



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 10:33 AM UTC

PDB ID : 8ZJI / pdb_00008zji
EMDB ID : EMD-60146
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 1)
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2024-05-15
Resolution : 4.23 Å(reported)
Based on initial model : 7DPA

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

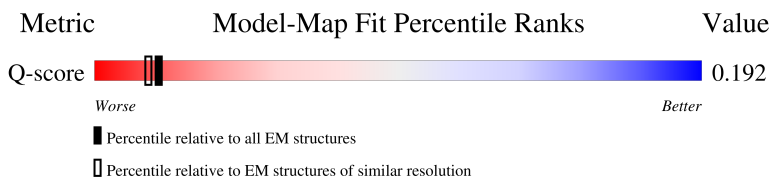
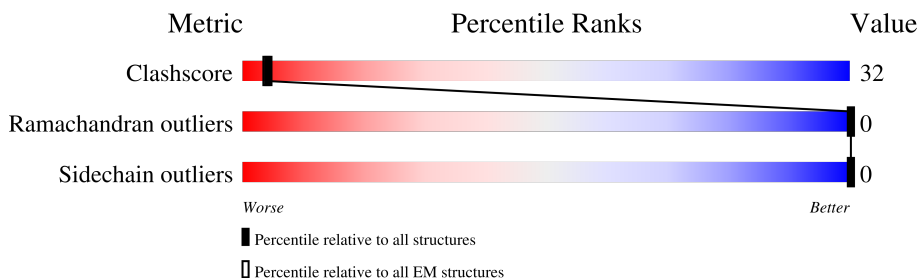
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.23 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4685 (3.74 - 4.73)

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	733	
1	D	733	
2	B	1648	
2	E	1648	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	184	 49% 47% .
3	F	184	 49% 47% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
3	F	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 16 discrepancies between the modelled and reference sequences:

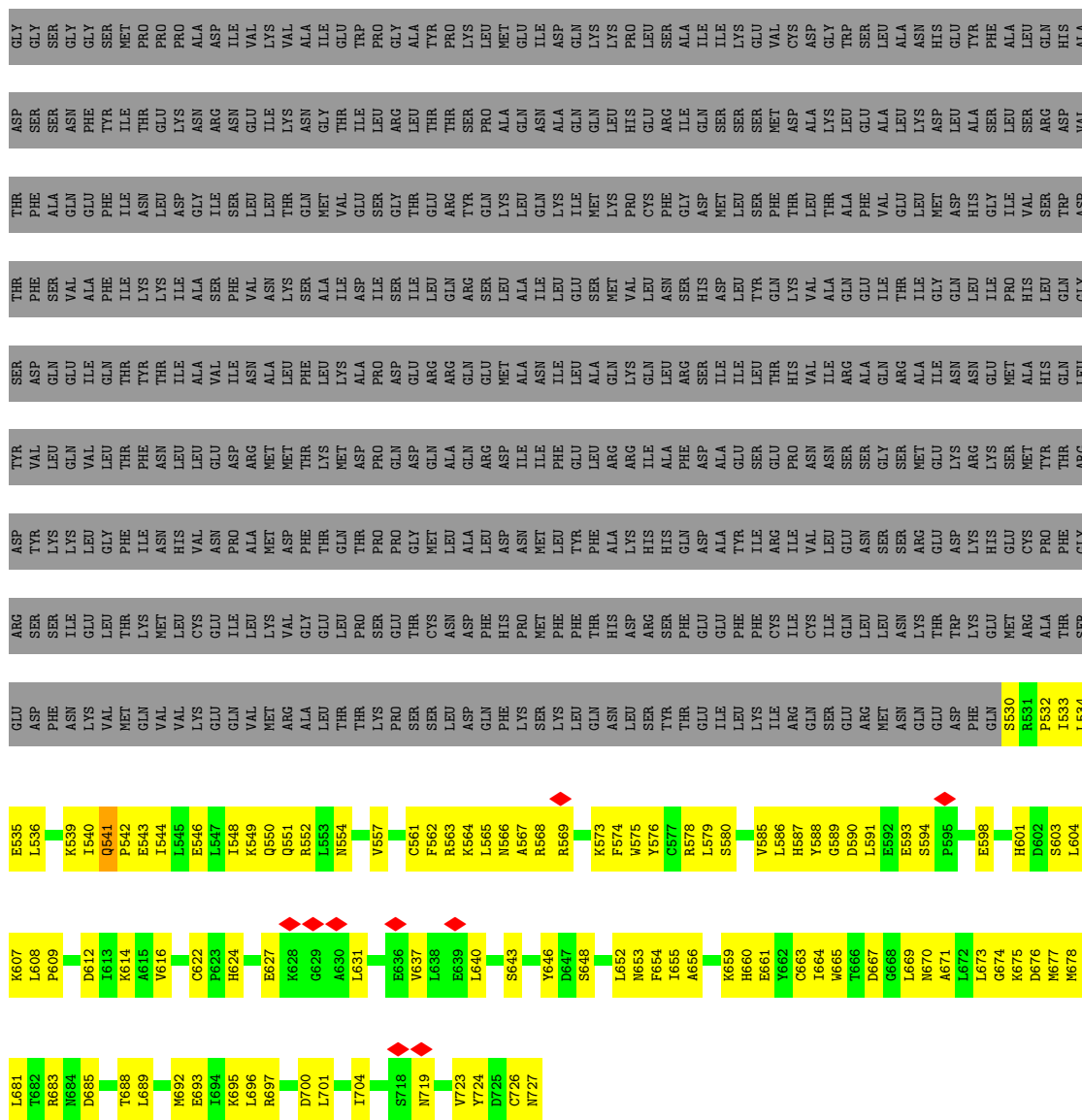
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

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: Engulfment and cell motility protein 1

Chain A: 



Chain D: 12% 15% 73%

Chain B:

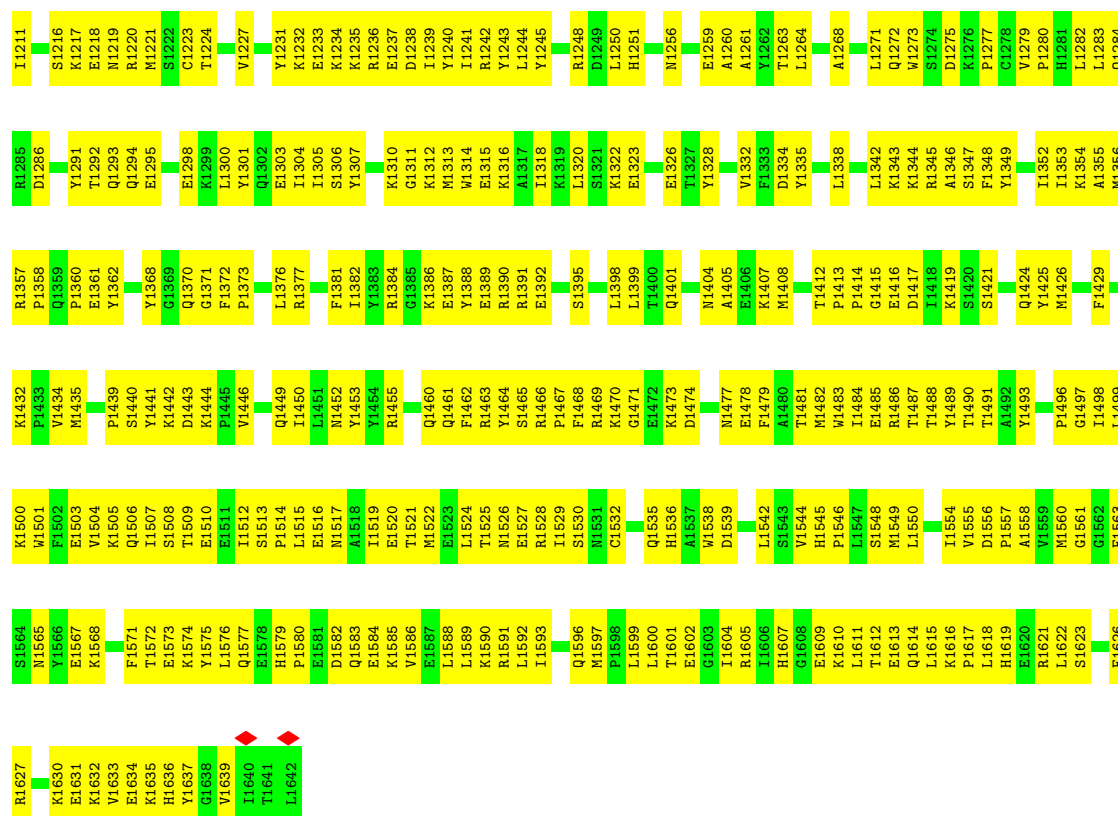
8% 42% 57%

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

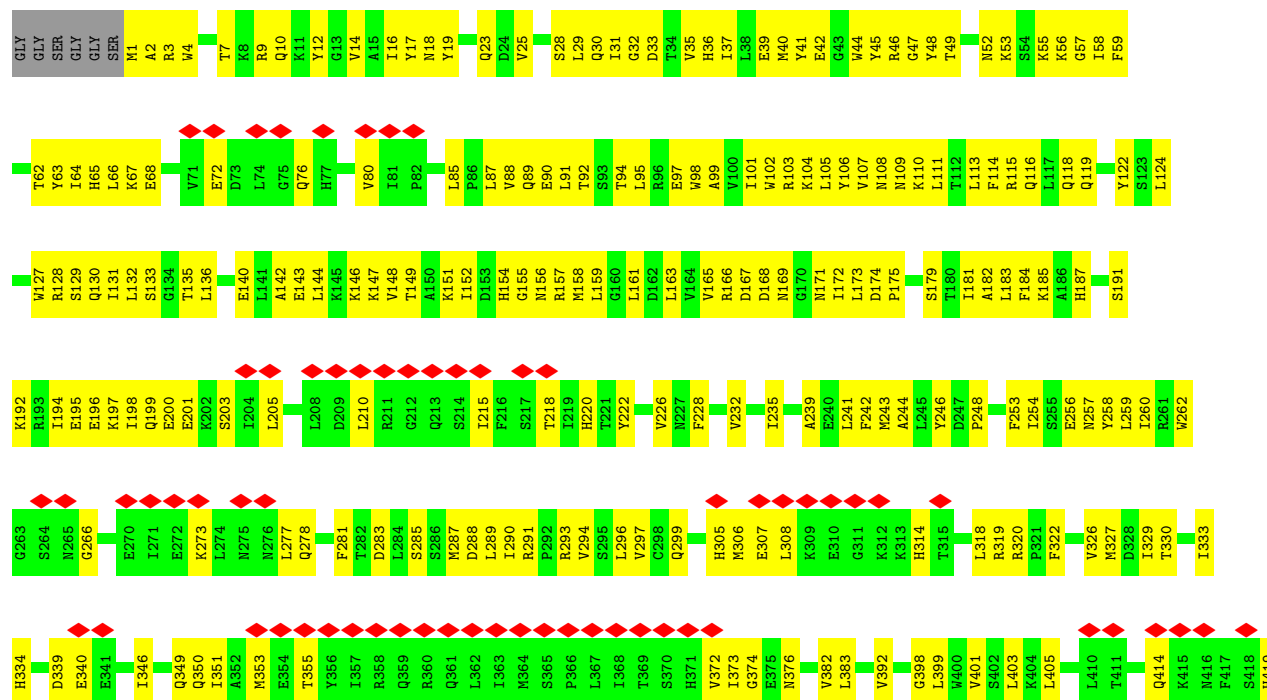
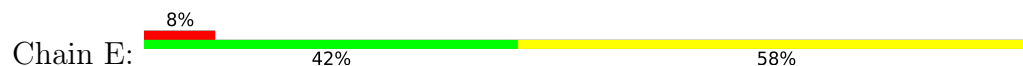
E61 T62 Y63 I64 H65 L66 K67 E68 V71 E72 D73 L74 G75 Q76 H77 V80 I81 P82 L85 P86 L87 V88 Q89 E90 L91 R92 S93 T94 L95 R96 E97 W98 A99 I100 V101 M102 Y103 K104 L105 Y106 V107 N108 M109 K110 L111 T112 F113 F114 R115 Q116 L117 Q118 Q119 L122 E123

L124 W127 R128 S129 Q130 L131 L132 S133 T135 L136 E140 L141 A142 E143 L144 K145 K146 K147 V148 T149 A150 K151 L152 D153 H154 G155 M156 L157 M158 L159 G160 G161 L162 D162 L163 V164 V165 R166 D167 D168 M171 L172 L173 D174 P175 S179 T180 L181 A182 L183 F184 K185 A186 H187 S191

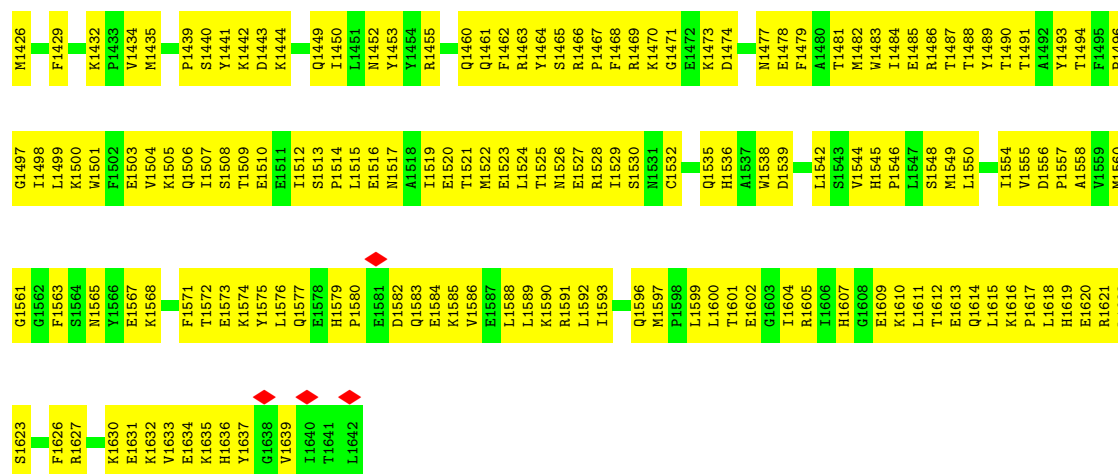
K1075	N1143	M992	I925	L852	Q710	L637	L569	A488	H419	T330	I260	K192
Y1076	H1144	F993	Q926	W853	H711	L638	L572	G489	L420	I333	R261	R193
G1077	D1077	K994	I927	R854	P714	G639	Y572	Y490	D421	H334	W262	I194
D1078	D985	L995	I928	R855	W715	L640	D575	E495	D422	G335	W665	E195
R1079	M1146	L996	N929	Q855	L716	N642	N576	Y496	R423	D339	G266	K197
M1081	M1147	I997	N930	R856	W717	W643	N577	V500	S424	E340	K269	I198
K1081	E1082	Y1002	R931	R857	W718	W644	K577	Q503	T425	E341	I271	Q199
E1082			R932	R858	W719	W645	K578	Y510	A426	I346	E272	E200
R1086		M1009	R933	C859	W720	N646	N579	E511	I427	I347	I272	E201
D1089		R1015	R934	T861	W721	W647	E580	Y511	A428	I348	E273	S203
W1090		Y1092	R935	R860	W722	W648	D581	K514	R429	Q349	K273	I204
W1091		Q1023	R936	R861	W723	W649	A582	W515	K430	Q350	L274	L205
W1092		F1024	R937	R862	W724	W650	A583	S516	M431	I351	W275	L206
W1093		R1019	R938	W864	S725	W651	K583	I517	G432	A352	L277	L208
Q1023		Q1023	R939	E865	S726	W652	F584	I518	I436	M353	L278	D209
F1024		F1024	R940	R866	A726	W653	W585	A518	I437	E354	Q278	L210
W1027		W1027	R941	L868	W727	W654	W586	I519	L438	T355	F281	R211
L1028		L1028	R942	F869	W728	W655	W587	E520	P439	I357	T282	Q212
L1029		L1029	R943	R870	W729	W656	L588	E521	P439	R358	D283	Q213
L1030		L1030	R944	R871	W730	W657	P589	E522	P439	Q359	S285	S214
F1031		F1031	R945	W872	W731	W658	G590	E523	G440	R361	S286	I215
Q1032		Q1032	R946	R873	W732	W659	G591	E524	V442	Q361	M287	F216
F1033		F1033	R947	C874	W733	W660	K592	E525	V442	Q362	D288	S217
R948		R948	R948	R875	W734	W661	M593	C525	V442	I363	L289	T218
I102		I102	R949	R876	W735	W662	E594	R532	V442	M364	R291	H220
M105		M105	R950	W877	W736	W663	E597	H331	K457	S365	R293	Y222
W106		W106	R951	W878	W737	W664	K598	H332	K458	P366	Y294	Y225
L107		L107	R952	W879	W738	W665	E599	H333	G459	L367	Y296	Y226
L108		L108	R953	W880	W739	W666	E599	H334	K460	I368	Y297	Y227
L109		L109	R954	W881	W740	W667	E599	H335	K461	I369	C398	F228
L110		L110	R955	W882	W741	W668	E599	H336	T462	S370	Q299	V232
L111		L111	R956	W883	W742	W669	E599	H337	T462	H371	H305	I235
L112		L112	R957	W884	W743	W670	E599	H338	T462	V372	M306	I235
L113		L113	R958	W885	W744	W671	E599	H339	T462	V372	E307	A239
L114		L114	R959	W886	W745	W672	E599	H340	T462	V372	E307	E240
L115		L115	R960	W887	W746	W673	E599	H341	T462	V372	E307	L241
L116		L116	R961	W888	W747	W674	E599	H342	T462	V372	E307	F242
L117		L117	R962	W889	W748	W675	E599	H343	T462	V372	E307	M243
L118		L118	R963	W890	W749	W676	E599	H344	T462	V372	E307	A244
L119		L119	R964	W891	W750	W677	E599	H345	T462	V372	E307	L245
L120		L120	R965	W892	W751	W678	E599	H346	T462	V372	E307	D247
L121		L121	R966	W893	W752	W679	E599	H347	T462	V372	E307	P248
L122		L122	R967	W894	W753	W680	E599	H348	T462	V372	E307	Q250
L123		L123	R968	W895	W754	W681	E599	H349	T462	V372	E307	F253
L124		L124	R969	W896	W755	W682	E599	H350	T462	V372	E307	I254
L125		L125	R970	W897	W756	W683	E599	H351	T462	V372	E307	S255
L126		L126	R971	W898	W757	W684	E599	H352	T462	V372	E307	E256
L127		L127	R972	W899	W758	W685	E599	H353	T462	V372	E307	N257
L128		L128	R973	W900	W759	W686	E599	H354	T462	V372	E307	L259
L129		L129	R974	W901	W760	W687	E599	H355	T462	V372	E307	
L130		L130	R975	W902	W761	W688	E599	H356	T462	V372	E307	
L131		L131	R976	W903	W762	W689	E599	H357	T462	V372	E307	
L132		L132	R977	W904	W763	W690	E599	H358	T462	V372	E307	
L133		L133	R978	W905	W764	W691	E599	H359	T462	V372	E307	
L134		L134	R979	W906	W765	W692	E599	H360	T462	V372	E307	
L135		L135	R980	W907	W766	W693	E599	H361	T462	V372	E307	
L136		L136	R981	W908	W767	W694	E599	H362	T462	V372	E307	
L137		L137	R982	W909	W768	W695	E599	H363	T462	V372	E307	
L138		L138	R983	W910	W769	W696	E599	H364	T462	V372	E307	
L139		L139	R984	W911	W770	W697	E599	H365	T462	V372	E307	
L140		L140	R985	W912	W771	W698	E599	H366	T462	V372	E307	
L141		L141	R986	W913	W772	W699	E599	H367	T462	V372	E307	
L142		L142	R987	W914	W773	W700	E599	H368	T462	V372	E307	
L143		L143	R988	W915	W774	W701	E599	H369	T462	V372	E307	
L144		L144	R989	W916	W775	W702	E599	H370	T462	V372	E307	
L145		L145	R990	W917	W776	W703	E599	H371	T462	V372	E307	
L146		L146	R991	W918	W777	W704	E599	H372	T462	V372	E307	
L147		L147	R992	W919	W778	W705	E599	H373	T462	V372	E307	
L148		L148	R993	W920	W779	W706	E599	H374	T462	V372	E307	
L149		L149	R994	W921	W780	W707	E599	H375	T462	V372	E307	
L150		L150	R995	W922	W781	W708	E599	H376	T462	V372	E307	
L151		L151	R996	W923	W782	W709	E599	H377	T462	V372	E307	
L152		L152	R997	W924	W783	W710	E599	H378	T462	V372	E307	
L153		L153	R998	W925	W784	W711	E599	H379	T462	V372	E307	
L154		L154	R999	W926	W785	W712	E599	H380	T462	V372	E307	
L155		L155	R1000	W927	W786	W713	E599	H381	T462	V372	E307	
L156		L156	R1001	W928	W787	W714	E599	H382	T462	V372	E307	
L157		L157	R1002	W929	W788	W715	E599	H383	T462	V372	E307	
L158		L158	R1003	W930	W789	W716	E599	H384	T462	V372	E307	
L159		L159	R1004	W931	W790	W717	E599	H385	T462	V372	E307	
L160		L160	R1005	W932	W791	W718	E599	H386	T462	V372	E307	
L161		L161	R1006	W933	W792	W719	E599	H387	T462	V372	E307	
L162		L162	R1007	W934	W793	W720	E599	H388	T462	V372	E307	
L163		L163	R1008	W935	W794	W721	E599	H389	T462	V372	E307	
L164		L164	R1009	W936	W795	W722	E599	H390	T462	V372	E307	
L165		L165	R1010	W937	W796	W723	E599	H391	T462	V372	E307	
L166		L166	R1011	W938	W797	W724	E599	H392	T462	V372	E307	
L167		L167	R1012	W939	W798	W725	E599	H393	T462	V372	E307	
L168		L168	R1013	W940	W799	W726	E599	H394	T462	V372	E307	
L169		L169	R1014	W941	W800	W727	E599	H395	T462	V372	E307	
L170		L170	R1015	W942	W801	W728	E599	H396	T462	V372	E307	
L171		L171	R1016	W943	W802	W729	E599	H397	T462	V372	E307	
L172		L172	R1017	W944	W803	W730	E599	H398	T462	V372	E307	
L173		L173	R1018	W945	W804	W731	E599	H399	T462	V372	E307	
L174		L174	R1019	W946	W805	W732	E599	H400	T462	V372	E307	
L175		L175	R1020	W947	W806	W733	E599	H401	T462	V372	E307	
L176		L176	R1021	W948	W807	W734	E599	H402	T462	V372	E307	
L177		L177	R1022	W949	W808	W735	E599	H403	T462	V372	E307	
L178		L178	R1023	W950	W809	W736	E599	H404	T462	V372	E307	
L179		L179	R1024	W951	W810	W737	E599	H405	T462	V372	E307	
L180		L180	R1025	W952	W811	W738	E599	H406	T462	V372	E307	
L181		L181	R1026	W953	W812	W739	E599	H407	T462	V372	E307	
L182		L182	R1027	W954	W813	W740	E599	H408	T462	V372	E307	
L183		L183	R1028	W955	W814	W741	E599	H409	T462	V372	E307	
L184		L184	R1029	W956	W815	W742	E599	H410	T462	V372	E307	
L185		L185	R1030	W957	W816	W743	E599	H411	T462	V372	E307	
L186		L186	R1031	W958	W817	W744	E599	H412	T462	V372	E307	
L187		L187	R1032	W959	W818	W745	E599	H413	T462	V372	E307	
L188		L188	R1033	W960	W819	W746	E599	H414	T462	V372	E307	
L189		L189	R1034	W961	W820	W747	E599	H415	T462	V372	E307	
L190		L190	R1035	W962	W821	W748	E599	H416	T462	V372	E307	
L191		L191	R1036	W963	W822	W749	E599	H417	T462	V372	E307	
L192		L192	R1037	W964	W823	W750	E599	H418	T462	V372	E307	
L193		L193	R1038	W965	W824	W751	E599	H419	T462	V372	E307	
L194		L194	R1039	W966	W825	W752	E599	H420	T462	V372	E307	
L195		L195	R1040	W967	W826	W753	E599	H421	T462	V		



• Molecule 2: Dedicator of cytokinesis protein 5

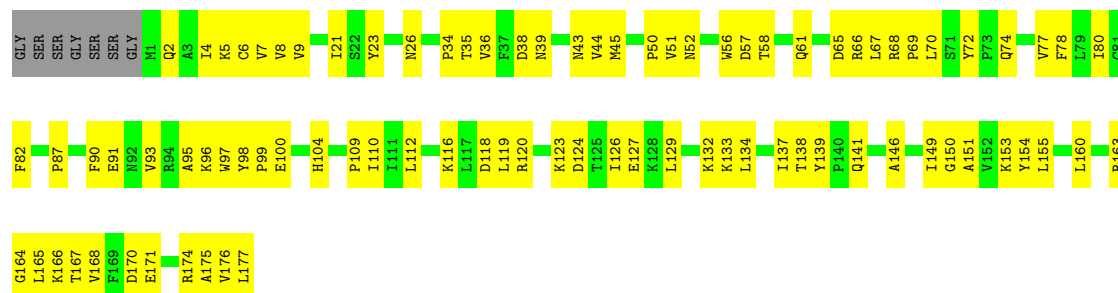


K1354	L1283	T1209	V1073	N992	Q926	S846	Q780	L631	G559	L420
A1355	Q1284	I1210	K1074	F993	L927	I847	S781	T632	A488	V421
M1356	D1285	I1211	K1075	K994	I928			Q633	G489	D422
P1357	D1286		K1076	D995	M929	L852	D782	L638	Y490	R423
Q1358		S1216	G1077	L996	E930	R853	K783	G639	E495	S424
P1359	Y1291	K1217	D1078	L997	R931	R854	G784	L640	Y496	T425
P1360	T1292	E1218	M1079		L932	Q855	D785	L641	K497	A126
E1361	Q1293	M1219	K1080	Y1002	L933	K856	E786	L642	S498	A428
Y1362	Q1294	K1220	K1081	M1009	R934	L857	F787	N643	V500	I427
	E1295	M1221	E1082		R935	N858	N788	R644	Q503	K430
Y1368		N1149	R1086	R1015	I936	R935	N789	S645		M431
G1369	E1298	C1223			N937	M860	S790	N646	Y510	G432
Q1370	A1299	T1224		R1019	R938	T861	S791	K577	Y511	I436
G1371	L1300	V1227	D1089		T939	K862	R792	K578	ES11	I437
P1372	Y1301		M1090	M1022	V940	I863	Q793	M579	K514	L438
P1373	Q1302	Y1231	Y1092	Q1023	G942	V864	L794	E580	V515	F439
L1376	E1303	K1232	N1093	F1024	M943	S866	L795	I650	I517	G440
R1377	I1304	K1233	L1094	A1025	N944	T867	A797	K651	ES16	V442
	I1305	E1234	G1095	E1026	R945	L868	F798	H652	I518	R443
F1381	Y1307	K1235	P1096	E1027	Q946	F869	N799	L654	ES20	M444
I1382	K1310	R1236	H1097	Q1027	Q947	R870	F799	K655	ES21	D445
R1384	G1311	D1237	K1098	L1028	S947	K871	N800	K656	ES22	I446
G1385	M1312	I1238	I1099	T1029	P948	Q870	M801	L657	ES23	
K1386	M1313	T1239	K1100	R1030	H949	S872	L802	L586	ES24	L450
E1387	W1314	Y1240	F1101	F1031	I950	E873	M802	L587	C525	I451
Y1388	E1315	I1241	F1102	F1032		C874	R804	L588	H526	F455
R1390	K1316	K1244		M1033	F953	R875	R805	V660	ES27	D456
A1317	A1317	Y1245	M1105	Q1035	V954	V877	P805	E664	H533	K457
I1318	L1172		V1106	Q1036	C956	L878			ES34	G458
G1319	L1176	L1177	G1107	S1037	R957	M957	E808	K667	ES35	K459
L1320	L1178	L1179	P1108	F1038	I958	P880	A809	F668	R532	K460
F1321	E1178	E1179	I1109	E1039	A959	L881	V810	N677	H534	T462
S1322	H1179	C1180	L1110	L1040	L960	T882	K812	Q670	S536	P463
E1323	E1181	R1181	V1112	W1043	L961	T883	K813	L673	Q637	K464
	K1182	K1182		M1044	Q962	D884	A816		ES38	M465
E1326	N1256		L1114	M1045	Q963	Q885		L676	ES39	V466
T1327	E1259	A1260	T1115	Y1046	M964	L890	Y819	F677	ES40	V468
Y1328	A1261	A1261	P1116	F1047	D965	K896	L820	N678	D541	T469
V1332	E1262	E1262	E1117	H1048	S967	H968	P821	I679	T608	V472
F1333	A1263	A1263	V1118	L1054	Y969	H969	S922	M680	S543	H473
D1334	L1263	L1264	E1119	T1055	S970	L905	I823	M681	ES44	D474
Y1335	L1264		R1121	T1056	H971	L905	I824	E682	R545	E475
	A1268		K1122	E1057	Y972	I909	N825	D826	A696	E476
L1338	L1271	L1271	A1123	S1058	I973	K828	D827	L606	R771	G477
G1339	Q1272	Q1272	T1124	L1059	S974	L910	K828	L607	K542	K478
L1342	M1273	M1273	I1125	E1062	T975	V912	L829	V607	S543	L480
K1343	G1273	G1273	P1126	T1063	F976	R915	V830	F609	ES44	E481
E1405	S1198	S1198	I1127	F1064		R915	F831	T610	R545	K482
E1406	L1199	L1199	F1128	S1065	R979	V912	D832	P611	R545	A483
K1407	L1200	L1200	F1129	Q1066		V912	P833	S612	G548	I484
M1408	L1201	L1201	D1130	Q1067	F985	V918	V934	R771	V549	H485
	L1204	L1204	M1131	A1067	L986	L986	L839	L697	D614	P486
P1413	L1205	L1205	M1132	A1068	M987	L986	T921	I700	S815	
G1415	D1206	D1206	Q1133	R1069	E988	L986	A922	I701	D614	
E1416	P1280	P1280	C1134	K1070	F989	L986	V923	I704	S815	
D1417	H1281	H1281	E1135	K1071	F990	L986	H924		D614	
I1418	Y1425	Y1425	F1136	I1072	I991	L986	Q945		S815	
S1421										
Q1424										
Y1425										



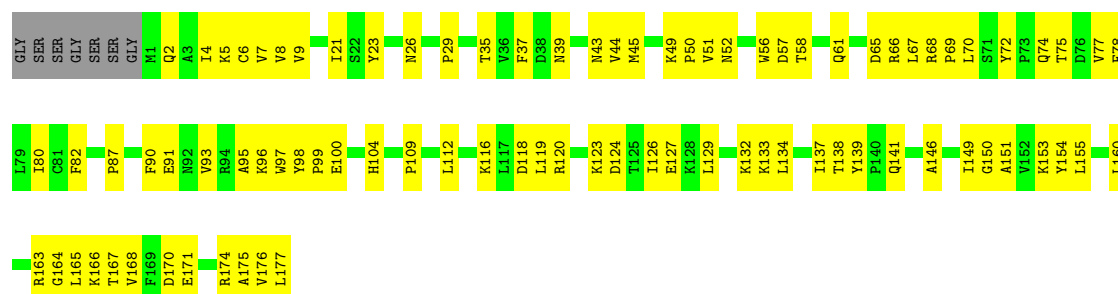
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C: 49% 47% .



• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F: 49% 47% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	133323	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/1641	0.46	0/2218
1	D	0.24	0/1641	0.46	0/2218
2	B	0.25	0/13722	0.47	0/18514
2	E	0.25	0/13722	0.47	0/18514
3	C	0.23	0/1415	0.47	0/1924
3	F	0.23	0/1415	0.47	0/1924
All	All	0.25	0/33556	0.47	0/45312

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	GLN	Peptide
1	D	541	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1608	0	1617	106	0
1	D	1608	0	1617	112	0
2	B	13436	0	13516	896	0
2	E	13436	0	13516	897	0
3	C	1385	0	1407	84	0
3	F	1385	0	1407	91	0
All	All	32858	0	33080	2123	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 32.

All (2123) 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)
2:B:1346:ALA:HB2	2:E:1342:LEU:HD11	1.27	1.09
1:A:536:LEU:HD21	2:B:17:TYR:HB2	1.40	1.03
1:A:697:ARG:HB3	2:B:31:ILE:HB	1.53	0.89
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.59	0.85
2:E:144:LEU:HD13	2:E:147:LYS:HE2	1.60	0.83
3:C:93:VAL:HA	3:C:97:TRP:HB2	1.59	0.83
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.61	0.83
1:D:535:GLU:O	1:D:539:LYS:HB3	1.79	0.82
2:E:883:THR:OG1	2:E:931:ARG:NH1	2.12	0.82
1:A:535:GLU:O	1:A:539:LYS:HB3	1.79	0.82
2:B:883:THR:OG1	2:B:931:ARG:NH1	2.12	0.82
2:E:166:ARG:NH1	2:E:167:ASP:OD1	2.12	0.81
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.12	0.81
2:B:802:MET:HA	2:B:813:LYS:HE3	1.62	0.81
2:B:1305:ILE:HD11	2:B:1320:LEU:HB2	1.62	0.81
2:B:1349:TYR:HB3	2:E:1335:TYR:HB3	1.61	0.81
2:B:144:LEU:HD13	2:B:147:LYS:HE2	1.60	0.80
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.61	0.80
2:E:1305:ILE:HD11	2:E:1320:LEU:HB2	1.62	0.80
2:E:1621:ARG:NH2	3:F:67:LEU:HD11	1.97	0.80
2:E:802:MET:HA	2:E:813:LYS:HE3	1.62	0.80
2:B:10:GLN:HG3	2:B:37:ILE:HB	1.65	0.79
2:B:681:MET:HE1	2:B:728:LEU:H	1.48	0.78
2:E:681:MET:HE1	2:E:728:LEU:H	1.48	0.78
2:B:788:ASN:O	2:B:792:ARG:NH1	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:GLN:HE22	2:B:421:VAL:HG12	1.49	0.78
2:E:242:PHE:HB2	2:E:299:GLN:HB2	1.64	0.78
2:B:1328:TYR:HA	2:B:1332:VAL:HG12	1.66	0.78
2:E:10:GLN:HB3	2:E:40:MET:HE1	1.66	0.78
2:B:10:GLN:HB3	2:B:40:MET:HE1	1.66	0.77
1:A:563:ARG:HB3	1:A:573:LYS:HE3	1.65	0.77
1:D:670:ASN:ND2	1:D:676:ASP:O	2.16	0.77
1:A:670:ASN:ND2	1:A:676:ASP:O	2.16	0.77
2:B:242:PHE:HB2	2:B:299:GLN:HB2	1.65	0.77
2:E:197:LYS:HA	2:E:200:GLU:HG2	1.66	0.77
2:E:414:GLN:HE22	2:E:421:VAL:HG12	1.49	0.77
2:E:1393:ASP:OD1	3:F:166:LYS:NZ	2.17	0.77
2:B:968:HIS:HA	2:B:971:HIS:HD2	1.50	0.77
2:E:788:ASN:O	2:E:792:ARG:NH1	2.16	0.77
2:E:10:GLN:HG3	2:E:37:ILE:HB	1.65	0.77
1:D:563:ARG:HB3	1:D:573:LYS:HE3	1.65	0.77
2:E:241:LEU:HB2	2:E:260:ILE:HB	1.67	0.77
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.67	0.77
2:B:445:ASP:HB2	2:B:627:CYS:HB2	1.66	0.76
2:B:278:GLN:HB2	2:B:425:THR:HG23	1.68	0.76
2:E:445:ASP:HB2	2:E:627:CYS:HB2	1.66	0.76
2:B:241:LEU:HB2	2:B:260:ILE:HB	1.67	0.76
3:C:23:TYR:HB2	3:C:165:LEU:HD21	1.64	0.76
3:F:23:TYR:HB2	3:F:165:LEU:HD21	1.65	0.76
2:E:968:HIS:HA	2:E:971:HIS:HD2	1.50	0.76
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.66	0.76
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.68	0.76
2:E:1310:LYS:O	2:E:1312:LYS:NZ	2.18	0.76
2:E:921:THR:O	2:E:925:ILE:N	2.18	0.75
2:E:1398:LEU:HD22	2:E:1426:MET:HE3	1.68	0.75
2:E:1473:LYS:HD3	2:E:1481:THR:HG21	1.68	0.75
2:B:1473:LYS:HD3	2:B:1481:THR:HG21	1.68	0.75
2:B:1579:HIS:HB3	2:B:1582:ASP:HB2	1.68	0.75
2:B:1398:LEU:HD22	2:B:1426:MET:HE3	1.68	0.75
2:B:7:THR:HB	2:B:40:MET:HE2	1.69	0.75
2:B:1346:ALA:CB	2:E:1342:LEU:HD11	2.14	0.75
2:B:1391:ARG:HD2	2:B:1429:PHE:HA	1.69	0.75
2:E:1388:TYR:OH	2:E:1390:ARG:NH1	2.20	0.75
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.69	0.74
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.68	0.74
2:B:921:THR:O	2:B:925:ILE:N	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1310:LYS:O	2:B:1312:LYS:NZ	2.18	0.74
3:C:146:ALA:O	3:C:150:GLY:N	2.20	0.74
2:E:874:CYS:HB2	2:E:878:LEU:HD13	1.68	0.74
2:E:1579:HIS:HB3	2:E:1582:ASP:HB2	1.68	0.74
2:B:874:CYS:HB2	2:B:878:LEU:HD13	1.68	0.74
3:F:146:ALA:O	3:F:150:GLY:N	2.20	0.74
2:E:278:GLN:HB2	2:E:425:THR:HG23	1.68	0.74
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.21	0.74
2:E:91:LEU:HD11	2:E:128:ARG:HG3	1.70	0.74
2:E:761:LYS:HE2	2:E:765:ARG:HH12	1.53	0.74
2:B:761:LYS:HE2	2:B:765:ARG:HH12	1.53	0.73
2:E:925:ILE:HA	2:E:928:ILE:HD12	1.69	0.73
2:E:1056:HIS:ND1	2:E:1057:GLU:OE2	2.21	0.73
2:E:1391:ARG:HD2	2:E:1429:PHE:HA	1.69	0.73
3:F:9:VAL:HG22	3:F:78:PHE:HZ	1.53	0.73
2:B:927:LEU:HB2	2:B:931:ARG:HH21	1.54	0.73
3:C:9:VAL:HG22	3:C:78:PHE:HZ	1.52	0.73
2:E:730:TYR:HB2	2:E:767:ILE:HG23	1.70	0.72
2:E:1260:ALA:O	2:E:1263:THR:OG1	2.07	0.72
2:E:7:THR:HB	2:E:40:MET:HE2	1.69	0.72
2:E:927:LEU:HB2	2:E:931:ARG:HH21	1.54	0.72
3:C:171:GLU:HA	3:C:174:ARG:HG2	1.71	0.72
1:A:552:ARG:HH12	1:A:664:ILE:HG12	1.54	0.72
2:B:1388:TYR:OH	2:B:1390:ARG:NH1	2.20	0.72
2:E:472:VAL:HG21	2:E:483:ALA:HB3	1.71	0.72
2:B:91:LEU:HD11	2:B:128:ARG:HG3	1.70	0.72
2:B:1441:TYR:HE2	2:B:1450:ILE:HG21	1.54	0.72
2:E:1487:THR:HA	2:E:1509:THR:HA	1.69	0.72
2:B:49:THR:OG1	2:B:52:ASN:OD1	2.08	0.72
2:B:946:GLN:HA	2:B:950:ILE:HG21	1.72	0.72
2:B:1260:ALA:O	2:B:1263:THR:OG1	2.07	0.72
2:E:946:GLN:HA	2:E:950:ILE:HG21	1.72	0.72
2:E:1034:ASP:OD1	2:E:1097:HIS:NE2	2.22	0.72
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.70	0.72
1:D:550:GLN:O	1:D:554:ASN:ND2	2.23	0.72
2:B:472:VAL:HG21	2:B:483:ALA:HB3	1.71	0.71
2:B:749:LYS:HG2	2:B:753:LEU:HD23	1.71	0.71
2:B:825:ASN:OD1	2:B:826:ASP:N	2.23	0.71
2:E:1275:ASP:O	2:E:1292:THR:OG1	2.06	0.71
2:B:1399:LEU:HD22	2:B:1405:ALA:HB1	1.73	0.71
2:B:1487:THR:HA	2:B:1509:THR:HA	1.69	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1478:GLU:HG3	2:E:1482:MET:HE2	1.72	0.71
2:B:1478:GLU:HG3	2:B:1482:MET:HE2	1.72	0.71
2:E:1259:GLU:N	2:E:1259:GLU:OE1	2.23	0.71
3:F:171:GLU:HA	3:F:174:ARG:HG2	1.71	0.71
1:A:589:GLY:HA3	1:A:604:LEU:HB2	1.72	0.71
2:B:95:LEU:HD21	2:B:124:LEU:HD22	1.72	0.71
2:B:1275:ASP:O	2:B:1292:THR:OG1	2.06	0.71
2:B:1284:GLN:HG2	2:B:1286:ASP:H	1.55	0.71
2:E:1441:TYR:HE2	2:E:1450:ILE:HG21	1.54	0.71
2:E:1284:GLN:HG2	2:E:1286:ASP:H	1.55	0.71
2:E:1575:TYR:O	2:E:1579:HIS:N	2.23	0.71
2:B:771:ARG:NH2	2:B:781:SER:OG	2.23	0.71
2:E:95:LEU:HD21	2:E:124:LEU:HD22	1.72	0.71
2:E:1399:LEU:HD22	2:E:1405:ALA:HB1	1.73	0.71
1:A:550:GLN:O	1:A:554:ASN:ND2	2.23	0.71
2:E:1245:TYR:HD2	2:E:1248:ARG:HH21	1.39	0.71
2:B:945:ARG:HH11	2:B:946:GLN:H	1.38	0.71
2:B:1386:LYS:HB3	2:B:1389:GLU:HG3	1.73	0.71
2:B:3:ARG:HH22	2:B:42:GLU:H	1.39	0.70
1:D:589:GLY:HA3	1:D:604:LEU:HB2	1.71	0.70
2:E:1470:LYS:HB3	2:E:1483:TRP:CD1	2.27	0.70
2:E:244:ALA:HB2	2:E:257:ASN:HA	1.73	0.70
2:E:3:ARG:HH22	2:E:42:GLU:H	1.39	0.70
2:E:749:LYS:HG2	2:E:753:LEU:HD23	1.71	0.70
2:E:771:ARG:NH2	2:E:781:SER:OG	2.23	0.70
1:A:566:ASN:HA	1:A:568:ARG:HE	1.56	0.70
2:B:349:GLN:HB2	2:B:392:VAL:HG13	1.74	0.70
2:B:1177:LEU:HD22	2:B:1181:ARG:HH22	1.56	0.70
2:B:1470:LYS:HB3	2:B:1483:TRP:CD1	2.27	0.70
1:D:552:ARG:HH12	1:D:664:ILE:HG12	1.54	0.70
1:D:566:ASN:HA	1:D:568:ARG:HE	1.57	0.70
2:E:500:VAL:HG13	2:E:534:ARG:HH21	1.57	0.70
2:B:1015:ARG:HE	2:B:1076:TYR:HD1	1.40	0.70
1:D:711:PRO:HD2	2:E:17:TYR:HE1	1.57	0.70
2:E:945:ARG:HH11	2:E:946:GLN:H	1.38	0.70
2:E:444:ASN:ND2	2:E:517:ILE:O	2.25	0.69
2:E:1177:LEU:HD22	2:E:1181:ARG:HH22	1.56	0.69
2:B:1575:TYR:O	2:B:1579:HIS:N	2.23	0.69
2:E:772:VAL:HA	2:E:775:LEU:HD12	1.74	0.69
2:E:1360:PRO:HA	2:E:1387:GLU:HA	1.74	0.69
1:A:573:LYS:N	1:A:593:GLU:OE2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ALA:HB2	2:B:257:ASN:HA	1.73	0.69
2:B:518:ALA:HB3	2:B:521:GLU:HB2	1.74	0.69
2:B:1248:ARG:HG3	2:B:1264:LEU:HD11	1.73	0.69
2:B:1618:LEU:HD23	2:B:1621:ARG:HH21	1.56	0.69
1:D:573:LYS:N	1:D:593:GLU:OE2	2.25	0.69
2:E:349:GLN:HB2	2:E:392:VAL:HG13	1.74	0.69
2:B:1439:PRO:HA	2:B:1442:LYS:HZ3	1.58	0.69
2:B:444:ASN:ND2	2:B:517:ILE:O	2.25	0.69
2:B:857:LEU:O	2:B:861:THR:OG1	2.09	0.69
2:B:1034:ASP:OD1	2:B:1097:HIS:NE2	2.22	0.69
2:E:518:ALA:HB3	2:E:521:GLU:HB2	1.74	0.69
2:E:825:ASN:OD1	2:E:826:ASP:N	2.23	0.69
2:E:1439:PRO:HA	2:E:1442:LYS:HZ3	1.58	0.69
2:E:49:THR:OG1	2:E:52:ASN:OD1	2.08	0.68
2:E:1248:ARG:HG3	2:E:1264:LEU:HD11	1.73	0.68
2:B:772:VAL:HA	2:B:775:LEU:HD12	1.74	0.68
2:B:1516:GLU:HA	2:B:1519:ILE:HD12	1.73	0.68
1:A:701:LEU:HA	1:A:704:ILE:HD12	1.75	0.68
2:B:695:ASP:OD1	2:B:740:TYR:OH	2.10	0.68
2:E:1386:LYS:HB3	2:E:1389:GLU:HG3	1.73	0.68
2:B:9:ARG:HD2	2:B:68:GLU:HG2	1.76	0.68
2:B:500:VAL:HG13	2:B:534:ARG:HH21	1.57	0.68
1:D:564:LYS:O	1:D:573:LYS:NZ	2.19	0.68
2:E:1516:GLU:HA	2:E:1519:ILE:HD12	1.73	0.68
2:B:1259:GLU:OE1	2:B:1259:GLU:N	2.23	0.68
2:E:1618:LEU:HD23	2:E:1621:ARG:HH21	1.56	0.68
3:F:61:GLN:O	3:F:68:ARG:NH2	2.26	0.68
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.11	0.68
3:C:170:ASP:HB3	3:C:174:ARG:HH21	1.59	0.68
2:E:695:ASP:OD1	2:E:740:TYR:OH	2.10	0.68
2:B:879:LEU:HD12	2:B:882:LEU:HB2	1.76	0.68
2:B:1245:TYR:HD2	2:B:1248:ARG:HH21	1.39	0.68
2:E:945:ARG:NH1	2:E:946:GLN:OE1	2.27	0.68
2:B:945:ARG:NH1	2:B:946:GLN:OE1	2.27	0.68
2:B:1154:LYS:HD2	2:B:1157:GLN:HE22	1.59	0.68
2:E:1154:LYS:HD2	2:E:1157:GLN:HE22	1.59	0.68
3:C:61:GLN:O	3:C:68:ARG:NH2	2.26	0.68
2:E:879:LEU:HD12	2:E:882:LEU:HB2	1.76	0.68
2:B:129:SER:HA	2:B:132:LEU:HD12	1.76	0.67
1:D:536:LEU:HD23	2:E:31:ILE:HD11	1.76	0.67
2:E:1218:GLU:OE1	2:E:1218:GLU:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:TYR:HB2	2:B:59:PHE:HE1	1.59	0.67
2:B:834:VAL:HB	2:B:873:GLU:HG2	1.77	0.67
2:B:1392:GLU:HB2	3:C:166:LYS:NZ	2.09	0.67
2:E:129:SER:HA	2:E:132:LEU:HD12	1.76	0.67
1:D:701:LEU:HA	1:D:704:ILE:HD12	1.75	0.67
2:E:730:TYR:HB3	2:E:770:SER:HB3	1.75	0.67
2:E:1015:ARG:HE	2:E:1076:TYR:HD1	1.40	0.67
2:B:351:ILE:HG12	2:B:382:VAL:HG21	1.77	0.67
2:B:1143:ASN:OD1	2:B:1145:HIS:ND1	2.28	0.67
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.28	0.67
2:B:1360:PRO:HA	2:B:1387:GLU:HA	1.74	0.67
2:E:853:VAL:HG23	2:E:854:ARG:HD3	1.76	0.67
2:B:90:GLU:O	2:B:94:THR:HG23	1.95	0.67
2:B:561:THR:HG21	2:B:631:LEU:HB3	1.76	0.67
2:B:730:TYR:HB3	2:B:770:SER:HB3	1.75	0.67
1:D:723:VAL:HG23	2:E:2:ALA:HB1	1.77	0.67
2:E:561:THR:HG21	2:E:631:LEU:HB3	1.76	0.67
2:B:1346:ALA:HB2	2:E:1342:LEU:CD1	2.17	0.67
2:B:1573:GLU:O	2:B:1577:GLN:NE2	2.28	0.67
2:E:19:TYR:HB2	2:E:59:PHE:HE1	1.59	0.67
2:E:1143:ASN:OD1	2:E:1145:HIS:ND1	2.28	0.67
2:E:94:THR:HG21	2:E:152:ILE:HD11	1.77	0.67
2:E:932:LEU:N	2:E:935:ARG:HH21	1.93	0.67
2:E:1573:GLU:O	2:E:1577:GLN:NE2	2.28	0.66
2:B:1114:LEU:O	2:B:1163:ARG:NH1	2.29	0.66
2:E:1233:GLU:O	2:E:1235:LYS:NZ	2.28	0.66
2:E:1462:PHE:HB2	2:E:1489:TYR:HB2	1.77	0.66
2:E:1486:ARG:O	2:E:1510:GLU:N	2.28	0.66
2:B:929:MET:HE1	2:B:968:HIS:O	1.96	0.66
2:B:1414:PRO:HB2	2:B:1419:LYS:HD3	1.78	0.66
1:D:536:LEU:HD21	2:E:17:TYR:HB2	1.77	0.66
2:E:929:MET:HE1	2:E:968:HIS:O	1.96	0.66
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.78	0.66
2:B:1486:ARG:O	2:B:1510:GLU:N	2.28	0.66
2:B:94:THR:HG21	2:B:152:ILE:HD11	1.77	0.66
2:B:1357:ARG:HH21	2:B:1453:TYR:HD1	1.44	0.66
2:E:103:ARG:HA	2:E:106:TYR:HE1	1.61	0.66
3:F:170:ASP:HB3	3:F:174:ARG:HH21	1.59	0.66
2:B:932:LEU:N	2:B:935:ARG:HH21	1.93	0.65
2:E:90:GLU:O	2:E:94:THR:HG23	1.95	0.65
2:E:834:VAL:HB	2:E:873:GLU:HG2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:857:LEU:O	2:E:861:THR:OG1	2.09	0.65
2:E:1357:ARG:HH21	2:E:1453:TYR:HD1	1.44	0.65
2:E:9:ARG:HD2	2:E:68:GLU:HG2	1.76	0.65
2:E:1114:LEU:O	2:E:1163:ARG:NH1	2.29	0.65
2:B:1233:GLU:O	2:B:1235:LYS:NZ	2.28	0.65
2:E:46:ARG:HB3	2:E:58:ILE:HG13	1.79	0.65
2:E:939:THR:O	2:E:943:MET:N	2.17	0.65
2:E:1059:LEU:HD12	2:E:1116:PRO:HB2	1.78	0.65
2:B:853:VAL:HG23	2:B:854:ARG:HD3	1.76	0.65
2:E:351:ILE:HG12	2:E:382:VAL:HG21	1.77	0.65
2:B:1277:PRO:HG3	2:B:1292:THR:HA	1.77	0.65
2:B:465:ASN:ND2	2:B:534:ARG:O	2.25	0.65
2:B:979:ARG:NH1	2:B:1031:PHE:O	2.30	0.65
2:B:1462:PHE:HB2	2:B:1489:TYR:HB2	1.77	0.65
2:E:1602:GLU:HG3	2:E:1605:ARG:CZ	2.27	0.65
2:B:1602:GLU:HG3	2:B:1605:ARG:CZ	2.27	0.65
2:E:1313:MET:HE1	2:E:1496:PRO:HG3	1.79	0.65
2:E:191:SER:HA	2:E:194:ILE:HD12	1.79	0.65
2:E:843:PHE:O	2:E:846:SER:OG	2.10	0.65
2:E:1059:LEU:O	2:E:1063:THR:OG1	2.11	0.65
2:E:1115:THR:O	2:E:1121:ARG:NH2	2.28	0.65
2:B:1353:ILE:HG23	2:E:1335:TYR:CD2	2.32	0.64
2:E:1277:PRO:HG3	2:E:1292:THR:HA	1.77	0.64
3:C:87:PRO:HA	3:C:90:PHE:CD2	2.32	0.64
2:B:1218:GLU:OE1	2:B:1218:GLU:N	2.27	0.64
2:B:1372:PHE:O	2:B:1377:ARG:NH2	2.28	0.64
2:B:1596:GLN:HE21	2:B:1600:LEU:HD21	1.61	0.64
2:E:1414:PRO:HB2	2:E:1419:LYS:HD3	1.78	0.64
2:E:1091:TRP:HA	2:E:1094:LEU:HD13	1.79	0.64
2:E:979:ARG:NH1	2:E:1031:PHE:O	2.30	0.64
2:E:1596:GLN:HE21	2:E:1600:LEU:HD21	1.61	0.64
3:F:77:VAL:HG12	3:F:109:PRO:HG2	1.80	0.64
2:B:970:SER:O	2:B:974:SER:OG	2.13	0.64
2:E:970:SER:O	2:E:974:SER:OG	2.13	0.64
2:B:1284:GLN:HE21	2:B:1286:ASP:HB2	1.63	0.64
2:B:1091:TRP:HA	2:B:1094:LEU:HD13	1.79	0.64
2:E:730:TYR:OH	2:E:771:ARG:NH1	2.31	0.64
2:E:785:ASP:OD1	2:E:786:GLU:N	2.31	0.64
2:B:191:SER:HA	2:B:194:ILE:HD12	1.79	0.63
2:B:730:TYR:OH	2:B:771:ARG:NH1	2.31	0.63
2:E:1391:ARG:NH2	3:F:29:PRO:HD3	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:GLN:HG2	2:E:58:ILE:HB	1.79	0.63
2:B:201:GLU:O	2:B:205:LEU:HB3	1.99	0.63
2:B:857:LEU:HA	2:B:860:MET:SD	2.38	0.63
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.26	0.63
3:C:129:LEU:HA	3:C:132:LYS:HG2	1.79	0.63
2:E:465:ASN:ND2	2:E:534:ARG:O	2.25	0.63
2:E:1524:LEU:HA	2:E:1527:GLU:CD	2.24	0.63
3:F:129:LEU:HA	3:F:132:LYS:HG2	1.79	0.63
2:E:465:ASN:O	2:E:534:ARG:NH1	2.31	0.63
2:E:857:LEU:HA	2:E:860:MET:SD	2.38	0.63
2:E:1623:SER:HB3	2:E:1627:ARG:HH12	1.64	0.63
2:B:1524:LEU:HA	2:B:1527:GLU:CD	2.24	0.63
2:E:1372:PHE:O	2:E:1377:ARG:NH2	2.28	0.63
2:B:103:ARG:HA	2:B:106:TYR:HE1	1.61	0.63
2:B:465:ASN:O	2:B:534:ARG:NH1	2.31	0.63
2:B:485:HIS:HB2	2:B:514:LYS:HB3	1.81	0.63
2:E:556:ASN:N	2:E:560:THR:O	2.32	0.63
3:F:44:VAL:N	3:F:51:VAL:O	2.27	0.63
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.78	0.63
2:B:87:LEU:HD23	2:B:91:LEU:HD23	1.81	0.63
2:E:1062:GLU:OE2	2:E:1080:ARG:NH1	2.32	0.63
3:F:87:PRO:HA	3:F:90:PHE:CD2	2.32	0.63
2:B:23:GLN:HG2	2:B:58:ILE:HB	1.79	0.63
2:B:785:ASP:OD1	2:B:786:GLU:N	2.31	0.63
2:E:127:TRP:HD1	2:E:130:GLN:NE2	1.97	0.63
2:E:1630:LYS:O	2:E:1634:GLU:HG2	1.99	0.63
2:B:1623:SER:HB3	2:B:1627:ARG:HH12	1.64	0.63
2:B:1630:LYS:O	2:B:1634:GLU:HG2	1.99	0.63
3:C:7:VAL:HA	3:C:56:TRP:HB2	1.80	0.63
3:F:120:ARG:HH12	3:F:139:TYR:HB2	1.64	0.63
2:B:939:THR:O	2:B:943:MET:N	2.17	0.62
2:B:1313:MET:HE1	2:B:1496:PRO:HG3	1.79	0.62
3:C:77:VAL:HG12	3:C:109:PRO:HG2	1.80	0.62
2:B:1062:GLU:OE2	2:B:1080:ARG:NH1	2.32	0.62
2:B:1362:TYR:HE1	2:B:1384:ARG:HG3	1.64	0.62
3:C:120:ARG:HH12	3:C:139:TYR:HB2	1.64	0.62
2:B:1323:GLU:HA	2:B:1326:GLU:HG2	1.80	0.62
2:E:1145:HIS:O	2:E:1149:ASN:ND2	2.32	0.62
2:E:968:HIS:HA	2:E:971:HIS:CD2	2.34	0.62
2:E:1323:GLU:HA	2:E:1326:GLU:HG2	1.80	0.62
2:B:1056:HIS:HD1	2:B:1057:GLU:H	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1219:ASN:OD1	2:E:1401:GLN:NE2	2.32	0.62
3:F:138:THR:H	3:F:141:GLN:NE2	1.98	0.62
2:E:87:LEU:HD23	2:E:91:LEU:HD23	1.81	0.62
3:F:7:VAL:HA	3:F:56:TRP:HB2	1.80	0.62
2:B:843:PHE:O	2:B:846:SER:OG	2.10	0.62
2:B:1145:HIS:O	2:B:1149:ASN:ND2	2.32	0.62
3:C:66:ARG:H	3:C:66:ARG:HD3	1.64	0.62
2:E:569:LEU:HD12	2:E:620:PHE:HD2	1.65	0.62
2:E:800:MET:HE1	2:E:804:ARG:HH21	1.64	0.62
2:E:1217:LYS:O	2:E:1221:MET:HG3	2.00	0.62
2:B:116:GLN:HG2	2:B:119:GLN:HE21	1.65	0.61
2:B:127:TRP:HD1	2:B:130:GLN:NE2	1.97	0.61
2:B:788:ASN:O	2:B:792:ARG:HG2	2.00	0.61
2:B:882:LEU:HA	2:B:885:GLN:HE21	1.65	0.61
2:E:882:LEU:HA	2:E:885:GLN:HE21	1.65	0.61
2:E:116:GLN:HG2	2:E:119:GLN:HE21	1.65	0.61
2:E:201:GLU:O	2:E:205:LEU:HB3	1.99	0.61
2:E:450:LEU:HB3	2:E:620:PHE:HZ	1.64	0.61
2:E:1284:GLN:HE21	2:E:1286:ASP:HB2	1.63	0.61
2:B:968:HIS:HA	2:B:971:HIS:CD2	2.34	0.61
2:E:1033:MET:HE1	2:E:1094:LEU:HA	1.81	0.61
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.83	0.61
2:E:1462:PHE:O	2:E:1489:TYR:N	2.33	0.61
3:F:66:ARG:H	3:F:66:ARG:HD3	1.64	0.61
2:B:940:VAL:HG13	2:B:992:MET:HE3	1.83	0.61
3:C:138:THR:H	3:C:141:GLN:NE2	1.98	0.61
2:E:940:VAL:HG13	2:E:992:MET:HE3	1.83	0.61
2:B:1388:TYR:CE2	3:C:44:VAL:HA	2.35	0.61
2:E:802:MET:HE1	2:E:847:ILE:HA	1.82	0.61
2:B:883:THR:HG21	2:B:931:ARG:HB3	1.82	0.61
2:B:1219:ASN:OD1	2:B:1401:GLN:NE2	2.32	0.61
1:D:548:ILE:O	1:D:552:ARG:HG2	2.00	0.61
1:D:578:ARG:O	1:D:587:HIS:N	2.31	0.61
1:D:692:MET:HA	1:D:695:LYS:HE2	1.83	0.61
2:E:485:HIS:HB2	2:E:514:LYS:HB3	1.81	0.61
2:E:809:ALA:HB1	2:E:812:ILE:HB	1.82	0.61
2:E:853:VAL:O	2:E:857:LEU:HG	2.00	0.61
1:A:548:ILE:O	1:A:552:ARG:HG2	2.00	0.61
3:C:43:ASN:ND2	3:C:52:ASN:OD1	2.34	0.61
2:E:473:HIS:ND1	2:E:477:GLY:O	2.32	0.61
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:VAL:O	2:B:857:LEU:HG	2.00	0.61
2:B:1462:PHE:O	2:B:1489:TYR:N	2.33	0.61
1:D:552:ARG:NH1	1:D:664:ILE:HG12	2.15	0.61
2:B:800:MET:HE1	2:B:804:ARG:HH21	1.64	0.61
2:B:802:MET:HE1	2:B:847:ILE:HA	1.82	0.61
2:B:1206:ASP:O	2:B:1210:ILE:HG12	2.01	0.61
2:B:1449:GLN:OE1	2:B:1449:GLN:N	2.29	0.61
3:C:132:LYS:HD2	3:C:134:LEU:HD12	1.83	0.61
2:E:144:LEU:HD22	2:E:147:LYS:HZ3	1.66	0.61
2:E:451:ILE:HD11	2:E:623:ALA:HB2	1.82	0.61
2:E:788:ASN:O	2:E:792:ARG:HG2	2.00	0.61
2:E:883:THR:HG21	2:E:931:ARG:HB3	1.82	0.61
2:E:1117:GLU:CD	2:E:1120:LEU:HG	2.26	0.61
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.64	0.61
2:B:1217:LYS:O	2:B:1221:MET:HG3	2.00	0.61
2:E:1056:HIS:HD1	2:E:1057:GLU:H	1.46	0.61
2:E:1362:TYR:HE1	2:E:1384:ARG:HG3	1.64	0.61
2:E:1478:GLU:OE2	2:E:1478:GLU:N	2.34	0.60
2:B:569:LEU:N	2:B:620:PHE:O	2.35	0.60
2:B:1135:GLU:O	2:B:1139:SER:N	2.34	0.60
2:B:1478:GLU:N	2:B:1478:GLU:OE2	2.34	0.60
2:E:1135:GLU:O	2:E:1139:SER:N	2.34	0.60
2:B:1033:MET:HE1	2:B:1094:LEU:HA	1.81	0.60
2:B:1117:GLU:CD	2:B:1120:LEU:HG	2.26	0.60
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.10	0.60
2:B:166:ARG:O	2:B:171:ASN:HA	2.02	0.60
3:F:132:LYS:HD2	3:F:134:LEU:HD12	1.83	0.60
2:B:1416:GLU:HA	2:B:1419:LYS:HG2	1.83	0.60
2:E:1525:THR:HG21	3:F:37:PHE:HE2	1.65	0.60
3:F:153:LYS:NZ	3:F:154:TYR:O	2.34	0.60
2:E:1300:LEU:O	2:E:1304:ILE:HG13	2.02	0.60
1:A:536:LEU:HD23	2:B:31:ILE:HD11	1.83	0.60
2:B:463:PRO:HD2	2:B:503:GLN:HB3	1.83	0.60
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.65	0.60
2:B:789:ASN:O	2:B:792:ARG:N	2.34	0.60
3:C:153:LYS:NZ	3:C:154:TYR:O	2.34	0.60
2:E:463:PRO:HD2	2:E:503:GLN:HB3	1.84	0.60
2:E:1117:GLU:OE1	2:E:1119:GLU:N	2.34	0.60
2:E:1206:ASP:O	2:E:1210:ILE:HG12	2.00	0.60
2:B:680:MET:HE3	2:B:693:VAL:HG21	1.84	0.60
2:B:1028:LEU:HA	2:B:1032:PHE:HD1	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:GLU:OE1	2:B:1111:GLU:N	2.25	0.60
2:B:1117:GLU:OE1	2:B:1119:GLU:N	2.34	0.60
2:B:1196:LEU:O	2:B:1199:SER:OG	2.18	0.60
2:B:910:LEU:O	2:B:963:GLN:NE2	2.32	0.60
2:B:1169:LYS:HA	2:B:1172:LEU:HD12	1.82	0.60
2:B:1560:MET:HE1	3:C:36:VAL:HG12	1.82	0.60
2:E:569:LEU:N	2:E:620:PHE:O	2.35	0.60
2:E:1028:LEU:HA	2:E:1032:PHE:HD1	1.66	0.60
1:A:552:ARG:NH1	1:A:664:ILE:HG12	2.15	0.59
1:A:692:MET:HA	1:A:695:LYS:HE2	1.83	0.59
2:E:797:ALA:HA	2:E:800:MET:HG3	1.83	0.59
2:E:896:LYS:HA	2:E:899:HIS:CE1	2.37	0.59
2:E:1120:LEU:O	2:E:1124:THR:OG1	2.10	0.59
3:F:43:ASN:ND2	3:F:52:ASN:OD1	2.34	0.59
2:B:844:ILE:HB	2:B:881:LEU:HD11	1.84	0.59
