



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 12:44 PM EDT

PDB ID : 10LK / pdb_000010lk
EMDB ID : EMD-75268
Title : Native flagellar filament from *Leptospira interrogans*
Authors : Brady, M.R.; San Martin, F.; Sindelar, C.V.; Buschiazzi, A.
Deposited on : 2026-01-26
Resolution : 4.40 Å (reported)
Based on initial model : .

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:

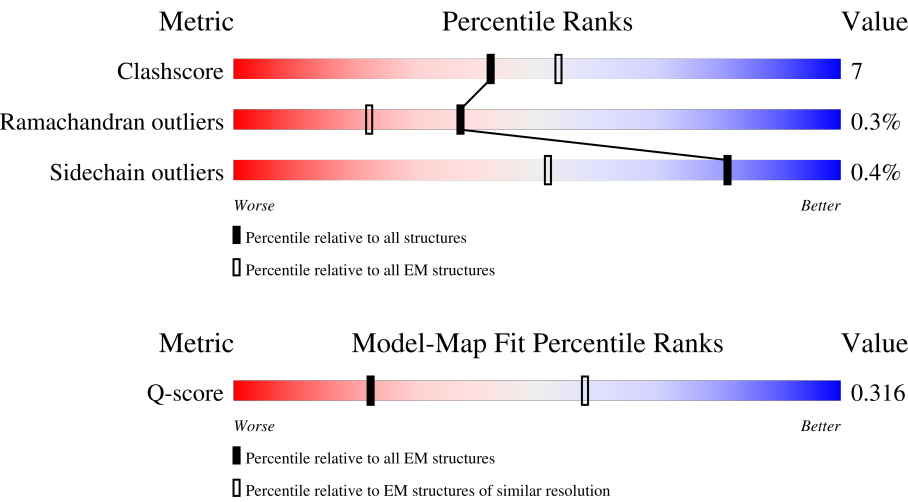
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	A4	281	
1	A5	281	
1	A6	281	
1	A7	281	

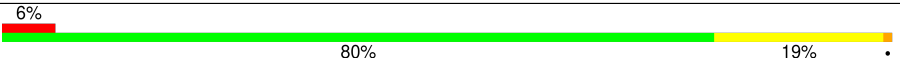
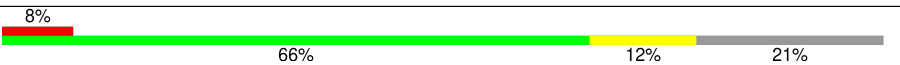
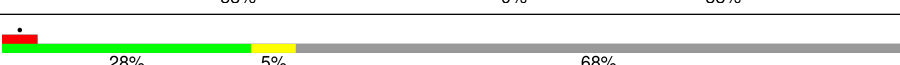
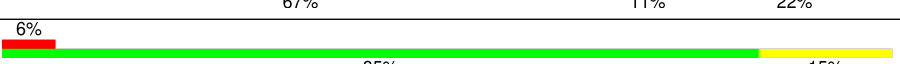
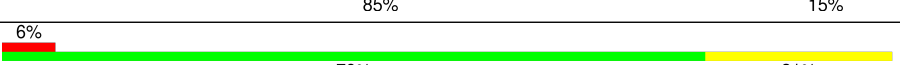
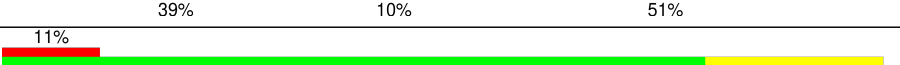
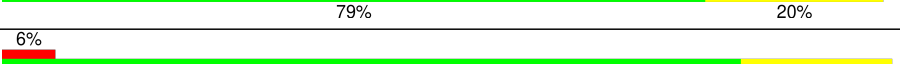
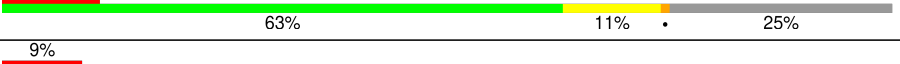
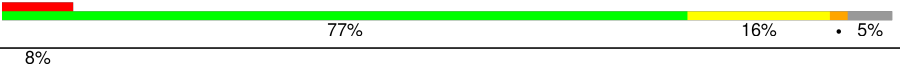
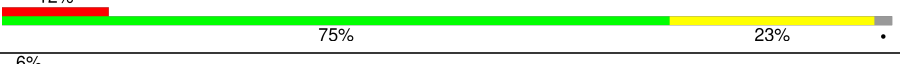
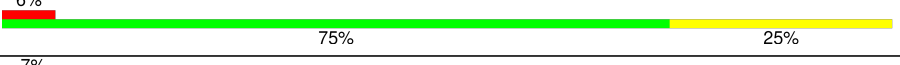
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	A8	281	
1	A9	281	
1	B3	281	
1	B4	281	
1	B5	281	
1	B6	281	
1	B7	281	
1	B8	281	
1	C3	281	
1	C4	281	
1	C5	281	
1	C6	281	
1	C7	281	
1	C8	281	
1	D3	281	
1	D4	281	
1	D5	281	
1	D6	281	
1	D7	281	
1	E2	281	
1	E3	281	
1	E4	281	
1	E5	281	
1	E6	281	
1	E7	281	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F2	281	
1	F3	281	
1	F4	281	
1	F5	281	
1	F6	281	
1	G1	281	
1	G2	281	
1	G6	281	
1	G7	281	
1	G8	281	
1	G9	281	
1	H6	281	
1	H7	281	
1	H8	281	
1	H9	281	
1	I5	281	
1	I6	281	
1	I7	281	
1	I8	281	
1	I9	281	
1	J5	281	
1	J6	281	
1	J7	281	
1	J8	281	
1	J9	281	

