



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:13 AM UTC

PDB ID : 7XR3 / pdb_00007xr3
EMDB ID : EMD-33404
Title : 3.4 Angstrom cryoEM D5 reconstruction of mud crab reovirus
Authors : Zhang, Q.F.; Gao, Y.Z.
Deposited on : 2022-05-09
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

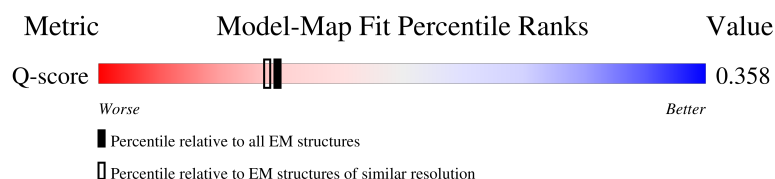
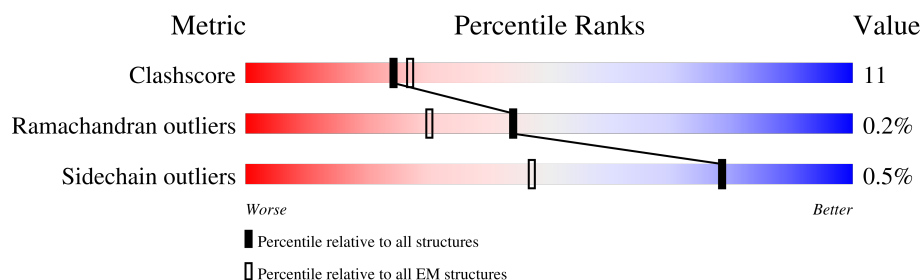
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	854	
1	B	854	
1	C	854	
1	D	854	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	854	29%74%19%7%
1	F	854	24%73%24%..
1	G	854	33%74%19%7%
1	H	854	30%78%21%.
1	I	854	28%72%21%7%
1	J	854	29%82%17%..
2	Z	1425	60%60%32%.7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 76250 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 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6516	4128	1128	1232	28		
1	B	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	C	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	D	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	E	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	F	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	G	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	H	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	I	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	J	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		

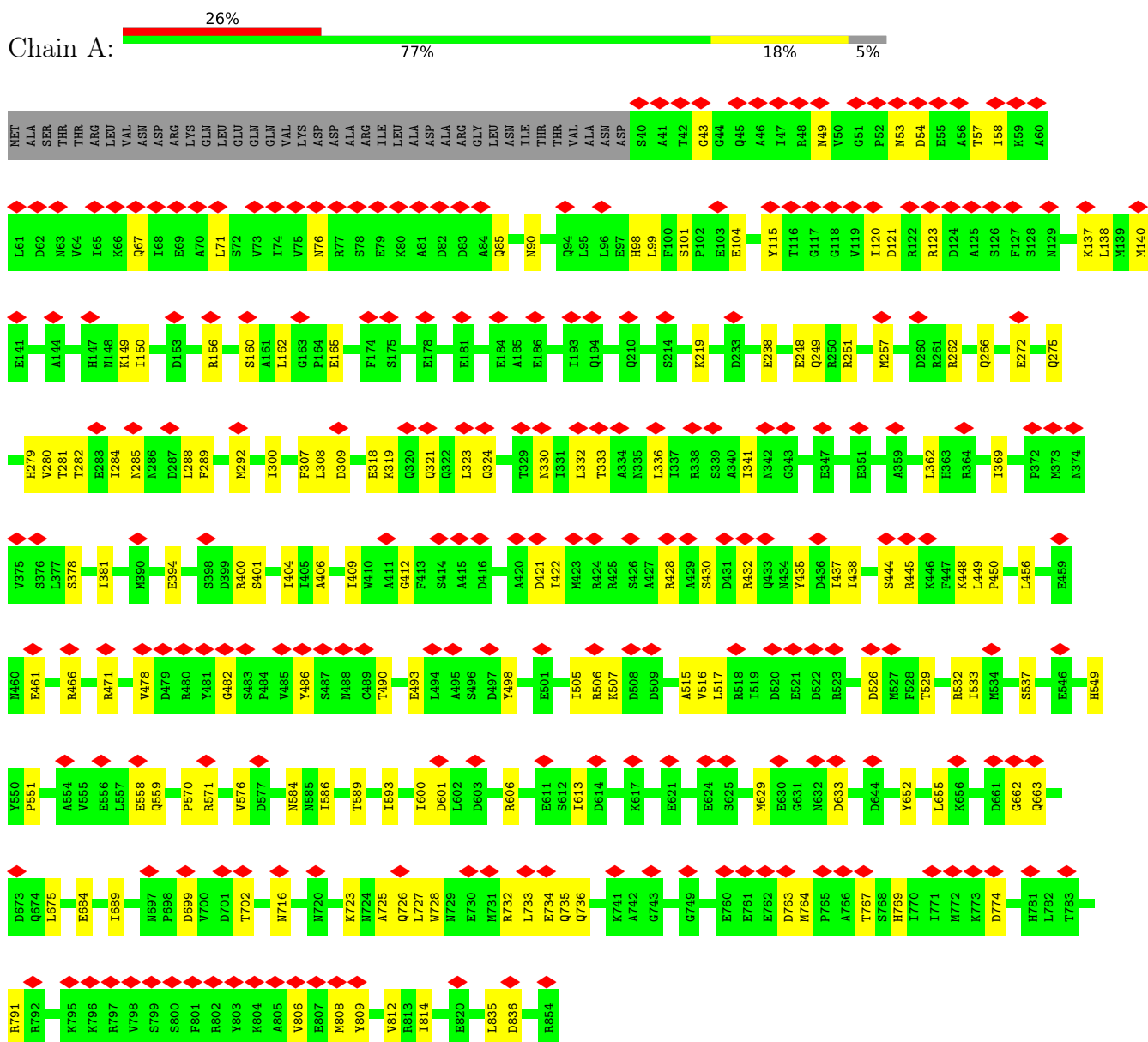
- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	1320	Total	C	N	O	S	0	0
			10516	6661	1799	2000	56		

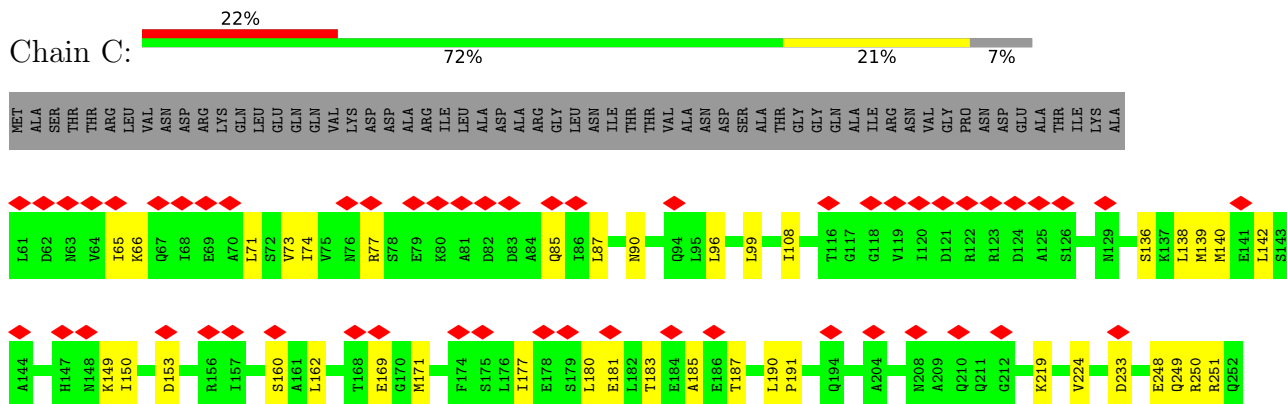
3 Residue-property plots

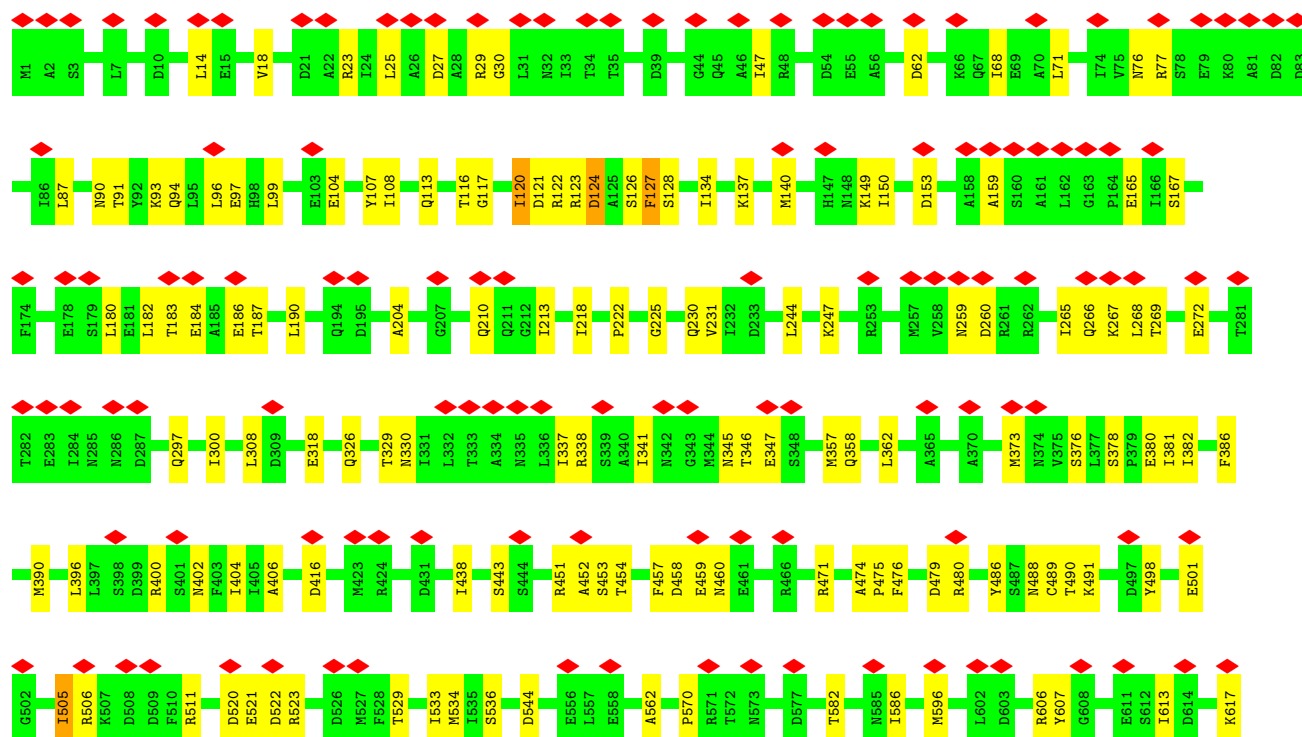
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

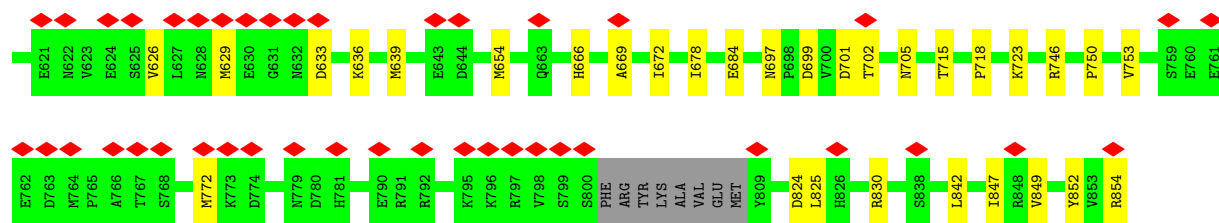
• Molecule 1: VP3



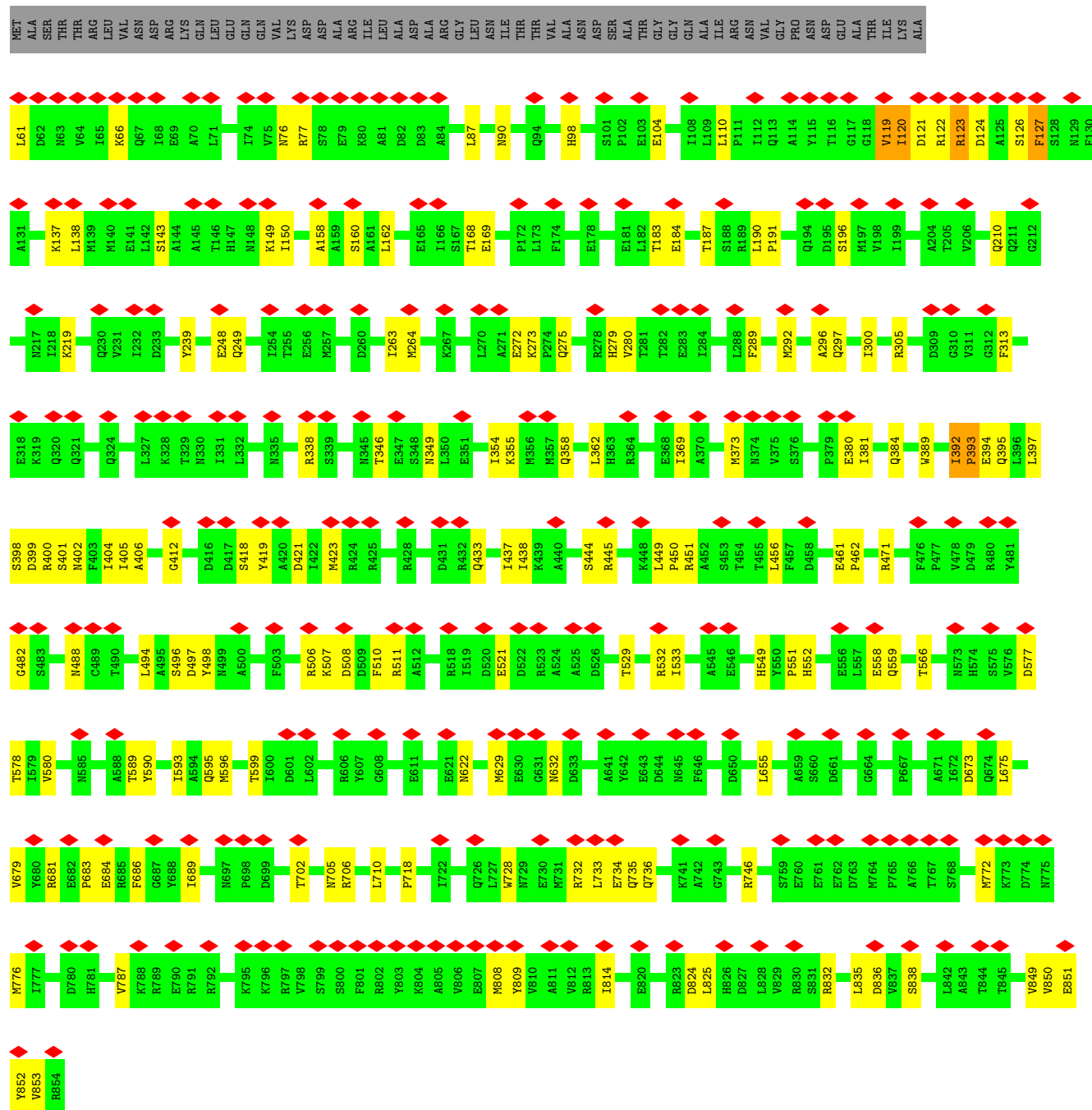
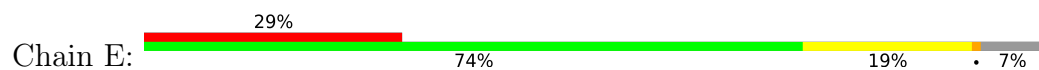
• Molecule 1: VP3



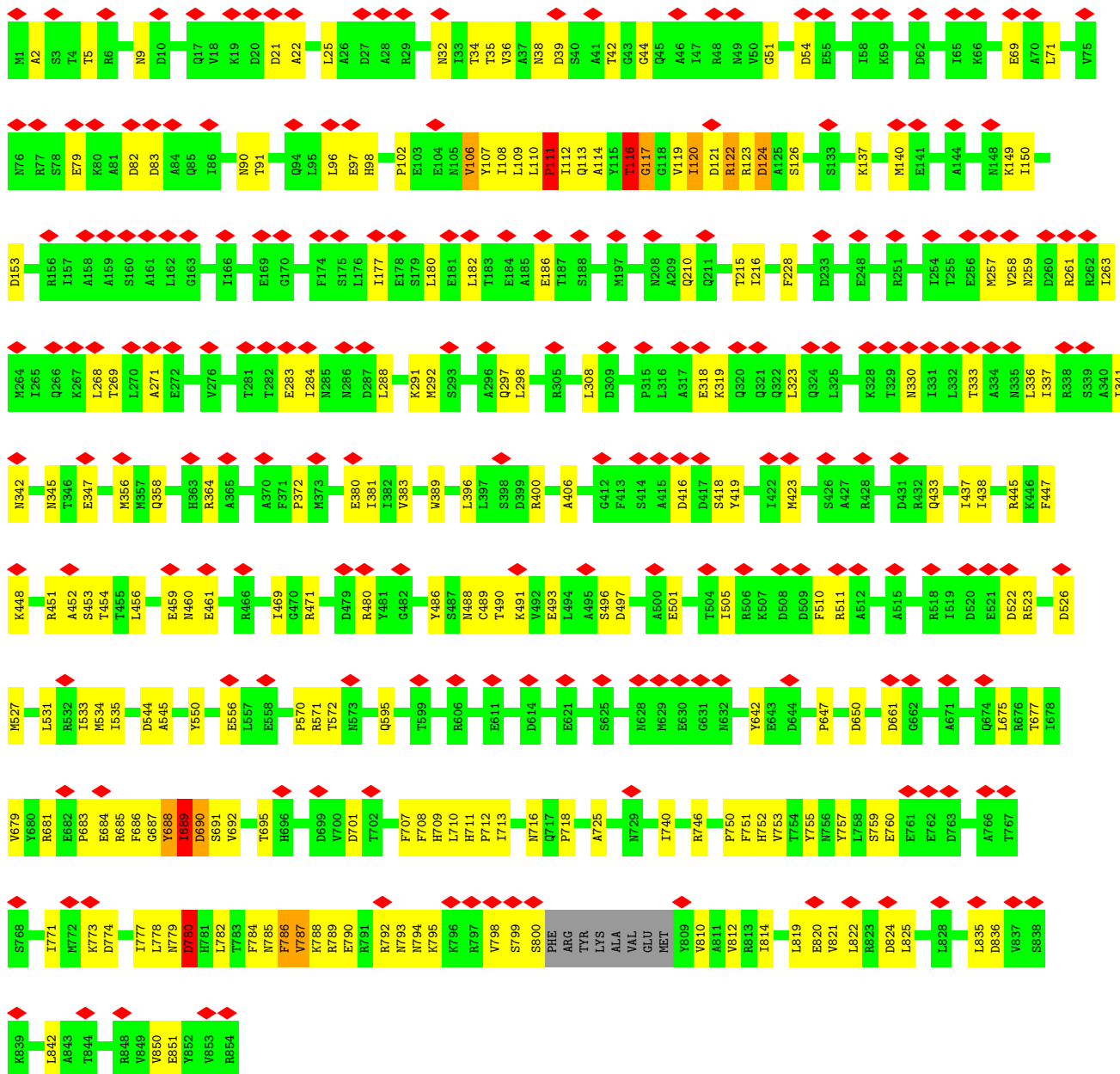
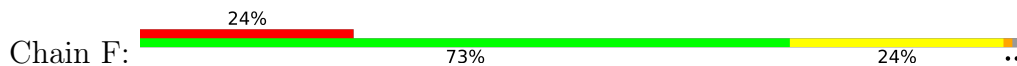




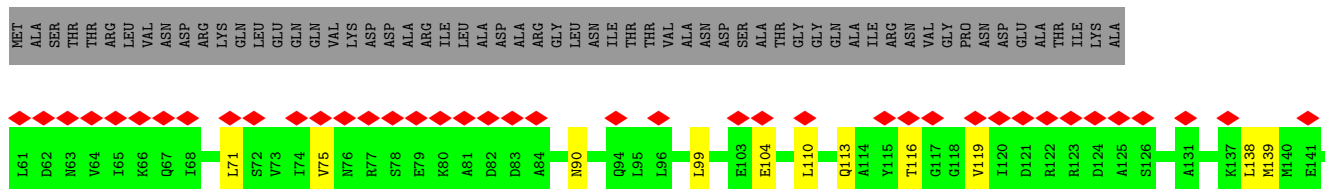
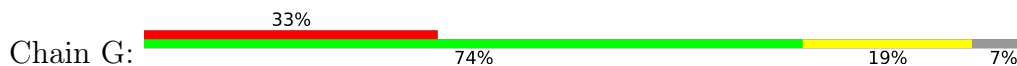
• Molecule 1: VP3

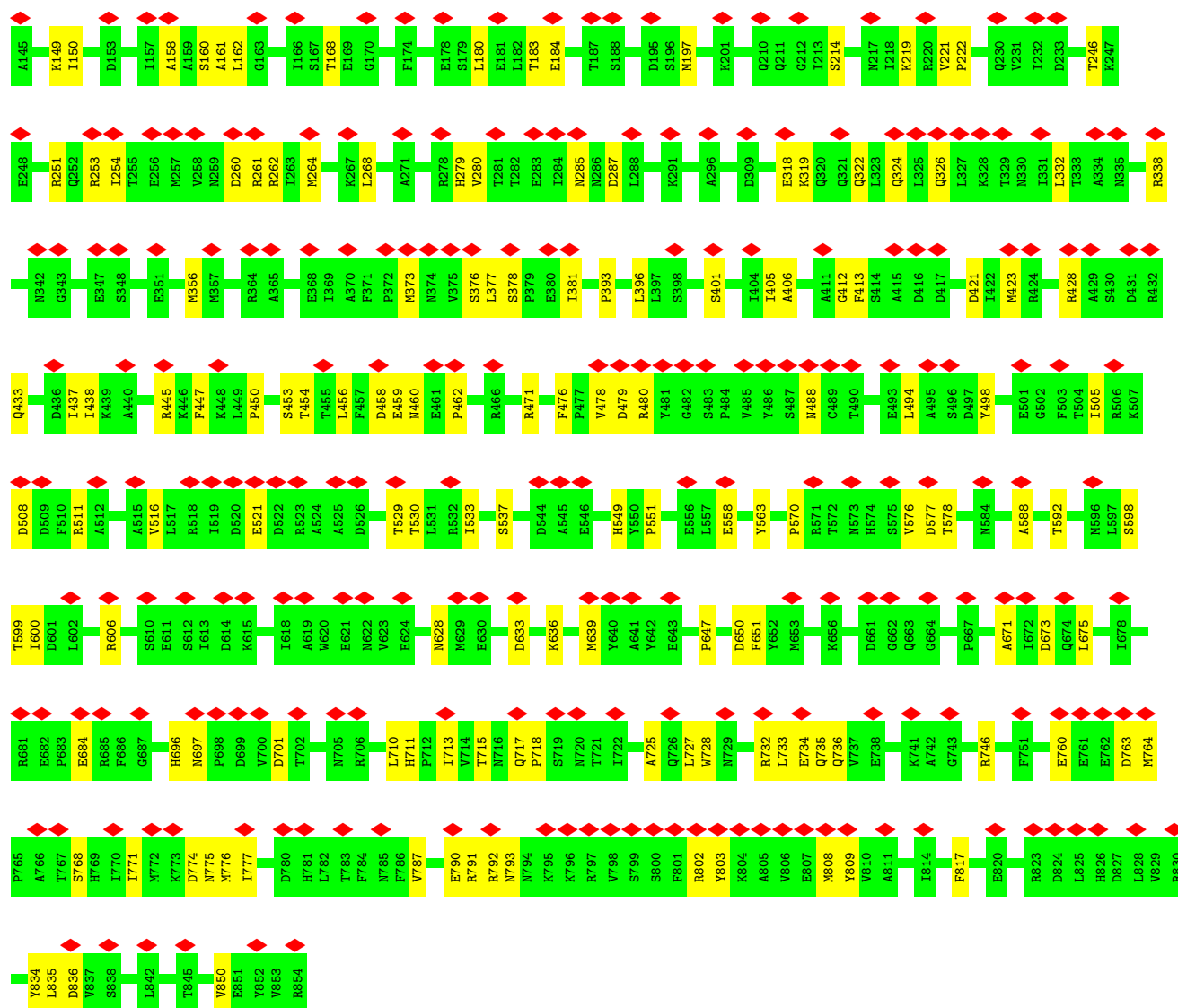


- Molecule 1: VP3

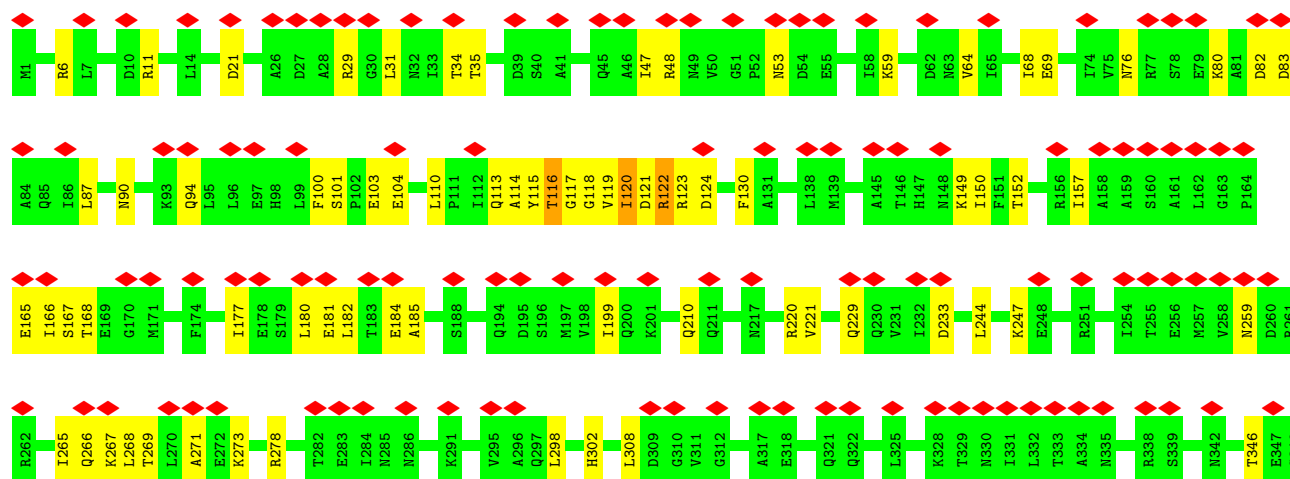
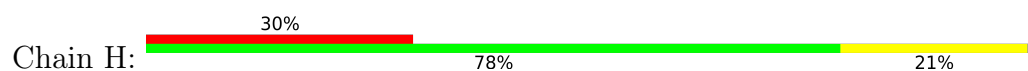