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	1.82	0.59
2:E:166:ARG:O	2:E:171:ASN:HA	2.02	0.59
2:E:1633:VAL:HA	2:E:1637:TYR:HB2	1.84	0.59
2:B:1468:PHE:CE2	2:B:1470:LYS:HB2	2.38	0.59
2:E:12:TYR:HB2	2:E:67:LYS:HB2	1.83	0.59
2:E:789:ASN:O	2:E:792:ARG:N	2.34	0.59
2:B:441:ASP:O	2:B:629:THR:OG1	2.20	0.59
2:B:473:HIS:ND1	2:B:477:GLY:O	2.32	0.59
2:B:530:THR:HA	2:B:549:VAL:HG22	1.85	0.59
2:B:1149:ASN:HA	2:B:1236:ARG:HH22	1.68	0.59
1:D:551:GLN:HG3	2:E:106:TYR:HD2	1.67	0.59
2:E:239:ALA:HB3	2:E:262:TRP:HB3	1.84	0.59
2:E:1601:THR:HB	2:E:1605:ARG:HH21	1.67	0.59
2:B:12:TYR:HB2	2:B:67:LYS:HB2	1.83	0.59
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	1.84	0.59
2:E:1468:PHE:CE2	2:E:1470:LYS:HB2	2.37	0.59
3:F:155:LEU:HD13	3:F:168:VAL:HA	1.85	0.59
2:B:790:SER:HA	2:B:793:GLN:NE2	2.18	0.59
2:B:879:LEU:HD23	2:B:931:ARG:HH22	1.67	0.59
2:B:896:LYS:HA	2:B:899:HIS:CE1	2.37	0.59
2:B:938:ARG:NH2	2:B:988:GLU:OE2	2.35	0.59
1:D:627:GLU:HG2	1:D:631:LEU:HB2	1.85	0.59
2:E:1067:ALA:O	2:E:1071:LYS:N	2.24	0.59
2:E:1416:GLU:HA	2:E:1419:LYS:HG2	1.83	0.59
2:E:1602:GLU:HA	2:E:1605:ARG:NE	2.18	0.59
2:B:451:ILE:HD11	2:B:623:ALA:HB2	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:ASN:N	2:B:560:THR:O	2.32	0.59
2:B:1506:GLN:NE2	2:B:1507:ILE:O	2.36	0.59
2:E:115:ARG:HA	2:E:118:GLN:HG3	1.85	0.59
2:E:790:SER:HA	2:E:793:GLN:NE2	2.18	0.59
2:E:1483:TRP:CE2	2:E:1514:PRO:HD3	2.37	0.59
1:A:564:LYS:O	1:A:573:LYS:NZ	2.19	0.59
2:B:1300:LEU:O	2:B:1304:ILE:HG13	2.02	0.59
2:E:879:LEU:HD23	2:E:931:ARG:HH22	1.67	0.59
2:E:1449:GLN:OE1	2:E:1449:GLN:N	2.29	0.59
2:B:1483:TRP:CE2	2:B:1514:PRO:HD3	2.37	0.59
1:D:530:SER:HA	1:D:533:ILE:HD12	1.85	0.59
1:A:667:ASP:OD1	1:A:678:MET:N	2.33	0.59
2:B:239:ALA:HB3	2:B:262:TRP:HB3	1.85	0.59
2:B:797:ALA:HA	2:B:800:MET:HG3	1.83	0.59
2:E:1169:LYS:HA	2:E:1172:LEU:HD12	1.83	0.59
2:B:115:ARG:HA	2:B:118:GLN:HG3	1.85	0.58
2:B:1121:ARG:O	2:B:1125:ILE:HD12	2.03	0.58
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.36	0.58
1:D:667:ASP:OD1	1:D:678:MET:N	2.33	0.58
2:E:938:ARG:NH2	2:E:988:GLU:OE2	2.35	0.58
2:B:1066:GLN:HA	2:B:1069:ARG:NH1	2.18	0.58
2:B:1067:ALA:O	2:B:1071:LYS:N	2.24	0.58
2:E:910:LEU:O	2:E:963:GLN:NE2	2.32	0.58
2:E:1506:GLN:NE2	2:E:1507:ILE:O	2.36	0.58
2:E:1593:ILE:O	2:E:1596:GLN:HB3	2.03	0.58
2:B:1491:THR:HA	2:B:1505:LYS:H	1.68	0.58
2:B:1601:THR:HB	2:B:1605:ARG:HH21	1.67	0.58
2:B:1615:LEU:O	2:B:1619:HIS:N	2.34	0.58
2:E:680:MET:HE3	2:E:693:VAL:HG21	1.84	0.58
2:E:1121:ARG:O	2:E:1125:ILE:HD12	2.03	0.58
2:E:1196:LEU:O	2:E:1199:SER:OG	2.18	0.58
2:E:1513:SER:O	2:E:1517:ASN:N	2.31	0.58
2:E:1599:LEU:HA	2:E:1602:GLU:OE1	2.04	0.58
2:B:870:ARG:HH11	2:B:873:GLU:HB3	1.69	0.58
3:C:155:LEU:HD13	3:C:168:VAL:HA	1.85	0.58
2:E:870:ARG:HH11	2:E:873:GLU:HB3	1.69	0.58
2:B:62:THR:HG23	2:B:63:TYR:HD1	1.68	0.58
2:B:1159:VAL:O	2:B:1208:ARG:NH1	2.37	0.58
2:B:1307:TYR:O	2:B:1311:GLY:N	2.36	0.58
2:E:844:ILE:HB	2:E:881:LEU:HD11	1.85	0.58
2:E:1315:GLU:OE1	2:E:1315:GLU:N	2.31	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:GLN:HA	1:A:554:ASN:HD22	1.69	0.58
2:B:1536:HIS:HA	2:B:1542:LEU:HD13	1.86	0.58
2:E:530:THR:HA	2:E:549:VAL:HG22	1.85	0.58
2:B:1032:PHE:HB3	2:B:1043:TRP:HH2	1.69	0.58
2:B:1593:ILE:O	2:B:1596:GLN:HB3	2.03	0.58
2:B:1602:GLU:HA	2:B:1605:ARG:NE	2.17	0.58
2:E:59:PHE:CE2	2:E:63:TYR:HB3	2.39	0.58
2:E:195:GLU:HA	2:E:198:ILE:HG12	1.86	0.58
2:E:1388:TYR:HE2	3:F:44:VAL:HG13	1.68	0.58
2:E:1452:ASN:OD1	2:E:1453:TYR:N	2.36	0.58
2:E:1536:HIS:HA	2:E:1542:LEU:HD13	1.86	0.58
1:A:530:SER:HA	1:A:533:ILE:HD12	1.85	0.58
2:E:37:ILE:HG21	2:E:45:TYR:HB3	1.86	0.58
2:E:1121:ARG:HG2	2:E:1125:ILE:HD11	1.86	0.58
2:E:1395:SER:O	2:E:1399:LEU:HG	2.04	0.58
2:E:133:SER:HB2	2:E:135:THR:HG23	1.85	0.58
2:E:1032:PHE:HB3	2:E:1043:TRP:HH2	1.69	0.58
2:B:37:ILE:HG21	2:B:45:TYR:HB3	1.86	0.57
2:B:870:ARG:NH1	2:B:873:GLU:HB3	2.20	0.57
2:B:1513:SER:O	2:B:1517:ASN:N	2.31	0.57
2:E:1588:LEU:HD23	2:E:1591:ARG:HH21	1.68	0.57
1:A:627:GLU:HG2	1:A:631:LEU:HB2	1.85	0.57
2:B:1315:GLU:OE1	2:B:1315:GLU:N	2.31	0.57
2:E:62:THR:HG23	2:E:63:TYR:HD1	1.68	0.57
2:E:1391:ARG:NH2	2:E:1392:GLU:OE2	2.37	0.57
2:B:446:ILE:HB	2:B:515:VAL:HB	1.86	0.57
2:B:1391:ARG:NH2	2:B:1392:GLU:OE2	2.37	0.57
2:B:1588:LEU:HD23	2:B:1591:ARG:HH21	1.68	0.57
1:D:564:LYS:HG3	1:D:575:TRP:NE1	2.20	0.57
2:E:1068:LYS:HA	2:E:1071:LYS:HE2	1.85	0.57
2:E:1095:GLY:H	2:E:1098:LYS:HE3	1.70	0.57
2:E:1368:TYR:O	2:E:1425:TYR:N	2.32	0.57
2:B:638:LEU:O	2:B:642:ASN:N	2.37	0.57
2:B:757:LEU:HD11	2:B:816:ALA:HA	1.87	0.57
2:B:1121:ARG:HG2	2:B:1125:ILE:HD11	1.86	0.57
1:D:551:GLN:HA	1:D:554:ASN:HD22	1.69	0.57
2:E:1149:ASN:HA	2:E:1236:ARG:HH22	1.68	0.57
2:E:1356:MET:HE1	2:E:1449:GLN:HG3	1.87	0.57
2:E:1515:LEU:HD22	2:E:1585:LYS:HB3	1.87	0.57
2:B:355:THR:HG21	2:B:372:VAL:HG22	1.86	0.57
2:B:1068:LYS:HA	2:B:1071:LYS:HE2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1392:GLU:HB2	3:C:166:LYS:HZ1	1.68	0.57
2:E:1390:ARG:NH2	3:F:23:TYR:O	2.37	0.57
2:B:254:ILE:HD12	2:B:294:VAL:HG13	1.86	0.57
2:B:860:MET:HE2	2:B:885:GLN:NE2	2.19	0.57
2:B:1133:GLN:HE22	2:B:1183:HIS:CD2	2.23	0.57
2:B:1395:SER:O	2:B:1399:LEU:HG	2.04	0.57
2:E:37:ILE:HA	2:E:47:GLY:HA3	1.86	0.57
2:E:860:MET:HE2	2:E:885:GLN:NE2	2.19	0.57
2:E:1066:GLN:HA	2:E:1069:ARG:NH1	2.18	0.57
2:E:1159:VAL:O	2:E:1208:ARG:NH1	2.37	0.57
2:E:1207:TYR:O	2:E:1211:ILE:HG12	2.05	0.57
2:E:1307:TYR:O	2:E:1311:GLY:N	2.36	0.57
2:B:59:PHE:CE2	2:B:63:TYR:HB3	2.39	0.57
2:E:246:TYR:HA	2:E:253:PHE:HA	1.87	0.57
2:B:1599:LEU:HA	2:B:1602:GLU:OE1	2.04	0.57
2:E:154:HIS:NE2	2:E:201:GLU:OE2	2.30	0.57
2:E:529:PHE:HE2	2:E:552:VAL:HG12	1.69	0.57
2:E:638:LEU:O	2:E:642:ASN:N	2.37	0.57
2:E:1522:MET:HE3	2:E:1526:ASN:HD21	1.70	0.57
3:F:90:PHE:CE2	3:F:137:ILE:HB	2.40	0.57
3:F:91:GLU:O	3:F:95:ALA:HB3	2.04	0.57
2:B:529:PHE:HE2	2:B:552:VAL:HG12	1.69	0.57
2:E:355:THR:HG21	2:E:372:VAL:HG22	1.86	0.57
2:E:1115:THR:HA	2:E:1163:ARG:HH22	1.70	0.57
1:D:536:LEU:HG	2:E:18:ASN:OD1	2.05	0.57
1:A:564:LYS:HG3	1:A:575:TRP:NE1	2.20	0.56
1:A:578:ARG:O	1:A:587:HIS:N	2.31	0.56
3:C:90:PHE:CE2	3:C:137:ILE:HB	2.40	0.56
1:A:578:ARG:HB3	1:A:587:HIS:HB2	1.88	0.56
2:B:133:SER:HB2	2:B:135:THR:HG23	1.85	0.56
2:B:154:HIS:NE2	2:B:201:GLU:OE2	2.30	0.56
2:B:938:ARG:HA	2:B:941:ILE:HD12	1.87	0.56
2:B:1466:ARG:NH1	2:B:1467:PRO:O	2.38	0.56
2:E:1117:GLU:OE2	2:E:1121:ARG:N	2.26	0.56
2:B:195:GLU:HA	2:B:198:ILE:HG12	1.86	0.56
2:B:730:TYR:CE1	2:B:771:ARG:HD3	2.40	0.56
2:B:771:ARG:HH21	2:B:784:GLY:HA2	1.70	0.56
2:B:1078:ASP:OD1	2:B:1081:LYS:N	2.37	0.56
2:B:1207:TYR:O	2:B:1211:ILE:HG12	2.05	0.56
2:B:1356:MET:HE1	2:B:1449:GLN:HG3	1.87	0.56
2:B:1515:LEU:HD22	2:B:1585:LYS:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1522:MET:HE3	2:B:1526:ASN:HD21	1.70	0.56
2:B:1617:PRO:HB2	2:B:1621:ARG:HH22	1.71	0.56
3:C:44:VAL:N	3:C:51:VAL:O	2.27	0.56
3:C:91:GLU:O	3:C:95:ALA:HB3	2.04	0.56
2:E:131:ILE:HD11	2:E:144:LEU:HG	1.88	0.56
2:E:182:ALA:HA	2:E:185:LYS:HG2	1.88	0.56
2:E:254:ILE:HD12	2:E:294:VAL:HG13	1.86	0.56
2:E:1499:LEU:HD11	2:E:1501:TRP:CZ2	2.40	0.56
2:E:1532:CYS:O	2:E:1535:GLN:NE2	2.38	0.56
2:B:297:VAL:HG22	2:B:326:VAL:HG22	1.87	0.56
1:D:607:LYS:NZ	1:D:608:LEU:O	2.38	0.56
2:E:156:ASN:HA	2:E:161:LEU:HD12	1.88	0.56
2:E:287:MET:HA	2:E:290:ILE:HG12	1.87	0.56
2:E:730:TYR:CE1	2:E:771:ARG:HD3	2.40	0.56
2:E:870:ARG:NH1	2:E:873:GLU:HB3	2.20	0.56
2:E:1078:ASP:OD1	2:E:1081:LYS:N	2.37	0.56
2:E:1160:GLU:OE2	2:E:1242:ARG:NH1	2.38	0.56
1:A:661:GLU:HA	1:A:664:ILE:HB	1.88	0.56
2:B:769:GLN:OE1	2:B:776:ARG:NH2	2.39	0.56
2:E:165:VAL:HG23	2:E:175:PRO:HD3	1.87	0.56
2:E:297:VAL:HG22	2:E:326:VAL:HG22	1.87	0.56
2:E:446:ILE:HB	2:E:515:VAL:HB	1.86	0.56
2:E:771:ARG:HH21	2:E:784:GLY:HA2	1.70	0.56
2:E:1111:GLU:OE1	2:E:1111:GLU:N	2.25	0.56
2:E:1344:LYS:O	2:E:1347:SER:OG	2.21	0.56
2:E:1491:THR:HA	2:E:1505:LYS:H	1.68	0.56
2:E:1617:PRO:HB2	2:E:1621:ARG:HH22	1.71	0.56
2:B:1160:GLU:OE2	2:B:1242:ARG:NH1	2.38	0.56
2:E:1048:HIS:CE1	2:E:1105:MET:HE1	2.40	0.56
2:B:30:GLN:N	2:B:33:ASP:OD2	2.39	0.56
1:D:659:LYS:NZ	1:D:680:ASP:OD2	2.37	0.56
2:E:694:PHE:HZ	2:E:737:LEU:HB3	1.70	0.56
2:E:1032:PHE:HA	2:E:1036:ALA:HB3	1.88	0.56
2:E:1381:PHE:HA	2:E:1503:GLU:HA	1.88	0.56
2:E:1466:ARG:NH1	2:E:1467:PRO:O	2.38	0.56
2:E:1583:GLN:O	2:E:1586:VAL:HG12	2.06	0.56
1:A:723:VAL:HG23	2:B:2:ALA:HB1	1.86	0.56
2:B:941:ILE:HA	2:B:992:MET:HE2	1.88	0.56
2:E:59:PHE:CZ	2:E:63:TYR:HB3	2.41	0.56
2:E:745:ASP:H	2:E:804:ARG:HH12	1.53	0.56
2:E:769:GLN:OE1	2:E:776:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:941:ILE:HA	2:E:992:MET:HE2	1.88	0.56
2:E:450:LEU:HD13	2:E:468:VAL:HB	1.88	0.56
2:B:182:ALA:HA	2:B:185:LYS:HG2	1.87	0.56
2:B:246:TYR:HA	2:B:253:PHE:HA	1.87	0.56
2:B:438:LEU:N	2:B:441:ASP:OD2	2.38	0.56
2:B:1177:LEU:O	2:B:1181:ARG:HG2	2.05	0.56
2:B:1344:LYS:O	2:B:1347:SER:OG	2.21	0.56
2:B:1371:GLY:C	2:B:1424:GLN:HE21	2.14	0.56
2:E:757:LEU:HD11	2:E:816:ALA:HA	1.87	0.56
2:E:828:LYS:HE2	2:E:833:PRO:HG3	1.88	0.56
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.86	0.55
2:B:745:ASP:H	2:B:804:ARG:HH12	1.53	0.55
2:B:1048:HIS:CE1	2:B:1105:MET:HE1	2.41	0.55
2:E:938:ARG:HA	2:E:941:ILE:HD12	1.87	0.55
2:E:1545:HIS:O	2:E:1548:SER:OG	2.21	0.55
3:F:8:VAL:O	3:F:58:THR:OG1	2.20	0.55
2:B:532:ARG:O	2:B:534:ARG:NH1	2.39	0.55
2:B:1499:LEU:HD11	2:B:1501:TRP:CZ2	2.40	0.55
2:E:438:LEU:N	2:E:441:ASP:OD2	2.38	0.55
1:A:607:LYS:NZ	1:A:608:LEU:O	2.38	0.55
2:B:165:VAL:HG23	2:B:175:PRO:HD3	1.87	0.55
2:B:1115:THR:HA	2:B:1163:ARG:HH22	1.70	0.55
2:B:1381:PHE:HA	2:B:1503:GLU:HA	1.88	0.55
2:E:30:GLN:N	2:E:33:ASP:OD2	2.39	0.55
2:E:532:ARG:O	2:E:534:ARG:NH1	2.39	0.55
2:E:973:ILE:HD13	2:E:976:PHE:CZ	2.41	0.55
3:F:67:LEU:HD13	3:F:70:LEU:HD12	1.89	0.55
2:B:287:MET:HA	2:B:290:ILE:HG12	1.87	0.55
2:B:694:PHE:HZ	2:B:737:LEU:HB3	1.70	0.55
2:B:855:GLN:OE1	2:B:855:GLN:N	2.28	0.55
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.22	0.55
2:E:1133:GLN:HE22	2:E:1183:HIS:CD2	2.23	0.55
2:E:1292:THR:HG23	2:E:1295:GLU:H	1.71	0.55
2:E:1465:SER:HA	2:E:1486:ARG:HG2	1.88	0.55
2:B:450:LEU:HD13	2:B:468:VAL:HB	1.88	0.55
2:B:973:ILE:HD13	2:B:976:PHE:CZ	2.41	0.55
2:B:1095:GLY:H	2:B:1098:LYS:HE3	1.70	0.55
2:B:1482:MET:HB3	2:B:1517:ASN:HD22	1.72	0.55
2:B:1545:HIS:O	2:B:1548:SER:OG	2.21	0.55
2:B:1583:GLN:O	2:B:1586:VAL:HG12	2.06	0.55
1:D:578:ARG:HB3	1:D:587:HIS:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1449:GLN:HA	2:E:1452:ASN:ND2	2.22	0.55
1:D:551:GLN:HG3	2:E:106:TYR:CD2	2.42	0.55
1:D:643:SER:OG	1:D:653:ASN:ND2	2.39	0.55
2:B:59:PHE:CZ	2:B:63:TYR:HB3	2.41	0.55
2:B:131:ILE:HD11	2:B:144:LEU:HG	1.88	0.55
2:B:1032:PHE:HA	2:B:1036:ALA:HB3	1.88	0.55
2:B:1532:CYS:O	2:B:1535:GLN:NE2	2.38	0.55
2:E:441:ASP:O	2:E:629:THR:OG1	2.20	0.55
2:E:472:VAL:HG12	2:E:527:ILE:HG12	1.89	0.55
2:E:866:SER:C	2:E:868:LEU:H	2.15	0.55
2:E:1177:LEU:O	2:E:1181:ARG:HG2	2.05	0.55
1:A:546:GLU:HA	1:A:549:LYS:HG2	1.88	0.55
2:B:1435:MET:SD	2:B:1455:ARG:HG2	2.47	0.55
2:B:1584:GLU:O	2:B:1588:LEU:HG	2.07	0.55
2:B:1618:LEU:O	2:B:1622:LEU:HG	2.07	0.55
2:E:1618:LEU:O	2:E:1622:LEU:HG	2.07	0.55
2:B:155:GLY:HA2	2:B:158:MET:SD	2.47	0.55
2:B:664:GLU:HA	2:B:667:LYS:HE3	1.88	0.55
3:C:67:LEU:HD13	3:C:70:LEU:HD12	1.89	0.55
1:D:546:GLU:HA	1:D:549:LYS:HG2	1.88	0.55
2:E:166:ARG:NH2	2:E:168:ASP:HB2	2.22	0.55
2:E:870:ARG:HH12	2:E:874:CYS:HB3	1.72	0.55
2:E:1238:ASP:HA	2:E:1241:ILE:HD12	1.88	0.55
2:B:657:LEU:HD12	2:B:660:VAL:HG21	1.88	0.55
2:B:1168:TYR:CE1	2:B:1172:LEU:HD11	2.42	0.55
2:B:1589:LEU:HD23	2:B:1592:LEU:HD12	1.89	0.55
2:E:1435:MET:SD	2:E:1455:ARG:HG2	2.47	0.55
1:A:576:TYR:HB2	1:A:598:GLU:HG2	1.90	0.54
2:B:17:TYR:OH	2:B:63:TYR:OH	2.19	0.54
2:B:870:ARG:HH12	2:B:874:CYS:HB3	1.72	0.54
2:B:1043:TRP:H	2:B:1043:TRP:HE3	1.55	0.54
2:B:1292:THR:HG23	2:B:1295:GLU:H	1.71	0.54
2:B:1536:HIS:CG	2:B:1542:LEU:HD22	2.42	0.54
2:B:1560:MET:SD	3:C:36:VAL:HA	2.47	0.54
1:D:614:LYS:HZ1	1:D:648:SER:H	1.55	0.54
2:E:288:ASP:HA	2:E:291:ARG:HE	1.73	0.54
2:E:1040:LEU:HD12	2:E:1097:HIS:CE1	2.42	0.54
1:A:561:CYS:SG	1:A:594:SER:OG	2.65	0.54
2:B:156:ASN:HA	2:B:161:LEU:HD12	1.88	0.54
2:B:866:SER:C	2:B:868:LEU:H	2.15	0.54
2:B:1040:LEU:HD12	2:B:1097:HIS:CE1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:O	3:C:58:THR:OG1	2.20	0.54
3:C:141:GLN:OE1	3:C:141:GLN:N	2.28	0.54
1:D:576:TYR:HB2	1:D:598:GLU:HG2	1.89	0.54
1:D:661:GLU:HA	1:D:664:ILE:HB	1.88	0.54
2:E:657:LEU:HD12	2:E:660:VAL:HG21	1.88	0.54
2:E:1168:TYR:CE1	2:E:1172:LEU:HD11	2.42	0.54
2:E:1371:GLY:C	2:E:1424:GLN:HE21	2.15	0.54
2:E:1415:GLY:O	2:E:1419:LYS:N	2.41	0.54
2:E:1584:GLU:O	2:E:1588:LEU:HG	2.07	0.54
2:B:1238:ASP:HA	2:B:1241:ILE:HD12	1.88	0.54
2:E:457:LYS:HG2	2:E:463:PRO:HA	1.89	0.54
2:E:664:GLU:HA	2:E:667:LYS:HE3	1.88	0.54
2:E:1536:HIS:CG	2:E:1542:LEU:HD22	2.42	0.54
2:E:1589:LEU:HD23	2:E:1592:LEU:HD12	1.89	0.54
2:B:19:TYR:O	2:B:28:SER:HA	2.08	0.54
2:B:472:VAL:HG12	2:B:527:ILE:HG12	1.89	0.54
2:B:828:LYS:HE2	2:B:833:PRO:HG3	1.88	0.54
2:E:1043:TRP:H	2:E:1043:TRP:HE3	1.55	0.54
3:F:65:ASP:HA	3:F:68:ARG:HG2	1.90	0.54
1:A:643:SER:OG	1:A:653:ASN:ND2	2.39	0.54
2:B:1623:SER:HB3	2:B:1627:ARG:NH1	2.23	0.54
1:D:561:CYS:SG	1:D:594:SER:OG	2.65	0.54
2:E:155:GLY:HA2	2:E:158:MET:SD	2.47	0.54
2:B:166:ARG:NH2	2:B:168:ASP:HB2	2.22	0.54
2:B:457:LYS:HG2	2:B:463:PRO:HA	1.89	0.54
1:D:697:ARG:HB3	2:E:31:ILE:HB	1.90	0.54
2:E:744:ALA:HA	2:E:753:LEU:HD22	1.90	0.54
2:E:1280:PRO:HA	2:E:1283:LEU:HD23	1.89	0.54
2:B:192:LYS:HG3	2:B:196:GLU:OE2	2.08	0.54
2:E:820:LEU:HG	2:E:821:PRO:HD3	1.90	0.54
2:B:1362:TYR:HD2	2:B:1462:PHE:HE2	1.56	0.54
1:A:567:ALA:HB3	1:A:573:LYS:HD3	1.90	0.54
1:A:643:SER:HA	1:A:652:LEU:O	2.08	0.54
2:B:259:LEU:HD22	2:B:486:PRO:HB2	1.90	0.54
2:B:649:ASN:O	2:B:653:ASN:N	2.29	0.54
2:B:1465:SER:HA	2:B:1486:ARG:HG2	1.88	0.54
2:E:192:LYS:HG3	2:E:196:GLU:OE2	2.08	0.54
2:E:1482:MET:HB3	2:E:1517:ASN:HD22	1.72	0.54
1:A:578:ARG:HH22	1:A:601:HIS:H	1.56	0.53
2:B:99:ALA:O	2:B:103:ARG:HG2	2.08	0.53
2:B:1368:TYR:O	2:B:1425:TYR:N	2.32	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1488:THR:N	2:B:1508:SER:O	2.41	0.53
1:D:551:GLN:OE1	1:D:552:ARG:NH2	2.38	0.53
2:E:460:LYS:HD2	2:E:464:LYS:HG2	1.90	0.53
1:A:659:LYS:NZ	1:A:680:ASP:OD2	2.37	0.53
2:B:1251:HIS:NE2	2:B:1498:ILE:O	2.42	0.53
2:B:1590:LYS:HB3	2:B:1639:VAL:HG12	1.90	0.53
3:C:69:PRO:HA	3:C:72:TYR:CD2	2.43	0.53
2:E:1058:SER:O	2:E:1062:GLU:HG3	2.08	0.53
2:B:281:PHE:HD1	2:B:428:ALA:HB3	1.74	0.53
2:B:288:ASP:HA	2:B:291:ARG:HE	1.72	0.53
2:B:868:LEU:O	2:B:871:GLN:HG3	2.09	0.53
2:B:1415:GLY:O	2:B:1419:LYS:N	2.41	0.53
1:D:567:ALA:HB3	1:D:573:LYS:HD3	1.90	0.53
2:E:19:TYR:O	2:E:28:SER:HA	2.08	0.53
2:E:273:LYS:O	2:E:277:LEU:HG	2.08	0.53
2:E:740:TYR:HA	2:E:749:LYS:HD3	1.90	0.53
2:E:1484:ILE:HB	2:E:1512:ILE:HD12	1.91	0.53
2:E:1488:THR:N	2:E:1508:SER:O	2.41	0.53
2:B:18:ASN:HA	2:B:29:LEU:O	2.09	0.53
2:B:460:LYS:HD2	2:B:464:LYS:HG2	1.90	0.53
2:B:1280:PRO:HA	2:B:1283:LEU:HD23	1.89	0.53
2:B:1466:ARG:O	2:B:1484:ILE:HA	2.09	0.53
2:E:99:ALA:O	2:E:103:ARG:HG2	2.08	0.53
2:E:960:LEU:O	2:E:964:MET:HG2	2.08	0.53
2:E:964:MET:O	2:E:1019:ARG:NH2	2.41	0.53
2:B:720:ILE:HG21	2:B:765:ARG:HG2	1.91	0.53
2:B:964:MET:O	2:B:1019:ARG:NH2	2.41	0.53
2:B:1490:THR:OG1	2:B:1506:GLN:HB3	2.08	0.53
2:E:589:PRO:HB3	2:E:594:GLU:HB3	1.90	0.53
2:E:632:THR:HG21	2:E:638:LEU:HD21	1.91	0.53
2:E:787:PHE:O	2:E:791:ILE:HG12	2.09	0.53
2:E:1392:GLU:OE1	2:E:1392:GLU:N	2.40	0.53
2:B:1392:GLU:OE1	2:B:1392:GLU:N	2.40	0.53
2:B:1527:GLU:O	2:B:1530:SER:N	2.41	0.53
3:C:65:ASP:HA	3:C:68:ARG:HG2	1.90	0.53
2:E:259:LEU:HD22	2:E:486:PRO:HB2	1.90	0.53
2:E:720:ILE:HG21	2:E:765:ARG:HG2	1.91	0.53
2:E:1390:ARG:NH2	3:F:26:ASN:OD1	2.42	0.53
2:E:1404:ASN:OD1	2:E:1424:GLN:HB2	2.08	0.53
2:B:14:VAL:HB	2:B:65:HIS:HB3	1.90	0.53
2:B:179:SER:OG	2:B:182:ALA:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:ALA:HA	2:B:753:LEU:HD22	1.90	0.53
2:B:909:ILE:HG13	2:B:910:LEU:HD12	1.91	0.53
2:B:1058:SER:O	2:B:1062:GLU:HG3	2.08	0.53
2:B:1332:VAL:HG13	2:B:1334:ASP:H	1.74	0.53
2:E:1615:LEU:O	2:E:1619:HIS:N	2.34	0.53
2:B:105:LEU:HD13	2:B:114:PHE:HD1	1.74	0.53
3:C:66:ARG:NH1	3:C:67:LEU:HD23	2.24	0.53
1:D:643:SER:HA	1:D:652:LEU:O	2.08	0.53
2:E:575:ASP:HB3	2:E:578:LYS:HB2	1.90	0.53
2:E:868:LEU:O	2:E:871:GLN:HG3	2.09	0.53
2:E:1490:THR:OG1	2:E:1506:GLN:HB3	2.08	0.53
2:E:1527:GLU:O	2:E:1530:SER:N	2.41	0.53
3:F:69:PRO:HA	3:F:72:TYR:CD2	2.43	0.53
2:B:589:PRO:HB3	2:B:594:GLU:HB3	1.90	0.53
2:B:1314:TRP:O	2:B:1318:ILE:HG12	2.09	0.53
2:E:166:ARG:HH22	2:E:168:ASP:HB2	1.74	0.53
2:E:1163:ARG:H	2:E:1208:ARG:HH12	1.57	0.53
2:B:7:THR:HG22	2:B:9:ARG:H	1.74	0.53
2:B:273:LYS:O	2:B:277:LEU:HG	2.08	0.53
2:B:1623:SER:HB3	2:B:1627:ARG:HH22	1.74	0.53
1:D:652:LEU:HB3	1:D:654:PHE:CE2	2.44	0.53
2:E:14:VAL:HB	2:E:65:HIS:HB3	1.90	0.53
2:E:97:GLU:O	2:E:101:ILE:HG13	2.09	0.53
2:B:306:MET:HB2	2:B:318:LEU:HD12	1.91	0.52
2:B:965:ASP:HB3	2:B:968:HIS:CG	2.44	0.52
2:B:1484:ILE:HB	2:B:1512:ILE:HD12	1.91	0.52
2:E:17:TYR:OH	2:E:63:TYR:OH	2.19	0.52
2:E:1623:SER:HB3	2:E:1627:ARG:NH1	2.23	0.52
3:F:66:ARG:NH1	3:F:67:LEU:HD23	2.24	0.52
2:B:740:TYR:HA	2:B:749:LYS:HD3	1.90	0.52
2:B:960:LEU:O	2:B:964:MET:HG2	2.08	0.52
2:B:1388:TYR:HD2	3:C:45:MET:HB3	1.73	0.52
2:E:965:ASP:HB3	2:E:968:HIS:CG	2.44	0.52
2:E:1362:TYR:HD2	2:E:1462:PHE:HE2	1.56	0.52
3:F:141:GLN:OE1	3:F:141:GLN:N	2.28	0.52
2:B:166:ARG:HH22	2:B:168:ASP:HB2	1.74	0.52
2:B:534:ARG:HG3	2:B:541:ASP:OD1	2.10	0.52
2:B:569:LEU:HB2	2:B:620:PHE:HB3	1.92	0.52
2:B:664:GLU:OE1	2:B:664:GLU:N	2.34	0.52
2:B:758:LYS:NZ	2:B:819:TYR:OH	2.43	0.52
1:D:578:ARG:HH22	1:D:601:HIS:H	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:179:SER:OG	2:E:182:ALA:HB3	2.09	0.52
2:E:855:GLN:OE1	2:E:855:GLN:N	2.28	0.52
2:E:1466:ARG:O	2:E:1484:ILE:HA	2.09	0.52
1:A:652:LEU:HB3	1:A:654:PHE:CE2	2.44	0.52
2:B:1231:TYR:O	2:B:1235:LYS:N	2.42	0.52
2:B:1404:ASN:OD1	2:B:1424:GLN:HB2	2.08	0.52
1:D:700:ASP:HB2	2:E:32:GLY:HA2	1.90	0.52
2:E:7:THR:HG22	2:E:9:ARG:H	1.74	0.52
2:E:758:LYS:NZ	2:E:819:TYR:OH	2.43	0.52
2:E:1251:HIS:NE2	2:E:1498:ILE:O	2.42	0.52
3:F:149:ILE:HG23	3:F:151:ALA:H	1.74	0.52
2:B:143:GLU:HG3	2:B:147:LYS:NZ	2.24	0.52
2:B:192:LYS:O	2:B:195:GLU:HG2	2.10	0.52
2:B:232:VAL:O	2:B:398:GLY:N	2.42	0.52
2:B:820:LEU:HG	2:B:821:PRO:HD3	1.90	0.52
2:B:1588:LEU:O	2:B:1592:LEU:HG	2.10	0.52
3:C:116:LYS:HB3	3:C:119:LEU:HB2	1.92	0.52
2:E:353:MET:HG3	2:E:374:GLY:O	2.10	0.52
2:E:1588:LEU:O	2:E:1592:LEU:HG	2.10	0.52
3:F:116:LYS:HB3	3:F:119:LEU:HB2	1.92	0.52
1:A:697:ARG:HE	2:B:30:GLN:HG2	1.75	0.52
2:B:876:GLU:N	2:B:876:GLU:OE1	2.43	0.52
2:B:1024:PHE:HA	2:B:1027:VAL:HG22	1.91	0.52
2:E:306:MET:HB2	2:E:318:LEU:HD12	1.91	0.52
2:B:144:LEU:HD22	2:B:147:LYS:HZ3	1.74	0.52
2:B:350:GLN:HE21	2:B:353:MET:HE1	1.75	0.52
2:B:575:ASP:HB3	2:B:578:LYS:HB2	1.90	0.52
2:B:632:THR:HG21	2:B:638:LEU:HD21	1.91	0.52
2:B:1113:THR:HG21	2:B:1128:PHE:HE2	1.75	0.52
2:B:1615:LEU:HA	2:B:1618:LEU:HD12	1.92	0.52
2:E:143:GLU:HG3	2:E:147:LYS:NZ	2.24	0.52
2:E:192:LYS:O	2:E:195:GLU:HG2	2.10	0.52
2:E:473:HIS:HB2	2:E:526:HIS:CE1	2.45	0.52
2:E:965:ASP:OD2	2:E:967:SER:OG	2.24	0.52
2:E:1024:PHE:HA	2:E:1027:VAL:HG22	1.91	0.52
2:E:1314:TRP:O	2:E:1318:ILE:HG12	2.09	0.52
2:B:1522:MET:HE1	2:B:1596:GLN:OE1	2.10	0.52
3:C:77:VAL:HG13	3:C:176:VAL:HG23	1.92	0.52
3:C:149:ILE:HG23	3:C:151:ALA:H	1.74	0.52
2:E:18:ASN:HA	2:E:29:LEU:O	2.09	0.52
2:E:165:VAL:O	2:E:171:ASN:ND2	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD11	1:A:653:ASN:HB2	1.92	0.52