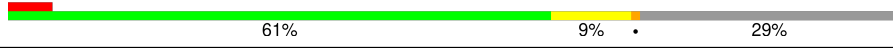
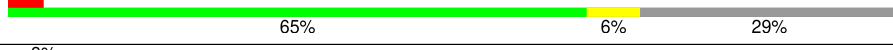
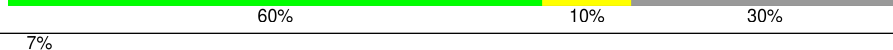
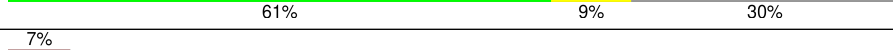
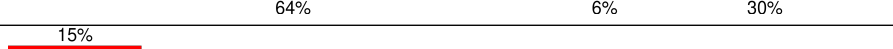
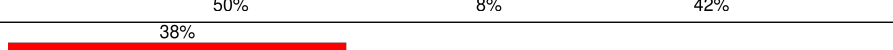
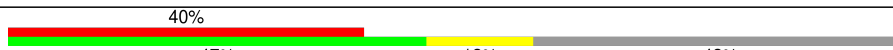
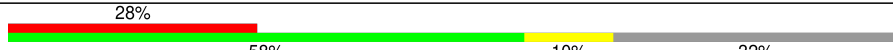
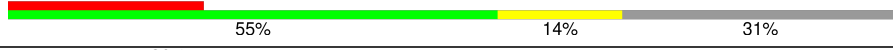
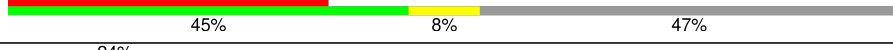
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K4	281	
1	K5	281	
1	K6	281	
1	K7	281	
1	K8	281	
1	K9	281	
1	h0	281	
1	h1	281	
1	i0	281	
1	j0	281	
2	L2	306	
2	L3	306	
2	L4	306	
2	L5	306	
2	L6	306	
2	M1	306	
2	M2	306	
2	M3	306	
2	M4	306	
2	M5	306	
2	N2	306	
2	N3	306	
2	N4	306	
2	N5	306	
2	N6	306	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O1	306	
2	O2	306	
2	O3	306	
2	O4	306	
2	O5	306	
2	P2	306	
2	P3	306	
2	P4	306	
2	P5	306	
2	P6	306	
2	p2	306	
2	p3	306	
2	p4	306	
2	p5	306	
3	Q1	276	
3	Q2	276	
3	Q3	276	
3	Q4	276	
3	R2	276	
3	R3	276	
3	R4	276	
3	R5	276	
3	S2	276	
3	S3	276	
3	S4	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	S5	276	
3	S6	276	
3	s3	276	
3	s4	276	
3	s5	276	
3	s6	276	
4	T1	315	
4	T2	315	
4	T3	315	
4	T4	315	
4	t1	315	
4	t2	315	
4	t3	315	
4	t4	315	
5	V1	239	
5	V2	239	
5	V3	239	
5	V4	239	
5	V5	239	
5	X1	239	
5	X2	239	
5	X3	239	
5	X4	239	
5	X5	239	
6	Y1	282	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	Y2	282	
6	Y3	282	
6	Y4	282	
6	Y5	282	
7	Z1	369	
7	Z2	369	
7	Z3	369	
7	Z4	369	
8	a2	237	
8	a3	237	
8	a4	237	
8	a5	237	
9	c1	146	
9	c2	146	
9	c3	146	
10	d2	291	
10	d3	291	
10	d4	291	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 248049 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 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A4	103	Total	C	N	O	S	0	0
			791	479	151	155	6		
1	A5	263	Total	C	N	O	S	0	0
			2054	1265	380	397	12		
1	A6	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	A7	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	A8	250	Total	C	N	O	S	0	0
			1945	1189	356	389	11		
1	A9	148	Total	C	N	O	S	0	0
			1151	711	201	233	6		
1	B3	64	Total	C	N	O	S	0	0
			500	311	94	91	4		
1	B4	147	Total	C	N	O	S	0	0
			1138	692	215	223	8		
1	B5	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	B6	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	B7	278	Total	C	N	O	S	0	0
			2162	1325	398	426	13		
1	B8	196	Total	C	N	O	S	0	0
			1541	947	282	304	8		
1	C3	103	Total	C	N	O	S	0	0
			791	479	151	155	6		
1	C4	246	Total	C	N	O	S	0	0
			1922	1179	358	373	12		
1	C5	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	C6	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	C7	250	Total	C	N	O	S	0	0
			1944	1191	353	389	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C8	159	Total	C	N	O	S	0	0
			1243	769	220	247	7		
1	D3	161	Total	C	N	O	S	0	0
			1263	767	245	241	10		
1	D4	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	D5	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	D6	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	D7	210	Total	C	N	O	S	0	0
			1638	1003	300	325	10		
1	E2	98	Total	C	N	O	S	0	0
			757	459	145	147	6		
1	E3	234	Total	C	N	O	S	0	0
			1832	1122	342	356	12		
1	E4	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	E5	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	E6	256	Total	C	N	O	S	0	0
			1995	1221	365	397	12		
1	E7	165	Total	C	N	O	S	0	0
			1292	798	232	255	7		
1	F2	131	Total	C	N	O	S	0	0
			1009	611	193	198	7		
1	F3	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	F4	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	F5	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	F6	221	Total	C	N	O	S	0	0
			1719	1049	314	346	10		
1	G1	261	Total	C	N	O	S	0	0
			2027	1241	371	403	12		
1	G2	174	Total	C	N	O	S	0	0
			1361	841	245	268	7		
1	G6	91	Total	C	N	O	S	0	0
			694	423	131	135	5		
1	G7	218	Total	C	N	O	S	0	0
			1710	1046	323	329	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G8	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	G9	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	H6	138	Total	C	N	O	S	0	0
			1067	648	203	208	8		
1	H7	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	H8	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	H9	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	I5	86	Total	C	N	O	S	0	0
			654	399	123	127	5		
1	I6	211	Total	C	N	O	S	0	0
			1655	1011	314	319	11		
1	I7	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	I8	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	I9	266	Total	C	N	O	S	0	0
			2063	1263	378	410	12		
1	J5	121	Total	C	N	O	S	0	0
			935	568	179	181	7		
1	J6	276	Total	C	N	O	S	0	0
			2151	1318	399	421	13		
1	J7	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	J8	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	J9	233	Total	C	N	O	S	0	0
			1812	1108	330	363	11		
1	K4	77	Total	C	N	O	S	0	0
			596	365	114	114	3		
1	K5	201	Total	C	N	O	S	0	0
			1578	965	301	301	11		
1	K6	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	K7	281	Total	C	N	O	S	0	0
			2190	1343	404	430	13		
1	K8	270	Total	C	N	O	S	0	0
			2100	1285	388	415	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K9	184	Total	C	N	O	S	0	0
			1442	889	260	286	7		
1	h0	235	Total	C	N	O	S	0	0
			1827	1115	333	368	11		
1	h1	109	Total	C	N	O	S	0	0
			819	503	142	171	3		
1	i0	178	Total	C	N	O	S	0	0
			1397	864	252	274	7		
1	j0	128	Total	C	N	O	S	0	0
			989	616	171	199	3		

