



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 09:51 pm GMT

PDB ID : 8BD7
EMDB ID : EMD-15977
Title : IFTB1 subcomplex of anterograde Intraflagellar transport trains (Chlamydomonas reinhardtii)
Authors : Lacey, S.E.; Foster, H.E.; Pigino, G.
Deposited on : 2022-10-18
Resolution : 9.90 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

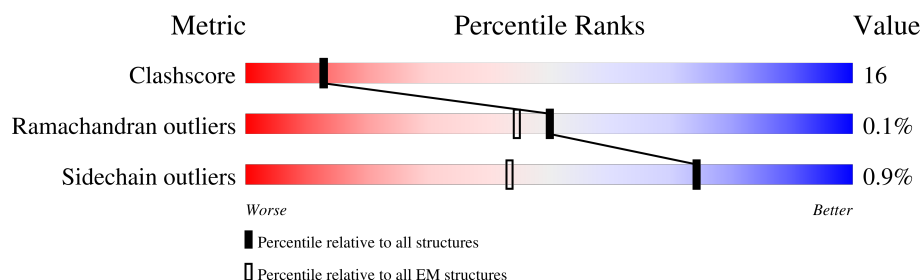
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	782	<div> <div>10%</div> <div>38%</div> <div>30%</div> <div>31%</div> </div>
1	H	782	<div> <div>10%</div> <div>37%</div> <div>31%</div> <div>31%</div> </div>
2	B	454	<div> <div>34%</div> <div>61%</div> <div>38%</div> </div>
2	J	454	<div> <div>35%</div> <div>64%</div> <div>36%</div> </div>
3	C	647	<div> <div>18%</div> <div>62%</div> <div>33%</div> </div>
3	K	647	<div> <div>21%</div> <div>62%</div> <div>34%</div> </div>
4	D	344	<div> <div>27%</div> <div>26%</div> <div>13%</div> <div>61%</div> </div>
4	N	344	<div> <div>28%</div> <div>25%</div> <div>13%</div> <div>61%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	555	
5	O	555	
6	F	683	
6	P	683	
7	G	641	
7	Q	641	
8	I	765	
8	R	765	
9	L	443	
9	T	443	
10	M	469	
10	U	469	
11	W	135	
11	Y	135	
12	X	510	
12	Z	510	
13	S	1755	
13	V	1755	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 86268 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 IFT88.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	539	Total	C	N	O	S	0	0
			4337	2747	762	795	33		
1	H	539	Total	C	N	O	S	0	0
			4337	2747	762	795	33		

- Molecule 2 is a protein called Osm-6-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	454	Total	C	N	O	S	0	0
			3553	2269	591	680	13		
2	J	454	Total	C	N	O	S	0	0
			3553	2269	591	680	13		

- Molecule 3 is a protein called IFT70.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	619	Total	C	N	O	S	0	0
			4978	3171	826	948	33		
3	K	619	Total	C	N	O	S	0	0
			4978	3171	826	948	33		

- Molecule 4 is a protein called Intraflagellar transport protein 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	133	Total	C	N	O	S	0	0
			1045	666	172	197	10		
4	N	133	Total	C	N	O	S	0	0
			1045	666	172	197	10		

- Molecule 5 is a protein called Intraflagellar transport protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	555	Total	C	N	O	S	0	0
			4465	2855	763	820	27		
5	O	555	Total	C	N	O	S	0	0
			4465	2855	763	820	27		

- Molecule 6 is a protein called Intraflagellar transport protein 81.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	335	Total	C	N	O	S	0	0
			2701	1692	476	526	7		
6	P	335	Total	C	N	O	S	0	0
			2701	1692	476	526	7		

- Molecule 7 is a protein called Intraflagellar transport protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	205	Total	C	N	O	S	0	0
			1674	1023	302	342	7		
7	Q	205	Total	C	N	O	S	0	0
			1674	1023	302	342	7		

- Molecule 8 is a protein called Intraflagellar transport protein 80.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	765	Total	C	N	O	S	0	0
			6025	3807	1053	1132	33		
8	R	765	Total	C	N	O	S	0	0
			6025	3807	1053	1132	33		

- Molecule 9 is a protein called Clusterin-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	303	Total	C	N	O	S	0	0
			2472	1547	439	476	10		
9	T	303	Total	C	N	O	S	0	0
			2472	1547	439	476	10		

- Molecule 10 is a protein called Intraflagellar transport protein 57.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	164	Total	C	N	O	S	0	0
			1328	812	247	264	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	164	Total	C	N	O	S	0	0
			1328	812	247	264	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	356	ALA	PHE	conflict	UNP Q2XQY7
U	356	ALA	PHE	conflict	UNP Q2XQY7

- Molecule 11 is a protein called Intraflagellar transport particle protein IFT20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	114	Total	C	N	O	S	0	0
			919	562	166	187	4		
11	Y	114	Total	C	N	O	S	0	0
			919	562	166	187	4		

- Molecule 12 is a protein called IFT54.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	106	Total	C	N	O	S	0	0
			849	524	155	164	6		
12	Z	106	Total	C	N	O	S	0	0
			849	524	155	164	6		

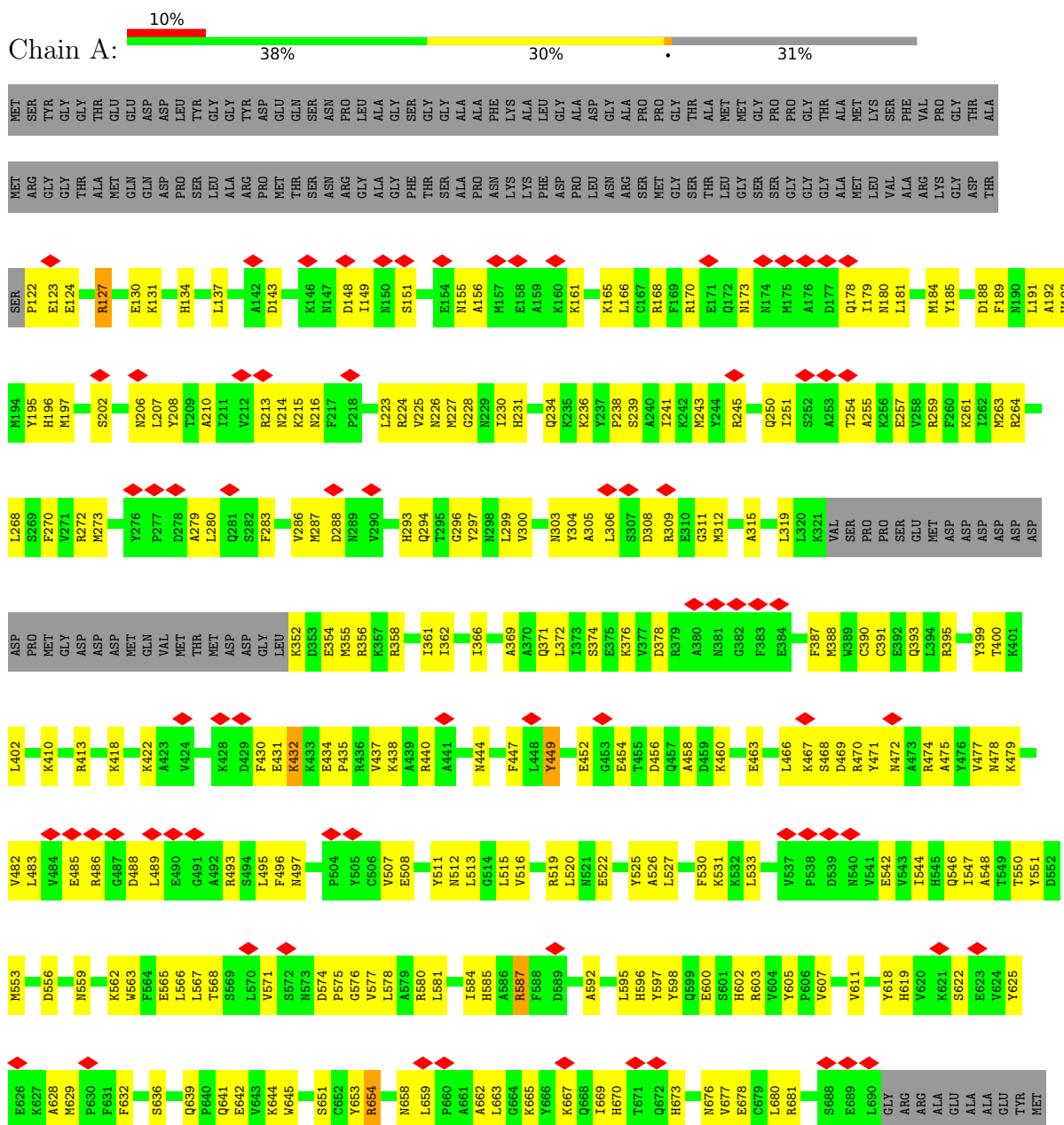
- Molecule 13 is a protein called Intraflagellar transport protein 172.

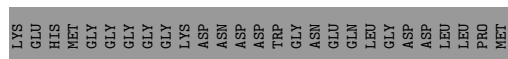
Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	1104	Total	C	N	O	S	0	0
			8788	5556	1532	1656	44		
13	V	1104	Total	C	N	O	S	0	0
			8788	5556	1532	1656	44		

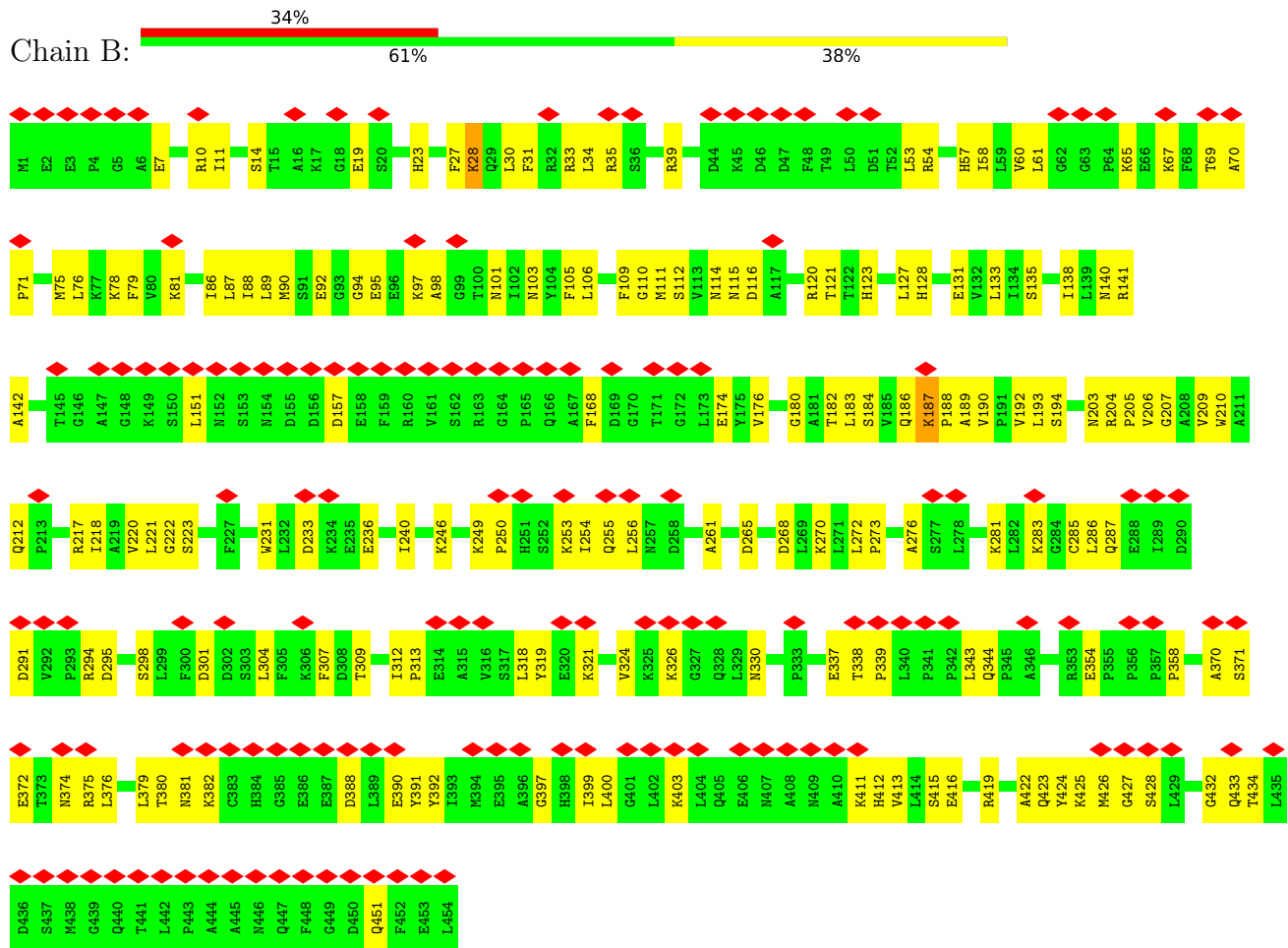
3 Residue-property plots

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.

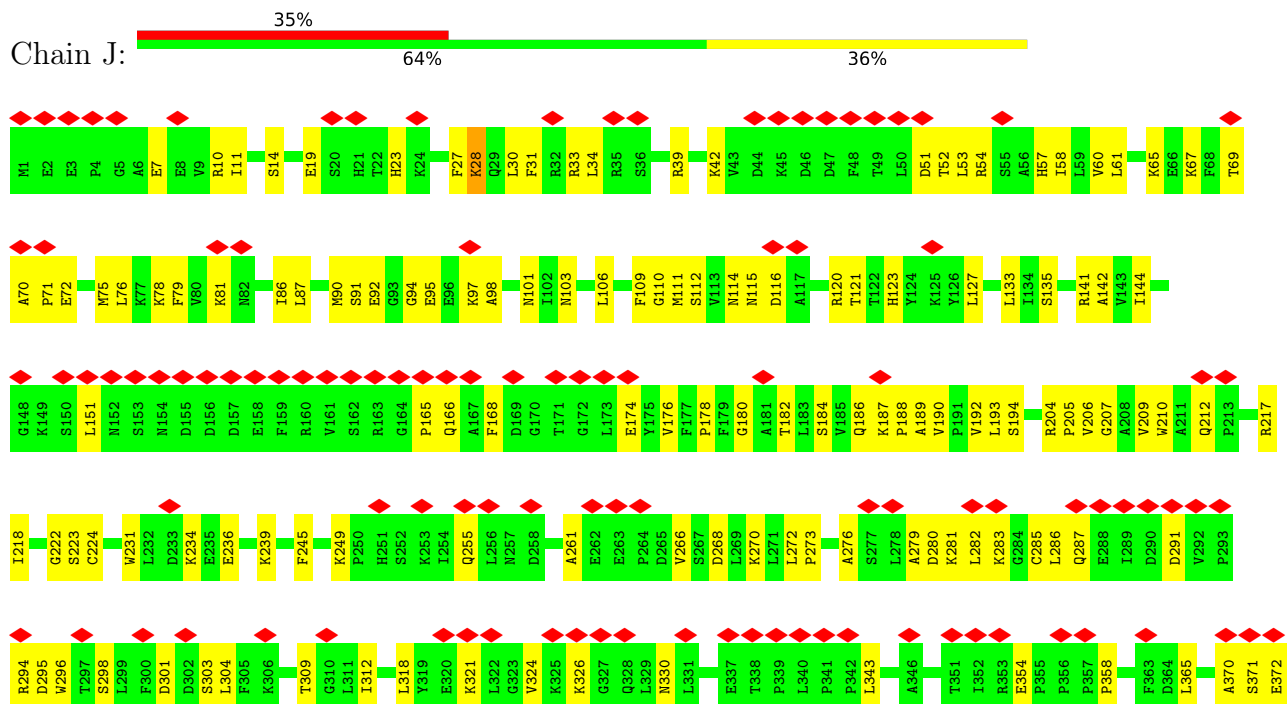
• Molecule 1: IFT88

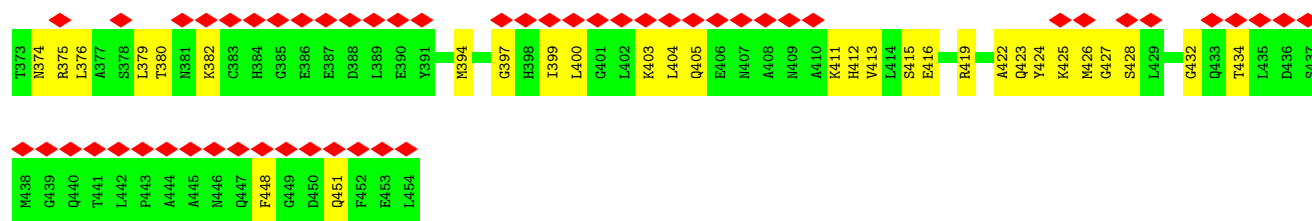




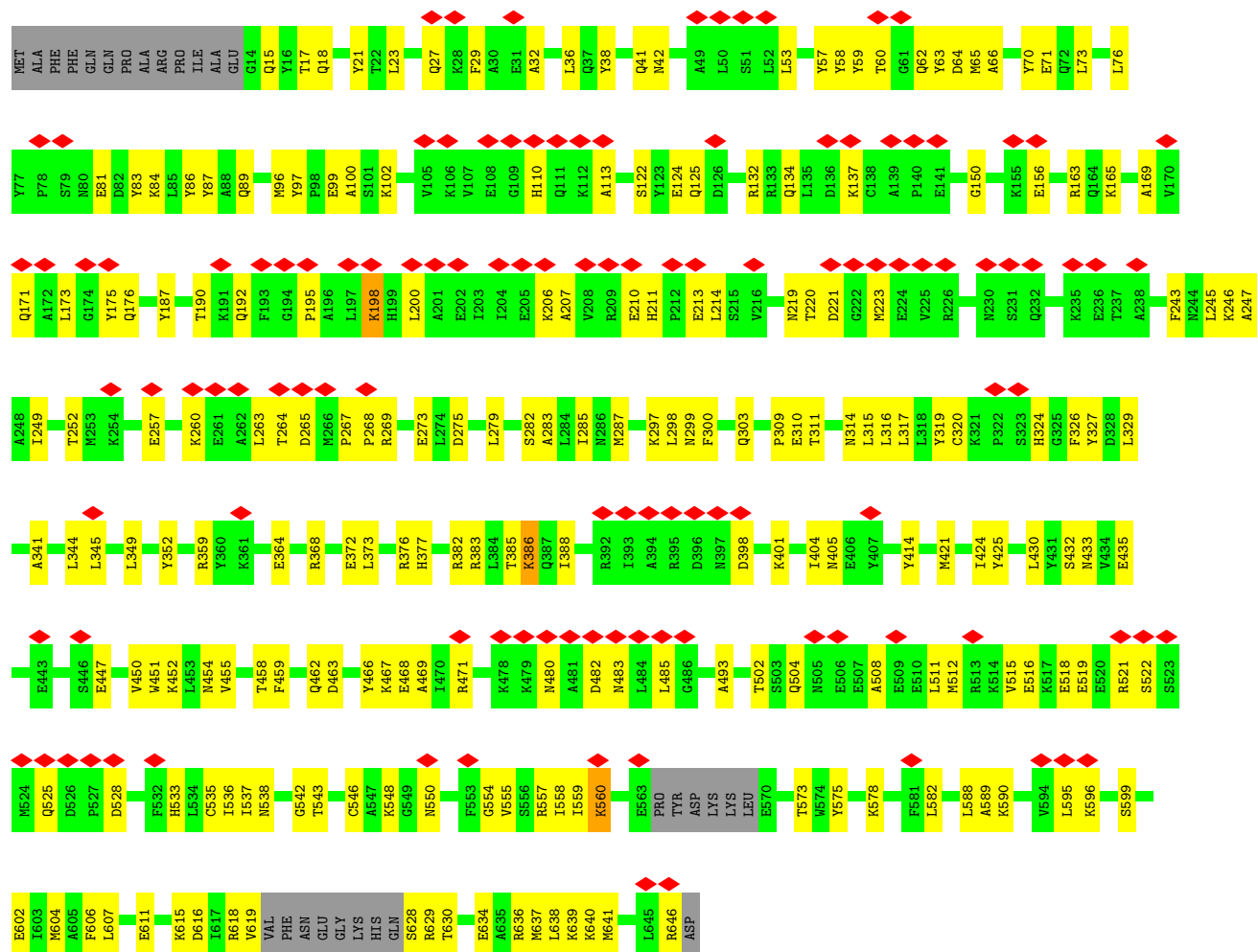


• Molecule 2: Osm-6-like protein

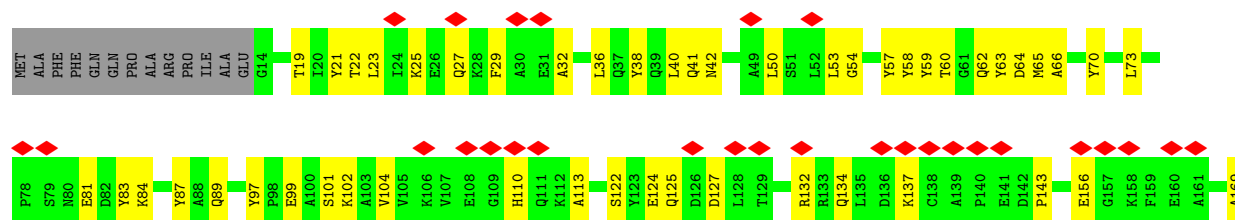


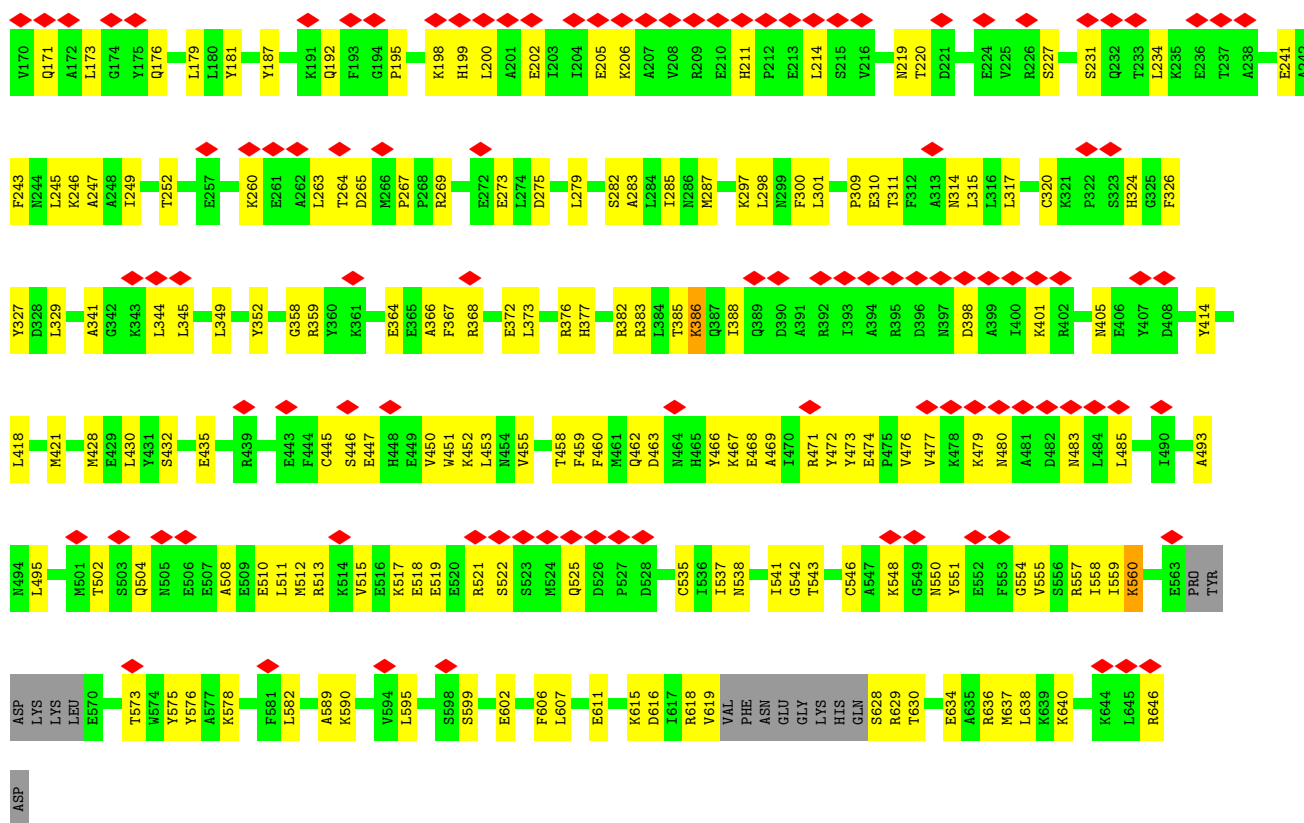


• Molecule 3: IFT70

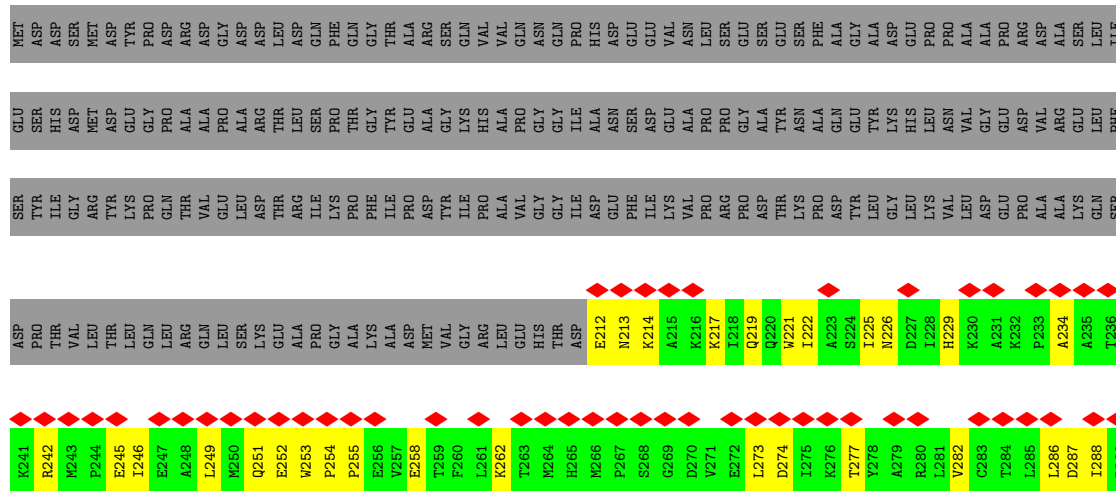


• Molecule 3: IFT70



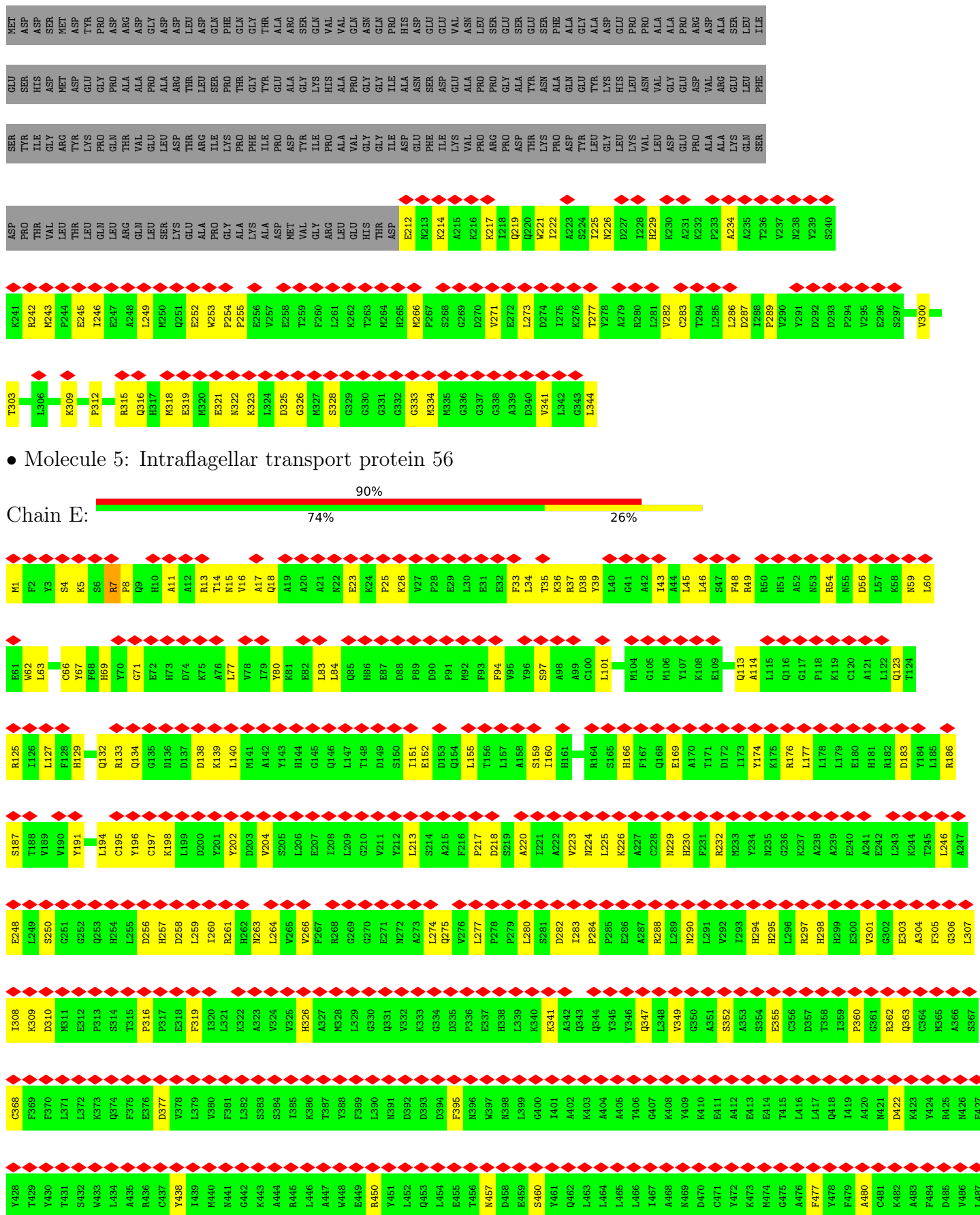


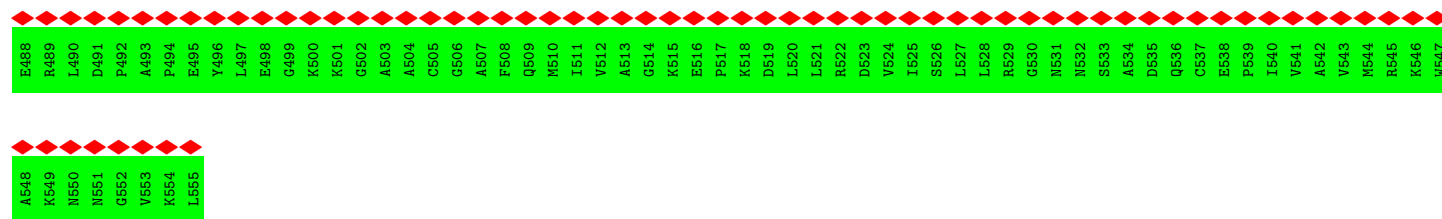
• Molecule 4: Intraflagellar transport protein 46



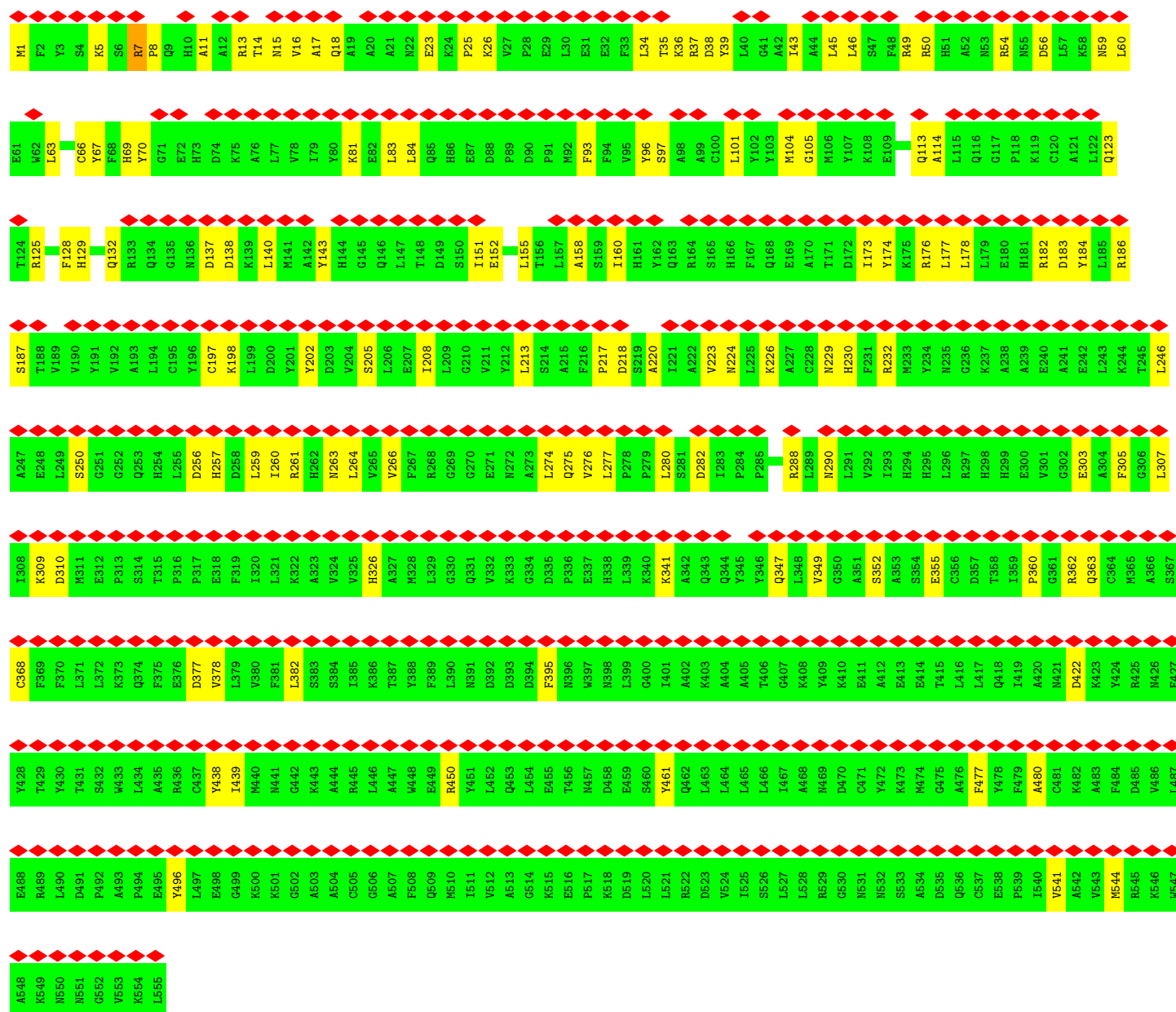
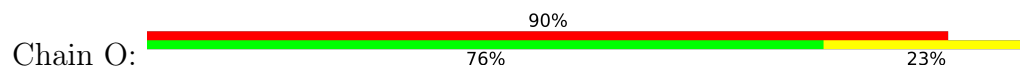
• Molecule 4: Intraflagellar transport protein 46



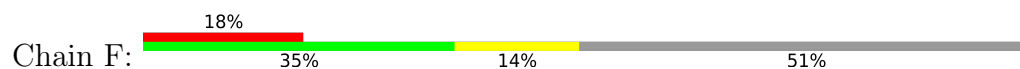


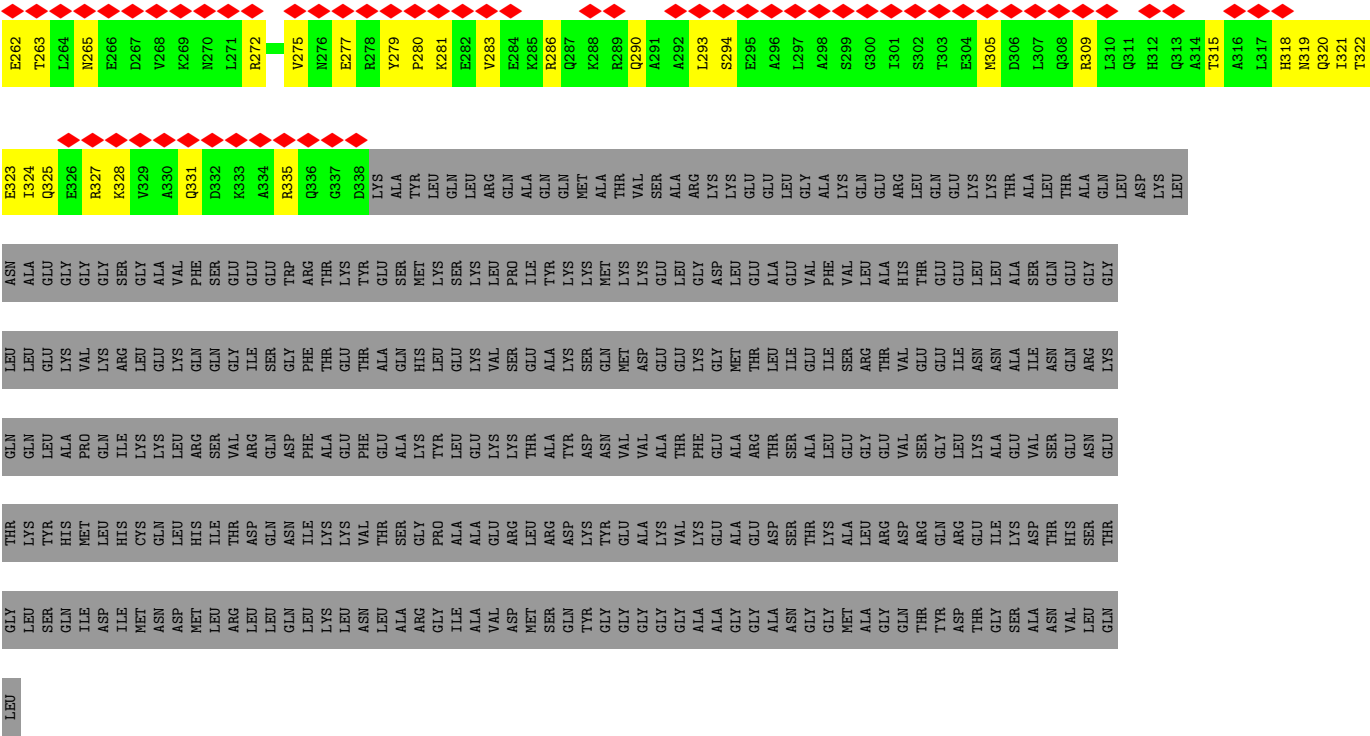


• Molecule 5: Intraflagellar transport protein 56

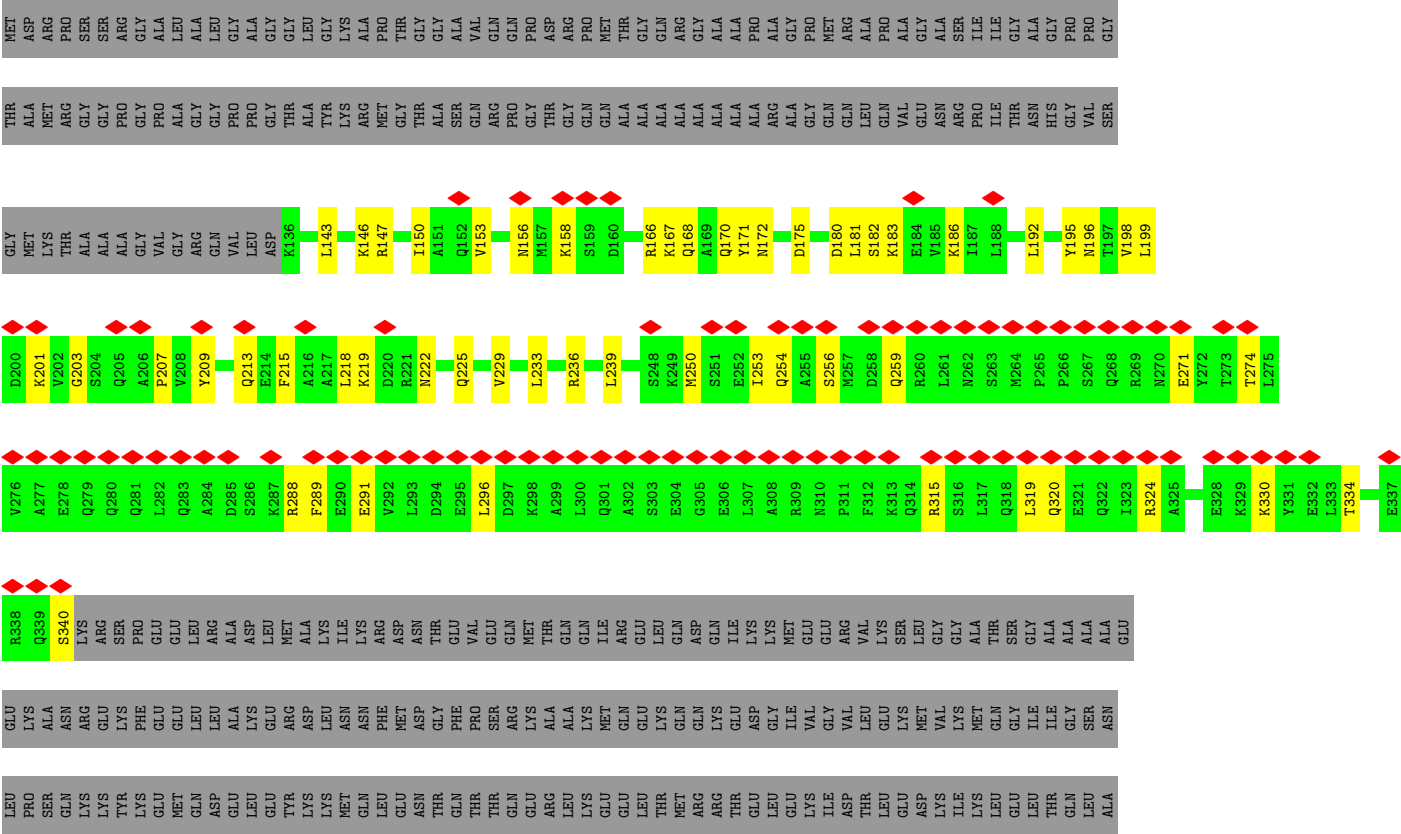


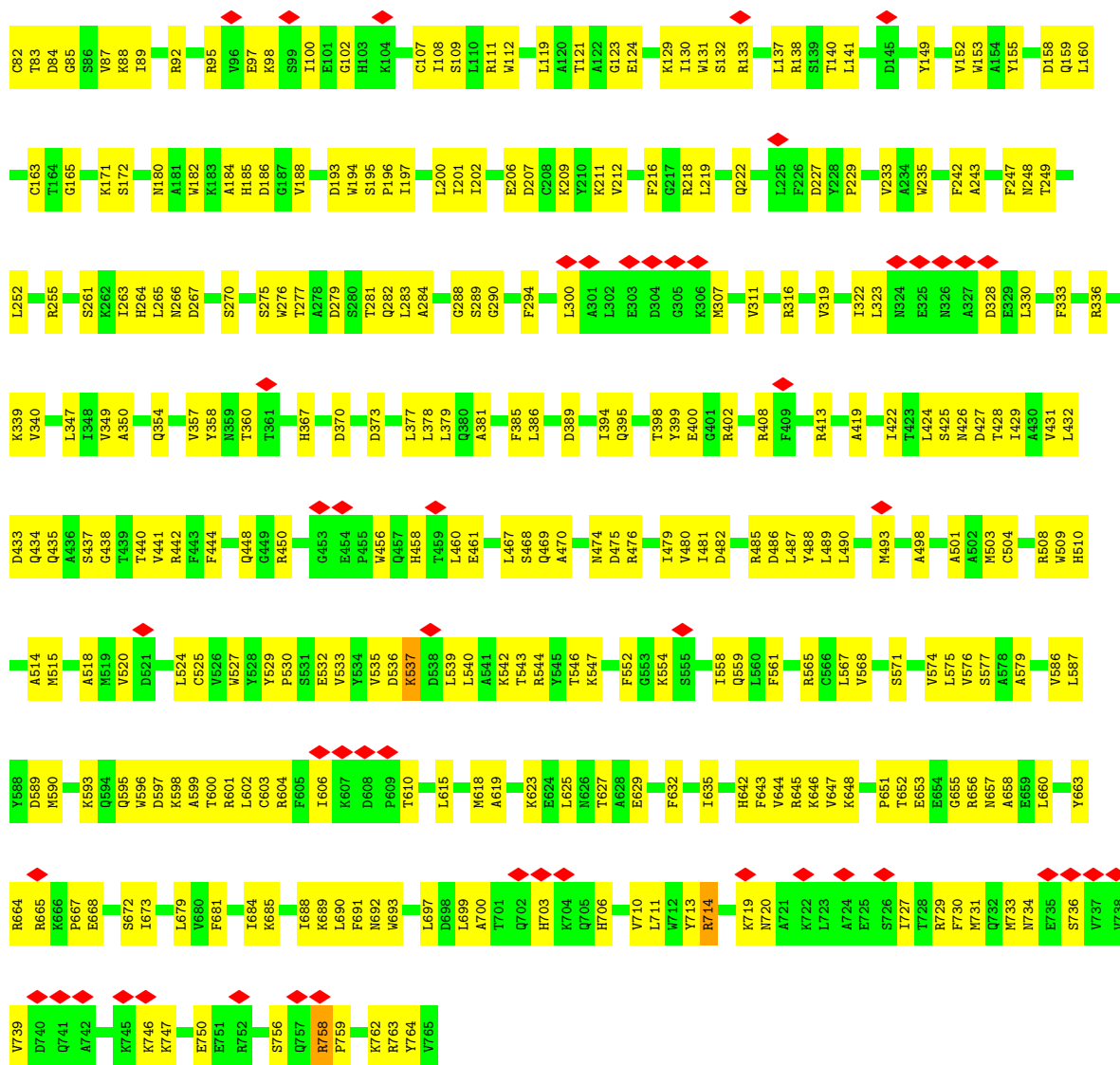
• Molecule 6: Intraflagellar transport protein 81