2:B:97:GLU:O	2:B:101:ILE:HG13	2.09	0.52
2:B:879:LEU:HD23	2:B:924:HIS:CE1	2.45	0.52
2:B:883:THR:CG2	2:B:931:ARG:HB3	2.40	0.52
2:E:534:ARG:HG3	2:E:541:ASP:OD1	2.10	0.52
2:E:1332:VAL:HG13	2:E:1334:ASP:H	1.74	0.52
2:E:1590:LYS:HB3	2:E:1639:VAL:HG12	1.90	0.52
2:E:1615:LEU:HA	2:E:1618:LEU:HD12	1.92	0.52
2:B:85:LEU:O	2:B:88:VAL:HG22	2.10	0.51
2:B:522:VAL:HA	2:B:525:CYS:HB2	1.92	0.51
2:B:1156:ASP:OD1	2:B:1242:ARG:NH2	2.44	0.51
2:B:1482:MET:HE1	3:C:34:PRO:HD2	1.92	0.51
2:B:1555:VAL:HG21	2:B:1622:LEU:HD22	1.93	0.51
2:E:876:GLU:OE1	2:E:876:GLU:N	2.43	0.51
2:B:1515:LEU:O	2:B:1519:ILE:HG13	2.11	0.51
2:E:46:ARG:HA	2:E:57:GLY:O	2.10	0.51
2:E:281:PHE:HD1	2:E:428:ALA:HB3	1.74	0.51
2:E:1464:TYR:O	2:E:1486:ARG:HA	2.11	0.51
2:E:1623:SER:HB3	2:E:1627:ARG:HH22	1.74	0.51
2:B:46:ARG:HA	2:B:57:GLY:O	2.10	0.51
2:E:105:LEU:HD13	2:E:114:PHE:HD1	1.74	0.51
2:E:716:LEU:O	2:E:720:ILE:HG13	2.10	0.51
2:B:25:VAL:HG11	2:B:56:LYS:HE2	1.93	0.51
2:B:167:ASP:OD1	2:B:167:ASP:N	2.44	0.51
2:B:226:VAL:HG22	2:B:403:LEU:HD22	1.92	0.51
2:E:85:LEU:O	2:E:88:VAL:HG22	2.10	0.51
2:B:787:PHE:O	2:B:791:ILE:HG12	2.09	0.51
2:B:1353:ILE:HD13	2:E:1335:TYR:HB2	1.93	0.51
2:E:962:GLN:NE2	2:E:963:GLN:HG3	2.26	0.51
2:E:1113:THR:HG21	2:E:1128:PHE:HE2	1.75	0.51
2:E:1165:ASP:O	2:E:1168:TYR:HB3	2.11	0.51
2:E:1525:THR:HA	2:E:1528:ARG:HH11	1.75	0.51
2:B:1368:TYR:N	2:B:1425:TYR:O	2.42	0.51
2:B:1557:PRO:HB2	2:B:1561:GLY:HA2	1.92	0.51
1:D:693:GLU:O	1:D:697:ARG:HG2	2.11	0.51
2:E:350:GLN:HE21	2:E:353:MET:HE1	1.75	0.51
2:E:883:THR:CG2	2:E:931:ARG:HB3	2.40	0.51
2:E:1231:TYR:CE2	2:E:1243:TYR:HE1	2.29	0.51
2:B:14:VAL:O	2:B:64:ILE:HA	2.11	0.51
2:B:1231:TYR:CE2	2:B:1243:TYR:HE1	2.29	0.51
2:E:232:VAL:O	2:E:398:GLY:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1256:ASN:ND2	2:E:1500:LYS:HD2	2.26	0.51
2:E:1417:ASP:N	2:E:1417:ASP:OD1	2.43	0.51
2:E:1557:PRO:HB2	2:E:1561:GLY:HA2	1.92	0.51
1:A:637:VAL:HG12	1:A:640:LEU:HD12	1.93	0.51
1:A:693:GLU:O	1:A:697:ARG:HG2	2.11	0.51
2:B:473:HIS:HB2	2:B:526:HIS:CE1	2.45	0.51
2:B:1197:VAL:O	2:B:1201:LEU:HG	2.11	0.51
2:B:1479:PHE:HZ	2:B:1560:MET:HE1	1.76	0.51
1:D:565:LEU:HD11	1:D:653:ASN:HB2	1.92	0.51
2:E:226:VAL:HG22	2:E:403:LEU:HD22	1.92	0.51
2:E:879:LEU:HD23	2:E:924:HIS:CE1	2.45	0.51
2:E:1485:GLU:OE1	2:E:1485:GLU:N	2.44	0.51
2:B:1163:ARG:H	2:B:1208:ARG:HH12	1.57	0.51
2:E:25:VAL:HG11	2:E:56:LYS:HE2	1.93	0.51
3:F:82:PHE:CD2	3:F:90:PHE:HE1	2.29	0.51
2:B:235:ILE:HG12	2:B:322:PHE:CE2	2.47	0.51
2:B:915:ARG:NH1	2:B:915:ARG:HA	2.26	0.51
2:B:1390:ARG:NH2	3:C:26:ASN:OD1	2.44	0.51
2:B:1485:GLU:OE1	2:B:1485:GLU:N	2.44	0.51
2:E:522:VAL:HA	2:E:525:CYS:HB2	1.92	0.51
2:E:670:GLN:HG3	2:E:719:TYR:CD1	2.45	0.51
2:E:810:VAL:HG13	2:E:852:LEU:HD21	1.93	0.51
2:B:353:MET:HG3	2:B:374:GLY:O	2.10	0.50
2:B:826:ASP:HA	2:B:829:LEU:HB2	1.92	0.50
3:C:82:PHE:CD1	3:C:112:LEU:HD11	2.47	0.50
2:E:184:PHE:HA	2:E:1009:MET:HE3	1.93	0.50
2:E:584:PHE:O	2:E:587:THR:OG1	2.26	0.50
2:E:915:ARG:NH1	2:E:915:ARG:HA	2.26	0.50
2:E:1471:GLY:O	2:E:1473:LYS:NZ	2.33	0.50
2:E:1522:MET:HE1	2:E:1596:GLN:OE1	2.10	0.50
2:E:1554:ILE:HD13	3:F:37:PHE:CE2	2.46	0.50
3:F:21:ILE:HD11	3:F:35:THR:HG23	1.93	0.50
2:B:64:ILE:HG22	2:B:66:LEU:HD22	1.92	0.50
2:B:670:GLN:HG3	2:B:719:TYR:CD1	2.45	0.50
2:B:716:LEU:O	2:B:720:ILE:HG13	2.10	0.50
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.11	0.50
2:B:1283:LEU:HD11	2:B:1291:TYR:HB2	1.92	0.50
3:C:21:ILE:HD11	3:C:35:THR:HG23	1.93	0.50
1:D:561:CYS:HA	1:D:576:TYR:HA	1.93	0.50
2:E:14:VAL:O	2:E:64:ILE:HA	2.11	0.50
2:E:569:LEU:HB2	2:E:620:PHE:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1283:LEU:HD11	2:E:1291:TYR:HB2	1.92	0.50
2:B:25:VAL:HG23	2:B:57:GLY:HA2	1.93	0.50
2:B:859:CYS:O	2:B:863:ILE:HG12	2.11	0.50
2:B:879:LEU:HG	2:B:931:ARG:HH12	1.77	0.50
2:E:80:VAL:HG12	2:E:85:LEU:HD11	1.94	0.50
2:E:215:ILE:O	2:E:218:THR:OG1	2.29	0.50
2:E:879:LEU:HG	2:E:931:ARG:HH12	1.76	0.50
2:E:1197:VAL:O	2:E:1201:LEU:HG	2.11	0.50
2:E:1231:TYR:O	2:E:1235:LYS:N	2.41	0.50
2:B:923:VAL:O	2:B:927:LEU:HG	2.11	0.50
2:B:1106:VAL:O	2:B:1109:ILE:HG22	2.12	0.50
2:B:1307:TYR:HD1	2:B:1310:LYS:HE2	1.77	0.50
2:B:1585:LYS:HG3	2:B:1588:LEU:HD12	1.93	0.50
2:E:25:VAL:HG23	2:E:57:GLY:HA2	1.93	0.50
2:E:465:ASN:O	2:E:533:HIS:HA	2.12	0.50
2:E:909:ILE:HG13	2:E:910:LEU:HD12	1.91	0.50
2:E:1275:ASP:OD2	2:E:1275:ASP:N	2.43	0.50
2:E:1585:LYS:HG3	2:E:1588:LEU:HD12	1.93	0.50
3:F:77:VAL:HG13	3:F:176:VAL:HG23	1.92	0.50
1:A:561:CYS:HA	1:A:576:TYR:HA	1.93	0.50
2:B:1464:TYR:O	2:B:1486:ARG:HA	2.11	0.50
2:B:1525:THR:HA	2:B:1528:ARG:HH11	1.75	0.50
2:E:923:VAL:O	2:E:927:LEU:HG	2.11	0.50
2:E:965:ASP:HB3	2:E:968:HIS:CD2	2.47	0.50
2:E:1479:PHE:HZ	2:E:1560:MET:HE1	1.76	0.50
1:A:590:ASP:H	1:A:604:LEU:HD22	1.77	0.50
2:B:465:ASN:O	2:B:533:HIS:HA	2.12	0.50
2:B:700:ILE:O	2:B:704:ILE:HG13	2.12	0.50
2:B:962:GLN:NE2	2:B:963:GLN:HG3	2.26	0.50
3:C:82:PHE:CD2	3:C:90:PHE:HE1	2.29	0.50
1:D:562:PHE:N	1:D:575:TRP:O	2.40	0.50
1:D:649:ASN:O	1:D:649:ASN:ND2	2.45	0.50
2:E:826:ASP:HA	2:E:829:LEU:HB2	1.92	0.50
2:E:1079:MET:HA	2:E:1082:GLU:OE2	2.11	0.50
2:B:1098:LYS:O	2:B:1102:ILE:HG13	2.11	0.50
2:B:1256:ASN:ND2	2:B:1500:LYS:HD2	2.26	0.50
2:E:48:TYR:HB3	2:E:53:LYS:HD2	1.94	0.50
2:E:468:VAL:H	2:E:498:SER:HG	1.59	0.50
2:E:1156:ASP:OD1	2:E:1242:ARG:NH2	2.44	0.50
3:F:82:PHE:CD1	3:F:112:LEU:HD11	2.47	0.50
2:B:584:PHE:O	2:B:587:THR:OG1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:LEU:O	2:B:882:LEU:N	2.45	0.50
1:D:590:ASP:H	1:D:604:LEU:HD22	1.77	0.50
2:E:64:ILE:HG22	2:E:66:LEU:HD22	1.92	0.50
2:E:235:ILE:HG12	2:E:322:PHE:CE2	2.47	0.50
2:E:1183:HIS:CG	2:E:1184:LYS:H	2.30	0.50
2:E:1555:VAL:HG21	2:E:1622:LEU:HD22	1.93	0.50
2:B:871:GLN:OE1	2:B:875:ARG:NH1	2.45	0.50
2:E:16:ILE:HG23	2:E:17:TYR:CD1	2.47	0.50
2:E:172:ILE:HD12	2:E:175:PRO:HG2	1.94	0.50
2:E:1098:LYS:O	2:E:1102:ILE:HG13	2.11	0.50
2:E:1128:PHE:O	2:E:1131:MET:HG2	2.12	0.50
2:E:1129:PHE:HA	2:E:1132:MET:HG3	1.94	0.50
2:E:1515:LEU:O	2:E:1519:ILE:HG13	2.11	0.50
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.30	0.49
1:D:555:ARG:HH22	2:E:109:ASN:HD21	1.58	0.49
2:E:1106:VAL:O	2:E:1109:ILE:HG22	2.12	0.49
2:B:80:VAL:HG12	2:B:85:LEU:HD11	1.93	0.49
2:B:156:ASN:HB3	2:B:161:LEU:HB2	1.94	0.49
2:B:373:ILE:HG23	2:B:376:ASN:HB2	1.93	0.49
2:B:810:VAL:HG13	2:B:852:LEU:HD21	1.93	0.49
2:B:965:ASP:HB3	2:B:968:HIS:CD2	2.47	0.49
2:B:1079:MET:HA	2:B:1082:GLU:OE2	2.11	0.49
2:E:4:TRP:CZ3	2:E:46:ARG:HG2	2.47	0.49
2:E:1054:LEU:HD11	2:E:1080:ARG:HB3	1.94	0.49
1:A:700:ASP:CG	2:B:14:VAL:HG13	2.36	0.49
2:B:4:TRP:CZ3	2:B:46:ARG:HG2	2.47	0.49
2:B:44:TRP:CE3	2:B:58:ILE:HG22	2.48	0.49
2:B:184:PHE:HA	2:B:1009:MET:HE3	1.93	0.49
2:B:194:ILE:O	2:B:198:ILE:HG23	2.12	0.49
2:E:194:ILE:O	2:E:198:ILE:HG23	2.12	0.49
2:E:859:CYS:O	2:E:863:ILE:HG12	2.11	0.49
1:A:541:GLN:O	1:A:544:ILE:HG22	2.12	0.49
1:A:551:GLN:OE1	1:A:552:ARG:NH2	2.38	0.49
2:B:7:THR:O	2:B:10:GLN:NE2	2.45	0.49
2:B:16:ILE:HG23	2:B:17:TYR:CD1	2.47	0.49
2:B:1040:LEU:HD22	2:B:1043:TRP:CH2	2.48	0.49
3:C:2:GLN:HE22	3:C:4:ILE:HD11	1.77	0.49
1:D:637:VAL:HG12	1:D:640:LEU:HD12	1.93	0.49
2:E:649:ASN:O	2:E:653:ASN:N	2.29	0.49
2:E:879:LEU:O	2:E:882:LEU:N	2.45	0.49
1:A:564:LYS:H	1:A:573:LYS:HD2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:TYR:HB3	2:B:53:LYS:HD2	1.93	0.49
2:B:721:TYR:OH	2:B:765:ARG:NE	2.46	0.49
2:B:959:ALA:O	2:B:962:GLN:NE2	2.46	0.49
2:B:1545:HIS:O	2:B:1549:MET:HG2	2.12	0.49
2:E:44:TRP:CE3	2:E:58:ILE:HG22	2.48	0.49
2:E:721:TYR:OH	2:E:765:ARG:NE	2.46	0.49
2:E:927:LEU:CB	2:E:931:ARG:HH21	2.25	0.49
2:E:1307:TYR:HD1	2:E:1310:LYS:HE2	1.77	0.49
1:A:563:ARG:HB2	1:A:655:ILE:O	2.12	0.49
2:B:308:LEU:HG	2:B:320:ARG:HH22	1.78	0.49
2:B:1471:GLY:O	2:B:1473:LYS:NZ	2.33	0.49
1:D:563:ARG:HB2	1:D:655:ILE:O	2.12	0.49
2:E:373:ILE:HG23	2:E:376:ASN:HB2	1.93	0.49
2:E:936:ILE:HD12	2:E:939:THR:HB	1.95	0.49
2:E:959:ALA:O	2:E:962:GLN:NE2	2.46	0.49
2:E:1154:LYS:HD2	2:E:1157:GLN:NE2	2.27	0.49
2:E:1388:TYR:CE2	3:F:44:VAL:HA	2.47	0.49
2:E:1460:GLN:HG2	2:E:1493:TYR:O	2.13	0.49
3:F:2:GLN:HE22	3:F:4:ILE:HD11	1.78	0.49
2:B:172:ILE:HD12	2:B:175:PRO:HG2	1.94	0.49
2:B:350:GLN:NE2	2:B:353:MET:HE1	2.28	0.49
2:B:1167:GLN:CD	2:B:1167:GLN:H	2.20	0.49
2:B:1632:LYS:O	2:B:1636:HIS:N	2.46	0.49
3:C:98:TYR:HE1	3:C:149:ILE:HD13	1.78	0.49
2:E:167:ASP:OD1	2:E:167:ASP:N	2.44	0.49
2:E:1167:GLN:CD	2:E:1167:GLN:H	2.20	0.49
1:A:680:ASP:OD1	1:A:680:ASP:N	2.45	0.49
2:B:526:HIS:CE1	2:B:586:LEU:HD21	2.48	0.49
2:B:1129:PHE:HA	2:B:1132:MET:HG3	1.94	0.49
2:E:95:LEU:HA	2:E:98:TRP:CD1	2.48	0.49
2:E:257:ASN:O	2:E:488:ALA:N	2.33	0.49
2:E:349:GLN:NE2	2:E:350:GLN:O	2.37	0.49
2:E:664:GLU:OE1	2:E:664:GLU:N	2.34	0.49
2:E:973:ILE:HD13	2:E:976:PHE:HZ	1.78	0.49
2:E:1038:PHE:O	2:E:1039:GLU:HG2	2.13	0.49
2:E:1545:HIS:O	2:E:1549:MET:HG2	2.12	0.49
2:E:1549:MET:HA	3:F:39:ASN:ND2	2.27	0.49
3:F:72:TYR:O	3:F:75:THR:OG1	2.24	0.49
1:A:588:TYR:N	1:A:603:SER:OG	2.46	0.49
2:B:319:ARG:O	2:B:500:VAL:N	2.45	0.49
2:B:1038:PHE:O	2:B:1039:GLU:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1128:PHE:O	2:B:1131:MET:HG2	2.12	0.49
2:B:1386:LYS:HG3	2:B:1387:GLU:H	1.78	0.49
2:E:1386:LYS:HG3	2:E:1387:GLU:H	1.77	0.49
2:E:1632:LYS:O	2:E:1636:HIS:N	2.46	0.49
3:F:98:TYR:HE1	3:F:149:ILE:HD13	1.78	0.49
2:B:102:TRP:CZ3	2:B:118:GLN:HG2	2.48	0.49
2:B:1054:LEU:HD11	2:B:1080:ARG:HB3	1.94	0.49
2:B:1282:LEU:HD12	2:B:1283:LEU:HD22	1.94	0.49
2:B:1460:GLN:HG2	2:B:1493:TYR:O	2.13	0.49
1:D:541:GLN:O	1:D:544:ILE:HG22	2.12	0.49
2:E:319:ARG:O	2:E:500:VAL:N	2.45	0.49
2:E:1040:LEU:HD22	2:E:1043:TRP:CH2	2.48	0.49
2:E:1358:PRO:HB2	2:E:1387:GLU:HB2	1.95	0.49
2:E:1362:TYR:CE1	2:E:1384:ARG:HG3	2.46	0.49
2:B:936:ILE:HD12	2:B:939:THR:HB	1.95	0.48
2:B:943:MET:HG2	2:B:953:PHE:CD2	2.48	0.48
2:B:1135:GLU:OE1	2:B:1139:SER:OG	2.31	0.48
3:C:7:VAL:HB	3:C:78:PHE:HD2	1.78	0.48
2:E:288:ASP:OD1	2:E:291:ARG:NH2	2.37	0.48
1:A:580:SER:HB2	1:A:585:VAL:HG22	1.95	0.48
2:B:25:VAL:HB	2:B:56:LYS:O	2.13	0.48
2:B:738:ASN:HD21	2:B:793:GLN:HG2	1.78	0.48
2:B:1408:MET:SD	2:B:1425:TYR:HB3	2.53	0.48
2:B:1565:ASN:O	2:B:1568:LYS:HG3	2.13	0.48
1:D:588:TYR:N	1:D:603:SER:OG	2.46	0.48
1:D:680:ASP:N	1:D:680:ASP:OD1	2.45	0.48
1:D:726:CYS:SG	1:D:727:ASN:N	2.86	0.48
2:E:7:THR:O	2:E:10:GLN:NE2	2.45	0.48
2:E:652:HIS:CD2	2:E:656:LYS:HD3	2.48	0.48
2:E:1368:TYR:N	2:E:1425:TYR:O	2.42	0.48
2:B:652:HIS:CD2	2:B:656:LYS:HD3	2.48	0.48
2:B:882:LEU:HA	2:B:885:GLN:NE2	2.28	0.48
1:D:665:TRP:O	1:D:669:LEU:HG	2.13	0.48
2:E:943:MET:HE2	2:E:950:ILE:HB	1.96	0.48
2:E:1118:VAL:O	2:E:1122:LYS:HG2	2.13	0.48
2:E:1565:ASN:O	2:E:1568:LYS:HG3	2.13	0.48
1:A:562:PHE:N	1:A:575:TRP:O	2.40	0.48
2:B:228:PHE:HA	2:B:401:VAL:HG12	1.96	0.48
2:B:556:ASN:ND2	2:B:561:THR:O	2.47	0.48
2:B:994:LYS:NZ	2:B:1048:HIS:HB3	2.28	0.48
2:E:254:ILE:O	2:E:431:MET:N	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:700:ILE:O	2:E:704:ILE:HG13	2.12	0.48
2:E:994:LYS:NZ	2:E:1048:HIS:HB3	2.28	0.48
2:E:1176:LEU:HD12	2:E:1177:LEU:N	2.29	0.48
2:B:215:ILE:O	2:B:218:THR:OG1	2.29	0.48
2:B:992:MET:O	2:B:996:LEU:HD23	2.13	0.48
2:B:1345:ARG:HG2	2:B:1349:TYR:CE2	2.49	0.48
3:C:39:ASN:H	3:C:57:ASP:HB3	1.77	0.48
2:E:926:GLN:O	2:E:929:MET:N	2.47	0.48
2:E:943:MET:HG2	2:E:953:PHE:CD2	2.48	0.48
2:E:1033:MET:HE3	2:E:1093:ASN:OD1	2.14	0.48
2:E:1345:ARG:HG2	2:E:1349:TYR:CE2	2.49	0.48
1:A:646:TYR:CE1	1:A:652:LEU:HG	2.49	0.48
2:B:697:LEU:O	2:B:701:ILE:HG12	2.14	0.48
2:B:1033:MET:HE3	2:B:1093:ASN:OD1	2.14	0.48
2:B:1101:PHE:CE2	2:B:1105:MET:HG3	2.49	0.48
2:B:1176:LEU:HD12	2:B:1177:LEU:N	2.29	0.48
2:B:1358:PRO:HB2	2:B:1387:GLU:HB2	1.95	0.48
3:C:80:ILE:HD11	3:C:97:TRP:HB3	1.96	0.48
1:D:536:LEU:HG	1:D:539:LYS:HE3	1.96	0.48
1:D:557:VAL:HA	1:D:579:LEU:HB3	1.96	0.48
1:D:652:LEU:HD22	1:D:654:PHE:CZ	2.49	0.48
2:E:25:VAL:HB	2:E:56:LYS:O	2.13	0.48
2:E:869:PHE:HA	2:E:918:VAL:HG13	1.96	0.48
2:E:1303:GLU:OE1	2:E:1303:GLU:HA	2.14	0.48
2:B:105:LEU:HD21	2:B:113:LEU:HD11	1.96	0.48
2:B:248:PRO:HD2	2:B:293:ARG:HG3	1.94	0.48
2:B:727:THR:O	2:B:774:TYR:HB2	2.14	0.48
2:B:1002:TYR:CE2	2:B:1009:MET:HB3	2.48	0.48
2:B:1307:TYR:CD1	2:B:1310:LYS:HE2	2.49	0.48
1:D:678:MET:HA	1:D:683:ARG:HH12	1.79	0.48
2:E:697:LEU:O	2:E:701:ILE:HG12	2.14	0.48
2:E:738:ASN:HD21	2:E:793:GLN:HG2	1.78	0.48
2:E:950:ILE:O	2:E:954:VAL:HG23	2.13	0.48
3:F:124:ASP:O	3:F:127:GLU:HG2	2.14	0.48
1:A:530:SER:O	1:A:534:LEU:N	2.36	0.48
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.48	0.48
2:B:421:VAL:HG13	2:B:425:THR:HG21	1.96	0.48
2:B:1328:TYR:HB3	2:B:1338:LEU:HD21	1.96	0.48
1:D:580:SER:HB2	1:D:585:VAL:HG22	1.95	0.48
2:E:156:ASN:HB3	2:E:161:LEU:HB2	1.94	0.48
2:E:308:LEU:HG	2:E:320:ARG:HH22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:526:HIS:CE1	2:E:586:LEU:HD21	2.48	0.48
2:E:992:MET:O	2:E:996:LEU:HD23	2.13	0.48
2:E:1301:TYR:O	2:E:1305:ILE:HG12	2.14	0.48
2:E:1408:MET:SD	2:E:1425:TYR:HB3	2.53	0.48
1:A:665:TRP:O	1:A:669:LEU:HG	2.13	0.48
1:A:678:MET:HA	1:A:683:ARG:HH12	1.79	0.48
2:B:1118:VAL:O	2:B:1122:LYS:HG2	2.13	0.48
2:B:1346:ALA:HB1	2:E:1339:GLY:HA2	1.96	0.48
2:B:1370:GLN:N	2:B:1421:SER:O	2.47	0.48
2:B:1607:HIS:NE2	2:B:1619:HIS:HB2	2.29	0.48
2:B:1633:VAL:O	2:B:1639:VAL:HG22	2.13	0.48
3:C:45:MET:HA	3:C:50:PRO:HA	1.96	0.48
3:C:124:ASP:O	3:C:127:GLU:HG2	2.14	0.48
2:E:181:ILE:HD11	2:E:956:CYS:HA	1.95	0.48
2:E:248:PRO:HD2	2:E:293:ARG:HG3	1.94	0.48
2:E:450:LEU:O	2:E:510:TYR:N	2.45	0.48
2:E:931:ARG:C	2:E:932:LEU:HD12	2.39	0.48
2:E:1101:PHE:CE2	2:E:1105:MET:HG3	2.49	0.48
2:E:1607:HIS:NE2	2:E:1619:HIS:HB2	2.29	0.48
3:F:39:ASN:H	3:F:57:ASP:HB3	1.77	0.48
1:A:536:LEU:HG	1:A:539:LYS:HE3	1.96	0.48
2:B:103:ARG:HA	2:B:106:TYR:CE1	2.46	0.48
2:B:1417:ASP:N	2:B:1417:ASP:OD1	2.43	0.48
2:E:350:GLN:NE2	2:E:353:MET:HE1	2.28	0.48
2:E:421:VAL:HG13	2:E:425:THR:HG21	1.96	0.48
2:E:1002:TYR:CE2	2:E:1009:MET:HB3	2.48	0.48
2:E:1282:LEU:HD12	2:E:1283:LEU:HD22	1.94	0.48
3:F:7:VAL:HB	3:F:78:PHE:HD2	1.78	0.48
1:A:652:LEU:HD22	1:A:654:PHE:CZ	2.49	0.47
2:B:950:ILE:O	2:B:954:VAL:HG23	2.13	0.47
2:B:1303:GLU:OE1	2:B:1303:GLU:HA	2.14	0.47
2:B:1524:LEU:HA	2:B:1527:GLU:OE2	2.14	0.47
1:D:536:LEU:CD2	2:E:31:ILE:HD11	2.43	0.47
2:E:102:TRP:CZ3	2:E:118:GLN:HG2	2.48	0.47
2:E:228:PHE:HA	2:E:401:VAL:HG12	1.96	0.47
2:E:1516:GLU:O	2:E:1520:GLU:OE1	2.32	0.47
1:A:726:CYS:SG	1:A:727:ASN:N	2.86	0.47
2:B:287:MET:SD	2:B:291:ARG:NH2	2.88	0.47
2:B:642:ASN:HA	2:B:644:ARG:HH22	1.79	0.47
2:B:869:PHE:HA	2:B:918:VAL:HG13	1.96	0.47
2:B:1469:ARG:HD2	2:B:1481:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:ARG:NH2	3:C:139:TYR:H	2.12	0.47
2:E:538:GLU:OE1	2:E:542:LYS:NZ	2.38	0.47
2:E:556:ASN:ND2	2:E:561:THR:O	2.47	0.47
2:E:1516:GLU:O	2:E:1519:ILE:HB	2.14	0.47
2:B:327:MET:HB2	2:B:346:ILE:HG23	1.97	0.47
2:B:450:LEU:O	2:B:510:TYR:N	2.45	0.47
2:B:926:GLN:O	2:B:929:MET:N	2.47	0.47
2:B:1522:MET:HE2	2:B:1593:ILE:HA	1.95	0.47
2:E:105:LEU:HD21	2:E:113:LEU:HD11	1.96	0.47
2:E:757:LEU:O	2:E:760:LEU:HD22	2.14	0.47
3:F:137:ILE:HG23	3:F:141:GLN:HG3	1.96	0.47
2:B:59:PHE:HD2	2:B:64:ILE:HG12	1.79	0.47
2:B:87:LEU:O	2:B:90:GLU:HG3	2.14	0.47
2:B:147:LYS:O	2:B:151:LYS:HG2	2.14	0.47
2:B:166:ARG:NH1	2:B:168:ASP:H	2.13	0.47
2:B:651:LYS:HB3	2:B:689:TYR:CE1	2.49	0.47
2:B:741:VAL:HG21	2:B:798:PHE:HD1	1.80	0.47
2:B:1144:PHE:HB2	2:B:1147:PHE:HB3	1.96	0.47
2:B:1563:PHE:O	2:B:1567:GLU:HG2	2.15	0.47
1:D:541:GLN:N	1:D:542:PRO:HD3	2.30	0.47
1:D:646:TYR:CE1	1:D:652:LEU:HG	2.49	0.47
2:E:87:LEU:O	2:E:90:GLU:HG3	2.14	0.47
2:E:92:THR:HA	2:E:95:LEU:HD12	1.97	0.47
2:E:285:SER:N	2:E:288:ASP:OD2	2.40	0.47
2:E:651:LYS:HB3	2:E:689:TYR:CE1	2.49	0.47
2:E:1633:VAL:O	2:E:1639:VAL:HG22	2.13	0.47
3:F:45:MET:HA	3:F:50:PRO:HA	1.96	0.47
3:F:120:ARG:NH2	3:F:139:TYR:H	2.12	0.47
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.96	0.47
2:B:905:LEU:O	2:B:909:ILE:HG12	2.15	0.47
2:B:1574:LYS:HA	2:B:1577:GLN:OE1	2.15	0.47
3:C:91:GLU:O	3:C:95:ALA:CB	2.63	0.47
2:E:59:PHE:HD2	2:E:64:ILE:HG12	1.80	0.47
2:E:166:ARG:HG2	2:E:173:LEU:HB2	1.96	0.47
2:E:287:MET:SD	2:E:291:ARG:NH2	2.88	0.47
2:E:469:THR:O	2:E:530:THR:OG1	2.31	0.47
2:E:882:LEU:HA	2:E:885:GLN:NE2	2.28	0.47
2:E:1144:PHE:HB2	2:E:1147:PHE:HB3	1.96	0.47
2:E:1328:TYR:HB3	2:E:1338:LEU:HD21	1.96	0.47
2:B:922:ALA:HA	2:B:925:ILE:HD12	1.97	0.47
2:B:1185:TYR:O	2:B:1188:SER:OG	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ILE:HG23	3:C:141:GLN:HG3	1.96	0.47
1:D:532:PRO:O	1:D:536:LEU:HD13	2.15	0.47
1:D:544:ILE:CD1	1:D:689:LEU:HB2	2.44	0.47
1:D:696:LEU:HD12	1:D:697:ARG:HD2	1.97	0.47
2:E:1307:TYR:CD1	2:E:1310:LYS:HE2	2.49	0.47
2:E:1469:ARG:HD2	2:E:1481:THR:OG1	2.14	0.47
3:F:9:VAL:HG13	3:F:78:PHE:CE2	2.50	0.47
3:F:80:ILE:HD11	3:F:97:TRP:HB3	1.96	0.47
1:A:532:PRO:O	1:A:536:LEU:HD13	2.15	0.47
2:B:89:GLN:O	2:B:92:THR:OG1	2.31	0.47
2:B:119:GLN:HA	2:B:122:TYR:CD1	2.50	0.47
2:B:185:LYS:HB2	2:B:185:LYS:HE3	1.57	0.47
2:B:259:LEU:HD23	2:B:490:TYR:CG	2.49	0.47
2:B:466:VAL:HG22	2:B:547:PHE:HZ	1.79	0.47
2:B:943:MET:HE2	2:B:950:ILE:HB	1.96	0.47
2:B:1097:HIS:HA	2:B:1100:LYS:NZ	2.30	0.47
2:B:1125:ILE:N	2:B:1126:PRO:HD2	2.30	0.47
2:B:1361:GLU:OE2	2:B:1388:TYR:HA	2.15	0.47
1:D:547:LEU:HG	2:E:106:TYR:OH	2.14	0.47
1:D:564:LYS:H	1:D:573:LYS:HD2	1.78	0.47
1:D:622:CYS:HB3	1:D:624:HIS:ND1	2.30	0.47
2:E:36:HIS:N	2:E:48:TYR:O	2.48	0.47
2:E:166:ARG:NH1	2:E:168:ASP:H	2.13	0.47
2:E:965:ASP:O	2:E:968:HIS:HB2	2.14	0.47
2:E:1183:HIS:HB3	2:E:1187:SER:OG	2.15	0.47
2:E:1370:GLN:N	2:E:1421:SER:O	2.47	0.47
2:E:1463:ARG:HD3	2:E:1486:ARG:HD2	1.97	0.47
2:E:1577:GLN:HA	2:E:1580:PRO:HG3	1.97	0.47
2:B:88:VAL:O	2:B:91:LEU:HG	2.15	0.47
2:B:181:ILE:HD11	2:B:956:CYS:HA	1.95	0.47
2:B:757:LEU:O	2:B:760:LEU:HD22	2.14	0.47
2:B:1627:ARG:HA	2:B:1630:LYS:HB2	1.96	0.47
1:D:640:LEU:HB3	1:D:656:ALA:H	1.80	0.47
2:E:105:LEU:HD23	2:E:110:LYS:HD2	1.96	0.47
2:E:147:LYS:O	2:E:151:LYS:HG2	2.14	0.47
2:E:741:VAL:HG21	2:E:798:PHE:HD1	1.80	0.47
2:E:844:ILE:HG21	2:E:881:LEU:HD21	1.96	0.47
2:E:1135:GLU:OE1	2:E:1139:SER:OG	2.31	0.47
2:E:1478:GLU:CG	2:E:1482:MET:HE2	2.44	0.47
2:E:1627:ARG:HA	2:E:1630:LYS:HB2	1.96	0.47
2:B:25:VAL:HG12	2:B:55:LYS:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:THR:HA	2:B:152:ILE:HG22	1.97	0.47
2:B:871:GLN:CD	2:B:875:ARG:HD3	2.39	0.47
2:B:927:LEU:CB	2:B:931:ARG:HH21	2.25	0.47
2:B:1516:GLU:O	2:B:1519:ILE:HB	2.15	0.47
2:E:642:ASN:HA	2:E:644:ARG:HH22	1.79	0.47
2:E:926:GLN:O	2:E:929:MET:HB3	2.15	0.47
3:F:91:GLU:O	3:F:95:ALA:CB	2.63	0.47
2:B:288:ASP:OD1	2:B:291:ARG:NH2	2.37	0.47
2:B:469:THR:O	2:B:530:THR:OG1	2.31	0.47
2:B:926:GLN:O	2:B:929:MET:HB3	2.15	0.47
2:B:965:ASP:O	2:B:968:HIS:HB2	2.14	0.47
2:B:1224:THR:HA	2:B:1227:VAL:HG12	1.97	0.47
2:B:1240:TYR:O	2:B:1244:LEU:HG	2.15	0.47
2:B:1516:GLU:O	2:B:1520:GLU:OE1	2.32	0.47
2:B:1613:GLU:OE2	2:B:1614:GLN:HG3	2.14	0.47
3:C:93:VAL:O	3:C:98:TYR:HB3	2.15	0.47
1:D:670:ASN:HB2	1:D:678:MET:HE1	1.97	0.47
2:E:88:VAL:O	2:E:91:LEU:HG	2.15	0.47
2:E:871:GLN:OE1	2:E:875:ARG:NH1	2.45	0.47
2:E:1059:LEU:HD23	2:E:1062:GLU:OE1	2.15	0.47
2:E:1522:MET:HE2	2:E:1593:ILE:HA	1.95	0.47
2:E:1524:LEU:HA	2:E:1527:GLU:OE2	2.14	0.47
1:A:557:VAL:HA	1:A:579:LEU:HB3	1.96	0.46
1:A:696:LEU:HD12	1:A:697:ARG:HD2	1.97	0.46
2:B:36:HIS:N	2:B:48:TYR:O	2.48	0.46
2:B:288:ASP:HA	2:B:291:ARG:NE	2.30	0.46
2:B:931:ARG:C	2:B:932:LEU:HD12	2.39	0.46
2:B:1183:HIS:HB3	2:B:1187:SER:OG	2.15	0.46
2:B:1231:TYR:CE2	2:B:1239:ILE:HD12	2.50	0.46