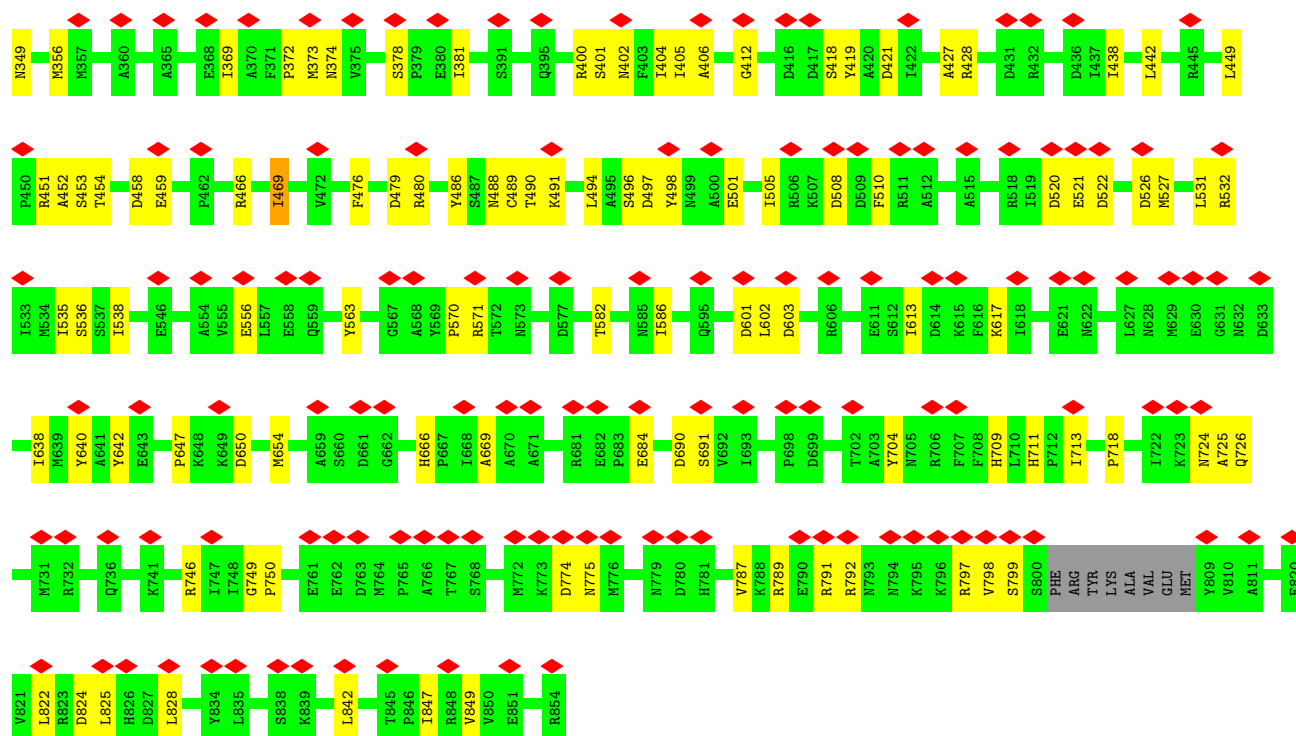
- Molecule 1: VP3



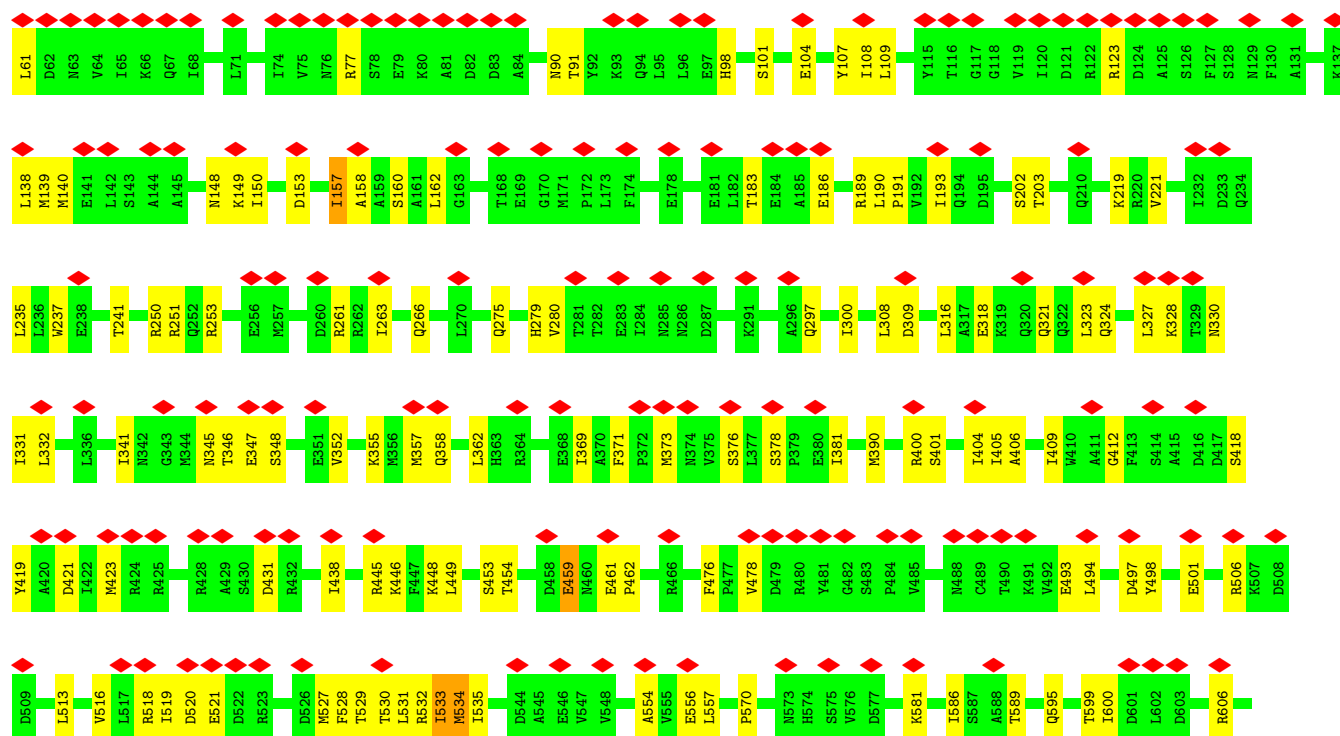


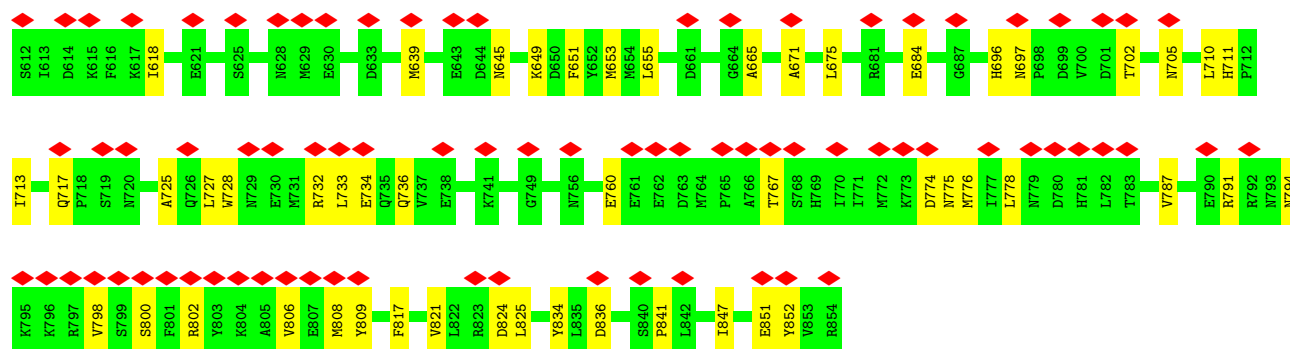
• Molecule 1: VP3



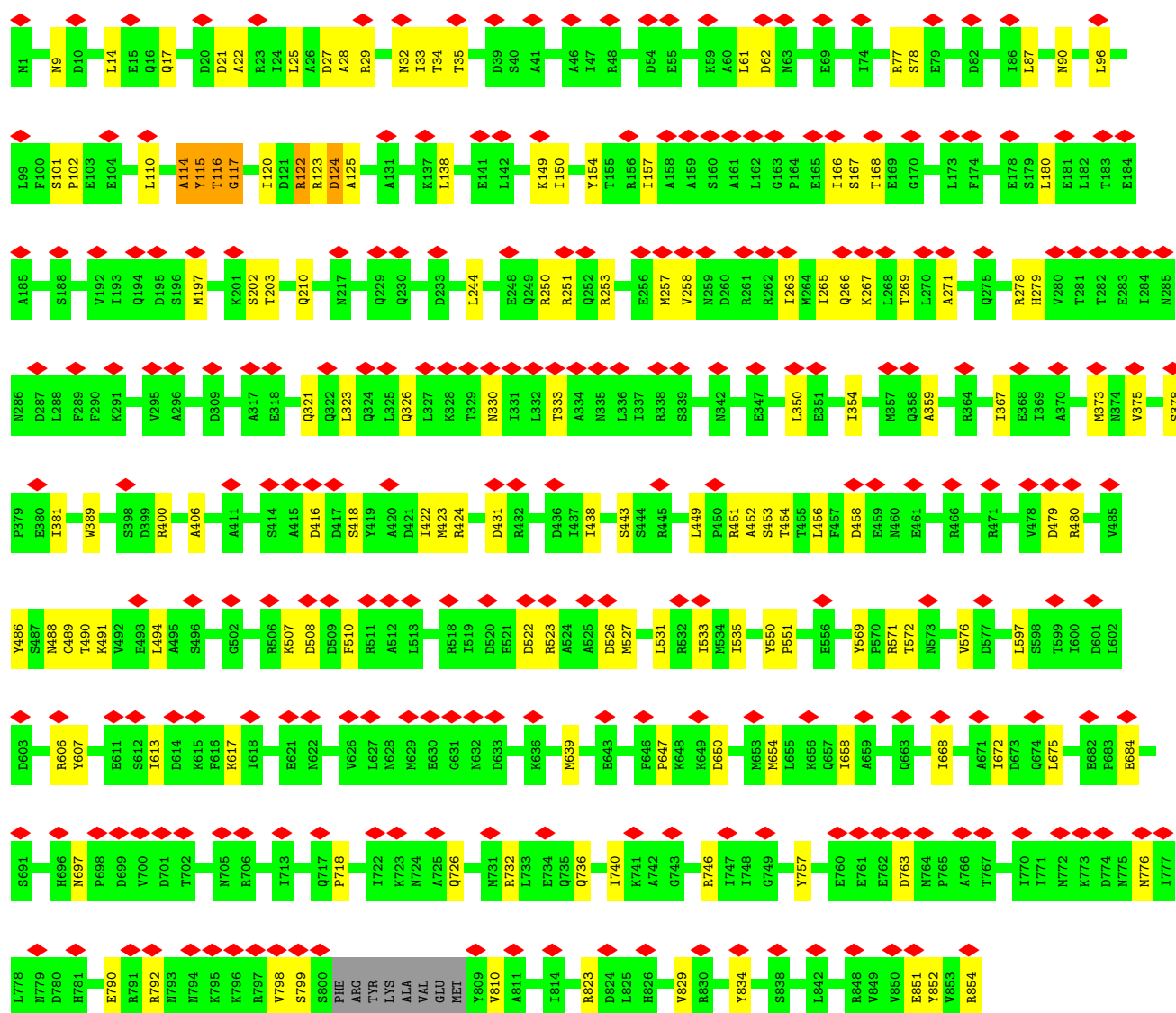
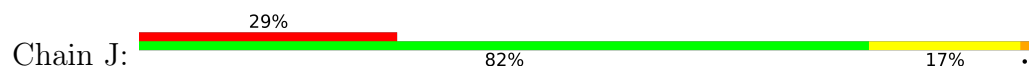


• Molecule 1: VP3





• Molecule 1: VP3



• Molecule 2: VP1



MET	ARG	ILE	MET	ALA	GLN	ARG	LEU	LYS	GLU	LEU	GLN	ARG	GLU	ILE	ASP	LYS	LYS	LYS	GLU	ARG	ILE	ALA	GLU	ALA	TYR	LEU	SER	SER	VAL	GLU	VAL	THR	ASN	SER	SER	PRO	SER	LEU	SER	ILE	LYS	GLN	ASP	ASP	ALA	LEU	THR	LEU	PRO	PRO	LYS	V52	S53	P54	F55	L56	D57	S58	T59	P60	
F61	T62	T63	L64	H65	H66	S67	G70	Q71	F72	L73	H74	S75	L76	D77	D78	E79	L80	A81	THR	ASP	THR	ALA	GLY	L83	C84	L85	L86	E87	E88	E89	L90	Q91	T92	Q93	D96	E97	Q98	L99	T100	A101	L102	K103	H104	F105	L106	T107	T110	G111	S112	P113	Q114	E115	I116	Q117	V119	D120	K121	E122	W123		
M124	K125	S126	H129	V130	P131	S132	F133	L134	G135	D136	V137	K138	L139	M140	F141	GLY	ASP	THR	ALA	GLY	L206	PHE	L207	ARG	R208	V209	V210	L211	R212	F213	V214	P215	K216	V217	D218	T219	T220	S221	ASN	SER	ASN	THR	ARG	LYS	ASP	ALA	THR	GLN	THR	ARG	SER	GLN	ILE	ARG	ASP	LYS	S190	Y181	V182	V183	Q184
K185	K186	H187	K188	V189	Q190	P192	L193	K194	P195	N196	T197	L198	Y199	V200	S201	K202	Y203	K204	G205	L206	P207	R208	V209	V210	L211	R212	F213	V214	P215	K216	V217	D218	T219	T220	S221	ASN	SER	ASN	THR	ARG	LYS	ASP	ALA	THR	GLN	THR	ARG	SER	GLN	ILE	ARG	ASP	LYS	S190	Y181	V182	V183	Q184			
P245	T246	W247	K248	Y249	T252	E253	A254	K255	E256	A257	F258	P259	D260	R261	S262	Y263	S264	D265	C266	L267	H268	P269	W270	T271	W272	E273	E274	W275	L276	E277	E278	W279	Q280	L286	T287	Q288	Y289	A290	H291	Q292	L293	V296	T297	L298	L299	Q300	D301	F302	N303	L304	G309	A310	S311	R312	V313						
R314	N315	I316	D317	M318	S319	T320	L321	P322	F323	S324	L325	N326	V327	L328	D329	H330	F331	E332	L333	Y334	G335	D336	A337	M338	K339	L340	A341	Y342	V343	R344	S345	G346	E347	W348	Y349	G350	L351	L352	R353	E354	I355	E356	Q357	E358	G359	M360	T361	V362	N363	E364	S365	E366	K367	V368	F369	A370	N371	P372	D373		
T374	Y375	V376	L377	N378	V379	K380	K381	L384	R385	R386	F387	Q388	Q389	E390	L391	A392	S393	M396	T397	P398	L399	T400	D401	E402	L403	L404	A405	I406	A407	F408	V409	H410	W411	N412	V415	T416	A417	E418	P419	Q422	V423	I424	K425	D426	D427	L428	L429	K430	S433	R434	Y435	D438	A439								
T440	F441	D442	Y443	N444	M445	K446	R447	S448	E449	M450	L451	V452	V453	T454	R455	G456	H457	L458	A459	A460	H461	K462	V463	L464	E465	C466	A467	L468	R469	I470	V471	E472	Y475	T476	D478	I479	Q480	D481	E482	T483	F484	K485	D486	I487	L488	I489	D490	L491	G492	L494	I495	M496	R497	D498	P499	I500					
Y501	G502	T503	T504	R507	D508	A509	T510	E511	V512	M513	K514	Q515	L516	M517	Y518	T519	Q520	G521	T522	F523	R525	R526	L527	M528	F529	K530	D533	Y534	S535	N536	F537	N538	E539	K540	K544	G545	E546	Q547	M548	T549	N550	P552	P553	T554	L555	L556	A557	T558	L559	H560	Y561	E562	E563	M564							
D565	K566	K567	R568	I569	D570	A571	L572	I573	N576	Q577	R578	A579	G580	N581	I582	L583	S584	Q585	S586	S587	I588	E589	R590	C591	R592	Y593	T594	D595	S596	L597	D598	L599	V600	G601	D602	A603	M604	R605	Y606	F607	L613	G618	F619	A620	S621	S622	D623	L624	L625	S626	G627	R628	I629	D630	S631	N632					
E633	S634	I635	E636	F637	T638	A641	H642	L643	R644	K645	E653	Q654	I655	S661	T662	V663	P664	R665	P666	S667	L668	P669	K670	V671	L672	L673	S674	G675	A676	K677	D678	T679	A680	S681	A682	S683	I684	E685	P686	L687	T688	F689	R690	I691	Y692	K693	T694	T695	P696	E697	Y698	R699	G700	E701	S702	L703					
N704	L705	V706	E707	S708	T709	V710	W711	M712	S713	T714	Q715	Y716	K717	W718	P719	N720	L721	R722	K723	A724	A725	E726	W727	L728	R729	S730	T731	V732	T733	W734	W735	Q736	E737	R738	L739	I740	S741	G742	G743	T744	R745	A746	V747	Q748	G749	G750	S751	G752	A753	R754	A755	V756	Y757	P758	T759	K760	Q761	P762	Y763		
H764	L765	A766	G767	S768	L769	F771	D775	T776	N779	A780	W781	K782	W783	Y784	R785	G786	W787	S788	N789	W790	Y791	G792	Q793	G794	L795	S796	N797	A798	T799	P800	H801	I802	G803	V804	P805	E806	I807	V810	D813	G814	N815	A816	L817	C818	L819	A820	L821	D822	V823	S824	A825	P826	D827								
K831	Y832	T833	E834	E838	N841	R842	D843	G844	S848	E849	L850	G855	E856	T857	V858	L859	E860	R861	M862	N863	P864	A865	D866	L867	N870	N874	T875	P876	P877	R878	Y879	Q882	T883	A884	L885	G886	D887	T888	L889	N890	L891	Q892	H893	D894	N895	R896	S897	G898	V899	P900	W901	T902									

R1362	R1363	G1364	P1365	P1366	L1367	P1368	I1369	I1370	D1371	R1372	T1373	L1374	N1375	R1376	L1377	L1378	M1383	L1384	M1385	F1386	M1389	G1390	K1391	S1392	I1393	D1394	S1395	T1396	K1397	I1398	D1399	P1400	T1401	L1402	S1403	W1404	R1405	A1406	I1407	L1408	E1409	S1410	N1411	D1412	Q1413	R1414	I1415	A1416	Q1417	L1418	S1419	E1420	L1421	L1422	T1423	A1424	V1425		
F1301	L1302	Q1303	V1304	M1305	S1306	V1307	Y1308	Q1309	L1310	P1311	D1312	T1313	L1314	T1315	H1316	E1317	M1318	L1319	A1320	A1321	V1322	V1323	A1324	I1325	E1326	L1327	Q1328	L1329	G1330	M1331	D1332	K1333	Y1334	A1335	V1336	D1337	M1338	G1339	V1340	Y1341	S1342	S1343	Q1344	A1345	I1348	R1349	I1350	N1351	D1352	A1353	L1354	M1355	D1356	S1357	I1358	T1359	Q1360	H1361	
S1229	D1230	L1231	K1232	Q1233	D1234	D1235	Y1236	Y1239	Q1245	R1248	N1256	D1257	S1258	R1259	I1260	T1261	S1262	F1263	D1264	P1265	K1266	G1267	K1268	L1269	Q1270	H1271	L1272	L1273	A1274	K1275	N1276	S1277	Q1278	I1279	L1280	P1281	I1282	H1283	F1284	D1285	I1286	E1287	F1288	Y1289	R1290	R1291	L1292	Y1293	L1294	Q1295	A1296	G1297	T1298	M1299	G1300				
H1167	L1168	M1169	R1170	Y1171	G1172	K1173	S1174	M1175	T1176	L1177	R1178	H1179	I1180	L1181	A1182	S1183	A1184	A1185	M1186	G1187	P1188	L1189	S1190	Q1191	T1192	E1193	K1194	M1195	V1196	N1197	A1198	Y1199	M1200	V1201	V1202	M1203	G1204	I1205	L1206	M1207	G1208	K1209	L1210	E1211	T1214	V1215	L1216	E1217	R1218	L1219	N1220	M1221	G1222	F1223	K1224	V1227	M1228		
H1107	G1108	S1109	S1110	F1111	G1112	W1113	M1114	F1115	D1116	D1117	M1118	L1119	I1120	K1121	T1122	A1123	M1124	S1125	I1126	G1127	A1128	I1129	S1130	D1131	S1132	S1133	Y1134	D1135	A1136	I1137	S1138	T1139	K1140	I1141	T1142	M1143	L1144	A1145	D1146	M1147	K1148	D1149	S1150	Q1151	Q1152	R1153	I1154	T1155	R1156	D1157	I1158	I1159	T1160	S1161	G1162	R1163	L1164	P1165	Q1166
I1041	R1042	D1043	I1044	T1045	D1046	I1049	D1054	E1055	T1056	R1057	L1058	K1059	M1059	K1060	Y1061	N1062	L1063	M1064	M1065	L1066	P1067	V1068	D1069	T1070	T1071	T1072	R1073	A1074	G1075	A1076	F1077	R1078	M1079	H1080	N1081	L1082	C1083	S1084	I1085	M1086	T1087	G1088	V1089	G1090	K1091	M1092	Y1093	L1094	L1098	N1099	N1100	K1101	L1102	I1103	A1104				
E976	Q979	D980	T981	A982	G983	T984	L985	G986	F987	A988	T989	L989	N990	A991	R992	G993	C994	M995	I996	G997	R998	S1001	E1002	Y1003	L1004	K1005	M1006	S1007	A1008	I1009	Y1010	G1011	M1012	I1013	K1014	M1017	Q1018	V1019	K1020	F1021	R1022	G1023	S1024	E1025	K1026	S1027	A1028	S1029	Y1030	H1031	F1032	G1033	V1034	K1037	V1038				
G903	T904	Q905	N906	D907	L908	V909	N910	N913	H914	H915	M916	D919	E920	K923	R924	E927	R930	Q931	G932	K933	I934	S935	I936	D937	D940	K941	H942	R946	V947	F948	G949	D950	D951	S952	T953	F954	I955	M956	D959	E960	S963	A964	E965	E966	V967	H968	L969	M970	C971	A972									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	128440	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	33.537	Depositor
Minimum map value	-21.310	Depositor
Average map value	0.081	Depositor
Map value standard deviation	1.814	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	872.0, 872.0, 872.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	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	0.25	0/6644	0.43	0/9015
1	B	0.27	0/6871	0.45	1/9322 (0.0%)
1	C	0.23	0/6499	0.40	0/8818
1	D	0.33	0/6871	0.50	3/9322 (0.0%)
1	E	0.27	0/6499	0.43	3/8818 (0.0%)
1	F	0.36	0/6871	0.54	8/9322 (0.1%)
1	G	0.21	0/6499	0.37	0/8818
1	H	0.25	0/6871	0.42	1/9322 (0.0%)
1	I	0.24	0/6499	0.42	3/8818 (0.0%)
1	J	0.27	0/6871	0.44	3/9322 (0.0%)
2	Z	0.51	0/10724	0.72	3/14518 (0.0%)
All	All	0.31	0/77719	0.49	25/105415 (0.0%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	THR	CB-CA-C	-7.23	97.49	110.36
1	F	780	ASP	N-CA-C	-7.03	103.81	112.88
1	E	392	ILE	O-C-N	-6.70	115.52	121.61
1	E	123	ARG	N-CA-C	-6.47	105.49	113.19
1	H	114	ALA	O-C-N	-6.16	115.16	123.10
1	D	127	PHE	CA-C-N	-6.15	109.85	122.58
1	D	127	PHE	C-N-CA	-6.15	109.85	122.58
1	F	116	THR	CB-CA-C	-6.03	98.42	110.42
1	F	111	PRO	N-CA-CB	-5.98	96.97	103.25
1	J	116	THR	CB-CA-C	-5.86	98.76	110.42
1	D	124	ASP	CB-CA-C	-5.71	102.66	111.74
2	Z	452	VAL	CA-C-N	-5.66	115.30	123.11
2	Z	452	VAL	C-N-CA	-5.66	115.30	123.11
1	I	534	MET	N-CA-C	-5.55	107.76	114.75
1	F	117	GLY	CA-C-O	-5.52	117.26	122.39
1	F	122	ARG	N-CA-C	-5.42	103.53	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	535	ILE	CA-C-N	-5.40	114.05	122.37
1	I	535	ILE	C-N-CA	-5.40	114.05	122.37
1	J	117	GLY	CA-C-O	-5.32	118.02	122.33
2	Z	894	ASP	CB-CA-C	-5.17	100.12	110.42
1	J	114	ALA	O-C-N	-5.16	116.45	122.96
1	F	688	TYR	CA-C-O	-5.13	116.40	121.02
1	F	106	VAL	O-C-N	5.12	128.41	123.03
1	F	786	PHE	CB-CA-C	-5.09	100.39	109.71
1	E	395	GLN	N-CA-C	-5.05	107.07	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6516	0	6517	110	0
1	B	6746	0	6755	164	0
1	C	6372	0	6375	132	0
1	D	6746	0	6755	130	0
1	E	6372	0	6375	133	0
1	F	6746	0	6755	192	0
1	G	6372	0	6375	123	0
1	H	6746	0	6755	146	0
1	I	6372	0	6375	144	0
1	J	6746	0	6755	115	0
2	Z	10516	0	10497	347	0
All	All	76250	0	76289	1637	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 11.