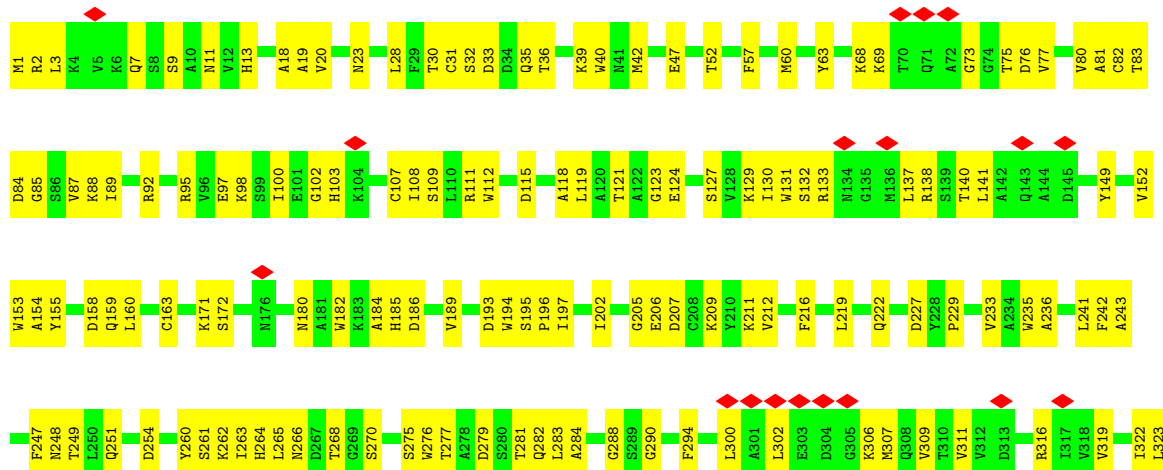


● Molecule 7: Intraflagellar transport protein 74



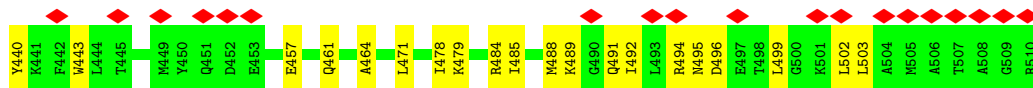
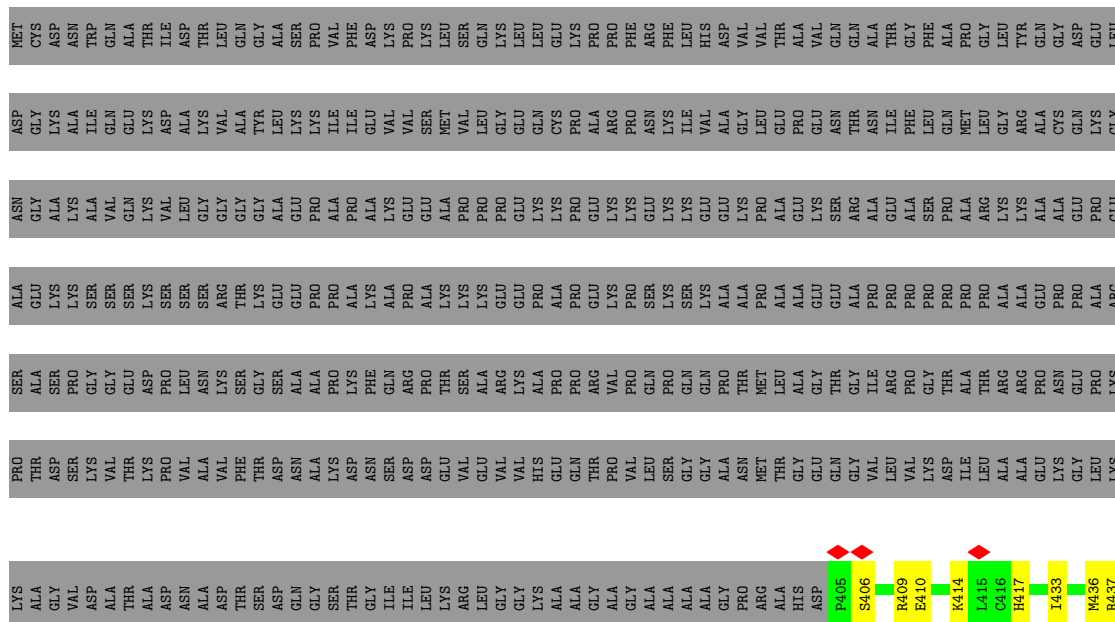


• Molecule 8: Intraflagellar transport protein 80





- Molecule 12: IFT54



- Molecule 13: Intraflagellar transport protein 172



A987	M916	R850	G780	S702	F621	L527	S445	L373	P301	N241	I181	W121
A988	F917	R851	G781	L707	L624	C530	V448	I374	M306	N242	W182	P122
B989	F918	A855	L782	A708	T625	D531	Q449	R376	T307	D243	K183	K123
K990	R920	E856	R785	Q709	P626	V536	E450	Y379	V308	E244	F184	D124
E993	R921	B857	Q788	G710	E627	P537	A451	T380	G309	R245	N185	R125
A994	R922	I858	V789	W711	D631	V541	R452	L381	S310	R246	F186	P126
E995	Q924	I860	W790	W712	W632	Q545	G453	L382	M311	E247	P187	N127
K996	R925	E861	M791	D713	L635	S546	I454	M383	T312	F248	A188	E128
E997	E926	E862	S792	I716	A636	R547	S458	D385	G313	T249	E189	V129
Y998	E927	E863	W793	L717	E637	N548	D466	L386	A314	T250	E190	V130
L999	T928	W794	H794	L718	N549	S549	L467	D387	V315	C251	G191	F131
A1000	T929	I795	W795	W719	L550	L550	Q468	T388	D316	G192	G192	G132
A1001	G930	W796	V796	Q720	A639	L550	T469	G389	M317	F253	T193	L133
G1002	G931	W797	W797	D721	T642	V654	W470	K390	Y318	N254	P194	A134
G1003	L932	T798	W798	W722	N643	S555	R471	L391	D319	P255	T195	A135
D1004	E933	T870	L801	W725	Q644	N564	L472	S392	A320	S256	S196	D136
D1005	E934	K872	D804	E726	L645	F565	Q473	P396	C321	G257	S197	G136
V1006	R937	M874	L807	A727	V646	P566	D474	W396	V322	D258	Q198	K137
D1007	Y938	D875	A801	D727	T647	I567	L475	D397	K323	T259	L199	R139
K1008	Y939	A877	L802	A728	A648	E569	D476	S398	R324	V260	V200	L140
A1011	A942	T878	D804	W731	R650	K568	A477	D399	H525	V261	H202	G141
M1012	A945	R879	L807	S734	C651	V571	P478	G400	G329	F262	V201	M142
Y1013	A946	H880	A808	T735	Y652	R576	T482	S401	E332	G263	S203	L143
K1014	R946	F881	S809	H736	L655	H577	L483	E402	F333	T264	C204	K144
N1015	D947	I882	L810	H737	L655	N578	A484	A405	T334	Y265	V205	M145
N1016	E950	S884	K812	A738	T658	H579	M487	F406	Y335	N266	P206	N146
M1018	R954	G885	A813	W739	F663	R580	H488	E407	S336	R267	Y207	K147
Y1019	A955	A886	C814	A740	L664	T581	D489	E408	V337	F268	S208	S148
D1020	T887	L815	L815	A741	V667	E582	T490	E409	R410	Y269	L209	Y149
D1021	K888	W816	E817	A742	D586	D586	D493	C412	K338	M270	G210	T150
Q1021	K889	E817	E817	L743	E587	E588	W494	M413	A340	Y271	W211	C151
M1022	K892	Y823	Y823	R744	Q673	G588	L495	M413	V341	T272	G212	Y152
Y1023	I895	M826	M826	Y747	Q676	E589	D498	H415	I342	F273	C214	A153
R1024	D896	S827	S827	W750	E577	N590	Q499	Y416	K344	N274	I215	H154
L1025	C897	R828	R828	E758	F678	T591	R500	L420	K347	I275	I216	P155
V1026	R898	R829	R829	A762	Q679	L596	G501	H421	T277	Q276	A217	E156
T1027	A965	S830	S830	Y766	D681	E598	H503	I422	A218	R277	A217	M157
Q1028	F900	F900	F900	E766	D682	E599	D508	V423	G219	N278	A218	S158
K1031	R966	A901	Q834	R767	Q683	L601	R507	G426	M350	D279	W280	Y159
E1032	G967	K902	S835	E767	T683	L601	D508	R427	R351	E281	D221	V160
K1033	Y968	A903	Y836	E768	D684	Q610	R511	N428	I352	E282	N222	V161
V1034	L969	G905	R838	D769	A685	D611	H512	L431	V353	A283	R223	L163
P1035	T970	I906	R838	W770	L691	Y612	L513	L435	L354	G284	V224	A164
E1036	E971	F907	H840	L771	N692	E613	L515	R435	K355	H285	V225	S165
E1037	E972	E908	A841	A772	A693	L616	S519	N440	S356	K286	F226	S166
H1038	M974	L910	R843	L773	Q694	Q617	G520	P441	V357	Q287	Y227	L167
T1041	K981	P912	K844	L774	K697	T618	R523	Y442	Y358	I288	D228	N168
A1042	A982	Y912	A845	G775	L619	L619	R523	L443	G359	D289	L229	G169
Q1043	A983	D847	T846	L776	L619	L619	R523	L443	Y360	N290	N230	Q170
Q1044	E984	L848	D847	Y777	W699	W699	R523	L443	E361	F291	G231	N171
E1046	F985	L848	D847	Y777	W699	W699	R523	L443	I362	Y292	R232	V172
V1047	E1048	L848	D847	Y777	W699	W699	R523	L443	E364	A293	E233	I173
L1051				K779	W699	W699	R523	L443	Y371	V294	I234	S174
									R372	S295	R235	G175
										A296	S236	H176
										A297	F237	M177
										S298	D238	D178
										W299	Y239	G179
										K300	S240	A180

TYR	K1094	Y1029	A960	I896	Y823	T754	T683	E608	R523	L443	R371	N241
ALA	Q1095	R1030	A961	D896	E824	G755	D684	E609	L527	I444	T372	N242
MET	V1096	K1031	R962	C897	H825	Q756	A685	D699	A446	A446	L373	D243
PHE	A1097	E1032	R963	R898	R828	E757	V688	Y612	V447	V447	A375	E244
LEU	Y1098	K1033	V964	Q899	S829	E758	R689	E613	Q449	Q449	R376	V245
ASP	A1099	V1034	A901	F900	Q834	V763	R689	E614	E450	E450	G309	R246
GLY	W1100	P1035	K902	A901	Q835	A615	A690	A615	A451	A451	S310	E247
ARG	A1101	P1035	Y963	K903	Y836	V616	M691	V616	A451	A451	M311	F248
PHE	L1102	H1038	R969	A904	R837	Q617	A693	Q617	D540	D540	T312	T249
ALA	T1103	I1041	T970	G905	R838	Q618	A694	T618	G453	G453	G313	T250
ALA	L1104	A1042	S972	I906	R839	E620	M696	E620	I454	I454	A314	C251
GLY	GLY	A1042	S972	Y907	H840	P621	K697	P621	A455	A455	D385	A252
ALA	GLY	Q1043	Y978	E908	A841	L624	Q698	L624	S456	S456	D387	F253
ASP	ASP	Q1044	R979	V909	R842	E627	R547	E627	E457	E457	M317	F254
PHE	ASP	L1045	A980	L910	R843	Q631	N648	Q631	S458	S458	Y318	N254
ILE	GLY	E1046	K981	P912	K844	Q632	L550	Q632	C389	C389	D319	P255
SER	ALA	V1047	A982	A915	A845	L635	C551	L635	K390	K390	A320	S256
GLY	LEU	E1048	A983	P916	L846	Q638	V552	Q638	L467	L467	K323	C257
LYS	LEU	E1053	A984	P917	L847	A639	Q553	A639	R471	R471	H325	D258
LYS	LEU	A1054	F985	Y918	L848	L640	V554	L640	D397	D397	V260	T259
MET	GLY	E1055	E986	F919	L849	A641	Y555	A641	Q395	Q395	R324	V261
ALA	GLY	K1056	A987	R920	L850	T642	S555	T642	D397	D397	H325	F262
CYS	LEU	H1057	A988	R921	R851	Q643	M564	Q643	L475	L475	K328	G263
ASP	LEU	K1058	H989	A923	R852	E649	F565	E649	A477	A477	G329	G264
MET	ASP	F1058	K990	Q924	E852	Y652	P566	Y652	P478	P478	K330	Y265
TYR	HIS	V1059	E993	Y925	F853	Y653	M566	Y653	Y479	Y479	F331	N266
MET	ALA	E1060	A994	Y926	R854	A653	V571	A653	T482	T482	T334	R267
ASN	GLY	A1061	E995	E927	V857	A653	K563	K563	L483	L483	Y335	F268
GLN	TYR	E1062	A996	T928	H857	T647	V572	T647	E409	E409	V336	Y269
ASP	ALA	K1062	K996	T929	L858	A643	V572	A643	R410	R410	S337	M270
ASP	GLY	D1063	E997	G930	E861	E649	H579	E649	V411	V411	K338	Y271
ALA	SER	W1064	Y998	A931	R864	Y652	R580	Y652	M412	M412	S339	T272
ALA	GLY	K1065	L999	A932	V867	A653	T581	A653	V414	V414	V341	T273
MET	ALA	S1066	E933	E934	L968	Y653	E582	Y653	L420	L420	V342	N274
ARG	PHE	A1067	E934	E934	T870	T658	E586	T658	L421	L421	K344	L275
ALA	GLN	V1068	R937	R937	R871	R662	D586	R662	Q499	Q499	T345	Q276
ARG	ALA	Q1069	Y938	Y939	K872	F663	I589	F663	R500	R500	L346	R277
TYR	GLY	M1070	Y939	Y939	M874	L664	N590	L664	G501	G501	K347	N278
ASP	MET	Y1071	A942	A942	D875	R666	T591	R666	H503	H503	T348	D279
THR	THR	R1072	D943	D943	A876	V667	V592	V667	G426	G426	M350	E281
ARG	ALA	Q1073	M944	M944	A877	Q673	T592	Q673	R427	R427	R351	E282
VAL	GLY	V1074	A945	A945	L878	A674	S593	A674	M428	M428	I352	A283
SER	ALA	Q1075	R946	R946	R879	R676	Y594	R676	L431	L431	V353	G284
ILE	HIS	W1077	D947	D947	H880	E677	A595	E677	R435	R435	L354	H285
LYS	LYS	E1078	E950	E950	F881	F678	L596	F678	M439	M439	K355	K286
LEU	LEU	D1079	S953	S953	E883	G679	L515	G679	N440	N440	V357	I288
PRO	PRO	A1080	R954	R954	E883	G680	L515	G680	P441	P441	G359	D289
SER	GLN	L1081	R955	R955	K889	D682	L515	D682	Y360	Y360	Y360	N290
VAL	VAL	R1082	A955	A955	K892	E763	L515	E763	I367	I367	I367	F291
GLU	GLU	V1083	K957	K957	K892	E763	L515	E763	Y368	Y368	Y368	Y292
HIS	HIS	A1084	W958	W958	K892	E763	L515	E763	H369	H369	H369	A293
VAL	VAL	K1085	E959	E959	K892	E763	L515	E763	V294	V294	V294	V294
GLU	GLU	V1086	E959	E959	K892	E763	L515	E763	S295	S295	S295	S295
SER	SER	G1088	E959	E959	K892	E763	L515	E763	A296	A296	A296	A296
GLN	GLN	G1089	E959	E959	K892	E763	L515	E763	A297	A297	A297	A297
ALA	ALA	V1090	E959	E959	K892	E763	L515	E763	S298	S298	S298	S298
ALA	ALA	A1092	E959	E959	K892	E763	L515	E763	P301	P301	P301	P301
ALA	ALA	S1093	E959	E959	K892	E763	L515	E763	P301	P301	P301	P301

Met	Tyr	Thr	Phe	Ser	Lys	Ala	Asn	Ile	Gln	Arg
		Cys	Ser	Val	Lys	Ala	Asn	Asn	Gln	Val
		His	Asp	Leu	Leu	Asn	Thr	Tyr	Ala	Ala
		Phe	Thr	Arg	Arg	Tyr	Phe	Gln	Gly	Glu
		Cys	Asp	Tyr	Asp	Ala	Ser	Arg	Gly	Arg
		Lys	Ile	Val	Met	Leu	Arg	His	Gly	Arg
		Lys	Pro	Gly	Met	Lys	Lys	Arg	Ser	Lys
		Lys	Tyr	Pro	Arg	His	Ile	Met	Gly	Gln
		Tyr	Asp	Thr	Arg	Ala	Glu	Gly	Gly	Trp
		Asp	Phe	Ile	Leu	Glu	Asp	Asp	Ala	Leu
		Thr	Thr	Pro	Val	Arg	Gln	Val	Ser	Pro
		Cys	Ile	Ala	Asn	Arg	Tyr	Val	Ala	Ala
		Val	Pro	Asp	Val	Phe	Asn	Val	Asp	Glu
		Val	Glu	Arg	Leu	Lys	Asn	Thr	Ala	Gly
		Thr	Arg	Ala	Arg	Gln	Tyr	Val	Val	Leu
		Gly	Ala	Phe	Ser	Gly	Leu	Ser	Ile	Phe
		Tyr	Tyr	Tyr	Gly	Asp	Gln	Glu	Asn	Ile
		Pro	Cys	Glu	Gly	Tyr	Gln	Arg	Lys	Lys
		Ile	Thr	Ala	Gly	Ala	Asn	Arg	Ala	Arg
		Gln	Glu	Gly	Ala	Gln	Gln	Gln	Ala	Lys
		Ser	Ser	Leu	Gly	Ala	Gln	Ile	Gly	Arg
		Tyr	Gln	Ala	Lys	Ala	Ala	Ile	Phe	Pro
		Asp	Arg	Trp	Tyr	Gln	Asp	Gly	Glu	Glu
		Arg	Glu	Tyr	Lys	Val	Glu	Arg	Arg	Ala
		Val	Asp	Glu	Val	Phe	Leu	His	Asn	Ala
		Phe	Val	Ala	Asp	Ala	Ser	Ala	Asn	Leu
		Lys	Asn	Arg	Lys	His	Arg	Ala	Tyr	Met
		Asn	Leu	Lys	Ala	Gly	Gly	Gly	Ala	Tyr
		Asn	Val	Asn	Phe	Ile	Gly	Glu	Arg	Arg
		Gly	Leu	Met	Gln	Thr	Gln	Leu	Ala	Asp
		Pro	Glu	Ala	Asn	Ala	His	His	Ile	Ala
		Glu	Ile	Phe	Tyr	Gln	Tyr	Glu	Glu	Arg
		Leu	Ser	Val	Tyr	Pro	Gln	Ser	Thr	Met
		Asn	Met	Met	Leu	Gln	Gln	Ile	Tyr	Trp
		Ala	Asp	Leu	Ala	Tyr	Ala	Asp	Leu	Asn
		Ile	Arg	Asn	Ala	Phe	Ile	Asp	Ser	Asp
		Arg	Ser	Arg	His	Glu	Glu	Ala	Leu	Ala
		Asp	Ser	Phe	Tyr	Leu	Met	Gln	Thr	Leu
		Met	Asp	Leu	Leu	Tyr	Tyr	Gly	Ala	Val
		Trp	Gln	Asp	Thr	Lys	Val	Ala	Gln	Arg
		Asn	Ser	Leu	Cys	Ser	Ala	Ile	Asp	Ala
		Lys	Leu	Ser	Ala	Ile	Arg	Arg	Thr	Glu
		Trp	Ala	Asp	Ala	Ala	Asp	Ala	Ser	Gln
		Val	Leu	Ala	Gln	Gly	Glu	Tyr	Asn	Tyr
		Glu	Lys	Met	Ala	Ala	Trp	Cys	Gln	Leu
		Ala	Ala	Asp	Lys	Val	Ala	Ala	Asp	Pro
		Phe	Cys	Glu	Glu	Leu	Lys	Gly	Gln	Thr
		Gly	Glu	Pro	Gln	His	Val	Arg	Leu	Lys
		Thr	His	Asp	Gly	Ala	His	Arg	Glu	Val
		Asp	Cys	Ser	Leu	Ser	Glu	Trp	His	Ala
		Pro	Gly	Ser	Lys	Gln	Leu	Lys	Cys	Glu
		Val	Lys	Ala	Asp	Gly	Ala	Lys	Trp	Val
		Thr	Pro	Ala	Ile	Asp	Ala	Ala	Gly	Gln
		Gly	Thr	Val	Ala	Arg	Gln	Ala	Gln	Met
		Met	Tyr	Ile	Ala	Asn	Gln	Thr	Ala	Glu
		Gln	Glu	Glu	Met	Pro	Gly	Leu	Ala	Leu
		Ala	Ala	Asn	Val	Val	Pro	Ala	Gln	Leu
		Pro	Met	Asp	Thr	Ala	Val	Gly	Leu	Met
		Thr	Met	Asp	Leu	Glu	Val	Thr	Leu	Thr
		Pro	Met	Asp	Thr	Ala	Val	Thr	Leu	Gly

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	18216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Warp/Relion/M - CTF Refinement in M	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	104	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.372	Depositor
Minimum map value	-0.388	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.466	Depositor
Map size (\AA)	775.68, 775.68, 775.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	3.03, 3.03, 3.03	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/4423	0.60	0/5956
1	H	0.32	1/4423 (0.0%)	0.62	0/5956
2	B	0.28	0/3635	0.57	0/4918
2	J	0.28	0/3635	0.59	0/4918
3	C	0.28	0/5080	0.56	0/6863
3	K	0.27	0/5080	0.57	0/6863
4	D	0.29	0/1068	0.61	0/1441
4	N	0.29	0/1068	0.62	0/1441
5	E	0.26	0/4570	0.52	0/6180
5	O	0.25	0/4570	0.51	0/6180
6	F	0.29	0/2740	0.62	0/3688
6	P	0.29	0/2740	0.64	0/3688
7	G	0.30	0/1687	0.65	0/2257
7	Q	0.33	0/1687	0.66	0/2257
8	I	0.28	0/6147	0.57	0/8333
8	R	0.27	0/6147	0.58	0/8333
9	L	0.28	0/2504	0.63	0/3356
9	T	0.35	2/2504 (0.1%)	0.65	0/3356
10	M	0.25	0/1343	0.59	0/1804
10	U	0.27	0/1343	0.60	0/1804
11	W	0.42	1/922 (0.1%)	0.64	0/1226
11	Y	0.33	0/922	0.62	0/1226
12	X	0.32	0/857	0.66	0/1144
12	Z	0.32	0/857	0.65	0/1144
13	S	0.27	0/8979	0.55	0/12160
13	V	0.28	0/8979	0.55	0/12160
All	All	0.29	4/87910 (0.0%)	0.58	0/118652