2:B:1521:THR:O	2:B:1524:LEU:HG	2.15	0.46
1:D:575:TRP:HB2	1:D:589:GLY:O	2.15	0.46
2:E:319:ARG:NH1	2:E:511:GLU:OE2	2.39	0.46
2:E:466:VAL:HG22	2:E:547:PHE:HZ	1.79	0.46
2:E:727:THR:O	2:E:774:TYR:HB2	2.14	0.46
2:E:1097:HIS:HA	2:E:1100:LYS:NZ	2.30	0.46
2:E:1521:THR:O	2:E:1524:LEU:HG	2.15	0.46
2:E:1563:PHE:O	2:E:1567:GLU:HG2	2.15	0.46
1:A:670:ASN:HB2	1:A:678:MET:HE1	1.97	0.46
1:A:719:ASN:O	2:B:1:MET:N	2.45	0.46
2:B:484:ILE:HD12	2:B:495:GLU:HA	1.97	0.46
2:B:643:TRP:HB2	2:B:650:ILE:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:GLN:HE21	2:B:711:HIS:CE1	2.33	0.46
2:B:973:ILE:HD13	2:B:976:PHE:HZ	1.78	0.46
2:B:1059:LEU:HD23	2:B:1062:GLU:OE1	2.15	0.46
3:C:39:ASN:OD1	3:C:56:TRP:HA	2.16	0.46
2:E:10:GLN:NE2	2:E:37:ILE:O	2.46	0.46
2:E:136:LEU:HD12	2:E:140:GLU:HG2	1.97	0.46
2:E:163:LEU:HD23	2:E:163:LEU:H	1.79	0.46
2:E:259:LEU:HD23	2:E:490:TYR:CG	2.49	0.46
2:E:339:ASP:N	2:E:339:ASP:OD1	2.48	0.46
2:E:875:ARG:HE	2:E:924:HIS:CD2	2.33	0.46
2:E:1335:TYR:O	2:E:1338:LEU:HB2	2.15	0.46
2:E:1399:LEU:HD11	2:E:1407:LYS:HE3	1.97	0.46
2:E:1434:VAL:HB	2:E:1461:GLN:HB2	1.97	0.46
2:E:1613:GLU:OE2	2:E:1614:GLN:HG3	2.14	0.46
1:A:622:CYS:HB3	1:A:624:HIS:ND1	2.30	0.46
2:B:35:VAL:HG23	2:B:37:ILE:HG13	1.97	0.46
2:B:319:ARG:NH1	2:B:511:GLU:OE2	2.39	0.46
2:B:630:LYS:HG2	2:B:668:PHE:HZ	1.80	0.46
1:D:647:ASP:OD1	3:F:163:ARG:NH2	2.49	0.46
2:E:327:MET:HB2	2:E:346:ILE:HG23	1.97	0.46
2:E:584:PHE:CE2	2:E:588:LEU:HD11	2.50	0.46
2:E:1354:LYS:HE3	2:E:1354:LYS:HB3	1.73	0.46
2:E:1574:LYS:HA	2:E:1577:GLN:OE1	2.15	0.46
1:A:544:ILE:CD1	1:A:689:LEU:HB2	2.45	0.46
2:B:307:GLU:HB2	2:B:314:HIS:CD2	2.51	0.46
2:B:647:SER:HA	2:B:650:ILE:HG13	1.97	0.46
2:B:844:ILE:HG21	2:B:881:LEU:HD21	1.96	0.46
2:B:943:MET:HG3	2:B:950:ILE:HD13	1.98	0.46
2:B:973:ILE:HA	2:B:976:PHE:CE1	2.51	0.46
3:C:9:VAL:HG13	3:C:78:PHE:CE2	2.50	0.46
2:E:119:GLN:HA	2:E:122:TYR:CD1	2.50	0.46
2:E:149:THR:HA	2:E:152:ILE:HG22	1.97	0.46
2:E:307:GLU:HB2	2:E:314:HIS:CD2	2.51	0.46
2:E:414:GLN:NE2	2:E:421:VAL:HG12	2.24	0.46
2:E:710:GLN:HE21	2:E:711:HIS:CE1	2.33	0.46
2:E:1231:TYR:CE2	2:E:1239:ILE:HD12	2.50	0.46
1:A:541:GLN:N	1:A:542:PRO:HD3	2.30	0.46
2:B:92:THR:HA	2:B:95:LEU:HD12	1.97	0.46
2:B:246:TYR:CZ	2:B:383:LEU:HD21	2.50	0.46
2:B:855:GLN:H	2:B:855:GLN:CD	2.21	0.46
2:B:862:LYS:O	2:B:865:GLU:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1335:TYR:O	2:B:1338:LEU:HB2	2.15	0.46
2:B:1343:LYS:HE2	2:E:1343:LYS:HD3	1.98	0.46
2:B:1434:VAL:HB	2:B:1461:GLN:HB2	1.97	0.46
1:D:697:ARG:HE	2:E:30:GLN:CD	2.24	0.46
2:E:985:PHE:HA	2:E:988:GLU:OE1	2.16	0.46
2:E:1027:VAL:HG12	2:E:1030:ARG:HH21	1.81	0.46
2:E:1469:ARG:HA	2:E:1481:THR:HB	1.98	0.46
2:B:163:LEU:HD23	2:B:163:LEU:H	1.79	0.46
2:B:718:THR:O	2:B:722:LYS:HE2	2.16	0.46
2:B:985:PHE:HA	2:B:988:GLU:OE1	2.16	0.46
2:B:1573:GLU:HG3	2:B:1577:GLN:NE2	2.31	0.46
3:C:5:LYS:HD2	3:C:74:GLN:O	2.16	0.46
2:E:484:ILE:HD12	2:E:495:GLU:HA	1.97	0.46
2:E:569:LEU:HD23	2:E:591:THR:HG22	1.98	0.46
2:E:871:GLN:CD	2:E:875:ARG:HD3	2.39	0.46
2:E:1499:LEU:HG	2:E:1501:TRP:H	1.81	0.46
2:E:1623:SER:HB3	2:E:1627:ARG:NH2	2.31	0.46
1:A:575:TRP:HB2	1:A:589:GLY:O	2.15	0.46
2:B:1030:ARG:HG3	2:B:1031:PHE:CE1	2.51	0.46
2:B:1220:ARG:HA	2:B:1223:CYS:SG	2.56	0.46
2:B:1301:TYR:O	2:B:1305:ILE:HG12	2.14	0.46
2:B:1362:TYR:CE1	2:B:1384:ARG:HG3	2.46	0.46
1:D:576:TYR:OH	1:D:601:HIS:O	2.34	0.46
2:E:945:ARG:NH1	2:E:947:SER:H	2.13	0.46
2:E:1189:SER:O	2:E:1192:VAL:HG22	2.16	0.46
2:E:1240:TYR:O	2:E:1244:LEU:HG	2.15	0.46
2:E:1259:GLU:HG3	2:E:1497:GLY:O	2.16	0.46
2:E:1318:ILE:HD11	2:E:1348:PHE:HB2	1.98	0.46
3:F:93:VAL:O	3:F:98:TYR:HB3	2.15	0.46
2:B:1463:ARG:HD3	2:B:1486:ARG:HD2	1.97	0.46
3:C:129:LEU:O	3:C:134:LEU:N	2.40	0.46
2:E:643:TRP:HB2	2:E:650:ILE:CD1	2.45	0.46
2:E:922:ALA:HA	2:E:925:ILE:HD12	1.97	0.46
2:E:1237:GLU:O	2:E:1240:TYR:HB3	2.15	0.46
2:E:1328:TYR:HB3	2:E:1338:LEU:CD2	2.46	0.46
2:E:1361:GLU:OE2	2:E:1388:TYR:HA	2.15	0.46
1:A:660:HIS:CG	1:A:661:GLU:N	2.84	0.46
2:B:985:PHE:O	2:B:989:THR:HG23	2.16	0.46
2:B:1119:GLU:HG2	2:B:1120:LEU:N	2.31	0.46
3:C:164:GLY:O	3:C:168:VAL:N	2.34	0.46
1:D:640:LEU:O	1:D:655:ILE:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:288:ASP:HA	2:E:291:ARG:NE	2.30	0.46
2:E:732:LYS:O	2:E:736:VAL:HG23	2.16	0.46
2:E:792:ARG:HH21	2:E:839:LEU:HD13	1.81	0.46
2:E:1125:ILE:N	2:E:1126:PRO:HD2	2.30	0.46
3:F:129:LEU:O	3:F:134:LEU:N	2.40	0.46
2:B:285:SER:N	2:B:288:ASP:OD2	2.40	0.46
2:B:330:THR:HG22	2:B:334:HIS:CE1	2.52	0.46
2:B:528:ARG:HD3	2:B:585:TYR:CZ	2.51	0.46
2:B:732:LYS:O	2:B:736:VAL:HG23	2.16	0.46
2:E:528:ARG:HD3	2:E:585:TYR:CZ	2.51	0.46
2:E:802:MET:HE1	2:E:847:ILE:CA	2.45	0.46
2:E:1600:LEU:O	2:E:1604:ILE:HG12	2.16	0.46
3:F:163:ARG:C	3:F:165:LEU:H	2.24	0.46
1:A:607:LYS:HE3	1:A:609:PRO:HA	1.98	0.45
2:B:85:LEU:HB3	2:B:89:GLN:HE22	1.81	0.45
2:B:146:LYS:HB2	2:B:146:LYS:HE2	1.80	0.45
2:B:296:LEU:HB2	2:B:329:ILE:HD13	1.98	0.45
2:B:875:ARG:HE	2:B:924:HIS:CD2	2.33	0.45
2:B:1081:LYS:HA	2:B:1120:LEU:HD23	1.98	0.45
2:B:1328:TYR:HB3	2:B:1338:LEU:CD2	2.46	0.45
2:E:111:LEU:HA	2:E:114:PHE:HB3	1.97	0.45
2:E:146:LYS:HB2	2:E:146:LYS:HE2	1.81	0.45
2:E:429:ARG:NE	2:E:445:ASP:OD2	2.46	0.45
2:E:905:LEU:O	2:E:909:ILE:HG12	2.15	0.45
2:E:972:TYR:HA	2:E:975:THR:OG1	2.16	0.45
3:F:39:ASN:OD1	3:F:56:TRP:HA	2.16	0.45
3:F:98:TYR:CE1	3:F:149:ILE:HD13	2.51	0.45
1:A:544:ILE:HD11	1:A:689:LEU:HB2	1.99	0.45
1:A:640:LEU:HB3	1:A:656:ALA:H	1.80	0.45
2:B:105:LEU:HD23	2:B:110:LYS:HD2	1.96	0.45
2:B:339:ASP:OD1	2:B:339:ASP:N	2.48	0.45
2:B:349:GLN:NE2	2:B:350:GLN:O	2.37	0.45
2:B:760:LEU:HD22	2:B:819:TYR:HB3	1.98	0.45
2:B:1023:GLN:O	2:B:1027:VAL:HG13	2.17	0.45
2:B:1189:SER:O	2:B:1192:VAL:HG22	2.16	0.45
2:B:1237:GLU:O	2:B:1240:TYR:HB3	2.16	0.45
2:E:718:THR:O	2:E:722:LYS:HE2	2.16	0.45
2:E:760:LEU:HD22	2:E:819:TYR:HB3	1.98	0.45
2:E:1484:ILE:HG22	2:E:1486:ARG:HG3	1.98	0.45
3:F:5:LYS:HD2	3:F:74:GLN:O	2.16	0.45
1:A:614:LYS:HZ1	1:A:648:SER:H	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:LEU:HD23	2:B:591:THR:HG22	1.97	0.45
2:B:792:ARG:HH21	2:B:839:LEU:HD13	1.81	0.45
2:B:1075:LYS:HB3	2:B:1075:LYS:HE3	1.60	0.45
2:B:1577:GLN:HA	2:B:1580:PRO:HG3	1.97	0.45
2:B:1623:SER:HB3	2:B:1627:ARG:NH2	2.31	0.45
3:C:98:TYR:CE1	3:C:149:ILE:HD13	2.51	0.45
3:C:174:ARG:HA	3:C:177:LEU:HB2	1.99	0.45
2:E:85:LEU:HB3	2:E:89:GLN:HE22	1.81	0.45
2:E:185:LYS:HB2	2:E:185:LYS:HE3	1.57	0.45
2:E:548:GLY:HA2	2:E:572:TYR:O	2.16	0.45
2:E:640:LEU:HD22	2:E:657:LEU:HD22	1.98	0.45
2:E:647:SER:HA	2:E:650:ILE:HG13	1.97	0.45
2:E:741:VAL:HG21	2:E:798:PHE:CD1	2.52	0.45
2:E:862:LYS:O	2:E:865:GLU:HB3	2.16	0.45
2:E:1224:THR:HA	2:E:1227:VAL:HG12	1.97	0.45
2:B:111:LEU:HA	2:B:114:PHE:HB3	1.97	0.45
2:B:654:LEU:HB3	2:B:692:LEU:HB3	1.97	0.45
2:B:1469:ARG:HA	2:B:1481:THR:HB	1.98	0.45
2:B:1482:MET:HE1	3:C:34:PRO:HG2	1.98	0.45
2:E:25:VAL:HG12	2:E:55:LYS:HE2	1.97	0.45
2:E:103:ARG:HA	2:E:106:TYR:CE1	2.46	0.45
2:E:246:TYR:CZ	2:E:383:LEU:HD21	2.50	0.45
2:E:943:MET:HG3	2:E:950:ILE:HD13	1.98	0.45
2:E:985:PHE:O	2:E:989:THR:HG23	2.16	0.45
2:E:1075:LYS:HE3	2:E:1075:LYS:HB3	1.60	0.45
2:E:1354:LYS:NZ	2:E:1355:ALA:HB2	2.31	0.45
2:E:1412:THR:HB	2:E:1413:PRO:HD3	1.98	0.45
2:E:1460:GLN:HE21	2:E:1494:THR:HG23	1.81	0.45
2:E:1573:GLU:HG3	2:E:1577:GLN:NE2	2.31	0.45
3:F:170:ASP:HB3	3:F:174:ARG:NH2	2.29	0.45
1:A:564:LYS:HE2	1:A:575:TRP:CD1	2.52	0.45
1:A:576:TYR:OH	1:A:601:HIS:O	2.34	0.45
2:B:1412:THR:HB	2:B:1413:PRO:HD3	1.97	0.45
2:E:973:ILE:HA	2:E:976:PHE:CE1	2.51	0.45
2:E:1030:ARG:HG3	2:E:1031:PHE:CE1	2.51	0.45
1:A:679:SER:HB3	1:A:681:LEU:HG	1.99	0.45
2:B:225:TYR:N	2:B:404:LYS:O	2.40	0.45
2:B:468:VAL:HG21	2:B:620:PHE:CZ	2.52	0.45
2:B:584:PHE:CE2	2:B:588:LEU:HD11	2.50	0.45
2:B:741:VAL:HG21	2:B:798:PHE:CD1	2.52	0.45
2:B:945:ARG:NH1	2:B:947:SER:H	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:TYR:HA	2:B:975:THR:OG1	2.16	0.45
2:B:1149:ASN:HA	2:B:1236:ARG:NH2	2.32	0.45
2:B:1248:ARG:HG3	2:B:1264:LEU:CD1	2.45	0.45
2:B:1399:LEU:HD11	2:B:1407:LYS:HE3	1.97	0.45
2:B:1605:ARG:O	2:B:1609:GLU:HG3	2.17	0.45
1:D:544:ILE:HD11	1:D:689:LEU:HB2	1.98	0.45
1:D:660:HIS:CG	1:D:661:GLU:N	2.84	0.45
1:D:679:SER:HB3	1:D:681:LEU:HG	1.99	0.45
2:E:719:TYR:CD1	2:E:723:HIS:HB2	2.51	0.45
2:E:1066:GLN:HA	2:E:1069:ARG:CZ	2.47	0.45
2:E:1166:GLU:O	2:E:1169:LYS:HG2	2.17	0.45
1:A:574:PHE:HB2	1:A:593:GLU:HA	1.99	0.45
2:B:414:GLN:NE2	2:B:421:VAL:HG12	2.25	0.45
2:B:673:LEU:HB3	2:B:677:PHE:CE2	2.52	0.45
2:B:809:ALA:O	2:B:813:LYS:HD3	2.16	0.45
2:B:929:MET:SD	2:B:964:MET:HE1	2.57	0.45
2:B:1381:PHE:CE1	2:B:1503:GLU:HB3	2.52	0.45
2:B:1478:GLU:CG	2:B:1482:MET:HE2	2.44	0.45
2:B:1550:LEU:O	2:B:1554:ILE:HG12	2.17	0.45
3:C:6:CYS:C	3:C:56:TRP:HD1	2.25	0.45
1:D:530:SER:O	1:D:534:LEU:N	2.36	0.45
1:D:564:LYS:HE2	1:D:575:TRP:CD1	2.52	0.45
2:E:694:PHE:CZ	2:E:737:LEU:HB3	2.51	0.45
2:E:1526:ASN:HA	2:E:1529:ILE:HD12	1.99	0.45
2:E:1549:MET:SD	3:F:39:ASN:OD1	2.75	0.45
3:F:174:ARG:HA	3:F:177:LEU:HB2	1.99	0.45
2:B:792:ARG:HE	2:B:839:LEU:HD11	1.82	0.45
2:B:802:MET:HE1	2:B:847:ILE:CA	2.45	0.45
2:E:283:ASP:HB2	2:E:430:LYS:HB3	1.99	0.45
2:B:879:LEU:O	2:B:880:PRO:C	2.60	0.45
2:B:965:ASP:HA	2:B:1019:ARG:HH21	1.82	0.45
2:B:1154:LYS:HD2	2:B:1157:GLN:NE2	2.27	0.45
2:E:746:ASP:CG	2:E:748:SER:HG	2.25	0.45
2:E:809:ALA:O	2:E:813:LYS:HD3	2.16	0.45
2:E:1388:TYR:OH	3:F:44:VAL:HG22	2.17	0.45
1:A:546:GLU:HB2	1:A:550:GLN:HE22	1.82	0.45
2:B:72:GLU:O	2:B:76:GLN:NE2	2.49	0.45
2:B:136:LEU:HD12	2:B:140:GLU:HG2	1.97	0.45
2:B:676:LEU:HD22	2:B:693:VAL:HG22	1.99	0.45
2:B:1600:LEU:O	2:B:1604:ILE:HG12	2.16	0.45
2:E:1119:GLU:HG2	2:E:1120:LEU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1345:ARG:HG2	2:E:1349:TYR:HE2	1.82	0.45
3:F:43:ASN:HA	3:F:52:ASN:HA	1.99	0.45
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.99	0.44
1:A:701:LEU:HD21	2:B:16:ILE:HA	1.98	0.44
2:B:719:TYR:CD1	2:B:723:HIS:HB2	2.51	0.44
2:B:757:LEU:HD21	2:B:816:ALA:N	2.33	0.44
2:B:932:LEU:H	2:B:935:ARG:HH21	1.62	0.44
2:B:993:PHE:O	2:B:997:ILE:HG22	2.17	0.44
2:B:1027:VAL:HG12	2:B:1030:ARG:HH21	1.81	0.44
2:B:1168:TYR:CZ	2:B:1172:LEU:HD11	2.53	0.44
2:B:1354:LYS:NZ	2:B:1355:ALA:HB2	2.31	0.44
2:B:1388:TYR:OH	3:C:44:VAL:HG22	2.18	0.44
2:B:1607:HIS:O	2:B:1611:LEU:N	2.50	0.44
3:C:170:ASP:HB3	3:C:174:ARG:NH2	2.29	0.44
1:D:564:LYS:HE3	1:D:590:ASP:CG	2.42	0.44
2:E:330:THR:HG22	2:E:334:HIS:CE1	2.51	0.44
2:E:932:LEU:H	2:E:935:ARG:HH21	1.62	0.44
2:E:1160:GLU:OE1	2:E:1243:TYR:OH	2.35	0.44
2:E:1220:ARG:HA	2:E:1223:CYS:SG	2.56	0.44
2:E:1381:PHE:CE1	2:E:1503:GLU:HB3	2.52	0.44
2:E:1605:ARG:O	2:E:1609:GLU:HG3	2.17	0.44
3:F:6:CYS:C	3:F:56:TRP:HD1	2.25	0.44
3:F:82:PHE:HD1	3:F:112:LEU:HD11	1.81	0.44
1:A:591:LEU:HD11	1:A:601:HIS:CE1	2.53	0.44
2:B:704:ILE:HA	2:B:709:PHE:HB2	1.99	0.44
2:B:940:VAL:HA	2:B:943:MET:HB3	1.98	0.44
2:B:1259:GLU:HG3	2:B:1497:GLY:O	2.16	0.44
2:E:35:VAL:HG23	2:E:37:ILE:HG13	1.97	0.44
2:E:468:VAL:HG21	2:E:620:PHE:CZ	2.52	0.44
2:E:654:LEU:HB3	2:E:692:LEU:HB3	1.97	0.44
2:E:704:ILE:HA	2:E:709:PHE:HB2	1.99	0.44
2:E:940:VAL:HA	2:E:943:MET:HB3	1.98	0.44
2:E:965:ASP:HA	2:E:1019:ARG:HH21	1.82	0.44
2:B:140:GLU:O	2:B:144:LEU:HD23	2.18	0.44
2:B:1179:HIS:O	2:B:1182:LYS:HG2	2.17	0.44
2:B:1220:ARG:HE	2:B:1250:LEU:CD2	2.31	0.44
2:B:1318:ILE:HD11	2:B:1348:PHE:HB2	1.98	0.44
2:E:1149:ASN:HA	2:E:1236:ARG:NH2	2.32	0.44
2:E:1220:ARG:HE	2:E:1250:LEU:CD2	2.31	0.44
2:E:1343:LYS:HE3	2:E:1343:LYS:HB2	1.76	0.44
2:E:1484:ILE:HB	2:E:1512:ILE:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:678:ASN:O	2:B:682:GLU:HG2	2.17	0.44
2:B:879:LEU:CD2	2:B:931:ARG:HH22	2.31	0.44
2:B:1354:LYS:HE3	2:B:1354:LYS:HB3	1.73	0.44
2:B:1484:ILE:HB	2:B:1512:ILE:HB	1.99	0.44
2:B:1484:ILE:HG22	2:B:1486:ARG:HG3	1.98	0.44
2:B:1611:LEU:HD13	2:B:1619:HIS:HB2	1.99	0.44
1:D:574:PHE:HB2	1:D:593:GLU:HA	1.99	0.44
2:E:792:ARG:HE	2:E:839:LEU:HD11	1.82	0.44
2:E:965:ASP:H	2:E:968:HIS:HB2	1.83	0.44
2:E:1124:THR:HG23	2:E:1127:ILE:HD12	1.99	0.44
2:E:1221:MET:HA	2:E:1224:THR:HG22	1.99	0.44
2:E:1550:LEU:O	2:E:1554:ILE:HG12	2.17	0.44
2:E:1611:LEU:HD13	2:E:1619:HIS:HB2	1.99	0.44
2:B:228:PHE:HE2	2:B:399:LEU:HD12	1.83	0.44
2:B:1557:PRO:HB2	2:B:1560:MET:O	2.17	0.44
1:D:670:ASN:OD1	1:D:675:LYS:HE3	2.18	0.44
2:E:155:GLY:O	2:E:159:LEU:HG	2.18	0.44
2:E:630:LYS:HG2	2:E:668:PHE:HZ	1.81	0.44
2:E:673:LEU:HB3	2:E:677:PHE:CE2	2.52	0.44
2:E:876:GLU:HG2	2:E:877:VAL:HG13	1.99	0.44
2:E:1362:TYR:HD2	2:E:1462:PHE:CE2	2.34	0.44
2:E:1432:LYS:HB3	2:E:1432:LYS:HE3	1.90	0.44
3:F:67:LEU:HD13	3:F:67:LEU:HA	1.74	0.44
2:B:283:ASP:HB2	2:B:430:LYS:HB3	1.99	0.44
2:B:333:ILE:O	2:B:405:LEU:HD22	2.18	0.44
2:B:548:GLY:HA2	2:B:572:TYR:O	2.16	0.44
2:B:630:LYS:HG2	2:B:668:PHE:CZ	2.53	0.44
2:B:640:LEU:HD22	2:B:657:LEU:HD22	1.98	0.44
2:B:909:ILE:HG13	2:B:910:LEU:N	2.33	0.44
2:B:1124:THR:HG23	2:B:1127:ILE:HD12	1.99	0.44
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.17	0.44
2:B:1538:TRP:CE2	2:B:1539:ASP:HB2	2.53	0.44
2:B:1558:ALA:HB3	3:C:38:ASP:OD2	2.17	0.44
1:D:607:LYS:HE3	1:D:609:PRO:HA	1.98	0.44
2:E:89:GLN:O	2:E:92:THR:OG1	2.31	0.44
2:B:174:ASP:O	2:B:183:LEU:HD21	2.17	0.44
2:B:243:MET:O	2:B:258:TYR:N	2.32	0.44
2:B:1066:GLN:HA	2:B:1069:ARG:CZ	2.47	0.44
2:B:1342:LEU:C	2:B:1342:LEU:HD12	2.43	0.44
2:B:1526:ASN:HA	2:B:1529:ILE:HD12	1.99	0.44
3:C:82:PHE:HD1	3:C:112:LEU:HD11	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ASP:O	2:E:183:LEU:HD21	2.17	0.44
2:E:630:LYS:HG2	2:E:668:PHE:CZ	2.53	0.44
2:E:879:LEU:CD2	2:E:931:ARG:HH22	2.31	0.44
2:E:964:MET:HE3	2:E:964:MET:HB3	1.82	0.44
2:E:1081:LYS:HA	2:E:1120:LEU:HD23	1.98	0.44
2:E:1133:GLN:OE1	2:E:1136:PHE:HD2	2.01	0.44
2:E:1168:TYR:CZ	2:E:1172:LEU:HD11	2.53	0.44
1:A:539:LYS:NZ	1:A:540:ILE:HD11	2.33	0.44
1:A:564:LYS:HE3	1:A:590:ASP:CG	2.42	0.44
2:B:562:LEU:O	2:B:633:GLN:NE2	2.51	0.44
2:B:1095:GLY:HA3	2:B:1096:PRO:HD3	1.90	0.44
2:B:1232:LYS:HB2	2:B:1240:TYR:CE2	2.53	0.44
2:E:220:HIS:NE2	2:E:436:ILE:HB	2.33	0.44
2:E:436:ILE:HG22	2:E:438:LEU:HD22	2.00	0.44
2:E:1179:HIS:O	2:E:1182:LYS:HG2	2.17	0.44
2:E:1273:TRP:HE3	2:E:1294:GLN:OE1	2.00	0.44
2:E:1607:HIS:O	2:E:1611:LEU:N	2.50	0.44
3:F:95:ALA:O	3:F:99:PRO:HG2	2.18	0.44
3:F:118:ASP:N	3:F:118:ASP:OD1	2.49	0.44
2:B:257:ASN:O	2:B:488:ALA:N	2.33	0.44
2:B:436:ILE:HG22	2:B:438:LEU:HD22	2.00	0.44
2:B:1273:TRP:HE3	2:B:1294:GLN:OE1	2.00	0.44
1:D:585:VAL:HG12	1:D:607:LYS:HD2	1.99	0.44
2:E:929:MET:SD	2:E:964:MET:HE1	2.57	0.44
1:A:576:TYR:CD1	1:A:591:LEU:HG	2.54	0.43
2:B:142:ALA:O	2:B:146:LYS:HG3	2.18	0.43
2:B:258:TYR:CE1	2:B:489:GLY:HA3	2.53	0.43
2:B:1439:PRO:HA	2:B:1442:LYS:NZ	2.31	0.43
3:C:43:ASN:HA	3:C:52:ASN:HA	1.99	0.43
1:D:591:LEU:HD11	1:D:601:HIS:CE1	2.53	0.43
2:E:72:GLU:O	2:E:76:GLN:NE2	2.49	0.43
2:E:228:PHE:HE2	2:E:399:LEU:HD12	1.83	0.43
2:E:258:TYR:HA	2:E:488:ALA:HB3	2.00	0.43
2:E:296:LEU:HB2	2:E:329:ILE:HD13	1.98	0.43
2:E:656:LYS:O	2:E:659:GLU:HG2	2.18	0.43
2:E:1382:ILE:HD11	2:E:1504:VAL:HB	1.99	0.43
2:E:1538:TRP:CE2	2:E:1539:ASP:HB2	2.53	0.43
2:E:1631:GLU:O	2:E:1635:LYS:HG3	2.18	0.43
2:B:111:LEU:O	2:B:115:ARG:HG2	2.18	0.43
2:B:720:ILE:HG12	2:B:766:PHE:CE1	2.53	0.43
2:B:876:GLU:HG2	2:B:877:VAL:HG13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:965:ASP:H	2:B:968:HIS:HB2	1.83	0.43
2:B:1133:GLN:OE1	2:B:1136:PHE:HD2	2.01	0.43
2:B:1440:SER:C	2:B:1441:TYR:HD1	2.27	0.43
2:B:1499:LEU:HG	2:B:1501:TRP:H	1.81	0.43
3:C:96:LYS:O	3:C:100:GLU:HG3	2.19	0.43
2:E:3:ARG:NH2	2:E:42:GLU:HG2	2.33	0.43
2:E:642:ASN:HA	2:E:644:ARG:NH2	2.33	0.43
2:E:874:CYS:SG	2:E:875:ARG:N	2.91	0.43
2:E:926:GLN:O	2:E:927:LEU:C	2.61	0.43
2:E:993:PHE:O	2:E:997:ILE:HG22	2.17	0.43
2:E:1557:PRO:HB2	2:E:1560:MET:O	2.17	0.43
1:A:670:ASN:OD1	1:A:675:LYS:HE3	2.18	0.43
2:B:744:ALA:HB3	2:B:804:ARG:NH1	2.34	0.43
2:B:875:ARG:NH1	2:B:921:THR:HB	2.33	0.43
2:B:957:MET:O	2:B:960:LEU:HB3	2.19	0.43
2:B:957:MET:O	2:B:961:LEU:HG	2.17	0.43
3:C:95:ALA:O	3:C:99:PRO:HG2	2.18	0.43
3:C:167:THR:O	3:C:170:ASP:N	2.51	0.43
1:D:576:TYR:CE1	1:D:591:LEU:HG	2.54	0.43
2:E:757:LEU:HD21	2:E:816:ALA:N	2.33	0.43
2:E:821:PRO:HA	2:E:824:ILE:HG23	2.01	0.43
2:E:1023:GLN:O	2:E:1027:VAL:HG13	2.17	0.43
2:E:1071:LYS:HE2	2:E:1071:LYS:HB2	1.89	0.43
2:E:1110:LEU:O	2:E:1114:LEU:HD23	2.19	0.43
2:E:1232:LYS:HB2	2:E:1240:TYR:CE2	2.53	0.43
2:E:1611:LEU:HD11	2:E:1616:LYS:HA	2.01	0.43
2:B:642:ASN:HA	2:B:644:ARG:NH2	2.34	0.43
2:B:642:ASN:O	2:B:646:ASN:N	2.50	0.43
2:B:1160:GLU:OE1	2:B:1243:TYR:OH	2.35	0.43
2:B:1382:ILE:HD11	2:B:1504:VAL:HB	1.99	0.43
2:B:1567:GLU:HA	2:B:1571:PHE:HB2	2.01	0.43
2:B:1593:ILE:O	2:B:1597:MET:HG2	2.18	0.43
2:B:1631:GLU:O	2:B:1635:LYS:HG3	2.18	0.43
2:E:111:LEU:O	2:E:115:ARG:HG2	2.18	0.43
2:E:333:ILE:O	2:E:405:LEU:HD22	2.18	0.43
2:E:805:PRO:O	2:E:808:GLU:HG2	2.18	0.43
3:F:164:GLY:O	3:F:168:VAL:N	2.33	0.43
1:A:543:GLU:HG2	1:A:544:ILE:N	2.34	0.43
1:A:585:VAL:HG12	1:A:607:LYS:HD2	1.99	0.43
2:B:41:TYR:CE2	2:B:44:TRP:HD1	2.37	0.43
2:B:821:PRO:HA	2:B:824:ILE:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:PHE:CG	2:B:832:ASP:N	2.87	0.43
2:B:870:ARG:NH1	2:B:874:CYS:HB3	2.34	0.43
2:B:1039:GLU:O	2:B:1040:LEU:HD23	2.18	0.43
2:B:1231:TYR:HE2	2:B:1243:TYR:HE1	1.66	0.43
2:B:1250:LEU:HA	2:B:1250:LEU:HD23	1.76	0.43
2:B:1545:HIS:N	2:B:1546:PRO:HD2	2.34	0.43
3:C:118:ASP:N	3:C:118:ASP:OD1	2.49	0.43
1:D:539:LYS:NZ	1:D:540:ILE:HD11	2.33	0.43
1:D:543:GLU:HG2	1:D:544:ILE:N	2.34	0.43
1:D:546:GLU:HB2	1:D:550:GLN:HE22	1.82	0.43
2:E:258:TYR:CE1	2:E:489:GLY:HA3	2.53	0.43
2:E:678:ASN:O	2:E:682:GLU:HG2	2.17	0.43
2:E:879:LEU:O	2:E:880:PRO:C	2.60	0.43
2:E:957:MET:O	2:E:961:LEU:HG	2.17	0.43
2:E:1233:GLU:HG3	2:E:1234:LYS:HD2	2.01	0.43
2:E:1342:LEU:C	2:E:1342:LEU:HD12	2.43	0.43
1:A:640:LEU:O	1:A:655:ILE:HA	2.16	0.43
2:B:3:ARG:NH2	2:B:42:GLU:HG2	2.33	0.43
2:B:1150:GLU:O	2:B:1154:LYS:HG2	2.19	0.43
2:B:1233:GLU:HG3	2:B:1234:LYS:HD2	2.01	0.43
2:B:1256:ASN:HB3	2:B:1259:GLU:OE1	2.18	0.43
2:B:1314:TRP:HB3	2:B:1348:PHE:HB3	2.01	0.43
2:B:1387:GLU:HG2	2:B:1388:TYR:N	2.34	0.43
2:B:1632:LYS:HD2	2:B:1636:HIS:HB2	2.01	0.43
3:C:77:VAL:HG11	3:C:175:ALA:HB3	2.00	0.43
2:E:243:MET:O	2:E:258:TYR:N	2.32	0.43
2:E:444:ASN:HB2	2:E:519:ILE:HG12	2.00	0.43
2:E:1301:TYR:HE2	2:E:1320:LEU:HD22	1.84	0.43
1:A:551:GLN:HG3	2:B:106:TYR:HD2	1.83	0.43
1:A:580:SER:HB2	1:A:585:VAL:CG2	2.49	0.43
2:B:258:TYR:HA	2:B:488:ALA:HB3	2.00	0.43
2:B:656:LYS:O	2:B:659:GLU:HG2	2.18	0.43
2:B:711:HIS:C	2:B:714:PRO:HD2	2.43	0.43
2:B:775:LEU:CD2	2:B:781:SER:HB2	2.49	0.43
2:B:1261:ALA:HB1	2:B:1304:ILE:HG23	2.00	0.43
3:C:167:THR:O	3:C:168:VAL:C	2.62	0.43
1:D:723:VAL:HB	2:E:3:ARG:H	1.84	0.43
2:E:140:GLU:N	2:E:140:GLU:OE1	2.52	0.43
2:E:140:GLU:O	2:E:144:LEU:HD23	2.18	0.43
2:E:1121:ARG:HD3	2:E:1168:TYR:HD2	1.84	0.43
3:F:77:VAL:HG11	3:F:175:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:160:LEU:HD12	3:F:160:LEU:HA	1.85	0.43
3:F:167:THR:O	3:F:170:ASP:N	2.51	0.43
2:B:220:HIS:NE2	2:B:436:ILE:HB	2.33	0.43
2:B:443:ARG:HG3	2:B:627:CYS:O	2.19	0.43
2:B:879:LEU:HG	2:B:931:ARG:NH1	2.34	0.43
2:B:1121:ARG:HD3	2:B:1168:TYR:HD2	1.84	0.43
2:B:1343:LYS:HE3	2:B:1343:LYS:HB2	1.76	0.43
2:B:1567:GLU:HA	2:B:1571:PHE:CD1	2.54	0.43
2:B:1630:LYS:HE3	2:B:1630:LYS:HB3	1.86	0.43
3:C:163:ARG:C	3:C:165:LEU:H	2.24	0.43
2:E:41:TYR:CE2	2:E:44:TRP:HD1	2.37	0.43
2:E:656:LYS:N	2:E:656:LYS:HD2	2.34	0.43
2:E:990:PHE:HB3	2:E:1045:ASN:OD1	2.19	0.43
2:E:1091:TRP:CD1	2:E:1127:ILE:HG23	2.54	0.43
2:E:1474:ASP:OD2	2:E:1477:ASN:HB2	2.19	0.43
