:378:VAL:HB	2.03	0.41
15:C:369:TYR:HD1	15:C:372:ARG:HE	1.69	0.41
17:E:56:ILE:HB	17:E:100:LEU:HB2	2.02	0.41
21:i:100:GLN:HE21	29:q:83:PHE:HE1	1.68	0.41
24:l:229:VAL:O	24:l:233:LEU:N	2.48	0.41
26:n:14:LEU:HD11	26:n:101:ALA:HB3	2.02	0.41
28:p:189:ILE:HG23	28:p:196:THR:HB	2.02	0.41
3:W:59:ASP:O	3:W:63:THR:OG1	2.32	0.41
3:W:316:ARG:CD	3:W:319:THR:OG1	2.66	0.41
4:X:74:ARG:HH12	4:X:112:GLU:HB3	1.86	0.41
12:f:675:PHE:O	12:f:679:LEU:CD1	2.69	0.41
15:C:90:HIS:CE1	16:D:109:SER:HB2	2.56	0.41
26:N:14:LEU:HD11	26:N:101:ALA:HB3	2.02	0.41
26:n:20:THR:HB	26:n:28:ASN:HB3	2.01	0.41
1:U:602:LEU:HD21	1:U:621:SER:HB2	2.03	0.41
2:V:92:ARG:HG2	2:V:96:ARG:HH22	1.86	0.41
2:V:228:ARG:HH21	2:V:257:ASN:HB3	1.86	0.41
3:W:219:THR:HB	3:W:222:LEU:HB3	2.03	0.41
3:W:352:LYS:HG3	3:W:355:LYS:HG2	2.02	0.41
4:X:122:ARG:HD2	4:X:125:LEU:HB2	2.03	0.41
8:b:3:LEU:HB3	8:b:105:HIS:HA	2.01	0.41
12:f:198:HIS:O	12:f:202:HIS:CB	2.69	0.41
12:f:221:ILE:HB	12:f:239:TYR:CZ	2.56	0.41
12:f:646:MET:HE2	12:f:646:MET:HB2	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:92:GLU:HB3	15:C:93:GLY:H	1.60	0.41
27:O:83:LEU:HA	27:O:83:LEU:HD23	1.88	0.41
30:R:55:TRP:NE1	31:S:97:TYR:OH	2.52	0.41
32:T:96:MET:HE1	32:T:106:LEU:HD12	2.03	0.41
26:n:138:TYR:O	26:n:142:THR:CB	2.69	0.41
1:U:160:LEU:HG	1:U:197:VAL:HG22	2.03	0.41
1:U:763:VAL:HA	1:U:766:PHE:HB3	2.03	0.41
2:V:62:HIS:O	2:V:66:GLU:CB	2.69	0.41
2:V:403:ILE:HD12	2:V:403:ILE:HA	1.97	0.41
3:W:142:ARG:NH2	3:W:178:GLU:OE1	2.54	0.41
3:W:390:GLU:O	3:W:394:SER:OG	2.35	0.41
4:X:213:GLN:HA	4:X:216:ILE:HB	2.03	0.41
4:X:225:TRP:O	4:X:229:TYR:CB	2.69	0.41
5:Y:89:GLU:HA	5:Y:92:GLU:HG2	2.03	0.41
8:b:22:LEU:HD22	8:b:177:PRO:O	2.16	0.41
8:b:35:ILE:HD11	8:b:184:ILE:HD11	2.03	0.41
8:b:37:CYS:O	8:b:41:THR:OG1	2.35	0.41
9:c:254:ASN:HB3	9:c:280:PRO:HB3	2.02	0.41
10:d:107:LEU:C	10:d:107:LEU:CD2	2.88	0.41
12:f:437:GLU:HB2	12:f:440:ILE:HB	2.02	0.41
12:f:609:VAL:HG12	14:B:74:MET:HE1	2.03	0.41
14:B:381:ASP:HA	14:B:384:ILE:HD12	2.03	0.41
14:B:407:LEU:HA	14:B:407:LEU:HD23	1.86	0.41
17:E:97:ARG:NH1	17:E:114:GLU:HB3	2.35	0.41
17:E:281:ARG:HE	17:E:283:ASP:HB2	1.86	0.41
17:E:291:ARG:HE	17:E:294:ARG:NH1	2.19	0.41
22:J:96:LEU:O	30:R:81:LYS:NZ	2.40	0.41
22:J:154:HIS:HD2	22:J:156:TRP:NE1	2.19	0.41
28:P:59:ASP:OD2	28:P:104:TYR:N	2.41	0.41
29:Q:23:SER:OG	29:Q:24:ASN:N	2.53	0.41
31:S:16:ALA:HB2	31:S:121:VAL:HG23	2.03	0.41
22:j:81:ARG:HA	22:j:84:ILE:HD12	2.03	0.41
29:q:23:SER:OG	29:q:24:ASN:N	2.53	0.41
29:q:117:TYR:HB3	29:q:125:ALA:HB3	2.02	0.41
30:r:9:ARG:NH2	30:r:146:ASP:OD1	2.51	0.41
3:W:87:ILE:HD12	3:W:91:SER:HB2	2.02	0.41
3:W:105:VAL:O	3:W:109:CYS:CB	2.63	0.41
3:W:328:LEU:HB3	3:W:337:ALA:HB1	2.03	0.41
7:a:145:LEU:HD12	7:a:147:GLY:N	2.36	0.41
7:a:337:GLN:HA	7:a:338:PRO:HD3	1.96	0.41
8:b:22:LEU:HG	8:b:179:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:41:THR:HB	10:d:44:THR:HG23	2.03	0.41
10:d:114:GLU:CA	10:d:117:THR:CG2	2.89	0.41
12:f:325:GLN:HE21	12:f:420:TRP:HE3	1.69	0.41
12:f:811:LEU:HD11	12:f:862:ILE:HD13	2.03	0.41
13:A:425:ALA:HA	14:B:339:PRO:HB2	2.03	0.41
16:D:68:LEU:O	16:D:72:PHE:CB	2.67	0.41
17:E:138:LEU:HD12	17:E:142:ILE:HG13	2.02	0.41
19:G:123:GLN:O	19:G:127:GLN:HB2	2.20	0.41
20:h:69:THR:HG22	20:h:72:ILE:HB	2.03	0.41
32:t:96:MET:HE1	32:t:106:LEU:HD12	2.03	0.41
1:U:326:ILE:O	1:U:330:SER:OG	2.32	0.40
2:V:266:GLN:HG2	2:V:299:GLN:CD	2.45	0.40
2:V:316:ALA:HA	2:V:317:PRO:HD3	1.93	0.40
3:W:89:LEU:O	3:W:93:ARG:HB2	2.21	0.40
4:X:83:ALA:HB2	20:H:229:TYR:CE1	2.55	0.40
4:X:346:GLN:HE21	4:X:349:HIS:CE1	2.38	0.40
5:Y:36:ALA:O	5:Y:40:GLU:CB	2.68	0.40
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.02	0.40
7:a:115:LYS:HD3	7:a:118:ILE:HD12	2.02	0.40
7:a:144:ASN:C	7:a:144:ASN:HD22	2.28	0.40
8:b:124:LEU:HD21	8:b:152:LYS:HB3	2.04	0.40
9:c:221:HIS:ND1	9:c:222:LYS:HG2	2.36	0.40
10:d:114:GLU:O	10:d:117:THR:HG23	2.21	0.40
10:d:203:PRO:HG2	10:d:205:LYS:HB3	2.04	0.40
12:f:761:MET:HE2	12:f:766:GLN:HG2	2.04	0.40
12:f:761:MET:CE	12:f:766:GLN:CA	2.91	0.40
12:f:810:ILE:HA	12:f:856:ALA:HB2	2.02	0.40
12:f:872:VAL:HG21	12:f:882:LEU:H	1.86	0.40
15:C:303:SER:HA	15:C:306:LEU:HB2	2.03	0.40
22:j:36:ARG:HB3	22:j:144:LEU:HD23	2.03	0.40
29:q:25:ILE:HG13	29:q:26:VAL:HG13	2.03	0.40
2:V:257:ASN:HD21	2:V:261:TYR:HE2	1.68	0.40
2:V:263:LEU:HD11	2:V:264:TYR:HB3	1.99	0.40
2:V:357:LEU:CD1	2:V:360:TYR:HD2	2.34	0.40
3:W:357:ARG:NH1	3:W:357:ARG:HG3	2.36	0.40
4:X:347:ILE:HA	4:X:350:ILE:HG22	2.02	0.40
5:Y:234:PRO:HA	5:Y:237:ARG:HG3	2.03	0.40
6:Z:14:LEU:HG	9:c:39:LEU:HB3	2.03	0.40
6:Z:231:GLN:O	6:Z:235:ASN:HB2	2.20	0.40
7:a:142:LEU:C	7:a:144:ASN:H	2.29	0.40
9:c:191:ALA:C	9:c:196:LEU:HD22	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:43:LEU:HD23	10:d:43:LEU:HA	1.98	0.40
12:f:206:ASP:OD2	12:f:245:ASN:ND2	2.55	0.40
14:B:135:ILE:HA	14:B:159:VAL:HB	2.03	0.40
14:B:357:ASP:O	14:B:360:THR:OG1	2.27	0.40
16:D:159:LYS:C	16:D:161:ASP:H	2.28	0.40
17:E:217:GLU:HA	17:E:220:ASN:HB2	2.02	0.40
18:F:91:SER:HA	18:F:126:THR:HA	2.03	0.40
24:L:94:ASP:OD1	24:L:95:SER:N	2.53	0.40
25:M:67:PHE:HB2	25:M:75:MET:HB3	2.02	0.40
22:j:109:ARG:O	22:j:113:SER:CB	2.70	0.40
25:m:36:ALA:HB3	25:m:165:ILE:HG13	2.02	0.40
1:U:202:VAL:HB	1:U:216:VAL:HG23	2.02	0.40
7:a:170:ALA:O	7:a:174:LYS:HB2	2.22	0.40
9:c:59:GLY:HA3	9:c:69:VAL:HA	2.03	0.40
12:f:441:LYS:HD2	12:f:477:MET:HE1	2.03	0.40
16:D:95:ALA:HA	16:D:101:ALA:HA	2.03	0.40
18:F:362:ARG:NE	18:F:388:THR:O	2.55	0.40
21:I:13:SER:CB	21:I:19:TYR:CZ	3.04	0.40
25:M:36:ALA:HB3	25:M:165:ILE:HG13	2.02	0.40
30:R:97:MET:HB3	30:R:116:SER:HB3	2.04	0.40
28:p:107:PRO:HG2	28:p:124:LEU:HB2	2.01	0.40
31:s:6:VAL:HG12	31:s:57:PHE:HE1	1.86	0.40
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.03	0.40
1:U:725:MET:HE3	1:U:725:MET:HB2	1.97	0.40
2:V:99:ARG:NH2	2:V:103:SER:OG	2.52	0.40
3:W:131:VAL:HA	3:W:144:ARG:HH22	1.87	0.40
3:W:144:ARG:HG3	3:W:147:LYS:NZ	2.36	0.40
3:W:165:ILE:HG12	3:W:169:LEU:HD21	2.03	0.40
4:X:192:SER:HA	4:X:195:THR:HG22	2.04	0.40
4:X:319:ILE:HA	4:X:322:HIS:HD2	1.85	0.40
4:X:368:MET:HE1	4:X:373:LYS:HD2	2.03	0.40
6:Z:14:LEU:HD22	9:c:43:LYS:HD3	2.03	0.40
7:a:33:LEU:HD13	7:a:36:GLN:H	1.86	0.40
8:b:89:GLY:HA2	8:b:92:VAL:HG12	2.03	0.40
10:d:4:GLN:HB3	10:d:25:ARG:HE	1.86	0.40
12:f:168:LYS:HD3	12:f:204:ALA:HB1	2.03	0.40
12:f:209:MET:HG3	12:f:211:ILE:H	1.86	0.40
12:f:279:GLU:HB2	12:f:281:ILE:HD11	2.02	0.40
17:E:322:LYS:HD3	17:E:326:ILE:HG13	2.03	0.40
20:H:69:THR:HG22	20:H:72:ILE:HB	2.03	0.40
22:J:81:ARG:HA	22:J:84:ILE:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:40:ARG:HD2	25:M:161:TRP:CE3	2.56	0.40
30:R:9:ARG:NH2	30:R:146:ASP:OD1	2.51	0.40
23:k:111:SER:HA	23:k:114:GLN:HG2	2.04	0.40
5:Y:186:LEU:HA	5:Y:189:VAL:HG12	2.02	0.40
5:Y:233:ARG:HH22	5:Y:306:GLN:HE21	1.68	0.40
9:c:50:PRO:HG3	17:E:84:ARG:HG2	2.03	0.40
9:c:162:LEU:HA	9:c:200:TYR:HB3	2.04	0.40
10:d:45:LYS:CG	10:d:45:LYS:O	2.70	0.40
16:D:143:LEU:HD13	16:D:143:LEU:HA	1.98	0.40
19:G:112:ASP:HB3	19:G:152:TYR:CZ	2.57	0.40
21:I:106:PRO:HB2	21:I:109:GLN:HG2	2.03	0.40
23:K:111:SER:HA	23:K:114:GLN:HG2	2.04	0.40
28:P:189:ILE:HG23	28:P:196:THR:HB	2.02	0.40
25:m:41:CYS:N	25:m:44:GLY:O	2.48	0.40
31:s:16:ALA:HB2	31:s:121:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	731 (91%)	72 (9%)	3 (0%)	30	60
2	V	506/533 (95%)	445 (88%)	55 (11%)	6 (1%)	10	40
3	W	454/456 (100%)	401 (88%)	49 (11%)	4 (1%)	14	45
4	X	378/422 (90%)	352 (93%)	25 (7%)	1 (0%)	36	65
5	Y	376/389 (97%)	336 (89%)	40 (11%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	31
7	a	371/376 (99%)	324 (87%)	42 (11%)	5 (1%)	9	38
8	b	189/377 (50%)	170 (90%)	18 (10%)	1 (0%)	24	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	c	285/309 (92%)	244 (86%)	39 (14%)	2 (1%)	18	50
10	d	255/349 (73%)	208 (82%)	46 (18%)	1 (0%)	30	60
11	e	36/70 (51%)	27 (75%)	9 (25%)	0	100	100
12	f	887/908 (98%)	698 (79%)	176 (20%)	13 (2%)	8	36
13	A	392/433 (90%)	340 (87%)	50 (13%)	2 (0%)	24	56
14	B	382/440 (87%)	338 (88%)	41 (11%)	3 (1%)	16	48
15	C	359/398 (90%)	332 (92%)	25 (7%)	2 (1%)	21	52
16	D	378/418 (90%)	327 (86%)	46 (12%)	5 (1%)	9	38
17	E	373/403 (93%)	338 (91%)	35 (9%)	0	100	100
18	F	372/439 (85%)	339 (91%)	33 (9%)	0	100	100
19	G	238/245 (97%)	230 (97%)	8 (3%)	0	100	100
19	g	238/245 (97%)	228 (96%)	9 (4%)	1 (0%)	30	60
20	H	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
20	h	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
21	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
21	i	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
22	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	48
22	j	237/247 (96%)	217 (92%)	18 (8%)	2 (1%)	16	48
23	K	224/240 (93%)	213 (95%)	11 (5%)	0	100	100
23	k	224/240 (93%)	213 (95%)	11 (5%)	0	100	100
24	L	236/268 (88%)	218 (92%)	17 (7%)	1 (0%)	30	60
24	l	236/268 (88%)	217 (92%)	19 (8%)	0	100	100
25	M	238/254 (94%)	221 (93%)	16 (7%)	1 (0%)	30	60
25	m	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
26	N	189/238 (79%)	181 (96%)	8 (4%)	0	100	100
26	n	189/238 (79%)	181 (96%)	8 (4%)	0	100	100
27	O	218/276 (79%)	210 (96%)	8 (4%)	0	100	100
27	o	218/276 (79%)	210 (96%)	8 (4%)	0	100	100
28	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
28	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
30	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
30	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
31	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
32	T	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
32	t	213/263 (81%)	201 (94%)	12 (6%)	0	100	100
All	All	13243/14859 (89%)	11994 (91%)	1188 (9%)	61 (0%)	26	56