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	56	ASP	C-N	8.35	1.53	1.34
9	T	72	VAL	C-N	6.69	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	268	GLU	C-N	-5.12	1.22	1.34
1	H	262	ILE	C-N	5.06	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4337	0	4306	191	0
1	H	4337	0	4306	201	0
2	B	3553	0	3523	158	0
2	J	3553	0	3523	146	0
3	C	4978	0	4912	161	0
3	K	4978	0	4912	154	0
4	D	1045	0	1039	44	0
4	N	1045	0	1039	44	0
5	E	4465	0	4396	109	0
5	O	4465	0	4396	93	0
6	F	2701	0	2731	81	0
6	P	2701	0	2731	80	0
7	G	1674	0	1673	46	0
7	Q	1674	0	1673	52	0
8	I	6025	0	5988	279	0
8	R	6025	0	5988	255	0
9	L	2472	0	2484	109	0
9	T	2472	0	2484	100	0
10	M	1328	0	1322	50	0
10	U	1328	0	1322	50	0
11	W	919	0	936	67	0
11	Y	919	0	936	52	0
12	X	849	0	863	49	0
12	Z	849	0	863	40	0
13	S	8788	0	8605	238	0
13	V	8788	0	8605	287	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	86268	0	85556	2793	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2793) 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)
9:L:136:ILE:HG21	12:X:410:GLU:CD	1.18	1.45
9:L:136:ILE:CG2	12:X:410:GLU:CD	1.98	1.30
9:L:136:ILE:HG21	12:X:410:GLU:OE2	1.21	1.27
9:L:136:ILE:CG2	12:X:410:GLU:OE1	2.02	1.07
9:T:133:PRO:HA	9:T:136:ILE:HG22	1.32	1.06
2:J:110:GLY:HA3	2:J:188:PRO:HG3	1.39	1.03
2:B:110:GLY:HA3	2:B:188:PRO:HG3	1.43	1.00
9:L:136:ILE:CG2	12:X:410:GLU:OE2	2.04	0.99
11:W:117:GLU:HA	13:V:781:GLY:HA3	1.45	0.98
9:L:136:ILE:HG23	12:X:410:GLU:OE1	1.60	0.96
2:J:189:ALA:HB2	2:J:210:TRP:HD1	1.35	0.89
9:L:106:LYS:HA	11:W:56:ASP:CB	2.04	0.87
2:J:189:ALA:HB2	2:J:210:TRP:CD1	2.09	0.85
13:V:756:GLN:HA	13:V:780:GLY:HA2	1.58	0.84
1:A:449:TYR:CD1	1:A:458:ALA:HB2	2.12	0.84
8:I:688:ILE:HD12	13:V:662:ARG:HH22	1.41	0.83
2:B:189:ALA:HB2	2:B:210:TRP:HD1	1.41	0.83
13:V:847:ASP:HB2	13:V:860:ILE:HA	1.59	0.82
2:J:106:LEU:HB3	2:J:111:MET:HB2	1.62	0.81
11:W:117:GLU:CA	13:V:781:GLY:HA3	2.10	0.80
2:B:428:SER:H	4:D:254:PRO:HD2	1.45	0.80
13:V:668:VAL:O	13:V:672:GLN:HB2	1.81	0.80
2:B:106:LEU:HB3	2:B:111:MET:HB2	1.64	0.80
2:J:428:SER:H	4:N:254:PRO:HD2	1.46	0.80
2:B:189:ALA:HB2	2:B:210:TRP:CD1	2.16	0.80
6:P:199:ASP:HB2	6:P:203:TYR:HB2	1.63	0.79
2:J:273:PRO:HA	9:T:269:LEU:HD13	1.65	0.79
1:H:449:TYR:CD1	1:H:458:ALA:HB2	2.18	0.78
11:W:120:LEU:HB3	13:V:781:GLY:HA2	1.64	0.78
8:I:596:TRP:HE1	8:I:627:THR:HG1	1.29	0.78
9:L:106:LYS:HA	11:W:56:ASP:HB3	1.64	0.78
11:W:56:ASP:HA	11:W:59:VAL:HG22	1.63	0.77
5:E:1:MET:HB3	5:E:194:LEU:HD22	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:ASP:HB2	6:F:203:TYR:HB2	1.65	0.77
1:A:449:TYR:CE2	1:A:454:GLU:HG3	2.19	0.77
8:I:651:PRO:HB2	8:I:764:TYR:H	1.50	0.77
12:Z:406:SER:HB2	12:Z:409:ARG:HH21	1.50	0.76
1:H:449:TYR:CE2	1:H:454:GLU:HG3	2.20	0.76
10:M:360:MET:SD	10:M:364:ARG:NH1	2.58	0.76
5:E:224:ASN:HD21	5:E:259:LEU:HD11	1.50	0.76
5:O:224:ASN:HD21	5:O:259:LEU:HD11	1.51	0.76
9:L:106:LYS:HA	11:W:56:ASP:HB2	1.68	0.75
9:T:136:ILE:CG1	12:Z:410:GLU:HG3	2.16	0.75
1:A:388:MET:SD	1:A:410:LYS:NZ	2.60	0.75
10:U:360:MET:SD	10:U:364:ARG:NH1	2.60	0.75
13:V:787:ALA:O	13:V:791:MET:HB2	1.87	0.75
11:W:124:LYS:HD3	13:V:779:LYS:HG2	1.68	0.75
9:T:133:PRO:CA	9:T:136:ILE:HG22	2.16	0.75
9:T:136:ILE:HG12	12:Z:410:GLU:HG3	1.69	0.74
8:I:3:LEU:HB2	8:I:263:ILE:HG13	1.70	0.74
8:R:651:PRO:HG2	8:R:763:ARG:HE	1.52	0.74
1:A:263:MET:HG2	1:A:286:VAL:HG21	1.67	0.74
1:H:449:TYR:CE1	1:H:458:ALA:HB2	2.23	0.74
5:O:277:LEU:HD11	5:O:280:LEU:HB2	1.68	0.74
8:R:688:ILE:HG12	8:R:710:VAL:HA	1.70	0.74
13:V:758:GLU:CD	13:V:782:LEU:HB2	2.09	0.74
11:W:117:GLU:HA	13:V:781:GLY:CA	2.16	0.73
8:I:629:GLU:O	13:V:724:ARG:NH1	2.20	0.73
13:V:332:GLU:HG3	13:V:344:LYS:HB2	1.71	0.73
8:I:651:PRO:HG2	8:I:763:ARG:HE	1.52	0.73
3:K:23:LEU:HB3	3:K:29:PHE:HB3	1.71	0.72
13:S:413:MET:HB3	13:S:420:LEU:HD11	1.72	0.72
13:S:440:ASN:HB3	13:S:443:LEU:HD23	1.71	0.72
3:K:459:PHE:HA	3:K:462:GLN:HB2	1.71	0.72
6:P:286:ARG:HD2	7:Q:296:LEU:HB2	1.70	0.72
3:C:23:LEU:HB3	3:C:29:PHE:HB3	1.69	0.72
13:V:413:MET:HB3	13:V:420:LEU:HD11	1.72	0.72
4:D:242:ARG:HH22	4:D:246:ILE:HG12	1.52	0.72
6:P:249:GLN:O	6:P:253:GLN:HB2	1.89	0.72
8:I:688:ILE:O	13:V:665:HIS:NE2	2.23	0.72
10:M:452:ARG:HH22	10:M:455:ARG:HH11	1.35	0.72
13:V:990:LYS:HD3	13:V:993:GLU:HB2	1.72	0.71
13:S:990:LYS:HD3	13:S:993:GLU:HB2	1.72	0.71
5:E:80:TYR:O	5:E:84:LEU:HB2	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:413:MET:HG3	13:S:422:ILE:HG22	1.72	0.71
3:C:171:GLN:HG2	5:E:303:GLU:HB3	1.72	0.71
13:S:179:GLY:HA2	13:S:206:PRO:HD3	1.73	0.71
3:C:29:PHE:HB2	3:C:32:ALA:HB3	1.73	0.71
8:I:354:GLN:HA	8:I:370:ASP:HA	1.73	0.71
11:W:124:LYS:HG2	13:V:779:LYS:HA	1.73	0.71
3:C:163:ARG:NH2	3:C:190:THR:OG1	2.19	0.71
1:H:418:LYS:HG2	9:T:274:GLN:HE21	1.55	0.70
2:J:270:LYS:NZ	9:T:268:GLU:OE1	2.20	0.70
8:I:759:PRO:HA	8:I:762:LYS:HB2	1.74	0.70
1:A:581:LEU:O	1:A:585:HIS:ND1	2.25	0.70
13:S:410:ARG:HE	13:S:448:VAL:HB	1.56	0.69
13:V:413:MET:HG3	13:V:422:ILE:HG22	1.73	0.69
8:R:433:ASP:HB3	8:R:440:THR:HB	1.74	0.69
13:V:841:ALA:HB1	13:V:844:LYS:HB3	1.74	0.69
8:I:645:ARG:HG2	13:V:722:ASN:HA	1.73	0.69
8:R:152:VAL:HG21	8:R:193:ASP:HA	1.73	0.69
3:C:459:PHE:HA	3:C:462:GLN:HB2	1.74	0.69
1:A:456:ASP:OD1	1:A:460:LYS:NZ	2.24	0.69
11:W:81:GLU:HA	11:W:84:LYS:HE2	1.74	0.69
8:I:152:VAL:HG21	8:I:193:ASP:HA	1.73	0.69
11:W:94:LEU:HD13	12:X:471:LEU:HG	1.75	0.69
8:R:354:GLN:HA	8:R:370:ASP:HA	1.75	0.69
8:R:759:PRO:HA	8:R:762:LYS:HB2	1.75	0.69
1:H:472:ASN:O	1:H:474:ARG:NH1	2.26	0.69
5:O:275:GLN:HG3	5:O:276:VAL:HG23	1.74	0.69
1:A:449:TYR:CE1	1:A:458:ALA:HB2	2.28	0.69
9:L:18:TYR:HB3	9:L:45:ARG:HH11	1.58	0.69
1:H:581:LEU:O	1:H:585:HIS:ND1	2.26	0.68
8:R:235:TRP:HA	8:R:242:PHE:HA	1.75	0.68
2:B:273:PRO:O	9:L:269:LEU:HD13	1.94	0.68
8:I:642:HIS:HB3	13:V:694:GLN:HA	1.76	0.68
11:W:117:GLU:HB3	13:V:780:GLY:O	1.93	0.68
8:R:155:TYR:OH	8:R:413:ARG:NH2	2.26	0.68
8:R:651:PRO:HB2	8:R:764:TYR:H	1.58	0.68
13:S:412:CYS:HB3	13:S:423:VAL:HB	1.76	0.68
13:S:847:ASP:OD2	13:S:864:TRP:NE1	2.26	0.68
8:I:85:GLY:HA2	8:I:107:CYS:HB2	1.74	0.68
13:V:440:ASN:HB3	13:V:443:LEU:HD23	1.74	0.68
9:T:204:ARG:HE	10:U:378:ASN:HB3	1.58	0.68
13:V:6:PHE:HB3	13:V:317:MET:HG3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:81:GLU:HA	3:K:84:LYS:HE2	1.76	0.68
13:V:503:HIS:HB3	13:V:515:LEU:HD11	1.76	0.68
1:H:642:GLU:HB3	1:H:645:TRP:HB3	1.76	0.68
6:P:305:MET:O	6:P:309:ARG:NH1	2.27	0.68
12:X:419:SER:HA	12:X:422:LEU:HD12	1.74	0.67
8:R:536:ASP:HA	8:R:665:ARG:HB2	1.76	0.67
13:V:410:ARG:HE	13:V:448:VAL:HB	1.60	0.67
2:B:381:ASN:HD21	4:D:234:ALA:H	1.40	0.67
3:K:616:ASP:HA	3:K:630:THR:HA	1.75	0.67
3:C:96:MET:HB3	3:C:99:GLU:HB2	1.75	0.67
13:V:224:VAL:HB	13:V:237:PHE:HB2	1.76	0.67
1:H:512:ASN:HA	1:H:515:LEU:HD12	1.76	0.67
8:I:235:TRP:HA	8:I:242:PHE:HA	1.75	0.67
8:I:679:LEU:HB2	8:I:758:ARG:HH22	1.60	0.67
13:V:412:CYS:HB3	13:V:423:VAL:HB	1.77	0.67
8:I:111:ARG:NH1	8:I:112:TRP:O	2.27	0.67
3:C:81:GLU:HA	3:C:84:LYS:HE2	1.75	0.67
3:K:29:PHE:HB2	3:K:32:ALA:HB3	1.75	0.67
13:V:443:LEU:HA	13:V:495:LEU:HD21	1.75	0.67
3:K:542:GLY:O	3:K:546:CYS:N	2.27	0.67
13:V:668:VAL:HA	13:V:691:MET:HE2	1.75	0.67
5:E:183:ASP:H	5:E:186:ARG:HB2	1.60	0.67
8:I:589:ASP:O	8:I:593:LYS:NZ	2.26	0.67
12:X:406:SER:HB2	12:X:409:ARG:HH21	1.59	0.67
4:N:221:TRP:O	4:N:225:ILE:HB	1.95	0.67
9:T:18:TYR:HB3	9:T:45:ARG:HH11	1.59	0.67
5:O:261:ARG:HE	5:O:264:LEU:HD21	1.60	0.67
10:U:411:ASN:HA	10:U:415:ALA:HB3	1.77	0.66
8:I:155:TYR:OH	8:I:413:ARG:NH2	2.28	0.66
8:I:386:LEU:HB2	8:I:424:LEU:HD22	1.76	0.66
13:S:841:ALA:HB1	13:S:844:LYS:HB3	1.77	0.66
1:H:279:ALA:HB3	1:H:302:CYS:SG	2.34	0.66
8:I:632:PHE:HB2	13:V:724:ARG:HH12	1.60	0.66
8:R:155:TYR:HB2	8:R:196:PRO:HB2	1.77	0.66
6:F:70:LYS:HG3	6:F:75:ARG:HH21	1.61	0.66
8:I:1:MET:O	8:I:261:SER:OG	2.14	0.66
13:V:757:GLU:HG3	13:V:779:LYS:HE2	1.76	0.66
1:A:544:ILE:HG21	1:A:566:LEU:HD22	1.76	0.66
8:R:85:GLY:HA2	8:R:107:CYS:HB2	1.76	0.66
4:D:249:LEU:HD23	4:D:251:GLN:HE21	1.61	0.66
13:S:874:MET:HA	13:S:877:ALA:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:193:ARG:HD3	10:U:371:THR:HA	1.77	0.66
12:Z:433:ILE:HG22	12:Z:437:ARG:HE	1.60	0.66
13:V:823:TYR:HB3	13:V:828:ARG:HB3	1.77	0.66
1:A:418:LYS:HG2	9:L:274:GLN:HE21	1.60	0.66
3:C:616:ASP:HA	3:C:630:THR:HA	1.76	0.66
5:O:114:ALA:O	5:O:123:GLN:NE2	2.29	0.66
1:A:508:GLU:HG2	2:B:283:LYS:HB3	1.76	0.66
1:A:294:GLN:NE2	2:B:301:ASP:OD1	2.29	0.66
2:B:390:GLU:HG3	2:B:391:TYR:HD1	1.60	0.66
8:I:697:LEU:HD11	8:I:729:ARG:HB3	1.78	0.66
8:R:3:LEU:HB2	8:R:263:ILE:HG13	1.77	0.66
13:V:652:TYR:HB3	13:V:663:PHE:HB3	1.77	0.66
1:A:202:SER:O	1:A:206:ASN:ND2	2.29	0.66
1:A:642:GLU:HB3	1:A:645:TRP:HB3	1.77	0.66
3:C:383:ARG:NH2	3:K:25:LYS:O	2.28	0.66
8:I:731:MET:HA	8:I:734:ASN:HB2	1.76	0.66
13:S:990:LYS:HB3	13:S:994:ALA:HB2	1.78	0.66
1:H:508:GLU:HG2	2:J:283:LYS:HB3	1.76	0.65
5:O:36:LYS:NZ	5:O:38:ASP:O	2.27	0.65
13:V:179:GLY:HA2	13:V:206:PRO:HD3	1.76	0.65
1:A:472:ASN:O	1:A:474:ARG:NH1	2.29	0.65
4:D:341:VAL:HB	4:D:344:LEU:HD12	1.79	0.65
11:W:61:ARG:HB3	12:X:440:TYR:HE2	1.61	0.65
2:J:133:LEU:HD22	2:J:176:VAL:HA	1.79	0.65
4:N:341:VAL:HB	4:N:344:LEU:HD12	1.78	0.65
11:Y:125:LEU:HD22	12:Z:502:LEU:HD13	1.79	0.65
1:H:456:ASP:OD1	1:H:460:LYS:NZ	2.29	0.65
13:V:990:LYS:HB3	13:V:994:ALA:HB2	1.79	0.65
8:I:524:LEU:HB3	8:I:547:LYS:HB3	1.79	0.65
1:H:170:ARG:HE	1:H:173:ASN:HB2	1.61	0.65
1:H:294:GLN:NE2	2:J:301:ASP:OD1	2.30	0.65
6:P:72:ILE:O	6:P:113:ARG:NH1	2.30	0.65
8:R:558:ILE:HA	8:R:568:VAL:HG12	1.79	0.65
2:B:65:LYS:HA	2:B:98:ALA:HB1	1.78	0.65
5:E:277:LEU:HD11	5:E:280:LEU:HB2	1.78	0.65
8:I:433:ASP:HB3	8:I:440:THR:HB	1.77	0.65
12:X:413:GLN:HB3	10:U:348:ARG:HD3	1.77	0.65
9:T:33:GLU:HB3	9:T:56:ILE:HG21	1.79	0.65
1:A:565:GLU:OE1	9:T:231:GLN:NE2	2.30	0.65
7:G:167:LYS:O	7:G:171:TYR:HB3	1.97	0.65
5:O:152:GLU:HA	5:O:155:LEU:HB2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:111:ARG:NH1	8:R:112:TRP:O	2.29	0.65
1:A:641:GLN:NE2	1:A:642:GLU:OE2	2.30	0.64
5:E:94:PHE:HD1	5:E:113:GLN:HE21	1.43	0.64
8:I:601:ARG:NH2	13:V:754:THR:OG1	2.30	0.64
1:H:202:SER:O	1:H:206:ASN:ND2	2.29	0.64
11:Y:124:LYS:HG3	11:Y:125:LEU:HD12	1.77	0.64
5:E:114:ALA:O	5:E:123:GLN:NE2	2.30	0.64
8:I:693:TRP:HE3	13:V:662:ARG:HG3	1.63	0.64
8:R:282:GLN:HB2	8:R:336:ARG:HH22	1.63	0.64
10:U:309:HIS:HE1	11:Y:38:ILE:HG12	1.62	0.64
13:V:690:ALA:O	13:V:722:ASN:ND2	2.30	0.64
6:F:72:ILE:O	6:F:113:ARG:NH1	2.29	0.64
9:L:130:GLY:O	9:L:134:LYS:N	2.30	0.64
13:S:405:HIS:HB2	13:S:413:MET:HB2	1.79	0.64
6:P:210:LEU:HG	6:P:214:GLN:HE22	1.63	0.64
6:F:238:TYR:HE2	7:G:239:LEU:HB3	1.62	0.64
13:V:266:ASN:HA	13:V:291:PHE:HB3	1.80	0.64
8:R:576:VAL:HG22	11:Y:92:ARG:HH12	1.62	0.64
5:E:125:ARG:NE	5:E:152:GLU:OE1	2.30	0.64
8:I:711:LEU:HD12	8:I:733:MET:HG3	1.78	0.64
1:H:227:MET:SD	1:H:243:MET:SD	2.95	0.64
8:R:219:LEU:HD21	8:R:222:GLN:HB2	1.80	0.64
8:R:688:ILE:HG21	8:R:706:HIS:HE1	1.61	0.64
1:A:184:MET:HG2	1:A:216:ASN:HD21	1.63	0.64
3:C:299:ASN:O	3:C:303:GLN:NE2	2.31	0.64
6:F:181:GLU:OE2	6:F:182:ARG:NH1	2.31	0.64
9:L:193:ARG:HD3	10:M:371:THR:HA	1.80	0.64
9:L:293:ARG:HH22	9:L:294:LEU:HG	1.62	0.64
13:S:847:ASP:HB2	13:S:860:ILE:HA	1.79	0.64
13:S:995:GLU:HB2	13:S:1006:VAL:HG13	1.80	0.64
1:H:537:VAL:HG21	10:U:460:GLN:HG2	1.80	0.64
13:V:133:LEU:HB2	13:V:139:ARG:HH12	1.62	0.64
3:C:383:ARG:NH2	3:K:27:GLN:OE1	2.31	0.63
13:V:667:VAL:HG12	13:V:691:MET:HG2	1.80	0.63
1:A:512:ASN:HA	1:A:515:LEU:HD12	1.79	0.63
9:L:290:MET:HG2	9:L:293:ARG:HH21	1.64	0.63
13:S:1052:ARG:HH22	10:U:359:LEU:HG	1.63	0.63
4:N:273:LEU:HB3	4:N:277:THR:HB	1.81	0.63
8:I:713:TYR:HB3	13:V:665:HIS:HD2	1.62	0.63
1:H:231:HIS:CD2	1:H:243:MET:SD	2.91	0.63
8:R:357:VAL:HB	8:R:367:HIS:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:689:LYS:HG3	13:V:666:LYS:HD3	1.81	0.63
2:J:419:ARG:HH11	4:N:344:LEU:HB3	1.63	0.63
6:P:315:THR:HA	6:P:318:HIS:CD2	2.33	0.63
8:R:679:LEU:HB2	8:R:758:ARG:HH22	1.62	0.63
9:T:130:GLY:O	9:T:134:LYS:N	2.32	0.63
9:T:133:PRO:HA	9:T:136:ILE:CG2	2.21	0.63
6:F:285:LYS:HD2	6:F:286:ARG:HH21	1.63	0.63
3:K:171:GLN:HG2	5:O:303:GLU:HB3	1.79	0.63
4:N:252:GLU:HG2	4:N:254:PRO:HD3	1.81	0.63
8:R:598:LYS:HE2	12:Z:496:ASP:HB3	1.79	0.63
8:I:598:LYS:HB2	12:X:499:LEU:HD23	1.81	0.63
13:S:811:ALA:O	13:S:838:ARG:NH1	2.31	0.63
1:H:447:PHE:CE2	2:J:286:LEU:HB2	2.33	0.63
2:J:343:LEU:HD21	3:K:317:LEU:HD21	1.80	0.63
6:P:70:LYS:HG3	6:P:75:ARG:HH21	1.63	0.63
8:I:536:ASP:HA	8:I:665:ARG:HB2	1.81	0.63
1:H:170:ARG:HD2	1:H:179:ILE:HG21	1.81	0.63
1:H:251:ILE:HG21	1:H:255:ALA:HB3	1.79	0.63
8:R:141:LEU:O	8:R:171:LYS:NZ	2.31	0.63
13:V:874:MET:HA	13:V:877:ALA:HB3	1.79	0.63
8:R:302:LEU:HD22	8:R:342:LEU:HD23	1.80	0.63
8:R:524:LEU:HB3	8:R:547:LYS:HB3	1.80	0.63
10:U:462:ALA:O	10:U:467:GLU:N	2.32	0.63
13:S:781:GLY:O	13:S:782:LEU:HD22	1.99	0.62
1:H:418:LYS:HD2	9:T:277:GLN:HE22	1.64	0.62
8:R:180:ASN:ND2	8:R:216:PHE:O	2.31	0.62
13:V:267:ARG:HD2	13:V:269:TYR:HE1	1.64	0.62
3:C:522:SER:O	3:C:525:GLN:NE2	2.32	0.62
8:I:756:SER:O	8:I:763:ARG:NH1	2.32	0.62
11:W:114:VAL:O	11:W:118:GLN:NE2	2.31	0.62
1:H:312:MET:HB3	1:H:373:ILE:HD11	1.81	0.62
1:H:485:GLU:OE1	1:H:486:ARG:NH1	2.33	0.62
9:T:259:PHE:HA	9:T:262:LEU:HD12	1.82	0.62
1:A:447:PHE:HB2	1:A:478:ASN:HD21	1.63	0.62
2:B:419:ARG:HH11	4:D:344:LEU:HB3	1.65	0.62
13:S:133:LEU:HB2	13:S:139:ARG:HH12	1.64	0.62
8:R:276:TRP:HA	8:R:283:LEU:HA	1.81	0.62
7:G:199:LEU:HD12	7:G:203:GLY:HA3	1.82	0.62
13:S:375:ALA:HB3	13:S:382:LEU:HB2	1.81	0.62
8:R:266:ASN:HA	11:Y:75:ARG:HH21	1.64	0.62
11:Y:94:LEU:HD13	12:Z:471:LEU:HG	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:210:LEU:HD11	7:G:218:LEU:HD21	1.80	0.62
8:I:714:ARG:HE	8:I:727:ILE:HD11	1.65	0.62
7:Q:199:LEU:HD12	7:Q:203:GLY:HA3	1.81	0.62
2:B:54:ARG:HE	2:B:79:PHE:HB2	1.64	0.62
2:J:189:ALA:HB1	2:J:209:VAL:O	2.00	0.62
4:N:321:GLU:O	4:N:325:ASP:N	2.30	0.62
8:R:379:LEU:HB2	8:R:386:LEU:HB3	1.79	0.62
13:V:896:ASP:OD1	13:V:921:ARG:NH1	2.32	0.62
5:E:151:ILE:HG12	5:E:177:LEU:HB3	1.80	0.62
6:F:196:LYS:NZ	7:G:203:GLY:O	2.33	0.62
10:M:411:ASN:HA	10:M:415:ALA:HB3	1.80	0.62
11:W:25:ASN:HA	11:W:28:LYS:HE2	1.81	0.62
13:S:503:HIS:HB3	13:S:515:LEU:HD11	1.79	0.62
5:E:26:LYS:HA	5:E:45:LEU:HB3	1.81	0.62
8:I:574:VAL:HG21	11:W:92:ARG:HD2	1.82	0.62
9:L:259:PHE:HA	9:L:262:LEU:HD12	1.82	0.62
11:W:56:ASP:OD1	11:W:57:GLN:N	2.33	0.62
3:K:247:ALA:HB2	3:K:263:LEU:HD21	1.82	0.62
3:K:502:THR:O	3:K:504:GLN:NE2	2.32	0.62
6:P:35:GLN:NE2	6:P:52:ASP:OD1	2.33	0.62
8:R:11:ASN:ND2	8:R:290:GLY:O	2.32	0.62
1:A:669:ILE:O	1:A:673:HIS:N	2.27	0.62
8:I:525:CYS:HA	8:I:546:THR:HA	1.81	0.62
10:M:462:ALA:O	10:M:467:GLU:N	2.33	0.62
13:S:443:LEU:HA	13:S:495:LEU:HD21	1.81	0.62
5:O:125:ARG:NE	5:O:152:GLU:OE1	2.31	0.62
3:C:134:GLN:HA	3:C:137:LYS:HE2	1.82	0.62
3:C:247:ALA:HB2	3:C:263:LEU:HD21	1.80	0.62
2:J:419:ARG:O	2:J:423:GLN:NE2	2.30	0.62
1:A:449:TYR:HD1	1:A:458:ALA:HB2	1.61	0.61
6:F:315:THR:HA	6:F:318:HIS:CD2	2.35	0.61
13:S:309:GLY:HA2	13:S:315:VAL:HA	1.81	0.61
1:H:447:PHE:HB2	1:H:478:ASN:HD21	1.65	0.61
1:A:625:TYR:HA	1:A:628:ALA:HB3	1.81	0.61
2:B:189:ALA:HB1	2:B:209:VAL:O	2.00	0.61
8:I:138:ARG:NH1	8:I:138:ARG:O	2.33	0.61
8:I:379:LEU:HB2	8:I:386:LEU:HB3	1.80	0.61
13:S:896:ASP:OD1	13:S:921:ARG:NH1	2.33	0.61
2:J:189:ALA:HB1	2:J:210:TRP:HA	1.82	0.61
2:B:419:ARG:O	2:B:423:GLN:NE2	2.32	0.61
2:B:434:THR:HG21	4:D:344:LEU:HD23	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:204:ARG:HE	10:M:378:ASN:HB3	1.66	0.61
13:S:697:LYS:HG3	13:S:698:GLN:HG2	1.83	0.61
3:K:134:GLN:HA	3:K:137:LYS:HE2	1.83	0.61
5:O:220:ALA:O	5:O:224:ASN:HB2	2.00	0.61
7:Q:183:LYS:O	7:Q:186:LYS:NZ	2.33	0.61
2:B:210:TRP:NE1	2:B:212:GLN:OE1	2.33	0.61
1:H:567:LEU:O	1:H:571:VAL:N	2.31	0.61
3:C:542:GLY:O	3:C:546:CYS:N	2.32	0.61
6:F:210:LEU:HG	6:F:214:GLN:HE22	1.64	0.61
8:I:339:LYS:HE3	8:I:377:LEU:HA	1.82	0.61
8:I:535:VAL:HG12	8:I:539:LEU:HD23	1.81	0.61
8:I:647:VAL:HG11	8:I:656:ARG:HA	1.82	0.61
2:J:65:LYS:HA	2:J:98:ALA:HB1	1.82	0.61
6:P:196:LYS:NZ	7:Q:203:GLY:O	2.33	0.61
8:R:309:VAL:HG12	8:R:319:VAL:HG22	1.82	0.61
9:L:213:ILE:HD13	9:L:216:LYS:HZ3	1.65	0.61
3:K:195:PRO:O	3:K:199:HIS:ND1	2.24	0.61
13:V:1077:TRP:HA	13:V:1081:LEU:HD23	1.83	0.61
2:B:90:MET:HB2	2:B:222:GLY:HA2	1.81	0.61
2:B:189:ALA:HB1	2:B:210:TRP:HA	1.83	0.61
13:S:823:TYR:HB3	13:S:828:ARG:HB3	1.82	0.61
3:K:455:VAL:HA	3:K:458:THR:HG22	1.83	0.61
8:R:470:ALA:H	8:R:509:TRP:HE1	1.48	0.61
8:R:535:VAL:HG12	8:R:539:LEU:HD23	1.82	0.61
8:R:711:LEU:HD12	8:R:733:MET:HG3	1.80	0.61
6:F:35:GLN:NE2	6:F:52:ASP:OD1	2.33	0.61
2:J:192:VAL:HG13	2:J:193:LEU:HG	1.82	0.61
6:P:70:LYS:HD2	6:P:75:ARG:HE	1.65	0.61
8:R:373:ASP:HB3	8:R:389:ASP:HB2	1.82	0.61
2:B:270:LYS:NZ	9:L:268:GLU:OE1	2.25	0.61
4:D:252:GLU:HG2	4:D:254:PRO:HD3	1.82	0.61
5:E:261:ARG:HE	5:E:264:LEU:HD21	1.66	0.61
8:I:711:LEU:HD22	8:I:739:VAL:HB	1.82	0.61
13:S:507:ARG:NH1	13:S:531:GLN:O	2.34	0.61
1:H:522:GLU:HB3	1:H:526:ALA:H	1.66	0.61
3:K:445:CYS:SG	3:K:446:SER:N	2.73	0.61
1:A:463:GLU:HB3	1:A:467:LYS:HZ3	1.65	0.60
8:I:141:LEU:O	8:I:171:LYS:NZ	2.32	0.60
13:V:375:ALA:HB3	13:V:382:LEU:HB2	1.83	0.60
13:V:758:GLU:HB2	13:V:780:GLY:HA3	1.83	0.60
1:A:522:GLU:HB3	1:A:526:ALA:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ILE:HD12	2:B:34:LEU:HD21	1.82	0.60
3:C:455:VAL:HA	3:C:458:THR:HG22	1.82	0.60
6:F:6:TYR:HB2	7:G:334:THR:HG21	1.83	0.60
13:S:926:TYR:HA	13:S:929:THR:HG22	1.83	0.60
1:A:231:HIS:CD2	1:A:243:MET:SD	2.94	0.60
11:Y:61:ARG:HB3	12:Z:440:TYR:HE2	1.66	0.60
13:V:668:VAL:O	13:V:672:GLN:CB	2.48	0.60
8:I:155:TYR:HB2	8:I:196:PRO:HB2	1.83	0.60
1:H:296:GLY:HA2	1:H:299:LEU:HD12	1.84	0.60
2:J:90:MET:HB2	2:J:222:GLY:HA2	1.82	0.60
13:V:737:HIS:NE2	13:V:747:TYR:OH	2.33	0.60
5:O:26:LYS:HA	5:O:45:LEU:HB3	1.81	0.60
8:R:386:LEU:HB2	8:R:424:LEU:HD22	1.82	0.60
12:X:433:ILE:HG22	12:X:437:ARG:HE	1.67	0.60
8:R:498:ALA:HB1	8:R:533:VAL:HG21	1.83	0.60
13:V:550:LEU:HB2	13:V:565:PHE:HB3	1.83	0.60
8:I:282:GLN:HB2	8:I:336:ARG:HH22	1.67	0.60
9:L:136:ILE:HD11	12:X:409:ARG:HH22	1.66	0.60
8:R:1:MET:O	8:R:261:SER:OG	2.15	0.60
8:R:756:SER:O	8:R:763:ARG:NH1	2.35	0.60
13:V:405:HIS:HB2	13:V:413:MET:HB2	1.83	0.60
1:A:181:LEU:HA	1:A:184:MET:HG3	1.83	0.60
3:C:220:THR:O	3:C:264:THR:OG1	2.19	0.60
2:J:426:MET:HB2	4:N:255:PRO:HA	1.83	0.60
3:C:60:THR:HG23	3:C:62:GLN:H	1.67	0.60
8:I:498:ALA:HB1	8:I:533:VAL:HG21	1.84	0.60
1:H:651:SER:O	1:H:654:ARG:NH1	2.35	0.60
1:H:663:LEU:HD23	1:H:667:LYS:HE2	1.83	0.60
5:O:37:ARG:HE	5:O:69:HIS:HB2	1.66	0.60
2:B:451:GLN:NE2	4:D:312:PRO:O	2.34	0.60
8:I:481:ILE:HG23	8:I:485:ARG:HA	1.84	0.60
13:S:613:GLU:OE1	13:S:650:ARG:NH1	2.34	0.60
2:J:354:GLU:OE2	3:K:89:GLN:NE2	2.35	0.60
3:K:310:GLU:O	3:K:314:ASN:ND2	2.35	0.60
3:K:522:SER:O	3:K:525:GLN:NE2	2.35	0.60
5:O:132:GLN:HB2	5:O:160:ILE:HD11	1.83	0.60
8:I:211:LYS:HG2	8:I:222:GLN:HA	1.83	0.59
13:S:408:ASN:HB2	13:S:411:VAL:HG22	1.83	0.59
5:O:25:PRO:O	5:O:49:ARG:NH1	2.34	0.59
9:T:104:LEU:HA	9:T:106:LYS:HG2	1.84	0.59
9:T:213:ILE:HD13	9:T:216:LYS:HZ3	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:309:GLY:HA2	13:V:315:VAL:HA	1.83	0.59
13:V:776:LEU:HD23	13:V:779:LYS:HD3	1.84	0.59
13:V:912:PRO:HB3	13:V:919:PHE:HE2	1.67	0.59
1:A:283:PHE:HA	1:A:286:VAL:HG22	1.85	0.59
8:I:357:VAL:HB	8:I:367:HIS:HB2	1.84	0.59
9:L:53:ALA:HB3	9:L:62:ARG:HH12	1.68	0.59
12:X:491:GLN:HG2	12:X:494:ARG:HH21	1.67	0.59
13:S:889:LYS:HA	13:S:892:LYS:HE2	1.84	0.59
12:Z:409:ARG:NH1	12:Z:410:GLU:OE1	2.35	0.59
13:V:790:VAL:HG23	13:V:791:MET:HG3	1.84	0.59
1:A:230:ILE:O	1:A:234:GLN:NE2	2.35	0.59
2:B:422:ALA:HB1	2:B:425:LYS:HE2	1.84	0.59
10:M:312:GLU:O	10:M:316:HIS:ND1	2.29	0.59
10:M:384:VAL:O	10:M:388:ASN:ND2	2.35	0.59
13:S:720:GLN:O	13:S:725:TRP:NE1	2.35	0.59
3:K:249:ILE:O	3:K:252:THR:OG1	2.20	0.59
1:A:300:VAL:HA	1:A:303:ASN:HD22	1.68	0.59
1:A:418:LYS:HD2	9:L:277:GLN:HE22	1.67	0.59
11:W:34:THR:HA	11:W:37:PHE:CE2	2.37	0.59
13:S:445:SER:HB2	13:S:495:LEU:O	2.03	0.59
13:S:848:LEU:HD23	13:S:860:ILE:HD11	1.83	0.59
4:N:318:MET:SD	4:N:322:ASN:ND2	2.76	0.59
2:B:10:ARG:HG2	2:B:39:ARG:HD2	1.84	0.59
6:F:321:ILE:HD11	7:G:330:LYS:HB2	1.85	0.59
8:I:699:LEU:O	8:I:703:HIS:HB2	2.03	0.59
9:L:133:PRO:HA	9:L:136:ILE:HB	1.83	0.59
13:S:550:LEU:HB2	13:S:565:PHE:HB3	1.85	0.59
1:H:230:ILE:O	1:H:234:GLN:NE2	2.36	0.59
2:J:451:GLN:NE2	4:N:312:PRO:O	2.35	0.59
8:R:339:LYS:HE3	8:R:377:LEU:HA	1.83	0.59
8:R:485:ARG:O	8:R:504:CYS:N	2.33	0.59
10:U:312:GLU:O	10:U:316:HIS:ND1	2.29	0.59
1:A:485:GLU:OE1	1:A:486:ARG:NH1	2.36	0.59
3:C:557:ARG:HA	3:C:560:LYS:HG3	1.83	0.59
2:J:282:LEU:O	10:U:453:ASN:ND2	2.35	0.59
2:B:190:VAL:HG13	2:B:261:ALA:HB2	1.84	0.59
3:C:163:ARG:HH22	3:C:190:THR:HG1	1.47	0.59
8:I:316:ARG:NH1	8:I:330:LEU:O	2.36	0.59
8:R:597:ASP:HB2	12:Z:503:LEU:HD12	1.83	0.59
13:V:371:ARG:NH1	13:V:385:ASP:OD2	2.36	0.59
13:V:861:GLU:OE1	13:V:880:HIS:ND1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLU:OE2	3:C:89:GLN:NE2	2.35	0.59
8:I:729:ARG:NH1	8:I:733:MET:SD	2.76	0.59
13:S:371:ARG:NH1	13:S:385:ASP:OD2	2.36	0.59
2:J:10:ARG:HG2	2:J:39:ARG:HD2	1.84	0.59
2:J:276:ALA:O	2:J:281:LYS:NZ	2.36	0.59
3:K:476:VAL:HA	3:K:479:LYS:HG2	1.84	0.59
1:A:170:ARG:HE	1:A:173:ASN:HB2	1.68	0.59
1:A:542:GLU:OE2	1:A:546:GLN:NE2	2.36	0.59
7:G:183:LYS:O	7:G:186:LYS:NZ	2.35	0.59
8:I:319:VAL:O	8:I:328:ASP:N	2.36	0.59
13:S:737:HIS:NE2	13:S:747:TYR:OH	2.34	0.59
3:K:195:PRO:HA	3:K:198:LYS:HG2	1.84	0.59
9:T:107:ALA:HB1	9:T:110:LYS:HB2	1.84	0.59
9:T:284:GLU:OE1	9:T:288:LYS:NZ	2.35	0.59
8:I:629:GLU:OE2	13:V:724:ARG:NH2	2.35	0.59
8:I:668:GLU:O	8:I:672:SER:HB3	2.03	0.59
13:S:846:ILE:HA	13:S:849:ALA:HB2	1.84	0.59
5:O:81:LYS:NZ	5:O:113:GLN:OE1	2.27	0.59
8:R:525:CYS:HA	8:R:546:THR:HA	1.84	0.59
13:S:788:GLN:O	13:S:792:SER:OG	2.15	0.58
8:R:574:VAL:HG21	11:Y:92:ARG:HD2	1.84	0.58
2:B:121:THR:O	9:L:258:ARG:NH2	2.36	0.58
13:S:137:LYS:O	13:S:139:ARG:NH1	2.37	0.58
1:H:355:MET:SD	1:H:356:ARG:NH1	2.76	0.58
3:K:243:PHE:HD1	3:K:246:LYS:HZ3	1.52	0.58
8:R:35:GLN:OE1	8:R:57:PHE:N	2.30	0.58
13:V:995:GLU:HB2	13:V:1006:VAL:HG13	1.85	0.58
5:E:37:ARG:HE	5:E:69:HIS:HB2	1.68	0.58
8:I:63:TYR:HB3	8:I:75:THR:HA	1.84	0.58
8:I:243:ALA:HB2	8:I:276:TRP:HE1	1.68	0.58
13:S:639:ALA:HB1	13:S:648:ALA:HA	1.86	0.58
2:J:54:ARG:HE	2:J:79:PHE:HB2	1.68	0.58
2:J:182:THR:HG22	2:J:206:VAL:HG12	1.84	0.58
8:R:129:LYS:HB3	8:R:137:LEU:HD11	1.84	0.58
8:R:379:LEU:HD12	8:R:386:LEU:HD22	1.84	0.58
13:V:507:ARG:NH1	13:V:531:GLN:O	2.35	0.58
5:E:39:TYR:O	5:E:43:ILE:N	2.31	0.58
7:G:320:GLN:OE1	7:G:324:ARG:NH1	2.36	0.58
10:M:441:VAL:HA	10:M:444:HIS:CD2	2.38	0.58
13:S:690:ALA:O	13:S:722:ASN:ND2	2.33	0.58
8:R:643:PHE:HE2	8:R:663:TYR:HB3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:379:ARG:NH1	10:U:382:GLU:OE1	2.37	0.58
1:A:663:LEU:HD23	1:A:667:LYS:HE2	1.85	0.58
1:A:678:GLU:HA	1:A:681:ARG:HE	1.68	0.58
8:I:270:SER:O	8:I:288:GLY:N	2.35	0.58
8:I:276:TRP:HA	8:I:283:LEU:HA	1.85	0.58
8:I:576:VAL:HG22	11:W:92:ARG:HH12	1.67	0.58
2:B:426:MET:HB2	4:D:255:PRO:HA	1.85	0.58
3:C:249:ILE:O	3:C:252:THR:OG1	2.21	0.58
8:R:688:ILE:HG21	8:R:706:HIS:CE1	2.38	0.58
9:T:228:SER:OG	10:U:404:MET:SD	2.55	0.58
8:I:379:LEU:HD12	8:I:386:LEU:HD22	1.83	0.58
2:J:190:VAL:HG13	2:J:261:ALA:HB2	1.85	0.58
8:R:270:SER:O	8:R:288:GLY:N	2.36	0.58
13:S:224:VAL:HB	13:S:237:PHE:HB2	1.85	0.58
13:V:821:GLU:O	13:V:825:HIS:ND1	2.28	0.58
13:V:926:TYR:HA	13:V:929:THR:HG22	1.85	0.58
1:A:257:GLU:HB3	3:C:646:ARG:HH22	1.67	0.58
8:I:597:ASP:HB2	12:X:503:LEU:HD12	1.86	0.58
1:H:483:LEU:HA	1:H:486:ARG:HB2	1.86	0.58
2:J:69:THR:HG23	2:J:71:PRO:HD2	1.86	0.58
8:R:138:ARG:NH1	8:R:138:ARG:O	2.37	0.58
8:R:316:ARG:NH1	8:R:330:LEU:O	2.37	0.58
1:A:659:LEU:HA	1:A:662:ALA:HB3	1.85	0.58
8:I:180:ASN:ND2	8:I:216:PHE:O	2.36	0.58
9:L:193:ARG:HH11	10:M:371:THR:HG23	1.69	0.58
1:H:268:LEU:HD22	2:J:304:LEU:HD21	1.86	0.58
9:T:59:GLU:OE1	9:T:87:TYR:OH	2.21	0.58
11:Y:118:GLN:O	11:Y:122:ILE:HG13	2.03	0.58
2:B:192:VAL:HG13	2:B:193:LEU:HG	1.84	0.57
6:F:13:LEU:O	6:F:17:SER:N	2.36	0.57
6:F:70:LYS:HD2	6:F:75:ARG:HE	1.68	0.57
13:S:266:ASN:HA	13:S:291:PHE:HB3	1.85	0.57
13:S:916:MET:HB3	13:S:920:ARG:HH12	1.69	0.57
1:H:625:TYR:HA	1:H:628:ALA:HB3	1.86	0.57
3:C:468:GLU:OE1	3:C:471:ARG:NH1	2.37	0.57
6:F:117:GLY:HA2	6:F:120:LEU:HB2	1.86	0.57
2:J:424:TYR:HA	4:N:255:PRO:HD3	1.86	0.57
6:P:117:GLY:HA2	6:P:120:LEU:HB2	1.86	0.57
8:R:533:VAL:HG23	8:R:537:LYS:HD3	1.86	0.57
2:B:11:ILE:HG12	2:B:58:ILE:HD12	1.87	0.57
2:B:141:ARG:HH22	2:B:151:LEU:HD21	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:846:ILE:HB	13:S:863:GLU:HG3	1.85	0.57
1:H:669:ILE:O	1:H:673:HIS:N	2.24	0.57
3:K:23:LEU:O	3:K:27:GLN:N	2.35	0.57
13:V:550:LEU:HD21	13:V:571:VAL:HG21	1.86	0.57
11:W:103:ARG:NH1	11:W:107:GLU:OE1	2.37	0.57
13:S:618:THR:HG23	13:S:619:LEU:HD12	1.86	0.57
1:H:277:PRO:HG3	1:H:303:ASN:HD22	1.69	0.57
1:H:592:ALA:O	1:H:596:HIS:HB2	2.04	0.57
2:J:210:TRP:NE1	2:J:212:GLN:OE1	2.37	0.57
9:T:53:ALA:HB3	9:T:62:ARG:HH12	1.70	0.57
2:B:273:PRO:HA	9:L:269:LEU:HD22	1.86	0.57
3:C:243:PHE:HD1	3:C:246:LYS:HZ3	1.52	0.57
3:C:604:MET:HA	3:C:639:LYS:HZ1	1.70	0.57
7:G:168:GLN:O	7:G:172:ASN:ND2	2.38	0.57
13:S:454:ILE:HD13	13:S:610:GLN:HB3	1.85	0.57
13:S:933:GLU:OE1	13:S:937:ARG:NH1	2.38	0.57
3:K:510:GLU:HA	3:K:513:ARG:HB2	1.86	0.57
10:U:357:GLU:OE2	10:U:361:GLN:NE2	2.37	0.57
10:U:441:VAL:HA	10:U:444:HIS:CD2	2.39	0.57
13:V:683:THR:O	13:V:689:ARG:NH2	2.38	0.57
6:F:249:GLN:O	6:F:253:GLN:HB2	2.04	0.57
10:M:346:GLN:HB2	10:M:350:LYS:HB2	1.87	0.57
13:S:141:GLY:HA2	13:S:148:SER:HA	1.85	0.57
13:S:719:TYR:HB2	13:S:728:ALA:HB2	1.87	0.57
1:H:239:SER:O	1:H:243:MET:HG3	2.04	0.57
3:K:320:CYS:HA	3:K:327:TYR:HE1	1.69	0.57
8:R:428:THR:HG23	8:R:467:LEU:HD13	1.86	0.57
9:T:193:ARG:HH11	10:U:371:THR:HG23	1.69	0.57
6:F:305:MET:O	6:F:309:ARG:NH1	2.37	0.57
13:S:861:GLU:OE1	13:S:880:HIS:ND1	2.37	0.57
3:K:463:ASP:HA	3:K:466:TYR:HE1	1.70	0.57
11:Y:108:GLU:HG3	12:Z:488:MET:HG3	1.86	0.57
13:V:180:ALA:HA	13:V:198:GLN:HE22	1.69	0.57
13:V:945:ALA:HB1	13:V:964:VAL:HB	1.86	0.57
3:C:502:THR:O	3:C:504:GLN:NE2	2.38	0.57
4:D:221:TRP:O	4:D:225:ILE:HB	2.04	0.57
7:G:167:LYS:O	7:G:171:TYR:CB	2.52	0.57
1:H:166:LEU:HD22	1:H:183:LEU:HD12	1.86	0.57
8:R:647:VAL:HG11	8:R:656:ARG:HA	1.87	0.57
9:T:290:MET:HG2	9:T:293:ARG:HH21	1.70	0.57
13:V:933:GLU:OE1	13:V:937:ARG:NH1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:SD	1:A:356:ARG:NH1	2.78	0.57
3:K:493:ALA:HB2	3:K:537:ILE:HA	1.87	0.57
11:Y:121:MET:SD	12:Z:499:LEU:HD13	2.44	0.57
3:C:38:TYR:O	3:C:42:ASN:ND2	2.38	0.57
3:C:607:LEU:HD22	3:C:639:LYS:HZ3	1.70	0.57
8:I:35:GLN:OE1	8:I:57:PHE:N	2.32	0.57
8:I:129:LYS:HB3	8:I:137:LEU:HD11	1.86	0.57
8:I:536:ASP:HB2	8:I:664:ARG:HG2	1.86	0.57
8:I:537:LYS:HD2	8:I:540:LEU:HD13	1.86	0.57
9:L:228:SER:OG	10:M:404:MET:SD	2.59	0.57
1:H:530:PHE:HA	1:H:533:LEU:HB2	1.87	0.57
6:P:13:LEU:O	6:P:17:SER:N	2.36	0.57
9:T:293:ARG:NH1	9:T:297:GLU:OE1	2.37	0.57
13:V:612:TYR:HE2	13:V:638:GLN:HB3	1.70	0.57
1:A:166:LEU:HD21	1:A:179:ILE:HB	1.87	0.56
2:B:69:THR:HG23	2:B:71:PRO:HD2	1.87	0.56
3:C:320:CYS:HA	3:C:327:TYR:HE1	1.70	0.56
5:E:152:GLU:HA	5:E:155:LEU:HB2	1.86	0.56
1:H:148:ASP:H	1:H:197:MET:HG3	1.69	0.56
2:J:121:THR:O	9:T:258:ARG:NH2	2.38	0.56
2:J:324:VAL:HG11	3:K:582:LEU:HD12	1.86	0.56
9:T:56:ILE:HG13	9:T:62:ARG:HH21	1.70	0.56
11:Y:121:MET:HA	11:Y:124:LYS:HG2	1.87	0.56
1:A:210:ALA:HA	1:A:213:ARG:HG2	1.85	0.56
1:A:449:TYR:CD2	1:A:454:GLU:HG3	2.40	0.56
3:C:23:LEU:O	3:C:27:GLN:N	2.36	0.56
3:C:604:MET:HG3	3:C:639:LYS:HZ2	1.69	0.56
8:I:381:ALA:O	8:I:399:TYR:OH	2.22	0.56
8:I:543:THR:HA	8:I:610:THR:HG23	1.87	0.56
13:S:549:ASN:ND2	13:S:564:MET:SD	2.78	0.56
2:J:11:ILE:HG12	2:J:58:ILE:HD12	1.87	0.56
2:J:412:HIS:O	2:J:416:GLU:N	2.38	0.56
6:P:325:GLN:HA	6:P:328:LYS:HG2	1.86	0.56
11:Y:79:LEU:O	12:Z:461:GLN:NE2	2.37	0.56
1:A:531:LYS:HD3	1:A:547:ILE:HD12	1.87	0.56
2:B:276:ALA:O	2:B:281:LYS:NZ	2.37	0.56
8:I:323:LEU:HD22	12:X:479:LYS:HZ1	1.70	0.56
13:S:142:MET:SD	13:S:144:LYS:NZ	2.78	0.56
13:S:380:THR:HA	13:S:395:PRO:HA	1.87	0.56
13:S:912:PRO:HB3	13:S:919:PHE:HE2	1.70	0.56
2:J:204:ARG:HD2	2:J:205:PRO:HD2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:434:THR:HG21	4:N:344:LEU:HD23	1.86	0.56
3:K:607:LEU:HD21	3:K:638:LEU:HB3	1.88	0.56
5:O:132:GLN:HA	5:O:140:LEU:HD11	1.87	0.56
6:P:6:TYR:HB2	7:Q:334:THR:HG21	1.87	0.56
8:R:33:ASP:OD1	9:T:7:ARG:NH2	2.27	0.56
8:R:306:LYS:HG3	8:R:307:MET:HE3	1.86	0.56
13:V:445:SER:HB2	13:V:495:LEU:O	2.05	0.56
13:V:663:PHE:HE2	13:V:696:ASN:HD21	1.52	0.56
1:A:474:ARG:HA	2:B:285:CYS:HB2	1.86	0.56
2:B:189:ALA:CB	2:B:210:TRP:HA	2.34	0.56
3:C:64:ASP:OD1	3:C:65:MET:N	2.38	0.56
3:C:169:ALA:O	3:C:173:LEU:CB	2.54	0.56
8:I:493:MET:N	8:I:493:MET:SD	2.79	0.56
10:M:458:GLN:NE2	10:M:468:GLU:OE2	2.38	0.56
8:R:468:SER:HB2	8:R:476:ARG:HA	1.86	0.56
13:V:408:ASN:HB2	13:V:411:VAL:HG22	1.87	0.56
3:C:36:LEU:HB3	3:C:53:LEU:HD11	1.87	0.56
3:C:269:ARG:NH2	3:C:273:GLU:O	2.38	0.56
8:I:219:LEU:HD21	8:I:222:GLN:HB2	1.87	0.56
10:M:379:ARG:NH1	10:M:382:GLU:OE1	2.39	0.56
13:S:901:ALA:HA	13:S:904:ALA:HB3	1.86	0.56
8:R:89:ILE:HD13	8:R:98:LYS:HB2	1.88	0.56
3:C:618:ARG:NH1	3:C:619:VAL:O	2.38	0.56
3:C:628:SER:OG	3:C:629:ARG:N	2.39	0.56
8:I:533:VAL:HG23	8:I:537:LYS:HD3	1.87	0.56
1:H:304:TYR:C	1:H:306:LEU:H	2.09	0.56
5:O:198:LYS:HG3	5:O:232:ARG:HH12	1.70	0.56
8:R:32:SER:OG	8:R:33:ASP:N	2.39	0.56
8:R:441:VAL:N	8:R:456:TRP:O	2.37	0.56
11:Y:59:VAL:HA	11:Y:62:LEU:HD12	1.87	0.56
4:D:304:LEU:O	4:D:308:PHE:HB2	2.05	0.56
4:D:321:GLU:O	4:D:325:ASP:N	2.33	0.56
10:M:357:GLU:OE2	10:M:361:GLN:NE2	2.39	0.56
8:R:699:LEU:O	8:R:703:HIS:HB2	2.05	0.56
11:Y:34:THR:HA	11:Y:37:PHE:CE2	2.40	0.56
13:V:139:ARG:HA	13:V:150:THR:HA	1.87	0.56
13:V:187:PRO:HD3	13:V:194:PRO:HB3	1.87	0.56
2:B:204:ARG:HD2	2:B:205:PRO:HD2	1.87	0.56
8:I:651:PRO:O	8:I:763:ARG:NH2	2.39	0.56
9:L:293:ARG:NH1	9:L:297:GLU:OE1	2.38	0.56
2:J:135:SER:HA	2:J:174:GLU:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:318:LEU:HA	2:J:321:LYS:HG2	1.87	0.56
5:O:151:ILE:HG12	5:O:177:LEU:HB3	1.87	0.56
8:I:11:ASN:ND2	8:I:290:GLY:O	2.39	0.56
8:I:525:CYS:SG	8:I:544:ARG:NH2	2.79	0.56
2:J:106:LEU:O	2:J:110:GLY:N	2.38	0.56
8:R:7:GLN:HE22	8:R:9:SER:HB2	1.71	0.56
8:R:23:ASN:ND2	8:R:75:THR:O	2.39	0.56
8:R:668:GLU:O	8:R:672:SER:HB3	2.06	0.56
1:A:268:LEU:HD22	2:B:304:LEU:HD21	1.87	0.56
3:C:385:THR:HA	3:C:388:ILE:HD12	1.88	0.56
5:E:198:LYS:HG3	5:E:232:ARG:HH12	1.69	0.56
8:I:265:LEU:O	11:W:75:ARG:NH2	2.38	0.56
8:I:266:ASN:HA	11:W:75:ARG:HH21	1.70	0.56
9:L:71:GLN:OE1	9:L:80:LYS:NZ	2.40	0.56
13:S:904:ALA:HB1	13:S:922:ILE:HG21	1.88	0.56
8:R:69:LYS:NZ	8:R:155:TYR:OH	2.39	0.56
8:R:138:ARG:HH22	13:V:435:ARG:HD2	1.71	0.56
8:R:587:LEU:HD23	8:R:614:THR:HG23	1.87	0.56
10:U:452:ARG:HH12	10:U:455:ARG:HH21	1.53	0.56
8:I:149:TYR:H	8:I:163:CYS:HB2	1.71	0.55
9:L:56:ILE:HG13	9:L:62:ARG:HH21	1.71	0.55
11:W:122:ILE:HD11	12:X:495:ASN:HA	1.88	0.55
8:R:487:LEU:N	8:R:501:ALA:O	2.38	0.55
3:C:401:LYS:O	3:C:405:ASN:ND2	2.39	0.55
3:C:425:TYR:O	3:C:430:LEU:N	2.35	0.55
13:S:139:ARG:HA	13:S:150:THR:HA	1.88	0.55
13:S:180:ALA:HA	13:S:198:GLN:HE22	1.71	0.55
2:J:370:ALA:O	2:J:375:ARG:NH2	2.39	0.55
3:K:63:TYR:HA	3:K:66:ALA:HB3	1.87	0.55
8:R:429:ILE:HB	8:R:444:PHE:HB2	1.87	0.55
8:R:481:ILE:HG23	8:R:485:ARG:HA	1.87	0.55
10:U:389:GLN:HA	10:U:392:HIS:CE1	2.40	0.55
13:V:697:LYS:HG3	13:V:698:GLN:HG2	1.88	0.55
1:A:565:GLU:O	9:T:231:GLN:NE2	2.39	0.55
2:B:103:ASN:HA	2:B:106:LEU:HB2	1.89	0.55
2:B:135:SER:HA	2:B:174:GLU:HA	1.88	0.55
5:E:60:LEU:HD11	5:E:83:LEU:HD13	1.88	0.55
8:I:23:ASN:ND2	8:I:75:THR:O	2.39	0.55
8:I:379:LEU:HD11	8:I:422:ILE:HG23	1.88	0.55
11:W:49:ASP:HA	11:W:52:VAL:HG22	1.89	0.55
13:S:945:ALA:HB1	13:S:964:VAL:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:220:THR:O	3:K:264:THR:OG1	2.24	0.55
7:Q:168:GLN:O	7:Q:172:ASN:ND2	2.39	0.55
10:U:384:VAL:O	10:U:388:ASN:ND2	2.40	0.55
11:Y:49:ASP:HA	11:Y:52:VAL:HG22	1.88	0.55