- Molecule 2 is a protein called Flagellar Coiling Protein A (FcpA).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	208	Total	C	N	O	S	0	0
			1678	1078	298	300	2		
2	L3	217	Total	C	N	O	S	0	0
			1768	1138	314	314	2		
2	L4	217	Total	C	N	O	S	0	0
			1768	1138	314	314	2		
2	L5	217	Total	C	N	O	S	0	0
			1768	1138	314	314	2		
2	L6	175	Total	C	N	O	S	0	0
			1444	932	256	254	2		
2	M1	90	Total	C	N	O		0	0
			724	465	128	131			
2	M2	221	Total	C	N	O	S	0	0
			1799	1158	319	320	2		
2	M3	221	Total	C	N	O	S	0	0
			1799	1158	319	320	2		
2	M4	221	Total	C	N	O	S	0	0
			1799	1158	319	320	2		
2	M5	216	Total	C	N	O	S	0	0
			1760	1132	313	313	2		
2	N2	190	Total	C	N	O	S	0	0
			1545	996	272	275	2		
2	N3	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		
2	N4	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		
2	N5	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N6	178	Total	C	N	O	S	0	0
			1464	943	263	256	2		
2	O1	63	Total	C	N	O		0	0
			507	323	90	94			
2	O2	216	Total	C	N	O	S	0	0
			1755	1130	313	310	2		
2	O3	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		
2	O4	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		
2	O5	216	Total	C	N	O	S	0	0
			1759	1133	313	311	2		
2	P2	179	Total	C	N	O	S	0	0
			1459	945	257	255	2		
2	P3	215	Total	C	N	O	S	0	0
			1750	1128	312	308	2		
2	P4	215	Total	C	N	O	S	0	0
			1750	1128	312	308	2		
2	P5	215	Total	C	N	O	S	0	0
			1750	1128	312	308	2		
2	P6	178	Total	C	N	O	S	0	0
			1463	942	264	255	2		
2	p2	215	Total	C	N	O	S	0	0
			1747	1124	312	309	2		
2	p3	217	Total	C	N	O	S	0	0
			1767	1139	314	312	2		
2	p4	216	Total	C	N	O	S	0	0
			1759	1133	313	311	2		
2	p5	216	Total	C	N	O	S	0	0
			1759	1133	313	311	2		

- Molecule 3 is a protein called Flagellar Coiling Protein B (FcpB).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q1	161	Total	C	N	O	S	0	0
			1339	854	236	243	6		
3	Q2	188	Total	C	N	O	S	0	0
			1567	997	274	289	7		
3	Q3	196	Total	C	N	O	S	0	0
			1633	1037	287	302	7		
3	Q4	192	Total	C	N	O	S	0	0
			1601	1018	280	296	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R2	183	Total	C	N	O	S	0	0
			1524	964	267	287	6		
3	R3	202	Total	C	N	O	S	0	0
			1677	1062	294	314	7		
3	R4	190	Total	C	N	O	S	0	0
			1588	1010	277	294	7		
3	R5	190	Total	C	N	O	S	0	0
			1585	1005	277	296	7		
3	S2	146	Total	C	N	O	S	0	0
			1228	784	214	225	5		
3	S3	187	Total	C	N	O	S	0	0
			1556	990	273	286	7		
3	S4	192	Total	C	N	O	S	0	0
			1602	1021	281	293	7		
3	S5	190	Total	C	N	O	S	0	0
			1581	1005	277	292	7		
3	S6	188	Total	C	N	O	S	0	0
			1569	997	275	290	7		
3	s3	192	Total	C	N	O	S	0	0
			1595	1013	279	296	7		
3	s4	189	Total	C	N	O	S	0	0
			1584	1009	275	293	7		
3	s5	192	Total	C	N	O	S	0	0
			1604	1022	279	296	7		
3	s6	166	Total	C	N	O	S	0	0
			1397	892	246	254	5		

- Molecule 4 is a protein called Flagellar filament sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T1	260	Total	C	N	O	S	0	0
			2058	1310	351	393	4		
4	T2	270	Total	C	N	O	S	0	0
			2141	1362	365	410	4		
4	T3	270	Total	C	N	O	S	0	0
			2141	1362	365	410	4		
4	T4	256	Total	C	N	O	S	0	0
			2035	1296	344	391	4		
4	t1	271	Total	C	N	O	S	0	0
			2150	1368	367	411	4		
4	t2	270	Total	C	N	O	S	0	0
			2141	1362	365	410	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	t3	270	Total	C	N	O	S	0	0
			2141	1362	365	410	4		
4	t4	268	Total	C	N	O	S	0	0
			2125	1351	363	408	3		

- Molecule 5 is a protein called Flagellar filament sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V1	173	Total	C	N	O	S	0	0
			1422	913	255	253	1		
5	V2	197	Total	C	N	O	S	0	0
			1621	1040	287	293	1		
5	V3	196	Total	C	N	O	S	0	0
			1613	1036	286	290	1		
5	V4	196	Total	C	N	O	S	0	0
			1613	1036	286	290	1		
5	V5	196	Total	C	N	O	S	0	0
			1613	1036	286	290	1		
5	X1	181	Total	C	N	O	S	0	0
			1484	949	265	269	1		
5	X2	197	Total	C	N	O	S	0	0
			1621	1040	287	293	1		
5	X3	197	Total	C	N	O	S	0	0
			1621	1040	287	293	1		
5	X4	197	Total	C	N	O	S	0	0
			1621	1040	287	293	1		
5	X5	195	Total	C	N	O	S	0	0
			1610	1033	285	291	1		

- Molecule 6 is a protein called FlaA2 associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y1	101	Total	C	N	O	S	0	0
			834	541	135	154	4		
6	Y2	222	Total	C	N	O	S	0	0
			1844	1177	316	346	5		
6	Y3	225	Total	C	N	O	S	0	0
			1876	1197	322	352	5		
6	Y4	224	Total	C	N	O	S	0	0
			1872	1195	321	351	5		
6	Y5	225	Total	C	N	O	S	0	0
			1876	1197	322	352	5		

- Molecule 7 is a protein called FlaA2-associated protein 1 (FlaAP).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z1	255	Total	C	N	O	S	0	0
			2173	1383	393	391	6		
7	Z2	255	Total	C	N	O	S	0	0
			2173	1383	393	391	6		
7	Z3	254	Total	C	N	O	S	0	0
			2162	1377	389	390	6		
7	Z4	255	Total	C	N	O	S	0	0
			2173	1383	393	391	6		

- Molecule 8 is a protein called DUF4468 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a2	172	Total	C	N	O	S	0	0
			1421	901	253	266	1		
8	a3	178	Total	C	N	O	S	0	0
			1460	924	260	275	1		
8	a4	178	Total	C	N	O	S	0	0
			1460	924	260	275	1		
8	a5	178	Total	C	N	O	S	0	0
			1460	924	260	275	1		