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	55	ARG
2	V	167	LEU
2	V	168	GLN
6	Z	149	THR
6	Z	150	PRO
7	a	145	LEU
7	a	152	HIS
7	a	186	LYS
8	b	22	LEU
9	c	158	ASP
12	f	281	ILE
12	f	766	GLN
12	f	789	SER
12	f	838	ARG
14	B	141	LYS
14	B	168	ASP
16	D	125	LYS
16	D	126	PRO
16	D	369	LYS
24	L	226	ASP
3	W	91	SER
3	W	315	MET
6	Z	151	THR
9	c	196	LEU
12	f	756	PRO
12	f	761	MET
14	B	278	ALA
16	D	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	M	186	CYS
1	U	52	GLU
7	a	151	VAL
12	f	476	THR
12	f	768	LEU
3	W	316	ARG
3	W	317	TRP
6	Z	224	HIS
7	a	69	HIS
10	d	109	GLN
12	f	118	ASN
12	f	681	TYR
22	J	200	GLN
19	g	134	LEU
22	j	198	VAL
22	j	200	GLN
2	V	496	PHE
4	X	392	PRO
6	Z	212	LEU
12	f	475	ASN
12	f	765	ALA
13	A	109	PRO
13	A	400	ARG
2	V	263	LEU
16	D	367	PRO
6	Z	99	PRO
12	f	643	PRO
1	U	174	PRO
15	C	90	HIS
2	V	29	PRO
22	J	198	VAL
2	V	497	PRO
15	C	127	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	683 (99%)	9 (1%)	61	71
2	V	415/459 (90%)	406 (98%)	9 (2%)	45	63
3	W	414/416 (100%)	400 (97%)	14 (3%)	32	55
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	83
5	Y	334/344 (97%)	332 (99%)	2 (1%)	78	79
6	Z	257/295 (87%)	242 (94%)	15 (6%)	18	45
7	a	333/336 (99%)	324 (97%)	9 (3%)	39	59
8	b	167/312 (54%)	164 (98%)	3 (2%)	51	67
9	c	252/267 (94%)	243 (96%)	9 (4%)	31	54
10	d	231/293 (79%)	223 (96%)	8 (4%)	32	54
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	743/763 (97%)	717 (96%)	26 (4%)	32	54
13	A	337/372 (91%)	334 (99%)	3 (1%)	70	75
14	B	339/385 (88%)	334 (98%)	5 (2%)	57	68
15	C	314/346 (91%)	305 (97%)	9 (3%)	37	57
16	D	333/366 (91%)	327 (98%)	6 (2%)	51	67
17	E	298/353 (84%)	295 (99%)	3 (1%)	68	74
18	F	296/379 (78%)	296 (100%)	0	100	100
19	G	193/209 (92%)	192 (100%)	1 (0%)	81	80
19	g	193/209 (92%)	190 (98%)	3 (2%)	55	68
20	H	164/190 (86%)	164 (100%)	0	100	100
20	h	164/190 (86%)	164 (100%)	0	100	100
21	I	193/220 (88%)	188 (97%)	5 (3%)	40	60
21	i	193/220 (88%)	193 (100%)	0	100	100
22	J	154/210 (73%)	149 (97%)	5 (3%)	34	56
22	j	152/210 (72%)	151 (99%)	1 (1%)	76	77
23	K	186/202 (92%)	186 (100%)	0	100	100
23	k	186/202 (92%)	186 (100%)	0	100	100
24	L	198/229 (86%)	195 (98%)	3 (2%)	57	68
24	l	198/229 (86%)	196 (99%)	2 (1%)	68	74
25	M	192/211 (91%)	191 (100%)	1 (0%)	81	80
25	m	192/211 (91%)	192 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	N	148/180 (82%)	148 (100%)	0	100	100
26	n	148/180 (82%)	148 (100%)	0	100	100
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	173/173 (100%)	173 (100%)	0	100	100
28	p	173/173 (100%)	173 (100%)	0	100	100
29	Q	164/171 (96%)	164 (100%)	0	100	100
29	q	164/171 (96%)	164 (100%)	0	100	100
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100
31	S	174/198 (88%)	174 (100%)	0	100	100
31	s	175/198 (88%)	175 (100%)	0	100	100
32	T	175/214 (82%)	175 (100%)	0	100	100
32	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11007/12597 (87%)	10855 (99%)	152 (1%)	57	70