1:A:530:PHE:HA	1:A:533:LEU:HB2	1.89	0.55
2:B:60:VAL:HG12	2:B:87:LEU:HB3	1.87	0.55
3:C:364:GLU:OE2	3:C:368:ARG:NH2	2.39	0.55
4:D:282:VAL:HG23	4:D:286:LEU:HD12	1.87	0.55
8:I:32:SER:OG	8:I:33:ASP:N	2.40	0.55
13:S:347:LYS:HG3	13:S:348:THR:HG23	1.87	0.55
8:R:700:ALA:HA	8:R:703:HIS:HB3	1.89	0.55
2:B:324:VAL:HG11	3:C:582:LEU:HD12	1.89	0.55
3:C:480:ASN:HD21	3:C:483:ASN:HB3	1.72	0.55
8:I:468:SER:HB2	8:I:476:ARG:HA	1.88	0.55
8:I:525:CYS:HB2	8:I:544:ARG:HE	1.70	0.55
13:S:554:TYR:HE1	13:S:596:LEU:HD21	1.71	0.55
13:S:874:MET:HB3	13:S:898:ARG:HD2	1.88	0.55
2:B:30:LEU:HA	2:B:33:ARG:HG2	1.87	0.55
3:K:628:SER:OG	3:K:629:ARG:N	2.39	0.55
10:U:346:GLN:HB2	10:U:350:LYS:HB2	1.89	0.55
1:A:584:ILE:HG23	1:A:587:ARG:HH21	1.72	0.55
1:A:632:PHE:O	1:A:645:TRP:NE1	2.37	0.55
3:C:219:ASN:HA	3:C:265:ASP:HA	1.88	0.55
9:L:5:GLU:HG2	9:L:94:VAL:HG21	1.87	0.55
1:H:641:GLN:NE2	1:H:642:GLU:OE2	2.40	0.55
2:J:30:LEU:HA	2:J:33:ARG:HG2	1.88	0.55
2:J:110:GLY:CA	2:J:188:PRO:HG3	2.25	0.55
2:J:268:ASP:OD1	9:T:272:TYR:OH	2.15	0.55
13:V:618:THR:HG23	13:V:619:LEU:HD12	1.88	0.55
13:S:652:TYR:HB3	13:S:663:PHE:HB3	1.87	0.55
2:J:186:GLN:O	2:J:188:PRO:HD2	2.07	0.55
3:K:38:TYR:O	3:K:42:ASN:ND2	2.40	0.55
7:Q:192:LEU:O	7:Q:196:ASN:HB2	2.05	0.55
7:Q:298:LYS:HA	7:Q:301:GLN:HG3	1.89	0.55
8:R:2:ARG:NE	8:R:261:SER:OG	2.36	0.55
13:V:549:ASN:ND2	13:V:564:MET:SD	2.80	0.55
13:V:716:ILE:HA	13:V:728:ALA:HB1	1.89	0.55
1:A:447:PHE:CE2	2:B:286:LEU:HB2	2.42	0.55
2:B:106:LEU:O	2:B:110:GLY:N	2.40	0.55
8:I:664:ARG:HH21	8:I:667:PRO:HA	1.72	0.55
9:T:253:GLN:HA	9:T:256:LEU:HG	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:323:LYS:HG3	13:V:335:TYR:HB2	1.89	0.55
13:V:811:ALA:O	13:V:838:ARG:NH1	2.40	0.55
2:B:133:LEU:HD22	2:B:176:VAL:HA	1.89	0.55
2:B:370:ALA:O	2:B:375:ARG:NH2	2.40	0.55
6:F:180:LYS:HA	6:F:183:LEU:HD12	1.89	0.55
8:I:28:LEU:HD22	8:I:40:TRP:HB2	1.89	0.55
13:S:422:ILE:HD11	13:S:475:LEU:HG	1.89	0.55
2:B:380:THR:OG1	4:D:234:ALA:O	2.22	0.54
3:C:467:LYS:HD3	3:C:502:THR:HG22	1.89	0.54
6:F:210:LEU:HD12	6:F:213:GLN:HE21	1.72	0.54
1:H:449:TYR:CD2	1:H:454:GLU:HG3	2.42	0.54
2:J:189:ALA:CB	2:J:210:TRP:HA	2.37	0.54
8:R:89:ILE:HG22	8:R:97:GLU:HB2	1.89	0.54
2:B:176:VAL:HG11	2:B:231:TRP:HB3	1.87	0.54
2:B:318:LEU:HA	2:B:321:LYS:HG2	1.89	0.54
2:B:434:THR:HA	4:D:262:LYS:HE2	1.89	0.54
3:C:63:TYR:HA	3:C:66:ALA:HB3	1.89	0.54
5:E:25:PRO:O	5:E:49:ARG:NH1	2.38	0.54
10:M:389:GLN:HA	10:M:392:HIS:CE1	2.41	0.54
1:H:358:ARG:HA	1:H:361:ILE:HD12	1.90	0.54
1:H:515:LEU:HD22	1:H:519:ARG:HH22	1.72	0.54
8:R:265:LEU:O	11:Y:75:ARG:NH2	2.39	0.54
10:U:310:LEU:O	10:U:314:HIS:ND1	2.39	0.54
11:Y:52:VAL:HA	11:Y:55:ILE:HG12	1.89	0.54
1:A:143:ASP:HA	1:A:149:ILE:HD11	1.89	0.54
1:A:264:ARG:HD2	2:B:304:LEU:HA	1.89	0.54
1:A:352:LYS:N	1:A:354:GLU:OE1	2.40	0.54
2:B:268:ASP:OD1	9:L:272:TYR:OH	2.19	0.54
2:B:433:GLN:NE2	4:D:258:GLU:OE2	2.39	0.54
5:E:152:GLU:HG3	5:E:155:LEU:HD22	1.88	0.54
5:E:294:HIS:O	5:E:297:ARG:NH1	2.39	0.54
8:I:3:LEU:HD11	8:I:252:LEU:HD22	1.89	0.54
8:I:690:LEU:HD21	13:V:695:LEU:HD11	1.89	0.54
13:S:498:ASN:HD21	13:S:502:THR:H	1.54	0.54
3:K:467:LYS:HD3	3:K:502:THR:HG22	1.89	0.54
8:R:247:PHE:HA	8:R:270:SER:HA	1.89	0.54
11:Y:123:GLN:NE2	11:Y:127:ASP:OD2	2.40	0.54
9:L:33:GLU:HB3	9:L:56:ILE:HG21	1.89	0.54
1:H:482:VAL:O	1:H:486:ARG:N	2.36	0.54
2:J:376:LEU:HD22	2:J:400:LEU:HD21	1.89	0.54
13:V:376:ARG:NH2	13:V:397:ASP:OD1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:89:ILE:HD13	8:I:98:LYS:HB2	1.90	0.54
13:S:228:ASP:OD1	13:S:232:ARG:N	2.35	0.54
2:J:405:GLN:HG2	2:J:413:VAL:HB	1.89	0.54
5:O:125:ARG:HG3	5:O:152:GLU:HB3	1.89	0.54
7:Q:167:LYS:O	7:Q:171:TYR:CB	2.56	0.54
1:A:371:GLN:O	1:A:374:SER:N	2.40	0.54
2:B:343:LEU:HD21	3:C:317:LEU:HD21	1.88	0.54
2:B:412:HIS:O	2:B:416:GLU:N	2.40	0.54
5:E:77:LEU:HD21	5:E:101:LEU:HG	1.89	0.54
8:I:529:TYR:HE2	8:I:618:MET:HB3	1.70	0.54
9:L:253:GLN:HA	9:L:256:LEU:HG	1.90	0.54
9:L:284:GLU:OE1	9:L:288:LYS:NZ	2.37	0.54
13:S:376:ARG:NH2	13:S:397:ASP:OD1	2.41	0.54
1:H:264:ARG:HD2	2:J:304:LEU:HA	1.90	0.54
1:H:305:ALA:HB3	9:T:299:LEU:HD22	1.90	0.54
1:H:474:ARG:HA	2:J:285:CYS:HB2	1.89	0.54
6:F:11:LEU:HG	6:F:18:TYR:HB2	1.90	0.54
8:I:434:GLN:HA	8:I:438:GLY:HA2	1.90	0.54
1:H:479:LYS:HB3	1:H:495:LEU:HD13	1.90	0.54
2:J:422:ALA:HB1	2:J:425:LYS:HE2	1.90	0.54
2:J:451:GLN:HG2	4:N:316:GLN:HB3	1.88	0.54
11:Y:103:ARG:NH1	11:Y:107:GLU:OE1	2.40	0.54
1:A:236:LYS:O	1:A:239:SER:OG	2.21	0.54
5:E:37:ARG:NH2	5:E:39:TYR:OH	2.40	0.54
5:E:56:ASP:HB3	5:E:59:ASN:HB2	1.90	0.54
9:L:110:LYS:HE3	12:X:436:MET:SD	2.47	0.54
13:S:1025:LEU:O	13:S:1028:GLN:NE2	2.40	0.54
2:J:419:ARG:HD3	4:N:344:LEU:HD13	1.88	0.54
3:K:463:ASP:N	3:K:463:ASP:OD1	2.41	0.54
3:K:480:ASN:HD21	3:K:483:ASN:HB3	1.73	0.54
3:K:518:GLU:HA	3:K:521:ARG:HE	1.73	0.54
8:R:87:VAL:HB	8:R:100:ILE:HG13	1.89	0.54
8:R:185:HIS:ND1	8:R:207:ASP:OD2	2.41	0.54
8:R:434:GLN:HA	8:R:438:GLY:HA2	1.90	0.54
9:T:240:GLU:HA	9:T:243:ARG:HD3	1.89	0.54
9:T:293:ARG:HH22	9:T:294:LEU:HG	1.72	0.54
1:A:305:ALA:HB3	9:L:299:LEU:HD22	1.90	0.54
2:B:57:HIS:HA	2:B:79:PHE:HZ	1.73	0.54
6:F:125:MET:O	6:F:130:ASN:ND2	2.41	0.54
9:L:243:ARG:NH2	10:M:414:ASP:O	2.40	0.54
11:W:66:LYS:HE3	11:W:70:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:471:TYR:HB3	6:P:182:ARG:HH22	1.72	0.54
5:O:7:ARG:HH12	5:O:256:ASP:HB3	1.72	0.54
8:R:537:LYS:HD2	8:R:540:LEU:HD13	1.89	0.54
8:R:591:ILE:HG21	8:R:618:MET:HG3	1.89	0.54
11:Y:94:LEU:HG	11:Y:98:GLN:HE22	1.73	0.54
13:V:373:LEU:HD23	13:V:386:LEU:HG	1.90	0.54
13:V:513:LEU:HB2	13:V:527:LEU:HB2	1.90	0.54
4:D:212:GLU:OE1	4:D:214:LYS:NZ	2.40	0.54
11:W:83:ARG:NH2	11:W:87:GLN:OE1	2.38	0.54
13:S:325:HIS:HB3	13:S:333:PHE:HB2	1.89	0.54
3:K:57:TYR:HA	3:K:60:THR:HG22	1.90	0.54
3:K:637:MET:O	3:K:640:LYS:NZ	2.38	0.54
6:P:144:ALA:O	6:P:147:GLN:NE2	2.41	0.54
8:R:729:ARG:HG2	8:R:732:GLN:HE21	1.73	0.54
9:T:214:GLU:HG3	9:T:217:LYS:HE3	1.89	0.54
4:D:246:ILE:HG13	4:D:304:LEU:HD22	1.89	0.53
5:E:13:ARG:HB3	5:E:250:SER:HA	1.89	0.53
5:E:176:ARG:HG3	5:E:177:LEU:HG	1.89	0.53
13:S:82:ILE:HB	13:S:90:PHE:HB2	1.89	0.53
13:S:267:ARG:NH1	13:S:269:TYR:OH	2.42	0.53
1:H:678:GLU:HA	1:H:681:ARG:HE	1.72	0.53
2:J:141:ARG:HH22	2:J:151:LEU:HD21	1.72	0.53
13:V:554:TYR:HE1	13:V:596:LEU:HD21	1.73	0.53
13:V:846:ILE:HB	13:V:863:GLU:HG3	1.90	0.53
1:A:178:GLN:HE21	1:A:181:LEU:HB3	1.73	0.53
1:A:304:TYR:CG	1:A:376:LYS:HE3	2.43	0.53
1:A:527:LEU:O	1:A:531:LYS:HG2	2.09	0.53
2:B:379:LEU:HD23	2:B:399:ILE:HD11	1.90	0.53
8:I:470:ALA:H	8:I:509:TRP:HE1	1.57	0.53
1:H:527:LEU:O	1:H:531:LYS:HG2	2.09	0.53
3:K:364:GLU:OE2	3:K:368:ARG:NH2	2.39	0.53
13:V:546:SER:OG	13:V:547:ARG:N	2.41	0.53
6:F:144:ALA:O	6:F:147:GLN:NE2	2.40	0.53
8:I:730:PHE:O	8:I:734:ASN:ND2	2.32	0.53
6:P:13:LEU:HB3	6:P:15:PRO:HD2	1.90	0.53
7:Q:250:MET:O	7:Q:254:GLN:HB2	2.08	0.53
8:R:536:ASP:HB2	8:R:664:ARG:HG2	1.88	0.53
9:T:175:ASP:HB3	9:T:177:VAL:HG22	1.91	0.53
10:U:453:ASN:HA	10:U:456:LEU:HD12	1.90	0.53
13:V:960:ALA:HA	13:V:963:ARG:HE	1.74	0.53
1:A:293:HIS:HA	1:A:319:LEU:HD21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ARG:NH2	2:B:233:ASP:OD1	2.41	0.53
9:L:214:GLU:HG3	9:L:217:LYS:HE3	1.89	0.53
1:H:670:HIS:HE1	1:H:676:ASN:HB3	1.73	0.53
5:O:43:ILE:HA	5:O:46:LEU:HB2	1.91	0.53
6:P:151:GLU:HA	6:P:154:LYS:HG2	1.89	0.53
8:R:87:VAL:N	8:R:100:ILE:O	2.40	0.53
13:V:442:TYR:O	13:V:495:LEU:HG	2.09	0.53
13:V:901:ALA:HA	13:V:904:ALA:HB3	1.90	0.53
5:E:220:ALA:HA	5:E:246:LEU:HD11	1.90	0.53
8:I:87:VAL:HB	8:I:100:ILE:HG13	1.89	0.53
12:X:488:MET:O	12:X:492:ILE:HG13	2.09	0.53
13:S:310:SER:HB2	13:S:314:ALA:H	1.73	0.53
1:H:483:LEU:HB3	1:H:488:ASP:HB2	1.90	0.53
1:H:632:PHE:O	1:H:645:TRP:NE1	2.39	0.53
2:J:51:ASP:OD1	2:J:52:THR:N	2.42	0.53
3:K:169:ALA:O	3:K:173:LEU:CB	2.57	0.53
8:R:107:CYS:HA	8:R:123:GLY:HA2	1.91	0.53
8:R:350:ALA:HB2	8:R:378:LEU:HD22	1.91	0.53
11:Y:47:LEU:HA	11:Y:50:LYS:HE3	1.91	0.53
13:V:729:ILE:HG12	13:V:743:LEU:HD11	1.91	0.53
2:B:182:THR:HG22	2:B:206:VAL:HG12	1.90	0.53
2:B:186:GLN:O	2:B:188:PRO:HD2	2.09	0.53
8:I:39:LYS:HG3	8:I:47:GLU:HB2	1.90	0.53
9:L:128:LEU:HD22	12:X:417:HIS:CG	2.43	0.53
1:H:189:PHE:HE2	2:J:309:THR:HG23	1.74	0.53
2:J:114:ASN:OD1	2:J:204:ARG:NH2	2.41	0.53
5:O:63:LEU:O	5:O:67:TYR:N	2.41	0.53
5:O:152:GLU:HG3	5:O:155:LEU:HD22	1.90	0.53
6:P:125:MET:O	6:P:130:ASN:ND2	2.42	0.53
13:V:310:SER:HB2	13:V:314:ALA:H	1.73	0.53
1:A:358:ARG:HA	1:A:361:ILE:HD12	1.91	0.53
1:A:567:LEU:O	1:A:571:VAL:N	2.28	0.53
8:I:485:ARG:O	8:I:504:CYS:N	2.39	0.53
9:L:265:LEU:O	9:L:269:LEU:HD12	2.08	0.53
13:S:89:VAL:HB	13:S:110:PHE:HB2	1.90	0.53
13:S:184:PHE:HD1	13:S:196:SER:HB2	1.73	0.53
13:S:187:PRO:HD3	13:S:194:PRO:HB3	1.90	0.53
13:S:636:ALA:HB2	13:S:655:LEU:HD11	1.89	0.53
1:H:371:GLN:O	1:H:374:SER:N	2.41	0.53
3:K:36:LEU:HB3	3:K:53:LEU:HD11	1.89	0.53
6:P:220:LEU:O	6:P:224:ILE:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:130:ILE:HD11	8:R:141:LEU:HB2	1.91	0.53
13:V:325:HIS:HB3	13:V:333:PHE:HB2	1.91	0.53
1:A:193:HIS:HA	1:A:196:HIS:HD1	1.74	0.53
7:G:166:ARG:HH21	7:G:170:GLN:HE22	1.55	0.53
8:I:87:VAL:N	8:I:100:ILE:O	2.41	0.53
9:L:243:ARG:O	9:L:246:GLY:N	2.42	0.53
10:M:451:LEU:HA	10:M:454:LYS:HG2	1.90	0.53
13:S:223:ARG:NE	13:S:236:SER:OG	2.39	0.53
13:S:546:SER:OG	13:S:547:ARG:N	2.42	0.53
3:K:468:GLU:HA	3:K:471:ARG:HG2	1.91	0.53
4:N:282:VAL:HG23	4:N:286:LEU:HD12	1.91	0.53
8:R:111:ARG:HG3	8:R:153:TRP:HD1	1.73	0.53
8:R:604:ARG:HH22	8:R:635:ILE:HG22	1.74	0.53
2:B:419:ARG:HD3	4:D:344:LEU:HD13	1.89	0.53
8:I:432:LEU:HD23	8:I:434:GLN:HG3	1.90	0.53
1:H:283:PHE:O	1:H:287:MET:HG2	2.08	0.53
3:K:58:TYR:O	3:K:63:TYR:OH	2.26	0.53
3:K:382:ARG:HA	3:K:385:THR:HG22	1.89	0.53
8:R:81:ALA:HA	8:R:87:VAL:HA	1.91	0.53
8:R:394:ILE:O	8:R:408:ARG:NH2	2.41	0.53
9:T:128:LEU:HD22	12:Z:417:HIS:CG	2.44	0.53
3:C:607:LEU:HD21	3:C:638:LEU:HB3	1.91	0.53
3:C:637:MET:O	3:C:640:LYS:NZ	2.38	0.53
6:F:203:TYR:OH	7:G:207:PRO:O	2.25	0.53
9:L:243:ARG:HH22	10:M:415:ALA:HA	1.74	0.53
3:K:599:SER:HA	3:K:602:GLU:HG2	1.91	0.53
2:B:194:SER:HA	2:B:205:PRO:HA	1.91	0.52
3:C:110:HIS:HB3	3:C:113:ALA:HB3	1.90	0.52
5:E:129:HIS:HA	5:E:132:GLN:HE21	1.74	0.52
8:I:598:LYS:HD2	8:I:602:LEU:HD23	1.91	0.52
9:L:240:GLU:HA	9:L:243:ARG:HD3	1.90	0.52
3:K:541:ILE:HG23	3:K:557:ARG:HE	1.74	0.52
5:O:155:LEU:HA	5:O:174:TYR:HE1	1.74	0.52
13:V:719:TYR:HB2	13:V:728:ALA:HB2	1.91	0.52
6:F:13:LEU:HB3	6:F:15:PRO:HD2	1.91	0.52
13:S:849:ALA:O	13:S:850:ARG:HD3	2.09	0.52
1:H:130:GLU:HG3	1:H:134:HIS:CE1	2.44	0.52
6:P:315:THR:O	6:P:319:ASN:ND2	2.42	0.52
8:R:63:TYR:HB3	8:R:75:THR:HA	1.90	0.52
8:R:109:SER:O	8:R:121:THR:OG1	2.26	0.52
9:T:204:ARG:NE	10:U:378:ASN:HB3	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:399:ASP:N	13:V:399:ASP:OD1	2.42	0.52
1:A:515:LEU:HD22	1:A:519:ARG:HH22	1.75	0.52
6:F:41:PHE:HA	6:F:44:ILE:HG12	1.90	0.52
8:I:111:ARG:HG3	8:I:153:TRP:HD1	1.74	0.52
8:I:373:ASP:HB3	8:I:389:ASP:HB2	1.91	0.52
9:L:277:GLN:HA	9:L:280:MET:HG2	1.91	0.52
13:S:931:ALA:HB1	13:S:934:GLU:HB2	1.90	0.52
1:H:542:GLU:OE2	1:H:546:GLN:NE2	2.42	0.52
3:K:508:ALA:HA	3:K:511:LEU:HB2	1.90	0.52
3:K:618:ARG:NH1	3:K:619:VAL:O	2.41	0.52
4:N:246:ILE:HG23	4:N:249:LEU:HD22	1.90	0.52
5:O:56:ASP:HB3	5:O:59:ASN:HB2	1.92	0.52
8:R:28:LEU:HD22	8:R:40:TRP:HB2	1.91	0.52
8:R:131:TRP:HA	8:R:137:LEU:HA	1.90	0.52
8:R:236:ALA:HB3	8:R:241:LEU:HB3	1.91	0.52
9:T:297:GLU:HA	9:T:300:ARG:HG2	1.91	0.52
10:U:452:ARG:NH1	10:U:455:ARG:HH21	2.06	0.52
13:V:545:GLN:NE2	13:V:546:SER:O	2.42	0.52
13:V:723:HIS:ND1	13:V:723:HIS:O	2.39	0.52
1:A:511:TYR:HD2	2:B:283:LYS:HB2	1.75	0.52
2:B:88:ILE:HB	2:B:220:VAL:HG12	1.91	0.52
3:C:200:LEU:HD11	3:C:245:LEU:HG	1.92	0.52
7:G:192:LEU:O	7:G:196:ASN:HB2	2.10	0.52
8:I:130:ILE:HD11	8:I:141:LEU:HB2	1.92	0.52
13:S:550:LEU:HD21	13:S:571:VAL:HG21	1.92	0.52
13:S:580:ARG:HA	13:S:601:ILE:HD13	1.90	0.52
2:J:372:GLU:HA	2:J:375:ARG:HG2	1.90	0.52
8:R:389:ASP:OD1	8:R:395:GLN:NE2	2.42	0.52
3:C:432:SER:O	3:C:435:GLU:HG2	2.10	0.52
3:C:480:ASN:ND2	3:C:483:ASN:O	2.42	0.52
8:I:487:LEU:N	8:I:501:ALA:O	2.40	0.52
8:I:644:VAL:HG21	13:V:724:ARG:HH21	1.74	0.52
12:X:432:ASP:O	12:X:436:MET:HG2	2.10	0.52
13:S:511:ARG:NH1	13:S:530:CYS:O	2.38	0.52
2:J:11:ILE:HD12	2:J:34:LEU:HD21	1.92	0.52
5:O:11:ALA:HB1	5:O:217:PRO:HB2	1.92	0.52
8:R:195:SER:HB3	8:R:235:TRP:CE2	2.44	0.52
8:R:319:VAL:O	8:R:328:ASP:N	2.36	0.52
9:T:243:ARG:O	9:T:246:GLY:N	2.42	0.52
13:V:141:GLY:HA2	13:V:148:SER:HA	1.90	0.52
13:V:846:ILE:HA	13:V:849:ALA:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:LEU:HD11	2:B:86:ILE:HG13	1.91	0.52
3:C:317:LEU:HA	3:C:320:CYS:HB2	1.92	0.52
5:E:274:LEU:HG	5:E:307:LEU:HD13	1.91	0.52
5:E:301:VAL:HA	5:E:304:ALA:HB3	1.91	0.52
13:S:828:ARG:HE	13:S:830:SER:HB3	1.74	0.52
13:S:911:ASP:OD1	13:S:911:ASP:N	2.43	0.52
1:H:280:LEU:CD2	1:H:302:CYS:HB3	2.39	0.52
1:H:474:ARG:NH2	1:H:508:GLU:OE1	2.42	0.52
1:H:493:ARG:O	1:H:497:ASN:ND2	2.43	0.52
5:O:5:LYS:HE2	5:O:257:HIS:CE1	2.45	0.52
6:P:48:HIS:HE2	6:P:65:LEU:HD21	1.73	0.52
8:R:85:GLY:O	8:R:102:GLY:N	2.35	0.52
2:B:112:SER:O	2:B:184:SER:N	2.42	0.52
6:F:315:THR:O	6:F:319:ASN:ND2	2.43	0.52
8:I:18:ALA:HB2	9:L:7:ARG:HH12	1.74	0.52
8:I:394:ILE:O	8:I:408:ARG:NH2	2.42	0.52
8:I:733:MET:HA	8:I:736:SER:HB3	1.91	0.52
11:W:115:LYS:O	12:X:495:ASN:ND2	2.43	0.52
2:J:425:LYS:HD3	4:N:286:LEU:HB3	1.91	0.52
4:N:309:LYS:O	4:N:315:ARG:NH1	2.40	0.52
8:R:589:ASP:O	8:R:593:LYS:NZ	2.43	0.52
1:A:251:ILE:HG21	1:A:255:ALA:HB3	1.91	0.52
2:B:413:VAL:HA	2:B:416:GLU:HB2	1.91	0.52
8:I:89:ILE:HG22	8:I:97:GLU:HB2	1.92	0.52
8:I:485:ARG:NH2	8:I:503:MET:O	2.43	0.52
8:I:706:HIS:HA	8:I:747:LYS:HD3	1.91	0.52
10:M:309:HIS:HE1	11:W:38:ILE:HG12	1.75	0.52
1:H:550:THR:HA	1:H:553:MET:SD	2.50	0.52
5:O:60:LEU:HD11	5:O:83:LEU:HD13	1.91	0.52
6:P:321:ILE:HA	6:P:324:ILE:HG12	1.91	0.52
13:V:187:PRO:HB3	13:V:194:PRO:HD3	1.91	0.52
3:C:482:ASP:OD1	3:C:483:ASN:N	2.43	0.52
5:E:34:LEU:HD12	5:E:35:THR:HG23	1.90	0.52
5:E:63:LEU:O	5:E:67:TYR:N	2.42	0.52
6:F:286:ARG:HD2	7:G:296:LEU:HB2	1.91	0.52
9:L:260:ARG:NH2	10:M:431:GLU:OE1	2.38	0.52
1:H:139:LYS:NZ	1:H:151:SER:O	2.43	0.52
5:O:220:ALA:HA	5:O:246:LEU:HD11	1.92	0.52
9:T:74:LEU:O	10:U:306:TRP:NE1	2.41	0.52
13:V:342:ILE:HG12	13:V:353:VAL:HG13	1.92	0.52
8:I:81:ALA:HA	8:I:87:VAL:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:107:CYS:HA	8:I:123:GLY:HA2	1.92	0.52
8:I:206:GLU:HA	8:I:229:PRO:HB3	1.92	0.52
8:I:714:ARG:O	8:I:714:ARG:NH1	2.41	0.52
13:S:443:LEU:O	13:S:495:LEU:HD11	2.10	0.52
1:H:240:ALA:HA	1:H:243:MET:CE	2.40	0.52
2:J:204:ARG:NH1	2:J:205:PRO:O	2.43	0.52
6:P:41:PHE:HA	6:P:44:ILE:HG12	1.91	0.52
8:R:68:LYS:HG3	8:R:73:GLY:HA2	1.92	0.52
8:R:608:ASP:HB3	8:R:611:MET:HG2	1.92	0.52
12:Z:406:SER:O	12:Z:410:GLU:HG2	2.10	0.52
1:A:636:SER:HB3	1:A:645:TRP:HD1	1.75	0.51
3:C:382:ARG:HA	3:C:385:THR:HG22	1.91	0.51
8:I:124:GLU:HG3	9:L:2:SER:HB2	1.91	0.51
8:I:558:ILE:HA	8:I:568:VAL:HG12	1.92	0.51
9:L:46:TYR:CZ	9:L:104:LEU:HB2	2.45	0.51
13:S:555:SER:N	13:S:627:GLU:OE1	2.30	0.51
7:Q:215:PHE:O	7:Q:219:LYS:HB2	2.10	0.51
9:T:71:GLN:OE1	9:T:80:LYS:NZ	2.43	0.51
13:V:383:MET:O	13:V:392:SER:N	2.39	0.51
2:B:110:GLY:CA	2:B:188:PRO:HG3	2.28	0.51
2:B:397:GLY:HA2	2:B:400:LEU:HD12	1.92	0.51
3:C:401:LYS:HA	3:C:404:ILE:HG12	1.90	0.51
5:E:132:GLN:HB2	5:E:160:ILE:HD11	1.93	0.51
5:E:220:ALA:O	5:E:224:ASN:HB2	2.10	0.51
8:I:109:SER:O	8:I:121:THR:OG1	2.27	0.51
8:I:428:THR:HG23	8:I:467:LEU:HD13	1.91	0.51
8:I:433:ASP:OD1	8:I:435:GLN:NE2	2.43	0.51
3:K:269:ARG:NH2	3:K:273:GLU:O	2.43	0.51
3:K:385:THR:HA	3:K:388:ILE:HD12	1.91	0.51
13:V:443:LEU:O	13:V:495:LEU:HD11	2.09	0.51
13:V:536:VAL:HG11	13:V:541:VAL:HB	1.92	0.51
1:A:312:MET:N	1:A:312:MET:SD	2.83	0.51
3:C:58:TYR:O	3:C:63:TYR:OH	2.22	0.51
3:C:310:GLU:O	3:C:314:ASN:ND2	2.44	0.51
3:C:373:LEU:O	3:C:377:HIS:ND1	2.35	0.51
6:F:324:ILE:HA	6:F:327:ARG:HG2	1.93	0.51
13:S:442:TYR:O	13:S:495:LEU:HG	2.11	0.51
6:P:140:GLU:HA	6:P:143:LYS:HE2	1.92	0.51
6:P:210:LEU:HD12	6:P:213:GLN:HE21	1.76	0.51
8:R:82:CYS:SG	8:R:83:THR:N	2.81	0.51
13:V:889:LYS:HA	13:V:892:LYS:HE2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:911:ASP:OD1	13:V:911:ASP:N	2.42	0.51
3:C:518:GLU:HA	3:C:521:ARG:HE	1.74	0.51
8:I:441:VAL:N	8:I:456:TRP:O	2.42	0.51
13:S:383:MET:O	13:S:392:SER:N	2.42	0.51
13:S:449:GLN:HB3	13:S:458:SER:HB2	1.92	0.51
1:H:511:TYR:HD2	2:J:283:LYS:HB2	1.76	0.51
5:O:223:VAL:HA	5:O:226:LYS:HE2	1.93	0.51
8:R:115:ASP:OD1	8:R:115:ASP:N	2.41	0.51
13:V:228:ASP:OD1	13:V:232:ARG:N	2.38	0.51
1:A:259:ARG:NH1	1:A:288:ASP:OD1	2.43	0.51
2:B:67:LYS:NZ	2:B:101:ASN:OD1	2.44	0.51
6:F:23:LEU:O	6:F:26:THR:OG1	2.28	0.51
7:G:209:TYR:O	7:G:213:GLN:NE2	2.33	0.51
8:I:602:LEU:HB2	8:I:606:ILE:HD13	1.93	0.51
11:W:109:GLN:HA	11:W:112:ILE:HD12	1.92	0.51
11:W:124:LYS:HD2	11:W:125:LEU:HG	1.92	0.51
13:S:799:ASP:HB3	13:S:802:LEU:H	1.76	0.51
1:H:449:TYR:CZ	1:H:454:GLU:HG3	2.46	0.51
1:H:602:HIS:HB2	1:H:611:VAL:HG11	1.91	0.51
6:P:181:GLU:OE2	6:P:182:ARG:NH1	2.43	0.51
3:C:15:GLN:OE1	3:C:18:GLN:NE2	2.40	0.51
5:E:422:ASP:OD1	5:E:422:ASP:N	2.43	0.51
8:I:130:ILE:HG22	8:I:138:ARG:HB3	1.93	0.51
1:H:531:LYS:HD3	1:H:547:ILE:HD12	1.92	0.51
7:Q:167:LYS:O	7:Q:171:TYR:HB3	2.10	0.51
8:R:379:LEU:HD11	8:R:422:ILE:HG23	1.92	0.51
8:R:381:ALA:O	8:R:399:TYR:OH	2.27	0.51
8:R:543:THR:HA	8:R:610:THR:HG23	1.93	0.51
8:R:567:LEU:HD11	8:R:575:LEU:HD12	1.92	0.51
6:F:83:LEU:HA	6:F:86:GLN:HG3	1.93	0.51
1:H:293:HIS:HA	1:H:319:LEU:HD21	1.93	0.51
3:K:341:ALA:HB1	3:K:345:LEU:HD11	1.93	0.51
6:P:11:LEU:HG	6:P:18:TYR:HB2	1.92	0.51
7:Q:143:LEU:O	7:Q:147:ARG:HG2	2.10	0.51
8:R:662:VAL:HG21	8:R:674:LEU:HD22	1.92	0.51
1:A:268:LEU:O	1:A:272:ARG:HG2	2.10	0.51
1:A:449:TYR:CZ	1:A:454:GLU:HG3	2.46	0.51
2:B:376:LEU:HD22	2:B:400:LEU:HD21	1.93	0.51
3:C:132:ARG:NH2	3:C:156:GLU:OE1	2.44	0.51
8:I:559:GLN:HB2	8:I:567:LEU:HG	1.92	0.51
9:L:136:ILE:HD12	12:X:410:GLU:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:4:ARG:O	13:S:319:ASP:N	2.40	0.51
13:V:352:ILE:HD11	13:V:391:LEU:HD21	1.93	0.51
13:V:360:TYR:CE2	13:V:379:TYR:HB3	2.46	0.51
3:C:213:GLU:HG2	3:C:214:LEU:HG	1.92	0.51
8:I:539:LEU:HD12	8:I:542:LYS:HD3	1.92	0.51
13:S:719:TYR:HE2	13:S:731:VAL:HG11	1.74	0.51
13:S:837:ARG:HG3	13:S:842:TYR:HB3	1.92	0.51
13:S:881:PHE:HA	13:S:884:SER:HB3	1.93	0.51
1:H:178:GLN:HE21	1:H:181:LEU:HB3	1.75	0.51
1:H:559:ASN:HA	1:H:562:LYS:HE2	1.92	0.51
2:J:403:LYS:HE2	4:N:326:GLY:HA2	1.93	0.51
3:K:231:SER:HB3	3:K:234:LEU:HD13	1.93	0.51
9:T:104:LEU:C	9:T:106:LYS:H	2.13	0.51
2:B:120:ARG:NH1	2:B:128:HIS:O	2.44	0.51
3:C:176:GLN:NE2	5:E:275:GLN:OE1	2.43	0.51
3:C:282:SER:HA	3:C:285:ILE:HG22	1.92	0.51
3:C:463:ASP:HA	3:C:466:TYR:HE1	1.76	0.51
13:S:231:GLY:O	13:S:232:ARG:NH1	2.44	0.51
13:S:513:LEU:HB2	13:S:527:LEU:HB2	1.93	0.51
1:H:304:TYR:O	1:H:304:TYR:HD1	1.94	0.51
1:H:304:TYR:O	1:H:306:LEU:N	2.44	0.51
3:K:401:LYS:O	3:K:405:ASN:ND2	2.44	0.51
5:O:461:TYR:HH	5:O:496:TYR:HH	1.56	0.51
8:R:251:GLN:HG3	8:R:262:LYS:HA	1.93	0.51
10:U:314:HIS:HA	10:U:317:LYS:HG2	1.93	0.51
13:V:493:ASP:OD1	13:V:493:ASP:N	2.44	0.51
1:A:559:ASN:HA	1:A:562:LYS:HE2	1.93	0.50
2:B:27:PHE:HB2	2:B:31:PHE:HE2	1.76	0.50
3:C:450:VAL:HG22	3:C:451:TRP:H	1.76	0.50
6:F:151:GLU:HA	6:F:154:LYS:HG2	1.93	0.50
8:I:2:ARG:NE	8:I:261:SER:OG	2.42	0.50
8:I:131:TRP:HA	8:I:137:LEU:HA	1.93	0.50
8:I:247:PHE:HA	8:I:270:SER:HA	1.93	0.50
13:S:667:VAL:HG12	13:S:691:MET:HG2	1.93	0.50
1:H:437:VAL:HG13	1:H:440:ARG:HH21	1.76	0.50
2:J:397:GLY:HA2	2:J:400:LEU:HD12	1.93	0.50
3:K:19:THR:O	3:K:23:LEU:HB2	2.10	0.50
3:K:480:ASN:ND2	3:K:483:ASN:O	2.44	0.50
3:K:559:ILE:HG21	3:K:602:GLU:HB2	1.93	0.50
5:O:197:CYS:SG	5:O:229:ASN:ND2	2.83	0.50
6:P:169:LEU:HA	6:P:172:LYS:HE2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:7:LYS:HE2	13:V:9:ILE:HG13	1.92	0.50
13:V:142:MET:SD	13:V:144:LYS:NZ	2.85	0.50
13:V:422:ILE:HG13	13:V:431:LEU:HB2	1.93	0.50
3:C:57:TYR:HA	3:C:60:THR:HG22	1.93	0.50
7:G:143:LEU:O	7:G:147:ARG:HG2	2.11	0.50
8:I:80:VAL:O	8:I:88:LYS:N	2.42	0.50
8:I:598:LYS:HE2	12:X:496:ASP:HB3	1.92	0.50
10:M:316:HIS:HB3	11:W:31:GLN:HE22	1.75	0.50
13:S:536:VAL:HG11	13:S:541:VAL:HB	1.93	0.50
1:H:434:GLU:O	1:H:438:LYS:N	2.42	0.50
1:H:508:GLU:OE2	1:H:512:ASN:ND2	2.45	0.50
2:J:60:VAL:HG12	2:J:87:LEU:HB3	1.92	0.50
4:N:266:MET:HE2	4:N:271:VAL:HA	1.91	0.50
6:P:28:LYS:HE2	6:P:36:LEU:HD22	1.92	0.50
8:R:18:ALA:HB2	9:T:7:ARG:HH12	1.76	0.50
8:R:202:ILE:HG22	8:R:212:VAL:HG22	1.92	0.50
8:R:619:ALA:O	8:R:623:LYS:N	2.44	0.50
11:Y:66:LYS:HE3	11:Y:70:ILE:HD11	1.92	0.50
8:I:448:GLN:O	8:I:450:ARG:NH1	2.44	0.50
8:I:460:LEU:HB3	8:I:482:ASP:HB2	1.93	0.50
13:S:292:TYR:HD2	13:S:311:MET:HG3	1.76	0.50
13:S:713:ASP:OD1	13:S:713:ASP:N	2.42	0.50
13:S:729:ILE:HG12	13:S:743:LEU:HD11	1.93	0.50
13:V:292:TYR:HD2	13:V:311:MET:HG3	1.76	0.50
13:V:713:ASP:OD1	13:V:713:ASP:N	2.42	0.50
13:V:758:GLU:H	13:V:780:GLY:HA3	1.76	0.50
2:B:273:PRO:HA	9:L:269:LEU:HD13	1.93	0.50
2:B:403:LYS:HE2	4:D:326:GLY:HA2	1.94	0.50
8:I:567:LEU:HD11	8:I:575:LEU:HD12	1.93	0.50
13:S:817:GLU:HA	13:S:835:SER:HB3	1.94	0.50
13:S:922:ILE:HA	13:S:925:HIS:HB3	1.94	0.50
2:J:165:PRO:O	2:J:166:GLN:NE2	2.45	0.50
2:J:413:VAL:HA	2:J:416:GLU:HB2	1.93	0.50
3:K:202:GLU:HA	3:K:205:GLU:HG3	1.93	0.50
6:P:210:LEU:HD11	7:Q:218:LEU:HD21	1.93	0.50
1:A:568:THR:OG1	9:T:231:GLN:OE1	2.27	0.50
5:E:290:ASN:O	5:E:294:HIS:HB3	2.11	0.50
7:G:271:GLU:HA	7:G:274:THR:HG22	1.93	0.50
8:I:138:ARG:HH22	13:S:435:ARG:HD2	1.76	0.50
8:I:688:ILE:HG12	8:I:710:VAL:HA	1.94	0.50
9:L:136:ILE:HG13	12:X:410:GLU:HG3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:53:SER:HA	11:W:56:ASP:OD2	2.11	0.50
13:S:140:LEU:HD21	13:S:186:PHE:HE1	1.77	0.50
7:Q:268:GLN:HG3	7:Q:271:GLU:OE2	2.12	0.50
12:Z:409:ARG:NH2	12:Z:410:GLU:OE1	2.44	0.50
13:V:1021:GLN:HA	13:V:1024:ARG:HB3	1.94	0.50
1:A:466:LEU:HD12	1:A:470:ARG:HD3	1.94	0.50
6:F:220:LEU:O	6:F:224:ILE:HG23	2.11	0.50
8:I:425:SER:OG	8:I:426:ASN:N	2.45	0.50
13:S:778:LEU:O	13:S:780:GLY:N	2.36	0.50
1:H:231:HIS:HD2	1:H:243:MET:SD	2.33	0.50
6:P:216:GLU:OE2	7:Q:226:ARG:NH2	2.37	0.50
8:R:118:ALA:HA	8:R:132:SER:HA	1.93	0.50
11:Y:101:LEU:HD22	12:Z:478:ILE:HG12	1.93	0.50
1:A:257:GLU:HB3	3:C:646:ARG:HH12	1.76	0.50
5:E:155:LEU:HA	5:E:174:TYR:HE1	1.77	0.50
6:F:169:LEU:HD11	7:G:175:ASP:HB3	1.94	0.50
8:I:429:ILE:HB	8:I:444:PHE:HB2	1.93	0.50
8:I:632:PHE:HA	8:I:635:ILE:HG12	1.93	0.50
9:L:274:GLN:O	9:L:277:GLN:NE2	2.42	0.50
13:S:24:TRP:HH2	13:S:45:GLU:HA	1.77	0.50
8:R:2:ARG:NH2	8:R:260:TYR:O	2.44	0.50
1:A:259:ARG:NH2	1:A:286:VAL:O	2.44	0.50
1:A:550:THR:HA	1:A:553:MET:SD	2.51	0.50
1:A:592:ALA:O	1:A:596:HIS:HB2	2.12	0.50
2:B:295:ASP:OD1	2:B:295:ASP:N	2.45	0.50
4:D:246:ILE:HA	4:D:249:LEU:HD13	1.94	0.50
5:E:36:LYS:NZ	5:E:38:ASP:O	2.29	0.50
6:F:286:ARG:HH11	7:G:296:LEU:HD22	1.77	0.50
8:I:66:SER:HA	8:I:69:LYS:HZ1	1.77	0.50
8:I:600:THR:O	8:I:604:ARG:NH1	2.45	0.50
9:L:175:ASP:HB3	9:L:177:VAL:HG22	1.92	0.50
13:S:1083:VAL:HA	13:S:1086:VAL:HG12	1.94	0.50
3:K:60:THR:HG23	3:K:62:GLN:H	1.76	0.50
3:K:450:VAL:HG22	3:K:451:TRP:H	1.77	0.50
5:O:36:LYS:HE2	5:O:38:ASP:HB3	1.94	0.50
7:Q:225:GLN:OE1	7:Q:228:ARG:NH2	2.44	0.50
8:R:323:LEU:HD22	12:Z:479:LYS:HZ1	1.77	0.50
9:T:166:ARG:HB3	10:U:344:LYS:HG2	1.94	0.50
9:T:281:GLU:HB3	9:T:285:ARG:NH1	2.27	0.50
13:V:586:ASP:HA	13:V:591:THR:HA	1.92	0.50
13:V:698:GLN:O	13:V:702:SER:N	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:1014:LYS:HB2	13:V:1033:LYS:HZ1	1.76	0.50
3:C:463:ASP:N	3:C:463:ASP:OD1	2.41	0.50
9:L:239:ASP:O	9:L:242:GLU:HG3	2.11	0.50
11:W:117:GLU:HA	13:V:781:GLY:O	2.12	0.50
13:S:471:ARG:HH21	13:S:473:GLN:HG3	1.77	0.50
2:J:194:SER:HA	2:J:205:PRO:HA	1.93	0.50
12:Z:491:GLN:HG2	12:Z:494:ARG:HH21	1.77	0.50
13:V:9:ILE:HD11	13:V:317:MET:HB2	1.93	0.50
13:V:777:TYR:HB3	13:V:786:ALA:HB2	1.94	0.50
5:E:306:GLY:HA2	5:E:309:LYS:HD3	1.93	0.49
8:I:207:ASP:OD1	8:I:207:ASP:N	2.45	0.49
8:I:518:ALA:HB3	8:I:527:TRP:HZ3	1.76	0.49
13:S:360:TYR:CE2	13:S:379:TYR:HB3	2.47	0.49
3:K:282:SER:HA	3:K:285:ILE:HG22	1.94	0.49
4:N:300:VAL:O	4:N:303:THR:OG1	2.25	0.49
5:O:84:LEU:HD21	5:O:93:PHE:HB2	1.94	0.49
12:Z:488:MET:O	12:Z:492:ILE:HG13	2.12	0.49
13:V:799:ASP:HB3	13:V:802:LEU:H	1.77	0.49
6:F:210:LEU:O	6:F:213:GLN:HG2	2.13	0.49
8:I:249:THR:HA	8:I:264:HIS:HA	1.94	0.49
11:W:101:LEU:HD22	12:X:478:ILE:HG12	1.94	0.49
13:S:549:ASN:HA	13:S:566:PRO:HA	1.95	0.49
1:H:304:TYR:CE2	2:J:296:TRP:HZ2	2.29	0.49
1:H:447:PHE:CD2	1:H:448:LEU:HG	2.46	0.49
3:K:317:LEU:HA	3:K:320:CYS:HB2	1.95	0.49
3:K:377:HIS:CD2	3:K:414:TYR:HB2	2.47	0.49
3:K:557:ARG:HA	3:K:560:LYS:HG3	1.93	0.49
8:R:532:GLU:HA	8:R:535:VAL:HB	1.94	0.49
9:T:150:LEU:HD21	11:Y:23:LYS:HG2	1.94	0.49
11:Y:111:LEU:HD21	12:Z:492:ILE:HG12	1.93	0.49
13:V:383:MET:HB3	13:V:392:SER:HB2	1.94	0.49
13:V:664:LEU:HD11	13:V:694:GLN:HE21	1.77	0.49
13:V:688:VAL:HG23	13:V:691:MET:HE3	1.93	0.49
13:V:837:ARG:HG3	13:V:842:TYR:HB3	1.94	0.49
1:A:170:ARG:HD2	1:A:179:ILE:HG21	1.93	0.49
3:C:38:TYR:HD1	3:C:41:GLN:HE21	1.60	0.49
3:C:485:LEU:O	3:C:533:HIS:NE2	2.45	0.49
8:I:586:VAL:HG12	8:I:598:LYS:HZ3	1.78	0.49
13:S:598:GLU:HA	13:S:601:ILE:HD12	1.94	0.49
2:J:14:SER:HB3	2:J:61:LEU:HD13	1.94	0.49
13:V:931:ALA:HB1	13:V:934:GLU:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:178:GLU:HA	9:L:181:ILE:HD12	1.94	0.49
13:S:508:ASP:OD1	13:S:512:HIS:N	2.44	0.49
13:S:729:ILE:HB	13:S:750:TRP:HE1	1.77	0.49
1:H:184:MET:HG2	1:H:216:ASN:HD21	1.77	0.49
8:R:425:SER:OG	8:R:426:ASN:N	2.46	0.49
13:V:347:LYS:HG3	13:V:348:THR:HG23	1.94	0.49
1:A:352:LYS:HA	3:C:636:ARG:HD3	1.93	0.49
1:A:508:GLU:OE2	1:A:512:ASN:ND2	2.45	0.49
4:D:217:LYS:HZ3	5:E:248:GLU:HG2	1.77	0.49
6:F:28:LYS:HE2	6:F:36:LEU:HD22	1.92	0.49
6:F:145:MET:HA	6:F:148:GLU:HB3	1.95	0.49
8:I:69:LYS:HE2	8:I:413:ARG:HH22	1.77	0.49
13:S:612:TYR:HE2	13:S:638:GLN:HB3	1.77	0.49
13:S:716:ILE:HA	13:S:728:ALA:HB1	1.94	0.49
13:S:758:GLU:HG3	13:S:782:LEU:H	1.77	0.49
1:H:466:LEU:HD12	1:H:470:ARG:HD3	1.93	0.49
1:H:618:TYR:HA	1:H:621:LYS:HG2	1.94	0.49
3:K:611:GLU:HB3	3:K:615:LYS:HE2	1.94	0.49
8:R:108:ILE:HD11	9:T:2:SER:HB3	1.94	0.49
13:V:218:ALA:HB2	13:V:224:VAL:HG22	1.95	0.49
13:V:847:ASP:OD1	13:V:848:LEU:N	2.45	0.49
3:C:341:ALA:HB1	3:C:345:LEU:HD11	1.95	0.49
8:I:347:LEU:HB3	8:I:358:TYR:HB2	1.94	0.49
13:S:43:PHE:HE1	13:S:49:LYS:HG3	1.77	0.49
1:H:659:LEU:HA	1:H:662:ALA:HB3	1.95	0.49
3:K:512:MET:HA	3:K:515:VAL:HG22	1.94	0.49
5:O:363:GLN:HG3	5:O:395:PHE:HZ	1.77	0.49
8:R:119:LEU:HB2	8:R:131:TRP:HB2	1.94	0.49
8:R:431:VAL:O	8:R:442:ARG:N	2.46	0.49
8:R:600:THR:O	8:R:604:ARG:HG2	2.11	0.49
9:T:124:VAL:HA	9:T:127:SER:HB3	1.94	0.49
13:V:904:ALA:HB1	13:V:922:ILE:HG21	1.94	0.49
3:C:246:LYS:HA	3:C:249:ILE:HG22	1.93	0.49
4:D:213:ASN:HD21	4:D:217:LYS:HE3	1.77	0.49
6:F:28:LYS:O	6:F:93:ARG:NH1	2.46	0.49
11:W:79:LEU:O	12:X:461:GLN:NE2	2.45	0.49
13:S:577:HIS:HE1	13:S:582:GLU:HG2	1.77	0.49
13:S:776:LEU:HD23	13:S:779:LYS:HD2	1.95	0.49
1:H:225:VAL:HG21	1:H:264:ARG:HH22	1.77	0.49
2:J:103:ASN:HA	2:J:106:LEU:HB2	1.95	0.49
2:J:112:SER:O	2:J:184:SER:N	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:212:GLU:OE1	4:N:214:LYS:NZ	2.38	0.49
6:P:10:SER:HB2	6:P:104:VAL:HG21	1.94	0.49
8:R:149:TYR:H	8:R:163:CYS:HB2	1.78	0.49
9:T:266:GLU:HA	9:T:269:LEU:HD12	1.93	0.49
13:V:184:PHE:HD1	13:V:196:SER:HB2	1.78	0.49
13:V:719:TYR:HE2	13:V:731:VAL:HG11	1.78	0.49
3:C:512:MET:HA	3:C:515:VAL:HG22	1.94	0.49
5:E:151:ILE:HA	5:E:177:LEU:HD13	1.94	0.49
13:S:332:GLU:HG3	13:S:344:LYS:HB2	1.95	0.49
13:S:960:ALA:HA	13:S:963:ARG:HE	1.78	0.49
1:H:143:ASP:OD1	1:H:151:SER:OG	2.31	0.49
1:H:584:ILE:HG23	1:H:587:ARG:HH21	1.78	0.49
2:J:106:LEU:HA	2:J:109:PHE:HB2	1.95	0.49
5:O:34:LEU:HD12	5:O:35:THR:HG23	1.94	0.49
8:R:529:TYR:HE2	8:R:618:MET:HB3	1.77	0.49
9:T:26:ASN:HB2	9:T:35:VAL:HG13	1.94	0.49
9:T:270:GLU:HG3	10:U:445:THR:HB	1.93	0.49
1:A:475:ALA:HA	1:A:478:ASN:HB2	1.95	0.49
2:B:114:ASN:OD1	2:B:204:ARG:NH2	2.42	0.49
2:B:120:ARG:HH22	2:B:127:LEU:HA	1.78	0.49
3:C:536:ILE:HG12	3:C:573:THR:HG21	1.95	0.49
8:I:467:LEU:O	8:I:469:GLN:NE2	2.40	0.49
8:I:587:LEU:HD11	8:I:615:LEU:HD13	1.94	0.49
13:S:174:SER:HB2	13:S:182:TRP:HB2	1.95	0.49
1:H:507:VAL:HG13	7:Q:201:LYS:HD3	1.95	0.49
2:J:72:GLU:HA	2:J:75:MET:HG3	1.94	0.49
6:P:9:ASP:OD1	6:P:19:GLN:NE2	2.35	0.49
7:Q:225:GLN:O	7:Q:229:VAL:HG23	2.13	0.49
8:R:39:LYS:HG3	8:R:47:GLU:HB2	1.95	0.49
13:V:422:ILE:HD11	13:V:475:LEU:HG	1.95	0.49
1:A:238:PRO:HA	1:A:241:ILE:HG12	1.95	0.49
2:B:128:HIS:HB3	2:B:131:GLU:HB2	1.95	0.49
3:C:99:GLU:OE1	3:C:102:LYS:NZ	2.37	0.49
8:I:41:ASN:HB3	8:I:45:GLU:HB3	1.95	0.49
8:I:186:ASP:OD1	8:I:186:ASP:N	2.45	0.49
8:I:195:SER:HB3	8:I:235:TRP:CE2	2.48	0.49
8:I:389:ASP:OD1	8:I:395:GLN:NE2	2.46	0.49
8:I:482:ASP:OD1	8:I:486:ASP:N	2.46	0.49
8:I:532:GLU:HA	8:I:535:VAL:HB	1.94	0.49
10:M:309:HIS:CE1	11:W:38:ILE:HG12	2.48	0.49
1:H:236:LYS:O	1:H:239:SER:OG	2.23	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:94:GLY:HA3	2:J:115:ASN:HA	1.95	0.49
4:N:319:GLU:OE1	4:N:323:LYS:NZ	2.39	0.49
5:O:13:ARG:NH2	5:O:16:VAL:O	2.46	0.49
5:O:151:ILE:HA	5:O:177:LEU:HD13	1.94	0.49
5:O:176:ARG:HG3	5:O:177:LEU:HG	1.94	0.49
8:R:243:ALA:HB2	8:R:276:TRP:HE1	1.77	0.49
8:R:489:LEU:N	8:R:498:ALA:O	2.41	0.49
9:T:223:GLN:O	9:T:226:ARG:HG3	2.12	0.49
1:A:449:TYR:HA	1:A:452:GLU:HG3	1.93	0.48
2:B:372:GLU:HA	2:B:375:ARG:HG2	1.94	0.48
2:B:424:TYR:HA	4:D:255:PRO:HD3	1.95	0.48
3:C:373:LEU:HD23	3:C:376:ARG:HH11	1.77	0.48
5:E:63:LEU:HA	5:E:66:CYS:HB2	1.94	0.48
6:F:93:ARG:NH2	6:F:97:TYR:OH	2.46	0.48
6:F:325:GLN:HA	6:F:328:LYS:HG2	1.95	0.48
8:I:333:PHE:HE2	8:I:349:VAL:HG11	1.77	0.48
13:S:924:GLN:OE1	13:S:939:TYR:OH	2.27	0.48
2:J:295:ASP:H	2:J:298:SER:HG	1.61	0.48
3:K:21:TYR:HE2	4:N:226:ASN:HD21	1.58	0.48
3:K:555:VAL:O	3:K:559:ILE:HG12	2.13	0.48
6:P:23:LEU:O	6:P:26:THR:OG1	2.20	0.48
8:R:448:GLN:O	8:R:450:ARG:NH1	2.46	0.48
8:R:559:GLN:HB2	8:R:567:LEU:HG	1.93	0.48
9:T:136:ILE:CD1	12:Z:410:GLU:HG3	2.43	0.48
1:A:143:ASP:OD1	1:A:151:SER:OG	2.31	0.48
3:C:21:TYR:HE2	4:D:226:ASN:HD21	1.60	0.48
3:C:493:ALA:HB2	3:C:537:ILE:HA	1.95	0.48
5:E:223:VAL:HB	5:E:246:LEU:HD22	1.94	0.48
8:I:36:THR:HG22	8:I:52:THR:HG23	1.94	0.48
8:I:370:ASP:OD1	8:I:370:ASP:N	2.46	0.48
8:I:485:ARG:HB2	8:I:503:MET:HA	1.94	0.48
13:S:255:PRO:HG3	13:S:301:PRO:HA	1.95	0.48
2:J:176:VAL:HG11	2:J:231:TRP:HB3	1.94	0.48
2:J:295:ASP:OD1	2:J:295:ASP:N	2.46	0.48
5:O:422:ASP:N	5:O:422:ASP:OD1	2.44	0.48
6:P:180:LYS:HA	6:P:183:LEU:HD12	1.95	0.48
6:P:335:ARG:HH12	7:Q:340:SER:HB3	1.76	0.48
8:R:36:THR:HG22	8:R:52:THR:HG23	1.95	0.48
8:R:206:GLU:HA	8:R:229:PRO:HB3	1.94	0.48
9:T:178:GLU:HA	9:T:181:ILE:HD12	1.94	0.48
13:V:138:VAL:HG23	13:V:151:CYS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:380:THR:HA	13:V:395:PRO:HA	1.95	0.48
3:C:383:ARG:HG3	3:C:386:LYS:HE3	1.95	0.48
8:I:89:ILE:O	8:I:97:GLU:N	2.46	0.48
13:S:800:PRO:O	13:S:804:ASP:HB2	2.14	0.48
1:H:466:LEU:HD22	1:H:479:LYS:HG2	1.95	0.48
2:J:27:PHE:HB2	2:J:31:PHE:HE2	1.78	0.48
5:O:54:ARG:HH21	5:O:83:LEU:HD11	1.77	0.48
8:R:249:THR:HA	8:R:264:HIS:HA	1.96	0.48
8:R:593:LYS:HB2	8:R:595:GLN:HE21	1.78	0.48
13:V:89:VAL:HB	13:V:110:PHE:HB2	1.94	0.48
13:V:829:SER:H	13:V:852:GLU:HA	1.78	0.48
13:V:867:TRP:O	13:V:870:THR:OG1	2.30	0.48
2:B:19:GLU:HA	2:B:65:LYS:HG3	1.95	0.48
3:C:398:ASP:N	3:C:398:ASP:OD1	2.46	0.48
13:S:581:THR:HG23	13:S:601:ILE:HG12	1.94	0.48
6:P:280:PRO:HA	6:P:283:VAL:HG22	1.94	0.48
8:R:89:ILE:O	8:R:97:GLU:N	2.46	0.48
8:R:480:VAL:HG13	8:R:488:TYR:HD1	1.77	0.48
13:V:447:VAL:HB	13:V:499:GLN:HA	1.94	0.48
13:V:939:TYR:HD1	13:V:944:MET:HG3	1.79	0.48
1:A:309:ARG:NH2	1:A:378:ASP:HB3	2.29	0.48
8:I:350:ALA:HB2	8:I:378:LEU:HD22	1.95	0.48
13:S:7:LYS:HE2	13:S:9:ILE:HG13	1.95	0.48
13:S:499:GLN:HG3	13:S:500:ARG:HD3	1.95	0.48
13:S:514:HIS:HB3	13:S:523:ARG:HG2	1.96	0.48
2:J:19:GLU:HA	2:J:65:LYS:HG3	1.95	0.48
2:J:78:LYS:HD3	2:J:81:LYS:HZ3	1.77	0.48
3:K:398:ASP:N	3:K:398:ASP:OD1	2.47	0.48