- Molecule 9 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c1	101	Total	C	N	O	S	0	0
			867	569	133	163	2		
9	c2	103	Total	C	N	O	S	0	0
			882	578	136	166	2		
9	c3	103	Total	C	N	O	S	0	0
			882	578	136	166	2		

- Molecule 10 is a protein called HEAT repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d2	248	Total	C	N	O	S	0	0
			1993	1272	334	380	7		
10	d3	240	Total	C	N	O	S	0	0
			1924	1227	321	369	7		
10	d4	245	Total	C	N	O	S	0	0
			1972	1258	328	379	7		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	T1	1	Total Ca 1 1	0
11	T2	1	Total Ca 1 1	0
11	T3	1	Total Ca 1 1	0
11	T4	1	Total Ca 1 1	0
11	V1	1	Total Ca 1 1	0
11	V2	1	Total Ca 1 1	0
11	V3	1	Total Ca 1 1	0
11	V4	1	Total Ca 1 1	0
11	V5	1	Total Ca 1 1	0
11	X1	1	Total Ca 1 1	0
11	X2	1	Total Ca 1 1	0
11	X3	1	Total Ca 1 1	0
11	X4	1	Total Ca 1 1	0
11	X5	1	Total Ca 1 1	0
11	t1	1	Total Ca 1 1	0
11	t2	1	Total Ca 1 1	0
11	t3	1	Total Ca 1 1	0
11	t4	1	Total Ca 1 1	0

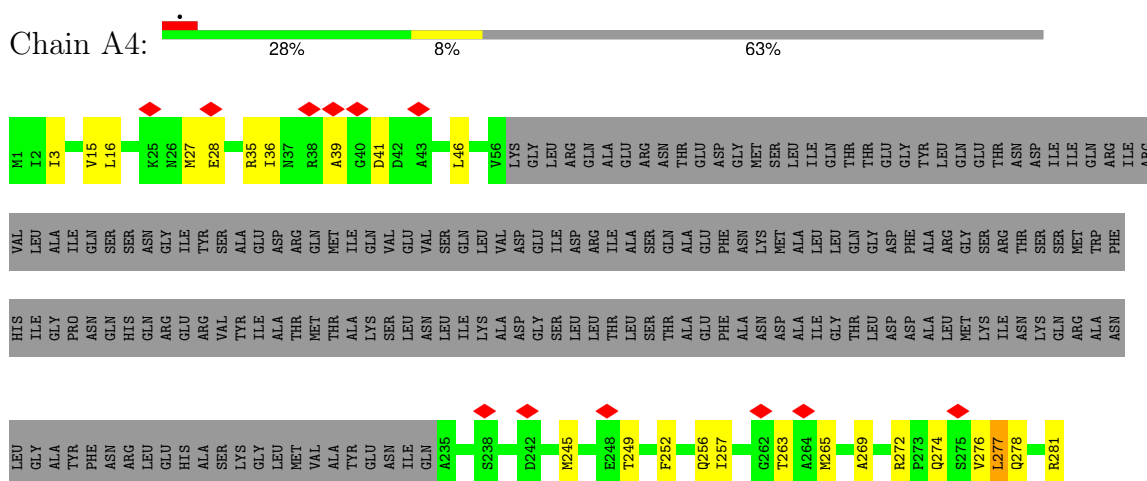
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	T1	2	Total 2	O 2	0
12	T2	2	Total 2	O 2	0
12	T3	2	Total 2	O 2	0
12	T4	2	Total 2	O 2	0
12	V1	2	Total 2	O 2	0
12	V2	2	Total 2	O 2	0
12	V3	2	Total 2	O 2	0
12	V4	2	Total 2	O 2	0
12	V5	2	Total 2	O 2	0
12	X1	2	Total 2	O 2	0
12	X2	2	Total 2	O 2	0
12	X3	2	Total 2	O 2	0
12	X4	2	Total 2	O 2	0
12	X5	2	Total 2	O 2	0
12	t1	2	Total 2	O 2	0
12	t2	2	Total 2	O 2	0
12	t3	2	Total 2	O 2	0
12	t4	2	Total 2	O 2	0

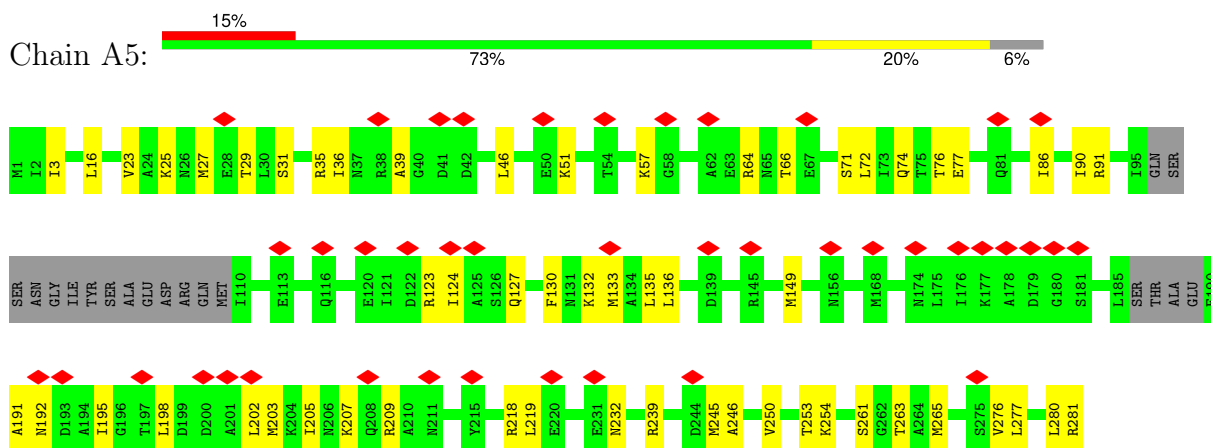
3 Residue-property plots [i](#)

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.