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	55	ARG
1	U	177	LEU
1	U	529	ILE
1	U	554	LEU
1	U	603	LEU
1	U	605	VAL
1	U	689	ILE
1	U	775	LEU
1	U	913	ILE
2	V	163	VAL
2	V	167	LEU
2	V	266	GLN
2	V	329	HIS
2	V	345	ARG
2	V	357	LEU
2	V	358	MET
2	V	362	LEU
2	V	437	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	86	ASN
3	W	87	ILE
3	W	88	MET
3	W	89	LEU
3	W	274	VAL
3	W	275	ILE
3	W	276	LEU
3	W	315	MET
3	W	316	ARG
3	W	355	LYS
3	W	357	ARG
3	W	359	VAL
3	W	361	HIS
3	W	364	ARG
4	X	80	ILE
5	Y	235	ASP
5	Y	287	LEU
6	Z	91	ILE
6	Z	141	VAL
6	Z	143	GLU
6	Z	145	HIS
6	Z	147	ASP
6	Z	149	THR
6	Z	151	THR
6	Z	152	SER
6	Z	153	LYS
6	Z	154	THR
6	Z	191	ILE
6	Z	192	THR
6	Z	193	ASN
6	Z	227	ILE
6	Z	236	LEU
7	a	143	ASN
7	a	145	LEU
7	a	149	THR
7	a	150	SER
7	a	151	VAL
7	a	183	VAL
7	a	186	LYS
7	a	188	LEU
7	a	190	VAL
8	b	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	b	52	ILE
8	b	71	ILE
9	c	49	VAL
9	c	69	VAL
9	c	83	SER
9	c	84	VAL
9	c	85	GLU
9	c	155	VAL
9	c	197	ASN
9	c	198	ARG
9	c	200	TYR
10	d	35	PHE
10	d	45	LYS
10	d	89	LEU
10	d	107	LEU
10	d	108	SER
10	d	117	THR
10	d	118	GLU
10	d	121	ARG
12	f	217	LEU
12	f	218	GLU
12	f	281	ILE
12	f	282	PHE
12	f	283	THR
12	f	344	VAL
12	f	679	LEU
12	f	681	TYR
12	f	712	LYS
12	f	713	PHE
12	f	755	ASP
12	f	757	ASN
12	f	759	LEU
12	f	763	ARG
12	f	764	LEU
12	f	768	LEU
12	f	769	THR
12	f	770	HIS
12	f	771	LEU
12	f	773	LYS
12	f	775	THR
12	f	787	LEU
12	f	788	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	f	822	VAL
12	f	838	ARG
12	f	840	LEU
13	A	400	ARG
13	A	401	ARG
13	A	403	ILE
14	B	125	THR
14	B	141	LYS
14	B	143	LEU
14	B	167	THR
14	B	168	ASP
15	C	48	GLN
15	C	49	ARG
15	C	89	VAL
15	C	90	HIS
15	C	92	GLU
15	C	109	THR
15	C	126	ILE
15	C	127	LEU
15	C	210	THR
16	D	124	LEU
16	D	125	LYS
16	D	231	VAL
16	D	354	LEU
16	D	369	LYS
16	D	370	ILE
17	E	115	VAL
17	E	138	LEU
17	E	384	LEU
19	G	222	VAL
21	I	20	GLN
21	I	22	GLU
21	I	225	ILE
21	I	226	ARG
21	I	228	LEU
22	J	53	LEU
22	J	54	GLN
22	J	56	GLU
22	J	159	ASN
22	J	200	GLN
24	L	103	LEU
24	L	161	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	L	227	ASP
25	M	187	ARG
19	g	134	LEU
19	g	222	VAL
19	g	224	ASN
22	j	159	ASN
24	l	103	LEU
24	l	161	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	111	GLN
1	U	241	ASN
1	U	338	HIS
1	U	345	ASN
1	U	355	ASN
1	U	377	HIS
1	U	389	ASN
1	U	415	HIS
1	U	595	ASN
1	U	604	HIS
1	U	685	GLN
1	U	768	GLN
1	U	777	HIS
2	V	62	HIS
2	V	78	HIS
2	V	319	HIS
2	V	329	HIS
2	V	400	HIS
2	V	401	ASN
2	V	427	GLN
2	V	452	ASN
2	V	487	HIS
3	W	53	GLN
3	W	86	ASN
3	W	96	GLN
3	W	106	GLN
3	W	356	ASN
3	W	361	HIS
3	W	362	ASN
3	W	399	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	430	GLN
3	W	440	ASN
4	X	198	ASN
4	X	207	GLN
4	X	213	GLN
4	X	262	ASN
4	X	322	HIS
4	X	329	ASN
4	X	333	GLN
4	X	406	ASN
5	Y	71	ASN
5	Y	306	GLN
5	Y	367	GLN
6	Z	109	ASN
6	Z	202	ASN
6	Z	223	ASN
6	Z	231	GLN
6	Z	273	HIS
6	Z	277	ASN
7	a	9	GLN
7	a	12	GLN
7	a	18	GLN
7	a	144	ASN
7	a	164	GLN
7	a	193	GLN
7	a	212	ASN
7	a	219	HIS
7	a	231	GLN
7	a	249	GLN
7	a	258	GLN
7	a	264	ASN
7	a	267	GLN
7	a	290	GLN
7	a	337	GLN
7	a	345	GLN
7	a	370	GLN
8	b	101	GLN
8	b	142	ASN
9	c	30	GLN
9	c	44	HIS
9	c	101	GLN
9	c	113	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	c	130	GLN
9	c	164	ASN
9	c	166	ASN
9	c	172	HIS
9	c	197	ASN
9	c	214	GLN
9	c	232	GLN
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
9	c	278	GLN
9	c	298	GLN
10	d	88	GLN
10	d	229	GLN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	171	GLN
12	f	213	GLN
12	f	238	ASN
12	f	245	ASN
12	f	291	GLN
12	f	396	ASN
12	f	405	HIS
12	f	457	ASN
12	f	475	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	619	HIS
12	f	715	HIS
12	f	737	ASN
12	f	782	HIS
12	f	808	ASN
12	f	826	GLN
12	f	866	GLN
13	A	44	GLN
13	A	54	GLN
13	A	247	GLN
13	A	304	ASN
13	A	433	ASN
14	B	81	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	B	84	GLN
14	B	241	ASN
14	B	242	GLN
15	C	32	GLN
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN
15	C	64	GLN
15	C	90	HIS
15	C	221	GLN
15	C	337	ASN
15	C	380	GLN
16	D	67	ASN
16	D	133	HIS
16	D	173	GLN
16	D	222	HIS
16	D	257	ASN
16	D	312	ASN
16	D	340	GLN
16	D	353	ASN
16	D	380	GLN
17	E	75	ASN
17	E	155	ASN
18	F	76	ASN
18	F	83	ASN
18	F	184	GLN
18	F	208	HIS
18	F	316	GLN
18	F	369	HIS
19	G	12	HIS
19	G	68	HIS
19	G	128	ASN
20	H	63	HIS
20	H	88	HIS
20	H	112	GLN
21	I	53	HIS
21	I	84	ASN
21	I	102	GLN
21	I	119	GLN
21	I	142	HIS
21	I	146	GLN
21	I	220	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	J	54	GLN
22	J	116	GLN
22	J	154	HIS
22	J	159	ASN
22	J	200	GLN
22	J	205	ASN
23	K	41	GLN
23	K	98	ASN
23	K	118	ASN
23	K	164	GLN
23	K	224	GLN
24	L	90	GLN
25	M	32	ASN
25	M	180	GLN
25	M	221	ASN
26	N	28	ASN
26	N	110	GLN
27	O	66	HIS
27	O	116	HIS
27	O	165	ASN
28	P	93	ASN
28	P	169	GLN
29	Q	8	GLN
29	Q	82	ASN
30	R	29	GLN
30	R	85	ASN
31	S	151	ASN
32	T	65	GLN
19	g	68	HIS
19	g	92	GLN
19	g	128	ASN
20	h	63	HIS
20	h	88	HIS
20	h	102	GLN
20	h	109	GLN
20	h	169	ASN
20	h	189	HIS
21	i	53	HIS
21	i	84	ASN
21	i	102	GLN
21	i	146	GLN
22	j	159	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	j	205	ASN
23	k	98	ASN
23	k	224	GLN
24	l	90	GLN
25	m	32	ASN
25	m	180	GLN
25	m	221	ASN
26	n	28	ASN
26	n	110	GLN
27	o	116	HIS
27	o	165	ASN
28	p	93	ASN
28	p	169	GLN
29	q	8	GLN
30	r	29	GLN
30	r	85	ASN
32	t	61	GLN
32	t	65	GLN
32	t	69	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
34	ATP	B	501	35	32,33,33	1.30	5 (15%)	48,52,52	1.76	11 (22%)
36	ADP	F	501	35	28,29,29	1.38	5 (17%)	43,45,45	1.79	10 (23%)
36	ADP	C	501	-	28,29,29	1.37	3 (10%)	43,45,45	2.02	9 (20%)
34	ATP	A	501	35	32,33,33	1.31	5 (15%)	48,52,52	1.78	10 (20%)
34	ATP	E	401	35	32,33,33	1.30	4 (12%)	48,52,52	1.82	8 (16%)
34	ATP	D	501	35	32,33,33	1.30	5 (15%)	48,52,52	1.77	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	B	501	35	-	0/22/38/38	0/3/3/3
36	ADP	F	501	35	-	6/16/32/32	0/3/3/3
36	ADP	C	501	-	-	3/16/32/32	0/3/3/3
34	ATP	A	501	35	-	1/22/38/38	0/3/3/3
34	ATP	E	401	35	-	6/22/38/38	0/3/3/3
34	ATP	D	501	35	-	6/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-C4	4.55	1.47	1.39
34	E	401	ATP	C5-C4	4.51	1.47	1.39
36	F	501	ADP	C5-C4	4.44	1.47	1.39
34	D	501	ATP	C5-C4	4.39	1.46	1.39
34	A	501	ATP	C5-C4	4.34	1.46	1.39
34	B	501	ATP	C5-C4	4.31	1.46	1.39
34	A	501	ATP	C5-N7	-2.80	1.34	1.39
36	F	501	ADP	C5-N7	-2.68	1.34	1.39
36	C	501	ADP	C5-N7	-2.60	1.34	1.39
36	C	501	ADP	C5-C6	2.58	1.48	1.41
34	B	501	ATP	C5-N7	-2.53	1.34	1.39
34	E	401	ATP	C5-C6	2.52	1.48	1.41
34	D	501	ATP	C5-N7	-2.52	1.34	1.39
34	E	401	ATP	C5-N7	-2.50	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	ATP	C5-C6	2.46	1.47	1.41
34	A	501	ATP	C5-C6	2.44	1.47	1.41
36	F	501	ADP	C5-C6	2.40	1.47	1.41
34	B	501	ATP	C5-C6	2.38	1.47	1.41
36	F	501	ADP	C4-N9	-2.30	1.32	1.37
34	B	501	ATP	C4-N9	-2.29	1.32	1.37
34	A	501	ATP	C4-N9	-2.25	1.33	1.37
34	D	501	ATP	C4-N9	-2.23	1.33	1.37
34	D	501	ATP	C8-N7	2.17	1.35	1.31
34	B	501	ATP	C8-N7	2.13	1.35	1.31
36	F	501	ADP	C8-N7	2.09	1.35	1.31
34	A	501	ATP	C8-N7	2.07	1.35	1.31
34	E	401	ATP	C8-N7	2.07	1.35	1.31