All (1637) 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)
1:I:357:MET:HE2	1:I:534:MET:HG2	1.26	1.07
2:Z:895:ASN:HB3	2:Z:905:GLN:OE1	1.66	0.96
1:F:98:HIS:HB2	1:F:112:ILE:HD11	1.44	0.96
2:Z:686:PRO:HG3	2:Z:717:LYS:HA	1.48	0.94
1:B:126:SER:HB3	1:B:129:ASN:OD1	1.68	0.93
1:E:119:VAL:HB	1:F:69:GLU:OE2	1.68	0.92
1:B:118:GLY:HA2	1:B:133:SER:OG	1.70	0.92
2:Z:462:LYS:HG3	2:Z:500:ILE:HD11	1.51	0.92
1:E:158:ALA:HB1	1:H:123:ARG:HH21	1.37	0.90
1:B:126:SER:C	1:B:128:SER:H	1.75	0.89
1:B:123:ARG:HB2	1:I:160:SER:CB	2.02	0.89
2:Z:459:LEU:HD23	2:Z:499:PRO:HD2	1.54	0.89
1:F:709:HIS:HB2	1:F:787:VAL:CG2	2.02	0.88
1:F:710:LEU:HB3	1:F:787:VAL:HG13	1.56	0.87
1:J:124:ASP:HB2	1:J:607:TYR:OH	1.75	0.86
1:D:126:SER:C	1:D:128:SER:H	1.85	0.85
2:Z:438:ASP:HB2	2:Z:456:GLY:HA3	1.61	0.83
1:B:124:ASP:HB3	1:B:607:TYR:OH	1.80	0.80
2:Z:314:ARG:HA	2:Z:459:LEU:HD22	1.64	0.80
1:F:108:ILE:HD12	1:F:819:LEU:HD11	1.63	0.80
1:F:308:LEU:HD13	1:F:570:PRO:HB3	1.64	0.80
1:E:263:ILE:HD11	1:H:373:MET:HE1	1.64	0.79
1:F:711:HIS:HD2	1:F:713:ILE:HB	1.48	0.79
1:J:479:ASP:OD1	1:J:480:ARG:N	2.16	0.79
1:E:120:ILE:HG22	1:E:121:ASP:H	1.47	0.78
1:F:689:ILE:HG13	1:F:691:SER:O	1.83	0.78
1:E:66:LYS:HD2	1:E:305:ARG:HE	1.48	0.78
1:B:479:ASP:OD1	1:B:480:ARG:N	2.16	0.78
2:Z:1153:ARG:HB2	2:Z:1309:GLN:HE22	1.49	0.78
1:J:34:THR:HG23	1:J:35:THR:HG23	1.66	0.78
1:G:733:LEU:HD12	1:G:734:GLU:H	1.49	0.77
2:Z:390:GLU:HB3	2:Z:391:ILE:HD12	1.67	0.77
1:B:123:ARG:HB2	1:I:160:SER:HB3	1.65	0.76
1:F:712:PRO:HG3	1:F:784:PHE:HB3	1.67	0.76
1:H:469:ILE:HD11	1:H:536:SER:HA	1.67	0.76
1:F:108:ILE:HD13	1:F:821:VAL:HG12	1.67	0.76
2:Z:457:HIS:HB2	2:Z:460:ALA:HB2	1.68	0.76
1:D:117:GLY:O	1:D:134:ILE:HG12	1.84	0.76
2:Z:522:THR:OG1	2:Z:523:GLN:OE1	2.04	0.75
1:E:160:SER:HB3	1:H:123:ARG:HB3	1.69	0.75
1:B:34:THR:HG23	1:B:35:THR:HG23	1.67	0.75
1:C:139:MET:HE3	1:C:671:ALA:HB1	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:710:LEU:H	1:F:787:VAL:HG22	1.52	0.74
1:G:717:GLN:OE1	1:G:717:GLN:N	2.19	0.74
1:H:521:GLU:N	1:H:521:GLU:OE1	2.21	0.74
2:Z:827:ASP:HA	2:Z:895:ASN:HD21	1.51	0.74
1:F:688:TYR:HA	1:F:751:PHE:O	1.88	0.74
1:I:357:MET:CE	1:I:534:MET:HG2	2.13	0.73
1:G:592:THR:HG22	1:H:53:ASN:H	1.51	0.73
1:B:308:LEU:HD13	1:B:570:PRO:HB3	1.70	0.73
1:D:126:SER:C	1:D:128:SER:N	2.44	0.73
1:G:160:SER:HB2	1:J:123:ARG:HB3	1.71	0.73
2:Z:819:LEU:HB2	2:Z:954:PHE:HB3	1.68	0.73
1:B:181:GLU:HG3	1:B:791:ARG:HE	1.54	0.73
1:F:688:TYR:O	1:F:689:ILE:C	2.32	0.73
2:Z:304:LEU:HD21	2:Z:328:LEU:HD11	1.71	0.73
1:B:11:ARG:HH11	1:C:618:ILE:HG23	1.53	0.72
1:C:318:GLU:OE1	1:C:318:GLU:N	2.21	0.72
1:F:459:GLU:OE2	1:F:480:ARG:NH1	2.22	0.72
1:H:121:ASP:HB2	1:H:124:ASP:OD1	1.89	0.72
2:Z:342:TYR:HA	2:Z:345:SER:HB3	1.71	0.72
1:H:526:ASP:OD2	1:H:571:ARG:NH2	2.22	0.72
1:E:596:MET:HE1	1:E:622:ASN:HB3	1.72	0.72
1:H:520:ASP:OD1	1:H:521:GLU:N	2.21	0.72
1:I:318:GLU:N	1:I:318:GLU:OE1	2.23	0.72
1:G:760:GLU:OE1	1:G:793:ASN:ND2	2.22	0.72
1:J:90:ASN:HB2	1:J:149:LYS:HB3	1.72	0.71
1:D:90:ASN:HB2	1:D:149:LYS:HB3	1.72	0.71
1:B:430:SER:HB3	1:B:433:GLN:HG3	1.72	0.71
1:G:790:GLU:OE1	1:G:792:ARG:NH2	2.23	0.71
2:Z:959:ASP:OD1	2:Z:960:GLU:N	2.24	0.71
1:C:347:GLU:OE1	2:Z:665:ARG:N	2.23	0.71
1:H:373:MET:HE3	1:H:374:ASN:H	1.56	0.71
1:B:126:SER:C	1:B:128:SER:N	2.36	0.70
1:F:120:ILE:HD13	1:F:750:PRO:HD2	1.73	0.70
1:A:318:GLU:N	1:A:318:GLU:OE1	2.23	0.70
1:H:269:THR:HG22	1:H:271:ALA:H	1.54	0.70
1:F:108:ILE:HD11	1:F:707:PHE:CZ	2.27	0.70
2:Z:512:VAL:HG11	2:Z:568:ARG:HB3	1.74	0.70
2:Z:924:ARG:NH2	2:Z:976:GLU:OE1	2.24	0.70
1:D:318:GLU:N	1:D:318:GLU:OE2	2.25	0.70
1:G:262:ARG:HE	1:G:462:PRO:HG3	1.55	0.70
1:D:346:THR:HG22	1:D:562:ALA:HB1	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:682:ALA:HB1	2:Z:758:PRO:HA	1.74	0.70
1:C:733:LEU:O	1:C:734:GLU:HG3	1.92	0.69
1:A:493:GLU:OE1	1:A:493:GLU:N	2.25	0.69
1:F:122:ARG:O	1:F:123:ARG:HB2	1.90	0.69
1:F:448:LYS:NZ	1:F:493:GLU:OE2	2.24	0.69
1:J:269:THR:HG22	1:J:271:ALA:H	1.55	0.69
1:C:90:ASN:HB2	1:C:149:LYS:HB3	1.73	0.69
1:F:34:THR:HG23	1:F:35:THR:HG23	1.73	0.69
1:I:297:GLN:HE21	1:I:358:GLN:HE22	1.37	0.69
1:A:219:LYS:HG3	1:A:836:ASP:HB2	1.73	0.69
1:A:257:MET:HE3	1:A:466:ARG:HG3	1.74	0.69
1:B:126:SER:O	1:B:128:SER:N	2.26	0.69
1:H:210:GLN:N	1:H:210:GLN:OE1	2.20	0.69
1:B:24:ILE:HD11	1:D:260:ASP:HB3	1.74	0.69
1:G:219:LYS:HG3	1:G:836:ASP:HB2	1.73	0.69
1:F:180:LEU:HD23	1:F:182:LEU:HD21	1.73	0.69
1:B:267:LYS:HZ2	1:B:268:LEU:N	1.90	0.69
1:J:378:SER:HB3	1:J:381:ILE:HG13	1.75	0.69
2:Z:418:GLU:OE2	2:Z:1057:ARG:NH2	2.24	0.69
1:A:309:ASP:HB2	2:Z:530:LYS:HD2	1.73	0.69
1:D:266:GLN:N	1:D:266:GLN:OE1	2.26	0.69
1:H:459:GLU:OE1	1:H:480:ARG:NH1	2.25	0.69
1:J:258:VAL:O	1:J:854:ARG:NH2	2.26	0.69
1:J:639:MET:HE3	1:J:658:ILE:HD11	1.75	0.68
1:F:683:PRO:HA	1:F:688:TYR:CE1	2.28	0.68
1:C:506:ARG:HD3	1:C:507:LYS:H	1.58	0.68
1:I:355:LYS:NZ	1:I:554:ALA:O	2.25	0.68
1:G:260:ASP:OD1	1:G:262:ARG:N	2.27	0.68
2:Z:920:GLU:OE2	2:Z:924:ARG:NH1	2.26	0.68
1:C:689:ILE:HD13	1:C:814:ILE:HD12	1.76	0.68
1:C:790:GLU:OE1	1:C:792:ARG:NH2	2.27	0.68
1:D:210:GLN:OE1	1:D:210:GLN:N	2.27	0.68
1:B:267:LYS:HZ2	1:B:268:LEU:H	1.42	0.67
1:D:120:ILE:HD11	1:D:750:PRO:HB2	1.74	0.67
1:G:459:GLU:OE1	1:G:459:GLU:N	2.28	0.67
1:B:123:ARG:HB2	1:I:160:SER:HB2	1.74	0.67
1:C:530:THR:HG21	1:C:571:ARG:HA	1.75	0.67
1:G:160:SER:CB	1:J:123:ARG:HB3	2.25	0.67
1:E:160:SER:CB	1:H:123:ARG:HB3	2.23	0.67
2:Z:129:HIS:HD2	2:Z:131:PRO:HD3	1.60	0.67
1:J:494:LEU:O	1:J:507:LYS:NZ	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:518:ARG:HG2	1:I:518:ARG:HH11	1.59	0.67
1:I:760:GLU:OE2	1:I:802:ARG:NH2	2.28	0.67
1:B:21:ASP:HA	1:B:24:ILE:HG22	1.76	0.67
1:C:319:LYS:NZ	1:C:516:VAL:O	2.28	0.67
1:F:107:TYR:HB2	1:F:822:LEU:HB2	1.77	0.67
2:Z:493:ARG:HH21	2:Z:582:ILE:HD11	1.60	0.67
2:Z:1362:ARG:HH21	2:Z:1366:PRO:HA	1.60	0.67
1:D:126:SER:O	1:D:128:SER:N	2.28	0.66
1:F:108:ILE:HD11	1:F:707:PHE:CE2	2.31	0.66
1:F:692:VAL:HG21	1:F:782:LEU:CD1	2.25	0.66
1:H:34:THR:HG23	1:H:35:THR:HG23	1.76	0.66
1:F:108:ILE:HG23	1:F:819:LEU:HD12	1.77	0.66
1:H:690:ASP:OD1	1:H:691:SER:N	2.29	0.66
1:J:851:GLU:N	1:J:851:GLU:OE1	2.28	0.66
1:D:14:LEU:O	1:D:18:VAL:HG12	1.95	0.66
1:E:272:GLU:N	1:E:272:GLU:OE2	2.28	0.66
1:G:261:ARG:NH1	1:J:431:ASP:OD2	2.28	0.66
1:B:269:THR:HG22	1:B:271:ALA:H	1.61	0.66
1:B:332:LEU:HD22	2:Z:1227:VAL:HG11	1.78	0.66
1:B:419:TYR:CZ	1:B:423:MET:HE1	2.31	0.66
1:E:456:LEU:HD23	1:E:471:ARG:HD3	1.76	0.66
1:H:647:PRO:HG2	1:H:650:ASP:HB2	1.77	0.66
1:A:378:SER:HB3	1:A:381:ILE:HG12	1.76	0.65
1:C:851:GLU:OE2	1:C:852:TYR:N	2.30	0.65
2:Z:441:PHE:CZ	2:Z:461:HIS:HA	2.32	0.65
2:Z:1045:THR:O	2:Z:1049:ILE:HG13	1.97	0.65
1:F:690:ASP:OD1	1:F:691:SER:N	2.29	0.65
1:I:529:THR:O	1:I:533:ILE:HG23	1.97	0.65
2:Z:387:PHE:HB2	2:Z:458:LEU:HD21	1.78	0.65
1:D:666:HIS:HD2	1:D:669:ALA:H	1.43	0.65
1:H:177:ILE:HD13	1:H:182:LEU:HD13	1.79	0.65
1:H:220:ARG:HG2	1:H:220:ARG:HH11	1.61	0.65
2:Z:259:PRO:HD2	2:Z:261:ARG:HH22	1.62	0.65
1:I:530:THR:HA	1:I:533:ILE:HG12	1.79	0.65
2:Z:554:THR:HG23	2:Z:998:ARG:HB3	1.79	0.65
1:J:267:LYS:HZ2	1:J:269:THR:H	1.42	0.65
1:F:711:HIS:CD2	1:F:713:ILE:HB	2.31	0.64
1:I:90:ASN:HB2	1:I:149:LYS:HB3	1.79	0.64
1:A:90:ASN:HB2	1:A:149:LYS:HB3	1.79	0.64
2:Z:61:PHE:HE2	2:Z:1060:LYS:HG2	1.61	0.64
1:A:532:ARG:NH1	1:D:501:GLU:OE1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:HZ2	1:D:269:THR:H	1.46	0.64
1:I:357:MET:HE2	1:I:534:MET:CG	2.16	0.64
2:Z:1021:PHE:HB3	2:Z:1044:ILE:HG21	1.79	0.64
1:G:732:ARG:NH1	1:H:267:LYS:O	2.30	0.64
1:I:139:MET:HE3	1:I:671:ALA:HB1	1.80	0.64
1:A:733:LEU:O	1:A:734:GLU:HG3	1.98	0.64
1:C:768:SER:OG	1:C:779:ASN:ND2	2.31	0.64
1:B:760:GLU:HG2	1:B:793:ASN:HD21	1.62	0.64
2:Z:719:PRO:HB2	2:Z:721:LEU:HG	1.80	0.64
1:B:431:ASP:OD2	1:I:261:ARG:NH2	2.31	0.64
1:C:732:ARG:HG3	1:C:733:LEU:O	1.98	0.64
1:A:526:ASP:OD2	1:A:571:ARG:NH2	2.30	0.64
2:Z:129:HIS:CD2	2:Z:131:PRO:HD3	2.33	0.64
1:E:90:ASN:HB2	1:E:149:LYS:HB3	1.80	0.63
1:E:297:GLN:NE2	1:E:358:GLN:OE1	2.31	0.63
1:G:732:ARG:NH2	1:G:734:GLU:OE2	2.31	0.63
1:H:21:ASP:OD2	1:I:123:ARG:NH2	2.32	0.63
1:B:116:THR:OG1	1:B:137:LYS:NZ	2.31	0.63
1:I:713:ILE:HD11	1:I:817:PHE:HB3	1.80	0.63
2:Z:80:LEU:HD11	2:Z:1103:ILE:HD11	1.80	0.63
2:Z:1233:GLN:HA	2:Z:1248:ARG:HD2	1.80	0.63
2:Z:1126:ILE:HB	2:Z:1197:ASN:HD21	1.61	0.63
2:Z:1207:ASN:OD1	2:Z:1208:GLY:N	2.32	0.63
1:F:526:ASP:OD2	1:F:571:ARG:NH2	2.31	0.63
1:G:696:HIS:CD2	1:G:697:ASN:HD22	2.17	0.63
2:Z:1141:ILE:HG13	2:Z:1144:LEU:HD22	1.80	0.63
1:C:248:GLU:OE2	1:C:249:GLN:NE2	2.31	0.63
1:F:269:THR:HG22	1:F:271:ALA:H	1.63	0.63
2:Z:513:MET:HG3	2:Z:594:THR:HG21	1.79	0.63
2:Z:1116:ASP:N	2:Z:1116:ASP:OD1	2.31	0.63
1:C:292:MET:HE1	1:C:590:TYR:CG	2.34	0.63
1:D:140:MET:HE1	1:D:626:VAL:HG13	1.81	0.63
1:B:682:GLU:OE1	1:B:818:GLN:NE2	2.26	0.63
1:I:824:ASP:OD1	1:I:825:LEU:N	2.31	0.63
1:J:122:ARG:HG2	1:J:726:GLN:HB2	1.80	0.63
1:H:122:ARG:HG2	1:H:726:GLN:HB2	1.79	0.63
2:Z:208:ARG:HG3	2:Z:209:VAL:HG23	1.80	0.63
1:B:103:GLU:O	1:B:791:ARG:NH1	2.32	0.62
1:G:90:ASN:HB2	1:G:149:LYS:HB3	1.81	0.62
2:Z:312:ARG:HE	2:Z:504:THR:HG21	1.64	0.62
1:B:250:ARG:O	1:B:254:ILE:HD12	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:O	1:C:255:THR:HG23	1.98	0.62
1:C:351:GLU:HA	2:Z:850:ILE:HG12	1.80	0.62
1:H:298:LEU:HD22	1:H:642:TYR:CE2	2.34	0.62
2:Z:799:ILE:HD12	2:Z:801:HIS:CE1	2.34	0.62
1:A:461:GLU:HG2	1:A:576:VAL:HG21	1.80	0.62
1:E:248:GLU:OE2	1:E:249:GLN:NE2	2.32	0.62
1:F:677:THR:O	1:F:681:ARG:HG2	1.99	0.62
1:H:29:ARG:NH1	1:H:29:ARG:HA	2.14	0.62
1:H:87:LEU:HD11	1:H:278:ARG:HB2	1.80	0.62
1:G:260:ASP:OD1	1:G:261:ARG:N	2.32	0.62
1:G:445:ARG:HD2	1:G:445:ARG:N	2.14	0.62
1:F:709:HIS:HB2	1:F:787:VAL:HG22	1.80	0.62
2:Z:396:MET:SD	2:Z:1029:SER:OG	2.57	0.62
1:A:689:ILE:HD13	1:A:814:ILE:HD12	1.80	0.62
2:Z:716:GLN:HB2	2:Z:1188:PRO:HD3	1.81	0.62
2:Z:733:THR:HG22	2:Z:762:PRO:HB2	1.80	0.62
1:C:380:GLU:CD	1:C:380:GLU:H	2.08	0.61
1:D:406:ALA:HB1	1:D:438:ILE:HG21	1.81	0.61
1:G:508:ASP:HB3	1:G:511:ARG:HH21	1.64	0.61
1:I:808:MET:HA	1:I:808:MET:HE2	1.81	0.61
2:Z:940:ASP:OD1	2:Z:940:ASP:N	2.34	0.61
1:B:288:LEU:O	1:B:291:LYS:NZ	2.33	0.61
1:A:123:ARG:HH22	1:J:17:GLN:NE2	1.99	0.61
2:Z:466:CYS:O	2:Z:470:ILE:HG13	2.01	0.61
1:C:169:GLU:HG3	1:C:832:ARG:HH21	1.64	0.61
1:D:308:LEU:HD13	1:D:570:PRO:HB3	1.82	0.61
1:A:323:LEU:HD23	1:A:341:ILE:HD13	1.81	0.61
2:Z:966:GLU:OE2	2:Z:966:GLU:N	2.31	0.61
1:B:31:LEU:HD23	1:B:31:LEU:H	1.66	0.61
1:G:733:LEU:O	1:G:734:GLU:HG3	2.01	0.61
2:Z:1386:PHE:HA	2:Z:1389:MET:HE3	1.82	0.61
1:F:792:ARG:HG3	1:F:792:ARG:HH11	1.65	0.61
2:Z:1043:ASP:OD1	2:Z:1044:ILE:N	2.34	0.61
1:A:506:ARG:NH2	1:I:328:LYS:HG3	2.15	0.60
1:G:445:ARG:HD2	1:G:445:ARG:H	1.66	0.60
1:B:378:SER:HB3	1:B:381:ILE:HG12	1.82	0.60
1:D:91:THR:HG22	1:D:153:ASP:HB3	1.83	0.60
2:Z:540:LYS:HD3	2:Z:1257:ASP:HB2	1.83	0.60
2:Z:894:ASP:CG	2:Z:896:ARG:H	2.08	0.60
1:E:210:GLN:N	1:E:210:GLN:OE1	2.31	0.60
1:H:488:ASN:OD1	1:H:489:CYS:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:MET:HE3	1:C:171:MET:H	1.65	0.60
1:D:116:THR:OG1	1:D:117:GLY:N	2.30	0.60
1:F:112:ILE:HG22	1:F:113:GLN:H	1.66	0.60
1:I:733:LEU:HD12	1:I:734:GLU:H	1.66	0.60
1:J:684:GLU:CD	1:J:684:GLU:H	2.09	0.60
1:I:808:MET:SD	1:I:809:TYR:N	2.70	0.60
2:Z:73:ILE:HD12	2:Z:74:HIS:H	1.65	0.60
1:C:800:SER:O	1:C:804:LYS:NZ	2.34	0.60
1:F:210:GLN:N	1:F:210:GLN:OE1	2.33	0.60
1:F:692:VAL:HG21	1:F:782:LEU:HD13	1.83	0.60
1:B:406:ALA:HB1	1:B:438:ILE:HG21	1.82	0.60
1:I:250:ARG:HG2	1:I:847:ILE:HD12	1.81	0.60
1:I:798:VAL:HG12	1:I:800:SER:H	1.67	0.60
1:D:94:GLN:OE1	1:D:94:GLN:N	2.25	0.59
1:H:29:ARG:HA	1:H:29:ARG:HH11	1.67	0.59
1:I:139:MET:HE1	1:I:235:LEU:HD21	1.84	0.59
1:I:330:ASN:OD1	1:I:331:ILE:N	2.35	0.59
1:E:121:ASP:O	1:E:122:ARG:HG2	2.01	0.59
1:E:401:SER:O	1:E:405:ILE:HG12	2.02	0.59
2:Z:60:PRO:C	2:Z:62:THR:H	2.10	0.59
1:A:248:GLU:OE2	1:A:249:GLN:NE2	2.35	0.59
1:F:453:SER:OG	1:F:454:THR:N	2.34	0.59
1:H:181:GLU:O	1:H:791:ARG:NH1	2.35	0.59
1:A:699:ASP:OD2	1:A:716:ASN:ND2	2.35	0.59
1:H:11:ARG:HE	1:I:618:ILE:HG23	1.68	0.59
1:C:733:LEU:HD12	1:C:734:GLU:H	1.66	0.59
1:G:104:GLU:HA	1:G:791:ARG:HH21	1.67	0.59
1:I:345:ASN:OD1	1:I:347:GLU:N	2.35	0.59
2:Z:801:HIS:CD2	2:Z:802:ILE:HG12	2.36	0.59
1:B:488:ASN:OD1	1:B:489:CYS:N	2.34	0.59
1:D:124:ASP:OD1	1:D:606:ARG:NH1	2.35	0.59
2:Z:311:SER:OG	2:Z:312:ARG:NH1	2.33	0.59
1:C:183:THR:HG23	1:C:185:ALA:H	1.67	0.59
1:G:406:ALA:HB1	1:G:438:ILE:HG21	1.84	0.59
1:G:138:LEU:HD23	1:G:675:LEU:HD21	1.84	0.58
2:Z:1079:MET:HE2	2:Z:1202:VAL:HG22	1.83	0.58
1:H:165:GLU:OE1	1:H:165:GLU:N	2.35	0.58
1:A:150:ILE:HG21	1:A:835:LEU:HD22	1.85	0.58
1:H:822:LEU:HD23	1:H:828:LEU:HD22	1.85	0.58
1:E:595:GLN:O	1:E:599:THR:HG22	2.04	0.58
1:F:25:LEU:HD23	1:H:76:ASN:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:GLU:OE1	1:F:79:GLU:N	2.37	0.58
1:C:160:SER:OG	1:F:123:ARG:NH2	2.35	0.58
1:F:291:LYS:NZ	1:F:661:ASP:OD1	2.37	0.58
1:H:459:GLU:OE2	1:H:532:ARG:NH1	2.36	0.58
1:J:359:ALA:HB2	1:J:367:ILE:HD11	1.86	0.58
1:A:593:ILE:HG21	1:A:655:LEU:HD13	1.86	0.58
1:B:524:ALA:HA	1:B:527:MET:HG3	1.86	0.58
1:D:378:SER:HB3	1:D:381:ILE:HG12	1.85	0.58
1:F:113:GLN:HG3	1:F:686:PHE:O	2.04	0.58
2:Z:549:THR:HG22	2:Z:551:GLU:H	1.67	0.58
1:I:104:GLU:N	1:I:104:GLU:OE1	2.37	0.58
1:G:736:GLN:NE2	1:G:775:ASN:OD1	2.32	0.58
1:I:345:ASN:OD1	1:I:346:THR:N	2.36	0.58
1:F:36:VAL:HG23	1:H:302:HIS:CE1	2.39	0.58
1:F:710:LEU:O	1:F:787:VAL:N	2.34	0.58
2:Z:534:TYR:CE1	2:Z:810:VAL:HG12	2.39	0.58
1:B:71:LEU:HG	1:J:14:LEU:HG	1.87	0.57
1:E:143:SER:HG	1:E:239:TYR:HH	1.52	0.57
1:I:77:ARG:NE	1:I:77:ARG:HA	2.18	0.57
1:C:628:ASN:OD1	1:C:636:LYS:NZ	2.36	0.57
1:I:406:ALA:HB1	1:I:438:ILE:HG21	1.86	0.57
2:Z:1269:LEU:HD11	2:Z:1286:ILE:HD13	1.86	0.57
1:A:160:SER:OG	1:D:123:ARG:NH2	2.37	0.57
1:A:289:PHE:HA	1:A:292:MET:HE2	1.85	0.57
1:B:99:LEU:HD22	1:B:180:LEU:HD11	1.87	0.57
1:H:94:GLN:HA	1:H:229:GLN:HE22	1.70	0.57
1:E:183:THR:O	1:E:187:THR:OG1	2.20	0.57
1:J:488:ASN:OD1	1:J:489:CYS:N	2.36	0.57
2:Z:569:ILE:HD11	2:Z:588:ILE:HG22	1.86	0.57
2:Z:1417:GLN:HG2	2:Z:1418:LEU:HD23	1.86	0.57
1:A:406:ALA:HB1	1:A:438:ILE:HG21	1.85	0.57
1:A:478:VAL:HG13	1:A:482:GLY:HA2	1.87	0.57
1:B:762:GLU:OE1	1:B:762:GLU:N	2.38	0.57
1:H:406:ALA:HB1	1:H:438:ILE:HG21	1.86	0.57
2:Z:386:ARG:O	2:Z:390:GLU:HB2	2.04	0.57
2:Z:438:ASP:CB	2:Z:456:GLY:HA3	2.34	0.57
2:Z:496:MET:HA	2:Z:496:MET:HE2	1.87	0.57
1:I:251:ARG:NH1	1:I:266:GLN:O	2.34	0.57
1:I:275:GLN:HG2	1:I:841:PRO:HG2	1.87	0.57
1:E:406:ALA:HB1	1:E:438:ILE:HG21	1.87	0.57
1:E:853:VAL:HG12	1:H:556:GLU:HG3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:ASP:HA	1:J:606:ARG:HD3	1.87	0.57
1:D:633:ASP:HB3	1:D:636:LYS:HB3	1.86	0.57
2:Z:210:VAL:HB	2:Z:1080:HIS:HB2	1.86	0.57
2:Z:483:THR:HA	2:Z:486:ASP:HB3	1.86	0.57
2:Z:661:SER:OG	2:Z:662:THR:N	2.38	0.57
1:D:23:ARG:NH1	1:F:461:GLU:OE1	2.28	0.56
1:D:479:ASP:OD1	1:D:480:ARG:N	2.27	0.56
1:F:108:ILE:HD13	1:F:821:VAL:CG1	2.35	0.56
2:Z:303:ASN:HA	2:Z:885:LEU:HD11	1.86	0.56
2:Z:827:ASP:HA	2:Z:895:ASN:ND2	2.20	0.56
1:B:96:LEU:HD23	1:B:96:LEU:H	1.70	0.56
1:D:318:GLU:OE1	2:Z:645:LYS:NZ	2.31	0.56
1:F:263:ILE:HD13	1:F:851:GLU:HB3	1.85	0.56
1:B:7:LEU:HD12	1:D:68:ILE:HD12	1.87	0.56
1:C:262:ARG:HH21	1:C:462:PRO:HB3	1.71	0.56
1:F:120:ILE:HD11	1:F:122:ARG:NH1	2.20	0.56
1:G:319:LYS:NZ	1:G:516:VAL:O	2.38	0.56
1:J:102:PRO:HA	1:J:790:GLU:HA	1.86	0.56
2:Z:113:PRO:O	2:Z:114:GLN:NE2	2.34	0.56
2:Z:893:HIS:O	2:Z:894:ASP:HB3	2.04	0.56
1:D:718:PRO:HG3	1:D:746:ARG:HE	1.69	0.56
1:E:184:GLU:OE1	1:E:184:GLU:N	2.39	0.56
1:F:2:ALA:O	1:F:5:THR:OG1	2.22	0.56
1:H:90:ASN:HB2	1:H:149:LYS:HB3	1.87	0.56
1:I:328:LYS:O	1:I:328:LYS:NZ	2.37	0.56
1:C:262:ARG:NH1	1:F:423:MET:HE3	2.20	0.56
1:G:647:PRO:HG2	1:G:650:ASP:OD1	2.06	0.56
1:H:247:LYS:HG3	1:H:847:ILE:HD11	1.87	0.56
1:I:309:ASP:OD1	1:I:309:ASP:N	2.34	0.56
2:Z:211:LEU:HD22	2:Z:1205:ILE:HD11	1.86	0.56
2:Z:445:MET:SD	2:Z:445:MET:N	2.78	0.56
1:D:522:ASP:OD1	1:D:523:ARG:N	2.38	0.56
1:E:305:ARG:HG3	1:E:354:ILE:HD13	1.87	0.56
1:G:139:MET:HE2	1:G:671:ALA:HB1	1.86	0.56
2:Z:194:LYS:HE3	2:Z:195:PRO:HD2	1.87	0.56
1:A:319:LYS:NZ	1:A:516:VAL:O	2.38	0.56
1:F:122:ARG:CZ	1:F:725:ALA:HB3	2.36	0.56
1:A:49:ASN:O	1:A:53:ASN:ND2	2.39	0.56
1:B:416:ASP:OD1	1:B:416:ASP:N	2.38	0.56
1:E:300:ILE:HD12	1:E:362:LEU:HD11	1.86	0.56
1:C:759:SER:OG	1:C:761:GLU:OE2	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:373:MET:SD	1:I:381:ILE:HG21	2.45	0.56
1:G:378:SER:HB3	1:G:381:ILE:HG12	1.88	0.56
1:I:140:MET:HE1	1:J:61:LEU:HD22	1.87	0.56
1:I:696:HIS:CD2	1:I:697:ASN:HD22	2.23	0.56
1:I:736:GLN:NE2	1:I:775:ASN:OD1	2.37	0.56
2:Z:286:LEU:HD22	2:Z:625:LEU:HD21	1.88	0.56
2:Z:314:ARG:CA	2:Z:459:LEU:HD22	2.35	0.55
1:B:214:SER:OG	1:B:249:GLN:NE2	2.35	0.55
1:E:126:SER:O	1:E:127:PHE:HB2	2.06	0.55
1:E:169:GLU:HG3	1:E:832:ARG:HH21	1.71	0.55
1:F:713:ILE:HD11	1:F:786:PHE:CE2	2.41	0.55
1:G:433:GLN:N	1:G:433:GLN:OE1	2.39	0.55
1:H:402:ASN:OD1	1:H:451:ARG:NH2	2.39	0.55
1:C:71:LEU:HA	1:C:74:ILE:HD12	1.87	0.55
1:E:577:ASP:OD1	1:E:578:THR:N	2.40	0.55
1:G:456:LEU:HD13	1:G:471:ARG:HD3	1.88	0.55
1:H:64:VAL:O	1:H:68:ILE:HG22	2.06	0.55
1:F:710:LEU:HB3	1:F:787:VAL:CG1	2.33	0.55
1:G:577:ASP:OD1	1:G:578:THR:N	2.39	0.55
1:H:372:PRO:HG2	1:H:381:ILE:HD11	1.88	0.55
2:Z:1002:GLU:HG3	2:Z:1007:SER:HB3	1.87	0.55
1:C:219:LYS:HG3	1:C:836:ASP:HB2	1.89	0.55
1:J:124:ASP:OD1	1:J:125:ALA:N	2.40	0.55
1:E:313:PHE:HB2	1:E:566:THR:HG21	1.89	0.55
1:E:733:LEU:O	1:E:734:GLU:HG3	2.07	0.55
1:I:529:THR:O	1:I:533:ILE:HG12	2.06	0.55
1:J:647:PRO:HG2	1:J:650:ASP:OD2	2.07	0.55
2:Z:798:ALA:HB1	2:Z:1341:TYR:CE1	2.42	0.55
1:E:532:ARG:NE	1:H:501:GLU:OE1	2.40	0.55
1:I:202:SER:OG	1:I:203:THR:N	2.39	0.55
1:J:453:SER:OG	1:J:454:THR:N	2.38	0.55
2:Z:286:LEU:HB3	2:Z:298:LEU:HD11	1.87	0.55
2:Z:508:ASP:OD2	2:Z:567:LYS:HE2	2.06	0.55
2:Z:1404:TRP:HA	2:Z:1407:ILE:HG22	1.88	0.55
1:B:123:ARG:NH2	1:I:160:SER:OG	2.40	0.55
1:B:318:GLU:O	1:B:322:GLN:HG3	2.07	0.55
1:F:406:ALA:HB1	1:F:438:ILE:HG21	1.89	0.55
1:H:116:THR:HG23	1:H:117:GLY:N	2.21	0.55
1:I:421:ASP:OD1	1:I:421:ASP:N	2.39	0.55
1:I:518:ARG:HG2	1:I:518:ARG:NH1	2.21	0.55
1:B:116:THR:C	1:B:137:LYS:HZ3	2.14	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:VAL:C	1:F:107:TYR:CG	2.85	0.54
1:F:345:ASN:HD21	1:F:347:GLU:HB2	1.72	0.54
1:I:684:GLU:CD	1:I:684:GLU:H	2.15	0.54
2:Z:1114:ASN:O	2:Z:1114:ASN:ND2	2.38	0.54
1:D:297:GLN:NE2	1:D:358:GLN:OE1	2.40	0.54
1:E:732:ARG:HG2	1:E:733:LEU:O	2.08	0.54
1:J:330:ASN:O	1:J:333:THR:OG1	2.21	0.54
1:B:603:ASP:OD1	1:B:603:ASP:N	2.37	0.54
1:F:488:ASN:OD1	1:F:489:CYS:N	2.39	0.54
1:F:689:ILE:HG23	1:F:689:ILE:O	2.06	0.54
1:F:709:HIS:HB2	1:F:787:VAL:HG23	1.89	0.54
2:Z:807:ILE:O	2:Z:810:VAL:HG22	2.07	0.54
1:D:231:VAL:HG11	1:D:678:ILE:HD11	1.88	0.54
1:H:267:LYS:HZ2	1:H:269:THR:H	1.55	0.54
2:Z:1337:ASP:O	2:Z:1339:GLY:N	2.41	0.54
1:J:257:MET:N	1:J:257:MET:HE2	2.22	0.54
1:B:251:ARG:HD3	1:B:268:LEU:HD11	1.88	0.54
1:C:717:GLN:N	1:C:717:GLN:OE1	2.41	0.54
1:D:267:LYS:NZ	1:D:269:THR:H	2.06	0.54
1:F:108:ILE:CG2	1:F:819:LEU:HD12	2.36	0.54
1:G:376:SER:OG	1:G:377:LEU:N	2.41	0.54
1:J:116:THR:OG1	1:J:117:GLY:N	2.38	0.54
1:J:523:ARG:O	1:J:527:MET:HG3	2.07	0.54
2:Z:1296:ALA:HB1	2:Z:1300:GLY:HA3	1.90	0.54
1:B:167:SER:HB2	1:B:221:VAL:HG12	1.89	0.54
1:C:611:GLU:OE1	1:C:611:GLU:N	2.41	0.54
2:Z:1411:ASN:O	2:Z:1415:ILE:HG12	2.08	0.54
1:B:372:PRO:HG2	1:B:381:ILE:HD11	1.90	0.54
1:B:709:HIS:CE1	1:B:789:ARG:HE	2.26	0.54
1:C:406:ALA:HB1	1:C:438:ILE:HG21	1.89	0.54
1:D:460:ASN:HB2	1:D:536:SER:HB3	1.89	0.54
1:G:633:ASP:N	1:G:633:ASP:OD1	2.40	0.54
1:H:101:SER:HB3	1:H:180:LEU:HD22	1.89	0.54
1:D:225:GLY:O	1:D:830:ARG:NH1	2.41	0.54
2:Z:320:THR:OG1	2:Z:321:LEU:N	2.40	0.54
1:A:115:TYR:OH	1:A:137:LYS:HD2	2.08	0.53
1:C:65:ILE:HD11	2:Z:842:ARG:HE	1.72	0.53
1:E:160:SER:OG	1:H:123:ARG:NH2	2.41	0.53
2:Z:67:SER:O	2:Z:71:GLN:NE2	2.40	0.53
2:Z:1300:GLY:O	2:Z:1304:VAL:HG23	2.08	0.53
2:Z:1311:PRO:HG2	2:Z:1314:LEU:HD21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:MET:HG3	1:A:809:TYR:N	2.22	0.53
2:Z:568:ARG:NH1	2:Z:591:CYS:SG	2.81	0.53
1:G:728:TRP:CH2	1:G:736:GLN:HB2	2.42	0.53
1:J:266:GLN:OE1	1:J:266:GLN:N	2.41	0.53
2:Z:519:THR:OG1	2:Z:520:GLN:OE1	2.25	0.53
2:Z:687:LEU:HD23	2:Z:723:LYS:NZ	2.23	0.53
2:Z:1160:THR:HG22	2:Z:1161:SER:H	1.73	0.53
2:Z:1375:ASN:OD1	2:Z:1376:ARG:N	2.42	0.53
1:D:684:GLU:CD	1:D:684:GLU:H	2.15	0.53
1:E:119:VAL:CB	1:F:69:GLU:OE2	2.50	0.53
1:F:102:PRO:HB3	1:F:789:ARG:O	2.09	0.53
1:H:442:LEU:HD22	1:H:449:LEU:HD12	1.90	0.53
2:Z:300:GLN:HG2	2:Z:886:GLY:HA3	1.89	0.53
2:Z:690:ARG:CG	2:Z:692:TYR:CE1	2.91	0.53
2:Z:739:ILE:HD13	2:Z:878:ARG:HB2	1.89	0.53
2:Z:1156:ARG:HB3	2:Z:1160:THR:HB	1.90	0.53
1:F:784:PHE:HE1	1:F:812:VAL:HG22	1.73	0.53
2:Z:546:GLU:OE2	2:Z:1236:TYR:HB3	2.09	0.53
2:Z:806:GLU:O	2:Z:810:VAL:HG13	2.09	0.53
2:Z:1198:ALA:O	2:Z:1202:VAL:HG23	2.08	0.53
1:H:82:ASP:OD1	1:H:83:ASP:N	2.42	0.53
2:Z:989:ILE:HD12	2:Z:990:ASN:H	1.74	0.53
2:Z:1025:GLU:OE1	2:Z:1026:LYS:HB2	2.08	0.53
1:C:160:SER:C	1:C:162:LEU:H	2.16	0.53
1:E:404:ILE:HD12	1:E:423:MET:HE1	1.90	0.53
1:E:689:ILE:HD13	1:E:814:ILE:HD12	1.89	0.53
1:F:364:ARG:NH2	1:F:544:ASP:OD1	2.42	0.53
1:F:688:TYR:O	1:F:690:ASP:N	2.42	0.53
1:G:701:ASP:HB3	1:G:715:THR:HG23	1.91	0.53
1:D:187:THR:HA	1:D:190:LEU:HD23	1.91	0.53
1:D:488:ASN:OD1	1:D:489:CYS:N	2.41	0.53
1:D:520:ASP:OD1	1:D:521:GLU:N	2.42	0.53
1:D:697:ASN:OD1	1:D:697:ASN:N	2.41	0.53
2:Z:401:ASP:O	2:Z:405:ASN:HB2	2.08	0.53
2:Z:637:PHE:HD1	2:Z:637:PHE:O	1.92	0.53
2:Z:1408:LEU:HD12	2:Z:1411:ASN:HD22	1.72	0.53
1:B:773:LYS:HE2	1:B:777:ILE:HD13	1.91	0.53
1:F:182:LEU:HB3	1:F:186:GLU:HB2	1.91	0.53
1:F:522:ASP:OD1	1:F:523:ARG:N	2.42	0.53
1:I:532:ARG:C	1:I:534:MET:H	2.17	0.53
2:Z:1187:GLY:HA2	2:Z:1190:SER:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASN:HB3	1:J:25:LEU:HD22	1.90	0.53
1:B:127:PHE:CE2	1:B:680:TYR:HE1	2.27	0.53
1:E:433:GLN:O	1:E:437:ILE:HG12	2.08	0.53
1:E:683:PRO:HD2	1:E:684:GLU:OE2	2.08	0.53
1:F:21:ASP:OD1	1:F:22:ALA:N	2.41	0.53
1:G:412:GLY:HA3	1:G:498:TYR:CE1	2.44	0.53
1:G:733:LEU:HD12	1:G:734:GLU:N	2.21	0.53
1:J:250:ARG:HH22	1:J:279:HIS:CG	2.27	0.53
1:B:120:ILE:HD11	1:B:122:ARG:NH2	2.24	0.52
1:B:318:GLU:H	1:B:318:GLU:CD	2.17	0.52
1:E:264:MET:HE3	1:E:850:VAL:HG21	1.92	0.52
1:E:824:ASP:OD1	1:E:825:LEU:N	2.43	0.52
1:F:215:THR:C	1:F:216:ILE:HD13	2.34	0.52
1:H:724:ASN:OD1	1:H:725:ALA:N	2.43	0.52
1:I:459:GLU:H	1:I:459:GLU:CD	2.17	0.52
1:I:725:ALA:C	1:I:727:LEU:H	2.17	0.52
2:Z:318:MET:N	2:Z:318:MET:HE2	2.24	0.52
1:B:25:LEU:HD12	1:B:25:LEU:O	2.08	0.52
1:B:87:LEU:O	1:B:842:LEU:HD23	2.10	0.52
1:B:257:MET:N	1:B:257:MET:HE2	2.25	0.52
1:B:582:THR:O	1:B:586:ILE:HG23	2.10	0.52
1:C:491:LYS:HB3	1:C:493:GLU:OE1	2.09	0.52
1:F:108:ILE:CD1	1:F:821:VAL:HG12	2.36	0.52
1:G:423:MET:HE1	1:G:428:ARG:HH22	1.75	0.52
1:G:736:GLN:HE22	1:G:776:MET:H	1.56	0.52
1:H:613:ILE:O	1:H:617:LYS:HG2	2.10	0.52
1:I:98:HIS:O	1:I:98:HIS:ND1	2.42	0.52
2:Z:326:ASN:OD1	2:Z:327:VAL:N	2.43	0.52
2:Z:411:TRP:O	2:Z:415:VAL:HG12	2.10	0.52
2:Z:788:SER:O	2:Z:789:ASN:C	2.53	0.52
1:B:181:GLU:O	1:B:791:ARG:NH2	2.35	0.52
2:Z:441:PHE:HZ	2:Z:461:HIS:HA	1.73	0.52
2:Z:1371:ASP:OD2	2:Z:1406:ALA:HB1	2.09	0.52
1:B:373:MET:HE1	1:I:263:ILE:HD11	1.90	0.52
1:C:461:GLU:HG2	1:C:576:VAL:HG21	1.92	0.52
1:C:759:SER:OG	1:C:760:GLU:N	2.42	0.52
1:I:530:THR:CA	1:I:533:ILE:HG12	2.40	0.52
2:Z:110:THR:HG22	2:Z:111:GLY:H	1.73	0.52
2:Z:462:LYS:HE3	2:Z:618:GLY:H	1.74	0.52
2:Z:1299:MET:HE3	2:Z:1299:MET:HA	1.91	0.52
1:B:414:SER:OG	1:B:417:ASP:O	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:GLU:O	1:E:384:GLN:HG3	2.09	0.52
1:E:444:SER:OG	1:E:445:ARG:N	2.43	0.52
1:F:718:PRO:HG3	1:F:746:ARG:HH21	1.73	0.52
1:B:613:ILE:O	1:B:617:LYS:HG2	2.09	0.52
1:F:210:GLN:HB3	1:F:283:GLU:HG3	1.91	0.52
1:I:157:ILE:HG23	1:I:158:ALA:H	1.74	0.52
2:Z:241:ASP:C	2:Z:243:LEU:H	2.17	0.52
2:Z:598:ASP:N	2:Z:598:ASP:OD1	2.42	0.52
1:C:586:ILE:HD11	1:C:634:PHE:CE2	2.44	0.52
1:E:123:ARG:O	1:E:124:ASP:HB2	2.10	0.52
1:E:629:MET:HG2	1:E:632:ASN:ND2	2.24	0.52
1:F:372:PRO:HG2	1:F:381:ILE:HD11	1.91	0.52
1:I:297:GLN:HE21	1:I:358:GLN:NE2	2.07	0.52
1:A:461:GLU:OE2	1:A:532:ARG:HD2	2.10	0.52
1:A:808:MET:HG3	1:A:809:TYR:H	1.75	0.52
1:B:453:SER:OG	1:B:454:THR:N	2.41	0.52
1:G:279:HIS:ND1	1:G:280:VAL:O	2.43	0.52
1:H:265:ILE:HD11	1:H:849:VAL:HG23	1.91	0.52
1:H:267:LYS:NZ	1:H:269:THR:H	2.08	0.52
1:I:308:LEU:HD21	1:I:534:MET:HE1	1.91	0.52
2:Z:1017:ASN:OD1	2:Z:1018:GLN:N	2.35	0.52
2:Z:1228:MET:HE3	2:Z:1391:LYS:HB2	1.92	0.52
1:A:430:SER:O	1:A:430:SER:OG	2.27	0.51
1:C:264:MET:HE3	1:C:850:VAL:HG11	1.92	0.51
1:G:628:ASN:OD1	1:G:636:LYS:NZ	2.43	0.51
1:J:790:GLU:OE2	1:J:792:ARG:NH1	2.43	0.51
2:Z:303:ASN:OD1	2:Z:304:LEU:N	2.43	0.51
1:E:160:SER:C	1:E:162:LEU:H	2.18	0.51
1:F:712:PRO:HD3	1:F:785:ASN:O	2.10	0.51
1:F:780:ASP:N	1:F:780:ASP:OD1	2.41	0.51
1:G:639:MET:HE1	1:G:651:PHE:CG	2.44	0.51
1:J:202:SER:OG	1:J:203:THR:N	2.43	0.51
1:B:157:ILE:HB	1:B:166:ILE:HB	1.92	0.51
1:C:254:ILE:HD13	1:D:47:ILE:HD13	1.91	0.51
1:D:113:GLN:OE1	1:D:753:VAL:O	2.28	0.51
1:D:182:LEU:HB3	1:D:186:GLU:HB2	1.92	0.51
1:F:284:ILE:HD11	1:F:595:GLN:HE21	1.75	0.51
1:G:318:GLU:O	1:G:322:GLN:HG3	2.11	0.51
1:H:418:SER:OG	1:H:419:TYR:N	2.43	0.51
1:I:639:MET:HE1	1:I:651:PHE:CG	2.45	0.51
1:E:418:SER:OG	1:E:421:ASP:OD1	2.21	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:GLU:HA	1:F:850:VAL:HG12	1.92	0.51
1:F:91:THR:HG22	1:F:153:ASP:HB3	1.92	0.51
2:Z:1073:ARG:N	2:Z:1073:ARG:HD2	2.25	0.51
1:B:120:ILE:HD11	1:B:122:ARG:CZ	2.41	0.51
1:B:267:LYS:NZ	1:B:269:THR:H	2.09	0.51
1:C:65:ILE:HD12	1:C:66:LYS:H	1.75	0.51
1:C:279:HIS:ND1	1:C:280:VAL:O	2.44	0.51
1:C:733:LEU:C	1:C:735:GLN:H	2.17	0.51
1:D:269:THR:HB	1:D:272:GLU:HB2	1.92	0.51
1:F:460:ASN:N	1:F:460:ASN:OD1	2.43	0.51
1:G:478:VAL:HG12	1:G:479:ASP:O	2.11	0.51
1:I:717:GLN:OE1	1:I:717:GLN:N	2.34	0.51
1:A:506:ARG:HH21	1:I:328:LYS:HG3	1.73	0.51
1:B:250:ARG:HG3	1:B:254:ILE:HD11	1.92	0.51
1:C:336:LEU:HD11	1:C:505:ILE:HD11	1.92	0.51
1:D:458:ASP:HB3	1:D:471:ARG:HG2	1.93	0.51
1:E:138:LEU:HD23	1:E:675:LEU:HD21	1.91	0.51
1:H:104:GLU:HA	1:H:791:ARG:HH21	1.76	0.51
1:H:400:ARG:O	1:H:404:ILE:HG12	2.10	0.51
1:B:697:ASN:OD1	1:B:697:ASN:N	2.44	0.51
1:F:687:GLY:O	1:F:752:HIS:HA	2.10	0.51
1:G:421:ASP:OD1	1:G:421:ASP:N	2.43	0.51
1:H:118:GLY:HA3	1:H:130:PHE:CE1	2.46	0.51
2:Z:129:HIS:ND1	2:Z:192:PRO:HG3	2.26	0.51
2:Z:462:LYS:HB3	2:Z:499:PRO:HB2	1.91	0.51
2:Z:488:LEU:HD22	2:Z:613:LEU:HD13	1.92	0.51
2:Z:1319:LEU:O	2:Z:1323:VAL:HG12	2.10	0.51
1:D:416:ASP:OD1	1:D:416:ASP:N	2.44	0.51
1:F:112:ILE:HG22	1:F:113:GLN:N	2.26	0.51
1:F:523:ARG:O	1:F:527:MET:HG3	2.11	0.51
1:F:790:GLU:HG3	1:F:793:ASN:OD1	2.11	0.51
1:J:101:SER:HB3	1:J:180:LEU:HD22	1.92	0.51
2:Z:88:TYR:OH	2:Z:204:LYS:O	2.28	0.51
1:C:250:ARG:HH21	1:C:254:ILE:HD11	1.76	0.51
1:E:150:ILE:HG21	1:E:835:LEU:HD22	1.93	0.51
1:F:708:PHE:HA	1:F:788:LYS:HA	1.92	0.51
1:I:710:LEU:H	1:I:787:VAL:HG23	1.76	0.51
2:Z:1316:HIS:HB3	2:Z:1369:ILE:HD11	1.92	0.51
1:J:613:ILE:O	1:J:617:LYS:HG2	2.11	0.51
1:J:718:PRO:HG3	1:J:746:ARG:HH21	1.76	0.51
2:Z:403:LEU:HG	2:Z:464:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:1117:ASP:OD1	2:Z:1117:ASP:N	2.44	0.51
1:E:736:GLN:NE2	1:E:776:MET:HB2	2.26	0.50
1:F:695:THR:HG21	1:F:716:ASN:ND2	2.26	0.50
1:G:119:VAL:HG13	1:H:69:GLU:OE2	2.11	0.50
1:G:262:ARG:NE	1:G:462:PRO:HG3	2.23	0.50
1:H:121:ASP:O	1:H:123:ARG:N	2.44	0.50
1:I:160:SER:C	1:I:162:LEU:H	2.19	0.50
1:D:230:GLN:OE1	1:D:830:ARG:HG3	2.11	0.50
1:F:433:GLN:O	1:F:437:ILE:HD12	2.11	0.50
1:F:753:VAL:HG11	1:F:755:TYR:CZ	2.46	0.50
1:H:122:ARG:CG	1:H:726:GLN:HB2	2.41	0.50
1:I:736:GLN:HE22	1:I:776:MET:H	1.59	0.50
1:J:443:SER:O	1:J:443:SER:OG	2.29	0.50
2:Z:796:SER:C	2:Z:798:ALA:H	2.18	0.50
2:Z:900:PRO:O	2:Z:901:TRP:HB3	2.10	0.50
1:C:478:VAL:HG21	1:C:527:MET:HE1	1.92	0.50
1:D:458:ASP:OD2	1:D:471:ARG:NH1	2.44	0.50
2:Z:119:VAL:HG23	2:Z:123:TRP:CE3	2.47	0.50
2:Z:481:ASP:OD1	2:Z:482:GLU:N	2.44	0.50
1:A:138:LEU:HD23	1:A:675:LEU:HD21	1.93	0.50
1:A:529:THR:O	1:A:533:ILE:HG23	2.11	0.50
1:G:264:MET:HE3	1:G:850:VAL:HG11	1.93	0.50
2:Z:89:GLU:O	2:Z:92:THR:OG1	2.24	0.50
2:Z:494:LEU:HD21	2:Z:582:ILE:HG21	1.94	0.50
2:Z:556:LEU:HD11	2:Z:971:CYS:SG	2.52	0.50
1:B:90:ASN:HB2	1:B:149:LYS:HB3	1.93	0.50
1:C:87:LEU:HD22	1:C:150:ILE:HD11	1.94	0.50
1:D:300:ILE:HG21	1:D:362:LEU:HD21	1.92	0.50
1:D:613:ILE:O	1:D:617:LYS:HG2	2.11	0.50
1:F:124:ASP:C	1:F:126:SER:H	2.17	0.50
1:F:533:ILE:HD11	1:F:572:THR:HG21	1.93	0.50
2:Z:288:GLN:HG2	2:Z:298:LEU:H	1.76	0.50
1:B:338:ARG:HG2	1:B:338:ARG:HH11	1.76	0.50
1:B:684:GLU:H	1:B:684:GLU:CD	2.20	0.50
1:D:443:SER:OG	1:D:488:ASN:ND2	2.44	0.50
1:D:639:MET:HE1	1:D:654:MET:SD	2.52	0.50
1:H:369:ILE:O	1:H:400:ARG:NH2	2.45	0.50
1:J:416:ASP:OD1	1:J:416:ASP:N	2.44	0.50
2:Z:76:ILE:HG13	2:Z:76:ILE:O	2.10	0.50
2:Z:876:PRO:HG2	2:Z:891:LEU:HD11	1.94	0.50
2:Z:1266:LYS:HE2	2:Z:1340:VAL:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:1307:TYR:OH	2:Z:1420:GLU:OE2	2.30	0.50
1:B:122:ARG:O	1:B:123:ARG:C	2.53	0.50
1:C:267:LYS:HD2	1:F:550:TYR:CZ	2.47	0.50
1:D:184:GLU:HA	1:D:184:GLU:OE1	2.11	0.50
1:E:593:ILE:HG21	1:E:655:LEU:HD13	1.92	0.50
1:F:759:SER:OG	1:F:760:GLU:N	2.45	0.50
1:H:121:ASP:C	1:H:123:ARG:N	2.69	0.50
1:H:704:TYR:HD2	1:H:713:ILE:HG21	1.76	0.50
1:I:378:SER:HB3	1:I:381:ILE:HG12	1.92	0.50
2:Z:1362:ARG:NH2	2:Z:1367:LEU:H	2.10	0.50
2:Z:1371:ASP:OD1	2:Z:1371:ASP:N	2.42	0.50
1:E:397:LEU:HD22	1:E:401:SER:HB2	1.93	0.50
1:G:183:THR:OG1	1:G:184:GLU:N	2.45	0.50
1:G:639:MET:HE1	1:G:651:PHE:CD1	2.46	0.50
1:I:419:TYR:HE1	1:I:423:MET:HE2	1.77	0.50
1:J:389:TRP:HE1	1:J:449:LEU:HB3	1.76	0.50
1:J:533:ILE:HD11	1:J:572:THR:HG21	1.94	0.50
2:Z:810:VAL:HG11	2:Z:955:ILE:HD13	1.94	0.50
1:A:85:GLN:OE1	1:B:49:ASN:ND2	2.44	0.50
1:A:449:LEU:HD23	1:A:450:PRO:HD2	1.94	0.50
1:B:283:GLU:C	1:B:284:ILE:HD12	2.37	0.50
1:C:684:GLU:CD	1:C:684:GLU:H	2.20	0.50
1:E:122:ARG:C	1:E:124:ASP:H	2.18	0.50
1:G:99:LEU:HG	1:G:180:LEU:HD21	1.93	0.50
1:H:48:ARG:HG3	1:H:48:ARG:HH11	1.75	0.50
1:J:526:ASP:OD2	1:J:569:TYR:OH	2.20	0.50
2:Z:257:ALA:C	2:Z:258:PHE:HD1	2.20	0.50
2:Z:1372:ARG:NH1	2:Z:1376:ARG:HH21	2.09	0.50
1:C:556:GLU:OE2	1:D:330:ASN:ND2	2.45	0.49
1:C:599:THR:HG23	1:C:600:ILE:HG12	1.94	0.49
1:H:150:ILE:HD11	1:H:244:LEU:HD11	1.92	0.49
1:H:582:THR:O	1:H:586:ILE:HG23	2.11	0.49
2:Z:668:LEU:HD12	2:Z:668:LEU:H	1.77	0.49
1:B:316:LEU:HD21	1:B:346:THR:HG23	1.94	0.49
1:B:639:MET:HE1	1:B:654:MET:HE3	1.95	0.49
1:B:731:MET:HG2	1:B:735:GLN:HB2	1.94	0.49
1:C:169:GLU:HG3	1:C:832:ARG:NH2	2.27	0.49
1:D:582:THR:O	1:D:586:ILE:HG23	2.12	0.49
1:E:98:HIS:O	1:E:98:HIS:ND1	2.45	0.49
1:E:338:ARG:HG2	1:E:338:ARG:HH11	1.77	0.49
1:E:850:VAL:HG12	1:F:42:THR:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:797:ARG:HD2	1:H:798:VAL:N	2.28	0.49
2:Z:1186:MET:SD	2:Z:1186:MET:N	2.85	0.49
1:A:300:ILE:HD12	1:A:362:LEU:HD21	1.94	0.49
1:H:346:THR:HB	1:H:349:ASN:ND2	2.28	0.49
1:I:767:THR:HG22	1:I:806:VAL:HB	1.93	0.49
2:Z:1087:THR:HG21	2:Z:1113:TRP:CG	2.47	0.49
2:Z:1186:MET:O	2:Z:1190:SER:N	2.44	0.49
1:A:606:ARG:HH21	1:J:9:ASN:HB2	1.77	0.49
1:B:79:GLU:O	1:B:848:ARG:NH1	2.45	0.49
1:G:160:SER:C	1:G:162:LEU:H	2.20	0.49
1:G:214:SER:OG	1:G:246:THR:OG1	2.22	0.49
2:Z:1285:ASP:O	2:Z:1289:VAL:HG23	2.10	0.49
1:D:457:PHE:CE1	1:D:459:GLU:HB2	2.48	0.49
1:E:219:LYS:HG3	1:E:836:ASP:HB2	1.94	0.49
1:G:725:ALA:C	1:G:727:LEU:H	2.21	0.49
2:Z:134:LEU:HB3	2:Z:698:TYR:HE2	1.77	0.49
2:Z:680:ALA:HB3	2:Z:683:SER:HB3	1.94	0.49
2:Z:1177:LEU:HA	2:Z:1180:ILE:HG12	1.94	0.49
1:A:279:HIS:ND1	1:A:280:VAL:O	2.46	0.49
1:B:633:ASP:HB3	1:B:636:LYS:HB3	1.95	0.49
1:C:138:LEU:HD22	1:C:675:LEU:HD21	1.94	0.49
1:F:297:GLN:NE2	1:F:358:GLN:OE1	2.43	0.49
1:F:712:PRO:CG	1:F:784:PHE:HB3	2.40	0.49
1:F:794:ASN:O	1:F:795:LYS:HG2	2.13	0.49
1:G:113:GLN:HE22	1:G:116:THR:HA	1.77	0.49
1:G:521:GLU:OE1	1:I:376:SER:OG	2.29	0.49
1:G:533:ILE:HB	1:G:576:VAL:HG22	1.94	0.49
2:Z:1066:LEU:HD23	2:Z:1083:CYS:HA	1.93	0.49
1:B:107:TYR:OH	1:B:186:GLU:OE2	2.29	0.49
1:F:710:LEU:N	1:F:787:VAL:HG22	2.23	0.49
1:H:774:ASP:OD1	1:H:774:ASP:N	2.46	0.49
1:I:418:SER:OG	1:I:419:TYR:N	2.46	0.49
1:A:600:ILE:HD11	1:B:61:LEU:HD13	1.94	0.49
1:B:356:MET:HE2	1:B:563:TYR:HE2	1.76	0.49
1:D:453:SER:OG	1:D:454:THR:N	2.45	0.49
1:H:103:GLU:CD	1:H:104:GLU:H	2.21	0.49
1:J:798:VAL:HG13	1:J:799:SER:H	1.78	0.49
2:Z:876:PRO:HG2	2:Z:891:LEU:CD1	2.42	0.49
2:Z:910:ASN:ND2	2:Z:950:ASP:O	2.46	0.49
2:Z:1126:ILE:HB	2:Z:1197:ASN:ND2	2.28	0.49
2:Z:1298:THR:HG23	2:Z:1299:MET:SD	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:THR:O	1:D:533:ILE:HG23	2.12	0.49
1:E:808:MET:HG3	1:E:809:TYR:H	1.77	0.49
1:G:197:MET:HE3	1:G:222:PRO:HB2	1.94	0.49
1:J:138:LEU:HD23	1:J:675:LEU:HD22	1.95	0.49
2:Z:273:GLU:CD	2:Z:273:GLU:H	2.20	0.49
1:B:824:ASP:OD1	1:B:825:LEU:N	2.44	0.49
1:C:726:GLN:HA	1:C:729:ASN:HB2	1.95	0.49
1:E:733:LEU:C	1:E:735:GLN:H	2.21	0.49
1:I:791:ARG:HA	1:I:794:ASN:ND2	2.28	0.49
1:A:262:ARG:HH22	1:D:376:SER:HA	1.77	0.48
1:A:369:ILE:HG13	1:A:401:SER:HB3	1.95	0.48
1:A:613:ILE:HD11	1:B:481:TYR:C	2.38	0.48
1:B:127:PHE:CE2	1:B:680:TYR:CE1	3.00	0.48
1:C:453:SER:OG	1:C:454:THR:N	2.45	0.48
1:D:347:GLU:HG3	2:Z:923:LYS:HB2	1.95	0.48
1:F:771:ILE:HB	1:F:777:ILE:HG22	1.95	0.48
1:F:784:PHE:CE1	1:F:812:VAL:HG22	2.48	0.48
1:G:401:SER:O	1:G:405:ILE:HG12	2.13	0.48
1:H:704:TYR:CD2	1:H:713:ILE:HG21	2.48	0.48
1:J:406:ALA:HB1	1:J:438:ILE:HG21	1.95	0.48
2:Z:61:PHE:CE2	2:Z:1060:LYS:HG2	2.45	0.48
2:Z:985:LEU:H	2:Z:985:LEU:HD23	1.77	0.48
1:A:412:GLY:HA3	1:A:498:TYR:CE1	2.48	0.48
1:B:116:THR:O	1:B:137:LYS:NZ	2.37	0.48
1:G:113:GLN:NE2	1:G:116:THR:HA	2.28	0.48
1:C:378:SER:HB2	1:C:381:ILE:HG12	1.96	0.48
1:D:260:ASP:HA	1:D:854:ARG:HH21	1.78	0.48
1:F:799:SER:OG	1:F:800:SER:N	2.46	0.48
1:H:167:SER:OG	1:H:168:THR:N	2.46	0.48
1:H:401:SER:O	1:H:405:ILE:HG12	2.13	0.48
1:H:479:ASP:OD1	1:H:480:ARG:N	2.40	0.48
1:I:91:THR:HG22	1:I:153:ASP:HB3	1.95	0.48
1:C:65:ILE:HD11	2:Z:842:ARG:HH21	1.79	0.48
1:C:305:ARG:HD2	2:Z:850:ILE:HD12	1.95	0.48
1:E:772:MET:HE1	1:E:776:MET:HE2	1.95	0.48
1:F:701:ASP:N	1:F:701:ASP:OD1	2.43	0.48
1:I:412:GLY:HA3	1:I:498:TYR:CE1	2.48	0.48
1:B:419:TYR:CE2	1:B:423:MET:HE1	2.48	0.48
1:C:847:ILE:HD12	1:C:847:ILE:H	1.78	0.48
1:D:107:TYR:C	1:D:108:ILE:HD13	2.39	0.48
1:F:342:ASN:ND2	1:F:342:ASN:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:480:ARG:HG3	1:G:480:ARG:HH11	1.77	0.48
1:G:558:GLU:OE1	1:G:558:GLU:N	2.44	0.48
1:G:808:MET:HG2	1:G:809:TYR:N	2.29	0.48
1:H:267:LYS:HZ2	1:H:268:LEU:N	2.11	0.48
1:J:490:THR:OG1	1:J:491:LYS:N	2.46	0.48
1:A:684:GLU:CD	1:A:684:GLU:H	2.21	0.48
1:B:115:TYR:CE2	1:B:138:LEU:HD11	2.49	0.48
1:C:668:ILE:O	1:C:672:ILE:HG13	2.14	0.48
1:D:77:ARG:NE	1:D:852:TYR:OH	2.37	0.48
1:G:479:ASP:CG	1:G:480:ARG:H	2.22	0.48
1:H:269:THR:O	1:H:273:LYS:HG3	2.14	0.48
1:J:87:LEU:HD21	1:J:278:ARG:HB2	1.96	0.48
2:Z:58:SER:O	2:Z:60:PRO:HD3	2.13	0.48
2:Z:188:LYS:HA	2:Z:704:ASN:HB3	1.95	0.48
2:Z:218:ASP:OD1	2:Z:218:ASP:N	2.46	0.48
2:Z:638:THR:O	2:Z:984:THR:OG1	2.31	0.48
2:Z:757:TYR:HB3	2:Z:879:TYR:CZ	2.48	0.48
2:Z:821:LEU:HB2	2:Z:989:ILE:CD1	2.43	0.48
2:Z:1013:ILE:C	2:Z:1014:LYS:HD2	2.38	0.48
2:Z:1013:ILE:O	2:Z:1014:LYS:HD2	2.13	0.48
2:Z:1233:GLN:HA	2:Z:1248:ARG:CD	2.43	0.48
2:Z:1363:ARG:HG2	2:Z:1363:ARG:HH11	1.79	0.48
1:A:444:SER:O	1:A:448:LYS:NZ	2.46	0.48
1:B:100:PHE:HE1	1:B:110:LEU:HD21	1.79	0.48
1:C:140:MET:HE1	1:D:62:ASP:CG	2.39	0.48
1:F:318:GLU:N	1:F:318:GLU:OE1	2.45	0.48
1:H:122:ARG:HB3	1:H:726:GLN:HB2	1.95	0.48
1:I:711:HIS:ND1	1:I:713:ILE:HB	2.29	0.48
1:A:160:SER:C	1:A:162:LEU:H	2.21	0.48
1:B:531:LEU:O	1:B:535:ILE:HG22	2.14	0.48
1:C:532:ARG:HE	1:F:501:GLU:CD	2.21	0.48
1:D:204:ALA:HB2	1:D:218:ILE:HD13	1.94	0.48
1:E:681:ARG:NE	1:E:681:ARG:HA	2.29	0.48
1:H:476:PHE:CG	1:H:527:MET:HE3	2.48	0.48
2:Z:747:VAL:HG11	2:Z:751:LYS:HG3	1.96	0.48
1:B:254:ILE:HD12	1:B:254:ILE:H	1.78	0.48
2:Z:817:ILE:HG22	2:Z:998:ARG:HG3	1.96	0.48
1:A:478:VAL:CG1	1:A:482:GLY:HA2	2.44	0.47
1:B:93:LYS:HB2	1:B:93:LYS:HE2	1.68	0.47
1:B:122:ARG:C	1:B:124:ASP:N	2.71	0.47
1:B:718:PRO:HG3	1:B:746:ARG:HE	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:MET:HE2	1:D:629:MET:N	2.29	0.47
1:E:120:ILE:HG22	1:E:121:ASP:N	2.24	0.47
1:F:25:LEU:HD12	1:F:25:LEU:O	2.14	0.47
1:F:835:LEU:HD12	1:F:836:ASP:H	1.79	0.47