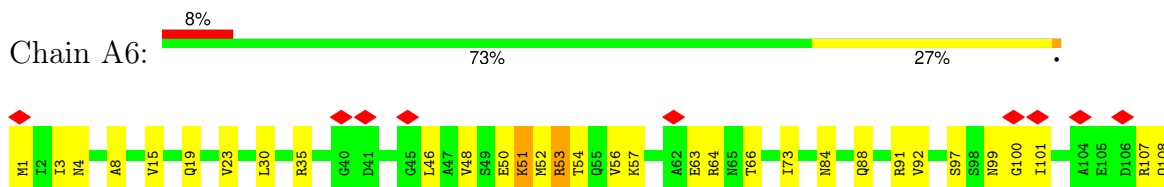
• Molecule 1: Flagellin

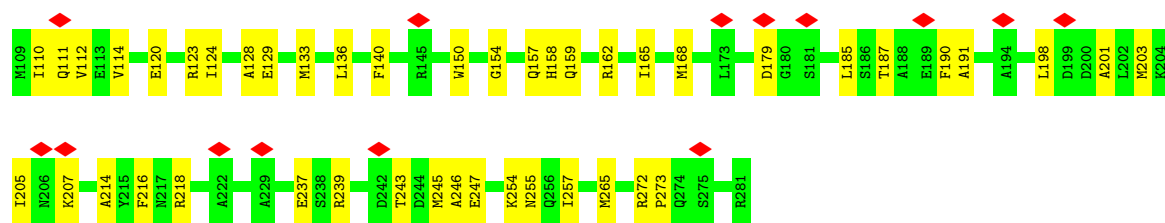


• Molecule 1: Flagellin

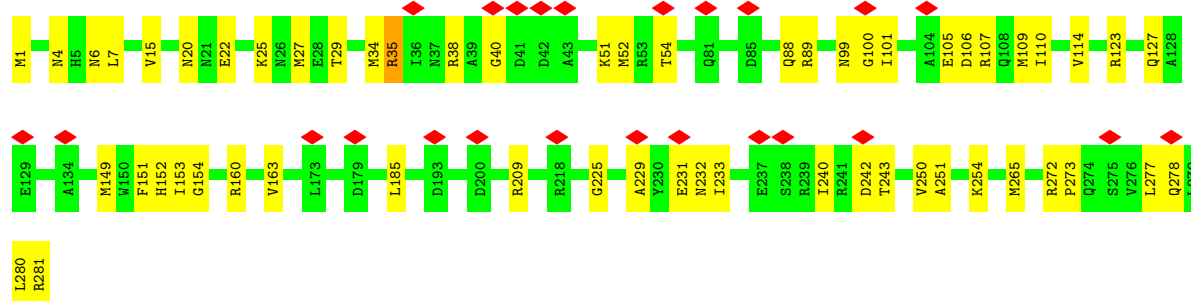
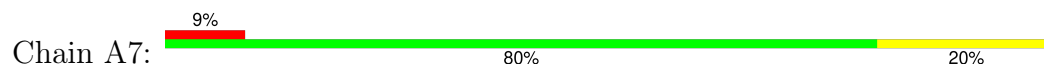


• Molecule 1: Flagellin

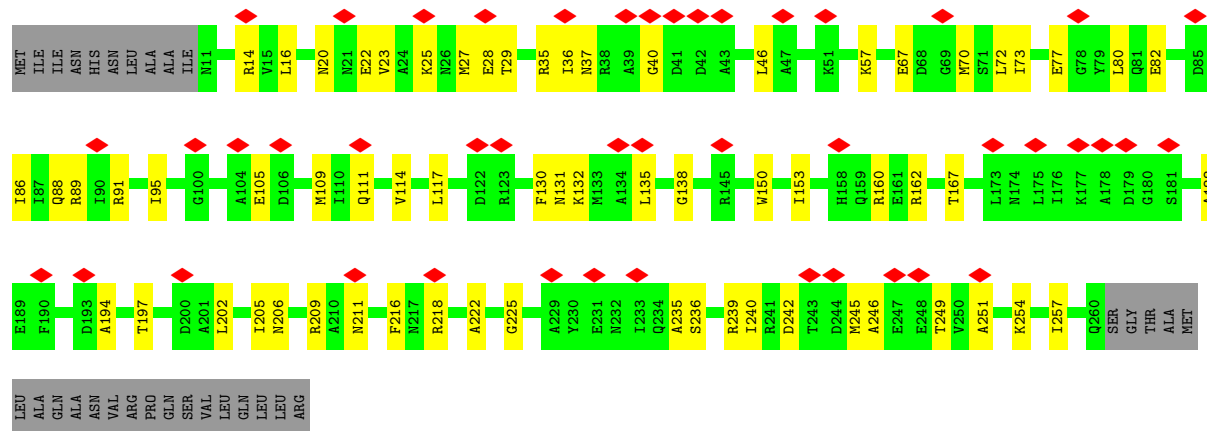




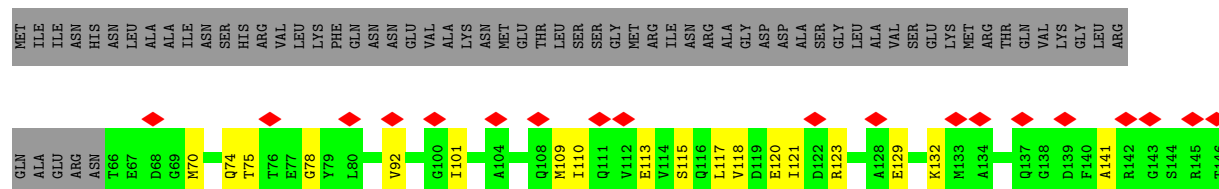
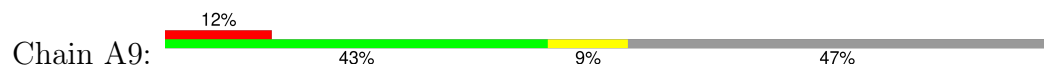
• Molecule 1: Flagellin



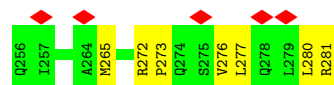
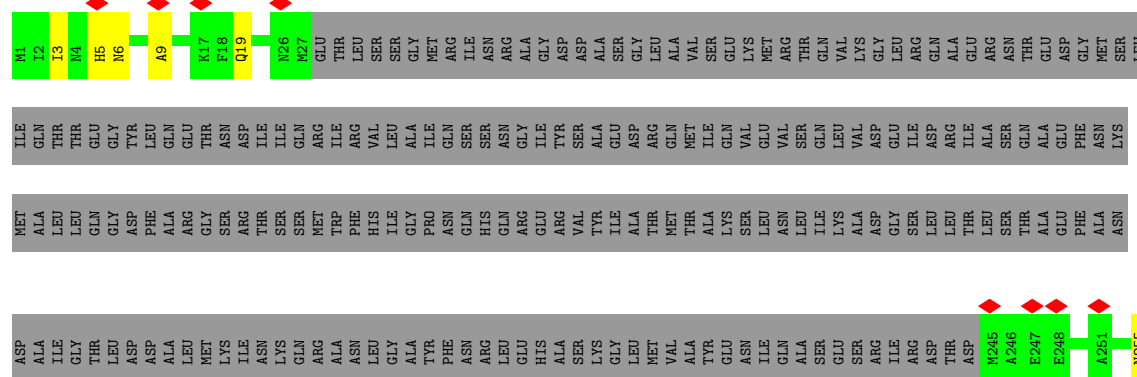
• Molecule 1: Flagellin