2:E:1483:TRP:HA	2:E:1512:ILE:O	2.19	0.43
3:F:90:PHE:HA	3:F:93:VAL:HG12	2.01	0.43
1:A:693:GLU:O	1:A:696:LEU:HG	2.19	0.43
2:B:694:PHE:CZ	2:B:737:LEU:HB3	2.51	0.43
2:B:964:MET:HB2	2:B:969:TYR:CE2	2.54	0.43
2:B:1121:ARG:HG2	2:B:1125:ILE:CD1	2.49	0.43
2:B:1221:MET:HA	2:B:1224:THR:HG22	1.99	0.43
2:B:1522:MET:CE	2:B:1596:GLN:HB2	2.49	0.43
3:C:9:VAL:HG12	3:C:58:THR:OG1	2.19	0.43
1:D:693:GLU:O	1:D:696:LEU:HG	2.19	0.43
2:E:562:LEU:O	2:E:633:GLN:NE2	2.51	0.43
2:E:724:PHE:CZ	2:E:726:ALA:HB3	2.54	0.43
2:E:957:MET:O	2:E:960:LEU:HB3	2.19	0.43
2:E:1193:PHE:O	2:E:1196:LEU:HB3	2.19	0.43
2:E:1200:LEU:O	2:E:1204:LEU:HD23	2.19	0.43
2:E:1261:ALA:HB1	2:E:1304:ILE:HG23	2.01	0.43
2:E:1482:MET:HB3	2:E:1517:ASN:ND2	2.34	0.43
2:E:1545:HIS:N	2:E:1546:PRO:HD2	2.34	0.43
1:A:576:TYR:CE1	1:A:591:LEU:HG	2.54	0.43
2:B:80:VAL:H	2:B:85:LEU:HD11	1.84	0.43
2:B:444:ASN:HB2	2:B:519:ILE:HG12	2.00	0.43
2:B:561:THR:HB	2:B:631:LEU:HD22	2.01	0.43
2:B:805:PRO:O	2:B:808:GLU:HG2	2.18	0.43
2:B:874:CYS:SG	2:B:875:ARG:N	2.91	0.43
3:C:90:PHE:HA	3:C:93:VAL:HG12	2.01	0.43
1:D:609:PRO:HB2	1:D:612:ASP:OD1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:472:VAL:O	2:E:479:LEU:HD12	2.19	0.43
2:E:768:ILE:HG23	2:E:830:VAL:HG11	2.01	0.43
2:E:860:MET:HG3	2:E:882:LEU:HD22	2.01	0.43
2:E:909:ILE:HG13	2:E:910:LEU:N	2.33	0.43
2:E:1499:LEU:HD21	2:E:1501:TRP:NE1	2.34	0.43
2:E:1593:ILE:O	2:E:1597:MET:HG2	2.18	0.43
2:B:155:GLY:O	2:B:159:LEU:HG	2.18	0.42
2:B:203:SER:HB3	2:B:210:LEU:HD12	2.01	0.42
2:B:472:VAL:O	2:B:479:LEU:HD12	2.19	0.42
2:B:1136:PHE:HB2	2:B:1186:LEU:HD23	2.01	0.42
2:B:1432:LYS:HB3	2:B:1432:LYS:HE3	1.90	0.42
2:B:1483:TRP:HA	2:B:1512:ILE:O	2.19	0.42
2:E:144:LEU:O	2:E:148:VAL:HG12	2.19	0.42
2:E:203:SER:HB3	2:E:210:LEU:HD12	2.01	0.42
2:E:720:ILE:HG12	2:E:766:PHE:CE1	2.53	0.42
2:E:879:LEU:HG	2:E:931:ARG:NH1	2.34	0.42
2:E:1136:PHE:HB2	2:E:1186:LEU:HD23	2.01	0.42
1:A:551:GLN:HG3	2:B:106:TYR:CD2	2.54	0.42
2:B:1099:ILE:C	2:B:1101:PHE:H	2.27	0.42
2:B:1474:ASP:OD2	2:B:1477:ASN:HB2	2.19	0.42
2:B:1589:LEU:HA	2:B:1592:LEU:HD12	2.00	0.42
2:B:1611:LEU:HD11	2:B:1616:LYS:HA	2.01	0.42
2:E:142:ALA:O	2:E:146:LYS:HG3	2.18	0.42
2:E:306:MET:HE1	2:E:534:ARG:O	2.19	0.42
2:E:676:LEU:HD22	2:E:693:VAL:HG22	2.00	0.42
2:E:711:HIS:C	2:E:714:PRO:HD2	2.44	0.42
2:E:800:MET:O	2:E:804:ARG:HG3	2.19	0.42
2:E:831:PHE:CG	2:E:832:ASP:N	2.87	0.42
2:E:1121:ARG:HG2	2:E:1125:ILE:CD1	2.49	0.42
2:E:1532:CYS:HA	2:E:1535:GLN:HG3	2.01	0.42
2:E:1567:GLU:HA	2:E:1571:PHE:HB2	2.01	0.42
3:F:96:LYS:O	3:F:100:GLU:HG3	2.19	0.42
2:B:561:THR:HG22	2:B:632:THR:O	2.20	0.42
2:B:768:ILE:HG23	2:B:830:VAL:HG11	2.01	0.42
2:B:800:MET:O	2:B:804:ARG:HG3	2.19	0.42
2:B:879:LEU:HD23	2:B:924:HIS:HE1	1.84	0.42
1:D:576:TYR:CD1	1:D:591:LEU:HG	2.54	0.42
1:D:647:ASP:CG	3:F:163:ARG:HH22	2.27	0.42
2:E:685:ASP:OD1	2:E:685:ASP:N	2.52	0.42
2:E:744:ALA:HB3	2:E:804:ARG:NH1	2.34	0.42
2:E:775:LEU:CD2	2:E:781:SER:HB2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:875:ARG:NH1	2:E:921:THR:HB	2.33	0.42
2:E:964:MET:HB2	2:E:969:TYR:CE2	2.54	0.42
2:E:1306:SER:O	2:E:1310:LYS:HG2	2.20	0.42
2:E:1372:PHE:CZ	2:E:1424:GLN:HB3	2.54	0.42
2:E:1544:VAL:HG12	2:E:1610:LYS:HB3	2.01	0.42
2:E:1589:LEU:HA	2:E:1592:LEU:HD12	2.00	0.42
2:B:98:TRP:HZ3	2:B:159:LEU:HD12	1.85	0.42
2:B:144:LEU:O	2:B:148:VAL:HG12	2.19	0.42
2:B:256:GLU:HG2	2:B:429:ARG:H	1.85	0.42
2:B:771:ARG:NH2	2:B:784:GLY:HA2	2.35	0.42
2:B:990:PHE:HB3	2:B:1045:ASN:OD1	2.19	0.42
2:B:1193:PHE:O	2:B:1196:LEU:HB3	2.19	0.42
2:B:1306:SER:HB3	2:B:1310:LYS:NZ	2.34	0.42
2:B:1345:ARG:HG2	2:B:1349:TYR:HE2	1.82	0.42
2:B:1362:TYR:HD2	2:B:1462:PHE:CE2	2.34	0.42
1:D:579:LEU:HA	1:D:586:LEU:HD13	2.01	0.42
1:D:685:ASP:HA	1:D:688:THR:HG22	2.01	0.42
2:E:36:HIS:O	2:E:48:TYR:N	2.52	0.42
2:E:962:GLN:O	2:E:1019:ARG:NH1	2.51	0.42
2:E:1039:GLU:O	2:E:1040:LEU:HD23	2.18	0.42
2:E:1250:LEU:HD23	2:E:1250:LEU:HA	1.75	0.42
2:E:1483:TRP:NE1	2:E:1514:PRO:HD3	2.34	0.42
2:E:1522:MET:CE	2:E:1596:GLN:HB2	2.49	0.42
2:B:556:ASN:HD22	2:B:560:THR:HG1	1.59	0.42
2:B:656:LYS:N	2:B:656:LYS:HD2	2.34	0.42
2:B:745:ASP:N	2:B:804:ARG:HH12	2.17	0.42
2:B:746:ASP:CG	2:B:748:SER:HG	2.25	0.42
2:B:860:MET:HG3	2:B:882:LEU:HD22	2.01	0.42
2:B:926:GLN:O	2:B:927:LEU:C	2.61	0.42
2:B:1091:TRP:CD1	2:B:1127:ILE:HG23	2.54	0.42
2:B:1200:LEU:O	2:B:1204:LEU:HD23	2.19	0.42
2:B:1275:ASP:OD2	2:B:1275:ASP:N	2.43	0.42
2:B:1499:LEU:HD21	2:B:1501:TRP:NE1	2.34	0.42
3:C:98:TYR:CE1	3:C:149:ILE:HB	2.54	0.42
1:D:591:LEU:HD13	1:D:591:LEU:HA	1.90	0.42
2:E:3:ARG:NH2	2:E:42:GLU:H	2.13	0.42
2:E:1440:SER:C	2:E:1441:TYR:HD1	2.27	0.42
3:F:9:VAL:HG12	3:F:58:THR:OG1	2.19	0.42
1:A:669:LEU:O	1:A:673:LEU:HG	2.19	0.42
2:B:165:VAL:O	2:B:171:ASN:ND2	2.33	0.42
2:B:306:MET:HE1	2:B:534:ARG:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:VAL:HG13	2:B:534:ARG:NH2	2.30	0.42
2:B:1279:VAL:O	2:B:1282:LEU:HG	2.20	0.42
2:B:1306:SER:O	2:B:1310:LYS:HG2	2.20	0.42
2:B:1463:ARG:HA	2:B:1487:THR:O	2.20	0.42
1:D:663:CYS:HB3	1:D:679:SER:HA	2.01	0.42
2:E:98:TRP:HZ3	2:E:159:LEU:HD12	1.84	0.42
2:E:760:LEU:CD2	2:E:819:TYR:HB3	2.50	0.42
2:E:799:ASN:HA	2:E:802:MET:HG3	2.02	0.42
2:E:1099:ILE:C	2:E:1101:PHE:H	2.27	0.42
2:E:1314:TRP:HB3	2:E:1348:PHE:HB3	2.01	0.42
3:F:98:TYR:CE1	3:F:149:ILE:HB	2.54	0.42
2:B:43:GLY:O	2:B:61:GLU:N	2.38	0.42
2:B:140:GLU:N	2:B:140:GLU:OE1	2.52	0.42
2:B:328:ASP:OD1	2:B:328:ASP:N	2.51	0.42
2:B:724:PHE:CZ	2:B:726:ALA:HB3	2.54	0.42
2:B:760:LEU:CD2	2:B:819:TYR:HB3	2.50	0.42
2:B:1072:ILE:HG13	2:B:1073:VAL:N	2.34	0.42
2:B:1205:LEU:HA	2:B:1208:ARG:HD3	2.01	0.42
2:B:1372:PHE:CZ	2:B:1424:GLN:HB3	2.54	0.42
1:D:669:LEU:O	1:D:673:LEU:HG	2.19	0.42
2:E:1105:MET:SD	2:E:1108:PRO:HG2	2.59	0.42
2:E:1157:GLN:HA	2:E:1160:GLU:HG2	2.02	0.42
2:E:1234:LYS:HD2	2:E:1234:LYS:N	2.35	0.42
2:E:1546:PRO:O	2:E:1549:MET:HB2	2.20	0.42
2:E:1567:GLU:HA	2:E:1571:PHE:CD1	2.54	0.42
1:A:568:ARG:HB2	1:A:569:ARG:HH11	1.85	0.42
2:B:36:HIS:O	2:B:48:TYR:N	2.52	0.42
2:B:1154:LYS:HA	2:B:1157:GLN:CD	2.45	0.42
2:B:1544:VAL:HG12	2:B:1610:LYS:HB3	2.02	0.42
1:D:568:ARG:HB2	1:D:569:ARG:HH11	1.85	0.42
1:D:580:SER:HB2	1:D:585:VAL:CG2	2.49	0.42
2:E:107:VAL:HG23	2:E:108:ASN:OD1	2.20	0.42
2:E:741:VAL:HG23	2:E:801:LEU:CD1	2.50	0.42
2:E:795:PHE:HD2	2:E:839:LEU:HD13	1.85	0.42
2:E:933:LEU:HD23	2:E:937:ASN:OD1	2.20	0.42
2:E:1154:LYS:HA	2:E:1157:GLN:CD	2.45	0.42
2:E:1256:ASN:HB3	2:E:1259:GLU:OE1	2.19	0.42
2:E:1463:ARG:HA	2:E:1487:THR:O	2.20	0.42
2:E:1632:LYS:HD2	2:E:1636:HIS:HB2	2.01	0.42
2:B:222:TYR:CG	2:B:289:LEU:HD11	2.55	0.42
2:B:1039:GLU:C	2:B:1040:LEU:HD23	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:LEU:O	2:B:1114:LEU:HD23	2.18	0.42
2:B:1349:TYR:HA	2:B:1352:ILE:HG22	2.02	0.42
3:C:129:LEU:O	3:C:133:LYS:N	2.53	0.42
2:E:33:ASP:O	2:E:35:VAL:HG13	2.20	0.42
2:E:561:THR:HB	2:E:631:LEU:HD22	2.01	0.42
2:E:772:VAL:O	2:E:776:ARG:HG2	2.20	0.42
2:E:921:THR:OG1	2:E:924:HIS:HB3	2.20	0.42
2:E:929:MET:HE1	2:E:968:HIS:C	2.45	0.42
1:A:579:LEU:HA	1:A:586:LEU:HD13	2.01	0.42
1:A:609:PRO:HB2	1:A:612:ASP:OD1	2.19	0.42
2:B:523:THR:O	2:B:555:MET:HE2	2.20	0.42
2:B:743:ASN:HB3	2:B:749:LYS:HD2	2.02	0.42
2:B:933:LEU:HD23	2:B:937:ASN:OD1	2.20	0.42
2:B:990:PHE:HE1	2:B:1046:TYR:HB2	1.85	0.42
2:B:1234:LYS:HD2	2:B:1234:LYS:N	2.35	0.42
2:B:1483:TRP:NE1	2:B:1514:PRO:HD3	2.34	0.42
2:E:256:GLU:HG2	2:E:429:ARG:H	1.85	0.42
2:E:990:PHE:HE1	2:E:1046:TYR:HB2	1.85	0.42
2:E:1117:GLU:OE2	2:E:1120:LEU:HG	2.19	0.42
2:E:1205:LEU:HA	2:E:1208:ARG:HD3	2.01	0.42
2:E:1306:SER:HB3	2:E:1310:LYS:NZ	2.35	0.42
2:E:1318:ILE:O	2:E:1322:LYS:HG2	2.20	0.42
2:E:1373:PRO:HD2	2:E:1376:LEU:HB2	2.01	0.42
2:E:1491:THR:HG23	2:E:1493:TYR:O	2.20	0.42
2:E:1535:GLN:OE1	2:E:1542:LEU:HD11	2.20	0.42
1:A:546:GLU:O	1:A:549:LYS:HG2	2.21	0.41
2:B:430:LYS:HE2	2:B:432:GLY:HA3	2.02	0.41
2:B:795:PHE:HD2	2:B:839:LEU:HD13	1.85	0.41
2:B:921:THR:OG1	2:B:924:HIS:HB3	2.20	0.41
2:B:1373:PRO:HD2	2:B:1376:LEU:HB2	2.02	0.41
2:B:1446:VAL:HG12	2:E:1333:PHE:CZ	2.54	0.41
2:E:98:TRP:CZ3	2:E:159:LEU:HD12	2.55	0.41
2:E:172:ILE:HA	2:E:175:PRO:HG2	2.02	0.41
2:E:222:TYR:CG	2:E:289:LEU:HD11	2.55	0.41
2:E:789:ASN:O	2:E:790:SER:C	2.62	0.41
2:E:1054:LEU:HD12	2:E:1054:LEU:HA	1.79	0.41
2:E:1102:ILE:HD11	2:E:1134:CYS:HB2	2.02	0.41
2:E:1150:GLU:O	2:E:1154:LYS:HG2	2.19	0.41
2:E:1231:TYR:HE2	2:E:1243:TYR:HE1	1.66	0.41
1:A:663:CYS:HB3	1:A:679:SER:HA	2.01	0.41
1:A:685:ASP:HA	1:A:688:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:SER:HA	2:B:430:LYS:HA	2.03	0.41
2:B:825:ASN:O	2:B:829:LEU:HD23	2.20	0.41
2:B:1105:MET:SD	2:B:1108:PRO:HG2	2.59	0.41
2:B:1117:GLU:OE2	2:B:1120:LEU:HG	2.19	0.41
2:B:1529:ILE:HG12	2:B:1550:LEU:HD21	2.02	0.41
3:C:129:LEU:HB3	3:C:134:LEU:O	2.20	0.41
2:E:1387:GLU:HG2	2:E:1388:TYR:N	2.34	0.41
2:E:1525:THR:HA	2:E:1528:ARG:NH1	2.35	0.41
3:F:153:LYS:HA	3:F:153:LYS:HD2	1.90	0.41
2:B:1301:TYR:HE2	2:B:1320:LEU:HD22	1.84	0.41
2:B:1576:LEU:HD22	2:B:1583:GLN:HB3	2.02	0.41
3:C:123:LYS:HA	3:C:126:ILE:HG12	2.03	0.41
2:E:443:ARG:HG3	2:E:627:CYS:O	2.19	0.41
2:E:1033:MET:C	2:E:1035:GLN:N	2.78	0.41
2:E:1072:ILE:HG13	2:E:1073:VAL:N	2.34	0.41
2:E:1216:SER:OG	2:E:1219:ASN:OD1	2.31	0.41
2:E:1362:TYR:CD2	2:E:1462:PHE:HE2	2.37	0.41
2:E:1466:ARG:HB3	2:E:1485:GLU:H	1.86	0.41
2:B:99:ALA:O	2:B:102:TRP:HB3	2.20	0.41
2:B:467:GLU:N	2:B:534:ARG:HH12	2.18	0.41
2:B:875:ARG:HG2	2:B:924:HIS:CE1	2.56	0.41
2:B:1033:MET:C	2:B:1035:GLN:N	2.78	0.41
2:B:1292:THR:O	2:B:1295:GLU:N	2.54	0.41
2:B:1532:CYS:HA	2:B:1535:GLN:HG3	2.01	0.41
2:B:1626:PHE:CD2	2:B:1627:ARG:HD3	2.55	0.41
2:E:305:HIS:CG	2:E:314:HIS:HB2	2.56	0.41
2:E:523:THR:O	2:E:555:MET:HE2	2.20	0.41
2:E:1066:GLN:OE1	2:E:1069:ARG:NH1	2.45	0.41
2:E:1556:ASP:HB2	2:E:1558:ALA:HB2	2.02	0.41
3:F:123:LYS:HA	3:F:126:ILE:HG12	2.03	0.41
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.94	0.41
2:B:10:GLN:NE2	2:B:37:ILE:O	2.46	0.41
2:B:1322:LYS:HD3	2:B:1345:ARG:NH1	2.36	0.41
2:B:1443:ASP:OD1	2:B:1444:LYS:HD2	2.21	0.41
1:D:676:ASP:O	1:D:677:MET:HE2	2.20	0.41
2:E:196:GLU:O	2:E:199:GLN:HG3	2.20	0.41
2:E:430:LYS:HE2	2:E:432:GLY:HA3	2.02	0.41
2:E:771:ARG:NH2	2:E:784:GLY:HA2	2.35	0.41
2:E:948:PRO:C	2:E:950:ILE:H	2.28	0.41
3:F:49:LYS:NZ	3:F:50:PRO:O	2.42	0.41
2:B:1157:GLN:HA	2:B:1160:GLU:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1216:SER:OG	2:B:1219:ASN:OD1	2.31	0.41
2:B:1525:THR:HA	2:B:1528:ARG:NH1	2.35	0.41
1:D:667:ASP:OD2	1:D:677:MET:HB3	2.20	0.41
2:E:561:THR:HG22	2:E:632:THR:O	2.20	0.41
2:E:745:ASP:N	2:E:804:ARG:HH12	2.17	0.41
2:E:820:LEU:O	2:E:823:ILE:HG12	2.21	0.41
2:E:1065:SER:OG	2:E:1068:LYS:HB2	2.21	0.41
2:E:1392:GLU:HA	2:E:1395:SER:HB3	2.02	0.41
2:E:1549:MET:HE1	3:F:56:TRP:CD2	2.56	0.41
2:E:1626:PHE:CD2	2:E:1627:ARG:HD3	2.56	0.41
2:B:196:GLU:O	2:B:199:GLN:HG3	2.20	0.41
2:B:262:TRP:CZ2	2:B:266:GLY:HA2	2.56	0.41
2:B:745:ASP:N	2:B:745:ASP:OD1	2.53	0.41
2:B:799:ASN:HA	2:B:802:MET:HG3	2.02	0.41
2:B:1236:ARG:HD3	2:B:1236:ARG:HA	1.87	0.41
2:B:1478:GLU:O	2:B:1482:MET:HG2	2.21	0.41
2:E:129:SER:O	2:E:132:LEU:HB2	2.21	0.41
2:E:340:GLU:CD	2:E:420:LEU:HD21	2.46	0.41
2:E:419:HIS:CD2	2:E:420:LEU:HG	2.56	0.41
2:E:467:GLU:N	2:E:534:ARG:HH12	2.18	0.41
2:E:825:ASN:O	2:E:829:LEU:HD23	2.20	0.41
2:E:875:ARG:HG2	2:E:924:HIS:CE1	2.56	0.41
2:E:1322:LYS:HD3	2:E:1345:ARG:NH1	2.36	0.41
3:F:129:LEU:HB3	3:F:134:LEU:O	2.20	0.41
1:A:564:LYS:HG3	1:A:575:TRP:CD1	2.56	0.41
2:B:4:TRP:CE3	2:B:46:ARG:HG2	2.56	0.41
2:B:305:HIS:CG	2:B:314:HIS:HB2	2.56	0.41
2:B:685:ASP:OD1	2:B:685:ASP:N	2.52	0.41
2:B:741:VAL:HG23	2:B:801:LEU:CD1	2.50	0.41
2:B:789:ASN:O	2:B:790:SER:C	2.63	0.41
2:B:839:LEU:O	2:B:842:LYS:HG2	2.20	0.41
2:B:860:MET:HE2	2:B:885:GLN:HE22	1.86	0.41
2:B:948:PRO:C	2:B:950:ILE:H	2.28	0.41
2:E:262:TRP:CZ2	2:E:266:GLY:HA2	2.56	0.41
2:E:676:LEU:HB3	2:E:693:VAL:HG13	2.03	0.41
2:E:745:ASP:N	2:E:745:ASP:OD1	2.53	0.41
2:E:1039:GLU:C	2:E:1040:LEU:HD23	2.45	0.41
2:E:1154:LYS:HA	2:E:1157:GLN:NE2	2.36	0.41
2:E:1349:TYR:HA	2:E:1352:ILE:HG22	2.02	0.41
2:E:1520:GLU:HA	2:E:1523:GLU:HG3	2.03	0.41
3:F:167:THR:O	3:F:168:VAL:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:TYR:HB2	2:B:4:TRP:O	2.21	0.41
2:B:3:ARG:HH22	2:B:42:GLU:HG2	1.86	0.41
2:B:3:ARG:NH2	2:B:42:GLU:H	2.13	0.41
2:B:107:VAL:HG23	2:B:108:ASN:OD1	2.20	0.41
2:B:157:ARG:HG3	2:B:194:ILE:HG23	2.03	0.41
2:B:187:HIS:CD2	2:B:1009:MET:HG2	2.56	0.41
2:B:486:PRO:HB3	2:B:496:TYR:HE1	1.86	0.41
2:B:772:VAL:O	2:B:776:ARG:HG2	2.20	0.41
2:B:929:MET:HE1	2:B:968:HIS:C	2.45	0.41
2:B:986:LEU:HD11	2:B:1024:PHE:HB3	2.03	0.41
2:B:1102:ILE:HD11	2:B:1134:CYS:HB2	2.02	0.41
2:B:1154:LYS:HA	2:B:1157:GLN:NE2	2.36	0.41
2:B:1220:ARG:HE	2:B:1250:LEU:HD21	1.86	0.41
2:B:1272:GLN:O	2:B:1293:GLN:HG3	2.21	0.41
2:B:1312:LYS:HE2	2:B:1312:LYS:HB2	1.89	0.41
2:B:1318:ILE:O	2:B:1322:LYS:HG2	2.20	0.41
2:B:1452:ASN:OD1	2:B:1452:ASN:C	2.64	0.41
2:B:1474:ASP:CG	2:B:1477:ASN:HB2	2.46	0.41
2:B:1556:ASP:HB2	2:B:1558:ALA:HB2	2.02	0.41
2:B:1633:VAL:O	2:B:1639:VAL:N	2.53	0.41
3:C:87:PRO:HG2	3:C:134:LEU:HB3	2.03	0.41
1:D:556:LEU:HD23	1:D:665:TRP:HD1	1.85	0.41
1:D:616:VAL:HG23	1:D:643:SER:C	2.46	0.41
1:D:717:PRO:HD2	2:E:1:MET:SD	2.61	0.41
2:E:99:ALA:O	2:E:102:TRP:HB3	2.20	0.41
2:E:116:GLN:O	2:E:119:GLN:HG3	2.21	0.41
2:E:157:ARG:HG3	2:E:194:ILE:HG23	2.03	0.41
2:E:163:LEU:HD13	2:E:194:ILE:HD11	2.03	0.41
2:E:486:PRO:HB3	2:E:496:TYR:HE1	1.86	0.41
2:E:719:TYR:HD1	2:E:723:HIS:HB2	1.86	0.41
2:E:839:LEU:O	2:E:842:LYS:HG2	2.20	0.41
2:E:1022:ASN:O	2:E:1026:GLU:OE1	2.39	0.41
2:E:1292:THR:O	2:E:1295:GLU:N	2.54	0.41
2:E:1295:GLU:O	2:E:1298:GLU:HG3	2.21	0.41
2:E:1576:LEU:HD22	2:E:1583:GLN:HB3	2.02	0.41
3:F:129:LEU:O	3:F:133:LYS:N	2.53	0.41
2:B:197:LYS:HA	2:B:200:GLU:CG	2.46	0.41
2:B:254:ILE:O	2:B:431:MET:N	2.40	0.41
2:B:651:LYS:HD2	2:B:652:HIS:N	2.36	0.41
2:B:701:ILE:HB	2:B:759:ALA:HB1	2.03	0.41
2:B:1063:THR:HA	2:B:1069:ARG:HH11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:SER:OG	2:B:1068:LYS:HB2	2.21	0.41
2:B:1086:ARG:HA	2:B:1089:ASP:OD2	2.21	0.41
1:D:531:ARG:HH21	1:D:534:LEU:HD12	1.86	0.41
2:E:4:TRP:CE3	2:E:46:ARG:HG2	2.56	0.41
2:E:80:VAL:H	2:E:85:LEU:HD11	1.84	0.41
2:E:166:ARG:HD3	2:E:173:LEU:HB2	2.03	0.41
2:E:456:ASP:H	2:E:618:ASP:CG	2.29	0.41
2:E:821:PRO:O	2:E:824:ILE:HG12	2.21	0.41
2:E:1063:THR:HA	2:E:1069:ARG:HH11	1.86	0.41
2:E:1066:GLN:CD	2:E:1069:ARG:HH12	2.29	0.41
2:E:1279:VAL:O	2:E:1282:LEU:HG	2.20	0.41
3:F:87:PRO:HG2	3:F:134:LEU:HB3	2.03	0.41
3:F:100:GLU:O	3:F:104:HIS:ND1	2.48	0.41
1:A:727:ASN:N	2:B:46:ARG:HH22	2.18	0.40
2:B:129:SER:O	2:B:132:LEU:HB2	2.21	0.40
2:B:340:GLU:CD	2:B:420:LEU:HD21	2.46	0.40
2:B:1535:GLN:OE1	2:B:1542:LEU:HD11	2.20	0.40
3:C:160:LEU:HD12	3:C:160:LEU:HA	1.85	0.40
2:E:166:ARG:NE	2:E:169:ASN:OD1	2.55	0.40
2:E:642:ASN:O	2:E:646:ASN:N	2.50	0.40
2:E:651:LYS:HD2	2:E:652:HIS:N	2.36	0.40
2:E:717:GLU:HA	2:E:720:ILE:HD12	2.03	0.40
2:E:743:ASN:HB3	2:E:749:LYS:HD2	2.02	0.40
2:E:856:LYS:NZ	2:E:885:GLN:OE1	2.54	0.40
2:E:890:LEU:HD22	2:E:935:ARG:HG3	2.03	0.40
2:E:1086:ARG:HA	2:E:1089:ASP:OD2	2.21	0.40
2:E:1544:VAL:CG1	2:E:1610:LYS:HB3	2.51	0.40
2:E:1573:GLU:OE1	2:E:1576:LEU:HD12	2.21	0.40
1:A:667:ASP:OD2	1:A:677:MET:HB3	2.20	0.40
2:B:634:ASN:OD1	2:B:637:LEU:N	2.49	0.40
2:B:821:PRO:O	2:B:824:ILE:HG12	2.21	0.40
2:B:912:VAL:O	2:B:915:ARG:HB2	2.21	0.40
2:B:962:GLN:O	2:B:1019:ARG:NH1	2.51	0.40
2:B:1205:LEU:HD13	2:B:1208:ARG:HD3	2.04	0.40
2:B:1376:LEU:HD23	2:B:1376:LEU:HA	1.87	0.40
2:B:1612:THR:HG23	2:B:1615:LEU:H	1.86	0.40
3:C:78:PHE:HD1	3:C:110:ILE:HD13	1.86	0.40
2:E:879:LEU:HD23	2:E:924:HIS:HE1	1.84	0.40
2:E:1512:ILE:HG23	2:E:1516:GLU:HB3	2.03	0.40
1:A:671:ALA:C	1:A:674:GLY:H	2.30	0.40
2:B:98:TRP:CZ3	2:B:159:LEU:HD12	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:GLU:HA	2:B:720:ILE:HD12	2.03	0.40
2:B:892:ASP:OD1	2:B:895:ASN:ND2	2.55	0.40
2:B:1295:GLU:O	2:B:1298:GLU:HG3	2.21	0.40
2:B:1470:LYS:HD3	2:B:1483:TRP:CE2	2.56	0.40
2:B:1572:THR:HB	2:B:1574:LYS:HE2	2.03	0.40
2:B:1573:GLU:OE1	2:B:1576:LEU:HD12	2.21	0.40
3:C:96:LYS:C	3:C:99:PRO:HD2	2.47	0.40
1:D:564:LYS:HE3	1:D:590:ASP:OD1	2.22	0.40
2:E:45:TYR:CZ	2:E:66:LEU:HD11	2.56	0.40
2:E:187:HIS:CD2	2:E:1009:MET:HG2	2.56	0.40
2:E:912:VAL:O	2:E:915:ARG:HB2	2.21	0.40
2:E:1272:GLN:O	2:E:1293:GLN:HG3	2.21	0.40
2:E:1316:LYS:O	2:E:1320:LEU:HG	2.22	0.40
3:F:72:TYR:HD2	3:F:104:HIS:HB3	1.85	0.40
1:A:616:VAL:HG23	1:A:643:SER:C	2.46	0.40
1:A:676:ASP:O	1:A:677:MET:HE2	2.20	0.40
2:B:33:ASP:O	2:B:35:VAL:HG13	2.20	0.40
2:B:181:ILE:HG21	2:B:907:SER:HB2	2.03	0.40
2:B:866:SER:C	2:B:868:LEU:N	2.79	0.40
2:B:1546:PRO:O	2:B:1549:MET:HB2	2.20	0.40
1:D:599:VAL:HA	1:D:600:PRO:HD3	1.92	0.40
2:E:104:LYS:O	2:E:108:ASN:ND2	2.55	0.40
2:E:455:PHE:CE2	2:E:466:VAL:HG11	2.57	0.40
2:E:986:LEU:HD11	2:E:1024:PHE:HB3	2.03	0.40
2:E:1058:SER:HA	2:E:1080:ARG:NH1	2.37	0.40
2:E:1443:ASP:OD1	2:E:1444:LYS:HD2	2.21	0.40
2:E:1478:GLU:O	2:E:1482:MET:HG2	2.21	0.40
2:E:1612:THR:HG23	2:E:1615:LEU:H	1.86	0.40
2:B:116:GLN:O	2:B:119:GLN:HG3	2.21	0.40
2:B:419:HIS:CD2	2:B:420:LEU:HG	2.56	0.40
2:B:719:TYR:HD1	2:B:723:HIS:HB2	1.86	0.40
2:B:929:MET:O	2:B:935:ARG:NH2	2.55	0.40
2:B:968:HIS:O	2:B:969:TYR:C	2.64	0.40
2:B:994:LYS:HZ2	2:B:1048:HIS:HB3	1.85	0.40
2:B:1081:LYS:NZ	2:B:1119:GLU:HG3	2.37	0.40
2:B:1113:THR:O	2:B:1121:ARG:HG3	2.22	0.40
2:B:1125:ILE:HD12	2:B:1125:ILE:H	1.86	0.40
2:B:1316:LYS:O	2:B:1320:LEU:HG	2.22	0.40
2:B:1482:MET:HB3	2:B:1517:ASN:ND2	2.34	0.40
2:B:1491:THR:HG23	2:B:1493:TYR:O	2.20	0.40
2:B:1544:VAL:CG1	2:B:1610:LYS:HB3	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:TYR:HD2	3:C:104:HIS:HB3	1.85	0.40
2:E:3:ARG:HH22	2:E:42:GLU:HG2	1.86	0.40
2:E:198:ILE:HA	2:E:201:GLU:OE1	2.22	0.40
2:E:728:LEU:HA	2:E:730:TYR:CE2	2.57	0.40
2:E:870:ARG:NH1	2:E:874:CYS:HB3	2.34	0.40
2:E:1572:THR:HB	2:E:1574:LYS:HE2	2.03	0.40
2:E:1617:PRO:HA	2:E:1620:GLU:HG3	2.04	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	196/733 (27%)	180 (92%)	16 (8%)	0	100	100
1	D	196/733 (27%)	180 (92%)	16 (8%)	0	100	100
2	B	1640/1648 (100%)	1539 (94%)	101 (6%)	0	100	100
2	E	1640/1648 (100%)	1540 (94%)	100 (6%)	0	100	100
3	C	175/184 (95%)	163 (93%)	12 (7%)	0	100	100
3	F	175/184 (95%)	163 (93%)	12 (7%)	0	100	100
All	All	4022/5130 (78%)	3765 (94%)	257 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/664 (28%)	183 (100%)	0	100	100
1	D	183/664 (28%)	183 (100%)	0	100	100
2	B	1495/1497 (100%)	1495 (100%)	0	100	100
2	E	1495/1497 (100%)	1495 (100%)	0	100	100
3	C	153/157 (98%)	153 (100%)	0	100	100
3	F	153/157 (98%)	153 (100%)	0	100	100
All	All	3662/4636 (79%)	3662 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	554	ASN
2	B	20	ASN
2	B	108	ASN
2	B	130	GLN
2	B	350	GLN
2	B	414	GLN
2	B	506	GLN
2	B	526	HIS
2	B	710	GLN
2	B	723	HIS
2	B	738	ASN
2	B	788	ASN
2	B	924	HIS
2	B	962	GLN
2	B	971	HIS
2	B	1060	GLN
2	B	1133	GLN
2	B	1203	ASN
2	B	1294	GLN
2	B	1460	GLN
2	B	1517	ASN
2	B	1526	ASN
2	B	1596	GLN
3	C	2	GLN
1	D	554	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	582	ASN
1	D	649	ASN
2	E	20	ASN
2	E	108	ASN
2	E	130	GLN
2	E	299	GLN
2	E	350	GLN
2	E	414	GLN
2	E	506	GLN
2	E	526	HIS
2	E	710	GLN
2	E	723	HIS
2	E	738	ASN
2	E	788	ASN
2	E	899	HIS
2	E	924	HIS
2	E	962	GLN
2	E	971	HIS
2	E	1060	GLN
2	E	1093	ASN
2	E	1133	GLN
2	E	1203	ASN
2	E	1424	GLN
2	E	1460	GLN
2	E	1506	GLN
2	E	1517	ASN
2	E	1526	ASN
2	E	1596	GLN
3	F	2	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.