1:G:460:ASN:HD21	1:J:424:ARG:HH12	1.62	0.47
2:Z:83:ILE:HD11	2:Z:1389:MET:SD	2.54	0.47
1:C:171:MET:HE1	1:C:224:VAL:HG12	1.96	0.47
1:E:76:ASN:HB3	1:E:77:ARG:HH12	1.79	0.47
1:F:713:ILE:HD11	1:F:786:PHE:CZ	2.49	0.47
2:Z:133:PHE:C	2:Z:135:GLY:H	2.22	0.47
2:Z:789:ASN:C	2:Z:789:ASN:HD22	2.22	0.47
1:B:337:ILE:HD13	1:B:383:VAL:HG22	1.97	0.47
1:E:168:THR:O	1:E:168:THR:OG1	2.27	0.47
1:E:733:LEU:HD23	1:E:734:GLU:HB3	1.96	0.47
2:Z:288:GLN:HE21	2:Z:297:THR:HA	1.78	0.47
2:Z:553:PRO:HB3	2:Z:1009:ILE:HD11	1.95	0.47
1:A:516:VAL:HG13	1:A:517:LEU:HD23	1.96	0.47
1:A:633:ASP:OD1	1:A:633:ASP:N	2.45	0.47
1:A:733:LEU:C	1:A:735:GLN:H	2.22	0.47
1:B:81:ALA:HB2	1:B:848:ARG:HH22	1.79	0.47
1:B:797:ARG:HD2	1:B:798:VAL:N	2.30	0.47
1:E:494:LEU:HB2	1:E:507:LYS:NZ	2.30	0.47
1:G:476:PHE:CD1	1:G:478:VAL:HB	2.50	0.47
1:H:704:TYR:CD2	1:H:713:ILE:HD13	2.49	0.47
1:I:445:ARG:HG3	1:I:446:LYS:HD3	1.97	0.47
1:C:713:ILE:HD11	1:C:817:PHE:CB	2.45	0.47
1:D:718:PRO:HG3	1:D:746:ARG:HH21	1.80	0.47
1:F:111:PRO:HD2	1:F:757:TYR:OH	2.15	0.47
1:G:71:LEU:O	1:G:75:VAL:HG22	2.14	0.47
1:I:77:ARG:HA	1:I:77:ARG:HE	1.78	0.47
1:I:138:LEU:HD22	1:I:675:LEU:HD21	1.96	0.47
1:I:400:ARG:O	1:I:404:ILE:HG12	2.14	0.47
2:Z:800:PRO:HG2	2:Z:1239:TYR:OH	2.15	0.47
2:Z:895:ASN:OD1	2:Z:895:ASN:N	2.48	0.47
1:A:98:HIS:O	1:A:98:HIS:ND1	2.48	0.47
1:B:454:THR:OG1	1:B:455:THR:N	2.47	0.47
1:F:54:ASP:N	1:F:54:ASP:OD1	2.48	0.47
1:F:288:LEU:HD23	1:F:288:LEU:H	1.80	0.47
1:G:732:ARG:HH21	1:G:735:GLN:HG2	1.79	0.47
1:H:31:LEU:H	1:H:31:LEU:HD23	1.80	0.47
2:Z:411:TRP:CD2	2:Z:425:LYS:HE3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:833:THR:HG21	2:Z:985:LEU:HD12	1.96	0.47
2:Z:916:MET:HG3	2:Z:981:THR:HG22	1.97	0.47
2:Z:1266:LYS:NZ	2:Z:1329:LEU:HD21	2.29	0.47
1:B:268:LEU:O	1:B:269:THR:OG1	2.27	0.47
1:B:418:SER:OG	1:B:421:ASP:OD2	2.22	0.47
1:B:460:ASN:HB2	1:B:536:SER:HB3	1.97	0.47
1:C:140:MET:HE1	1:D:62:ASP:OD1	2.15	0.47
1:C:346:THR:HB	1:C:349:ASN:ND2	2.30	0.47
1:F:416:ASP:OD1	1:F:416:ASP:N	2.42	0.47
1:I:149:LYS:C	1:I:150:ILE:HD13	2.39	0.47
2:Z:203:TYR:CE1	2:Z:204:LYS:HG3	2.50	0.47
2:Z:298:LEU:HD22	2:Z:888:ILE:HD12	1.96	0.47
2:Z:516:LEU:O	2:Z:518:TYR:N	2.47	0.47
2:Z:913:ASN:HA	2:Z:916:MET:HE3	1.97	0.47
2:Z:1004:LEU:O	2:Z:1004:LEU:HD12	2.15	0.47
1:B:248:GLU:OE1	1:B:273:LYS:HB3	2.14	0.47
1:C:99:LEU:HG	1:C:180:LEU:HD11	1.97	0.47
1:C:300:ILE:HD12	1:C:362:LEU:HD11	1.96	0.47
1:F:298:LEU:HD21	1:F:642:TYR:CG	2.49	0.47
1:I:327:LEU:HD23	1:I:327:LEU:HA	1.77	0.47
2:Z:362:VAL:O	2:Z:363:ASN:C	2.57	0.47
2:Z:690:ARG:HG3	2:Z:692:TYR:CD1	2.49	0.47
1:B:167:SER:OG	1:B:168:THR:N	2.47	0.47
1:B:701:ASP:O	1:B:702:THR:OG1	2.31	0.47
1:G:251:ARG:HD2	1:G:268:LEU:HG	1.95	0.47
1:A:558:GLU:HG2	1:A:559:GLN:N	2.29	0.47
1:B:115:TYR:CG	1:B:138:LEU:HD13	2.49	0.47
1:B:373:MET:HE3	1:B:374:ASN:H	1.79	0.47
1:B:740:ILE:HD13	1:B:810:VAL:HG21	1.97	0.47
1:C:760:GLU:OE1	1:C:793:ASN:ND2	2.46	0.47
1:E:412:GLY:HA3	1:E:498:TYR:CE1	2.49	0.47
1:E:728:TRP:CH2	1:E:736:GLN:HB2	2.50	0.47
1:F:531:LEU:O	1:F:535:ILE:HG22	2.14	0.47
1:G:160:SER:HB2	1:J:123:ARG:C	2.39	0.47
2:Z:692:TYR:HA	2:Z:711:GLU:HG3	1.96	0.47
2:Z:1266:LYS:HZ1	2:Z:1329:LEU:HD21	1.79	0.47
1:A:140:MET:HE1	1:B:62:ASP:HA	1.97	0.46
1:D:27:ASP:OD1	1:D:27:ASP:N	2.45	0.46
1:F:150:ILE:HG21	1:F:842:LEU:HD21	1.97	0.46
1:G:160:SER:HB2	1:J:123:ARG:O	2.14	0.46
1:G:537:SER:O	1:G:537:SER:OG	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:ILE:HD12	1:I:423:MET:HE1	1.97	0.46
1:J:167:SER:OG	1:J:168:THR:N	2.47	0.46
1:D:347:GLU:CG	2:Z:923:LYS:HB2	2.46	0.46
1:E:196:SER:O	1:E:196:SER:OG	2.34	0.46
1:E:684:GLU:CD	1:E:684:GLU:H	2.23	0.46
1:G:450:PRO:HA	1:G:488:ASN:OD1	2.15	0.46
1:G:480:ARG:NH2	1:J:418:SER:OG	2.48	0.46
1:I:645:ASN:OD1	1:J:326:GLN:NE2	2.49	0.46
1:A:445:ARG:HD3	1:A:445:ARG:N	2.30	0.46
1:B:773:LYS:HG3	1:B:774:ASP:H	1.80	0.46
1:E:529:THR:O	1:E:533:ILE:HG23	2.16	0.46
1:J:251:ARG:NH2	1:J:265:ILE:O	2.49	0.46
1:J:269:THR:HG22	1:J:271:ALA:N	2.29	0.46
1:J:697:ASN:OD1	1:J:697:ASN:N	2.47	0.46
2:Z:259:PRO:O	2:Z:261:ARG:NH1	2.48	0.46
1:B:267:LYS:HZ1	1:B:269:THR:H	1.62	0.46
1:B:412:GLY:HA3	1:B:498:TYR:CE1	2.51	0.46
1:C:494:LEU:HB2	1:C:507:LYS:HZ2	1.79	0.46
1:C:694:LEU:HB2	1:C:745:VAL:HG13	1.97	0.46
1:F:778:LEU:C	1:F:779:ASN:O	2.56	0.46
1:I:369:ILE:HG21	1:I:557:LEU:HD13	1.98	0.46
2:Z:206:LEU:HD23	2:Z:208:ARG:NH2	2.29	0.46
2:Z:722:MET:HE3	2:Z:722:MET:HB3	1.82	0.46
2:Z:907:ASP:OD1	2:Z:908:LEU:N	2.49	0.46
1:A:400:ARG:O	1:A:404:ILE:HG12	2.16	0.46
1:D:247:LYS:HG3	1:D:847:ILE:HD11	1.98	0.46
1:E:279:HIS:ND1	1:E:280:VAL:O	2.47	0.46
1:F:798:VAL:HG13	1:F:799:SER:H	1.80	0.46
1:G:150:ILE:HG21	1:G:835:LEU:HD22	1.97	0.46
2:Z:680:ALA:HB3	2:Z:683:SER:CB	2.46	0.46
1:B:116:THR:O	1:B:137:LYS:HD3	2.15	0.46
1:H:266:GLN:HE22	1:H:268:LEU:HA	1.81	0.46
1:H:453:SER:OG	1:H:454:THR:N	2.48	0.46
2:Z:578:ARG:NH2	2:Z:579:ALA:HA	2.30	0.46
1:B:2:ALA:H	1:B:5:THR:HG23	1.81	0.46
1:C:639:MET:HE1	1:C:651:PHE:CG	2.51	0.46
1:D:400:ARG:O	1:D:404:ILE:HG12	2.15	0.46
1:D:505:ILE:HD12	1:D:505:ILE:HA	1.76	0.46
1:G:161:ALA:HB3	1:J:123:ARG:O	2.16	0.46
1:I:183:THR:HG22	1:I:186:GLU:HG3	1.97	0.46
1:I:728:TRP:CH2	1:I:736:GLN:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:423:MET:HA	1:J:423:MET:HE3	1.97	0.46
2:Z:138:LYS:HD2	2:Z:1129:ILE:HD13	1.97	0.46
1:E:497:ASP:OD2	1:E:506:ARG:NH1	2.49	0.46
1:F:177:ILE:HD13	1:F:182:LEU:HD12	1.98	0.46
1:I:586:ILE:O	1:I:589:THR:HG22	2.16	0.46
1:J:732:ARG:O	1:J:736:GLN:HG3	2.15	0.46
2:Z:802:ILE:HD11	2:Z:1257:ASP:HA	1.97	0.46
2:Z:1118:ASN:HB3	2:Z:1210:LEU:HD22	1.98	0.46
1:B:798:VAL:HG23	1:B:799:SER:H	1.81	0.46
1:D:669:ALA:O	1:D:672:ILE:HG22	2.15	0.46
1:G:262:ARG:HB2	1:G:262:ARG:NH1	2.31	0.46
1:J:494:LEU:HD21	1:J:510:PHE:CD2	2.50	0.46
1:J:523:ARG:HG3	1:J:527:MET:HE3	1.98	0.46
1:J:823:ARG:HD2	1:J:823:ARG:HA	1.78	0.46
2:Z:920:GLU:O	2:Z:924:ARG:HG2	2.16	0.46
1:B:124:ASP:N	1:B:124:ASP:OD1	2.47	0.46
1:C:321:GLN:HA	1:C:321:GLN:OE1	2.16	0.46
1:E:400:ARG:O	1:E:404:ILE:HG12	2.16	0.46
1:G:599:THR:HG23	1:G:600:ILE:HG12	1.96	0.46
1:H:709:HIS:HB2	1:H:787:VAL:HG23	1.96	0.46
1:J:114:ALA:O	1:J:115:TYR:O	2.34	0.46
1:J:736:GLN:O	1:J:740:ILE:HG13	2.15	0.46
2:Z:569:ILE:HD13	2:Z:592:ARG:HH21	1.80	0.46
2:Z:687:LEU:HD23	2:Z:723:LYS:HZ1	1.78	0.46
1:A:763:ASP:OD1	1:A:764:MET:N	2.49	0.45
1:A:835:LEU:HD12	1:A:835:LEU:HA	1.79	0.45
1:C:519:ILE:HG22	1:C:521:GLU:H	1.80	0.45
1:E:77:ARG:CZ	1:E:578:THR:HG23	2.46	0.45
1:F:380:GLU:OE1	1:F:380:GLU:N	2.49	0.45
1:F:490:THR:OG1	1:F:491:LYS:N	2.49	0.45
1:H:522:ASP:OD1	1:H:522:ASP:N	2.49	0.45
1:I:732:ARG:HG3	1:I:733:LEU:N	2.31	0.45
1:A:537:SER:O	1:A:537:SER:OG	2.32	0.45
1:A:767:THR:HG21	1:A:806:VAL:HG23	1.97	0.45
1:C:443:SER:O	1:C:443:SER:OG	2.27	0.45
1:F:647:PRO:HG2	1:F:650:ASP:OD2	2.17	0.45
1:G:160:SER:HB2	1:J:123:ARG:CB	2.45	0.45
2:Z:275:TRP:HE1	2:Z:310:ALA:HB2	1.81	0.45
2:Z:1258:SER:C	2:Z:1259:ARG:HG3	2.41	0.45
1:B:104:GLU:OE1	1:B:104:GLU:N	2.47	0.45
1:B:794:ASN:OD1	1:B:795:LYS:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:851:GLU:OE2	1:E:852:TYR:N	2.48	0.45
1:I:189:ARG:O	1:I:193:ILE:HG12	2.16	0.45
2:Z:266:CYS:SG	2:Z:268:HIS:CE1	3.10	0.45
2:Z:1220:ASN:O	2:Z:1221:MET:HE2	2.16	0.45
2:Z:1348:ILE:HG22	2:Z:1350:ILE:HG12	1.98	0.45
1:A:54:ASP:O	1:A:58:ILE:HG23	2.16	0.45
1:A:156:ARG:HD3	1:A:165:GLU:OE2	2.16	0.45
1:B:599:THR:HG21	1:B:672:ILE:HG21	1.97	0.45
1:C:737:VAL:O	1:C:740:ILE:HG13	2.16	0.45
1:C:772:MET:SD	1:C:808:MET:HE1	2.56	0.45
1:D:329:THR:HB	1:D:338:ARG:HH12	1.81	0.45
1:E:369:ILE:HD12	1:E:401:SER:HB3	1.97	0.45
1:G:480:ARG:HG3	1:G:480:ARG:NH1	2.31	0.45
1:G:768:SER:O	1:G:768:SER:OG	2.29	0.45
1:H:490:THR:OG1	1:H:491:LYS:N	2.49	0.45
1:H:684:GLU:CD	1:H:684:GLU:H	2.25	0.45
1:H:709:HIS:CE1	1:H:789:ARG:HE	2.35	0.45
1:I:497:ASP:OD2	1:I:506:ARG:NE	2.49	0.45
2:Z:1104:ALA:O	2:Z:1108:GLY:N	2.49	0.45
1:A:104:GLU:H	1:A:104:GLU:CD	2.24	0.45
1:A:400:ARG:HG3	1:A:428:ARG:HD2	1.98	0.45
1:A:725:ALA:C	1:A:727:LEU:H	2.25	0.45
1:B:194:GLN:O	1:B:194:GLN:NE2	2.50	0.45
1:C:160:SER:HB3	1:F:123:ARG:HB3	1.99	0.45
1:D:267:LYS:HZ2	1:D:269:THR:N	2.12	0.45
1:I:449:LEU:HD23	1:I:449:LEU:HA	1.76	0.45
1:J:96:LEU:HD23	1:J:96:LEU:H	1.81	0.45
1:J:508:ASP:OD1	1:J:508:ASP:C	2.59	0.45
1:D:93:LYS:NZ	1:D:93:LYS:HB3	2.32	0.45
1:E:389:TRP:O	1:E:451:ARG:NH1	2.49	0.45
1:F:336:LEU:HD21	1:F:505:ILE:HG22	1.99	0.45
1:F:456:LEU:HD13	1:F:471:ARG:HE	1.81	0.45
1:I:219:LYS:HG3	1:I:836:ASP:HB2	1.98	0.45
1:I:791:ARG:HA	1:I:794:ASN:HD22	1.81	0.45
1:J:150:ILE:HD11	1:J:244:LEU:HD11	1.98	0.45
2:Z:259:PRO:N	2:Z:261:ARG:HH12	2.15	0.45
1:C:529:THR:O	1:C:533:ILE:HG23	2.17	0.45
1:D:701:ASP:HB3	1:D:715:THR:CG2	2.47	0.45
1:F:2:ALA:HB1	1:G:673:ASP:OD2	2.16	0.45
1:F:90:ASN:HB3	1:F:149:LYS:HB3	1.98	0.45
1:F:740:ILE:HD13	1:F:810:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:SER:C	1:J:123:ARG:O	2.60	0.45
1:G:711:HIS:ND1	1:G:713:ILE:HB	2.31	0.45
1:H:199:ILE:HG12	1:H:221:VAL:HG22	1.99	0.45
1:H:378:SER:HB3	1:H:381:ILE:HG12	1.98	0.45
1:I:530:THR:HA	1:I:533:ILE:CG1	2.45	0.45
1:B:122:ARG:O	1:B:124:ASP:N	2.49	0.45
1:B:761:GLU:N	1:B:761:GLU:OE1	2.50	0.45
1:E:272:GLU:HA	1:E:275:GLN:HG3	1.99	0.45
1:E:482:GLY:HA2	1:E:521:GLU:HG3	1.99	0.45
1:F:708:PHE:HB3	1:F:787:VAL:O	2.16	0.45
1:H:244:LEU:HD23	1:H:244:LEU:HA	1.80	0.45
1:H:412:GLY:HA3	1:H:498:TYR:CE1	2.52	0.45
2:Z:690:ARG:HG3	2:Z:692:TYR:CE1	2.51	0.45
2:Z:971:CYS:SG	2:Z:972:ALA:N	2.90	0.45
1:A:284:ILE:HG23	1:A:288:LEU:HD23	1.99	0.45
1:F:121:ASP:N	1:F:121:ASP:OD1	2.50	0.45
1:G:373:MET:HA	1:G:373:MET:HE3	1.99	0.45
1:H:157:ILE:HB	1:H:166:ILE:HB	1.98	0.45
1:J:210:GLN:N	1:J:210:GLN:OE1	2.50	0.45
1:D:259:ASN:N	1:D:259:ASN:OD1	2.49	0.45
1:D:265:ILE:HD11	1:D:849:VAL:HA	1.98	0.45
1:F:108:ILE:HD12	1:F:819:LEU:CD1	2.38	0.45
1:F:228:PHE:CE1	1:F:685:ARG:HG3	2.52	0.45
1:F:356:MET:HE2	1:F:356:MET:HB2	1.76	0.45
1:G:588:ALA:O	1:G:592:THR:HG23	2.17	0.45
1:G:718:PRO:HG3	1:G:746:ARG:CZ	2.47	0.45
1:H:508:ASP:OD1	1:H:508:ASP:C	2.60	0.45
1:I:108:ILE:HD12	1:I:821:VAL:HG12	1.99	0.45
1:I:649:LYS:O	1:I:653:MET:HG2	2.17	0.45
2:Z:349:TYR:HB2	2:Z:370:ALA:O	2.17	0.45
2:Z:989:ILE:HD12	2:Z:990:ASN:N	2.32	0.45
2:Z:1187:GLY:N	2:Z:1188:PRO:HD2	2.31	0.45
2:Z:1189:LEU:H	2:Z:1189:LEU:HD23	1.82	0.45
1:B:18:VAL:HA	1:B:21:ASP:OD1	2.17	0.44
1:B:696:HIS:CE1	1:B:740:ILE:HG22	2.52	0.44
1:C:224:VAL:HG13	1:C:828:LEU:HG	1.98	0.44
1:C:261:ARG:HH21	1:F:400:ARG:HG3	1.82	0.44
1:D:452:ALA:HA	1:D:486:TYR:HD1	1.82	0.44
1:D:702:THR:HA	1:D:705:ASN:ND2	2.32	0.44
1:E:123:ARG:O	1:E:123:ARG:HD3	2.17	0.44
1:G:221:VAL:HG11	1:G:834:TYR:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:300:ILE:HD12	1:I:362:LEU:HD21	1.98	0.44
1:A:421:ASP:OD1	1:A:422:ILE:N	2.50	0.44
1:A:486:TYR:HD2	1:A:490:THR:HG22	1.81	0.44
1:C:177:ILE:HD12	1:C:187:THR:HG22	1.98	0.44
1:C:177:ILE:HD11	1:C:190:LEU:HD12	1.99	0.44
1:C:262:ARG:HH11	1:F:423:MET:HE3	1.82	0.44
1:C:639:MET:HE1	1:C:651:PHE:CD1	2.53	0.44
1:D:167:SER:OG	1:D:222:PRO:O	2.22	0.44
1:D:386:PHE:O	1:D:390:MET:HG2	2.16	0.44
1:D:490:THR:OG1	1:D:491:LYS:N	2.50	0.44
1:D:498:TYR:HB3	1:D:505:ILE:HG22	1.99	0.44
1:E:122:ARG:C	1:E:124:ASP:N	2.74	0.44
1:E:169:GLU:HG3	1:E:832:ARG:NH2	2.32	0.44
1:E:394:GLU:HG3	1:E:402:ASN:HD21	1.82	0.44
1:E:398:SER:OG	1:E:399:ASP:N	2.51	0.44
1:F:116:THR:OG1	1:F:117:GLY:N	2.44	0.44
1:G:447:PHE:HD1	1:G:494:LEU:HD12	1.82	0.44
1:G:710:LEU:HD13	1:G:803:TYR:CG	2.52	0.44
1:H:718:PRO:HG3	1:H:746:ARG:HE	1.83	0.44
2:Z:312:ARG:NE	2:Z:504:THR:HG21	2.32	0.44
2:Z:584:SER:O	2:Z:588:ILE:HG23	2.17	0.44
2:Z:1383:MET:HG3	2:Z:1393:ILE:HD11	1.98	0.44
1:A:507:LYS:HB2	1:A:507:LYS:NZ	2.32	0.44
1:B:79:GLU:HA	1:B:850:VAL:HG12	1.98	0.44
1:B:385:CYS:SG	1:B:408:VAL:HG11	2.58	0.44
1:C:136:SER:O	1:C:140:MET:HG3	2.18	0.44
1:E:292:MET:HG2	1:E:590:TYR:CE2	2.53	0.44
1:G:529:THR:O	1:G:533:ILE:HG23	2.17	0.44
1:H:458:ASP:OD1	1:H:458:ASP:C	2.60	0.44
1:J:253:ARG:O	1:J:257:MET:HE3	2.17	0.44
1:J:531:LEU:O	1:J:535:ILE:HG22	2.17	0.44
2:Z:486:ASP:O	2:Z:489:ILE:N	2.50	0.44
2:Z:735:ASN:ND2	2:Z:877:PRO:HD3	2.32	0.44
1:A:655:LEU:HD23	1:A:655:LEU:HA	1.77	0.44
1:D:701:ASP:HB3	1:D:715:THR:HG23	1.99	0.44
1:E:596:MET:CE	1:E:622:ASN:HB3	2.44	0.44
2:Z:517:MET:HG3	2:Z:518:TYR:CD2	2.53	0.44
1:D:124:ASP:HB2	1:D:607:TYR:OH	2.17	0.44
1:E:392:ILE:O	1:E:393:PRO:O	2.35	0.44
1:F:308:LEU:HD21	1:F:534:MET:HE3	2.00	0.44
1:F:418:SER:OG	1:F:419:TYR:N	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ARG:HE	1:I:606:ARG:HH12	1.65	0.44
1:H:617:LYS:HD2	1:H:640:TYR:CZ	2.53	0.44
1:I:371:PHE:CE2	1:I:557:LEU:HD22	2.53	0.44
1:J:350:LEU:O	1:J:354:ILE:HG12	2.18	0.44
2:Z:371:ASN:ND2	2:Z:373:ASP:HB3	2.32	0.44
2:Z:691:ILE:HG23	2:Z:713:SER:HA	1.99	0.44
2:Z:834:GLU:O	2:Z:838:GLU:HB2	2.18	0.44
1:A:394:GLU:OE1	1:A:435:TYR:OH	2.23	0.44
1:B:767:THR:HB	1:B:783:THR:HG23	1.99	0.44
1:C:160:SER:O	1:C:162:LEU:N	2.51	0.44
1:C:450:PRO:HA	1:C:488:ASN:OD1	2.18	0.44
1:D:150:ILE:HG21	1:D:842:LEU:HD21	1.98	0.44
1:D:506:ARG:HA	1:D:506:ARG:HD3	1.84	0.44
1:E:160:SER:HB2	1:H:123:ARG:HB3	2.00	0.44
1:F:137:LYS:HE2	1:F:137:LYS:HB2	1.88	0.44
1:F:711:HIS:HD2	1:F:713:ILE:CB	2.23	0.44
1:I:461:GLU:HG3	1:I:462:PRO:HD2	2.00	0.44
1:I:528:PHE:HD1	1:I:531:LEU:HD23	1.83	0.44
2:Z:206:LEU:HD23	2:Z:208:ARG:HH21	1.83	0.44
2:Z:356:GLU:OE2	2:Z:362:VAL:HG11	2.18	0.44
2:Z:1059:TRP:CE2	2:Z:1091:LYS:HE2	2.51	0.44
2:Z:1119:LEU:O	2:Z:1122:THR:HG22	2.18	0.44
1:A:549:HIS:CD2	1:A:551:PRO:HD2	2.53	0.44
1:A:769:HIS:HB3	1:A:812:VAL:HG21	2.00	0.44
1:B:508:ASP:C	1:B:508:ASP:OD1	2.61	0.44
1:E:419:TYR:OH	1:E:423:MET:HE2	2.16	0.44
1:E:496:SER:O	1:E:507:LYS:NZ	2.51	0.44
1:E:508:ASP:HB3	1:E:511:ARG:HH21	1.82	0.44
1:F:751:PHE:CD1	1:F:780:ASP:HA	2.53	0.44
1:H:603:ASP:OD1	1:H:603:ASP:N	2.38	0.44
1:J:197:MET:HE3	1:J:829:VAL:HG22	2.00	0.44
2:Z:785:ARG:HD2	2:Z:785:ARG:HA	1.86	0.44
2:Z:907:ASP:OD1	2:Z:907:ASP:C	2.60	0.44
1:A:281:THR:OG1	1:A:282:THR:N	2.51	0.44
1:A:515:ALA:HB2	1:C:502:GLY:HA3	2.00	0.44
1:B:172:PRO:O	1:B:175:SER:OG	2.34	0.44
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.85	0.44
1:D:723:LYS:HE3	1:D:723:LYS:HA	2.00	0.44
1:E:706:ARG:HG2	1:E:706:ARG:HH11	1.83	0.44
1:E:710:LEU:HG	1:E:787:VAL:HG21	1.98	0.44
1:F:9:ASN:ND2	1:G:606:ARG:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:LEU:HD23	1:F:97:GLU:N	2.32	0.44
1:G:549:HIS:CD2	1:G:551:PRO:HD2	2.53	0.44
1:H:113:GLN:OE1	1:H:116:THR:HB	2.17	0.44
1:H:531:LEU:O	1:H:535:ILE:HG22	2.17	0.44
1:H:798:VAL:HG13	1:H:799:SER:H	1.82	0.44
1:I:148:ASN:N	1:I:148:ASN:OD1	2.50	0.44
1:I:851:GLU:CD	1:I:852:TYR:H	2.26	0.44
1:J:378:SER:H	1:J:381:ILE:HD12	1.83	0.44
2:Z:391:ILE:HD12	2:Z:391:ILE:N	2.33	0.44
2:Z:516:LEU:HB3	2:Z:519:THR:HG23	1.99	0.44
2:Z:884:ALA:O	2:Z:885:LEU:HG	2.18	0.44
1:A:272:GLU:HG2	1:A:275:GLN:NE2	2.33	0.44
1:B:622:ASN:OD1	1:B:622:ASN:C	2.61	0.44
1:F:257:MET:HE2	1:F:257:MET:N	2.33	0.44
1:F:760:GLU:HB3	1:F:793:ASN:ND2	2.33	0.44
1:H:100:PHE:HE1	1:H:110:LEU:HD21	1.82	0.44
2:Z:87:GLU:OE1	2:Z:1093:TYR:N	2.50	0.44
2:Z:690:ARG:HG2	2:Z:692:TYR:HE1	1.83	0.44
2:Z:802:ILE:HD11	2:Z:1256:ASN:O	2.18	0.44
2:Z:843:ASP:N	2:Z:843:ASP:OD1	2.50	0.44
2:Z:1156:ARG:HB2	2:Z:1161:SER:HB3	1.98	0.44
1:A:448:LYS:HD2	1:A:493:GLU:OE2	2.17	0.43
1:E:679:VAL:HA	1:E:686:PHE:CE2	2.53	0.43
1:F:824:ASP:OD1	1:F:825:LEU:N	2.51	0.43
1:H:59:LYS:HE3	1:H:59:LYS:HB3	1.92	0.43
1:H:496:SER:OG	1:H:497:ASP:N	2.51	0.43
1:J:32:ASN:OD1	1:J:33:ILE:N	2.51	0.43
2:Z:54:PRO:O	2:Z:56:LEU:N	2.48	0.43
2:Z:213:PHE:HB2	2:Z:1076:ALA:O	2.18	0.43
2:Z:1335:ALA:O	2:Z:1339:GLY:HA2	2.18	0.43
1:C:690:ASP:OD1	1:C:690:ASP:N	2.50	0.43
1:D:183:THR:N	1:D:186:GLU:OE1	2.49	0.43
1:H:80:LYS:HE2	1:H:80:LYS:HB3	1.93	0.43
1:H:538:ILE:HD13	1:H:538:ILE:HA	1.85	0.43
1:H:798:VAL:HG13	1:H:799:SER:N	2.33	0.43
1:I:639:MET:HE2	1:I:639:MET:HB2	1.74	0.43
1:I:736:GLN:NE2	1:I:776:MET:H	2.16	0.43
2:Z:188:LYS:HE3	2:Z:703:LEU:HG	2.00	0.43
2:Z:1189:LEU:O	2:Z:1192:ILE:HG13	2.18	0.43
1:B:711:HIS:ND1	1:B:713:ILE:HB	2.33	0.43
1:C:644:ASP:OD1	1:C:644:ASP:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD23	1:D:87:LEU:HA	1.78	0.43
1:F:445:ARG:HE	1:F:445:ARG:HB3	1.61	0.43
1:G:458:ASP:OD2	1:G:471:ARG:NH2	2.51	0.43
1:G:701:ASP:HB3	1:G:715:THR:CG2	2.48	0.43
1:I:330:ASN:OD1	1:I:332:LEU:HG	2.18	0.43
1:I:405:ILE:O	1:I:409:ILE:HG12	2.18	0.43
1:J:157:ILE:HB	1:J:166:ILE:HB	2.01	0.43
2:Z:1228:MET:HG3	2:Z:1393:ILE:HG22	2.01	0.43
1:A:54:ASP:HA	1:A:57:THR:HG22	2.00	0.43
1:A:321:GLN:O	1:A:324:GLN:HG3	2.18	0.43
1:A:629:MET:HE3	1:A:629:MET:O	2.18	0.43
1:B:178:GLU:OE1	1:B:179:SER:N	2.50	0.43
1:B:346:THR:HB	1:B:349:ASN:ND2	2.33	0.43
1:B:491:LYS:HA	1:B:491:LYS:HD3	1.81	0.43
1:B:533:ILE:HB	1:B:576:VAL:HG22	2.01	0.43
1:C:190:LEU:N	1:C:191:PRO:HD2	2.33	0.43
1:C:394:GLU:OE2	1:C:395:GLN:NE2	2.51	0.43
1:E:394:GLU:HG3	1:E:402:ASN:ND2	2.34	0.43
1:F:109:LEU:N	1:F:820:GLU:O	2.50	0.43
1:G:453:SER:OG	1:G:454:THR:N	2.51	0.43
1:H:184:GLU:OE1	1:H:185:ALA:N	2.52	0.43
1:H:466:ARG:HG3	1:H:466:ARG:HH11	1.84	0.43
1:I:476:PHE:HD2	1:I:478:VAL:HB	1.82	0.43
1:J:110:LEU:HD13	1:J:757:TYR:CD1	2.53	0.43
1:J:606:ARG:HG2	1:J:607:TYR:CD2	2.54	0.43
2:Z:516:LEU:C	2:Z:518:TYR:H	2.25	0.43
2:Z:607:PHE:CD2	2:Z:1014:LYS:HB3	2.53	0.43
1:A:43:GLY:HA2	2:Z:75:SER:OG	2.18	0.43
1:A:437:ILE:HD13	1:A:437:ILE:HA	1.84	0.43
1:E:104:GLU:H	1:E:104:GLU:CD	2.26	0.43
1:H:220:ARG:HG2	1:H:220:ARG:NH1	2.30	0.43
1:H:356:MET:HE2	1:H:563:TYR:CE2	2.53	0.43
2:Z:344:ARG:HD3	2:Z:344:ARG:C	2.44	0.43
2:Z:487:ILE:HD12	2:Z:590:ARG:HB3	2.00	0.43
1:A:728:TRP:CH2	1:A:736:GLN:HB2	2.54	0.43
1:B:422:ILE:HD13	1:B:422:ILE:HA	1.93	0.43
1:C:253:ARG:HA	1:C:253:ARG:HD3	1.82	0.43
1:C:527:MET:HG3	1:C:569:TYR:CG	2.53	0.43
1:D:244:LEU:HD23	1:D:244:LEU:HA	1.83	0.43
1:F:795:LYS:HE3	1:F:795:LYS:HB3	1.79	0.43
1:G:221:VAL:HG11	1:G:834:TYR:HE2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:763:ASP:OD1	1:G:763:ASP:N	2.45	0.43
1:H:182:LEU:HD12	1:H:182:LEU:H	1.83	0.43
1:I:323:LEU:HD13	1:I:341:ILE:HD13	2.01	0.43
1:J:451:ARG:HA	1:J:451:ARG:HD2	1.73	0.43
2:Z:1079:MET:HE1	2:Z:1201:VAL:HG22	2.00	0.43
1:B:373:MET:HE1	1:I:263:ILE:CD1	2.49	0.43
1:C:65:ILE:HD12	1:C:66:LYS:N	2.34	0.43
1:H:121:ASP:C	1:H:123:ARG:H	2.26	0.43
1:I:253:ARG:HA	1:I:253:ARG:HD3	1.84	0.43
1:I:501:GLU:OE1	1:I:501:GLU:N	2.52	0.43
1:J:120:ILE:HG23	1:J:120:ILE:O	2.17	0.43
1:J:263:ILE:HD13	1:J:851:GLU:HB3	2.00	0.43
2:Z:273:GLU:O	2:Z:277:GLU:HG2	2.18	0.43
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.76	0.43
1:B:490:THR:OG1	1:B:491:LYS:N	2.52	0.43
1:C:853:VAL:HG12	1:F:556:GLU:HG3	2.01	0.43
1:D:666:HIS:CD2	1:D:669:ALA:H	2.31	0.43
1:E:397:LEU:HD22	1:E:401:SER:CB	2.48	0.43
1:E:702:THR:HA	1:E:705:ASN:OD1	2.18	0.43
1:E:836:ASP:OD1	1:E:838:SER:OG	2.31	0.43
1:F:258:VAL:HG22	1:F:258:VAL:O	2.18	0.43
1:F:319:LYS:HD2	1:F:319:LYS:HA	1.81	0.43
1:I:533:ILE:HG13	1:I:533:ILE:O	2.18	0.43
2:Z:213:PHE:HE2	2:Z:215:PRO:HB3	1.84	0.43
2:Z:693:LYS:HB3	2:Z:710:VAL:O	2.19	0.43
2:Z:1343:SER:O	2:Z:1344:GLN:C	2.62	0.43
1:A:308:LEU:HD13	1:A:570:PRO:HB3	2.00	0.43
1:A:725:ALA:O	1:A:726:GLN:HB2	2.18	0.43
1:D:122:ARG:C	1:D:124:ASP:H	2.27	0.43
1:D:491:LYS:N	1:D:491:LYS:HD3	2.33	0.43
1:E:110:LEU:HD13	1:E:110:LEU:HA	1.91	0.43
1:E:373:MET:SD	1:E:381:ILE:HG21	2.58	0.43
1:H:498:TYR:HB3	1:H:505:ILE:HG13	2.00	0.43
1:I:528:PHE:CD1	1:I:531:LEU:HD23	2.54	0.43
1:J:27:ASP:OD1	1:J:28:ALA:N	2.52	0.43
1:J:533:ILE:HB	1:J:576:VAL:HG22	2.01	0.43
2:Z:764:HIS:HA	2:Z:900:PRO:HG3	1.99	0.43
2:Z:1305:MET:O	2:Z:1305:MET:HG3	2.18	0.43
1:B:253:ARG:O	1:B:257:MET:HE3	2.18	0.43
1:B:318:GLU:CD	1:B:318:GLU:N	2.75	0.43
1:C:73:VAL:HG12	1:C:77:ARG:HH21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:HIS:CD2	1:E:551:PRO:HD2	2.54	0.43
1:E:673:ASP:OD1	1:E:673:ASP:C	2.62	0.43
1:F:423:MET:HE2	1:F:423:MET:HB2	1.93	0.43
1:F:496:SER:OG	1:F:497:ASP:N	2.51	0.43
1:G:437:ILE:HD13	1:G:437:ILE:HA	1.83	0.43
1:H:267:LYS:HZ2	1:H:269:THR:N	2.17	0.43
1:H:654:MET:HE3	1:H:654:MET:HB3	1.70	0.43
1:I:419:TYR:CE1	1:I:423:MET:HE2	2.53	0.43
1:I:431:ASP:OD1	1:I:431:ASP:C	2.61	0.43
1:J:776:MET:HE2	1:J:776:MET:HB3	1.89	0.43
2:Z:472:GLU:O	2:Z:476:THR:HG22	2.19	0.43
2:Z:1092:MET:HE2	2:Z:1104:ALA:HB2	2.00	0.43
1:A:99:LEU:HD23	1:A:99:LEU:H	1.84	0.42
1:C:108:ILE:HD12	1:C:821:VAL:HG12	2.01	0.42
1:E:397:LEU:HD23	1:E:397:LEU:HA	1.86	0.42
1:H:122:ARG:CB	1:H:726:GLN:HB2	2.49	0.42
1:H:617:LYS:HD2	1:H:640:TYR:OH	2.19	0.42
1:H:690:ASP:OD1	1:H:690:ASP:C	2.62	0.42
1:I:321:GLN:NE2	2:Z:1403:SER:OG	2.41	0.42
1:I:702:THR:HA	1:I:705:ASN:OD1	2.18	0.42
1:J:452:ALA:HA	1:J:486:TYR:HD1	1.84	0.42
2:Z:266:CYS:SG	2:Z:268:HIS:HE1	2.42	0.42
2:Z:470:ILE:HD13	2:Z:492:GLY:HA3	2.01	0.42
1:B:614:ASP:OD1	1:B:614:ASP:N	2.51	0.42
1:C:614:ASP:OD1	1:C:614:ASP:C	2.62	0.42
1:C:643:GLU:OE2	1:C:648:LYS:HE3	2.19	0.42
1:C:769:HIS:HB3	1:C:812:VAL:HG21	2.01	0.42
1:D:99:LEU:HG	1:D:180:LEU:HD11	2.00	0.42
1:E:851:GLU:OE2	1:E:852:TYR:CD1	2.73	0.42
1:F:120:ILE:HD12	1:F:121:ASP:N	2.33	0.42
1:F:261:ARG:HD2	1:F:851:GLU:HG3	2.01	0.42
1:G:771:ILE:HB	1:G:777:ILE:HG13	2.01	0.42
1:I:448:LYS:HB2	1:I:493:GLU:OE1	2.19	0.42
1:I:520:ASP:O	1:I:521:GLU:HB3	2.19	0.42
1:J:522:ASP:OD1	1:J:523:ARG:N	2.52	0.42
2:Z:183:VAL:HG13	2:Z:706:VAL:HG13	2.01	0.42
2:Z:276:LEU:O	2:Z:280:GLN:HB3	2.18	0.42
2:Z:570:ASP:HA	2:Z:573:ILE:HG22	2.01	0.42
2:Z:947:VAL:HG12	2:Z:952:SER:HB3	2.01	0.42
2:Z:1043:ASP:OD1	2:Z:1043:ASP:C	2.62	0.42
1:A:76:ASN:HB3	2:Z:815:MET:HE1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD13	1:A:471:ARG:HD3	2.00	0.42
1:B:100:PHE:CE1	1:B:110:LEU:HD21	2.54	0.42
1:C:412:GLY:HA3	1:C:498:TYR:CE1	2.54	0.42
1:D:29:ARG:HD2	1:D:30:GLY:H	1.84	0.42
1:D:159:ALA:HB2	1:D:165:GLU:OE1	2.20	0.42
1:F:268:LEU:O	1:F:269:THR:OG1	2.29	0.42
1:F:292:MET:HE1	1:F:545:ALA:HA	2.01	0.42
1:J:458:ASP:OD1	1:J:458:ASP:C	2.61	0.42
2:Z:300:GLN:NE2	2:Z:887:ASP:H	2.17	0.42
1:A:120:ILE:HD12	1:A:121:ASP:H	1.84	0.42
1:A:432:ARG:HB3	1:A:432:ARG:CZ	2.49	0.42
1:A:733:LEU:HD22	1:A:774:ASP:C	2.44	0.42
1:B:126:SER:CB	1:B:129:ASN:OD1	2.54	0.42
1:B:712:PRO:HD2	1:B:786:PHE:CE1	2.55	0.42
1:C:371:PHE:CZ	1:C:404:ILE:HG21	2.54	0.42
1:D:137:LYS:HE3	1:D:137:LYS:HB2	1.80	0.42
1:H:120:ILE:HD11	1:H:122:ARG:NH1	2.34	0.42
1:H:775:ASN:OD1	1:H:775:ASN:N	2.53	0.42
1:I:101:SER:HB2	1:I:107:TYR:HD1	1.85	0.42
1:I:655:LEU:HD23	1:I:655:LEU:HA	1.74	0.42
1:J:740:ILE:HD13	1:J:810:VAL:HG21	2.00	0.42
2:Z:385:ARG:O	2:Z:389:GLN:HG3	2.19	0.42
2:Z:802:ILE:O	2:Z:805:PRO:HD3	2.19	0.42
2:Z:821:LEU:HB2	2:Z:989:ILE:HD13	2.01	0.42
1:A:422:ILE:HD12	1:A:422:ILE:HA	1.87	0.42
1:C:96:LEU:H	1:C:96:LEU:HD12	1.85	0.42
1:C:449:LEU:HD23	1:C:449:LEU:HA	1.92	0.42
1:D:213:ILE:HD13	1:D:213:ILE:HA	1.83	0.42
1:D:474:ALA:C	1:D:476:PHE:H	2.26	0.42
1:E:558:GLU:HG2	1:E:559:GLN:N	2.34	0.42
1:F:505:ILE:HD11	1:F:510:PHE:CZ	2.54	0.42
1:G:253:ARG:HA	1:G:253:ARG:HD3	1.77	0.42
1:G:684:GLU:OE1	1:G:684:GLU:N	2.49	0.42
1:H:308:LEU:HD12	1:H:570:PRO:HB3	2.01	0.42
1:I:493:GLU:O	1:I:494:LEU:HD13	2.20	0.42
1:J:373:MET:HE2	1:J:373:MET:HA	2.00	0.42
2:Z:107:THR:HG23	2:Z:112:SER:HA	2.02	0.42
2:Z:767:GLY:HA3	2:Z:900:PRO:HG2	2.01	0.42
1:A:115:TYR:CD2	1:A:138:LEU:HD13	2.54	0.42
1:A:808:MET:HE3	1:A:809:TYR:H	1.85	0.42
1:C:494:LEU:HB2	1:C:507:LYS:NZ	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLU:OE1	1:D:104:GLU:N	2.52	0.42
1:E:77:ARG:NH2	1:E:578:THR:HG23	2.35	0.42
1:F:126:SER:O	1:F:126:SER:OG	2.37	0.42
1:F:751:PHE:HD1	1:F:780:ASP:HA	1.85	0.42
1:F:798:VAL:HG13	1:F:799:SER:N	2.34	0.42
1:G:254:ILE:HD13	1:H:47:ILE:HD12	2.00	0.42
1:H:104:GLU:HA	1:H:791:ARG:NH2	2.34	0.42
1:I:61:LEU:HD23	1:J:321:GLN:HE22	1.84	0.42
1:J:154:TYR:HB3	1:J:834:TYR:CE2	2.55	0.42
2:Z:818:CYS:SG	2:Z:1001:SER:HB2	2.59	0.42
2:Z:1041:ILE:HD12	2:Z:1041:ILE:HA	1.86	0.42
1:A:101:SER:OG	1:A:791:ARG:NH2	2.53	0.42
1:C:405:ILE:O	1:C:409:ILE:HG12	2.20	0.42
1:D:182:LEU:HD12	1:D:182:LEU:H	1.85	0.42
1:D:521:GLU:N	1:D:521:GLU:OE1	2.44	0.42
1:F:38:ASN:HB2	1:H:642:TYR:HE1	1.85	0.42
1:G:356:MET:HE2	1:G:356:MET:HB2	1.74	0.42
1:H:268:LEU:O	1:H:269:THR:OG1	2.29	0.42
1:H:792:ARG:H	1:H:792:ARG:HG3	1.56	0.42
1:J:323:LEU:HD12	1:J:323:LEU:HA	1.91	0.42
2:Z:313:VAL:HG23	2:Z:459:LEU:HD13	2.01	0.42
2:Z:724:ALA:O	2:Z:725:ALA:C	2.62	0.42
2:Z:1066:LEU:HD12	2:Z:1066:LEU:HA	1.81	0.42
2:Z:1317:GLU:HA	2:Z:1369:ILE:HD12	2.02	0.42
1:A:330:ASN:OD1	1:A:332:LEU:HB2	2.19	0.42
1:A:584:ASN:HB3	1:B:50:VAL:HG11	2.01	0.42
1:A:732:ARG:HG2	1:A:733:LEU:O	2.19	0.42
1:C:537:SER:O	1:C:537:SER:OG	2.37	0.42
1:C:645:ASN:OD1	1:D:326:GLN:NE2	2.43	0.42
1:D:380:GLU:CD	1:D:380:GLU:H	2.27	0.42
1:F:124:ASP:OD1	1:F:124:ASP:N	2.52	0.42
1:H:825:LEU:HD23	1:H:825:LEU:HA	1.88	0.42
1:I:109:LEU:HD23	1:I:109:LEU:HA	1.87	0.42
1:I:713:ILE:HD11	1:I:817:PHE:CB	2.48	0.42
1:J:672:ILE:HD12	1:J:672:ILE:HA	1.87	0.42
2:Z:267:ILE:HD13	2:Z:497:ARG:HD3	2.02	0.42
2:Z:494:LEU:HD13	2:Z:494:LEU:HA	1.91	0.42
2:Z:1176:ILE:O	2:Z:1180:ILE:HG23	2.20	0.42
1:A:336:LEU:HD21	1:A:505:ILE:CD1	2.49	0.42
1:F:337:ILE:HD13	1:F:383:VAL:HG22	2.01	0.42
1:G:332:LEU:HD21	2:Z:1418:LEU:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:639:MET:HE1	1:I:651:PHE:CD1	2.55	0.42
1:I:774:ASP:OD1	1:I:774:ASP:C	2.63	0.42
2:Z:273:GLU:OE1	2:Z:273:GLU:N	2.46	0.42
1:A:330:ASN:HB3	1:A:333:THR:HG22	2.02	0.42
1:B:346:THR:O	1:B:346:THR:OG1	2.35	0.42
1:F:111:PRO:HB2	1:F:684:GLU:HB3	2.01	0.42
1:F:124:ASP:C	1:F:126:SER:N	2.78	0.42
1:F:690:ASP:OD1	1:F:690:ASP:C	2.63	0.42
1:I:369:ILE:HD12	1:I:401:SER:HB3	2.02	0.42
1:J:21:ASP:OD1	1:J:22:ALA:N	2.53	0.42
1:J:597:LEU:HD23	1:J:597:LEU:HA	1.84	0.42
2:Z:459:LEU:O	2:Z:463:VAL:HG23	2.20	0.42
2:Z:1372:ARG:CZ	2:Z:1376:ARG:HH21	2.33	0.42
1:A:251:ARG:NH1	1:A:266:GLN:O	2.52	0.41
1:G:376:SER:O	1:G:377:LEU:HD23	2.20	0.41
1:I:345:ASN:OD1	1:I:345:ASN:C	2.62	0.41
2:Z:430:LYS:O	2:Z:430:LYS:HD3	2.19	0.41
1:A:601:ASP:OD2	1:A:652:TYR:OH	2.35	0.41
1:B:259:ASN:OD1	1:B:259:ASN:N	2.52	0.41
1:C:85:GLN:NE2	1:C:277:MET:SD	2.93	0.41
1:C:181:GLU:O	1:C:791:ARG:NH1	2.53	0.41
1:C:433:GLN:OE1	1:C:433:GLN:N	2.53	0.41
1:D:308:LEU:HD21	1:D:534:MET:HE3	2.02	0.41
1:E:87:LEU:HD13	1:E:150:ILE:HG13	2.03	0.41
1:G:168:THR:O	1:G:168:THR:OG1	2.23	0.41
1:J:29:ARG:HD3	1:J:29:ARG:HA	1.86	0.41
2:Z:105:PHE:CE1	2:Z:404:LEU:HD21	2.54	0.41
2:Z:655:ILE:HD11	2:Z:841:MET:HG2	2.02	0.41
2:Z:668:LEU:HA	2:Z:671:VAL:HG12	2.02	0.41
2:Z:760:LYS:HB3	2:Z:762:PRO:HD2	2.02	0.41
1:B:121:ASP:OD1	1:B:121:ASP:N	2.49	0.41
1:C:233:ASP:OD2	1:C:832:ARG:HD3	2.21	0.41
1:D:268:LEU:O	1:D:269:THR:OG1	2.31	0.41
1:D:396:LEU:HD21	1:D:475:PRO:HA	2.02	0.41
1:D:402:ASN:OD1	1:D:451:ARG:NH2	2.54	0.41
1:D:511:ARG:H	1:D:511:ARG:HG2	1.59	0.41
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.84	0.41
1:F:102:PRO:HA	1:F:790:GLU:HA	2.01	0.41
1:F:452:ALA:HA	1:F:486:TYR:HD1	1.84	0.41
1:G:413:PHE:HE1	1:G:498:TYR:HB2	1.85	0.41
1:J:77:ARG:HG3	1:J:852:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:654:MET:O	1:J:658:ILE:HG13	2.20	0.41
1:J:798:VAL:HG13	1:J:799:SER:N	2.35	0.41
2:Z:459:LEU:HD23	2:Z:499:PRO:CD	2.39	0.41
2:Z:629:ILE:HD13	2:Z:629:ILE:HA	1.89	0.41
2:Z:1049:ILE:HG13	2:Z:1049:ILE:H	1.70	0.41
2:Z:1376:ARG:HH11	2:Z:1376:ARG:HB3	1.86	0.41
1:B:159:ALA:HB2	1:B:165:GLU:OE1	2.20	0.41
1:E:190:LEU:N	1:E:191:PRO:HD2	2.35	0.41
1:F:469:ILE:HD13	1:F:469:ILE:HA	1.89	0.41
1:G:324:GLN:OE1	1:G:338:ARG:NH1	2.53	0.41
1:H:421:ASP:OD1	1:H:421:ASP:N	2.53	0.41
2:Z:315:ASN:HA	2:Z:459:LEU:HB2	2.03	0.41
2:Z:328:LEU:HB3	2:Z:375:TYR:HB3	2.03	0.41
2:Z:404:LEU:HD23	2:Z:405:ASN:N	2.35	0.41
1:A:67:GLN:OE1	1:A:71:LEU:HD21	2.20	0.41
1:A:238:GLU:OE1	1:A:238:GLU:C	2.63	0.41
1:B:104:GLU:N	1:B:104:GLU:CD	2.78	0.41
1:B:798:VAL:HG23	1:B:799:SER:N	2.35	0.41
1:C:728:TRP:CH2	1:C:736:GLN:HB2	2.55	0.41
1:C:764:MET:HE3	1:C:764:MET:HB3	1.95	0.41
1:D:140:MET:HE2	1:D:140:MET:HB2	1.85	0.41
1:E:289:PHE:HA	1:E:292:MET:HE2	2.03	0.41
1:E:461:GLU:HG3	1:E:462:PRO:HD2	2.02	0.41
1:E:494:LEU:HD11	1:E:510:PHE:CD2	2.56	0.41
1:F:71:LEU:HD23	1:F:71:LEU:HA	1.74	0.41
1:F:259:ASN:OD1	1:F:259:ASN:N	2.53	0.41
1:F:689:ILE:O	1:F:690:ASP:C	2.61	0.41
1:G:326:GLN:HA	1:G:326:GLN:OE1	2.20	0.41
1:H:666:HIS:CD2	1:H:669:ALA:H	2.38	0.41
1:I:221:VAL:HG11	1:I:834:TYR:CE2	2.56	0.41
1:I:308:LEU:HD13	1:I:570:PRO:HB3	2.02	0.41
1:I:324:GLN:OE1	2:Z:1365:PRO:HG3	2.21	0.41
1:J:550:TYR:N	1:J:551:PRO:HD2	2.35	0.41
2:Z:458:LEU:HD23	2:Z:458:LEU:O	2.21	0.41
1:C:394:GLU:C	1:C:394:GLU:OE1	2.63	0.41
1:C:644:ASP:HB2	1:D:326:GLN:HE21	1.85	0.41
1:D:71:LEU:HD23	1:D:71:LEU:HA	1.88	0.41
1:D:699:ASP:C	1:D:699:ASP:OD1	2.64	0.41
1:E:851:GLU:CD	1:E:852:TYR:H	2.27	0.41
1:F:39:ASP:OD1	1:F:39:ASP:N	2.52	0.41
1:F:330:ASN:O	1:F:333:THR:OG1	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:447:PHE:HE1	1:F:496:SER:HB3	1.86	0.41
1:G:261:ARG:O	1:J:400:ARG:NH1	2.52	0.41
1:I:348:SER:O	1:I:352:VAL:HG23	2.19	0.41
1:I:581:LYS:HE2	1:I:581:LYS:HB2	1.75	0.41
1:J:367:ILE:N	1:J:367:ILE:HD13	2.34	0.41
1:J:456:LEU:HD23	1:J:456:LEU:HA	1.84	0.41
2:Z:440:THR:HG21	2:Z:455:ARG:HG3	2.03	0.41
1:B:10:ASP:OD1	1:B:10:ASP:C	2.63	0.41
1:C:153:ASP:OD1	1:C:153:ASP:C	2.63	0.41
1:C:851:GLU:OE2	1:C:852:TYR:CD1	2.73	0.41
1:D:373:MET:HE2	1:D:373:MET:HA	2.03	0.41
1:D:378:SER:OG	1:D:380:GLU:OE1	2.33	0.41
1:E:61:LEU:HD13	1:E:61:LEU:HA	1.92	0.41
1:E:137:LYS:HE2	1:E:137:LYS:HB2	1.94	0.41
1:E:494:LEU:C	1:E:507:LYS:HZ1	2.29	0.41
1:F:323:LEU:HD21	1:F:341:ILE:HD12	2.03	0.41
1:G:393:PRO:HG2	1:G:396:LEU:HD22	2.01	0.41
1:H:34:THR:OG1	1:H:35:THR:N	2.53	0.41
1:I:237:TRP:O	1:I:241:THR:HG23	2.21	0.41
1:I:453:SER:OG	1:I:454:THR:N	2.54	0.41
1:I:513:LEU:O	1:I:516:VAL:HG12	2.21	0.41
1:I:556:GLU:H	1:I:556:GLU:HG2	1.57	0.41
2:Z:119:VAL:HG22	2:Z:119:VAL:O	2.20	0.41
2:Z:187:HIS:NE2	2:Z:705:LEU:HD11	2.35	0.41
2:Z:527:ILE:HB	2:Z:1011:GLY:HA3	2.02	0.41
1:A:409:ILE:HD13	1:A:409:ILE:HA	1.95	0.41
1:B:61:LEU:O	1:B:65:ILE:HG22	2.21	0.41
1:B:763:ASP:C	1:B:763:ASP:OD1	2.63	0.41
1:D:345:ASN:HB2	2:Z:919:ASP:OD1	2.21	0.41
1:D:772:MET:HE2	1:D:772:MET:HB3	1.87	0.41
1:F:111:PRO:HB2	1:F:684:GLU:CB	2.51	0.41
1:F:140:MET:HE2	1:F:140:MET:HB3	1.88	0.41
1:F:675:LEU:O	1:F:679:VAL:HG23	2.20	0.41
1:I:279:HIS:ND1	1:I:280:VAL:O	2.54	0.41
2:Z:208:ARG:NH1	2:Z:1115:PHE:HB3	2.35	0.41
2:Z:320:THR:O	2:Z:321:LEU:HD22	2.21	0.41
2:Z:428:LEU:HD23	2:Z:428:LEU:HA	1.83	0.41
2:Z:661:SER:OG	2:Z:663:VAL:HG23	2.21	0.41
2:Z:690:ARG:HA	2:Z:690:ARG:HD2	1.81	0.41
1:C:287:ASP:N	1:C:287:ASP:OD1	2.51	0.41
1:C:386:PHE:CE1	1:C:409:ILE:HD12	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PHE:HE1	1:C:449:LEU:HD11	1.85	0.41
1:C:731:MET:HG2	1:C:732:ARG:N	2.36	0.41
1:E:280:VAL:HG21	1:F:51:GLY:HA3	2.02	0.41
1:F:32:ASN:OD1	1:F:32:ASN:N	2.40	0.41
1:F:291:LYS:HB2	1:F:291:LYS:HE2	1.81	0.41
1:F:389:TRP:CD2	1:F:451:ARG:HD3	2.55	0.41
1:G:713:ILE:HD11	1:G:817:PHE:CB	2.50	0.41
1:G:774:ASP:OD1	1:G:774:ASP:C	2.64	0.41
1:H:233:ASP:OD1	1:H:233:ASP:N	2.52	0.41
1:I:733:LEU:HG	1:I:734:GLU:OE2	2.21	0.41
1:I:778:LEU:HD23	1:I:778:LEU:HA	1.89	0.41
1:J:78:SER:HB2	1:J:851:GLU:CD	2.46	0.41
1:J:244:LEU:HD23	1:J:244:LEU:HA	1.87	0.41
1:J:373:MET:O	1:J:375:VAL:HG23	2.20	0.41
1:J:526:ASP:OD2	1:J:571:ARG:NH1	2.53	0.41
1:J:763:ASP:OD1	1:J:763:ASP:C	2.64	0.41
2:Z:114:GLN:HE22	2:Z:196:ASN:CG	2.28	0.41
2:Z:404:LEU:HA	2:Z:408:PHE:HD1	1.86	0.41
2:Z:1130:SER:HB2	2:Z:1193:GLU:HG3	2.03	0.41
2:Z:1193:GLU:HA	2:Z:1196:VAL:HG12	2.02	0.41
2:Z:1256:ASN:OD1	2:Z:1257:ASP:N	2.54	0.41
2:Z:1394:ASP:OD1	2:Z:1394:ASP:N	2.52	0.41
2:Z:1400:PRO:HA	2:Z:1403:SER:HB3	2.02	0.41
1:A:586:ILE:O	1:A:589:THR:HG22	2.21	0.41
1:C:498:TYR:HB3	1:C:505:ILE:HB	2.03	0.41
1:E:369:ILE:CD1	1:E:397:LEU:HD21	2.51	0.41
1:E:718:PRO:HG3	1:E:746:ARG:CZ	2.51	0.41
1:F:531:LEU:O	1:F:531:LEU:HD12	2.21	0.41
1:G:158:ALA:HB1	1:J:123:ARG:NH2	2.36	0.41
1:G:356:MET:HE3	1:G:563:TYR:CE2	2.56	0.41
1:G:530:THR:HG21	1:G:570:PRO:HB2	2.03	0.41
1:G:764:MET:HE2	1:G:802:ARG:O	2.21	0.41
1:H:427:ALA:O	1:H:428:ARG:HG2	2.21	0.41
1:I:316:LEU:HD12	1:I:316:LEU:HA	1.88	0.41
2:Z:79:GLU:O	2:Z:83:ILE:HG13	2.21	0.41
1:B:268:LEU:H	1:B:268:LEU:HD12	1.86	0.40
1:B:320:GLN:OE1	1:B:342:ASN:ND2	2.54	0.40
1:B:517:LEU:HD23	1:B:517:LEU:HA	1.87	0.40
1:D:308:LEU:HD11	1:D:357:MET:HG2	2.04	0.40
1:E:126:SER:O	1:E:127:PHE:CB	2.67	0.40
1:E:450:PRO:HA	1:E:488:ASN:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ASP:OD1	1:F:83:ASP:N	2.54	0.40
1:H:452:ALA:HA	1:H:486:TYR:HD1	1.87	0.40
1:I:519:ILE:HG21	1:I:527:MET:HE1	2.02	0.40
2:Z:60:PRO:C	2:Z:62:THR:N	2.74	0.40
2:Z:139:LEU:HD11	2:Z:697:GLU:HA	2.03	0.40
2:Z:581:ASN:OD1	2:Z:581:ASN:N	2.54	0.40
2:Z:1098:LEU:HD23	2:Z:1384:LEU:HB3	2.03	0.40
2:Z:1154:ILE:HG22	2:Z:1173:LYS:HG2	2.02	0.40
2:Z:1206:LEU:HD12	2:Z:1206:LEU:HA	1.86	0.40
1:A:702:THR:HG22	1:A:702:THR:O	2.21	0.40
1:B:675:LEU:HD13	1:B:675:LEU:HA	1.95	0.40
1:C:736:GLN:NE2	1:C:776:MET:HB2	2.36	0.40
1:D:337:ILE:O	1:D:341:ILE:HG22	2.21	0.40
1:D:596:MET:HE2	1:D:596:MET:HA	2.03	0.40
1:E:66:LYS:HE2	1:E:66:LYS:HB2	1.83	0.40
1:E:589:THR:OG1	1:E:632:ASN:OD1	2.34	0.40
1:E:733:LEU:HD23	1:E:734:GLU:N	2.36	0.40
1:F:122:ARG:O	1:F:123:ARG:CB	2.62	0.40
1:F:773:LYS:HG3	1:F:774:ASP:H	1.85	0.40
1:G:505:ILE:HD13	1:G:505:ILE:HA	1.80	0.40
1:H:180:LEU:HA	1:H:180:LEU:HD23	1.85	0.40
1:H:638:ILE:HD13	1:H:638:ILE:HA	1.93	0.40
1:I:599:THR:HG23	1:I:600:ILE:HG12	2.03	0.40
1:J:668:ILE:HD13	1:J:668:ILE:HA	1.97	0.40
2:Z:769:LEU:HD23	2:Z:769:LEU:HA	1.91	0.40
2:Z:1301:PHE:CD1	2:Z:1319:LEU:HD12	2.55	0.40
1:A:307:PHE:O	1:A:308:LEU:HD23	2.22	0.40
1:A:662:GLY:O	1:A:663:GLN:HG2	2.22	0.40
1:A:723:LYS:HE2	1:A:723:LYS:HB2	1.82	0.40
1:B:400:ARG:O	1:B:404:ILE:HG13	2.21	0.40
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.93	0.40
1:D:76:ASN:OD1	1:D:76:ASN:N	2.54	0.40
1:D:544:ASP:OD1	1:D:544:ASP:O	2.39	0.40
1:D:824:ASP:OD1	1:D:825:LEU:N	2.54	0.40
1:E:160:SER:OG	1:H:123:ARG:CZ	2.69	0.40
1:E:273:LYS:HE2	1:E:273:LYS:HB2	1.91	0.40
1:E:296:ALA:O	1:E:300:ILE:HG13	2.20	0.40
1:E:313:PHE:HB2	1:E:566:THR:CG2	2.52	0.40
1:E:355:LYS:HD3	1:E:552:HIS:O	2.20	0.40
1:F:451:ARG:HD2	1:F:451:ARG:HA	1.79	0.40
1:G:285:ASN:OD1	1:G:287:ASP:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:356:MET:HE2	1:H:563:TYR:HE2	1.87	0.40
1:H:601:ASP:O	1:H:602:LEU:HD23	2.22	0.40
1:A:285:ASN:OD1	1:A:285:ASN:N	2.49	0.40
1:B:1:MET:N	1:B:1:MET:SD	2.93	0.40
1:B:197:MET:HB3	1:B:222:PRO:HG2	2.03	0.40
1:B:232:ILE:HD13	1:B:232:ILE:HA	1.90	0.40
1:B:749:GLY:HA2	1:B:750:PRO:HD3	1.97	0.40
1:C:317:ALA:HA	1:C:320:GLN:OE1	2.21	0.40
1:C:763:ASP:OD1	1:C:764:MET:N	2.55	0.40
1:E:577:ASP:HA	1:E:580:VAL:HG22	2.02	0.40
1:E:849:VAL:O	1:F:44:GLY:HA3	2.21	0.40
1:F:110:LEU:CD2	1:F:708:PHE:HZ	2.34	0.40
1:F:308:LEU:CD2	1:F:534:MET:HE3	2.51	0.40
1:F:356:MET:SD	1:F:396:LEU:HD23	2.62	0.40
1:F:511:ARG:H	1:F:511:ARG:HG2	1.69	0.40
1:F:755:TYR:CE1	1:F:814:ILE:HD13	2.55	0.40
1:G:110:LEU:HD23	1:G:110:LEU:HA	1.87	0.40
1:H:87:LEU:O	1:H:842:LEU:HD13	2.21	0.40
1:H:494:LEU:HD21	1:H:510:PHE:HD2	1.87	0.40
1:H:749:GLY:HA2	1:H:750:PRO:HD3	1.97	0.40
1:H:824:ASP:OD1	1:H:825:LEU:N	2.54	0.40
1:I:190:LEU:N	1:I:191:PRO:HD2	2.36	0.40
1:I:595:GLN:HG3	1:I:665:ALA:O	2.21	0.40
1:J:422:ILE:HD13	1:J:422:ILE:HA	1.95	0.40
2:Z:105:PHE:HE1	2:Z:404:LEU:HD21	1.86	0.40
2:Z:879:TYR:O	2:Z:889:ILE:HA	2.22	0.40
2:Z:1266:LYS:CE	2:Z:1340:VAL:O	2.69	0.40
1:B:538:ILE:HD13	1:B:538:ILE:HA	1.81	0.40
1:D:96:LEU:HD12	1:D:97:GLU:H	1.87	0.40
1:D:140:MET:CE	1:D:626:VAL:HG13	2.49	0.40
1:E:346:THR:HB	1:E:349:ASN:ND2	2.37	0.40
1:E:494:LEU:HB2	1:E:507:LYS:HZ1	1.87	0.40
1:G:710:LEU:HG	1:G:787:VAL:HG21	2.04	0.40
1:H:259:ASN:OD1	1:H:259:ASN:N	2.52	0.40
1:H:711:HIS:ND1	1:H:713:ILE:HB	2.36	0.40
1:I:140:MET:HG2	1:J:62:ASP:OD1	2.22	0.40
2:Z:1398:ILE:HD12	2:Z:1398:ILE:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	813/854 (95%)	741 (91%)	72 (9%)	0	100	100
1	B	842/854 (99%)	775 (92%)	65 (8%)	2 (0%)	43	72
1	C	792/854 (93%)	721 (91%)	71 (9%)	0	100	100
1	D	842/854 (99%)	785 (93%)	56 (7%)	1 (0%)	48	78
1	E	792/854 (93%)	719 (91%)	70 (9%)	3 (0%)	30	60
1	F	842/854 (99%)	761 (90%)	76 (9%)	5 (1%)	21	52
1	G	792/854 (93%)	726 (92%)	66 (8%)	0	100	100
1	H	842/854 (99%)	786 (93%)	55 (6%)	1 (0%)	48	78
1	I	792/854 (93%)	733 (93%)	58 (7%)	1 (0%)	48	78
1	J	842/854 (99%)	777 (92%)	64 (8%)	1 (0%)	48	78
2	Z	1314/1425 (92%)	1162 (88%)	144 (11%)	8 (1%)	21	52
All	All	9505/9965 (95%)	8686 (91%)	797 (8%)	22 (0%)	44	72