8:R:130:ILE:HG22	8:R:138:ARG:HB3	1.96	0.48
8:R:347:LEU:HB3	8:R:358:TYR:HB2	1.95	0.48
13:V:1083:VAL:HA	13:V:1086:VAL:HG12	1.96	0.48
2:B:337:GLU:OE2	3:C:454:ASN:ND2	2.47	0.48
3:C:122:SER:HA	3:C:125:GLN:HG2	1.95	0.48
6:F:78:VAL:HG11	6:F:83:LEU:HD11	1.96	0.48
8:I:431:VAL:HB	8:I:442:ARG:HB2	1.94	0.48
13:S:554:TYR:CZ	13:S:600:LEU:HD13	2.48	0.48
1:H:181:LEU:HA	1:H:184:MET:HG3	1.95	0.48
1:H:670:HIS:NE2	1:H:679:CYS:SG	2.84	0.48
3:K:132:ARG:NH2	3:K:156:GLU:OE1	2.47	0.48
3:K:460:PHE:O	3:K:466:TYR:OH	2.23	0.48
5:O:14:THR:OG1	5:O:17:ALA:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:44:ILE:HD11	6:P:68:PHE:HZ	1.78	0.48
7:Q:209:TYR:O	7:Q:213:GLN:NE2	2.34	0.48
8:R:505:ASP:OD1	8:R:505:ASP:N	2.46	0.48
12:Z:409:ARG:CZ	12:Z:410:GLU:OE1	2.62	0.48
13:V:471:ARG:HH21	13:V:473:GLN:HG3	1.79	0.48
13:V:508:ASP:OD1	13:V:512:HIS:N	2.46	0.48
1:A:280:LEU:HD11	1:A:303:ASN:OD1	2.14	0.48
2:B:186:GLN:O	2:B:188:PRO:CD	2.61	0.48
5:E:282:ASP:OD1	5:E:288:ARG:NH1	2.46	0.48
6:F:169:LEU:HA	6:F:172:LYS:HE2	1.95	0.48
8:I:437:SER:OG	8:I:461:GLU:OE2	2.30	0.48
8:I:596:TRP:CE2	12:X:503:LEU:HD11	2.49	0.48
9:L:161:ARG:HA	9:L:164:ARG:HE	1.77	0.48
13:S:198:GLN:NE2	13:S:200:VAL:O	2.47	0.48
1:H:268:LEU:O	1:H:272:ARG:HG2	2.13	0.48
1:H:511:TYR:CZ	1:H:515:LEU:HD11	2.48	0.48
3:K:543:THR:HA	3:K:546:CYS:HB2	1.95	0.48
8:R:479:ILE:HB	8:R:487:LEU:HD11	1.95	0.48
11:Y:122:ILE:HD11	12:Z:495:ASN:HA	1.94	0.48
13:V:514:HIS:HB3	13:V:523:ARG:HG2	1.96	0.48
13:V:729:ILE:HB	13:V:750:TRP:HE1	1.78	0.48
1:A:434:GLU:O	1:A:438:LYS:N	2.45	0.48
2:B:53:LEU:HB3	2:B:54:ARG:HH11	1.77	0.48
2:B:427:GLY:N	4:D:254:PRO:O	2.41	0.48
3:C:260:LYS:HA	3:C:285:ILE:HD11	1.95	0.48
5:E:132:GLN:HA	5:E:140:LEU:HD11	1.96	0.48
8:I:700:ALA:HA	8:I:703:HIS:HB3	1.94	0.48
9:L:204:ARG:NE	10:M:378:ASN:HB3	2.28	0.48
2:J:186:GLN:O	2:J:188:PRO:CD	2.61	0.48
3:K:275:ASP:O	3:K:279:LEU:N	2.41	0.48
3:K:474:GLU:HA	3:K:477:VAL:HB	1.96	0.48
5:O:129:HIS:HA	5:O:132:GLN:HG2	1.95	0.48
7:Q:150:ILE:HA	7:Q:153:VAL:HG22	1.96	0.48
8:R:211:LYS:HG2	8:R:222:GLN:HA	1.95	0.48
8:R:518:ALA:HB3	8:R:527:TRP:HZ3	1.78	0.48
13:V:30:ARG:NH1	13:V:77:SER:O	2.47	0.48
1:A:210:ALA:O	1:A:214:ASN:ND2	2.47	0.48
2:B:7:GLU:O	2:B:39:ARG:N	2.47	0.48
2:B:426:MET:HE1	4:D:287:ASP:H	1.78	0.48
4:D:318:MET:O	4:D:322:ASN:ND2	2.47	0.48
8:I:489:LEU:N	8:I:498:ALA:O	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:384:GLY:HA3	13:S:391:LEU:HD23	1.95	0.48
5:O:13:ARG:HH11	5:O:18:GLN:HG2	1.79	0.48
6:P:210:LEU:O	6:P:213:GLN:HG2	2.14	0.48
8:R:587:LEU:HD11	8:R:615:LEU:HD13	1.95	0.48
9:T:235:PRO:HD2	9:T:237:TYR:CZ	2.48	0.48
6:F:48:HIS:HE2	6:F:65:LEU:HD21	1.77	0.48
6:F:127:GLU:HA	6:F:130:ASN:HB2	1.95	0.48
6:F:186:LYS:O	6:F:190:ALA:HB2	2.14	0.48
13:S:867:TRP:O	13:S:870:THR:OG1	2.31	0.48
1:H:542:GLU:OE2	1:H:545:HIS:ND1	2.47	0.48
1:H:658:ASN:O	1:H:662:ALA:N	2.45	0.48
3:K:432:SER:O	3:K:435:GLU:HG2	2.14	0.48
7:Q:271:GLU:HA	7:Q:274:THR:HG22	1.96	0.48
13:V:549:ASN:HA	13:V:566:PRO:HA	1.96	0.48
1:A:228:GLY:HA2	1:A:231:HIS:CD2	2.48	0.47
3:C:96:MET:O	3:C:100:ALA:N	2.34	0.47
13:S:373:LEU:HD23	13:S:386:LEU:HG	1.94	0.47
13:S:664:LEU:HD11	13:S:694:GLN:HE21	1.79	0.47
13:S:874:MET:HG3	13:S:878:ILE:HG23	1.95	0.47
13:S:960:ALA:HB2	13:S:963:ARG:HH21	1.79	0.47
1:H:143:ASP:HA	1:H:149:ILE:HD11	1.96	0.47
13:V:531:GLN:N	13:V:545:GLN:O	2.41	0.47
13:V:560:ASP:OD1	13:V:561:ASN:N	2.47	0.47
13:V:849:ALA:O	13:V:850:ARG:HD3	2.14	0.47
1:A:148:ASP:H	1:A:197:MET:HG3	1.80	0.47
1:A:308:ASP:N	1:A:308:ASP:OD1	2.44	0.47
1:A:483:LEU:HA	1:A:486:ARG:HB2	1.95	0.47
2:B:187:LYS:NZ	2:B:261:ALA:HB1	2.29	0.47
4:D:219:GLN:HA	4:D:222:ILE:HD12	1.96	0.47
5:E:14:THR:OG1	5:E:17:ALA:O	2.33	0.47
8:I:153:TRP:HA	8:I:160:LEU:HG	1.96	0.47
8:I:202:ILE:HG22	8:I:212:VAL:HG22	1.95	0.47
1:H:240:ALA:HA	1:H:243:MET:HE2	1.96	0.47
1:H:259:ARG:O	1:H:263:MET:HG3	2.14	0.47
6:P:78:VAL:HG11	6:P:83:LEU:HD11	1.96	0.47
11:Y:109:GLN:HA	11:Y:112:ILE:HD12	1.95	0.47
13:V:498:ASN:HD21	13:V:502:THR:H	1.60	0.47
1:A:155:ASN:OD1	1:A:156:ALA:N	2.47	0.47
2:B:425:LYS:HZ2	4:D:288:ILE:HB	1.79	0.47
3:C:221:ASP:OD1	3:C:221:ASP:N	2.44	0.47
5:E:43:ILE:HA	5:E:46:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:335:ARG:HH12	7:G:340:SER:HB3	1.80	0.47
8:I:252:LEU:HA	8:I:252:LEU:HD12	1.74	0.47
8:I:300:LEU:HB2	8:I:311:VAL:HB	1.96	0.47
8:I:322:ILE:HG23	12:X:479:LYS:HZ2	1.80	0.47
8:I:480:VAL:HG13	8:I:488:TYR:HD1	1.79	0.47
1:H:576:GLY:HA3	2:J:272:LEU:HD23	1.95	0.47
2:J:7:GLU:O	2:J:39:ARG:N	2.46	0.47
8:R:211:LYS:HE2	8:R:222:GLN:HG3	1.96	0.47
8:R:275:SER:O	8:R:284:ALA:N	2.48	0.47
9:T:239:ASP:O	9:T:242:GLU:HG3	2.13	0.47
11:Y:108:GLU:O	11:Y:112:ILE:HG13	2.14	0.47
13:V:554:TYR:CZ	13:V:600:LEU:HD13	2.50	0.47
1:A:577:VAL:HA	1:A:580:ARG:HE	1.79	0.47
5:E:223:VAL:HA	5:E:226:LYS:HE2	1.97	0.47
8:I:322:ILE:HG23	12:X:479:LYS:NZ	2.29	0.47
13:S:342:ILE:HG12	13:S:353:VAL:HG22	1.95	0.47
13:S:493:ASP:OD1	13:S:494:TRP:N	2.47	0.47
13:S:899:GLN:HG2	13:S:900:PHE:H	1.80	0.47
1:H:352:LYS:N	1:H:354:GLU:OE1	2.47	0.47
3:K:219:ASN:HA	3:K:265:ASP:HA	1.97	0.47
8:R:366:PRO:HG2	8:R:368:ILE:HD11	1.95	0.47
9:T:277:GLN:HA	9:T:280:MET:HG3	1.96	0.47
1:A:283:PHE:O	1:A:287:MET:HG2	2.13	0.47
1:A:304:TYR:CD2	1:A:376:LYS:HE3	2.48	0.47
8:I:82:CYS:SG	8:I:83:THR:N	2.83	0.47
12:X:409:ARG:HA	12:X:412:VAL:HG22	1.96	0.47
1:H:308:ASP:OD1	1:H:308:ASP:N	2.47	0.47
3:K:298:LEU:HD23	3:K:301:LEU:HD12	1.97	0.47
5:O:183:ASP:H	5:O:186:ARG:HB2	1.80	0.47
6:P:83:LEU:HA	6:P:86:GLN:HG3	1.97	0.47
6:P:224:ILE:HG22	7:Q:229:VAL:HG22	1.97	0.47
7:Q:272:TYR:HA	7:Q:275:LEU:HD12	1.96	0.47
8:R:277:THR:N	8:R:282:GLN:O	2.39	0.47
8:R:389:ASP:OD1	8:R:389:ASP:N	2.46	0.47
8:R:433:ASP:OD1	8:R:435:GLN:NE2	2.47	0.47
13:V:639:ALA:HB1	13:V:648:ALA:HA	1.96	0.47
1:A:437:VAL:HG13	1:A:440:ARG:HH21	1.79	0.47
3:C:207:ALA:HA	3:C:210:GLU:HG3	1.96	0.47
3:C:555:VAL:O	3:C:559:ILE:HG12	2.14	0.47
7:G:146:LYS:HB3	7:G:147:ARG:NH2	2.30	0.47
8:I:182:TRP:HE1	8:I:184:ALA:HB2	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:499:LEU:HA	12:X:502:LEU:HG	1.96	0.47
1:H:270:PHE:HD2	1:H:279:ALA:HB2	1.78	0.47
8:R:756:SER:HB3	8:R:763:ARG:HH12	1.79	0.47
13:V:159:TYR:HB3	13:V:177:MET:HB2	1.96	0.47
1:A:576:GLY:HA3	2:B:272:LEU:HD23	1.96	0.47
3:C:169:ALA:O	3:C:173:LEU:HB3	2.14	0.47
3:C:599:SER:HA	3:C:602:GLU:HG2	1.97	0.47
5:E:13:ARG:NH2	5:E:16:VAL:O	2.48	0.47
8:I:95:ARG:NE	8:I:97:GLU:OE2	2.48	0.47
8:I:153:TRP:CE3	8:I:160:LEU:HD11	2.50	0.47
8:I:158:ASP:OD1	8:I:158:ASP:N	2.42	0.47
8:I:568:VAL:HG22	8:I:576:VAL:HB	1.96	0.47
8:I:593:LYS:HE2	8:I:595:GLN:NE2	2.30	0.47
9:L:16:LEU:O	9:L:45:ARG:NE	2.47	0.47
13:S:12:PRO:HG3	13:S:314:ALA:HB2	1.96	0.47
13:S:399:ASP:OD1	13:S:399:ASP:N	2.44	0.47
1:H:136:LEU:HD11	1:H:158:GLU:HG3	1.97	0.47
1:H:304:TYR:C	1:H:306:LEU:N	2.68	0.47
1:H:544:ILE:HG21	1:H:566:LEU:HD22	1.97	0.47
2:J:57:HIS:HA	2:J:79:PHE:HZ	1.79	0.47
5:O:69:HIS:NE2	5:O:187:SER:OG	2.43	0.47
5:O:347:GLN:HG2	5:O:368:CYS:HB2	1.96	0.47
6:P:222:THR:O	6:P:226:THR:HG23	2.15	0.47
8:R:20:VAL:HG12	8:R:30:THR:HG22	1.95	0.47
8:R:460:LEU:HB3	8:R:482:ASP:HB2	1.96	0.47
8:R:474:ASN:HA	8:R:493:MET:HE1	1.95	0.47
8:R:730:PHE:O	8:R:734:ASN:ND2	2.38	0.47
9:T:5:GLU:HG2	9:T:94:VAL:HG21	1.96	0.47
13:V:415:HIS:HA	13:V:420:LEU:HA	1.96	0.47
2:B:92:GLU:O	2:B:97:LYS:NZ	2.41	0.47
3:C:543:THR:HA	3:C:546:CYS:HB2	1.97	0.47
8:I:218:ARG:HH21	8:I:219:LEU:HB3	1.79	0.47
13:S:341:VAL:O	13:S:354:LEU:N	2.40	0.47
13:S:402:GLU:HG2	13:S:414:VAL:HB	1.97	0.47
13:S:836:TYR:HB2	13:S:845:ALA:HB2	1.96	0.47
8:R:207:ASP:OD1	8:R:207:ASP:N	2.43	0.47
13:V:978:TYR:HD2	13:V:1001:ALA:HA	1.80	0.47
13:V:998:TYR:OH	13:V:1008:LYS:NZ	2.46	0.47
1:A:208:TYR:HB3	1:A:223:LEU:HD11	1.96	0.47
3:C:223:MET:N	3:C:223:MET:SD	2.88	0.47
8:I:596:TRP:NE1	8:I:627:THR:OG1	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:698:GLN:O	13:S:702:SER:N	2.39	0.47
13:S:719:TYR:HD2	13:S:728:ALA:HA	1.80	0.47
2:J:92:GLU:O	2:J:97:LYS:NZ	2.41	0.47
2:J:180:GLY:HA2	2:J:223:SER:HB2	1.97	0.47
4:N:333:GLY:O	4:N:334:MET:C	2.53	0.47
5:O:63:LEU:HA	5:O:66:CYS:HB2	1.96	0.47
11:Y:72:LEU:O	11:Y:76:VAL:HG13	2.15	0.47
13:V:324:ARG:HH22	13:V:332:GLU:HB2	1.80	0.47
13:V:459:LYS:HG3	13:V:475:LEU:HB2	1.97	0.47
13:V:577:HIS:HE1	13:V:582:GLU:HG2	1.80	0.47
1:A:227:MET:SD	1:A:243:MET:SD	3.12	0.47
2:B:295:ASP:H	2:B:298:SER:HG	1.63	0.47
8:I:216:PHE:HZ	13:V:547:ARG:HH22	1.63	0.47
8:I:277:THR:N	8:I:282:GLN:O	2.39	0.47
3:K:458:THR:O	3:K:462:GLN:N	2.46	0.47
3:K:559:ILE:HD12	3:K:606:PHE:HB2	1.95	0.47
6:P:186:LYS:O	6:P:190:ALA:HB2	2.15	0.47
7:Q:180:ASP:OD1	7:Q:181:LEU:N	2.48	0.47
7:Q:195:TYR:HA	7:Q:198:VAL:HG22	1.97	0.47
1:A:511:TYR:CZ	1:A:515:LEU:HD11	2.50	0.46
2:B:140:ASN:HD21	2:B:256:LEU:HD12	1.79	0.46
3:C:243:PHE:HA	3:C:246:LYS:HG2	1.96	0.46
5:E:7:ARG:HH12	5:E:256:ASP:HB3	1.81	0.46
5:E:196:TYR:HB3	5:E:204:VAL:HG13	1.96	0.46
6:F:306:ASP:N	6:F:306:ASP:OD1	2.45	0.46
8:I:27:GLU:HB3	8:I:92:ARG:NH2	2.29	0.46
8:I:275:SER:O	8:I:284:ALA:N	2.48	0.46
8:I:692:ASN:H	13:V:662:ARG:H	1.62	0.46
9:L:221:GLU:O	9:L:225:LYS:HG2	2.15	0.46
1:H:311:GLY:O	1:H:315:ALA:HB3	2.15	0.46
3:K:573:THR:HA	3:K:576:TYR:HB2	1.97	0.46
5:O:14:THR:HG23	5:O:18:GLN:HE22	1.80	0.46
5:O:173:ILE:HG13	5:O:176:ARG:HH21	1.80	0.46
8:R:129:LYS:HA	8:R:140:THR:HA	1.96	0.46
8:R:227:ASP:OD1	8:R:227:ASP:N	2.48	0.46
9:T:107:ALA:HA	11:Y:59:VAL:HG21	1.97	0.46
13:V:402:GLU:HG3	13:V:416:TYR:HB2	1.96	0.46
13:V:916:MET:HB3	13:V:920:ARG:HH12	1.80	0.46
1:A:670:HIS:HE1	1:A:676:ASN:HB3	1.80	0.46
2:B:432:GLY:H	4:D:254:PRO:HB3	1.80	0.46
8:I:129:LYS:HA	8:I:140:THR:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:514:ALA:HB1	8:I:530:PRO:HG3	1.96	0.46
13:S:415:HIS:HD2	13:S:420:LEU:HB2	1.80	0.46
2:J:116:ASP:OD1	2:J:116:ASP:N	2.48	0.46
2:J:394:MET:HB2	2:J:404:LEU:HD11	1.96	0.46
2:J:427:GLY:N	4:N:254:PRO:O	2.36	0.46
5:O:349:VAL:O	5:O:352:SER:OG	2.28	0.46
8:R:577:SER:HB2	11:Y:97:LYS:NZ	2.31	0.46
9:T:200:GLU:O	9:T:204:ARG:HG2	2.16	0.46
13:V:8:SER:OG	13:V:316:ASP:OD2	2.32	0.46
13:V:616:VAL:HG12	13:V:632:TRP:HZ3	1.80	0.46
13:V:816:TYR:HE2	13:V:834:GLN:HB3	1.80	0.46
1:A:471:TYR:HB3	6:F:182:ARG:HH22	1.80	0.46
1:A:482:VAL:O	1:A:486:ARG:N	2.43	0.46
2:B:133:LEU:HD22	2:B:176:VAL:HG22	1.98	0.46
7:G:233:LEU:HD22	7:G:236:ARG:HH21	1.80	0.46
8:I:479:ILE:HB	8:I:487:LEU:HD11	1.97	0.46
9:L:96:GLU:OE2	9:L:99:LYS:NZ	2.34	0.46
12:X:485:ILE:O	12:X:489:LYS:HG2	2.15	0.46
2:J:67:LYS:NZ	2:J:101:ASN:OD1	2.48	0.46
2:J:106:LEU:O	2:J:111:MET:N	2.42	0.46
8:R:254:ASP:HB2	8:R:260:TYR:HE1	1.79	0.46
9:T:221:GLU:O	9:T:225:LYS:HG2	2.15	0.46
9:T:240:GLU:HA	9:T:243:ARG:HB2	1.98	0.46
13:V:82:ILE:HB	13:V:90:PHE:HB2	1.96	0.46
13:V:758:GLU:HG2	13:V:777:TYR:HA	1.98	0.46
2:B:106:LEU:O	2:B:111:MET:N	2.47	0.46
2:B:203:ASN:HB2	2:B:265:ASP:HB3	1.98	0.46
5:E:363:GLN:HG3	5:E:395:PHE:HZ	1.80	0.46
7:G:143:LEU:HG	7:G:147:ARG:NH1	2.31	0.46
8:I:200:LEU:HB2	8:I:255:ARG:HH11	1.80	0.46
9:L:166:ARG:HB3	10:M:344:LYS:HG2	1.97	0.46
11:W:115:LYS:HG2	12:X:495:ASN:ND2	2.31	0.46
1:H:228:GLY:HA2	1:H:231:HIS:CD2	2.50	0.46
1:H:304:TYR:CD2	2:J:296:TRP:HZ2	2.33	0.46
2:J:365:LEU:HD22	4:N:225:ILE:HG23	1.96	0.46
3:K:297:LYS:HA	3:K:300:PHE:HD2	1.80	0.46
5:O:128:PHE:CE1	5:O:143:TYR:HB3	2.50	0.46
5:O:178:LEU:HG	5:O:182:ARG:HH21	1.81	0.46
9:T:280:MET:O	9:T:283:GLN:HG3	2.16	0.46
13:V:540:ASP:OD1	13:V:540:ASP:N	2.46	0.46
13:V:795:ASN:OD1	13:V:796:VAL:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:924:GLN:OE1	13:V:939:TYR:OH	2.30	0.46
2:B:94:GLY:HA3	2:B:115:ASN:HA	1.98	0.46
2:B:388:ASP:HA	2:B:392:TYR:HB3	1.98	0.46
3:C:559:ILE:HD12	3:C:606:PHE:HB2	1.97	0.46
7:G:225:GLN:O	7:G:229:VAL:HG23	2.15	0.46
8:I:398:THR:HG22	8:I:402:ARG:H	1.81	0.46
13:S:218:ALA:HB2	13:S:224:VAL:HG22	1.98	0.46
13:S:616:VAL:HG12	13:S:632:TRP:HZ3	1.81	0.46
13:S:781:GLY:C	13:S:782:LEU:HD22	2.35	0.46
13:S:957:LYS:HG2	13:S:960:ALA:HB3	1.98	0.46
2:J:312:ILE:HB	3:K:589:ALA:HB1	1.98	0.46
6:P:196:LYS:HG3	6:P:198:PRO:HD3	1.97	0.46
6:P:272:ARG:HA	6:P:275:VAL:HG12	1.97	0.46
8:R:186:ASP:OD1	8:R:186:ASP:N	2.48	0.46
3:C:458:THR:O	3:C:462:GLN:N	2.47	0.46
8:I:68:LYS:HG3	8:I:73:GLY:HA2	1.96	0.46
11:W:117:GLU:HG2	13:V:756:GLN:HG2	1.97	0.46
13:S:363:GLU:OE1	13:S:376:ARG:NH1	2.48	0.46
13:S:402:GLU:HG3	13:S:416:TYR:HB2	1.97	0.46
6:P:238:TYR:HE2	7:Q:239:LEU:HB3	1.80	0.46
13:V:140:LEU:HD21	13:V:186:PHE:HE1	1.80	0.46
1:A:189:PHE:HE2	2:B:309:THR:HG23	1.81	0.46
2:B:106:LEU:HA	2:B:109:PHE:HB2	1.96	0.46
2:B:291:ASP:N	2:B:291:ASP:OD1	2.43	0.46
5:E:14:THR:HG23	5:E:18:GLN:HE22	1.79	0.46
6:F:328:LYS:HA	6:F:331:GLN:HG3	1.97	0.46
8:I:347:LEU:N	8:I:358:TYR:O	2.38	0.46
11:W:56:ASP:CA	11:W:59:VAL:HG22	2.40	0.46
12:X:407:SER:O	12:X:411:LEU:HG	2.16	0.46
13:S:1069:GLN:NE2	13:S:1073:GLN:OE1	2.49	0.46
1:H:257:GLU:OE1	3:K:646:ARG:NH2	2.45	0.46
2:J:54:ARG:HH21	2:J:76:LEU:HA	1.80	0.46
3:K:428:MET:HG2	3:K:430:LEU:HG	1.97	0.46
8:R:80:VAL:O	8:R:88:LYS:N	2.47	0.46
9:T:16:LEU:O	9:T:45:ARG:NE	2.48	0.46
9:T:110:LYS:HE3	12:Z:436:MET:HG2	1.97	0.46
13:V:945:ALA:HB3	13:V:969:LEU:HD23	1.97	0.46
1:A:231:HIS:HD2	1:A:243:MET:SD	2.37	0.46
2:B:330:ASN:HD21	3:C:548:LYS:HB2	1.80	0.46
5:E:5:LYS:HE2	5:E:257:HIS:CE1	2.51	0.46
7:G:153:VAL:HA	7:G:156:ASN:ND2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:108:ILE:HD11	9:L:2:SER:HB3	1.97	0.46
9:L:200:GLU:O	9:L:204:ARG:HG2	2.16	0.46
1:H:254:THR:OG1	1:H:255:ALA:N	2.47	0.46
1:H:283:PHE:HA	1:H:286:VAL:HG22	1.98	0.46
2:J:141:ARG:HH21	2:J:168:PHE:HA	1.80	0.46
9:T:70:ALA:HB2	9:T:83:ILE:HD11	1.97	0.46
1:A:454:GLU:OE2	10:M:443:SER:OG	2.25	0.46
2:B:71:PRO:O	2:B:75:MET:HG3	2.16	0.46
2:B:358:PRO:O	3:C:59:TYR:OH	2.33	0.46
3:C:17:THR:OG1	3:C:18:GLN:OE1	2.32	0.46
3:C:559:ILE:HG21	3:C:602:GLU:HB2	1.98	0.46
5:E:125:ARG:HG3	5:E:152:GLU:HB3	1.97	0.46
6:F:210:LEU:O	6:F:214:GLN:NE2	2.49	0.46
9:L:74:LEU:O	10:M:306:TRP:NE1	2.47	0.46
10:M:398:LEU:HB3	10:M:402:LYS:NZ	2.31	0.46
13:S:412:CYS:O	13:S:423:VAL:N	2.46	0.46
13:S:422:ILE:HG13	13:S:431:LEU:HB2	1.97	0.46
13:S:545:GLN:NE2	13:S:546:SER:O	2.44	0.46
13:S:945:ALA:HB3	13:S:969:LEU:HD23	1.98	0.46
1:H:180:ASN:OD1	1:H:181:LEU:N	2.49	0.46
1:H:496:PHE:CE2	1:H:516:VAL:HG21	2.51	0.46
3:K:211:HIS:CE1	3:K:214:LEU:HB2	2.51	0.46
5:O:326:HIS:CD2	5:O:341:LYS:HD2	2.51	0.46
6:P:328:LYS:HA	6:P:331:GLN:HG3	1.98	0.46
8:R:153:TRP:CE3	8:R:160:LEU:HD11	2.50	0.46
8:R:158:ASP:N	8:R:158:ASP:OD1	2.43	0.46
8:R:527:TRP:HA	8:R:544:ARG:HA	1.98	0.46
8:R:539:LEU:HD12	8:R:542:LYS:HD3	1.97	0.46
8:R:729:ARG:HA	8:R:732:GLN:HG3	1.98	0.46
13:V:402:GLU:HG2	13:V:414:VAL:HB	1.98	0.46
13:V:653:ALA:HA	13:V:662:ARG:HA	1.98	0.46
1:A:224:ARG:O	1:A:243:MET:HE1	2.15	0.46
1:A:306:LEU:HG	9:L:296:GLU:OE1	2.16	0.46
5:E:226:LYS:O	5:E:230:HIS:ND1	2.49	0.46
1:H:395:ARG:HG2	1:H:400:THR:HA	1.96	0.46
2:J:178:PRO:O	2:J:223:SER:OG	2.29	0.46
2:J:291:ASP:OD1	2:J:291:ASP:N	2.43	0.46
2:J:358:PRO:O	3:K:59:TYR:OH	2.34	0.46
3:K:64:ASP:OD1	3:K:65:MET:N	2.41	0.46
5:O:37:ARG:NH2	5:O:39:TYR:OH	2.49	0.46
5:O:223:VAL:HB	5:O:246:LEU:HD22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:711:LEU:HD22	8:R:739:VAL:HB	1.98	0.46
13:V:12:PRO:HG3	13:V:314:ALA:HB2	1.97	0.46
13:V:511:ARG:NH1	13:V:530:CYS:O	2.45	0.46
2:B:123:HIS:CG	9:L:258:ARG:HH12	2.34	0.45
8:I:529:TYR:CD1	8:I:532:GLU:HG2	2.50	0.45
8:I:619:ALA:O	8:I:623:LYS:N	2.48	0.45
8:I:688:ILE:HG13	8:I:713:TYR:HD2	1.81	0.45
1:H:239:SER:O	1:H:242:LYS:HG2	2.16	0.45
3:K:326:PHE:HB3	3:K:329:LEU:HD11	1.98	0.45
5:O:274:LEU:HG	5:O:307:LEU:HD13	1.97	0.45
7:Q:166:ARG:HH21	7:Q:170:GLN:HE22	1.62	0.45
8:R:398:THR:HG22	8:R:402:ARG:H	1.81	0.45
8:R:425:SER:HB2	8:R:467:LEU:HB3	1.97	0.45
13:V:26:PRO:HA	13:V:301:PRO:HG3	1.97	0.45
1:A:188:ASP:O	1:A:208:TYR:OH	2.24	0.45
1:A:270:PHE:HD2	1:A:279:ALA:HB2	1.82	0.45
1:A:578:LEU:HD23	1:A:597:TYR:HA	1.99	0.45
8:I:425:SER:OG	8:I:476:ARG:NE	2.48	0.45
8:I:458:HIS:NE2	8:I:480:VAL:HG21	2.31	0.45
8:I:510:HIS:HB2	8:I:515:MET:HB2	1.98	0.45
2:J:28:LYS:HA	2:J:31:PHE:HD2	1.81	0.45
2:J:120:ARG:HH22	2:J:127:LEU:HA	1.81	0.45
2:J:380:THR:OG1	4:N:234:ALA:O	2.21	0.45
3:K:541:ILE:HG23	3:K:557:ARG:NE	2.31	0.45
5:O:1:MET:HE3	5:O:155:LEU:HB3	1.98	0.45
7:Q:137:ASN:N	7:Q:137:ASN:OD1	2.49	0.45
10:U:451:LEU:HA	10:U:454:LYS:HG2	1.98	0.45
13:V:577:HIS:CE1	13:V:582:GLU:HG2	2.51	0.45
2:B:141:ARG:HH21	2:B:168:PHE:HA	1.81	0.45
3:C:175:TYR:H	5:E:275:GLN:HE22	1.64	0.45
3:C:275:ASP:O	3:C:279:LEU:N	2.42	0.45
5:E:13:ARG:HH11	5:E:18:GLN:HG2	1.81	0.45
5:E:54:ARG:HH21	5:E:83:LEU:HD11	1.81	0.45
5:E:326:HIS:CD2	5:E:341:LYS:HD2	2.51	0.45
8:I:76:ASP:O	8:I:92:ARG:N	2.49	0.45
9:L:124:VAL:HA	9:L:127:SER:HB3	1.98	0.45
10:M:453:ASN:HA	10:M:456:LEU:HD12	1.98	0.45
11:W:56:ASP:O	11:W:59:VAL:HG22	2.16	0.45
11:W:119:GLU:HB2	12:X:495:ASN:ND2	2.30	0.45
13:S:1053:GLU:HA	13:S:1056:LYS:HE2	1.98	0.45
1:H:600:GLU:HG2	1:H:603:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:659:LEU:HD22	1:H:686:LEU:HD21	1.97	0.45
2:J:76:LEU:HD11	2:J:86:ILE:HG13	1.99	0.45
3:K:187:TYR:O	3:K:192:GLN:N	2.47	0.45
5:O:377:ASP:N	5:O:377:ASP:OD1	2.49	0.45
8:R:467:LEU:O	8:R:469:GLN:NE2	2.43	0.45
13:V:1100:TRP:HA	13:V:1103:THR:HG22	1.98	0.45
1:A:600:GLU:HA	1:A:603:ARG:HG3	1.97	0.45
2:B:283:LYS:HZ1	10:M:457:LEU:HD22	1.82	0.45
2:B:371:SER:OG	2:B:374:ASN:OD1	2.31	0.45
5:E:34:LEU:HA	5:E:39:TYR:HE1	1.82	0.45
7:G:180:ASP:OD1	7:G:181:LEU:N	2.49	0.45
9:L:235:PRO:HD2	9:L:237:TYR:CE1	2.52	0.45
11:W:108:GLU:HG3	12:X:488:MET:HG3	1.97	0.45
13:S:138:VAL:HG23	13:S:151:CYS:HB2	1.97	0.45
13:S:631:GLN:HE22	13:S:635:LEU:HD11	1.81	0.45
1:H:226:ASN:O	1:H:230:ILE:HG12	2.16	0.45
1:H:309:ARG:NH2	1:H:378:ASP:HB3	2.31	0.45
2:J:123:HIS:CG	9:T:258:ARG:HH12	2.34	0.45
3:K:349:LEU:HA	3:K:352:TYR:HB2	1.98	0.45
4:N:312:PRO:HA	4:N:315:ARG:HB2	1.98	0.45
5:O:96:TYR:OH	5:O:184:TYR:OH	2.23	0.45
7:Q:256:SER:HA	7:Q:259:GLN:HE22	1.81	0.45
8:R:182:TRP:HE1	8:R:184:ALA:HB2	1.80	0.45
8:R:701:THR:HG23	8:R:729:ARG:HH21	1.81	0.45
9:T:122:ILE:HD11	11:Y:48:VAL:HG21	1.99	0.45
13:V:228:ASP:HB3	13:V:234:ILE:HD11	1.98	0.45
2:B:78:LYS:HD3	2:B:81:LYS:HZ3	1.81	0.45
3:C:73:LEU:HD22	3:C:83:TYR:CZ	2.52	0.45
3:C:535:CYS:HA	3:C:538:ASN:ND2	2.32	0.45
8:I:685:LYS:HA	8:I:688:ILE:HG22	1.99	0.45
9:L:107:ALA:HB1	9:L:110:LYS:HB2	1.99	0.45
9:L:108:THR:HG23	11:W:59:VAL:HG23	1.98	0.45
9:L:223:GLN:O	9:L:226:ARG:HG3	2.16	0.45
13:S:26:PRO:HA	13:S:301:PRO:HG3	1.97	0.45
13:S:469:THR:HA	13:S:487:ASN:HA	1.98	0.45
5:O:15:ASN:ND2	5:O:250:SER:O	2.48	0.45
5:O:39:TYR:HB3	5:O:43:ILE:HG13	1.99	0.45
8:R:63:TYR:HB2	8:R:77:VAL:O	2.17	0.45
8:R:159:GLN:HA	8:R:172:SER:HA	1.98	0.45
1:A:226:ASN:O	1:A:230:ILE:HG12	2.16	0.45
2:B:210:TRP:HB3	2:B:218:ILE:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:GLU:HB2	3:C:87:TYR:CE1	2.51	0.45
5:E:377:ASP:OD1	5:E:377:ASP:N	2.49	0.45
6:F:178:GLU:O	6:F:181:GLU:HG3	2.17	0.45
8:I:63:TYR:HB2	8:I:77:VAL:O	2.16	0.45
8:I:319:VAL:HB	8:I:328:ASP:HB3	1.98	0.45
8:I:536:ASP:O	8:I:539:LEU:N	2.38	0.45
13:S:776:LEU:CD2	13:S:779:LYS:HD2	2.47	0.45
1:H:263:MET:HG2	1:H:286:VAL:HG21	1.99	0.45
1:H:575:PRO:HG3	1:H:605:TYR:HB3	1.99	0.45
1:H:619:HIS:ND1	1:H:624:VAL:HG13	2.32	0.45
8:R:249:THR:OG1	8:R:251:GLN:OE1	2.18	0.45
8:R:601:ARG:HA	8:R:601:ARG:HD3	1.71	0.45
13:V:274:ASN:HD21	13:V:281:GLU:HG2	1.82	0.45
13:V:499:GLN:HG3	13:V:500:ARG:HD3	1.98	0.45
1:A:548:ALA:HB2	1:A:563:TRP:HB2	1.99	0.45
2:B:95:GLU:OE1	2:B:103:ASN:ND2	2.49	0.45
2:B:180:GLY:HA2	2:B:223:SER:HB2	1.98	0.45
3:C:297:LYS:HA	3:C:300:PHE:HD2	1.82	0.45
3:C:425:TYR:HB3	3:C:430:LEU:HB2	1.98	0.45
5:E:304:ALA:HA	5:E:307:LEU:HD12	1.98	0.45
13:S:176:HIS:HB2	13:S:180:ALA:HB3	1.98	0.45
13:S:586:ASP:HA	13:S:591:THR:HA	1.97	0.45
3:K:127:ASP:OD1	3:K:127:ASP:N	2.45	0.45
3:K:143:PRO:HG2	3:K:173:LEU:HD13	1.99	0.45
3:K:367:PHE:CE1	3:K:421:MET:HB2	2.52	0.45
3:K:373:LEU:HD23	3:K:376:ARG:HH11	1.82	0.45
3:K:559:ILE:HG13	3:K:602:GLU:HG3	1.98	0.45
7:Q:233:LEU:HD22	7:Q:236:ARG:HH21	1.82	0.45
8:R:13:HIS:NE2	8:R:30:THR:OG1	2.33	0.45
8:R:282:GLN:HE21	8:R:294:PHE:HB3	1.81	0.45
13:V:892:LYS:HA	13:V:895:ILE:HD12	1.98	0.45
1:A:296:GLY:HA2	1:A:299:LEU:HD12	1.99	0.45
3:C:97:TYR:CZ	3:C:124:GLU:HG2	2.51	0.45
3:C:195:PRO:HA	3:C:198:LYS:HG3	1.99	0.45
3:C:265:ASP:OD1	3:C:265:ASP:N	2.50	0.45
6:F:321:ILE:HA	6:F:324:ILE:HG12	1.98	0.45
1:H:479:LYS:HZ2	1:H:482:VAL:HG11	1.81	0.45
3:K:38:TYR:HD1	3:K:41:GLN:HE21	1.65	0.45
5:O:263:ASN:HA	5:O:266:VAL:HG22	1.99	0.45
6:P:210:LEU:O	6:P:214:GLN:NE2	2.50	0.45
6:P:262:GLU:HA	6:P:265:ASN:HD22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:290:GLN:O	6:P:294:SER:N	2.49	0.45
9:T:46:TYR:CZ	9:T:104:LEU:HB2	2.51	0.45
11:Y:93:MET:O	11:Y:97:LYS:HG2	2.16	0.45
13:V:137:LYS:O	13:V:139:ARG:NH1	2.50	0.45
13:V:449:GLN:HB3	13:V:458:SER:HB2	1.97	0.45
13:V:902:LYS:O	13:V:906:ILE:HG12	2.16	0.45
1:A:477:VAL:HG13	1:A:496:PHE:CE1	2.52	0.45
1:A:489:LEU:HD12	1:A:520:LEU:HD13	1.98	0.45
1:A:493:ARG:O	1:A:497:ASN:ND2	2.50	0.45
5:E:8:PRO:HG2	5:E:69:HIS:CG	2.52	0.45
6:F:139:LYS:HD3	6:F:139:LYS:HA	1.73	0.45
8:I:119:LEU:HB2	8:I:131:TRP:HB2	1.98	0.45
8:I:193:ASP:HB2	8:I:233:VAL:HG23	1.99	0.45
9:L:168:VAL:HA	9:L:171:HIS:CE1	2.52	0.45
10:M:314:HIS:HA	10:M:317:LYS:HG2	1.99	0.45
13:S:274:ASN:HD21	13:S:281:GLU:HG2	1.82	0.45
1:H:257:GLU:HB3	3:K:646:ARG:HH22	1.81	0.45
1:H:478:ASN:O	1:H:482:VAL:HG23	2.17	0.45
2:J:326:LYS:HD2	2:J:326:LYS:HA	1.74	0.45
3:K:634:GLU:O	3:K:638:LEU:N	2.48	0.45
6:P:169:LEU:HD11	7:Q:175:ASP:HB3	1.99	0.45
8:R:42:MET:HE2	8:R:42:MET:N	2.32	0.45
8:R:510:HIS:HB2	8:R:515:MET:HB2	1.99	0.45
9:T:73:MET:SD	9:T:81:LEU:HB2	2.56	0.45
11:Y:81:GLU:HA	11:Y:84:LYS:HE2	1.98	0.45
12:Z:457:GLU:O	12:Z:461:GLN:HG2	2.17	0.45
13:V:774:ILE:HA	13:V:777:TYR:HB2	1.98	0.45
13:V:848:LEU:HD23	13:V:860:ILE:HD11	1.97	0.45
1:A:444:ASN:ND2	2:B:287:GLN:OE1	2.50	0.45
3:C:634:GLU:O	3:C:638:LEU:N	2.49	0.45
5:E:159:SER:OG	5:E:195:CYS:SG	2.72	0.45
6:F:290:GLN:O	6:F:294:SER:N	2.50	0.45
8:I:69:LYS:NZ	8:I:155:TYR:OH	2.35	0.45
13:S:77:SER:O	13:S:77:SER:OG	2.33	0.45
13:S:693:ALA:HB1	13:S:699:TRP:HB2	1.98	0.45
1:H:435:PRO:HA	1:H:438:LYS:HB2	1.99	0.45
2:J:54:ARG:NH2	2:J:75:MET:SD	2.90	0.45
2:J:427:GLY:HA2	4:N:253:TRP:HA	1.98	0.45
4:N:219:GLN:HA	4:N:222:ILE:HD12	1.99	0.45
8:R:522:GLN:HE22	8:R:554:LYS:HA	1.81	0.45
8:R:536:ASP:O	8:R:539:LEU:N	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:922:ILE:HA	13:V:925:HIS:HB3	1.99	0.45
3:C:150:GLY:HA2	3:C:165:LYS:HD3	1.99	0.44
5:E:4:SER:HB3	5:E:133:ARG:HE	1.81	0.44
13:S:160:VAL:HA	13:S:176:HIS:HA	1.99	0.44
1:H:258:VAL:HA	1:H:261:LYS:HD2	1.99	0.44
3:K:298:LEU:HD22	3:K:315:LEU:HD13	1.99	0.44
8:R:482:ASP:OD1	8:R:482:ASP:N	2.49	0.44
9:T:123:ASP:HA	10:U:306:TRP:N	2.32	0.44
12:Z:485:ILE:O	12:Z:489:LYS:HG2	2.17	0.44
13:V:330:LYS:O	13:V:346:LEU:N	2.43	0.44
1:A:496:PHE:CE2	1:A:516:VAL:HG21	2.52	0.44
2:B:69:THR:OG1	2:B:70:ALA:N	2.48	0.44
2:B:391:TYR:OH	5:E:26:LYS:NZ	2.33	0.44
3:C:326:PHE:HB3	3:C:329:LEU:HD11	1.99	0.44
4:D:309:LYS:O	4:D:315:ARG:NH1	2.48	0.44
6:F:44:ILE:HD11	6:F:68:PHE:HZ	1.82	0.44
9:L:283:GLN:O	9:L:286:ARG:NH1	2.50	0.44
13:S:375:ALA:O	13:S:382:LEU:N	2.44	0.44
1:H:387:PHE:HB2	1:H:410:LYS:HZ2	1.82	0.44
1:H:399:TYR:HB3	1:H:402:LEU:HD13	1.98	0.44
5:O:138:ASP:OD1	5:O:138:ASP:N	2.51	0.44
8:R:427:ASP:N	8:R:427:ASP:OD1	2.49	0.44
9:T:243:ARG:HH22	10:U:415:ALA:HA	1.82	0.44
13:V:67:ILE:H	13:V:85:SER:HB3	1.82	0.44
13:V:873:GLN:NE2	13:V:875:ASP:OD1	2.51	0.44
1:A:430:PHE:O	1:A:432:LYS:N	2.51	0.44
1:A:474:ARG:NH2	1:A:508:GLU:OE1	2.50	0.44
1:A:602:HIS:HB2	1:A:611:VAL:HG11	1.98	0.44
3:C:298:LEU:HD22	3:C:315:LEU:HD13	1.99	0.44
5:E:349:VAL:O	5:E:352:SER:OG	2.30	0.44
8:I:652:THR:O	8:I:656:ARG:NH1	2.50	0.44
13:S:677:GLU:HB2	13:S:685:ALA:HA	1.98	0.44
8:R:19:ALA:HB3	8:R:31:CYS:HB2	1.98	0.44
8:R:76:ASP:O	8:R:92:ARG:N	2.49	0.44
8:R:695:ARG:HA	8:R:695:ARG:HD2	1.70	0.44
13:V:374:ILE:HG12	13:V:383:MET:SD	2.58	0.44
13:V:1080:ALA:HA	13:V:1083:VAL:HG12	2.00	0.44
1:A:254:THR:OG1	1:A:255:ALA:N	2.49	0.44
1:A:467:LYS:HZ2	6:F:304:GLU:CD	2.21	0.44
3:C:377:HIS:CD2	3:C:414:TYR:HB2	2.53	0.44
3:C:575:TYR:HA	3:C:578:LYS:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:273:LEU:HB3	4:D:277:THR:HB	2.00	0.44
8:I:85:GLY:O	8:I:102:GLY:N	2.34	0.44
8:I:196:PRO:HD2	8:I:197:ILE:HD12	1.99	0.44
13:S:902:LYS:O	13:S:906:ILE:HG12	2.17	0.44
1:H:449:TYR:CD1	1:H:449:TYR:C	2.91	0.44
5:O:26:LYS:HB3	5:O:26:LYS:HE2	1.80	0.44
5:O:282:ASP:OD1	5:O:288:ARG:NH1	2.50	0.44
8:R:69:LYS:HE2	8:R:413:ARG:HH22	1.83	0.44
8:R:153:TRP:HA	8:R:160:LEU:HG	1.99	0.44
8:R:340:VAL:HG22	8:R:349:VAL:HG23	1.99	0.44
8:R:596:TRP:CE2	12:Z:503:LEU:HD11	2.53	0.44
13:V:106:ILE:HB	13:V:109:LYS:HZ1	1.82	0.44
13:V:568:LYS:HD2	13:V:568:LYS:HA	1.76	0.44
13:V:868:LEU:HB2	13:V:877:ALA:HB2	1.98	0.44
2:B:14:SER:HB3	2:B:61:LEU:HD13	2.00	0.44
3:C:554:GLY:O	3:C:558:ILE:HG12	2.18	0.44
8:I:501:ALA:HB1	8:I:520:VAL:HG21	1.99	0.44
8:I:554:LYS:O	8:I:571:SER:OG	2.26	0.44
9:L:280:MET:O	9:L:283:GLN:HG3	2.18	0.44
13:S:790:VAL:HG23	13:S:791:MET:SD	2.57	0.44
13:S:1052:ARG:NH1	10:U:362:GLN:OE1	2.50	0.44
1:H:161:LYS:HZ1	1:H:168:ARG:HH22	1.65	0.44
1:H:244:TYR:CZ	1:H:265:ASN:HB3	2.53	0.44
1:H:369:ALA:HA	1:H:372:LEU:HG	1.99	0.44
3:K:243:PHE:HA	3:K:246:LYS:HG2	1.99	0.44
5:O:5:LYS:HG2	5:O:105:GLY:HA2	2.00	0.44
7:Q:294:ASP:C	7:Q:298:LYS:HZ1	2.20	0.44
8:R:432:LEU:HD23	8:R:434:GLN:HG3	2.00	0.44
8:R:456:TRP:HE1	8:R:458:HIS:CE1	2.36	0.44
9:T:101:ALA:O	9:T:105:TYR:HB2	2.17	0.44
9:T:134:LYS:NZ	10:U:311:ASP:OD2	2.34	0.44
11:Y:119:GLU:HB2	12:Z:495:ASN:HD21	1.81	0.44
13:V:412:CYS:O	13:V:423:VAL:N	2.49	0.44
13:V:748:LEU:O	13:V:752:LEU:HB3	2.17	0.44
5:E:1:MET:HB2	5:E:191:TYR:HD1	1.83	0.44
6:F:170:LYS:HD2	6:F:170:LYS:HA	1.80	0.44
8:I:340:VAL:HG22	8:I:349:VAL:HG23	2.00	0.44
9:L:299:LEU:O	9:L:303:ARG:N	2.51	0.44
12:X:455:ALA:HA	12:X:458:LEU:HG	2.00	0.44
13:S:106:ILE:HB	13:S:109:LYS:HZ1	1.82	0.44
1:H:208:TYR:HB3	1:H:223:LEU:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:519:ARG:HE	2:J:279:ALA:HB1	1.83	0.44
2:J:53:LEU:HB3	2:J:54:ARG:HH11	1.82	0.44
3:K:50:LEU:HB3	3:K:73:LEU:HD21	1.98	0.44
3:K:73:LEU:HD22	3:K:83:TYR:CZ	2.52	0.44
5:O:36:LYS:HA	5:O:217:PRO:HD2	2.00	0.44
5:O:310:ASP:N	5:O:310:ASP:OD1	2.50	0.44
8:R:196:PRO:HD2	8:R:197:ILE:HD12	2.00	0.44
8:R:525:CYS:HB2	8:R:544:ARG:HE	1.83	0.44
10:U:434:ASP:HA	10:U:437:VAL:HG22	1.99	0.44
1:A:273:MET:SD	1:A:273:MET:N	2.87	0.44
1:A:399:TYR:HB3	1:A:402:LEU:HD13	1.99	0.44
3:C:169:ALA:O	3:C:173:LEU:HB2	2.17	0.44
3:C:211:HIS:CE1	3:C:214:LEU:HB2	2.52	0.44
5:E:266:VAL:HG21	5:E:290:ASN:HD21	1.82	0.44
6:F:213:GLN:HE21	7:G:218:LEU:HD11	1.83	0.44
12:X:457:GLU:O	12:X:461:GLN:HG2	2.18	0.44
12:X:501:LYS:O	12:X:505:MET:HG2	2.18	0.44
1:H:181:LEU:HG	1:H:185:TYR:HD2	1.83	0.44
1:H:410:LYS:HE3	1:H:413:ARG:NH2	2.33	0.44
1:H:592:ALA:HA	1:H:595:LEU:HG	2.00	0.44
3:K:169:ALA:O	3:K:173:LEU:HB2	2.18	0.44
3:K:169:ALA:O	3:K:173:LEU:HB3	2.17	0.44
3:K:283:ALA:O	3:K:287:MET:HG2	2.18	0.44
3:K:447:GLU:HB3	3:K:452:LYS:HG3	2.00	0.44
5:O:8:PRO:HG2	5:O:69:HIS:CG	2.53	0.44
8:R:343:GLY:HA3	8:R:380:GLN:NE2	2.33	0.44
8:R:440:THR:HA	8:R:457:GLN:HA	2.00	0.44
11:Y:65:GLU:HB3	12:Z:443:TRP:HB3	1.98	0.44
13:V:174:SER:HB2	13:V:182:TRP:HB2	2.00	0.44
2:B:236:GLU:O	2:B:240:ILE:N	2.49	0.44
3:C:309:PRO:HB3	3:C:344:LEU:HG	1.99	0.44
5:E:39:TYR:HB3	5:E:43:ILE:HG13	2.00	0.44
6:F:280:PRO:HA	6:F:283:VAL:HG22	2.00	0.44
7:G:315:ARG:O	7:G:319:LEU:HB2	2.17	0.44
8:I:132:SER:HB3	8:I:138:ARG:HB2	2.00	0.44
8:I:474:ASN:OD1	8:I:475:ASP:N	2.50	0.44
8:I:508:ARG:NH1	8:I:561:PHE:HB3	2.33	0.44
9:L:59:GLU:OE1	9:L:87:TYR:OH	2.29	0.44
9:L:186:ALA:HB1	10:M:363:TYR:HD2	1.83	0.44
1:H:304:TYR:O	1:H:304:TYR:CD1	2.70	0.44
4:N:242:ARG:NH2	4:N:245:GLU:HA	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:226:LYS:O	5:O:230:HIS:ND1	2.51	0.44
6:P:186:LYS:HZ3	7:Q:192:LEU:HB3	1.83	0.44
7:Q:153:VAL:HA	7:Q:156:ASN:ND2	2.33	0.44
8:R:425:SER:OG	8:R:476:ARG:NE	2.51	0.44
10:U:342:LEU:HA	10:U:345:LEU:HB2	2.00	0.44
12:Z:410:GLU:O	12:Z:414:LYS:N	2.43	0.44
13:V:819:ALA:O	13:V:822:LEU:HB3	2.18	0.44
1:A:180:ASN:OD1	1:A:181:LEU:N	2.51	0.44
1:A:369:ALA:HA	1:A:372:LEU:HG	2.00	0.44
1:A:422:LYS:HD2	1:A:422:LYS:HA	1.79	0.44
2:B:427:GLY:HA2	4:D:253:TRP:HA	2.00	0.44
6:F:275:VAL:HG22	7:G:289:PHE:CZ	2.53	0.44
13:S:1100:TRP:HA	13:S:1103:THR:HG22	1.99	0.44
2:J:188:PRO:O	2:J:210:TRP:CD1	2.71	0.44
2:J:210:TRP:HB3	2:J:218:ILE:HG12	1.99	0.44
5:O:101:LEU:HA	5:O:104:MET:SD	2.58	0.44
8:R:347:LEU:N	8:R:358:TYR:O	2.41	0.44
8:R:395:GLN:OE1	8:R:408:ARG:NH2	2.51	0.44
8:R:627:THR:HA	8:R:630:VAL:HG12	1.99	0.44
11:Y:83:ARG:NH2	11:Y:87:GLN:OE1	2.40	0.44
13:V:489:ASP:OD1	13:V:490:THR:N	2.50	0.44
13:V:790:VAL:HG12	13:V:798:TRP:CE2	2.53	0.44
13:V:817:GLU:HA	13:V:835:SER:HB3	1.99	0.44
13:V:848:LEU:HD22	13:V:854:PRO:HA	2.00	0.44
13:V:864:TRP:HE3	13:V:880:HIS:CE1	2.36	0.44
1:A:653:TYR:HE2	1:A:665:LYS:HG2	1.83	0.43
2:B:411:LYS:HD3	2:B:415:SER:HB3	2.00	0.43
3:C:190:THR:HG1	3:C:192:GLN:CD	2.15	0.43
3:C:257:GLU:O	3:C:260:LYS:HB2	2.18	0.43
3:C:349:LEU:HA	3:C:352:TYR:HB2	2.00	0.43
5:E:97:SER:HB2	5:E:113:GLN:NE2	2.33	0.43
8:I:282:GLN:HE21	8:I:294:PHE:HB3	1.84	0.43
1:H:304:TYR:HB2	1:H:308:ASP:OD1	2.18	0.43
2:J:426:MET:HE1	4:N:287:ASP:H	1.82	0.43
6:P:322:THR:O	6:P:325:GLN:HG3	2.18	0.43
8:R:248:ASN:O	8:R:265:LEU:N	2.51	0.43
8:R:370:ASP:N	8:R:370:ASP:OD1	2.47	0.43
1:A:193:HIS:ND1	2:B:309:THR:OG1	2.51	0.43
1:A:311:GLY:O	1:A:315:ALA:HB3	2.18	0.43
1:A:677:VAL:HA	1:A:680:LEU:HD12	2.00	0.43
2:B:183:LEU:O	2:B:204:ARG:NH1	2.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:238:TYR:CE2	7:G:239:LEU:HB3	2.50	0.43
8:I:227:ASP:OD1	8:I:227:ASP:N	2.51	0.43
8:I:720:ASN:ND2	13:V:649:GLU:HG3	2.32	0.43
9:L:123:ASP:HA	10:M:306:TRP:N	2.33	0.43
11:W:83:ARG:NH1	11:W:87:GLN:HG2	2.34	0.43
1:H:198:ASN:O	1:H:200:ASN:N	2.47	0.43
3:K:517:LYS:HA	3:K:517:LYS:HD2	1.78	0.43
5:O:97:SER:HB2	5:O:113:GLN:HE22	1.83	0.43
6:P:324:ILE:HA	6:P:327:ARG:HE	1.83	0.43
8:R:398:THR:HG23	8:R:400:GLU:H	1.82	0.43
8:R:602:LEU:HB2	8:R:606:ILE:HD13	2.00	0.43
9:T:90:ASP:N	9:T:90:ASP:OD1	2.51	0.43
13:V:367:ILE:HG13	13:V:373:LEU:HA	2.00	0.43
13:V:580:ARG:HA	13:V:601:ILE:HD13	1.99	0.43
2:B:28:LYS:HA	2:B:31:PHE:HD2	1.83	0.43
2:B:186:GLN:C	2:B:188:PRO:HD3	2.38	0.43
5:E:7:ARG:HE	5:E:71:GLY:HA2	1.83	0.43
5:E:166:HIS:ND1	5:E:169:GLU:OE1	2.51	0.43
5:E:174:TYR:HH	5:E:195:CYS:HG	1.62	0.43
5:E:438:TYR:OH	5:E:450:ARG:NH1	2.52	0.43
7:G:195:TYR:HA	7:G:198:VAL:HG22	2.00	0.43
8:I:307:MET:HE3	8:I:360:THR:HB	2.00	0.43
13:S:568:LYS:HD2	13:S:568:LYS:HA	1.76	0.43
1:H:304:TYR:CE2	2:J:296:TRP:CZ2	3.07	0.43
1:H:551:TYR:OH	1:H:559:ASN:ND2	2.46	0.43
2:J:69:THR:OG1	2:J:70:ALA:N	2.49	0.43
8:R:47:GLU:HG3	13:V:900:PHE:CE2	2.53	0.43
8:R:505:ASP:OD1	8:R:519:MET:HB3	2.19	0.43
10:U:452:ARG:NE	10:U:456:LEU:HG	2.34	0.43
1:A:312:MET:HG3	1:A:376:LYS:HZ2	1.83	0.43
1:A:390:CYS:HA	1:A:393:GLN:HE21	1.83	0.43
1:A:605:TYR:CZ	1:A:607:VAL:HB	2.53	0.43
4:D:308:PHE:CE2	4:D:314:PHE:HB3	2.53	0.43
8:I:60:MET:HG2	8:I:80:VAL:HG22	1.99	0.43
13:S:841:ALA:O	13:S:845:ALA:N	2.51	0.43
1:H:470:ARG:HB2	1:H:475:ALA:HB3	2.00	0.43
3:K:70:TYR:HB3	3:K:87:TYR:HB2	2.00	0.43
3:K:101:SER:HA	3:K:104:VAL:HG12	2.00	0.43
3:K:418:LEU:HD12	3:K:421:MET:SD	2.59	0.43
4:N:318:MET:O	4:N:322:ASN:ND2	2.51	0.43
6:P:170:LYS:HD2	6:P:170:LYS:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:213:GLN:HE21	7:Q:218:LEU:HD11	1.83	0.43
9:T:166:ARG:HD3	9:T:166:ARG:HA	1.66	0.43
13:V:836:TYR:HB2	13:V:845:ALA:HB2	2.01	0.43
2:B:89:LEU:HD13	2:B:221:LEU:HB2	2.00	0.43
3:C:641:MET:SD	3:C:641:MET:N	2.89	0.43
4:D:226:ASN:O	4:D:229:HIS:NE2	2.51	0.43
6:F:224:ILE:HG22	7:G:229:VAL:HG22	2.00	0.43
6:F:272:ARG:HA	6:F:275:VAL:HG12	1.99	0.43
8:I:460:LEU:HD12	8:I:460:LEU:HA	1.92	0.43
8:I:600:THR:O	8:I:604:ARG:HG2	2.17	0.43
8:I:601:ARG:HD3	8:I:601:ARG:HA	1.56	0.43
8:I:646:LYS:HD3	8:I:646:LYS:HA	1.59	0.43
9:L:53:ALA:O	9:L:62:ARG:NH2	2.47	0.43