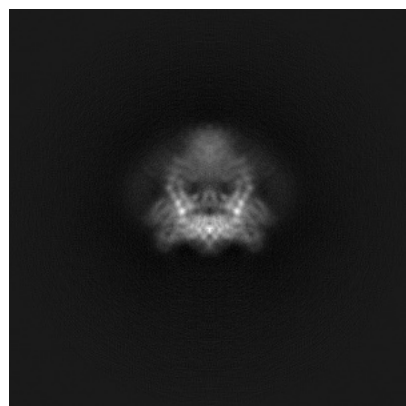
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60146. These allow visual inspection of the internal detail of the map and identification of artifacts.

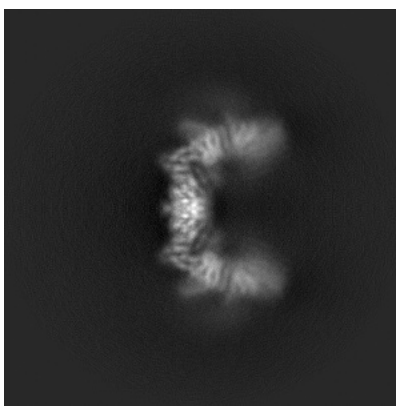
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

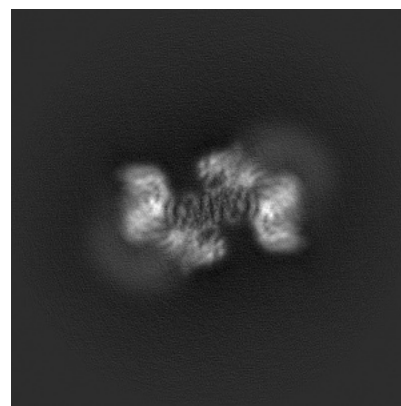
6.1.1 Primary map



X

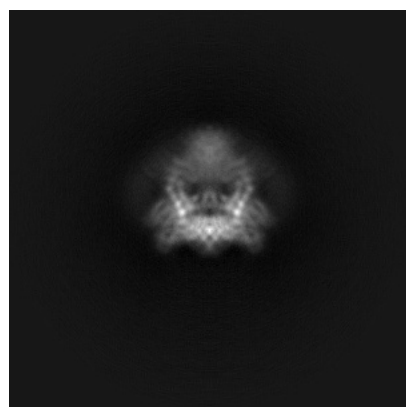


Y

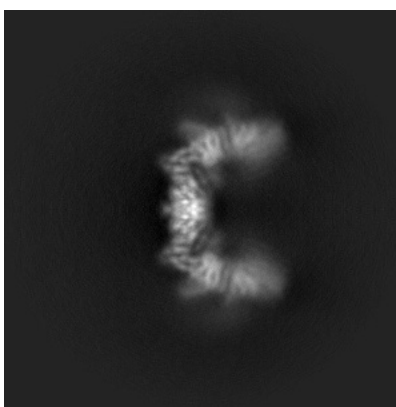


Z

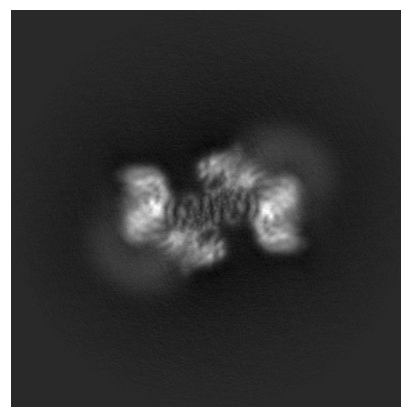
6.1.2 Raw map



X



Y

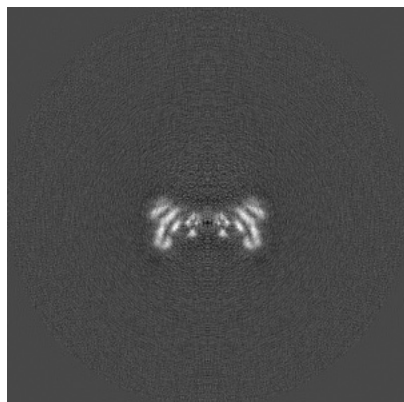


Z

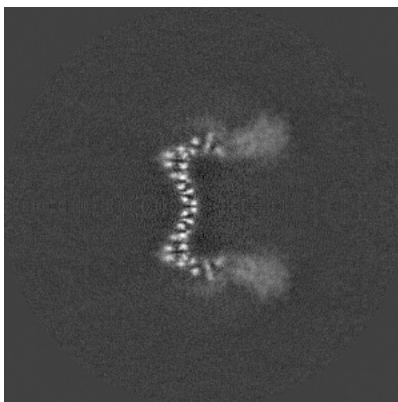
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

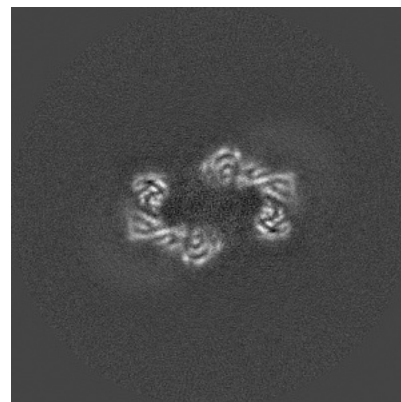
6.2.1 Primary map



X Index: 170

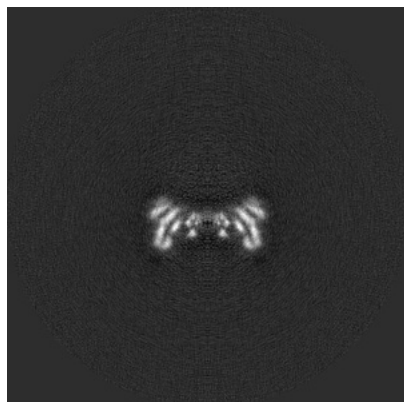


Y Index: 170

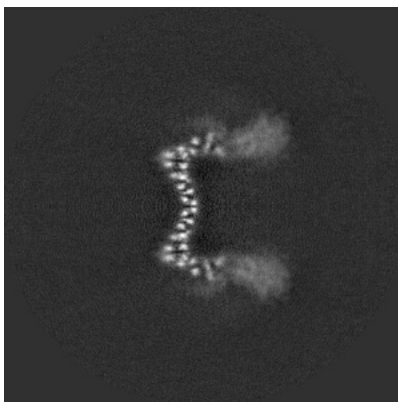


Z Index: 170

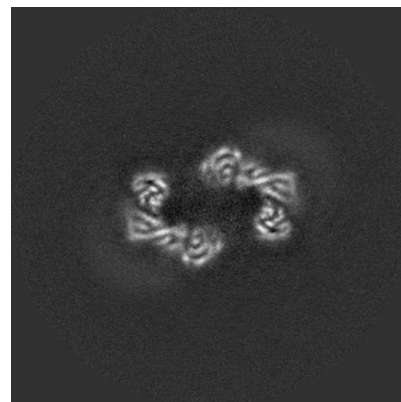
6.2.2 Raw map



X Index: 170



Y Index: 170

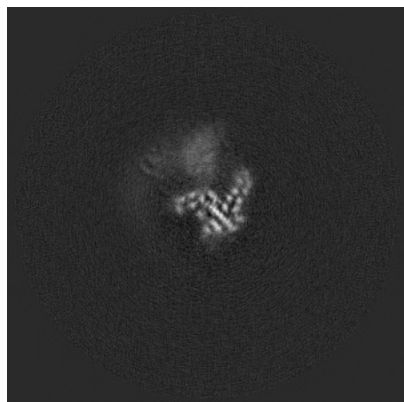


Z Index: 170

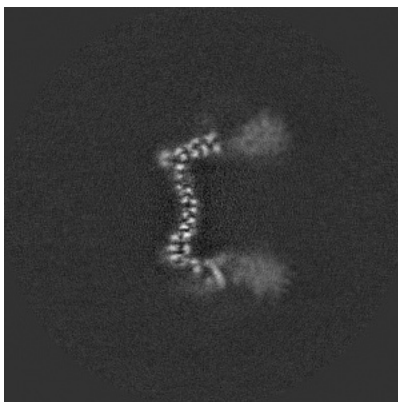
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