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	127	PHE
1	F	689	ILE
1	J	115	TYR
2	Z	894	ASP
2	Z	901	TRP
1	B	115	TYR
1	D	127	PHE
1	F	114	ALA
2	Z	1338	MET
1	H	115	TYR
2	Z	61	PHE
2	Z	242	ASP
1	F	111	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	116	THR
2	Z	1343	SER
1	B	127	PHE
1	E	120	ILE
1	F	690	ASP
1	I	533	ILE
2	Z	134	LEU
2	Z	55	PHE
1	E	393	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	718/751 (96%)	718 (100%)	0	100	100
1	B	744/751 (99%)	743 (100%)	1 (0%)	88	88
1	C	704/751 (94%)	703 (100%)	1 (0%)	88	88
1	D	744/751 (99%)	739 (99%)	5 (1%)	76	77
1	E	704/751 (94%)	703 (100%)	1 (0%)	88	88
1	F	744/751 (99%)	737 (99%)	7 (1%)	70	75
1	G	704/751 (94%)	703 (100%)	1 (0%)	88	88
1	H	744/751 (99%)	738 (99%)	6 (1%)	73	76
1	I	704/751 (94%)	701 (100%)	3 (0%)	84	81
1	J	744/751 (99%)	742 (100%)	2 (0%)	86	83
2	Z	1167/1263 (92%)	1149 (98%)	18 (2%)	57	68
All	All	8421/8773 (96%)	8376 (100%)	45 (0%)	78	80