11:W:94:LEU:HD12	11:W:94:LEU:HA	1.79	0.43
13:S:762:ALA:HB2	13:S:785:ARG:HH11	1.83	0.43
13:S:775:GLY:O	13:S:779:LYS:HG3	2.18	0.43
13:S:962:GLN:HB2	13:S:966:ARG:NH2	2.33	0.43
13:S:1021:GLN:HA	13:S:1024:ARG:HB3	2.00	0.43
1:H:131:LYS:HA	1:H:131:LYS:HD3	1.83	0.43
1:H:288:ASP:OD1	1:H:288:ASP:N	2.46	0.43
7:Q:143:LEU:HG	7:Q:147:ARG:NH1	2.33	0.43
8:R:322:ILE:HG23	12:Z:479:LYS:NZ	2.33	0.43
9:T:136:ILE:HD13	12:Z:410:GLU:HG3	1.99	0.43
13:V:368:TYR:CD1	13:V:374:ILE:HD12	2.52	0.43
13:V:471:ARG:CZ	13:V:482:THR:HB	2.48	0.43
1:A:449:TYR:O	1:A:452:GLU:HG2	2.19	0.43
5:E:310:ASP:OD1	5:E:310:ASP:N	2.51	0.43
8:I:248:ASN:O	8:I:265:LEU:N	2.52	0.43
13:S:531:GLN:N	13:S:545:GLN:O	2.47	0.43
1:H:125:GLN:O	1:H:129:MET:HG2	2.19	0.43
1:H:161:LYS:HD2	1:H:161:LYS:HA	1.85	0.43
1:H:238:PRO:HA	1:H:241:ILE:HG12	2.01	0.43
3:K:309:PRO:HB3	3:K:344:LEU:HG	2.00	0.43
3:K:368:ARG:O	3:K:372:GLU:HG3	2.19	0.43
6:P:290:GLN:HA	6:P:293:LEU:HB2	2.00	0.43
7:Q:158:LYS:HA	7:Q:158:LYS:HD2	1.72	0.43
7:Q:174:MET:SD	7:Q:177:ARG:NH2	2.89	0.43
8:R:476:ARG:HA	8:R:476:ARG:HD3	1.85	0.43
2:B:188:PRO:O	2:B:210:TRP:CD1	2.71	0.43
2:B:326:LYS:HD2	2:B:326:LYS:HA	1.79	0.43
3:C:187:TYR:CD2	3:C:195:PRO:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:SER:HB2	6:F:104:VAL:HG21	2.00	0.43
8:I:643:PHE:HA	13:V:695:LEU:HD23	2.01	0.43
9:L:134:LYS:HD3	9:L:134:LYS:HA	1.88	0.43
3:K:97:TYR:CZ	3:K:124:GLU:HG2	2.54	0.43
3:K:535:CYS:HA	3:K:538:ASN:ND2	2.33	0.43
5:O:355:GLU:HG2	5:O:360:PRO:HG2	2.01	0.43
8:R:60:MET:HG2	8:R:80:VAL:HG22	2.01	0.43
8:R:300:LEU:HB3	8:R:311:VAL:HB	2.00	0.43
8:R:596:TRP:HA	8:R:599:ALA:HB3	2.00	0.43
8:R:658:ALA:HB2	8:R:673:ILE:HG13	2.01	0.43
9:T:214:GLU:HA	9:T:217:LYS:HG2	2.00	0.43
11:Y:115:LYS:HG2	12:Z:495:ASN:ND2	2.34	0.43
13:V:25:ALA:HA	13:V:73:PHE:HD2	1.83	0.43
13:V:609:ASP:OD2	13:V:614:ARG:NH1	2.52	0.43
1:A:130:GLU:O	1:A:134:HIS:ND1	2.51	0.43
1:A:531:LYS:NZ	1:A:547:ILE:HG23	2.34	0.43
5:E:26:LYS:HE2	5:E:26:LYS:HB3	1.83	0.43
5:E:62:TRP:HD1	5:E:63:LEU:HD22	1.84	0.43
8:I:691:PHE:N	13:V:665:HIS:HE1	2.16	0.43
13:S:489:ASP:OD1	13:S:490:THR:N	2.50	0.43
13:S:816:TYR:HE2	13:S:834:GLN:HB3	1.84	0.43
1:H:507:VAL:O	1:H:511:TYR:HB3	2.19	0.43
1:H:541:VAL:HA	1:H:544:ILE:HD13	1.99	0.43
1:H:574:ASP:OD2	1:H:577:VAL:N	2.46	0.43
1:H:595:LEU:HA	1:H:598:TYR:CD2	2.53	0.43
2:J:95:GLU:OE1	2:J:103:ASN:ND2	2.52	0.43
2:J:133:LEU:HD22	2:J:176:VAL:HG22	2.01	0.43
8:R:522:GLN:NE2	8:R:553:GLY:O	2.51	0.43
10:U:417:PRO:HA	10:U:420:ARG:NE	2.34	0.43
13:V:9:ILE:HG21	13:V:43:PHE:CE2	2.54	0.43
13:V:176:HIS:HB2	13:V:180:ALA:HB3	2.00	0.43
13:V:555:SER:N	13:V:627:GLU:OE1	2.31	0.43
1:A:130:GLU:HG3	1:A:134:HIS:CE1	2.54	0.43
1:A:192:ALA:N	1:A:208:TYR:OH	2.52	0.43
1:A:395:ARG:HG2	1:A:400:THR:HA	2.00	0.43
1:A:435:PRO:HA	1:A:438:LYS:HB2	2.00	0.43
2:B:116:ASP:OD1	2:B:116:ASP:N	2.51	0.43
3:C:485:LEU:HD21	3:C:519:GLU:HA	2.01	0.43
3:C:528:ASP:OD1	3:C:528:ASP:N	2.49	0.43
3:C:596:LYS:HD2	3:C:596:LYS:HA	1.88	0.43
7:G:150:ILE:HA	7:G:153:VAL:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:29:PHE:CZ	8:I:39:LYS:HE2	2.54	0.43
8:I:377:LEU:HD12	8:I:419:ALA:HB2	2.01	0.43
9:L:122:ILE:HD11	11:W:48:VAL:HG21	2.00	0.43
11:W:66:LYS:NZ	11:W:73:ARG:HH22	2.17	0.43
1:H:475:ALA:HA	1:H:478:ASN:HB2	2.01	0.43
1:H:577:VAL:HA	1:H:580:ARG:HE	1.84	0.43
2:J:318:LEU:HA	2:J:321:LYS:HZ2	1.84	0.43
3:K:554:GLY:O	3:K:558:ILE:HG12	2.19	0.43
5:O:50:ARG:HG2	5:O:54:ARG:HD3	2.01	0.43
8:R:130:ILE:O	8:R:138:ARG:N	2.52	0.43
9:T:186:ALA:HB2	10:U:364:ARG:NH1	2.34	0.43
9:T:204:ARG:HA	9:T:204:ARG:HD3	1.88	0.43
1:A:206:ASN:OD1	1:A:207:LEU:N	2.52	0.43
1:A:225:VAL:HG21	1:A:264:ARG:HH22	1.84	0.43
1:A:447:PHE:HE2	2:B:286:LEU:HB2	1.82	0.43
1:A:449:TYR:CD1	1:A:449:TYR:C	2.91	0.43
6:F:16:PHE:HE1	6:F:40:VAL:HA	1.84	0.43
8:I:565:ARG:HA	8:I:579:ALA:HA	2.00	0.43
8:I:601:ARG:HG3	13:V:755:GLY:HA3	2.00	0.43
8:I:643:PHE:HB3	8:I:660:LEU:HA	2.00	0.43
8:I:655:GLY:HA2	8:I:658:ALA:HB3	2.01	0.43
9:L:26:ASN:HB2	9:L:35:VAL:HG13	2.01	0.43
11:W:79:LEU:HB3	12:X:461:GLN:HE21	1.84	0.43
11:W:121:MET:SD	12:X:499:LEU:HD13	2.59	0.43
13:S:154:HIS:CE1	13:S:156:GLU:HB2	2.54	0.43
1:H:444:ASN:ND2	2:J:287:GLN:OE1	2.51	0.43
1:H:619:HIS:CG	1:H:628:ALA:HB2	2.54	0.43
8:R:103:HIS:NE2	8:R:127:SER:O	2.51	0.43
8:R:124:GLU:HG3	9:T:2:SER:HB2	2.00	0.43
8:R:385:PHE:HE2	8:R:399:TYR:HA	1.84	0.43
13:V:878:ILE:O	13:V:882:ILE:HG12	2.19	0.43
1:A:161:LYS:HA	1:A:161:LYS:HD2	1.79	0.42
1:A:241:ILE:HG13	1:A:245:ARG:HH12	1.83	0.42
3:C:267:PRO:HA	3:C:268:PRO:HD3	1.88	0.42
3:C:550:ASN:OD1	3:C:550:ASN:N	2.52	0.42
5:E:260:ILE:HA	5:E:263:ASN:HD21	1.84	0.42
8:I:587:LEU:HA	8:I:590:MET:HG2	2.01	0.42
9:L:105:TYR:CE1	11:W:60:GLU:HG2	2.54	0.42
3:K:181:TYR:OH	3:K:241:GLU:HG2	2.18	0.42
5:O:438:TYR:OH	5:O:450:ARG:NH1	2.52	0.42
8:R:688:ILE:CG2	8:R:706:HIS:HE1	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:243:ARG:NH2	10:U:414:ASP:O	2.52	0.42
13:V:198:GLN:NE2	13:V:200:VAL:O	2.52	0.42
13:V:1076:GLN:HG3	13:V:1079:ASP:H	1.84	0.42
1:A:239:SER:O	1:A:243:MET:HG3	2.20	0.42
1:A:261:LYS:HG2	1:A:264:ARG:HH21	1.84	0.42
2:B:204:ARG:NH1	2:B:205:PRO:O	2.52	0.42
5:E:266:VAL:HG21	5:E:290:ASN:ND2	2.34	0.42
11:W:125:LEU:HA	11:W:125:LEU:HD23	1.70	0.42
13:S:235:ARG:NH1	13:S:280:TRP:O	2.52	0.42
13:S:471:ARG:CZ	13:S:482:THR:HB	2.49	0.42
13:S:892:LYS:HG3	13:S:918:TYR:CE2	2.54	0.42
13:S:898:ARG:NH2	13:S:899:GLN:OE1	2.52	0.42
1:H:262:ILE:O	1:H:266:ILE:HG12	2.19	0.42
3:K:246:LYS:HA	3:K:249:ILE:HG22	2.01	0.42
3:K:265:ASP:OD1	3:K:265:ASP:N	2.52	0.42
3:K:452:LYS:NZ	3:K:472:TYR:O	2.33	0.42
5:O:213:LEU:HD11	5:O:226:LYS:HE3	2.01	0.42
6:P:139:LYS:HD3	6:P:139:LYS:HA	1.71	0.42
6:P:320:GLN:O	6:P:323:GLU:HG2	2.18	0.42
8:R:458:HIS:NE2	8:R:480:VAL:HG21	2.34	0.42
9:T:186:ALA:HB1	10:U:363:TYR:HD2	1.83	0.42
3:C:368:ARG:O	3:C:372:GLU:HG3	2.20	0.42
6:F:37:LEU:HD13	6:F:37:LEU:HA	1.90	0.42
6:F:322:THR:O	6:F:325:GLN:HG3	2.19	0.42
7:G:233:LEU:HD23	7:G:236:ARG:HE	1.85	0.42
7:G:256:SER:HA	7:G:259:GLN:HE22	1.84	0.42
8:I:33:ASP:OD1	9:L:7:ARG:NH2	2.29	0.42
8:I:84:ASP:OD1	8:I:84:ASP:N	2.48	0.42
8:I:130:ILE:O	8:I:138:ARG:N	2.52	0.42
8:I:398:THR:HG23	8:I:400:GLU:H	1.83	0.42
8:I:651:PRO:HB3	8:I:656:ARG:HH22	1.84	0.42
9:L:12:VAL:HG12	9:L:16:LEU:HD12	2.01	0.42
10:M:434:ASP:HA	10:M:437:VAL:HG22	2.00	0.42
13:S:919:PHE:HD2	13:S:942:ALA:HB2	1.83	0.42
1:H:210:ALA:O	1:H:214:ASN:ND2	2.52	0.42
1:H:264:ARG:HB2	2:J:303:SER:O	2.19	0.42
1:H:391:CYS:O	1:H:395:ARG:HG3	2.20	0.42
6:P:66:ILE:HD13	6:P:66:ILE:HA	1.94	0.42
6:P:122:PHE:CE2	6:P:142:ILE:HD11	2.54	0.42
8:R:248:ASN:OD1	8:R:268:THR:N	2.48	0.42
13:V:864:TRP:HE3	13:V:880:HIS:HE1	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:OD1	1:A:215:LYS:N	2.49	0.42
2:B:424:TYR:HD2	4:D:308:PHE:HE1	1.68	0.42
3:C:430:LEU:HD13	3:C:433:ASN:HD21	1.84	0.42
3:C:459:PHE:HB2	3:C:469:ALA:HB2	2.00	0.42
8:I:209:LYS:HE2	8:I:209:LYS:HB3	1.85	0.42
8:I:604:ARG:CZ	8:I:635:ILE:HA	2.50	0.42
8:I:646:LYS:HB3	8:I:689:LYS:HD3	2.00	0.42
8:I:648:LYS:HA	8:I:656:ARG:HH21	1.85	0.42
13:S:410:ARG:HH21	13:S:448:VAL:H	1.66	0.42
1:H:619:HIS:HD1	1:H:624:VAL:HG13	1.85	0.42
3:K:450:VAL:O	3:K:453:LEU:HG	2.19	0.42
6:P:186:LYS:HB3	6:P:186:LYS:HE3	1.77	0.42
8:R:593:LYS:HE2	8:R:595:GLN:NE2	2.34	0.42
9:T:161:ARG:HA	9:T:164:ARG:HE	1.84	0.42
13:V:962:GLN:HB2	13:V:966:ARG:NH2	2.34	0.42
1:A:387:PHE:HE2	1:A:413:ARG:HH12	1.67	0.42
2:B:23:HIS:CD2	2:B:23:HIS:H	2.36	0.42
2:B:157:ASP:N	2:B:157:ASP:OD1	2.53	0.42
2:B:382:LYS:HE3	5:E:23:GLU:HB3	2.00	0.42
3:C:421:MET:HA	3:C:424:ILE:HB	2.02	0.42
3:C:559:ILE:HG13	3:C:602:GLU:HG3	2.00	0.42
3:C:588:LEU:HD21	3:C:595:LEU:HD23	2.01	0.42
5:E:8:PRO:O	5:E:69:HIS:HB3	2.20	0.42
5:E:187:SER:HB3	5:E:191:TYR:CE2	2.55	0.42
5:E:263:ASN:HA	5:E:266:VAL:HG22	2.02	0.42
8:I:658:ALA:HB2	8:I:673:ILE:HG13	2.01	0.42
10:M:444:HIS:O	10:M:447:LEU:HB3	2.19	0.42
11:W:87:GLN:O	11:W:91:GLU:HG2	2.20	0.42
13:S:577:HIS:CE1	13:S:582:GLU:HG2	2.53	0.42
13:S:709:GLN:OE1	13:S:711:LYS:NZ	2.46	0.42
13:S:1080:ALA:HA	13:S:1083:VAL:HG12	2.01	0.42
2:J:411:LYS:HB3	2:J:415:SER:HB3	2.02	0.42
8:R:710:VAL:HG12	8:R:730:PHE:CE1	2.55	0.42
9:T:5:GLU:HG2	9:T:94:VAL:HG11	2.01	0.42
13:V:18:LYS:NZ	13:V:20:THR:HG22	2.34	0.42
13:V:1025:LEU:O	13:V:1028:GLN:NE2	2.49	0.42
1:A:522:GLU:HG2	1:A:525:TYR:HD2	1.84	0.42
1:A:546:GLN:NE2	2:B:276:ALA:HB3	2.35	0.42
2:B:294:ARG:HE	2:B:298:SER:HB2	1.85	0.42
3:C:467:LYS:HB2	3:C:467:LYS:HE2	1.83	0.42
5:E:197:CYS:SG	5:E:229:ASN:ND2	2.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:252:TYR:O	6:F:256:SER:OG	2.30	0.42
9:L:151:TYR:HA	9:L:154:LEU:HG	2.01	0.42
10:M:372:ASP:O	10:M:376:THR:OG1	2.25	0.42
10:M:398:LEU:HB3	10:M:402:LYS:HZ3	1.84	0.42
1:H:148:ASP:N	1:H:197:MET:HG3	2.35	0.42
1:H:390:CYS:HA	1:H:393:GLN:HE21	1.84	0.42
2:J:91:SER:HB2	2:J:224:CYS:HB3	2.01	0.42
8:R:84:ASP:N	8:R:84:ASP:OD1	2.49	0.42
13:V:631:GLN:HE22	13:V:635:LEU:HD11	1.84	0.42
13:V:783:PRO:HB2	13:V:810:LEU:HD23	2.00	0.42
13:V:960:ALA:HB2	13:V:963:ARG:HH21	1.84	0.42
1:A:479:LYS:HB3	1:A:495:LEU:HD13	2.01	0.42
1:A:595:LEU:HA	1:A:598:TYR:CD2	2.55	0.42
1:A:644:LYS:HB3	1:A:644:LYS:HE2	1.86	0.42
1:A:658:ASN:O	1:A:662:ALA:N	2.42	0.42
2:B:105:PHE:HB3	2:B:109:PHE:CD2	2.54	0.42
2:B:358:PRO:HB3	3:C:86:TYR:CZ	2.54	0.42
4:D:274:ASP:H	4:D:277:THR:HB	1.84	0.42
5:E:218:ASP:OD1	5:E:218:ASP:N	2.53	0.42
8:I:643:PHE:CE2	8:I:663:TYR:HB3	2.54	0.42
9:L:90:ASP:N	9:L:90:ASP:OD1	2.51	0.42
13:S:847:ASP:OD1	13:S:848:LEU:N	2.52	0.42
13:S:915:ALA:HA	13:S:918:TYR:CD2	2.55	0.42
1:H:558:LYS:HE2	1:H:558:LYS:HB2	1.90	0.42
3:K:459:PHE:HB2	3:K:469:ALA:HB2	2.01	0.42
8:R:466:ALA:HB3	8:R:479:ILE:HD11	2.01	0.42
11:Y:113:LYS:H	11:Y:113:LYS:HD2	1.84	0.42
13:V:947:ASP:O	13:V:950:GLU:HG3	2.20	0.42
1:A:226:ASN:HA	2:B:307:PHE:CE1	2.55	0.42
2:B:400:LEU:HD21	4:D:305:TYR:HE2	1.85	0.42
5:E:33:PHE:HA	5:E:36:LYS:HD3	2.00	0.42
8:I:747:LYS:O	8:I:750:GLU:HG3	2.19	0.42
1:H:174:ASN:N	1:H:174:ASN:OD1	2.53	0.42
1:H:192:ALA:N	1:H:208:TYR:OH	2.53	0.42
1:H:464:MET:HG2	1:H:467:LYS:HZ3	1.85	0.42
5:O:266:VAL:HG21	5:O:290:ASN:HD21	1.84	0.42
7:Q:146:LYS:HB3	7:Q:147:ARG:NH2	2.34	0.42
8:R:47:GLU:O	13:V:929:THR:OG1	2.38	0.42
8:R:121:THR:HG22	8:R:131:TRP:CZ3	2.55	0.42
8:R:423:THR:OG1	8:R:465:ILE:O	2.32	0.42
11:Y:62:LEU:HD11	12:Z:436:MET:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:919:PHE:HD2	13:V:942:ALA:HB2	1.82	0.42
1:A:124:GLU:O	1:A:127:ARG:HD3	2.20	0.42
1:A:551:TYR:CE2	1:A:556:ASP:HB3	2.55	0.42
3:C:283:ALA:O	3:C:287:MET:HG2	2.20	0.42
3:C:316:LEU:HD13	3:C:319:TYR:HD2	1.85	0.42
5:E:295:HIS:HA	5:E:298:HIS:HD2	1.84	0.42
6:F:217:GLU:HG3	7:G:222:ASN:CG	2.39	0.42
8:I:129:LYS:HB2	8:I:131:TRP:CZ3	2.55	0.42
8:I:185:HIS:ND1	8:I:207:ASP:OD2	2.52	0.42
8:I:456:TRP:HE1	8:I:458:HIS:CE1	2.37	0.42
10:M:398:LEU:HA	10:M:401:VAL:HG12	2.01	0.42
13:S:137:LYS:HB3	13:S:153:ALA:HA	2.01	0.42
13:S:159:TYR:O	13:S:177:MET:N	2.53	0.42
13:S:727:ASP:N	13:S:727:ASP:OD1	2.53	0.42
13:S:908:GLU:HB2	13:S:938:TYR:CZ	2.55	0.42
1:H:422:LYS:HD2	1:H:422:LYS:HA	1.81	0.42
2:J:186:GLN:C	2:J:188:PRO:HD3	2.39	0.42
2:J:205:PRO:HD2	2:J:266:VAL:HG23	2.01	0.42
3:K:40:LEU:HD21	3:K:50:LEU:HG	2.02	0.42
6:P:260:LEU:O	6:P:263:THR:OG1	2.30	0.42
8:R:437:SER:OG	8:R:461:GLU:OE2	2.38	0.42
9:T:145:LYS:HG2	10:U:322:LYS:NZ	2.35	0.42
11:Y:66:LYS:NZ	11:Y:73:ARG:HH22	2.18	0.42
13:V:631:GLN:O	13:V:635:LEU:HG	2.20	0.42
13:V:677:GLU:HB2	13:V:685:ALA:HA	2.01	0.42
13:V:981:LYS:HE3	13:V:985:PHE:CZ	2.55	0.42
1:A:507:VAL:HG13	7:G:201:LYS:HD3	2.02	0.42
3:C:383:ARG:O	3:C:386:LYS:HG3	2.20	0.42
3:C:447:GLU:HB3	3:C:452:LYS:HG3	2.01	0.42
5:E:347:GLN:HG2	5:E:368:CYS:HB2	2.01	0.42
6:F:290:GLN:HA	6:F:293:LEU:HD12	2.01	0.42
8:I:81:ALA:HB1	8:I:107:CYS:HB3	2.01	0.42
8:I:211:LYS:HE2	8:I:222:GLN:HG3	2.01	0.42
8:I:218:ARG:HE	8:I:219:LEU:N	2.17	0.42
8:I:267:ASP:O	8:I:289:SER:OG	2.32	0.42
8:I:385:PHE:HE2	8:I:399:TYR:HA	1.84	0.42
8:I:598:LYS:HE2	12:X:496:ASP:CG	2.40	0.42
13:S:323:LYS:HG3	13:S:335:TYR:HB2	2.02	0.42
13:S:487:ASN:OD1	13:S:487:ASN:N	2.53	0.42
13:S:868:LEU:HD22	13:S:873:GLN:HB3	2.00	0.42
13:S:974:MET:N	13:S:974:MET:SD	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:ASP:O	1:H:208:TYR:OH	2.28	0.42
1:H:477:VAL:HG13	1:H:496:PHE:CE1	2.55	0.42
1:H:531:LYS:NZ	1:H:547:ILE:HG23	2.34	0.42
4:N:246:ILE:HA	4:N:249:LEU:HD13	2.02	0.42
5:O:439:ILE:HD12	5:O:439:ILE:HA	1.96	0.42
8:R:684:ILE:HD11	8:R:700:ALA:HB2	2.01	0.42
8:R:714:ARG:HE	8:R:727:ILE:HD11	1.85	0.42
9:T:134:LYS:HD3	9:T:134:LYS:HA	1.87	0.42
9:T:193:ARG:NH2	9:T:197:ASN:OD1	2.53	0.42
13:V:37:ASP:OD1	13:V:37:ASP:N	2.52	0.42
13:V:356:SER:OG	13:V:360:TYR:N	2.53	0.42
13:V:774:ILE:O	13:V:778:LEU:HG	2.20	0.42
1:A:496:PHE:HB3	1:A:513:LEU:HB2	2.01	0.41
3:C:508:ALA:HA	3:C:511:LEU:HB2	2.01	0.41
6:F:252:TYR:CE2	7:G:253:ILE:HD12	2.55	0.41
7:G:250:MET:O	7:G:254:GLN:HB2	2.20	0.41
8:I:121:THR:HG22	8:I:131:TRP:CZ3	2.55	0.41
8:I:159:GLN:HA	8:I:172:SER:HA	2.02	0.41
8:I:347:LEU:O	8:I:358:TYR:N	2.51	0.41
8:I:625:LEU:HD11	8:I:653:GLU:HA	2.02	0.41
2:J:432:GLY:H	4:N:254:PRO:HB3	1.85	0.41
3:K:99:GLU:OE1	3:K:102:LYS:NZ	2.37	0.41
3:K:102:LYS:HE2	3:K:102:LYS:HB3	1.90	0.41
5:O:260:ILE:HA	5:O:263:ASN:HD21	1.86	0.41
5:O:477:PHE:HA	5:O:480:ALA:HB3	2.01	0.41
6:P:64:ARG:HD2	6:P:64:ARG:HA	1.73	0.41
7:Q:143:LEU:HG	7:Q:147:ARG:HH11	1.84	0.41
7:Q:288:ARG:O	7:Q:291:GLU:HG2	2.20	0.41
10:U:452:ARG:HE	10:U:456:LEU:HG	1.85	0.41
12:Z:406:SER:HB2	12:Z:409:ARG:NH2	2.27	0.41
1:A:574:ASP:OD2	1:A:577:VAL:N	2.47	0.41
1:A:639:GLN:NE2	1:A:641:GLN:HE21	2.18	0.41
1:A:651:SER:O	1:A:654:ARG:NH1	2.53	0.41
2:B:343:LEU:HB3	2:B:344:GLN:H	1.79	0.41
5:E:477:PHE:HA	5:E:480:ALA:HB3	2.01	0.41
6:F:176:LEU:HD12	7:G:182:SER:HB3	2.02	0.41
7:G:158:LYS:HD2	7:G:158:LYS:HA	1.73	0.41
7:G:288:ARG:O	7:G:291:GLU:HG2	2.20	0.41
9:L:145:LYS:HG2	10:M:322:LYS:NZ	2.35	0.41
10:M:449:LEU:O	10:M:453:ASN:ND2	2.53	0.41
10:M:450:SER:HA	10:M:453:ASN:HD21	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:111:LEU:HD21	12:X:492:ILE:HG12	2.01	0.41
13:S:807:LEU:HD11	13:S:823:TYR:HE1	1.85	0.41
1:H:318:LYS:HB3	1:H:318:LYS:HE3	1.94	0.41
2:J:141:ARG:HA	2:J:144:ILE:HD12	2.02	0.41
2:J:330:ASN:HD21	3:K:548:LYS:HB2	1.84	0.41
2:J:371:SER:OG	2:J:374:ASN:OD1	2.33	0.41
3:K:227:SER:HA	3:K:267:PRO:HB2	2.02	0.41
3:K:383:ARG:O	3:K:386:LYS:HG3	2.21	0.41
3:K:383:ARG:HG3	3:K:386:LYS:HE3	2.02	0.41
6:P:221:SER:O	6:P:224:ILE:HG12	2.20	0.41
8:R:279:ASP:HB2	8:R:281:THR:HG22	2.01	0.41
9:T:32:PHE:HB3	9:T:62:ARG:HG2	2.00	0.41
9:T:168:VAL:HA	9:T:171:HIS:CE1	2.55	0.41
11:Y:66:LYS:HD3	12:Z:443:TRP:CZ3	2.55	0.41
11:Y:83:ARG:NH1	11:Y:87:GLN:HG2	2.35	0.41
13:V:215:ILE:HG23	13:V:227:TYR:HB2	2.02	0.41
13:V:231:GLY:O	13:V:232:ARG:NH1	2.53	0.41
13:V:731:VAL:HA	13:V:734:SER:HB3	2.01	0.41
5:E:11:ALA:HB1	5:E:217:PRO:HB2	2.02	0.41
5:E:197:CYS:SG	5:E:225:LEU:HB3	2.61	0.41
5:E:202:TYR:HE2	5:E:232:ARG:HD2	1.83	0.41
7:G:215:PHE:O	7:G:219:LYS:HB2	2.20	0.41
9:L:4:ARG:HG3	9:L:95:LYS:HZ2	1.84	0.41
9:L:186:ALA:HB2	10:M:364:ARG:NH1	2.35	0.41
11:W:83:ARG:CZ	12:X:464:ALA:HB2	2.51	0.41
11:W:113:LYS:H	11:W:113:LYS:HD2	1.85	0.41
13:S:37:ASP:OD1	13:S:37:ASP:N	2.52	0.41
13:S:878:ILE:O	13:S:882:ILE:HG12	2.20	0.41
1:H:183:LEU:HD23	1:H:183:LEU:HA	1.86	0.41
1:H:280:LEU:HD13	1:H:280:LEU:HA	1.91	0.41
1:H:465:ALA:O	1:H:470:ARG:HB3	2.21	0.41
5:O:13:ARG:HB3	5:O:250:SER:HA	2.01	0.41
6:P:203:TYR:OH	7:Q:207:PRO:O	2.26	0.41
8:R:590:MET:HA	8:R:593:LYS:HZ3	1.85	0.41
9:T:43:VAL:O	9:T:47:TYR:N	2.48	0.41
10:U:309:HIS:CE1	11:Y:38:ILE:HG12	2.50	0.41
10:U:312:GLU:HG2	10:U:316:HIS:HE1	1.85	0.41
11:Y:44:MET:O	11:Y:47:LEU:HG	2.19	0.41
13:V:853:PHE:CD1	13:V:854:PRO:HD2	2.56	0.41
1:A:122:PRO:HB2	1:A:123:GLU:H	1.66	0.41
1:A:362:ILE:O	1:A:366:ILE:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:TYR:HA	3:C:63:TYR:HE1	1.84	0.41
5:E:283:ILE:HB	5:E:284:PRO:HD3	2.03	0.41
5:E:316:PRO:HA	5:E:319:PHE:HB2	2.01	0.41
6:F:186:LYS:HB3	6:F:186:LYS:HE3	1.82	0.41
8:I:20:VAL:HG12	8:I:30:THR:HG22	2.01	0.41
9:L:78:ARG:HH21	11:W:49:ASP:HB2	1.84	0.41
11:W:117:GLU:HG3	13:V:782:LEU:HD22	2.02	0.41
13:S:415:HIS:HA	13:S:420:LEU:HA	2.02	0.41
1:H:404:ASN:HD21	1:H:433:LYS:HD3	1.85	0.41
1:H:666:TYR:HD2	1:H:683:LEU:HD22	1.85	0.41
2:J:448:PHE:CD1	4:N:312:PRO:HG2	2.55	0.41
3:K:297:LYS:HA	3:K:300:PHE:CD2	2.55	0.41
9:T:74:LEU:O	9:T:78:ARG:HA	2.21	0.41
13:V:154:HIS:CE1	13:V:156:GLU:HB2	2.56	0.41
13:V:752:LEU:HA	13:V:757:GLU:HB3	2.02	0.41
13:V:993:GLU:HA	13:V:996:LYS:HB2	2.03	0.41
13:V:1046:GLU:HA	13:V:1054:ALA:HB2	2.00	0.41
1:A:250:GLN:OE1	1:A:250:GLN:N	2.43	0.41
1:A:288:ASP:OD1	1:A:288:ASP:N	2.48	0.41
3:C:512:MET:O	3:C:516:GLU:N	2.54	0.41
5:E:15:ASN:ND2	5:E:250:SER:O	2.53	0.41
5:E:34:LEU:HA	5:E:39:TYR:CE1	2.55	0.41
9:L:137:LYS:HE2	10:M:316:HIS:HA	2.01	0.41
11:W:72:LEU:O	11:W:76:VAL:HG13	2.21	0.41
11:W:83:ARG:HA	11:W:83:ARG:HD2	1.89	0.41
1:H:313:LYS:O	1:H:317:ILE:HG12	2.21	0.41
1:H:452:GLU:OE1	10:U:443:SER:HA	2.21	0.41
2:J:23:HIS:H	2:J:23:HIS:CD2	2.38	0.41
2:J:236:GLU:HB2	2:J:239:LYS:HE3	2.01	0.41
2:J:379:LEU:HD23	2:J:399:ILE:HD11	2.02	0.41
3:K:58:TYR:HA	3:K:63:TYR:HE1	1.86	0.41
4:N:214:LYS:HA	4:N:217:LYS:HD3	2.02	0.41
4:N:328:SER:O	4:N:328:SER:OG	2.37	0.41
7:Q:304:GLU:HA	7:Q:307:LEU:HG	2.01	0.41
13:V:579:HIS:CE1	13:V:601:ILE:HG22	2.56	0.41
13:V:868:LEU:HD22	13:V:873:GLN:HB3	2.01	0.41
2:B:309:THR:HG22	2:B:313:PRO:HG2	2.03	0.41
2:B:428:SER:N	4:D:254:PRO:HD2	2.24	0.41
3:C:73:LEU:HA	3:C:76:LEU:HG	2.01	0.41
5:E:138:ASP:OD1	5:E:138:ASP:N	2.52	0.41
6:F:196:LYS:HG3	6:F:198:PRO:HD3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:240:GLU:HA	9:L:243:ARG:HB2	2.03	0.41
10:M:394:ILE:HA	10:M:397:THR:HG22	2.03	0.41
13:S:537:PRO:HB2	13:S:576:ARG:HD3	2.01	0.41
13:S:993:GLU:HA	13:S:996:LYS:HB2	2.03	0.41
1:H:546:GLN:NE2	2:J:276:ALA:HB3	2.35	0.41
1:H:578:LEU:HD23	1:H:597:TYR:HA	2.02	0.41
2:J:142:ALA:HB1	2:J:255:GLN:HG2	2.03	0.41
3:K:199:HIS:O	3:K:202:GLU:HG3	2.20	0.41
3:K:473:TYR:HB3	3:K:495:LEU:HD11	2.02	0.41
3:K:538:ASN:HA	3:K:541:ILE:HG22	2.02	0.41
5:O:137:ASP:HA	5:O:140:LEU:HD12	2.02	0.41
5:O:202:TYR:HE2	5:O:232:ARG:HD2	1.85	0.41
5:O:305:PHE:O	5:O:309:LYS:HG2	2.20	0.41
5:O:378:VAL:HG12	5:O:382:LEU:HD23	2.03	0.41
6:P:16:PHE:HE1	6:P:40:VAL:HA	1.85	0.41
6:P:321:ILE:HD11	7:Q:330:LYS:HB2	2.01	0.41
13:V:598:GLU:HA	13:V:601:ILE:HD12	2.03	0.41
13:V:706:LEU:HD21	13:V:719:TYR:HE1	1.86	0.41
13:V:915:ALA:HA	13:V:918:TYR:CD2	2.56	0.41
1:A:191:LEU:HD12	1:A:195:TYR:CZ	2.56	0.41
1:A:444:ASN:OD1	2:B:286:LEU:HD12	2.21	0.41
1:A:618:TYR:O	1:A:622:SER:OG	2.26	0.41
5:E:305:PHE:HA	5:E:308:ILE:HG22	2.01	0.41
8:I:604:ARG:NH2	8:I:635:ILE:HA	2.36	0.41
9:L:26:ASN:HD22	9:L:34:LEU:HB3	1.85	0.41
13:S:183:LYS:HE3	13:S:197:SER:HB2	2.02	0.41
13:S:254:ASN:OD1	13:S:255:PRO:HD2	2.20	0.41
1:H:496:PHE:HB3	1:H:513:LEU:HB2	2.02	0.41
1:H:618:TYR:O	1:H:622:SER:OG	2.25	0.41
2:J:245:PHE:O	2:J:249:LYS:HB2	2.19	0.41
3:K:73:LEU:HD13	3:K:83:TYR:CE1	2.56	0.41
3:K:200:LEU:HD11	3:K:245:LEU:HG	2.03	0.41
3:K:260:LYS:HA	3:K:285:ILE:HD11	2.02	0.41
3:K:551:TYR:HB2	3:K:595:LEU:HD21	2.03	0.41
4:N:242:ARG:NH1	4:N:243:MET:HG2	2.35	0.41
6:P:212:LYS:HD3	6:P:212:LYS:HA	1.58	0.41
6:P:277:GLU:O	6:P:281:LYS:NZ	2.47	0.41
8:R:651:PRO:O	8:R:763:ARG:NH2	2.51	0.41
8:R:697:LEU:HG	8:R:729:ARG:HD3	2.03	0.41
9:T:110:LYS:HA	9:T:113:ASP:HB2	2.03	0.41
11:Y:83:ARG:CZ	12:Z:464:ALA:HB2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:770:TYR:HA	13:V:773:ALA:HB3	2.02	0.41
2:B:249:LYS:NZ	2:B:250:PRO:O	2.36	0.41
2:B:338:THR:HA	2:B:339:PRO:HD3	1.95	0.41
3:C:324:HIS:HB3	3:C:326:PHE:CD2	2.56	0.41
8:I:389:ASP:OD1	8:I:389:ASP:N	2.52	0.41
13:S:443:LEU:HD13	13:S:495:LEU:HD21	2.02	0.41
13:S:731:VAL:HA	13:S:734:SER:HB3	2.02	0.41
2:J:448:PHE:HB3	4:N:316:GLN:HG2	2.03	0.41
3:K:176:GLN:HB2	3:K:179:LEU:HB2	2.03	0.41
3:K:468:GLU:OE1	3:K:471:ARG:NE	2.41	0.41
3:K:550:ASN:OD1	3:K:550:ASN:N	2.53	0.41
3:K:575:TYR:HA	3:K:578:LYS:HB2	2.02	0.41
6:P:16:PHE:HB3	6:P:18:TYR:HD2	1.86	0.41
8:R:95:ARG:NE	8:R:97:GLU:OE2	2.54	0.41
8:R:431:VAL:HB	8:R:442:ARG:HB2	2.01	0.41
10:U:389:GLN:HG3	10:U:393:ARG:NH1	2.36	0.41
13:V:759:GLN:O	13:V:763:VAL:HG23	2.21	0.41
13:V:895:ILE:O	13:V:898:ARG:HG2	2.21	0.41
1:A:297:TYR:HD2	2:B:301:ASP:HB2	1.86	0.41
1:A:575:PRO:HG3	1:A:605:TYR:HB3	2.02	0.41
3:C:70:TYR:HB3	3:C:87:TYR:HB2	2.03	0.41
3:C:364:GLU:O	3:C:368:ARG:HG2	2.21	0.41
4:D:300:VAL:O	4:D:303:THR:OG1	2.29	0.41
5:E:123:GLN:HE22	5:E:127:LEU:HD22	1.85	0.41
5:E:355:GLU:HG2	5:E:360:PRO:HG2	2.03	0.41
6:F:73:LYS:HA	6:F:75:ARG:HH22	1.85	0.41
6:F:261:LEU:HD12	6:F:261:LEU:HA	1.85	0.41
7:G:236:ARG:NH2	6:P:22:LEU:HB3	2.36	0.41
8:I:5:VAL:HG11	8:I:265:LEU:HD22	2.03	0.41
8:I:165:GLY:HA2	8:I:188:VAL:HG13	2.02	0.41
8:I:458:HIS:NE2	8:I:490:LEU:HD11	2.35	0.41
8:I:679:LEU:HG	8:I:681:PHE:H	1.84	0.41
9:L:106:LYS:CA	11:W:56:ASP:HB3	2.44	0.41
9:L:122:ILE:HD13	9:L:122:ILE:HA	1.88	0.41
9:L:179:ARG:NH2	10:M:359:LEU:HD13	2.36	0.41
10:M:389:GLN:HG3	10:M:393:ARG:NH1	2.36	0.41
13:S:67:ILE:H	13:S:85:SER:HB3	1.85	0.41
13:S:712:VAL:HG11	13:S:738:ALA:H	1.85	0.41
13:S:737:HIS:CG	13:S:740:ALA:HB2	2.56	0.41
13:S:1056:LYS:HA	13:S:1059:VAL:HG12	2.03	0.41
1:H:464:MET:HA	1:H:467:LYS:HZ3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:551:TYR:CE2	1:H:556:ASP:HB3	2.56	0.41
1:H:605:TYR:CE1	1:H:607:VAL:HB	2.55	0.41
2:J:280:ASP:OD1	2:J:280:ASP:N	2.44	0.41
2:J:419:ARG:HB3	4:N:344:LEU:HD13	2.02	0.41
3:K:110:HIS:HB3	3:K:113:ALA:HB3	2.02	0.41
3:K:122:SER:HA	3:K:125:GLN:HG2	2.03	0.41
3:K:430:LEU:HD23	3:K:430:LEU:HA	1.94	0.41
3:K:590:LYS:HD2	3:K:590:LYS:HA	1.72	0.41
5:O:39:TYR:HB2	5:O:70:TYR:CD1	2.56	0.41
6:P:279:TYR:HB2	7:Q:289:PHE:CZ	2.56	0.41
8:R:193:ASP:HB2	8:R:233:VAL:HG23	2.02	0.41
8:R:508:ARG:HH12	8:R:510:HIS:HA	1.85	0.41
8:R:596:TRP:HE1	8:R:627:THR:HB	1.86	0.41
8:R:600:THR:HG22	8:R:635:ILE:HG23	2.02	0.41
8:R:614:THR:O	8:R:618:MET:HG2	2.21	0.41
11:Y:115:LYS:O	12:Z:495:ASN:ND2	2.54	0.41
13:V:267:ARG:HD3	13:V:285:HIS:ND1	2.36	0.41
13:V:500:ARG:NH2	13:V:539:SER:O	2.54	0.41
13:V:581:THR:HG23	13:V:601:ILE:HG12	2.03	0.41
13:V:664:LEU:HG	13:V:692:MET:HE3	2.03	0.41
1:A:466:LEU:HD22	1:A:479:LYS:HG2	2.02	0.41
2:B:138:ILE:HG13	2:B:193:LEU:HD23	2.02	0.41
2:B:142:ALA:HB1	2:B:255:GLN:HG2	2.03	0.41
3:C:557:ARG:HB2	3:C:560:LYS:HE3	2.03	0.41
5:E:45:LEU:HA	5:E:48:PHE:CD2	2.57	0.41
5:E:457:ASN:H	5:E:460:SER:HB3	1.86	0.41
6:F:324:ILE:HG22	6:F:327:ARG:CZ	2.51	0.41
11:W:58:GLN:O	11:W:62:LEU:HG	2.21	0.41
13:S:495:LEU:N	13:S:495:LEU:HD23	2.35	0.41
13:S:778:LEU:C	13:S:780:GLY:H	2.21	0.41
1:H:574:ASP:OD1	2:J:272:LEU:N	2.54	0.41
1:H:653:TYR:HE2	1:H:665:LYS:HG2	1.86	0.41
2:J:23:HIS:CD2	2:J:42:LYS:HG2	2.56	0.41
4:N:226:ASN:O	4:N:229:HIS:NE2	2.54	0.41
5:O:125:ARG:O	5:O:129:HIS:ND1	2.34	0.41
5:O:205:SER:HA	5:O:208:ILE:HG22	2.03	0.41
7:Q:147:ARG:HA	7:Q:150:ILE:HG12	2.02	0.41
7:Q:199:LEU:HA	7:Q:203:GLY:HA3	2.02	0.41
8:R:514:ALA:HB1	8:R:530:PRO:HG3	2.02	0.41
13:V:338:LYS:HA	13:V:338:LYS:HD3	1.88	0.41
13:V:727:ASP:N	13:V:727:ASP:OD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:847:ASP:CG	13:V:860:ILE:HD13	2.41	0.41
2:B:318:LEU:HA	2:B:321:LYS:HZ2	1.86	0.40
4:D:225:ILE:HD13	4:D:225:ILE:HA	1.96	0.40
5:E:213:LEU:HD11	5:E:226:LYS:HE3	2.03	0.40
8:I:599:ALA:O	8:I:602:LEU:HG	2.20	0.40
9:L:110:LYS:HA	9:L:113:ASP:HB2	2.02	0.40
9:L:145:LYS:HG2	10:M:322:LYS:HZ3	1.86	0.40
13:S:778:LEU:C	13:S:780:GLY:N	2.74	0.40
13:S:981:LYS:HE3	13:S:985:PHE:CZ	2.56	0.40
1:H:224:ARG:NH1	1:H:243:MET:O	2.46	0.40
1:H:664:GLY:HA2	1:H:667:LYS:HE3	2.02	0.40
2:J:193:LEU:HB2	2:J:207:GLY:HA3	2.03	0.40
3:K:54:GLY:O	3:K:70:TYR:OH	2.34	0.40
3:K:311:THR:HA	3:K:314:ASN:HD22	1.86	0.40
6:P:324:ILE:HA	6:P:327:ARG:HG2	2.02	0.40
7:Q:186:LYS:HZ1	7:Q:187:ILE:HD11	1.85	0.40
8:R:576:VAL:HG22	11:Y:92:ARG:NH1	2.33	0.40
9:T:5:GLU:H	9:T:5:GLU:HG3	1.68	0.40
13:V:582:GLU:HA	13:V:595:ALA:HA	2.04	0.40
13:V:1028:GLN:H	13:V:1028:GLN:HG2	1.77	0.40
1:A:127:ARG:O	1:A:131:LYS:HG2	2.21	0.40
1:A:181:LEU:HG	1:A:185:TYR:CD2	2.56	0.40
1:A:479:LYS:HD2	1:A:479:LYS:HA	1.79	0.40
2:B:337:GLU:H	2:B:337:GLU:HG3	1.74	0.40
3:C:611:GLU:HB3	3:C:615:LYS:HE2	2.03	0.40
6:F:164:LYS:HD3	6:F:294:SER:HA	2.02	0.40
7:G:199:LEU:HA	7:G:203:GLY:HA3	2.04	0.40
13:S:407:GLU:HB2	13:S:441:PRO:HB3	2.03	0.40
1:H:211:ILE:HA	1:H:214:ASN:HD21	1.86	0.40
1:H:362:ILE:O	1:H:366:ILE:HG23	2.22	0.40
6:P:252:TYR:CE2	7:Q:253:ILE:HD12	2.56	0.40
8:R:138:ARG:HH12	13:V:435:ARG:NH1	2.19	0.40
8:R:154:ALA:HB2	8:R:194:TRP:CZ3	2.55	0.40
8:R:347:LEU:O	8:R:358:TYR:N	2.50	0.40
13:V:56:LYS:H	13:V:56:LYS:HG2	1.73	0.40
13:V:401:SER:HB3	13:V:416:TYR:HD1	1.87	0.40
13:V:542:ILE:O	13:V:552:VAL:HA	2.20	0.40
1:A:131:LYS:HA	1:A:131:LYS:HD3	1.85	0.40
1:A:391:CYS:O	1:A:395:ARG:HG3	2.22	0.40
1:A:600:GLU:HG2	1:A:603:ARG:HH21	1.85	0.40
1:A:619:HIS:CG	1:A:628:ALA:HB2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:PRO:HD2	3:C:59:TYR:HE1	1.86	0.40
4:D:242:ARG:NH2	4:D:245:GLU:HA	2.35	0.40
8:I:7:GLN:HE21	8:I:7:GLN:HB2	1.68	0.40
8:I:64:PRO:HG2	8:I:67:SER:HB3	2.04	0.40
8:I:527:TRP:HA	8:I:544:ARG:HA	2.04	0.40
9:L:74:LEU:O	9:L:78:ARG:HA	2.21	0.40
9:L:137:LYS:HD2	9:L:137:LYS:HA	1.78	0.40
9:L:214:GLU:HA	9:L:217:LYS:HG2	2.03	0.40
9:L:256:LEU:O	9:L:260:ARG:HG3	2.21	0.40
11:W:24:TYR:CZ	11:W:28:LYS:HD3	2.56	0.40
11:W:122:ILE:HG12	12:X:498:THR:OG1	2.21	0.40
13:S:25:ALA:HB2	13:S:30:ARG:HB3	2.04	0.40
13:S:892:LYS:HA	13:S:895:ILE:HD12	2.02	0.40
1:H:303:ASN:OD1	9:T:299:LEU:CD1	2.70	0.40
2:J:382:LYS:HE3	5:O:23:GLU:HB3	2.04	0.40
3:K:324:HIS:HB3	3:K:326:PHE:CD2	2.57	0.40
5:O:218:ASP:OD1	5:O:218:ASP:N	2.53	0.40
6:P:86:GLN:HE21	6:P:86:GLN:HB2	1.76	0.40
7:Q:172:ASN:HA	7:Q:175:ASP:OD2	2.21	0.40
8:R:129:LYS:HB2	8:R:131:TRP:CZ3	2.56	0.40
8:R:392:ALA:O	8:R:408:ARG:NH1	2.36	0.40
8:R:596:TRP:NE1	12:Z:503:LEU:HD11	2.36	0.40
8:R:712:TRP:HB2	8:R:744:VAL:HG11	2.03	0.40
9:T:137:LYS:HE2	10:U:316:HIS:HA	2.02	0.40
9:T:143:ILE:HG23	11:Y:23:LYS:NZ	2.37	0.40
11:Y:24:TYR:O	11:Y:28:LYS:HG2	2.22	0.40
13:V:80:LEU:HD13	13:V:94:LEU:HB3	2.03	0.40
13:V:161:VAL:HG11	13:V:207:TYR:HA	2.04	0.40
1:A:134:HIS:HA	1:A:137:LEU:HG	2.03	0.40
1:A:161:LYS:HG3	1:A:165:LYS:HE3	2.03	0.40
1:A:306:LEU:HD21	9:L:296:GLU:HG2	2.02	0.40
1:A:468:SER:OG	1:A:469:ASP:N	2.52	0.40
1:A:483:LEU:HD13	1:A:488:ASP:HB3	2.03	0.40
2:B:193:LEU:HB2	2:B:207:GLY:HA3	2.03	0.40
2:B:246:LYS:HB3	2:B:254:ILE:HD11	2.02	0.40
3:C:430:LEU:HD23	3:C:430:LEU:HA	1.94	0.40
3:C:518:GLU:HG2	3:C:521:ARG:CZ	2.52	0.40
5:E:54:ARG:HA	5:E:54:ARG:HD2	1.92	0.40
5:E:94:PHE:HD1	5:E:113:GLN:NE2	2.15	0.40
5:E:134:GLN:OE1	5:E:139:LYS:NZ	2.34	0.40
6:F:328:LYS:O	6:F:331:GLN:NE2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:38:HIS:CE1	8:I:46:PRO:HB2	2.56	0.40
8:I:194:TRP:HA	8:I:201:ILE:HA	2.04	0.40
8:I:279:ASP:HB2	8:I:281:THR:HG22	2.02	0.40
8:I:427:ASP:OD1	8:I:427:ASP:N	2.53	0.40
8:I:552:PHE:CD1	8:I:568:VAL:HG21	2.56	0.40
8:I:600:THR:HA	8:I:603:CYS:HB2	2.03	0.40
8:I:684:ILE:HD11	8:I:700:ALA:HB2	2.04	0.40
9:L:128:LEU:HD22	12:X:417:HIS:CD2	2.56	0.40
9:L:134:LYS:HZ3	10:M:312:GLU:HA	1.86	0.40
10:M:434:ASP:O	10:M:438:ARG:HD3	2.22	0.40
11:W:117:GLU:O	11:W:121:MET:HG3	2.22	0.40
12:X:412:VAL:HG23	12:X:413:GLN:N	2.36	0.40
13:S:56:LYS:H	13:S:56:LYS:HG2	1.73	0.40
13:S:306:MET:SD	13:S:318:TYR:HB2	2.61	0.40
13:S:337:SER:OG	13:S:338:LYS:N	2.55	0.40
13:S:1051:LEU:HD21	10:U:362:GLN:OE1	2.21	0.40
1:H:201:TYR:CE1	1:H:230:ILE:HD12	2.56	0.40
1:H:352:LYS:HA	3:K:636:ARG:HD3	2.04	0.40
2:J:54:ARG:HD2	2:J:79:PHE:CD1	2.56	0.40
2:J:176:VAL:HG21	2:J:234:LYS:HB3	2.03	0.40
2:J:294:ARG:NH2	2:J:298:SER:O	2.42	0.40
5:O:541:VAL:HA	5:O:544:MET:HG2	2.03	0.40
6:P:139:LYS:HD3	6:P:142:ILE:HD12	2.03	0.40
11:Y:104:LEU:O	11:Y:107:GLU:HG2	2.21	0.40
13:V:145:ASN:OD1	13:V:145:ASN:N	2.55	0.40
13:V:248:PHE:CD1	13:V:262:PHE:HB3	2.57	0.40
13:V:343:VAL:HB	13:V:352:ILE:HG23	2.04	0.40
2:B:312:ILE:HB	3:C:589:ALA:HB1	2.04	0.40
2:B:319:TYR:OH	3:C:582:LEU:O	2.35	0.40
3:C:311:THR:HA	3:C:314:ASN:HD22	1.85	0.40
3:C:590:LYS:HD2	3:C:590:LYS:HA	1.79	0.40
5:E:258:ASP:HB3	5:E:261:ARG:HB2	2.04	0.40
6:F:173:ILE:HD13	6:F:173:ILE:HA	1.96	0.40
8:I:577:SER:HB2	11:W:97:LYS:NZ	2.36	0.40
9:L:66:LEU:HA	9:L:69:VAL:HG22	2.02	0.40
10:M:452:ARG:HE	10:M:456:LEU:HG	1.87	0.40
11:W:118:GLN:O	11:W:122:ILE:HG13	2.21	0.40
13:S:770:TYR:O	13:S:774:ILE:HG12	2.22	0.40
13:S:851:ARG:HB3	13:S:855:ALA:HB2	2.03	0.40
13:S:947:ASP:O	13:S:950:GLU:HG3	2.22	0.40
1:H:191:LEU:HD12	1:H:195:TYR:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:22:THR:HA	3:K:25:LYS:HB2	2.03	0.40
3:K:358:GLY:HA3	3:K:366:ALA:HB2	2.03	0.40
3:K:485:LEU:HD21	3:K:519:GLU:HA	2.03	0.40
4:N:283:CYS:SG	4:N:289:PRO:HB3	2.61	0.40
5:O:158:ALA:HB2	5:O:173:ILE:HG21	2.04	0.40
8:R:189:VAL:HA	8:R:205:GLY:HA2	2.04	0.40
8:R:209:LYS:HE2	8:R:209:LYS:HB3	1.85	0.40
8:R:515:MET:SD	8:R:584:PRO:HB2	2.61	0.40
8:R:747:LYS:O	8:R:750:GLU:HG3	2.21	0.40
10:U:367:ARG:HH22	10:U:370:PHE:HD2	1.68	0.40
10:U:372:ASP:O	10:U:376:THR:OG1	2.23	0.40
13:V:900:PHE:O	13:V:903:ALA:N	2.54	0.40
13:V:908:GLU:HB2	13:V:938:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/782 (68%)	472 (88%)	61 (11%)	2 (0%)	30	68
1	H	535/782 (68%)	474 (89%)	57 (11%)	4 (1%)	19	57
2	B	452/454 (100%)	391 (86%)	60 (13%)	1 (0%)	44	78
2	J	452/454 (100%)	393 (87%)	58 (13%)	1 (0%)	44	78
3	C	613/647 (95%)	580 (95%)	33 (5%)	0	100	100
3	K	613/647 (95%)	582 (95%)	31 (5%)	0	100	100
4	D	131/344 (38%)	116 (88%)	15 (12%)	0	100	100
4	N	131/344 (38%)	117 (89%)	14 (11%)	0	100	100
5	E	553/555 (100%)	508 (92%)	45 (8%)	0	100	100
5	O	553/555 (100%)	513 (93%)	40 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	333/683 (49%)	324 (97%)	9 (3%)	0	100	100
6	P	333/683 (49%)	323 (97%)	10 (3%)	0	100	100
7	G	203/641 (32%)	192 (95%)	11 (5%)	0	100	100
7	Q	203/641 (32%)	191 (94%)	12 (6%)	0	100	100
8	I	763/765 (100%)	697 (91%)	65 (8%)	1 (0%)	48	83
8	R	763/765 (100%)	704 (92%)	58 (8%)	1 (0%)	48	83
9	L	301/443 (68%)	279 (93%)	22 (7%)	0	100	100
9	T	301/443 (68%)	276 (92%)	25 (8%)	0	100	100
10	M	162/469 (34%)	158 (98%)	4 (2%)	0	100	100
10	U	162/469 (34%)	158 (98%)	4 (2%)	0	100	100
11	W	112/135 (83%)	112 (100%)	0	0	100	100
11	Y	112/135 (83%)	112 (100%)	0	0	100	100
12	X	104/510 (20%)	104 (100%)	0	0	100	100
12	Z	104/510 (20%)	102 (98%)	2 (2%)	0	100	100
13	S	1102/1755 (63%)	1034 (94%)	67 (6%)	1 (0%)	48	83
13	V	1102/1755 (63%)	1030 (94%)	72 (6%)	0	100	100
All	All	10728/16366 (66%)	9942 (93%)	775 (7%)	11 (0%)	50	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	MET
1	H	629	MET
1	A	431	GLU
1	H	304	TYR
1	H	305	ALA
1	H	431	GLU
2	B	187	LYS
13	S	779	LYS
2	J	187	LYS
8	I	537	LYS
8	R	537	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/627 (73%)	451 (99%)	6 (1%)	65	77
1	H	457/627 (73%)	451 (99%)	6 (1%)	65	77
2	B	388/388 (100%)	384 (99%)	4 (1%)	73	82
2	J	388/388 (100%)	386 (100%)	2 (0%)	86	89
3	C	534/558 (96%)	529 (99%)	5 (1%)	75	83
3	K	534/558 (96%)	530 (99%)	4 (1%)	81	87
4	D	114/288 (40%)	114 (100%)	0	100	100
4	N	114/288 (40%)	114 (100%)	0	100	100
5	E	469/469 (100%)	467 (100%)	2 (0%)	89	91
5	O	469/469 (100%)	467 (100%)	2 (0%)	89	91
6	F	296/581 (51%)	294 (99%)	2 (1%)	81	87
6	P	296/581 (51%)	294 (99%)	2 (1%)	81	87
7	G	185/526 (35%)	185 (100%)	0	100	100
7	Q	185/526 (35%)	185 (100%)	0	100	100
8	I	648/648 (100%)	641 (99%)	7 (1%)	70	80
8	R	648/648 (100%)	642 (99%)	6 (1%)	75	83
9	L	261/358 (73%)	258 (99%)	3 (1%)	70	80
9	T	261/358 (73%)	258 (99%)	3 (1%)	70	80
10	M	144/380 (38%)	139 (96%)	5 (4%)	31	51
10	U	144/380 (38%)	139 (96%)	5 (4%)	31	51
11	W	101/120 (84%)	100 (99%)	1 (1%)	73	82
11	Y	101/120 (84%)	101 (100%)	0	100	100
12	X	90/401 (22%)	89 (99%)	1 (1%)	70	80
12	Z	90/401 (22%)	89 (99%)	1 (1%)	70	80
13	S	915/1431 (64%)	905 (99%)	10 (1%)	70	80
13	V	915/1431 (64%)	906 (99%)	9 (1%)	73	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9204/13550 (68%)	9118 (99%)	86 (1%)	74	83