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	501	ADP	C5-C4-N3	-6.73	117.45	126.72
34	E	401	ATP	C5-C4-N3	-6.12	118.29	126.72
34	A	501	ATP	C5-C4-N3	-5.76	118.79	126.72
36	C	501	ADP	N3-C4-N9	5.67	136.82	127.17
34	D	501	ATP	C5-C4-N3	-5.65	118.93	126.72
36	F	501	ADP	C5-C4-N3	-5.57	119.05	126.72
34	B	501	ATP	C5-C4-N3	-5.54	119.08	126.72
34	E	401	ATP	N3-C4-N9	5.12	135.88	127.17
34	A	501	ATP	N3-C4-N9	4.64	135.07	127.17
34	D	501	ATP	N3-C4-N9	4.63	135.05	127.17
34	B	501	ATP	N3-C4-N9	4.61	135.00	127.17
36	F	501	ADP	N3-C4-N9	4.51	134.83	127.17
36	C	501	ADP	C2-N3-C4	4.02	121.65	111.83
34	E	401	ATP	C2-N3-C4	3.84	121.21	111.83
34	D	501	ATP	C2-N3-C4	3.70	120.86	111.83
34	B	501	ATP	C2-N3-C4	3.61	120.66	111.83
34	A	501	ATP	C4-C5-N7	-3.48	106.60	110.58
34	A	501	ATP	C2-N3-C4	3.48	120.33	111.83
34	B	501	ATP	N3-C2-N1	-3.46	123.34	128.58
36	F	501	ADP	C2-N3-C4	3.45	120.27	111.83
34	D	501	ATP	N3-C2-N1	-3.32	123.55	128.58
34	E	401	ATP	N3-C2-N1	-3.27	123.63	128.58
34	D	501	ATP	C4-C5-N7	-3.23	106.89	110.58
36	F	501	ADP	C4-C5-N7	-3.19	106.94	110.58
36	C	501	ADP	C4-C5-N7	-3.18	106.95	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	501	ADP	N3-C2-N1	-3.15	123.82	128.58
34	B	501	ATP	C4-N9-C8	3.13	109.02	105.74
34	B	501	ATP	C4-C5-N7	-3.11	107.03	110.58
34	E	401	ATP	C4-C5-N7	-3.06	107.08	110.58
34	D	501	ATP	C4-N9-C8	3.02	108.91	105.74
36	F	501	ADP	N3-C2-N1	-2.98	124.08	128.58
34	A	501	ATP	C4-N9-C8	2.96	108.84	105.74
34	A	501	ATP	N3-C2-N1	-2.91	124.17	128.58
36	C	501	ADP	C3'-C2'-C1'	2.89	106.92	101.46
34	E	401	ATP	C4-N9-C8	2.72	108.59	105.74
36	F	501	ADP	C4-N9-C8	2.72	108.59	105.74
34	A	501	ATP	C5-N7-C8	2.66	107.63	103.45
36	C	501	ADP	C4-N9-C8	2.64	108.50	105.74
34	A	501	ATP	C3'-C2'-C1'	2.62	106.43	101.46
36	C	501	ADP	C5-N7-C8	2.55	107.45	103.45
34	B	501	ATP	C3'-C2'-C1'	2.43	106.06	101.46
34	D	501	ATP	C5-N7-C8	2.39	107.20	103.45
34	B	501	ATP	C5-N7-C8	2.37	107.17	103.45
34	E	401	ATP	C5-N7-C8	2.32	107.10	103.45
34	E	401	ATP	C3'-C2'-C1'	2.27	105.76	101.46
36	F	501	ADP	C5-N7-C8	2.27	107.02	103.45
36	C	501	ADP	C1'-N9-C8	-2.26	122.08	127.09
34	A	501	ATP	C2'-C1'-N9	-2.25	107.71	113.30
34	A	501	ATP	N9-C8-N7	-2.23	110.78	113.94
36	F	501	ADP	C2'-C1'-N9	-2.20	107.84	113.30
34	B	501	ATP	N9-C8-N7	-2.16	110.87	113.94
34	D	501	ATP	C6-C5-N7	2.15	136.23	132.09
36	F	501	ADP	C3'-C2'-C1'	2.14	105.52	101.46
36	F	501	ADP	O3B-PB-O2B	2.10	115.68	107.80
34	D	501	ATP	N9-C8-N7	-2.08	110.98	113.94
34	B	501	ATP	C2-N1-C6	2.06	122.11	118.73
34	D	501	ATP	C3'-C2'-C1'	2.02	105.29	101.46
34	B	501	ATP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	E	401	ATP	PB-O3B-PG-O2G
34	E	401	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	C	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	O4'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'
34	D	501	ATP	C2'-C1'-N9-C8
36	F	501	ADP	C2'-C1'-N9-C8
34	D	501	ATP	PA-O3A-PB-O1B
34	D	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	O4'-C1'-N9-C8
34	E	401	ATP	PB-O3B-PG-O1G
34	D	501	ATP	O4'-C1'-N9-C4
36	F	501	ADP	O4'-C1'-N9-C8
36	F	501	ADP	O4'-C1'-N9-C4
36	F	501	ADP	C2'-C1'-N9-C4
34	D	501	ATP	PA-O3A-PB-O2B
34	A	501	ATP	PA-O3A-PB-O1B

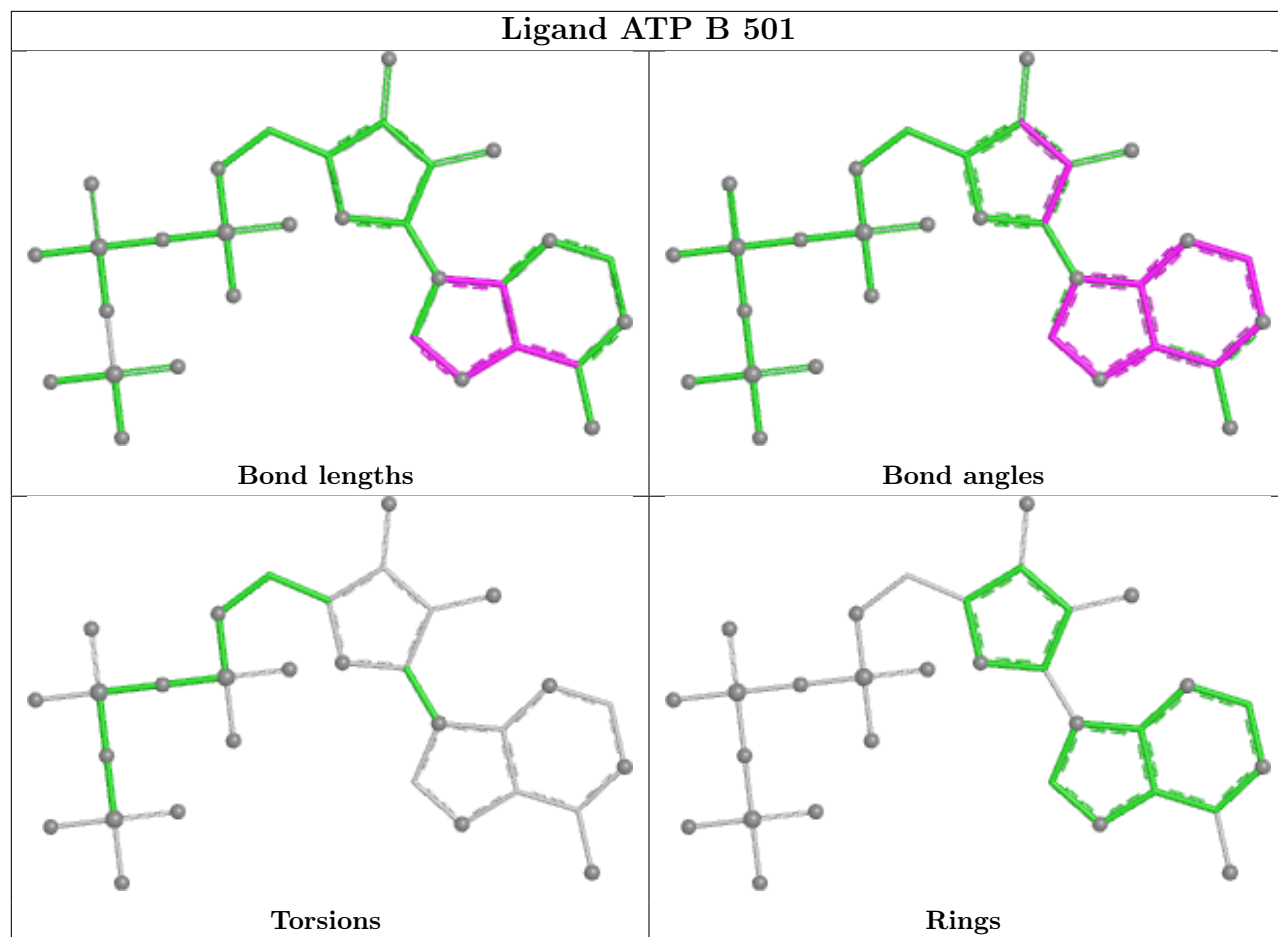
There are no ring outliers.

6 monomers are involved in 8 short contacts:

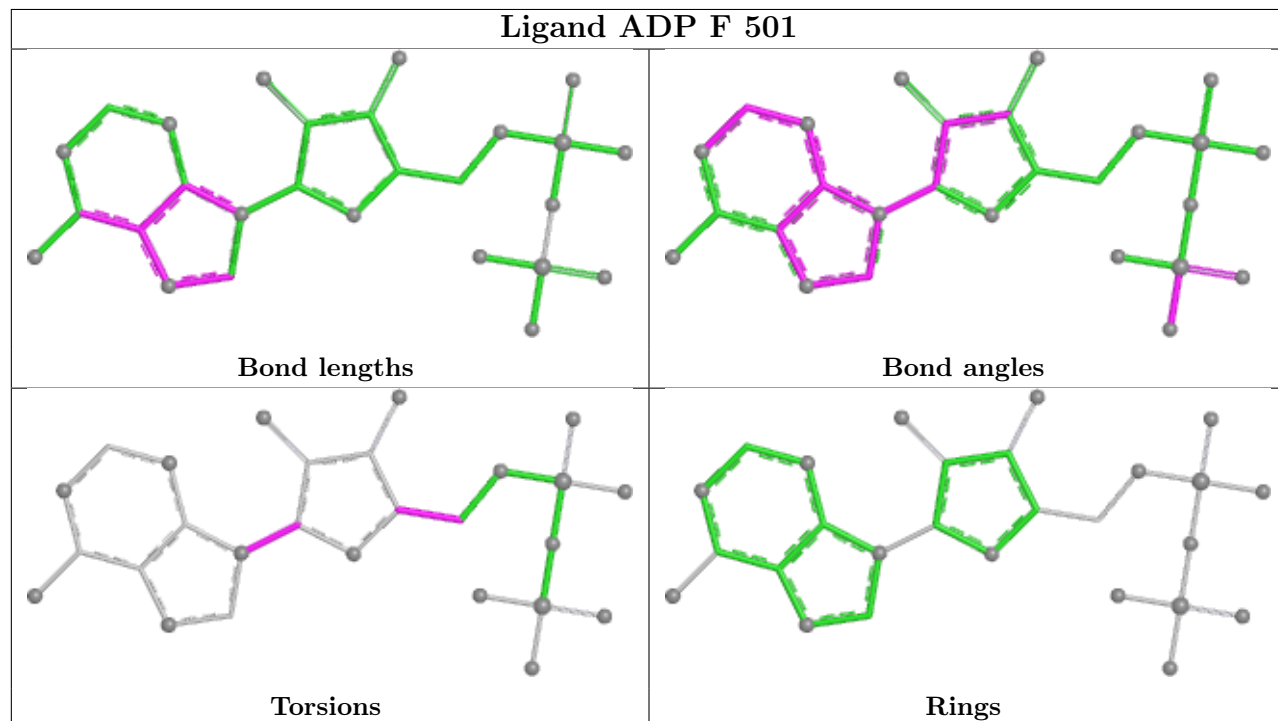
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	501	ATP	1	0
36	F	501	ADP	1	0
36	C	501	ADP	1	0
34	A	501	ATP	1	0
34	E	401	ATP	3	0
34	D	501	ATP	1	0