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	ILE
1	C	398	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	25	LEU
1	D	120	ILE
1	D	121	ASP
1	D	382	ILE
1	D	505	ILE
1	E	119	VAL
1	F	111	PRO
1	F	119	VAL
1	F	120	ILE
1	F	124	ASP
1	F	689	ILE
1	F	780	ASP
1	F	787	VAL
1	G	598	SER
1	H	116	THR
1	H	119	VAL
1	H	120	ILE
1	H	122	ARG
1	H	152	THR
1	H	469	ILE
1	I	157	ILE
1	I	390	MET
1	I	459	GLU
1	J	122	ARG
1	J	124	ASP
2	Z	133	PHE
2	Z	330	HIS
2	Z	333	LEU
2	Z	453	VAL
2	Z	459	LEU
2	Z	537	PHE
2	Z	731	THR
2	Z	732	VAL
2	Z	804	VAL
2	Z	806	GLU
2	Z	807	ILE
2	Z	892	GLN
2	Z	895	ASN
2	Z	899	VAL
2	Z	936	ILE
2	Z	940	ASP
2	Z	1116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Z	1141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	217	ASN
1	A	434	ASN
1	A	716	ASN
1	A	736	GLN
1	B	76	ASN
1	B	113	GLN
1	B	210	GLN
1	B	217	ASN
1	B	342	ASN
1	B	349	ASN
1	B	374	ASN
1	B	574	HIS
1	B	584	ASN
1	B	674	GLN
1	B	696	HIS
1	C	67	GLN
1	C	266	GLN
1	C	297	GLN
1	C	358	GLN
1	C	384	GLN
1	C	395	GLN
1	C	434	ASN
1	C	468	GLN
1	C	552	HIS
1	C	709	HIS
1	C	716	ASN
1	C	736	GLN
1	D	85	GLN
1	D	113	GLN
1	D	129	ASN
1	D	217	ASN
1	D	279	HIS
1	D	297	GLN
1	D	335	ASN
1	D	349	ASN
1	D	358	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	645	ASN
1	D	696	HIS
1	E	105	ASN
1	E	194	GLN
1	E	361	GLN
1	E	384	GLN
1	E	402	ASN
1	E	696	HIS
1	F	17	GLN
1	F	113	GLN
1	F	326	GLN
1	F	552	HIS
1	F	574	HIS
1	F	711	HIS
1	F	752	HIS
1	F	769	HIS
1	F	818	GLN
1	G	275	GLN
1	G	286	ASN
1	G	342	ASN
1	G	595	GLN
1	G	696	HIS
1	G	697	ASN
1	G	752	HIS
1	G	818	GLN
1	H	16	GLN
1	H	266	GLN
1	H	349	ASN
1	H	663	GLN
1	H	666	HIS
1	H	717	GLN
1	I	217	ASN
1	I	286	ASN
1	I	358	GLN
1	I	361	GLN
1	I	697	ASN
1	I	736	GLN
1	I	826	HIS
1	J	17	GLN
1	J	76	ASN
1	J	363	HIS
1	J	434	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	584	ASN
1	J	666	HIS
1	J	736	GLN
2	Z	71	GLN
2	Z	104	HIS
2	Z	114	GLN
2	Z	268	HIS
2	Z	330	HIS
2	Z	405	ASN
2	Z	410	HIS
2	Z	515	GLN
2	Z	538	ASN
2	Z	736	GLN
2	Z	748	GLN
2	Z	789	ASN
2	Z	1099	ASN
2	Z	1191	GLN
2	Z	1197	ASN
2	Z	1276	ASN
2	Z	1309	GLN
2	Z	1316	HIS
2	Z	1331	ASN
2	Z	1344	GLN
2	Z	1411	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