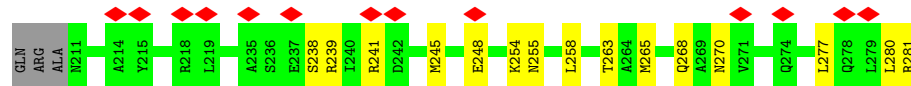
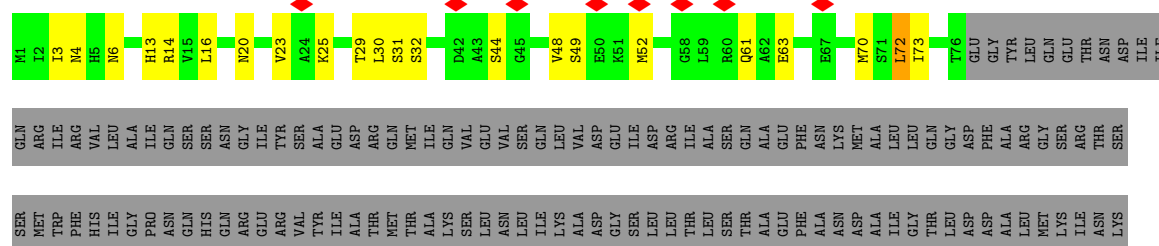
• Molecule 1: Flagellin



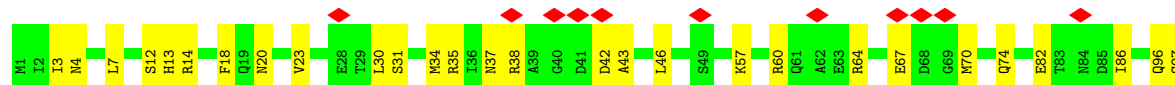
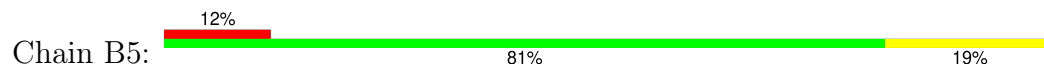
- Molecule 1: Flagellin

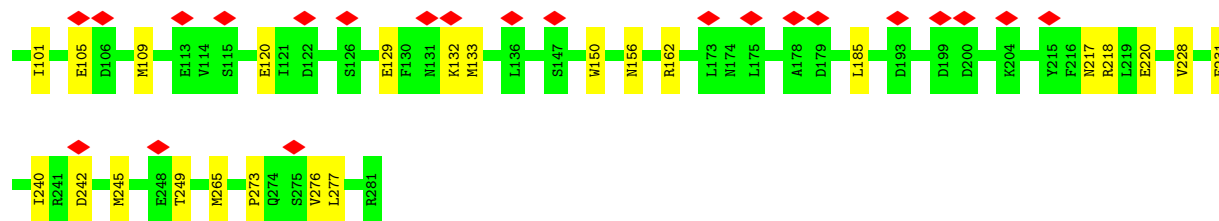


- Molecule 1: Flagellin

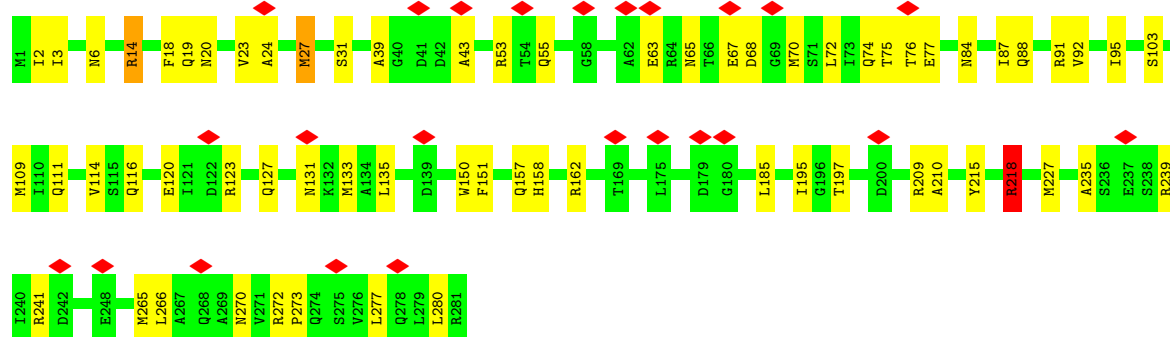
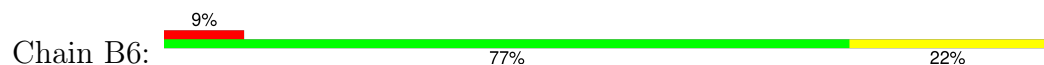


- Molecule 1: Flagellin

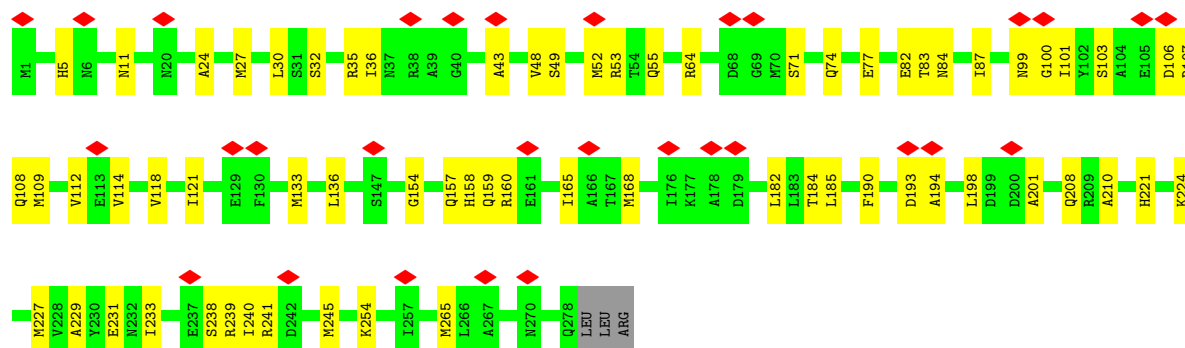
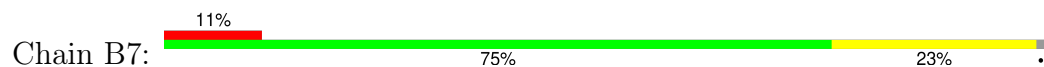