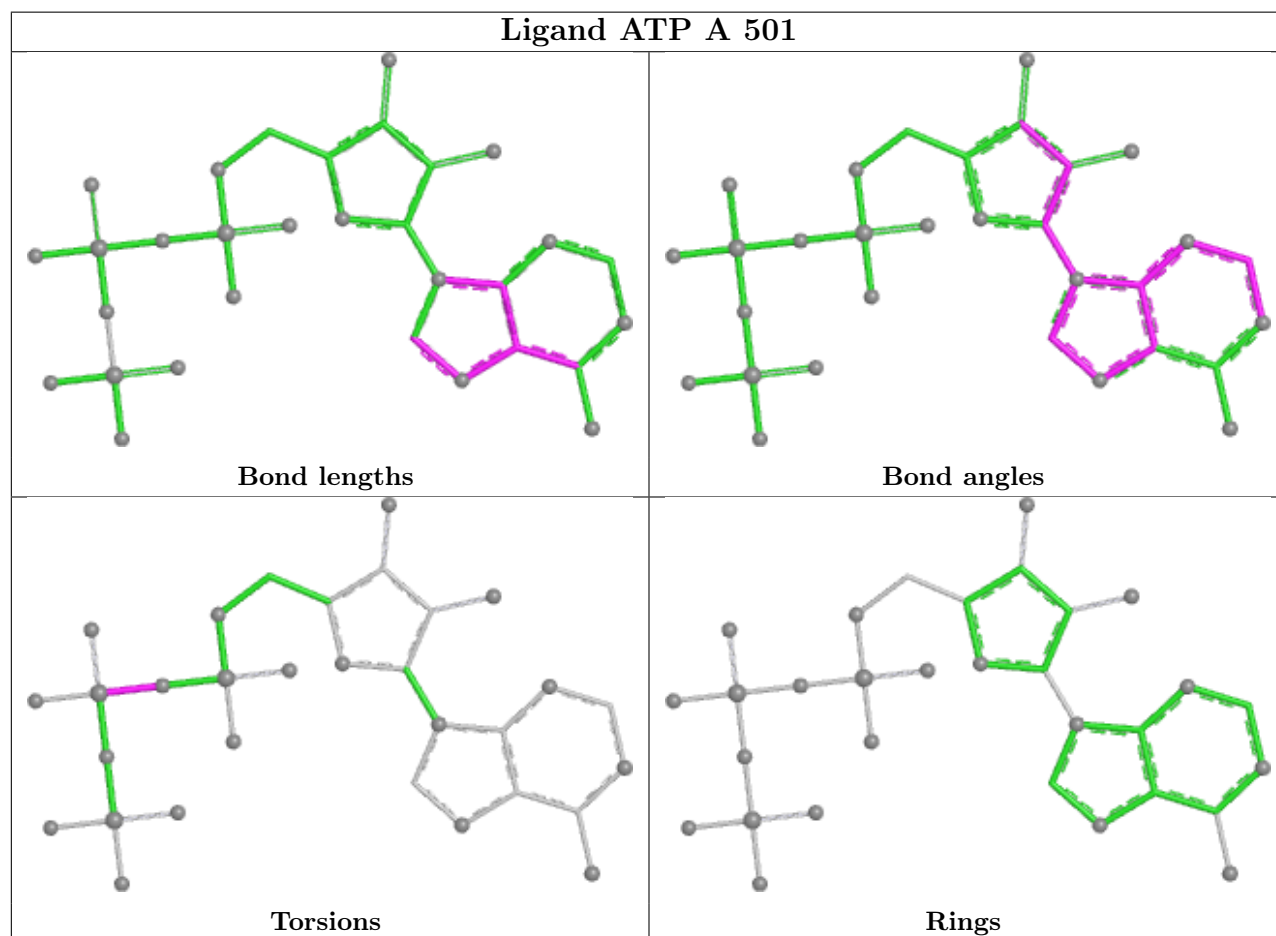
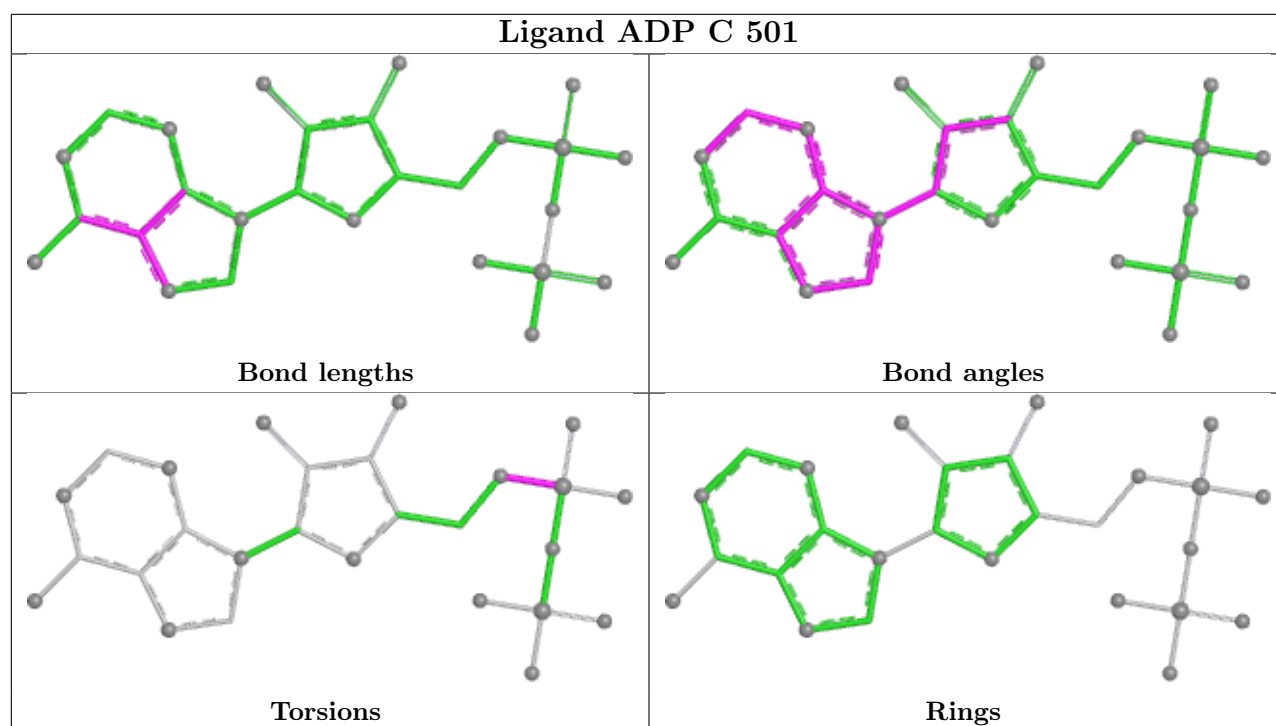
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