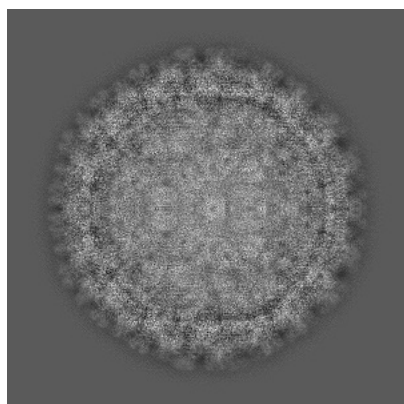
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33404. These allow visual inspection of the internal detail of the map and identification of artifacts.

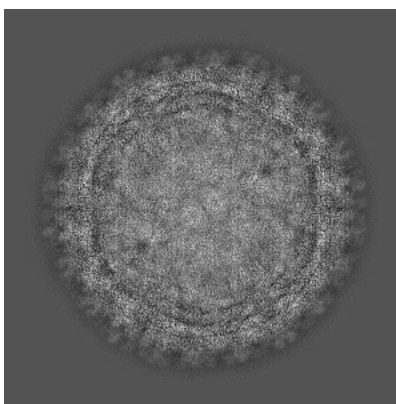
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

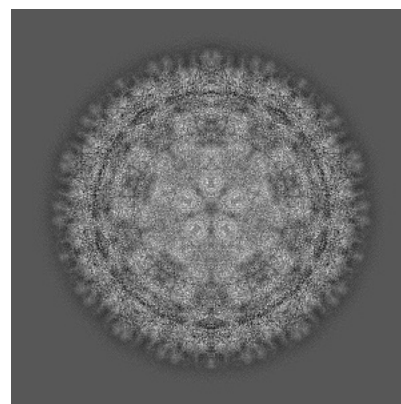
6.1.1 Primary map



X

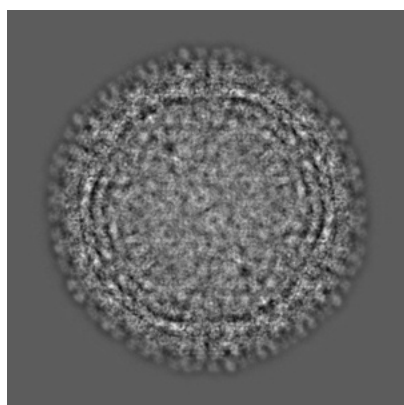


Y

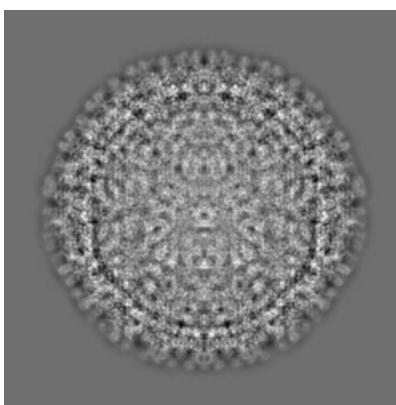


Z

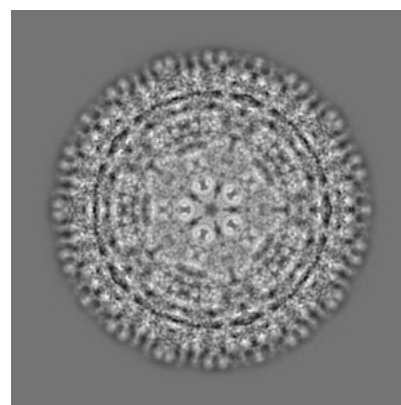
6.1.2 Raw map



X



Y

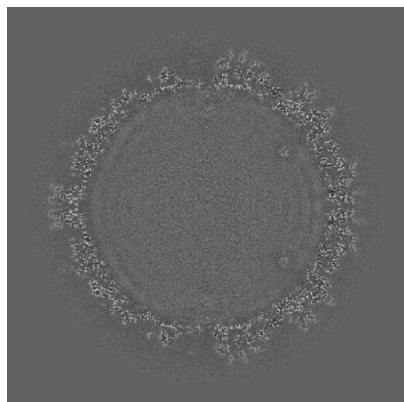


Z

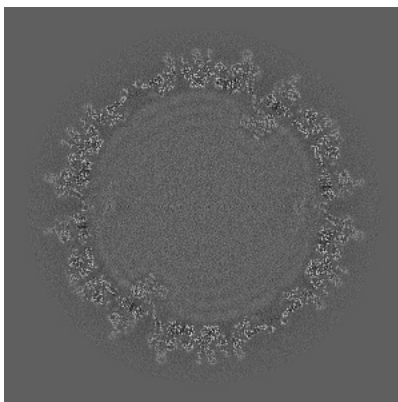
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

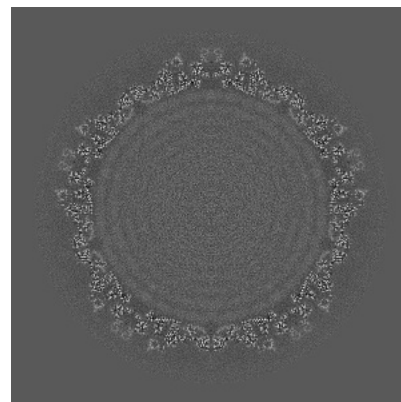
6.2.1 Primary map



X Index: 400

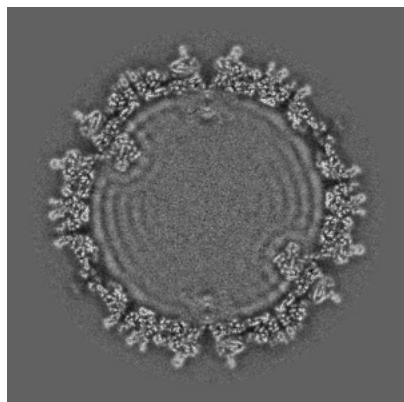


Y Index: 400

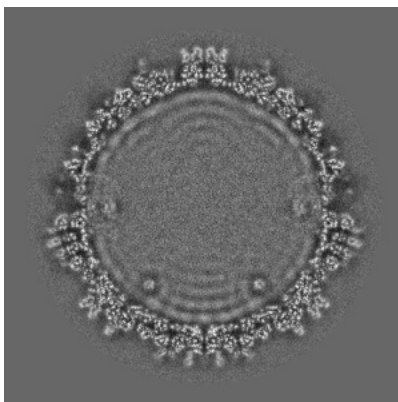


Z Index: 400

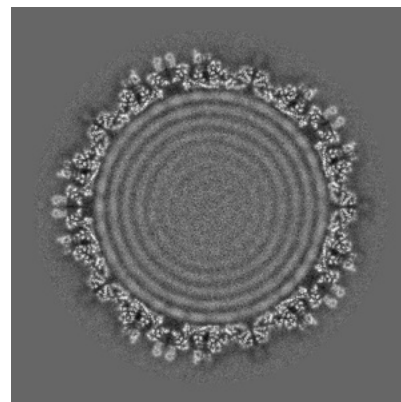
6.2.2 Raw map



X Index: 400



Y Index: 400

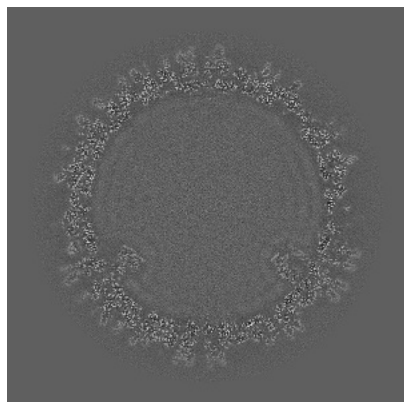


Z Index: 400

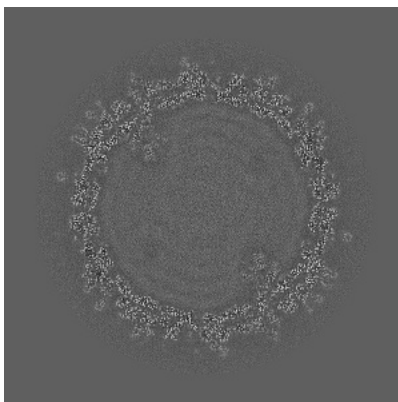
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

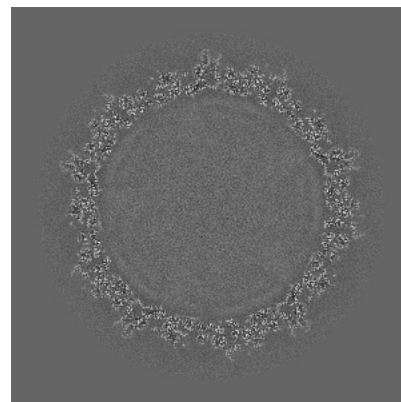
6.3.1 Primary map



X Index: 358

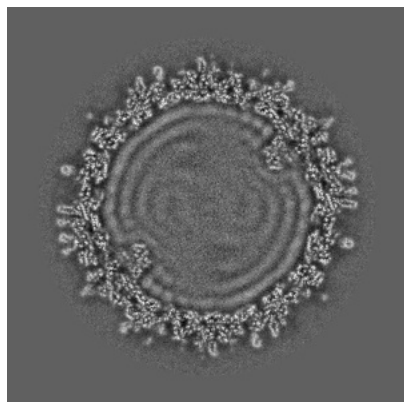


Y Index: 292

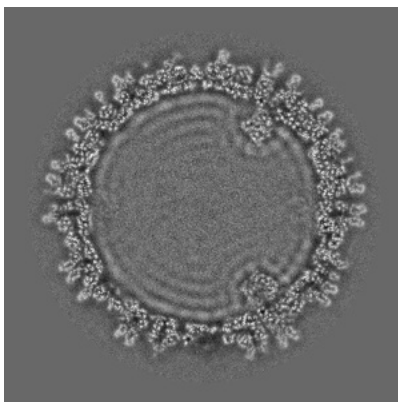


Z Index: 336

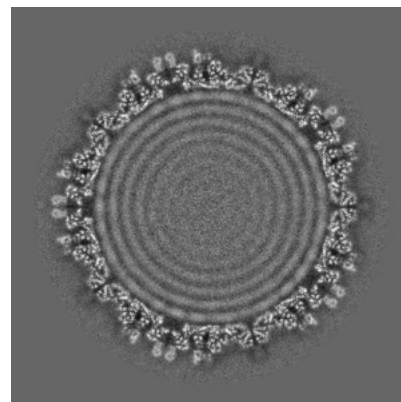
6.3.2 Raw map



X Index: 293



Y Index: 354

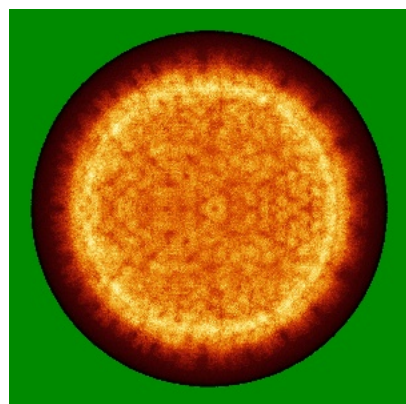


Z Index: 400

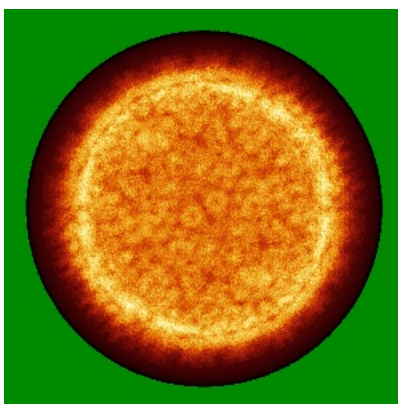
The images above show the largest variance slices of the map in three orthogonal directions.