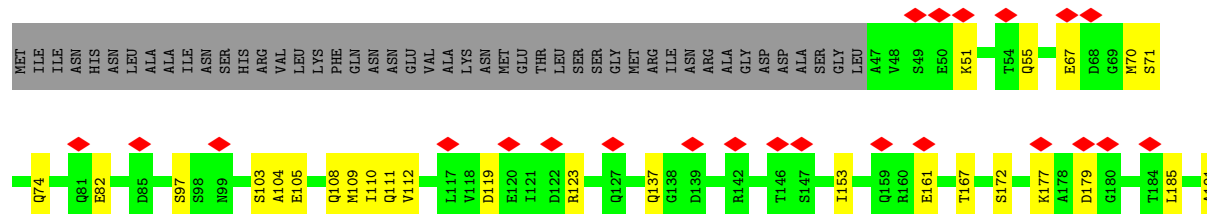
• Molecule 1: Flagellin

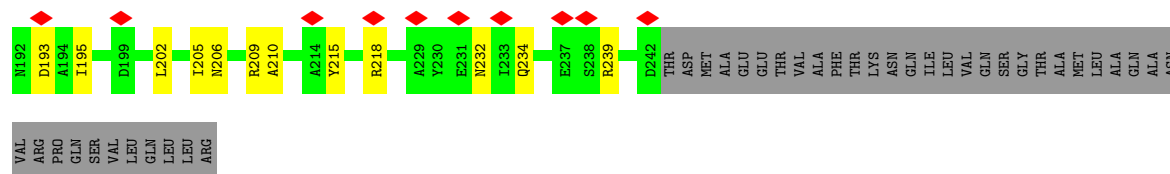


• Molecule 1: Flagellin



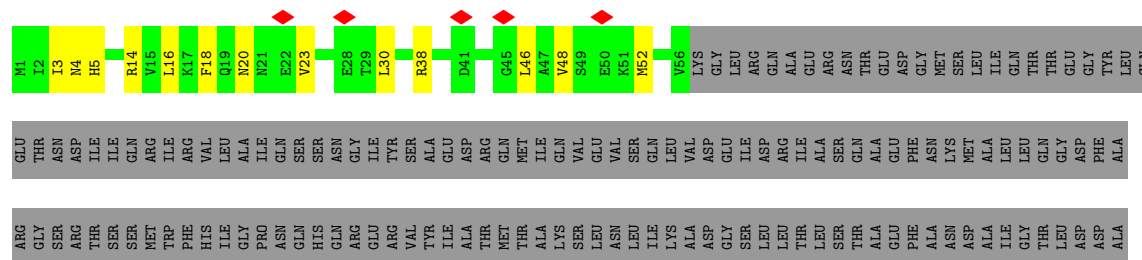
• Molecule 1: Flagellin





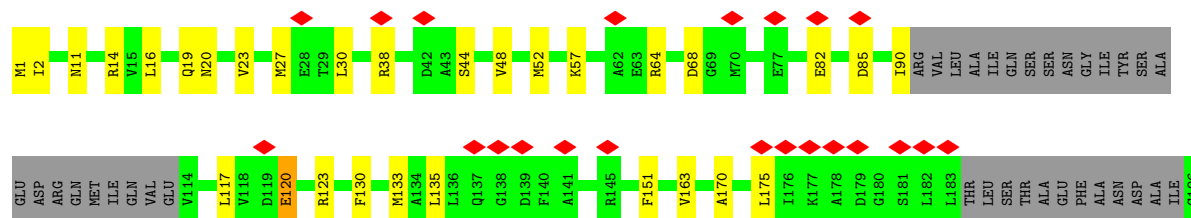
• Molecule 1: Flagellin

Chain C3: 30% 7% 63%



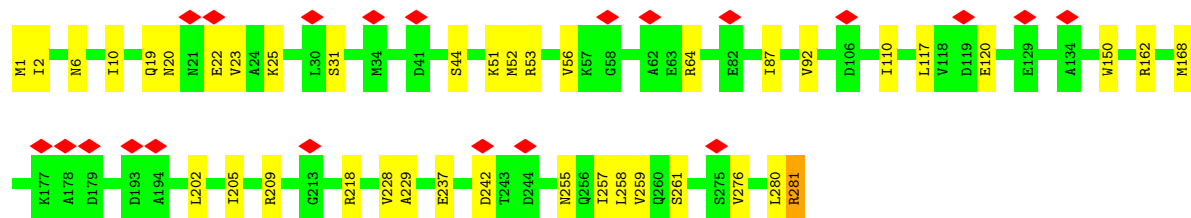
• Molecule 1: Flagellin

Chain C4: 11% 70% 17% 12%

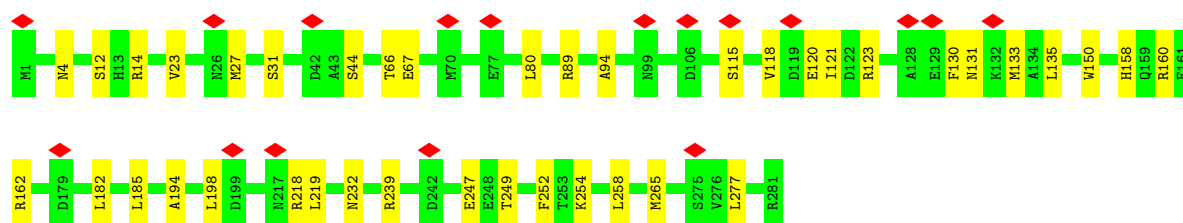
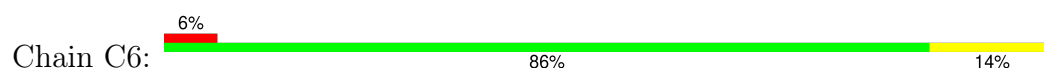