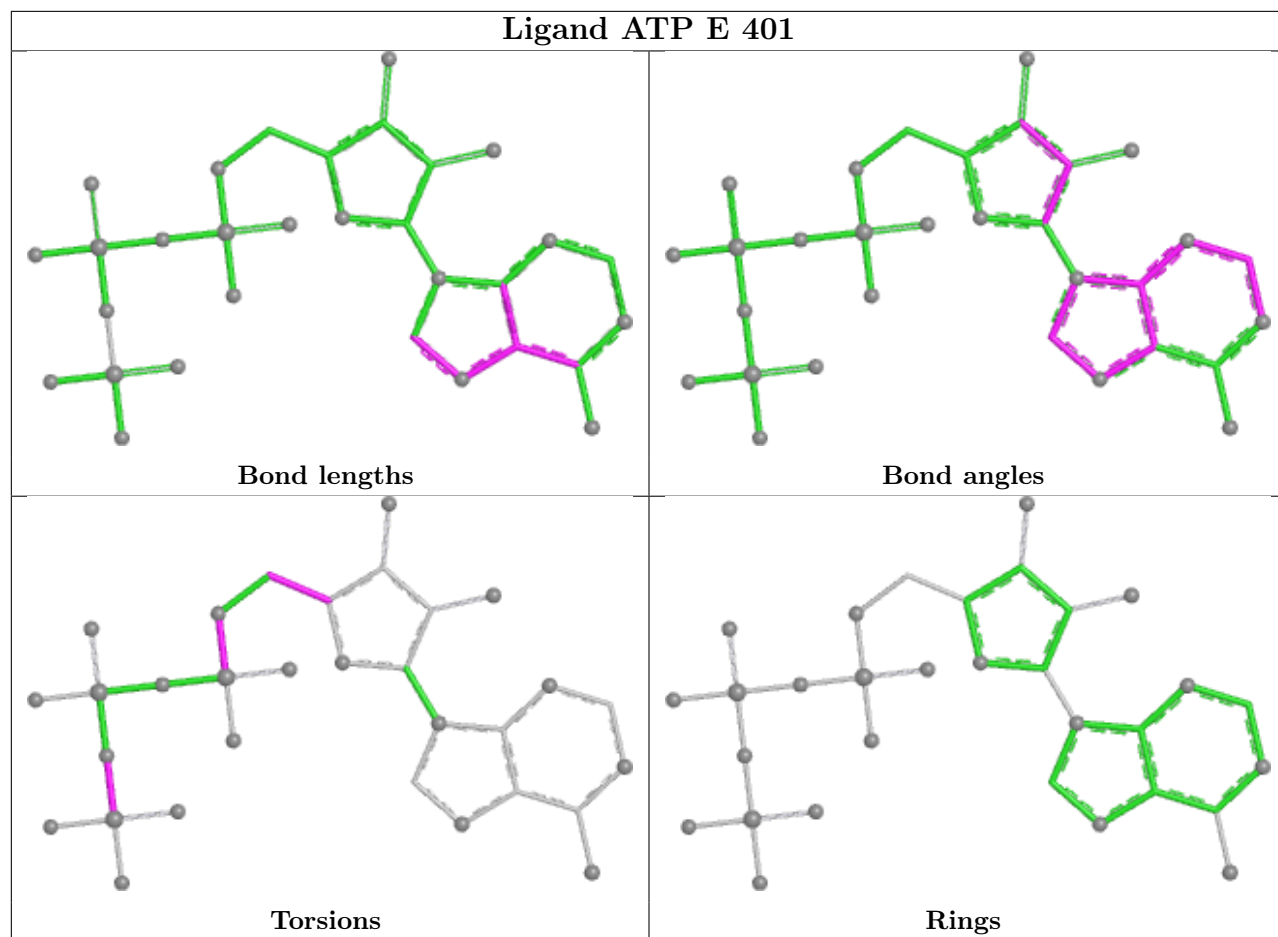
Ligand ATP B 501

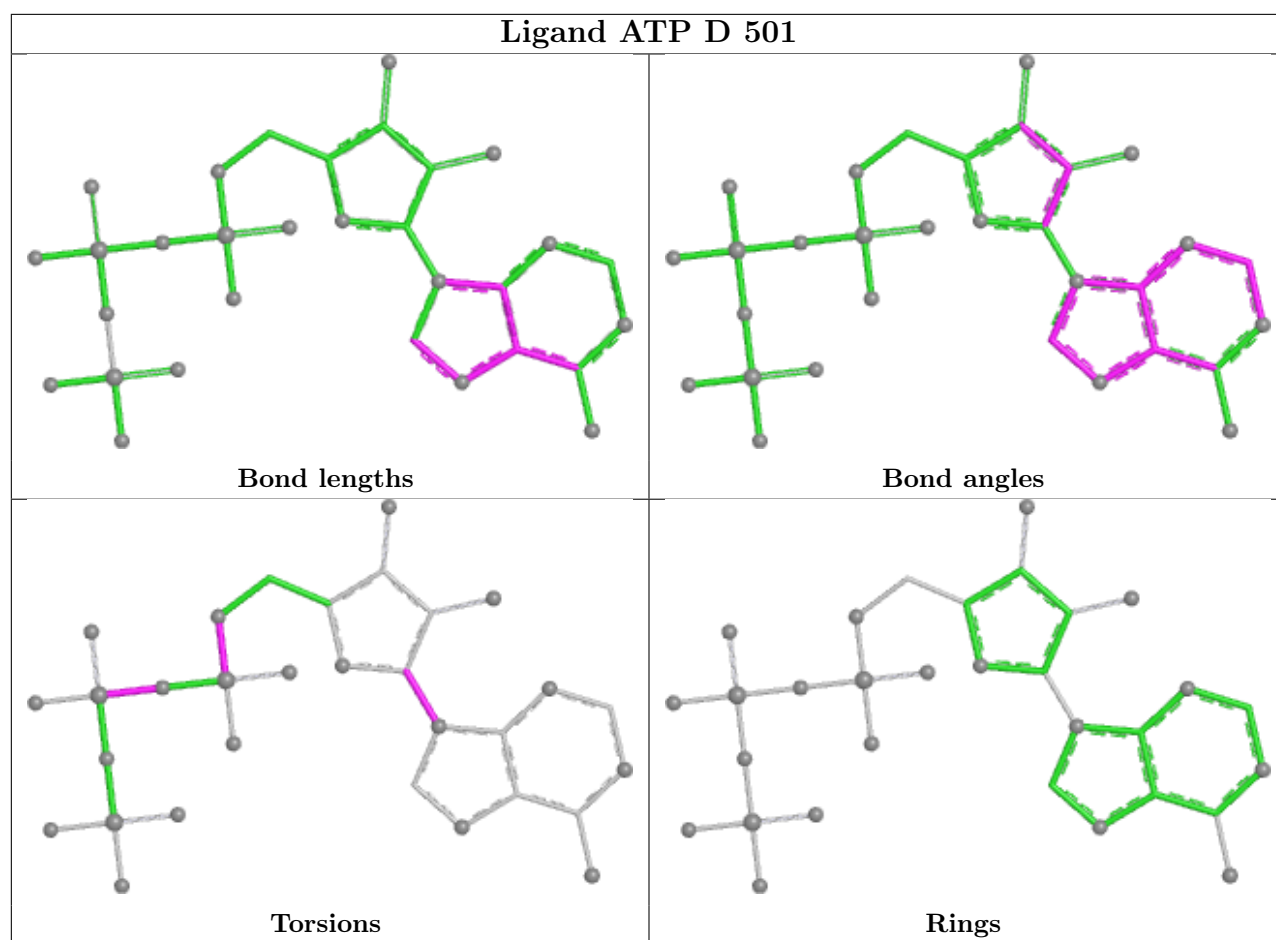


Ligand ADP F 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

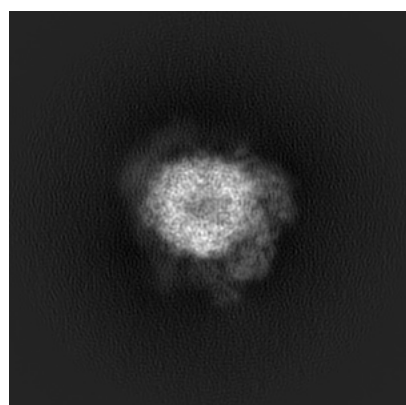
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14201. These allow visual inspection of the internal detail of the map and identification of artifacts.

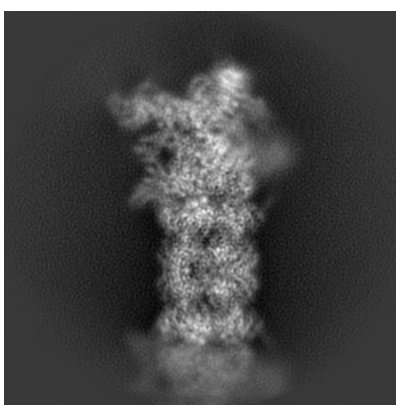
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

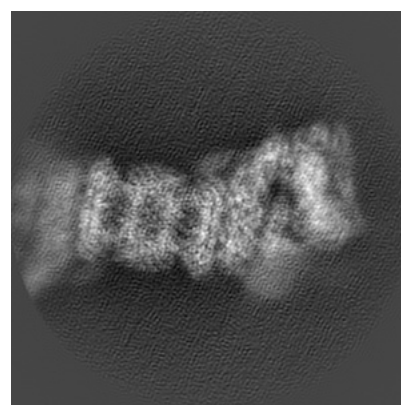
6.1.1 Primary map



X



Y

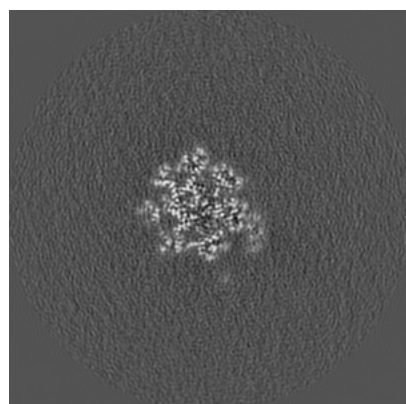


Z

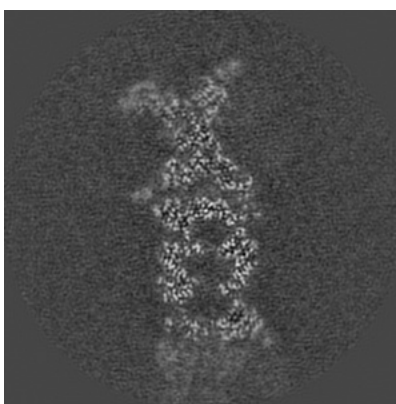
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

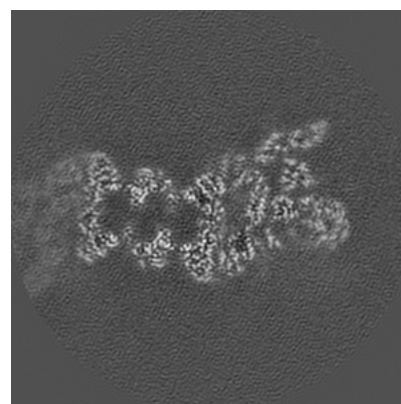
6.2.1 Primary map



X Index: 160



Y Index: 160

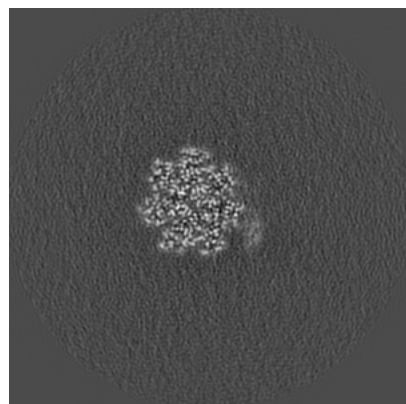


Z Index: 160

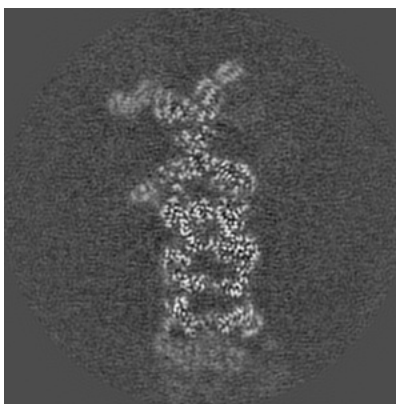
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

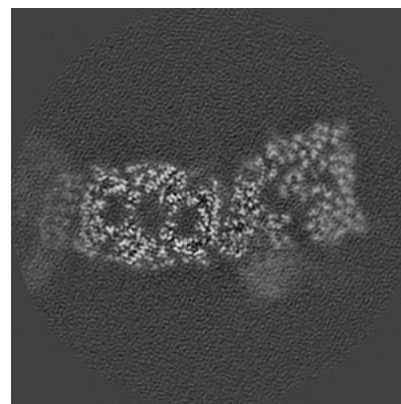
6.3.1 Primary map



X Index: 154



Y Index: 165

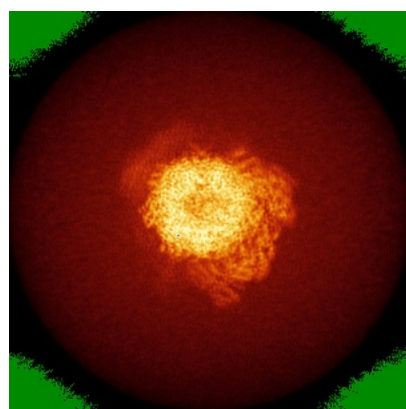


Z Index: 176

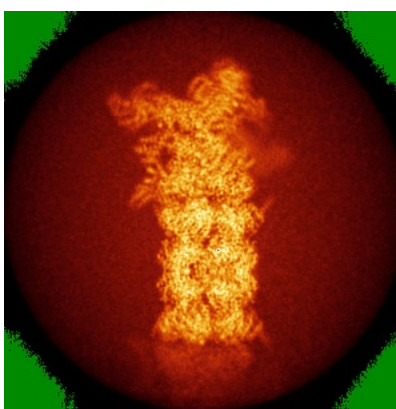
The images above show the largest variance slices of the map in three orthogonal directions.

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

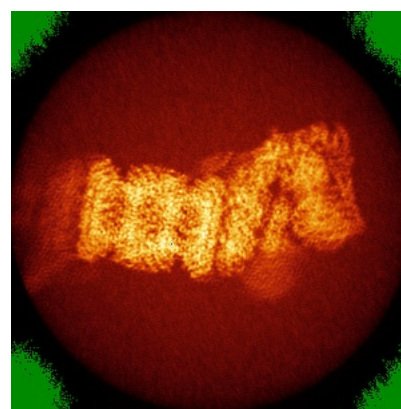
6.4.1 Primary map



X



Y

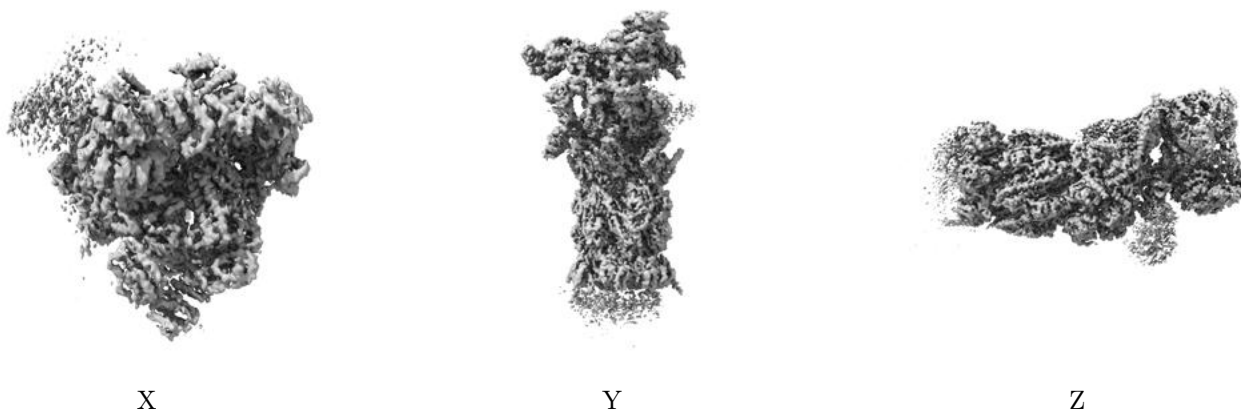


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0394. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