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

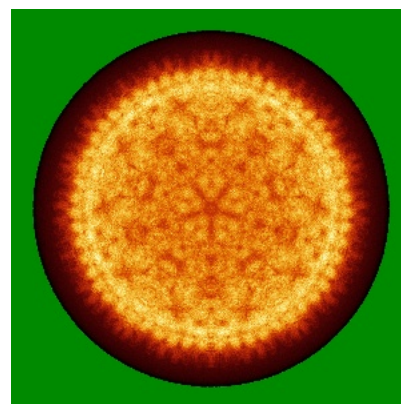
6.4.1 Primary map



X

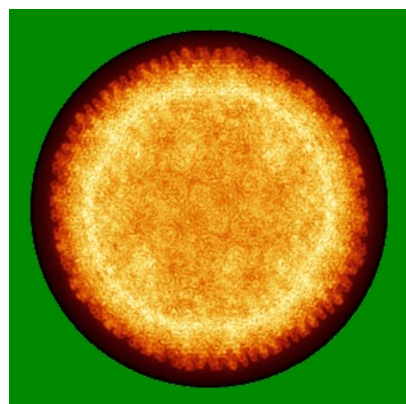


Y

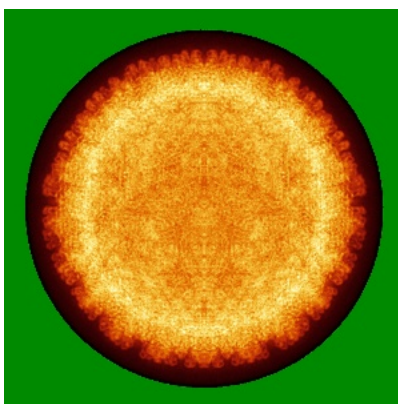


Z

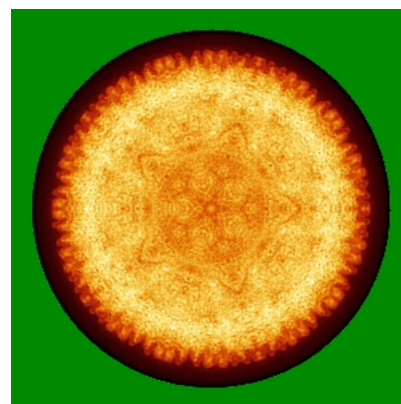
6.4.2 Raw map



X



Y

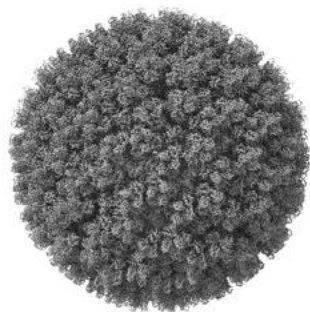


Z

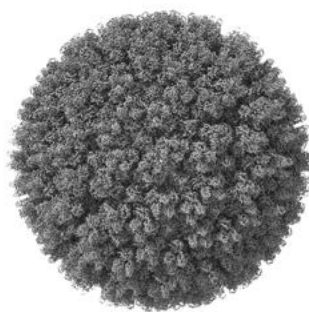
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

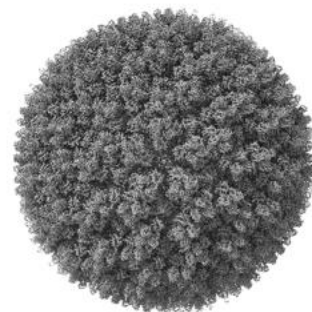
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. 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



X



Y



Z

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.

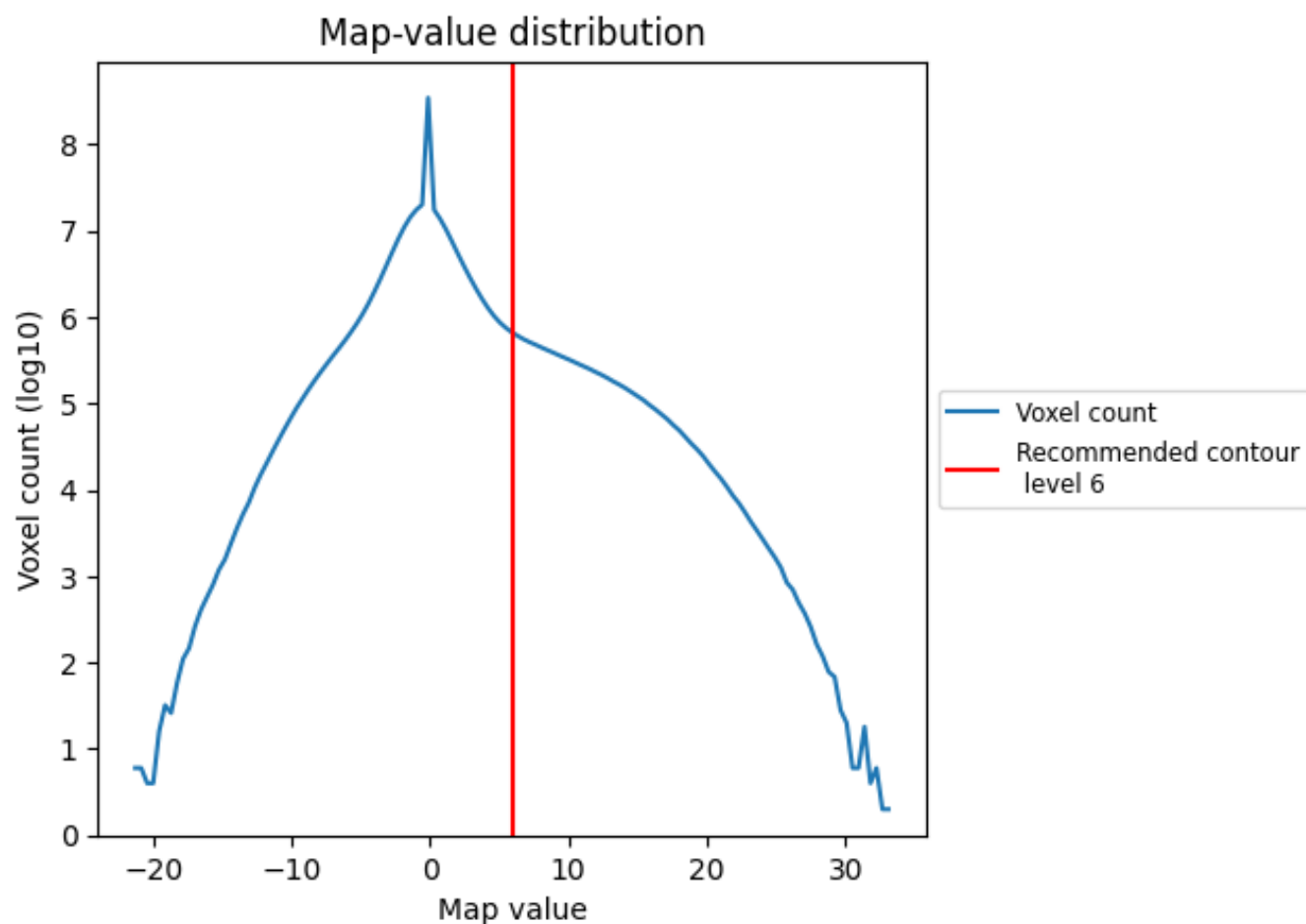
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

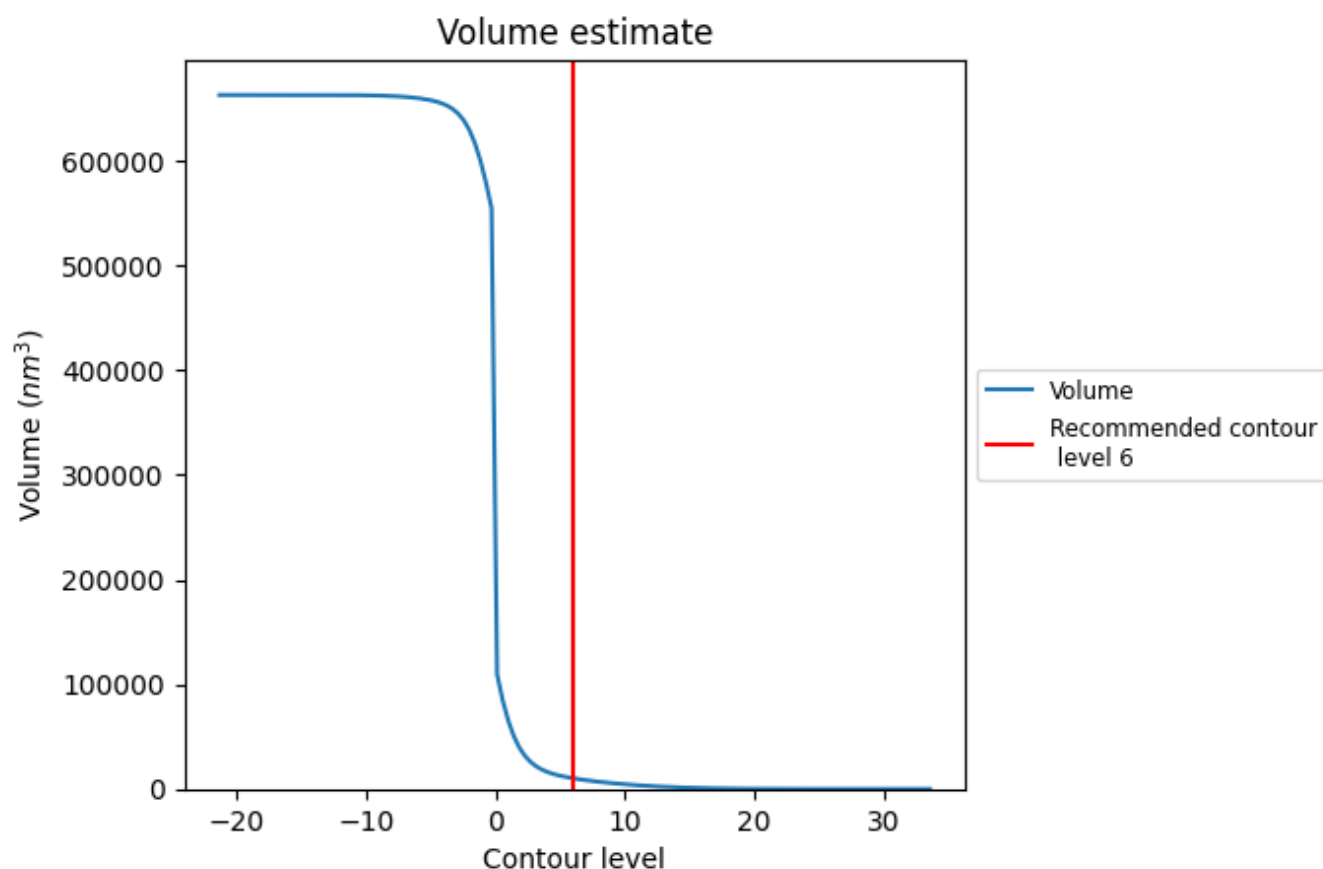
This section contains the results of statistical analysis of the map.

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.

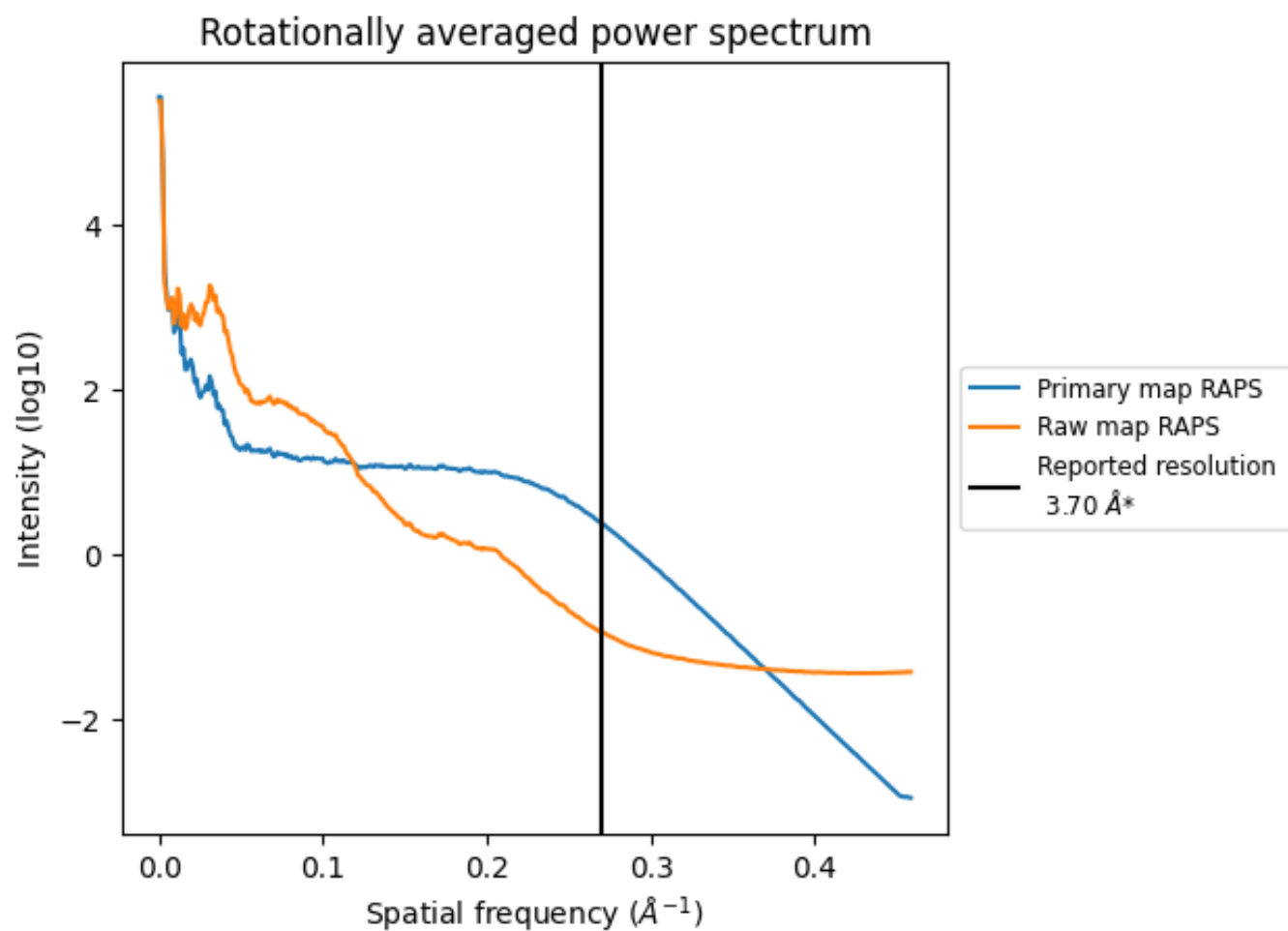
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101620 nm^3 ; this corresponds to an approximate mass of 9180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

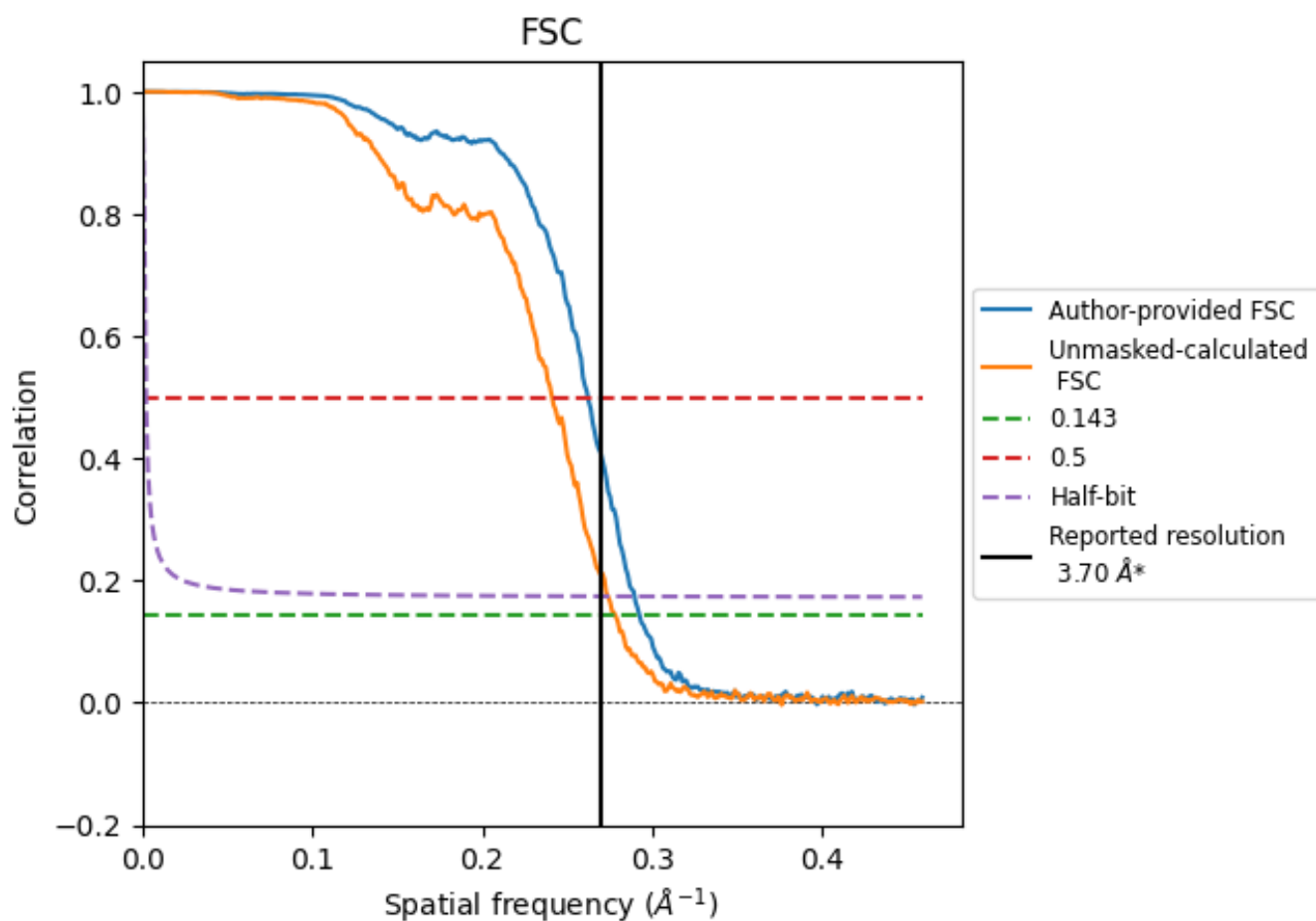


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.42	3.82	3.45
Unmasked-calculated*	3.59	4.15	3.65

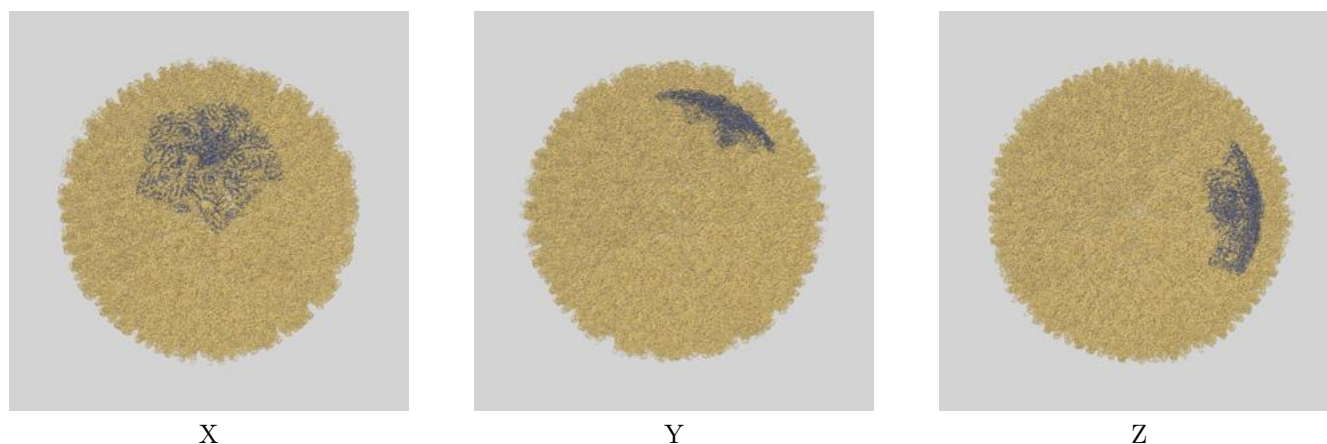
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

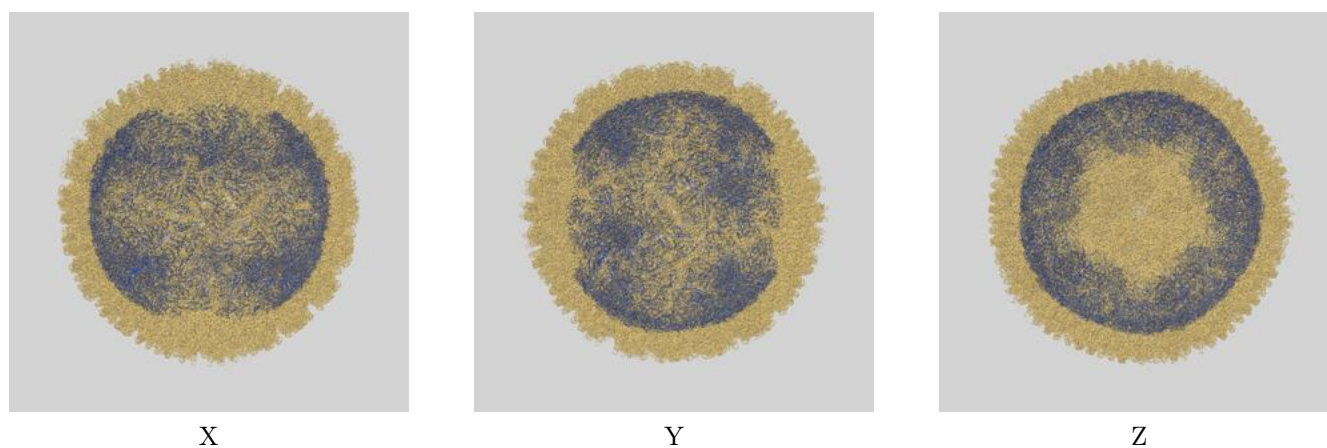
This section contains information regarding the fit between EMDB map EMD-33404 and PDB model 7XR3. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

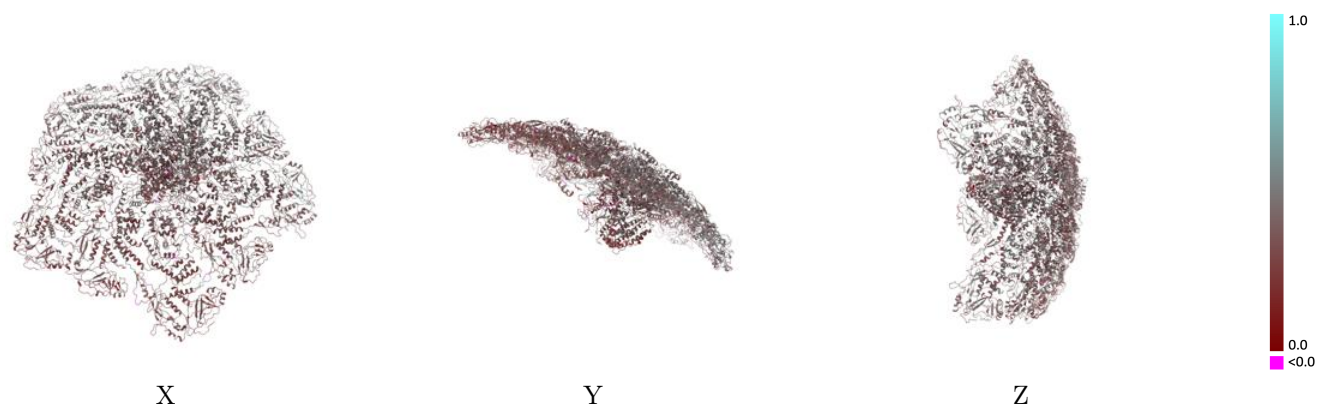


9.1.2 Map-model assembly overlay [i](#)



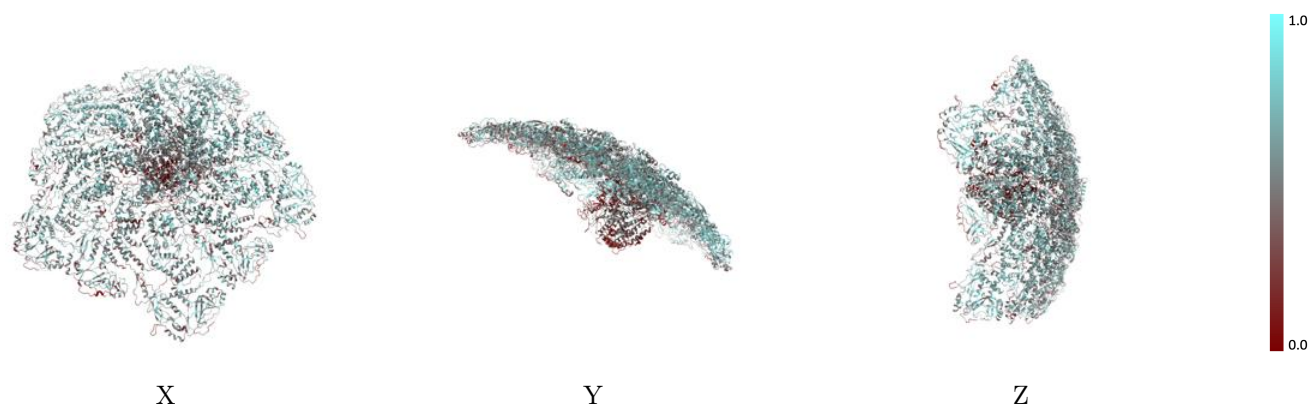
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



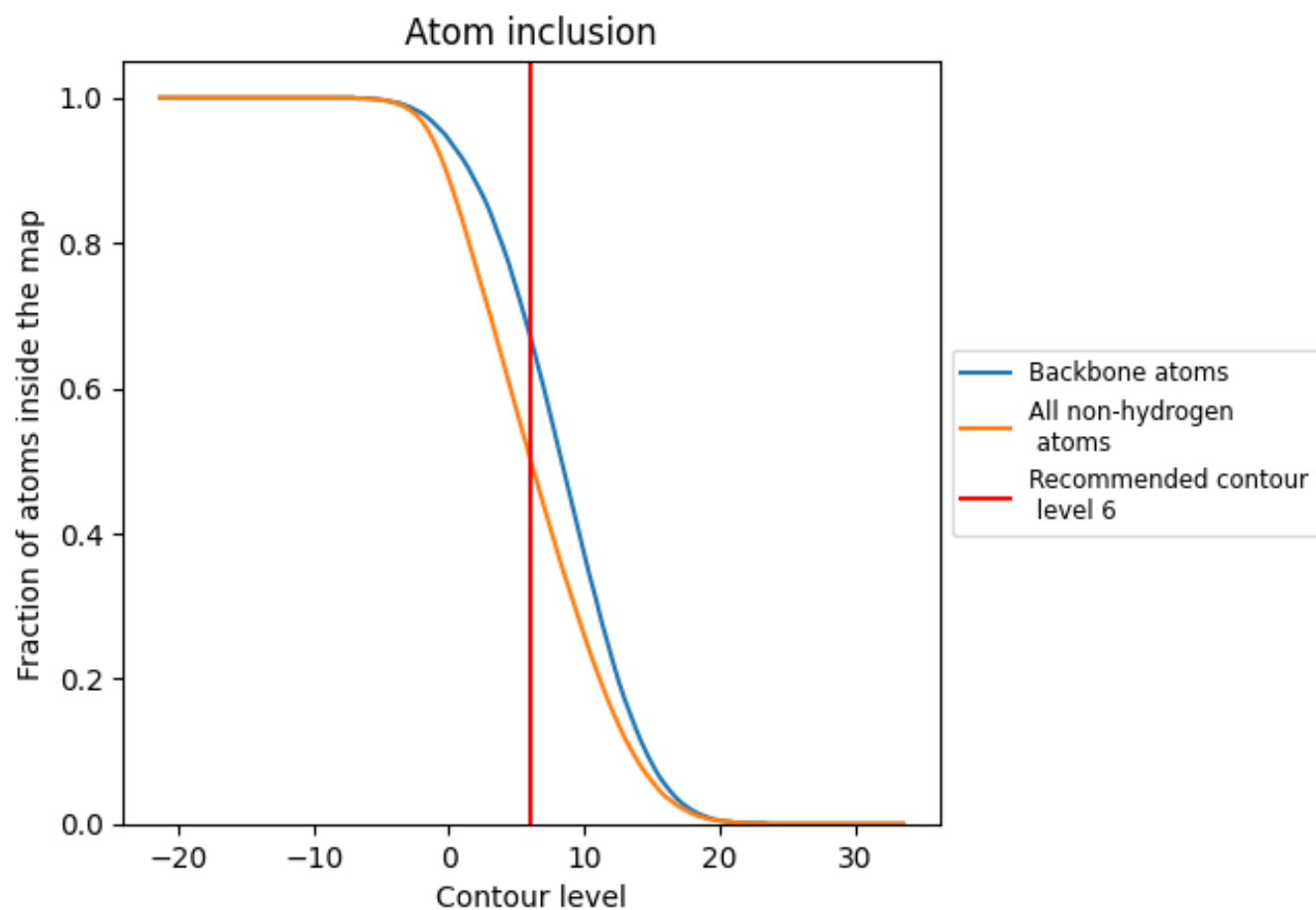
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.3580
A	0.5410	0.3990
B	0.5700	0.3920
C	0.5580	0.3950
D	0.5790	0.4090
E	0.5080	0.3430
F	0.5540	0.3670
G	0.4850	0.3300
H	0.5060	0.3160
I	0.5160	0.3590
J	0.5180	0.3340
Z	0.3130	0.3130

1.0

0.0

<0.0