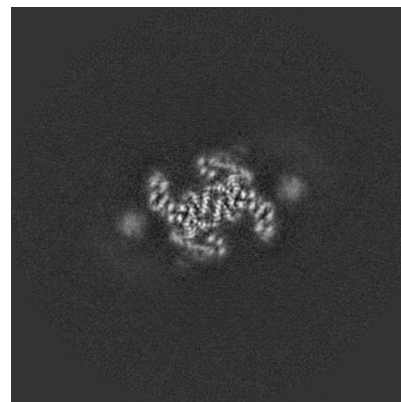
6.3.1 Primary map



X Index: 120

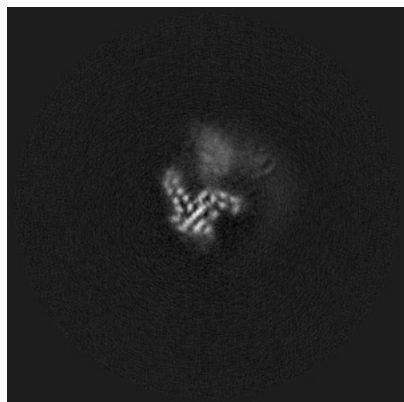


Y Index: 167

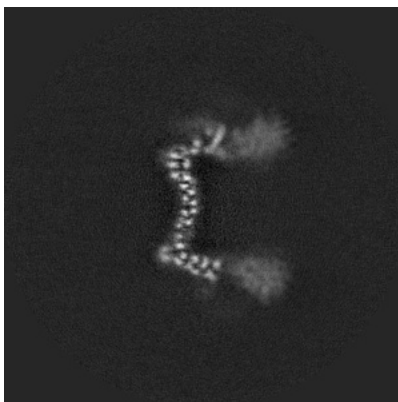


Z Index: 153

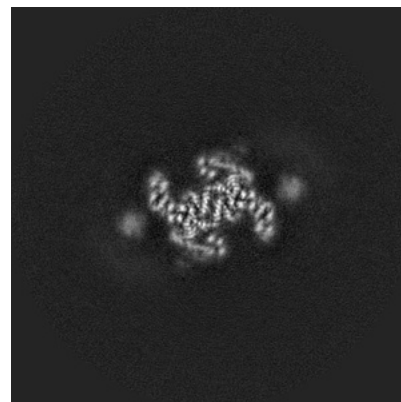
6.3.2 Raw map



X Index: 220



Y Index: 173

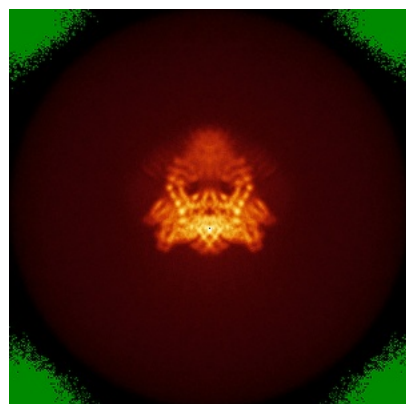


Z Index: 153

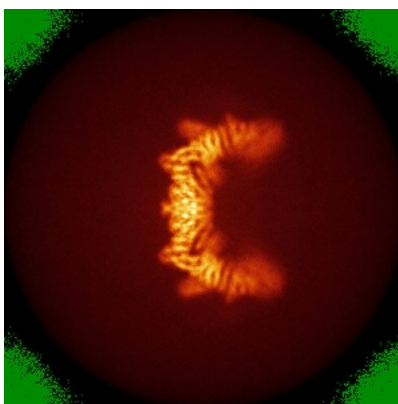
The images above show the largest variance slices of the map in three orthogonal directions.

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

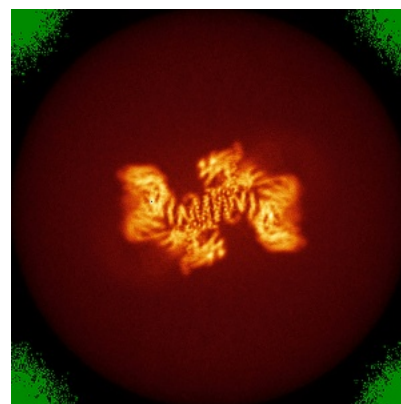
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

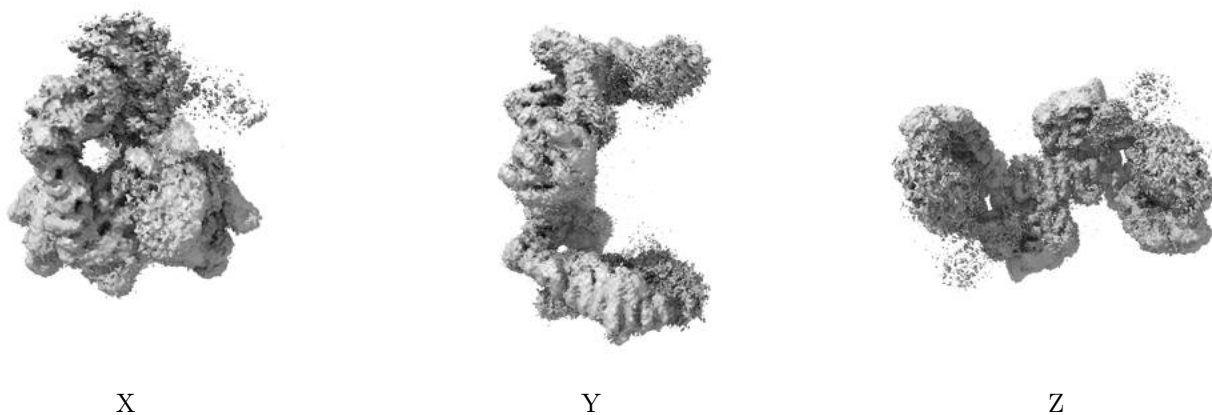


Z

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

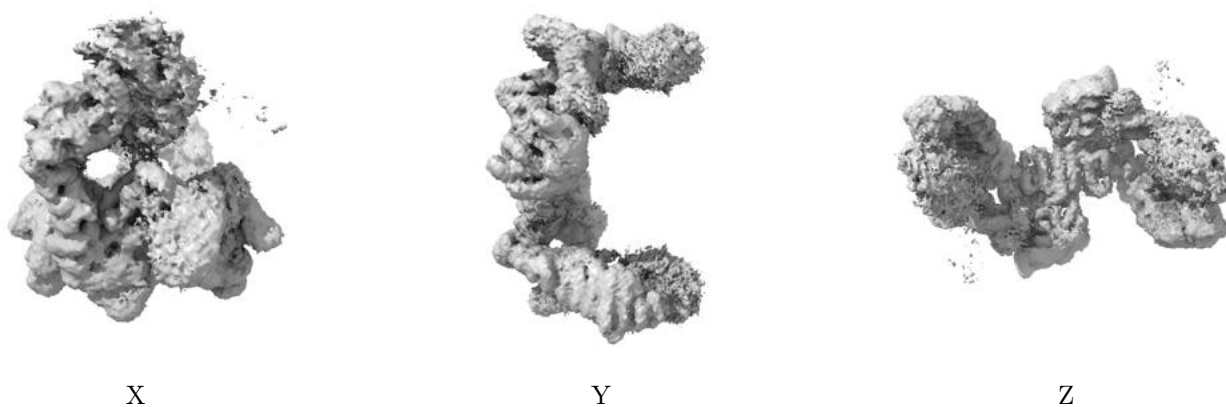
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

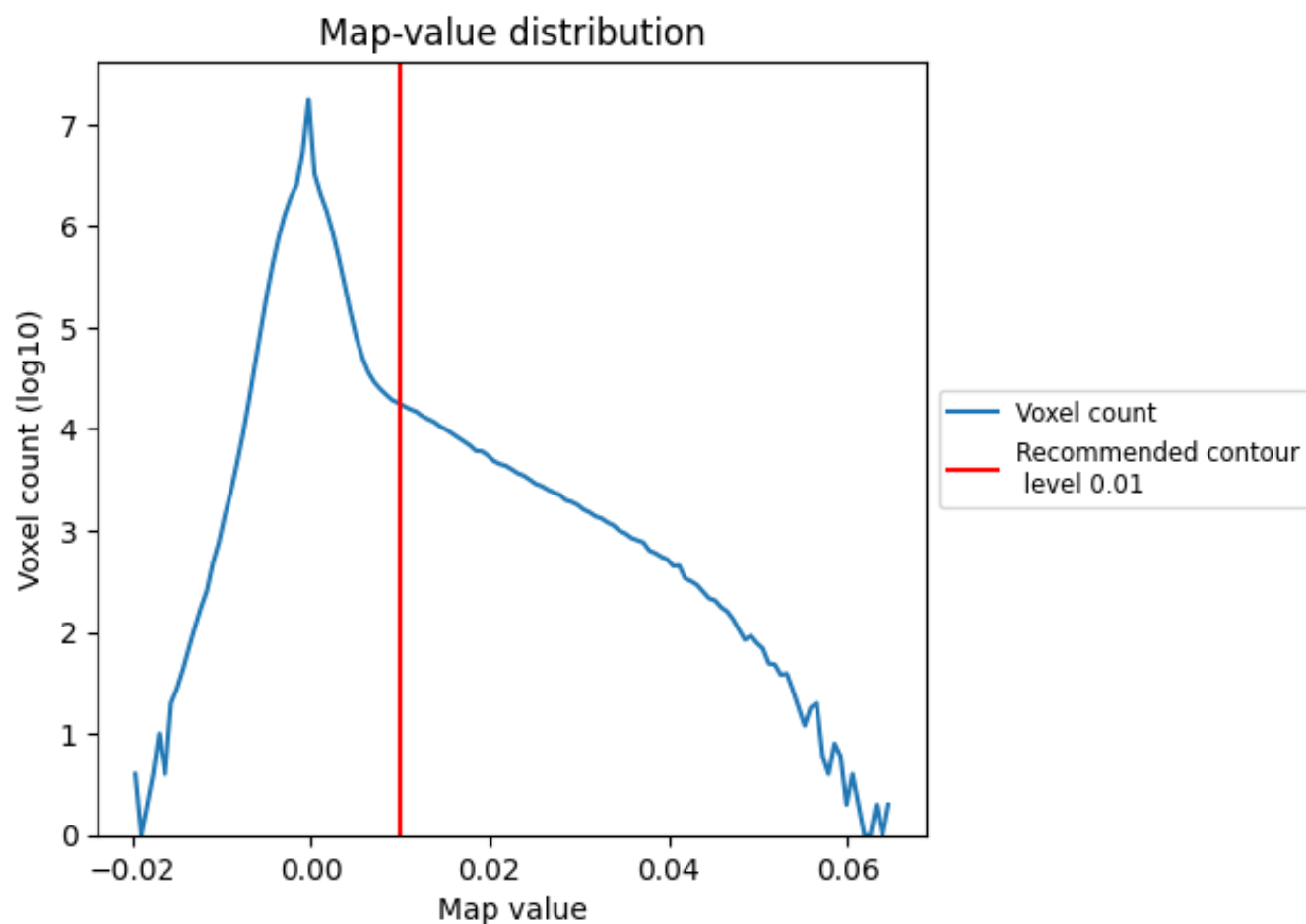
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

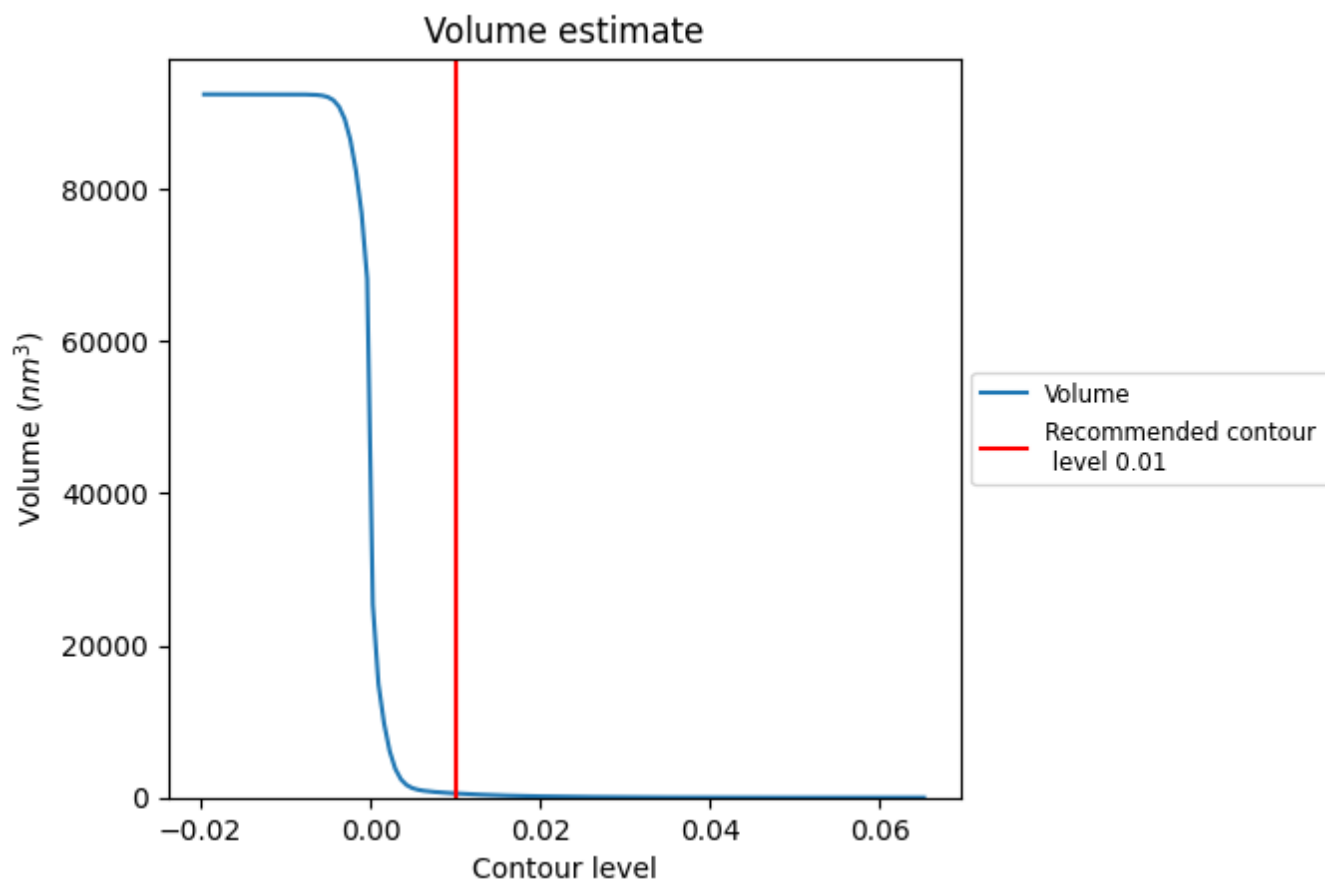
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

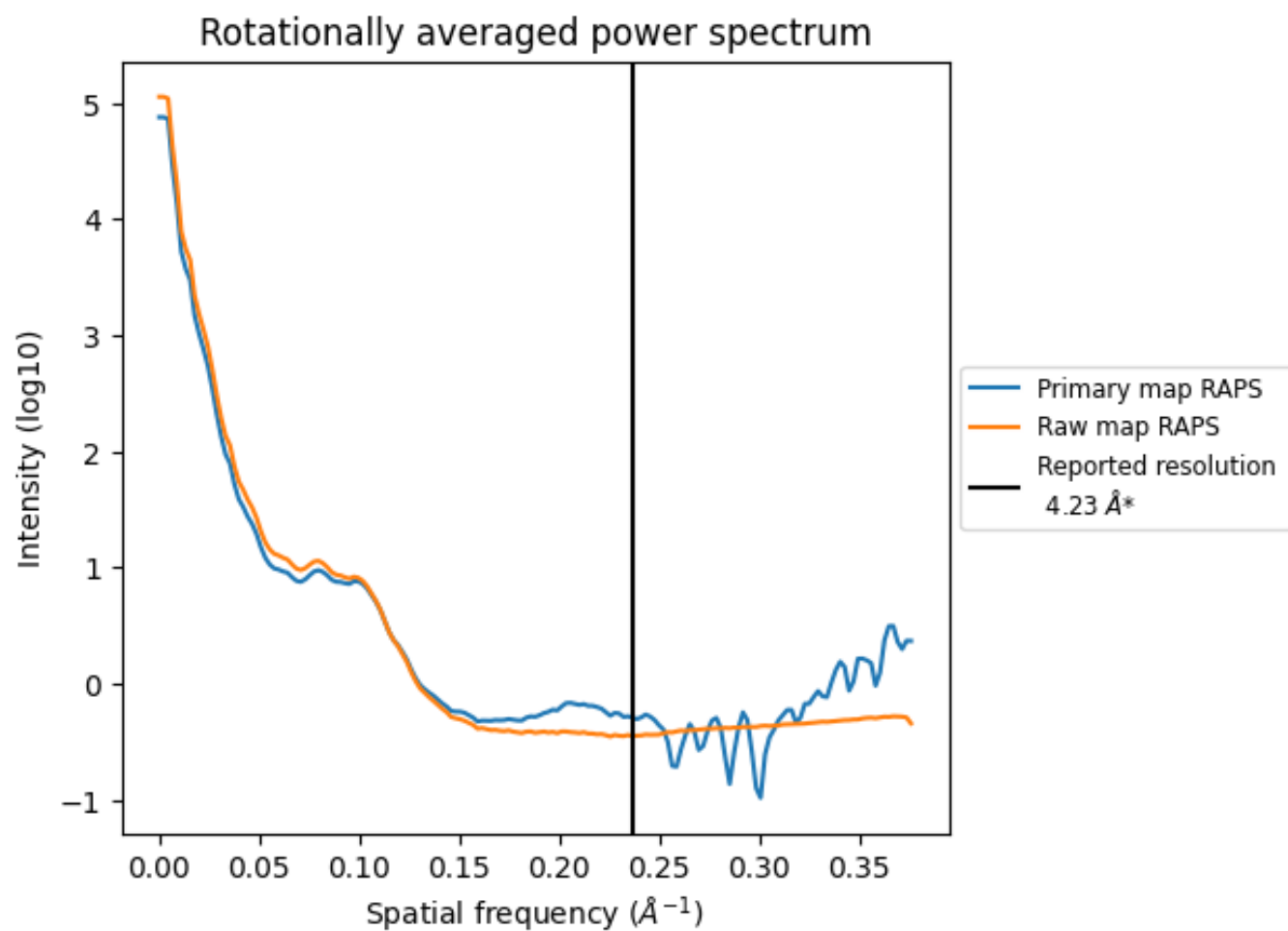
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 546 nm³; this corresponds to an approximate mass of 494 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 ⓘ

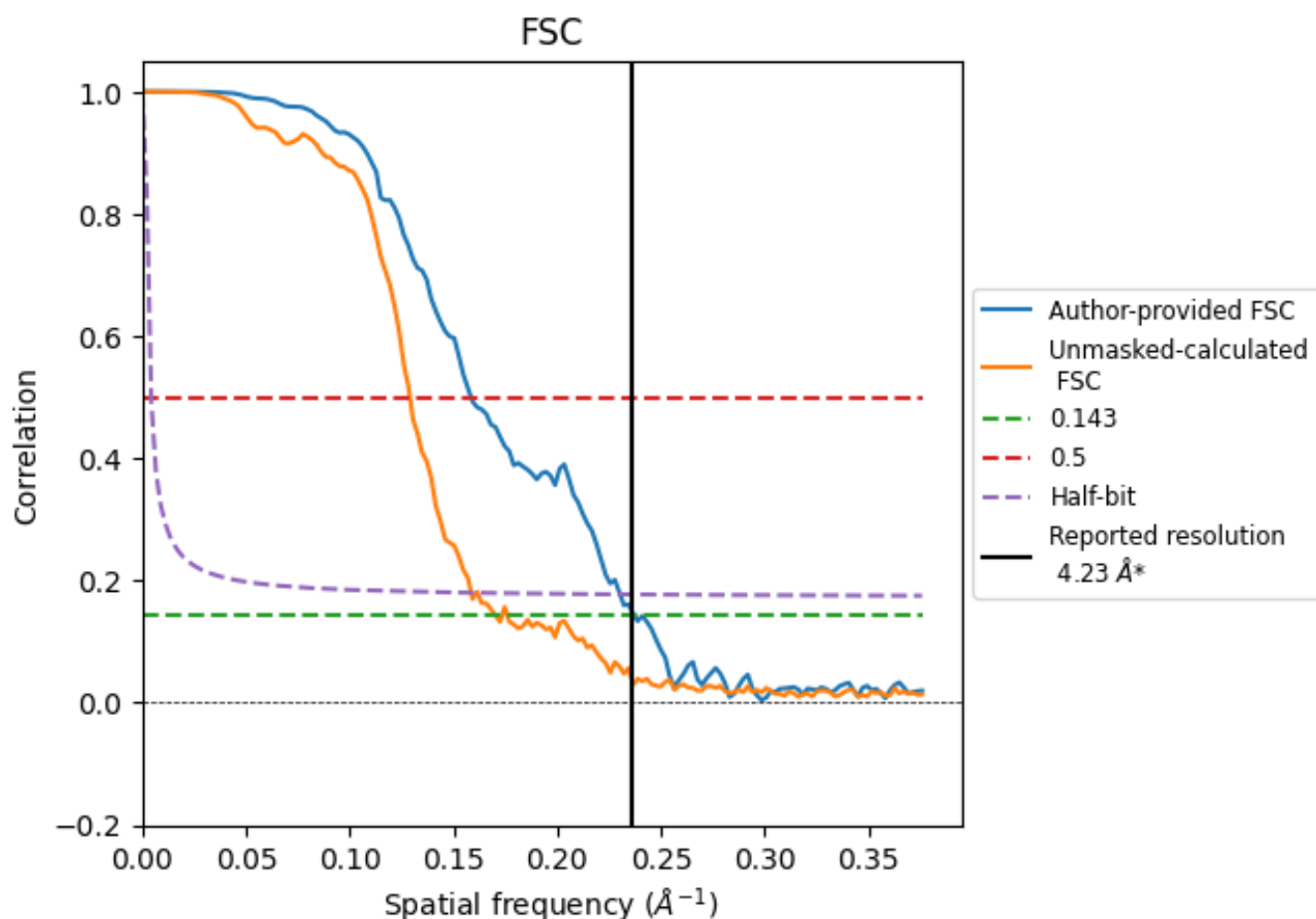


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.236 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

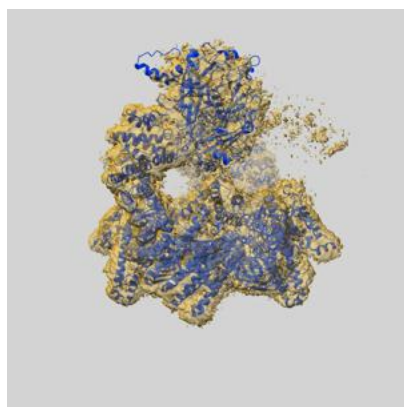
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.22	6.31	4.34
Unmasked-calculated*	5.88	7.75	6.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.88 differs from the reported value 4.23 by more than 10 %

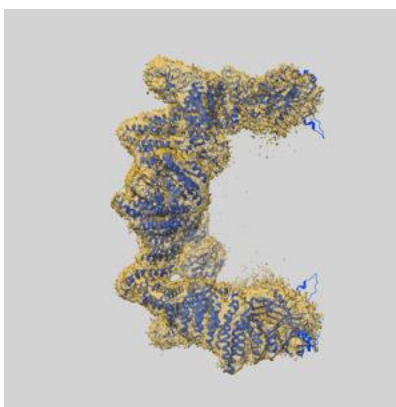
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60146 and PDB model 8ZJI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

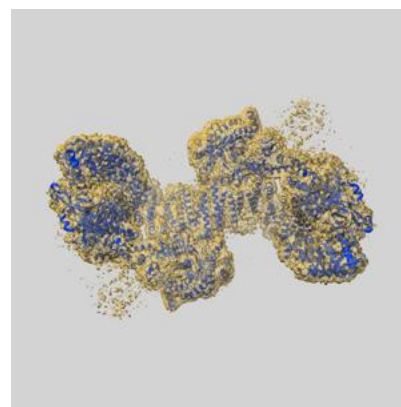
9.1 Map-model overlay [i](#)



X



Y



Z

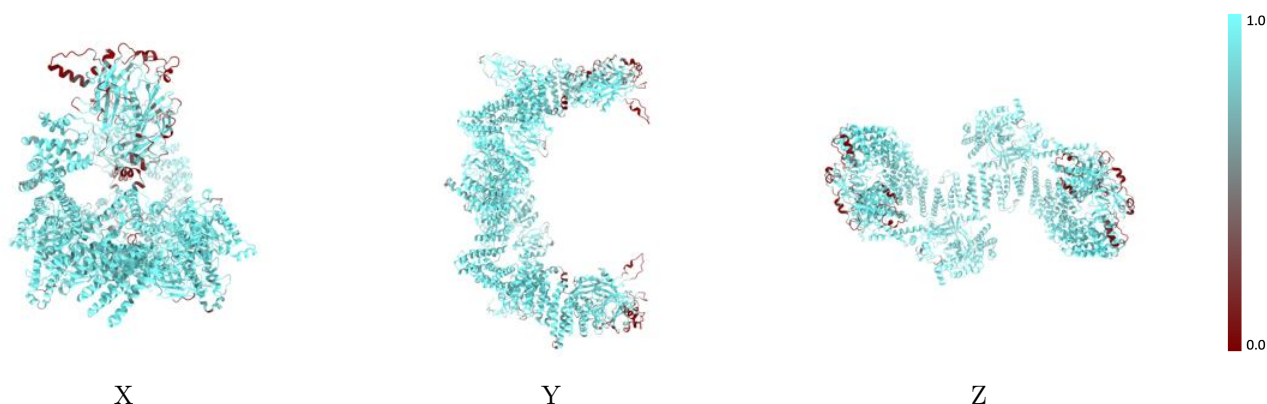
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



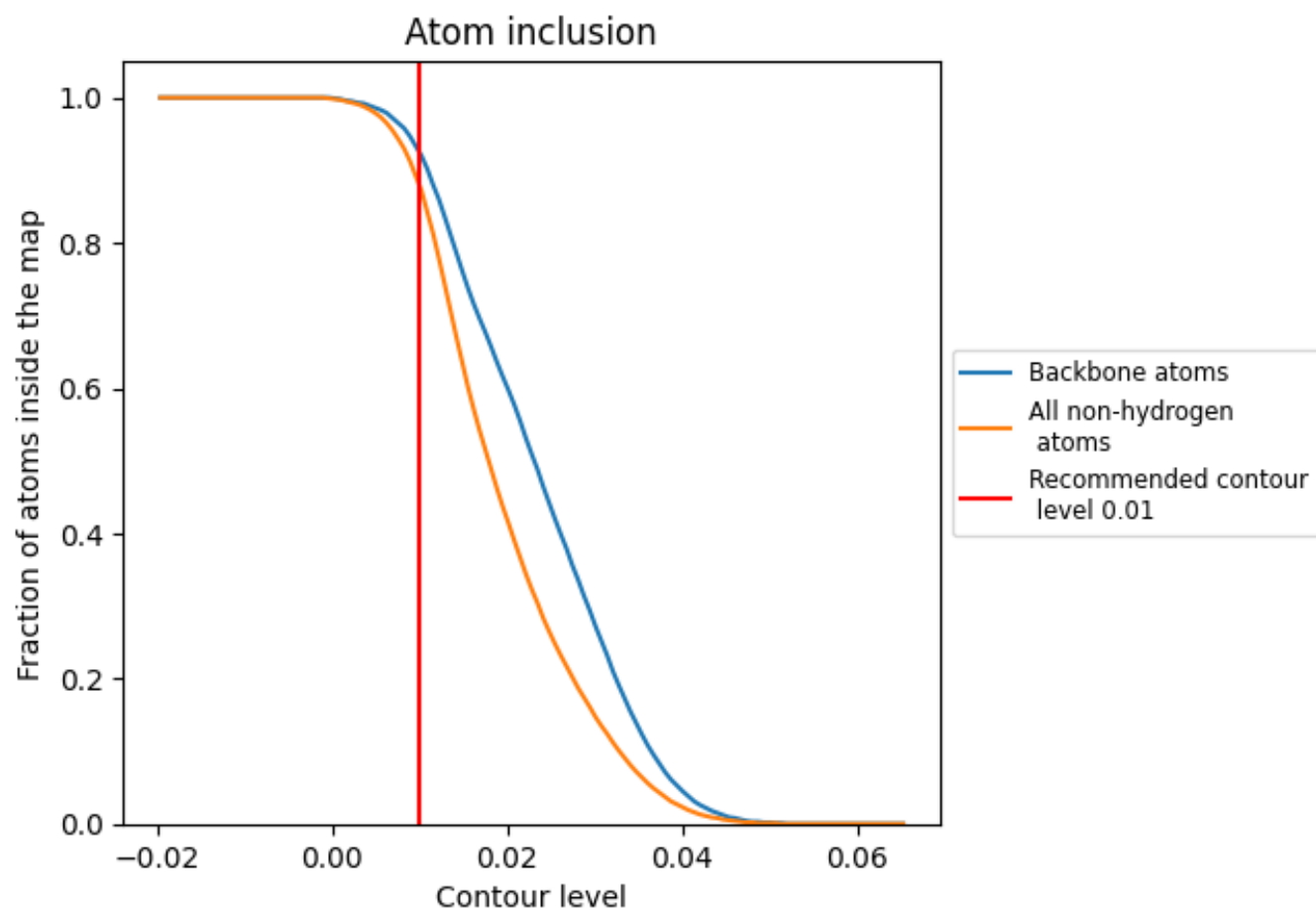
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.1920
A	0.9060	0.1590
B	0.8680	0.1910
C	0.9700	0.2480
D	0.9130	0.1580
E	0.8650	0.1900
F	0.9720	0.2490

1.0

0.0

<0.0