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	168	ARG
1	A	432	LYS
1	A	449	TYR
1	A	587	ARG
1	A	654	ARG
2	B	28	LYS
2	B	35	ARG
2	B	217	ARG
2	B	253	LYS
3	C	198	LYS
3	C	206	LYS
3	C	359	ARG
3	C	386	LYS
3	C	560	LYS
5	E	7	ARG
5	E	362	ARG
6	F	85	ARG
6	F	233	LYS
8	I	7	GLN
8	I	133	ARG
8	I	657	ASN
8	I	714	ARG
8	I	719	LYS
8	I	746	LYS
8	I	758	ARG
9	L	78	ARG
9	L	179	ARG
9	L	286	ARG
10	M	322	LYS
10	M	387	ARG
10	M	408	LYS
10	M	422	LYS
10	M	430	LYS
11	W	124	LYS
12	X	484	ARG
13	S	18	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	S	139	ARG
13	S	147	LYS
13	S	183	LYS
13	S	351	ARG
13	S	410	ARG
13	S	495	LEU
13	S	500	ARG
13	S	812	LYS
13	S	850	ARG
1	H	127	ARG
1	H	168	ARG
1	H	432	LYS
1	H	449	TYR
1	H	587	ARG
1	H	654	ARG
2	J	28	LYS
2	J	217	ARG
3	K	206	LYS
3	K	359	ARG
3	K	386	LYS
3	K	560	LYS
5	O	7	ARG
5	O	362	ARG
6	P	85	ARG
6	P	86	GLN
8	R	133	ARG
8	R	657	ASN
8	R	714	ARG
8	R	719	LYS
8	R	746	LYS
8	R	758	ARG
9	T	78	ARG
9	T	179	ARG
9	T	238	MET
10	U	322	LYS
10	U	387	ARG
10	U	408	LYS
10	U	422	LYS
10	U	430	LYS
12	Z	484	ARG
13	V	18	LYS
13	V	139	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	V	147	LYS
13	V	183	LYS
13	V	410	ARG
13	V	495	LEU
13	V	500	ARG
13	V	812	LYS
13	V	850	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	A	303	ASN
1	A	641	GLN
2	B	23	HIS
2	B	381	ASN
2	B	405	GLN
3	C	176	GLN
3	C	314	ASN
5	E	113	GLN
5	E	132	GLN
5	E	224	ASN
5	E	275	GLN
6	F	214	GLN
8	I	38	HIS
8	I	594	GLN
9	L	274	GLN
9	L	277	GLN
10	M	453	ASN
10	M	458	GLN
13	S	198	GLN
13	S	549	ASN
13	S	631	GLN
1	H	231	HIS
1	H	234	GLN
2	J	23	HIS
3	K	280	HIS
3	K	314	ASN
4	N	226	ASN
4	N	322	ASN
5	O	224	ASN
5	O	290	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	P	86	GLN
6	P	214	GLN
8	R	7	GLN
8	R	198	ASN
8	R	595	GLN
8	R	732	GLN
9	T	274	GLN
9	T	277	GLN
13	V	198	GLN
13	V	549	ASN
13	V	631	GLN
13	V	694	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](#)