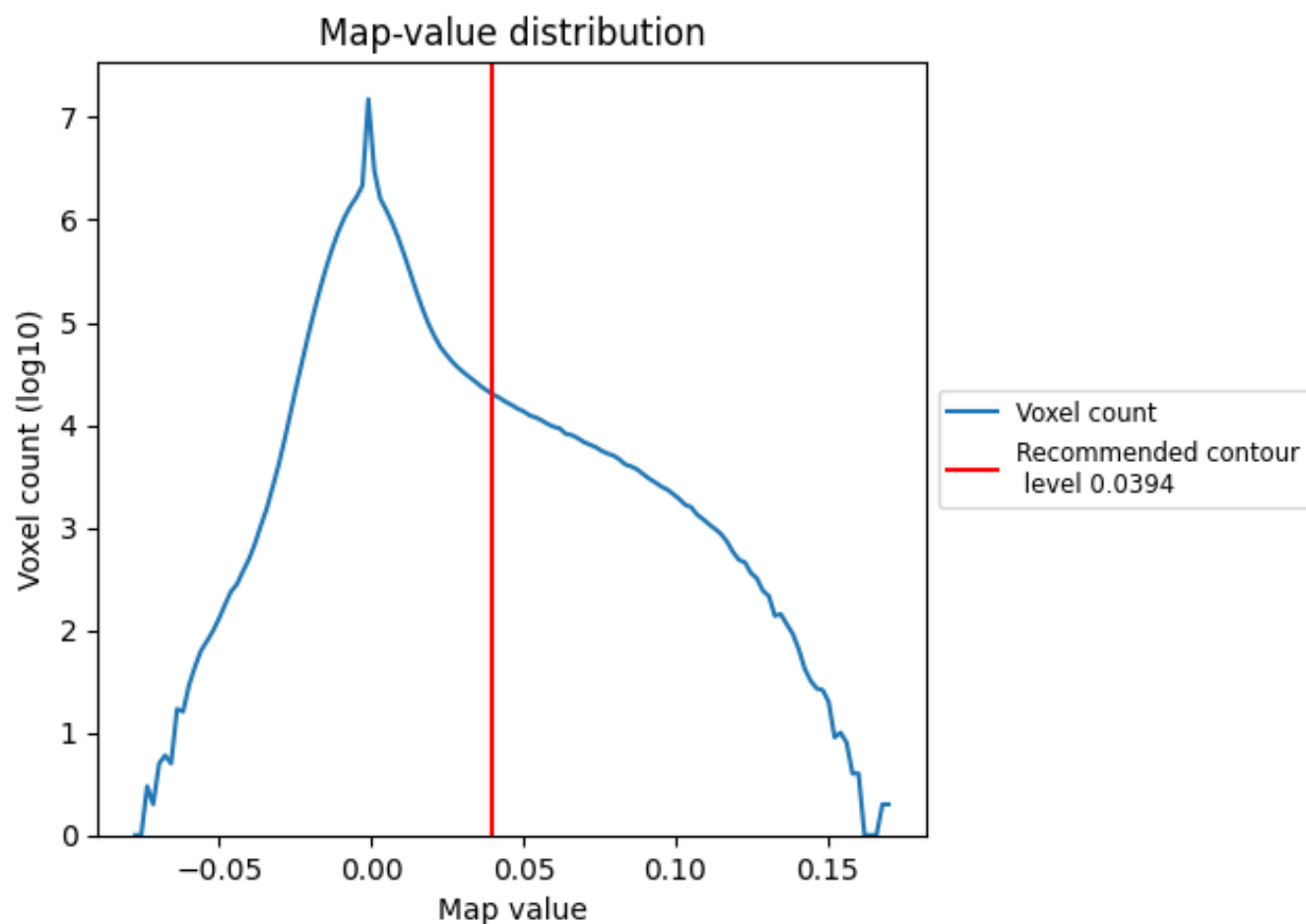
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

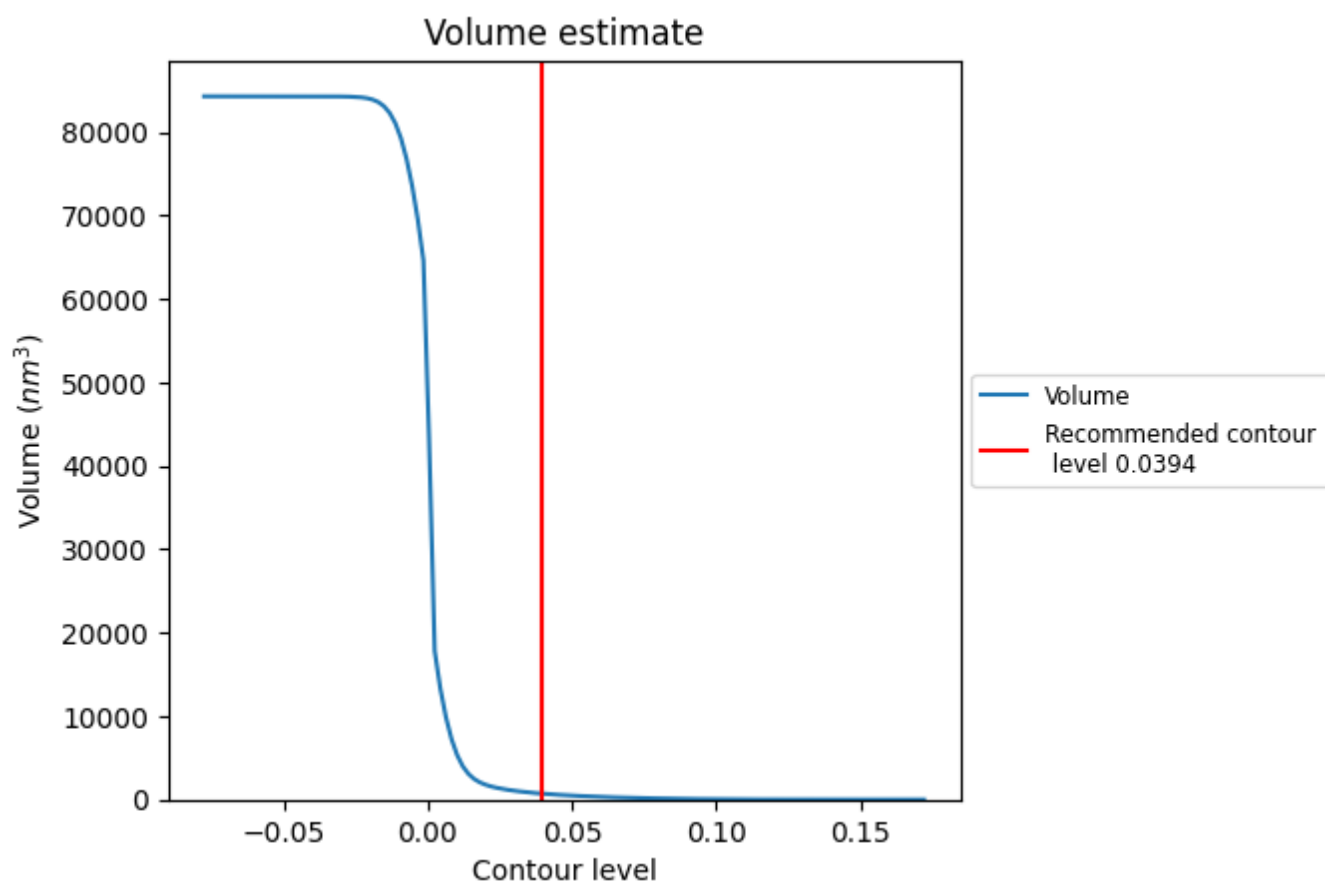
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

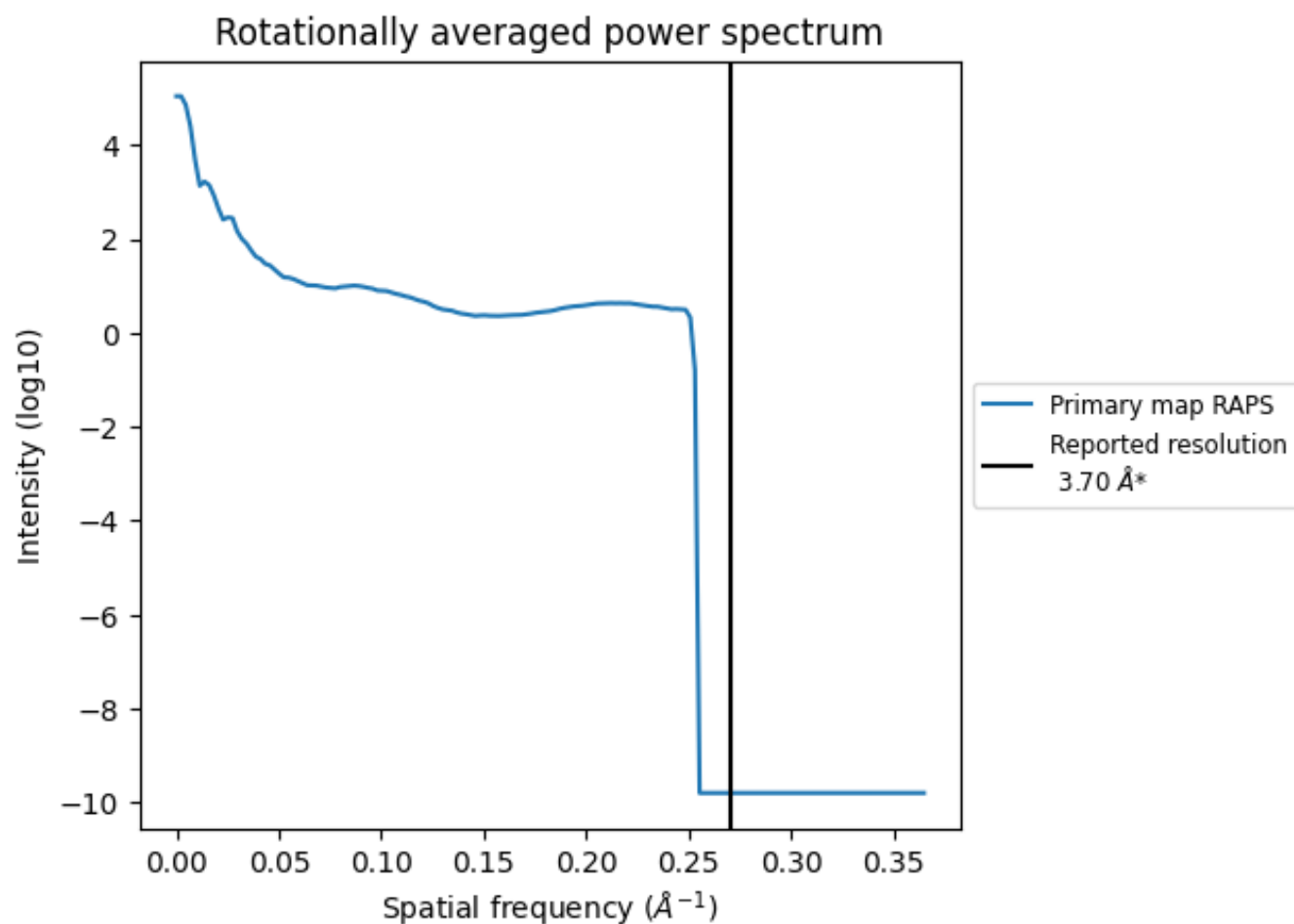
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 717 nm³; this corresponds to an approximate mass of 648 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 0.270 Å⁻¹