There are no ligands in this entry.

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.

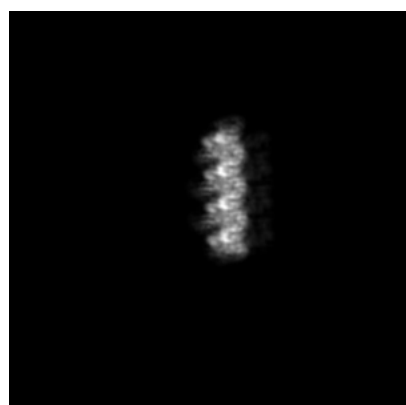
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15977. These allow visual inspection of the internal detail of the map and identification of artifacts.

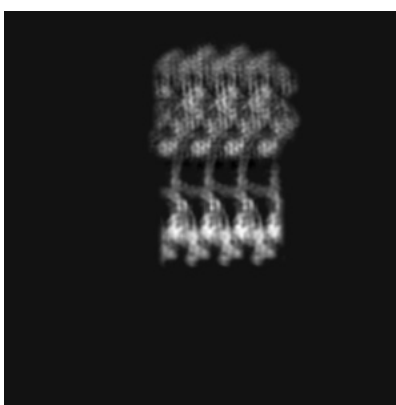
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

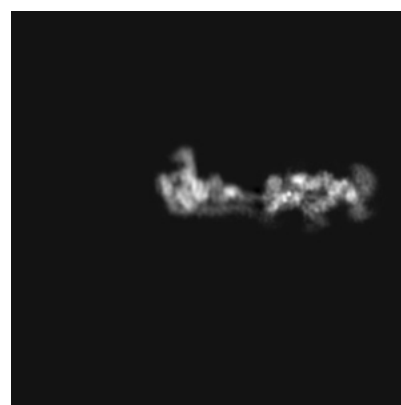
6.1.1 Primary map



X



Y

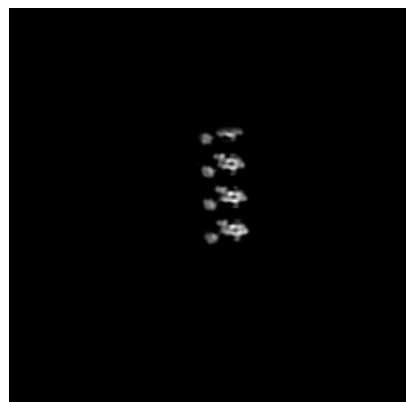


Z

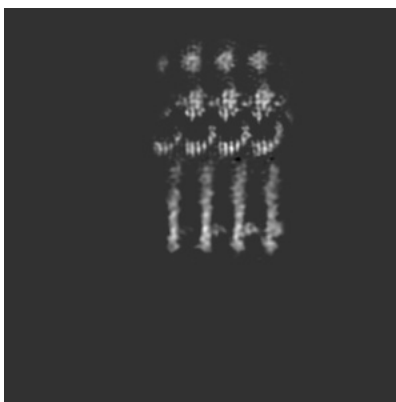
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

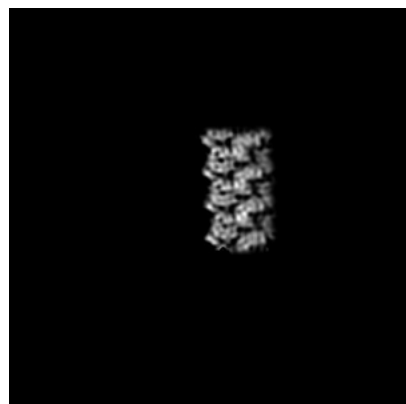


Z Index: 128

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

6.3 Largest variance slices [i](#)

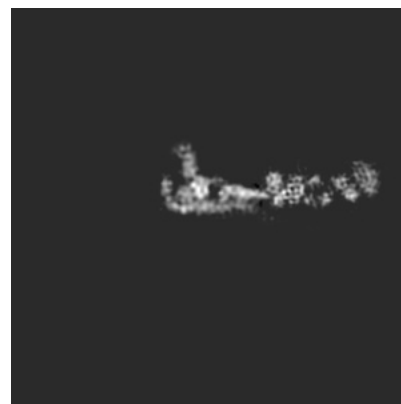
6.3.1 Primary map



X Index: 113



Y Index: 138

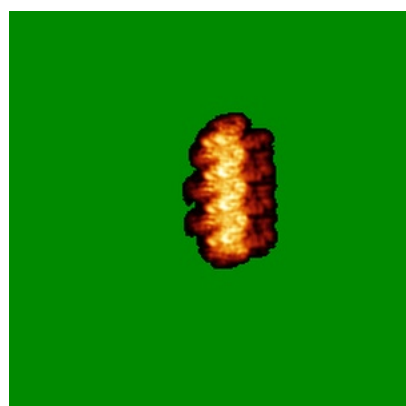


Z Index: 130

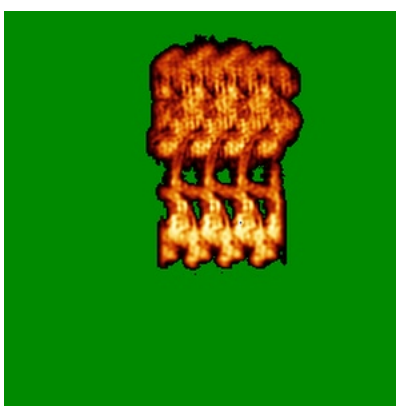
The images above show the largest variance slices of the map in three orthogonal directions.

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

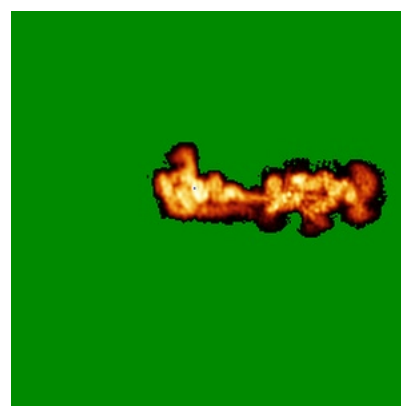
6.4.1 Primary map



X



Y

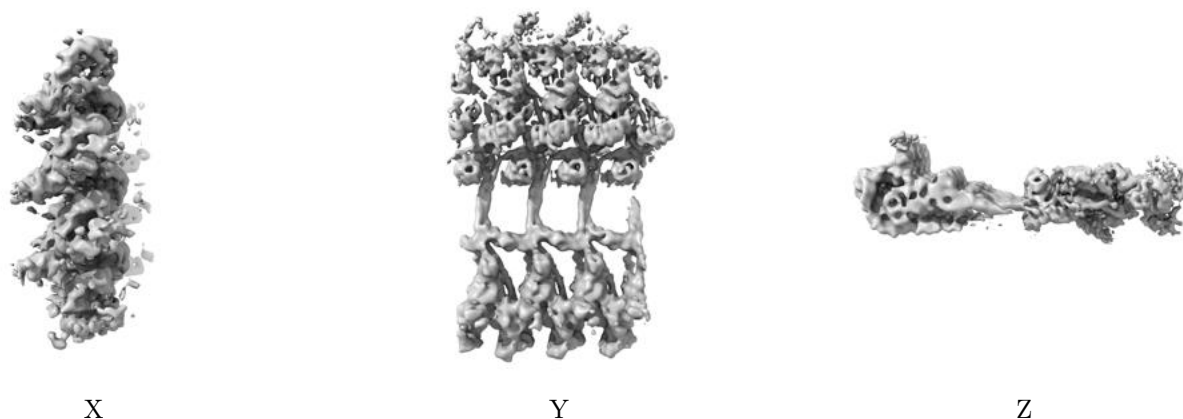


Z

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 0.466. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

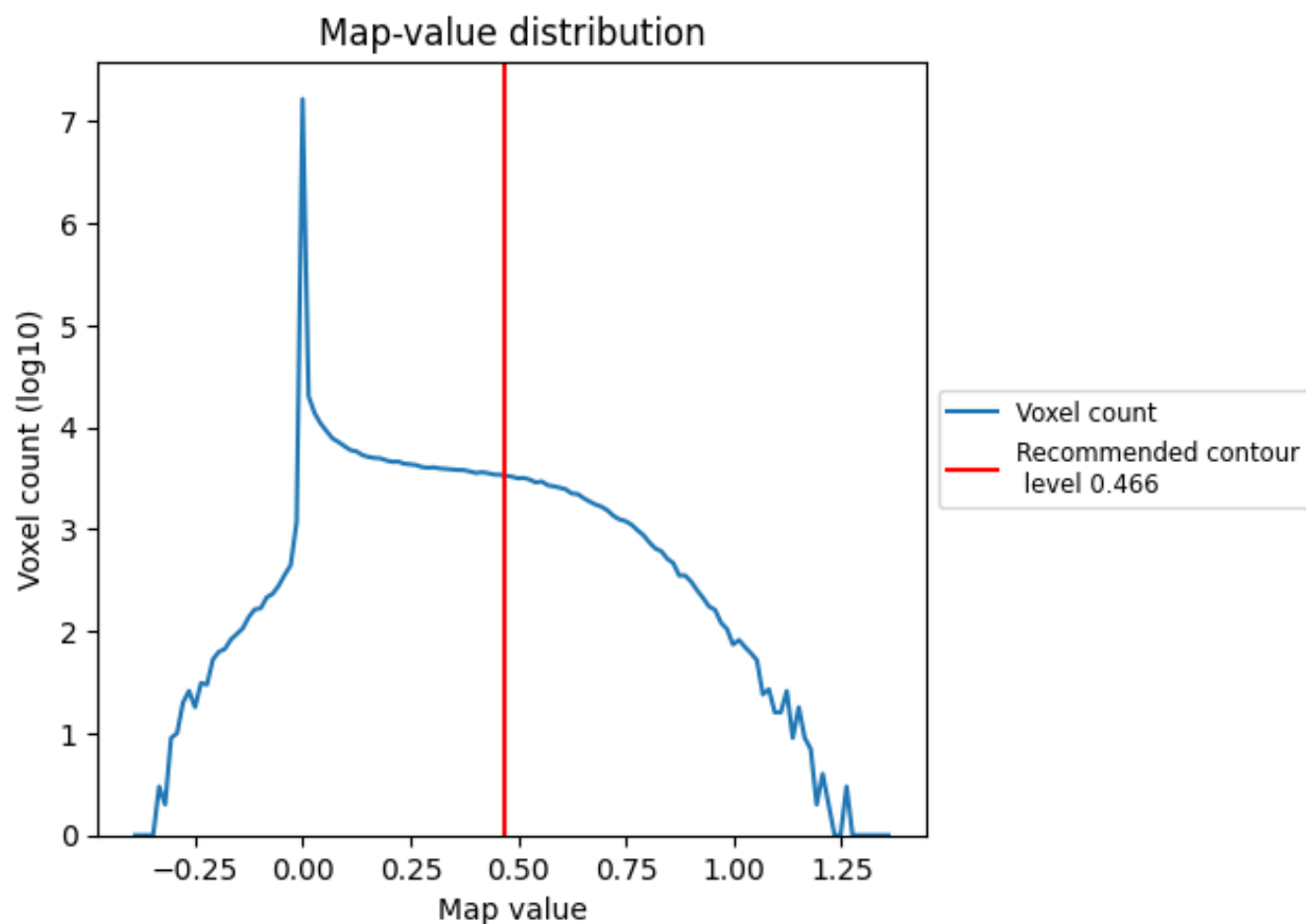
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

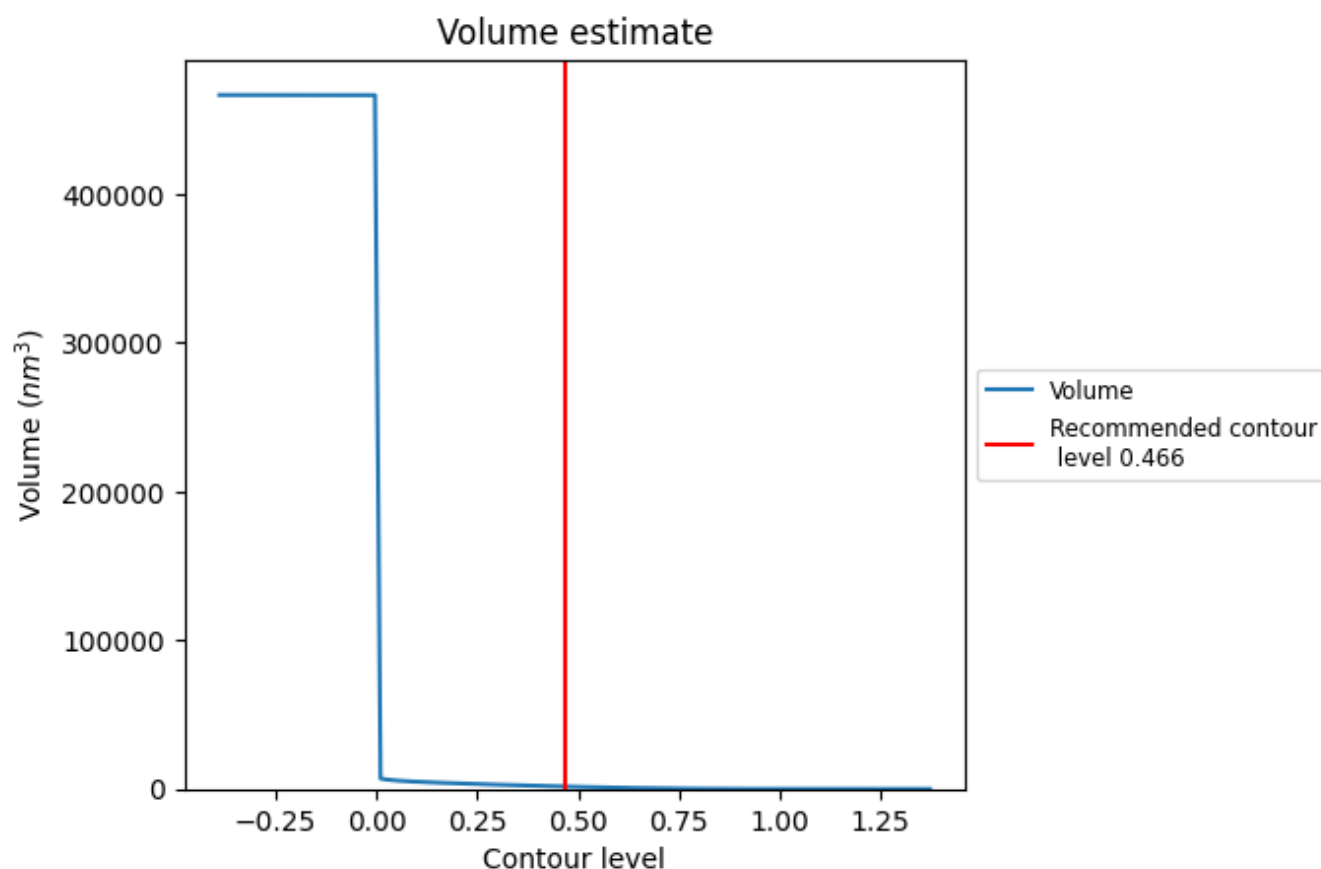
This section contains the results of statistical analysis of the map.

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.

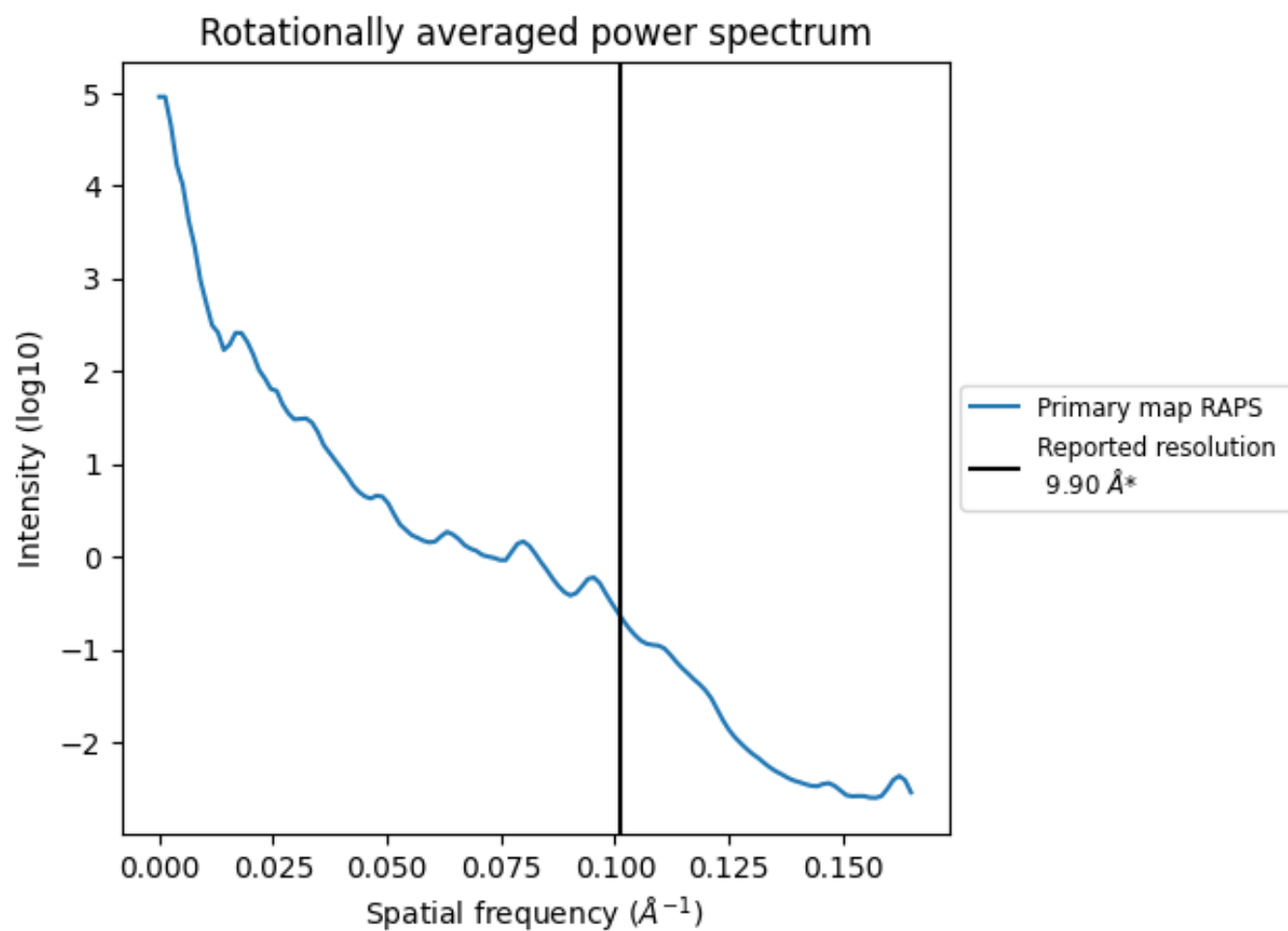
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1645 nm^3 ; this corresponds to an approximate mass of 1486 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 0.101 Å⁻¹

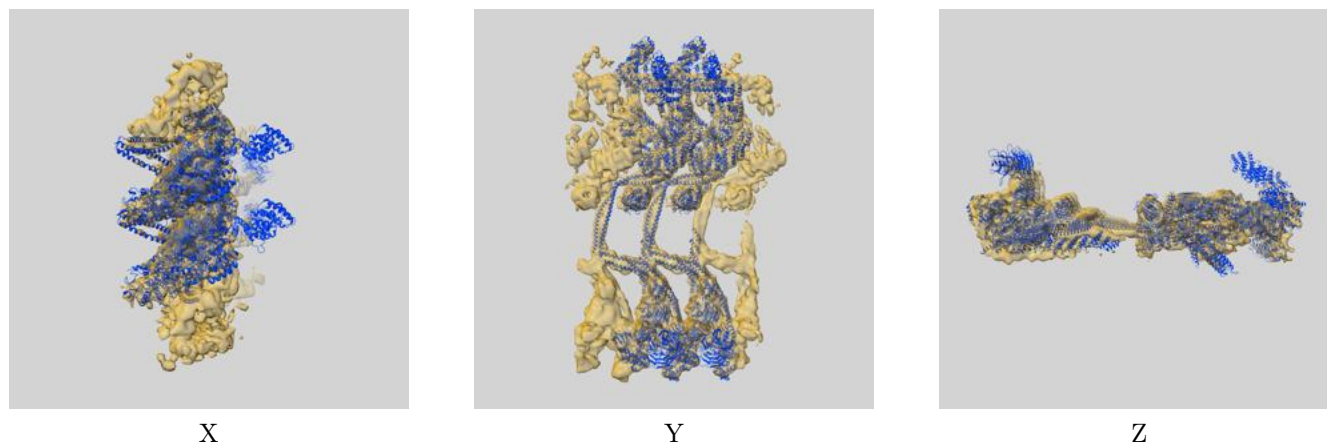
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

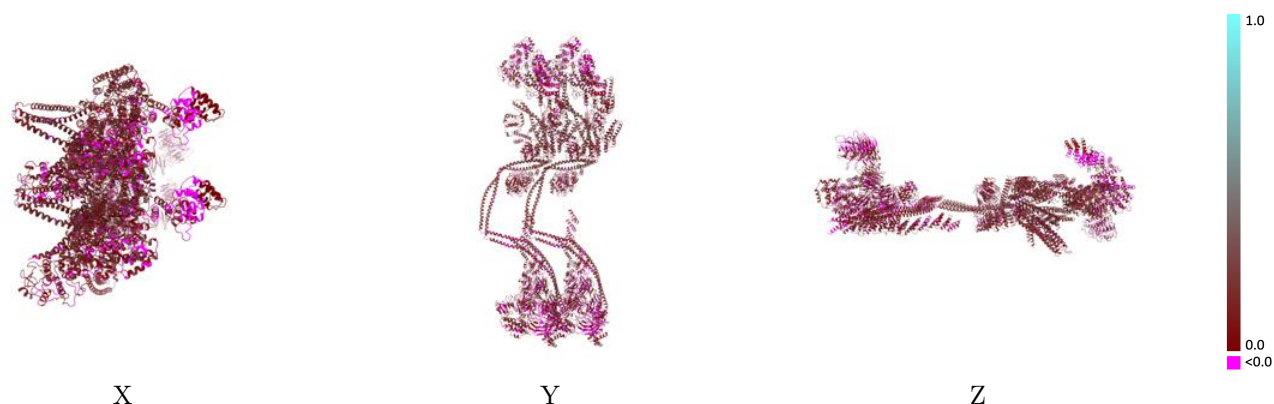
This section contains information regarding the fit between EMDB map EMD-15977 and PDB model 8BD7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



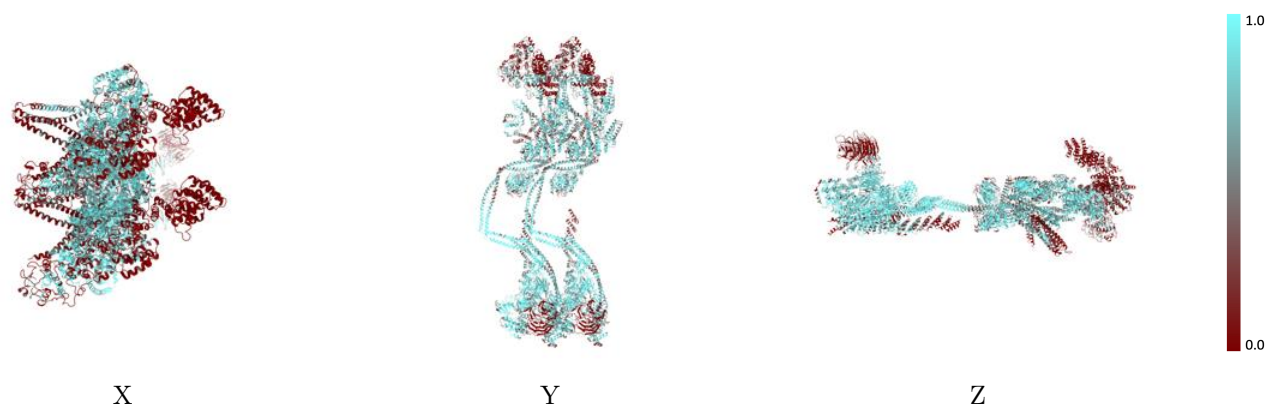
The images above show the 3D surface view of the map at the recommended contour level 0.466 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



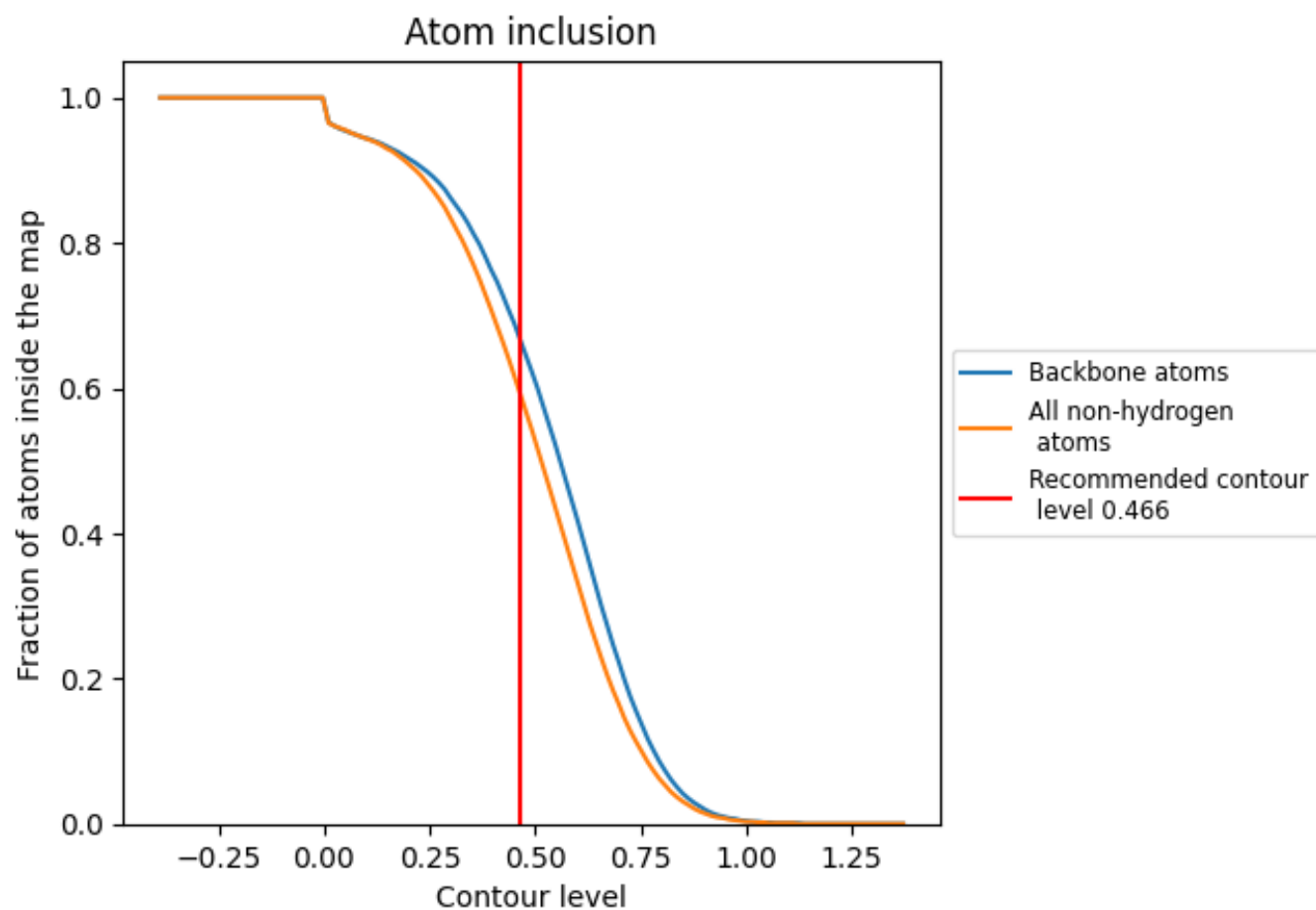
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.466).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.466) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5900	 0.1160
A	 0.7580	 0.1590
B	 0.5930	 0.1360
C	 0.7070	 0.1610
D	 0.2980	 0.0960
E	 0.1130	 0.0420
F	 0.5210	 0.1690
G	 0.4670	 0.1840
H	 0.7500	 0.1580
I	 0.8760	 0.1030
J	 0.5710	 0.1220
K	 0.6770	 0.1590
L	 0.8300	 0.1370
M	 0.7730	 0.1540
N	 0.2730	 0.0760
O	 0.0990	 0.0410
P	 0.5200	 0.1620
Q	 0.4430	 0.1720
R	 0.8590	 0.0980
S	 0.4670	 0.0810
T	 0.8340	 0.1350
U	 0.7860	 0.1600
V	 0.4690	 0.0790
W	 0.7630	 0.1070
X	 0.6990	 0.1260
Y	 0.7600	 0.1010
Z	 0.7260	 0.1260