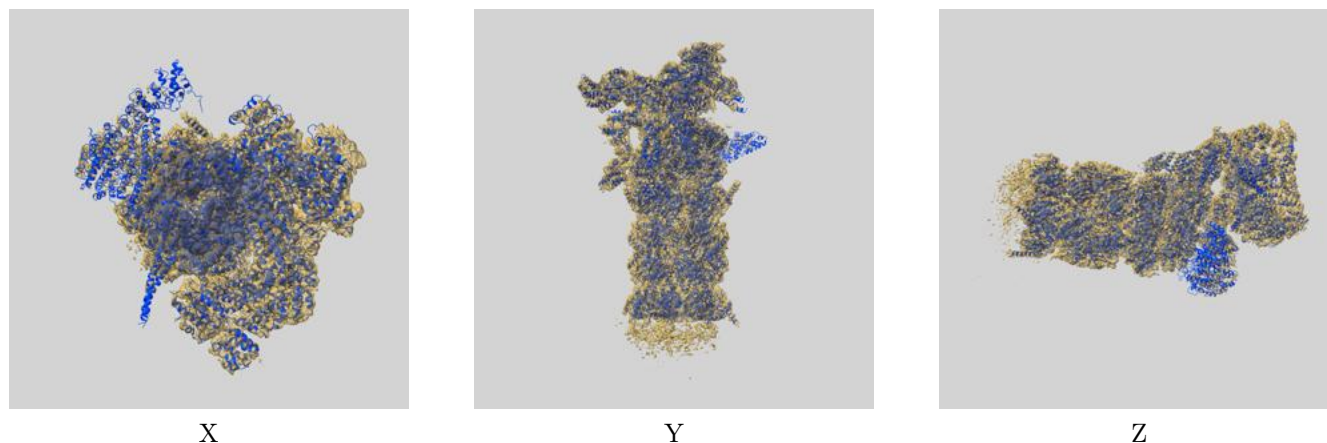
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

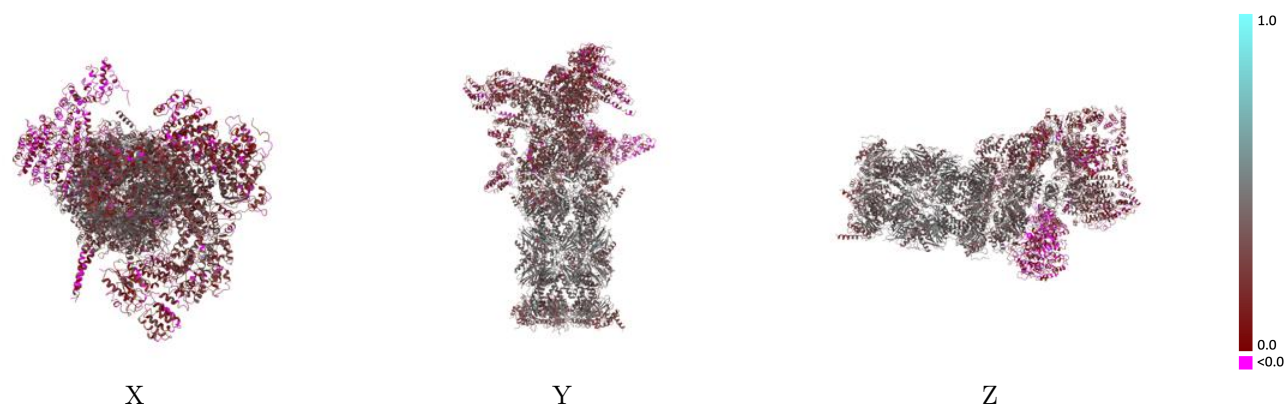
This section contains information regarding the fit between EMDB map EMD-14201 and PDB model 7QXN. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



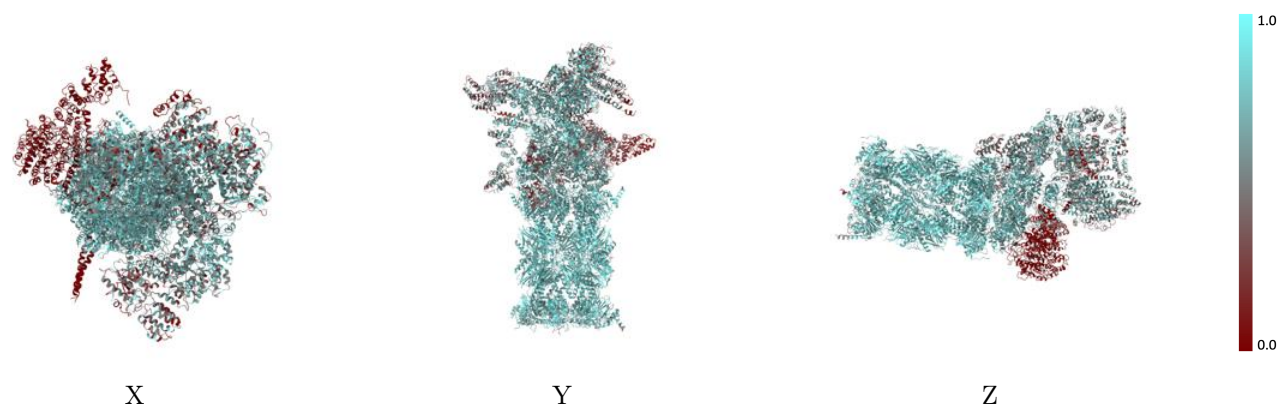
The images above show the 3D surface view of the map at the recommended contour level 0.0394 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



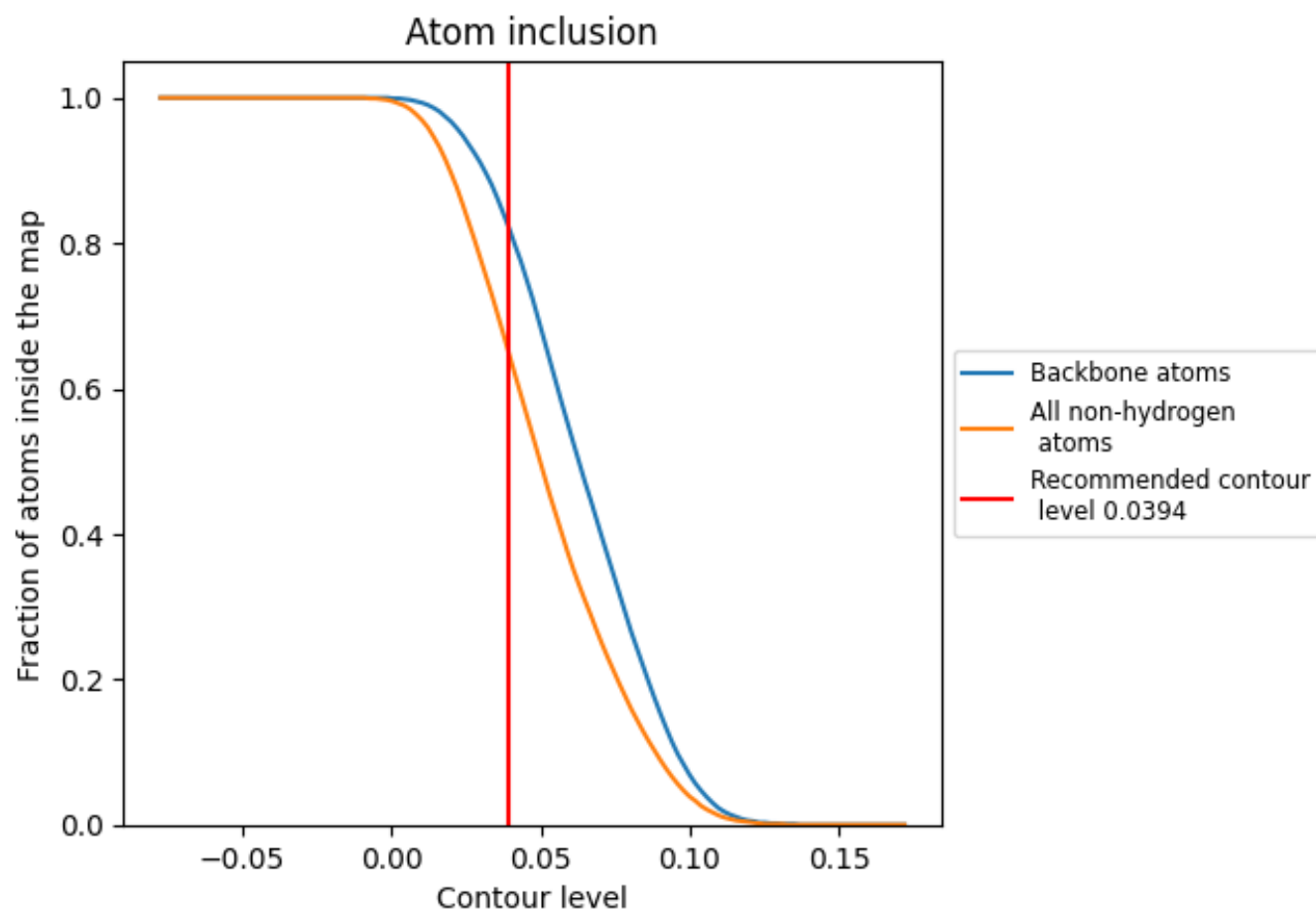
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0394).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.0394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.3190
A	 0.6810	 0.3510
B	 0.6280	 0.3260
C	 0.7050	 0.3540
D	 0.6960	 0.3530
E	 0.6960	 0.3440
F	 0.7030	 0.3630
G	 0.8000	 0.4100
H	 0.7980	 0.4130
I	 0.7730	 0.3880
J	 0.7850	 0.3870
K	 0.7830	 0.4010
L	 0.8060	 0.4150
M	 0.7880	 0.4030
N	 0.8280	 0.4300
O	 0.8250	 0.4290
P	 0.8200	 0.4350
Q	 0.8240	 0.4210
R	 0.8490	 0.4440
S	 0.8290	 0.4380
T	 0.8390	 0.4360
U	 0.5540	 0.2170
V	 0.4750	 0.1770
W	 0.5700	 0.2100
X	 0.4650	 0.2630
Y	 0.6530	 0.2480
Z	 0.6040	 0.2940
a	 0.5190	 0.2120
b	 0.3910	 0.1780
c	 0.6570	 0.3130
d	 0.4880	 0.1680
e	 0.4490	 0.1280
f	 0.0360	 0.0660
g	 0.7360	 0.3870
h	 0.7530	 0.3930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7100	 0.3650
j	 0.7280	 0.3530
k	 0.7290	 0.3820
l	 0.7540	 0.3880
m	 0.7390	 0.3780
n	 0.8190	 0.4240
o	 0.8150	 0.4260
p	 0.8160	 0.4340
q	 0.8090	 0.4180
r	 0.8250	 0.4230
s	 0.8130	 0.4180
t	 0.8370	 0.4280