• Molecule 1: Flagellin

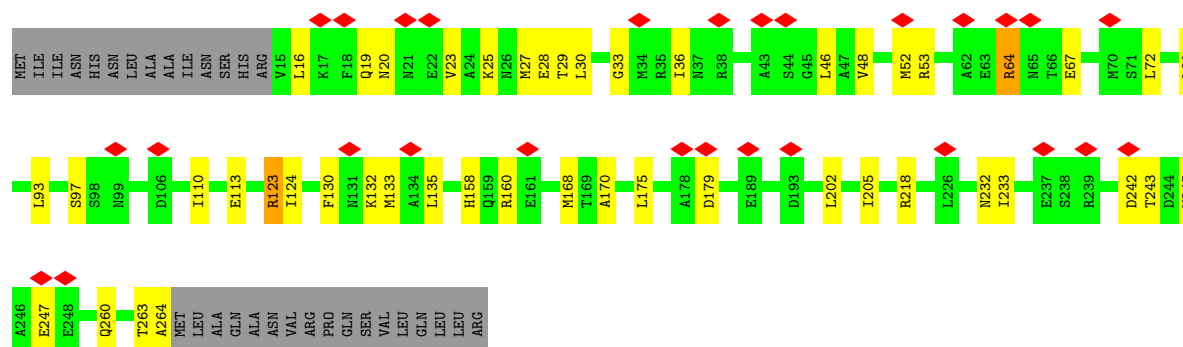
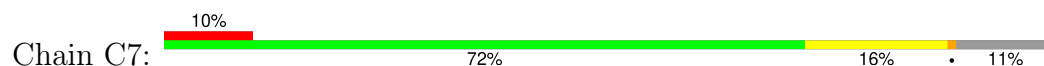
Chain C5: 7% 86% 14%



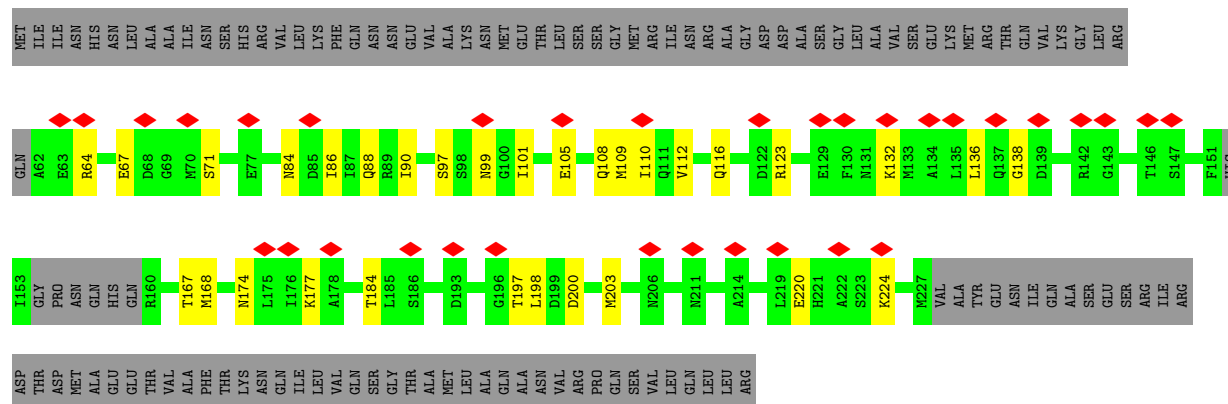
• Molecule 1: Flagellin



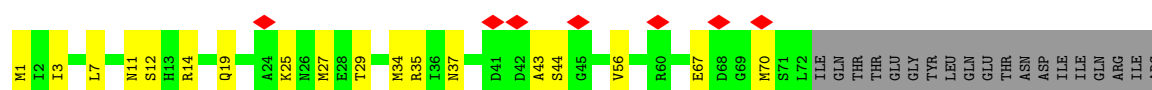
• Molecule 1: Flagellin

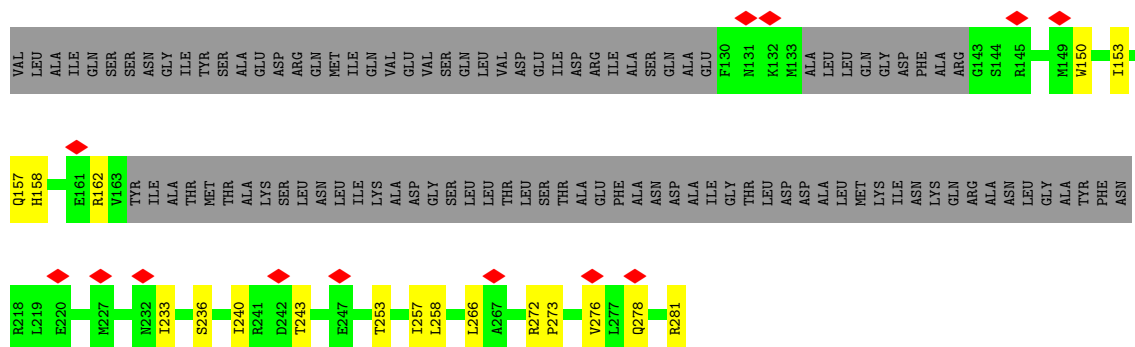


• Molecule 1: Flagellin

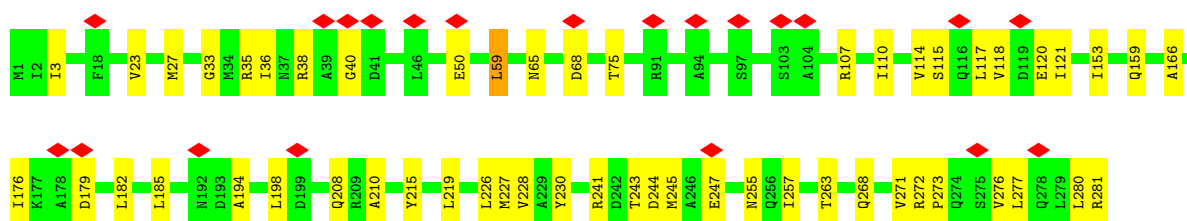
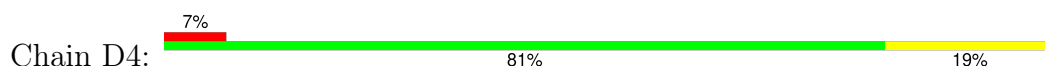


• Molecule 1: Flagellin

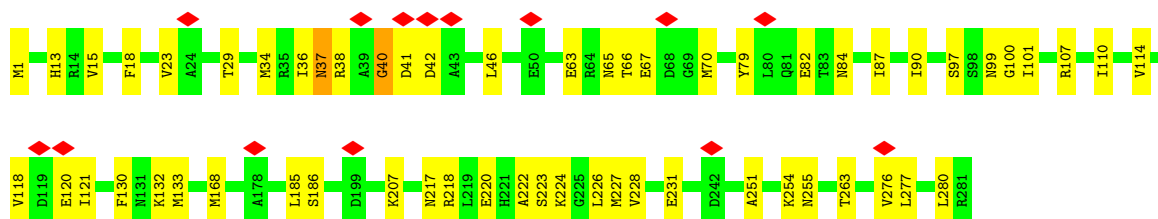
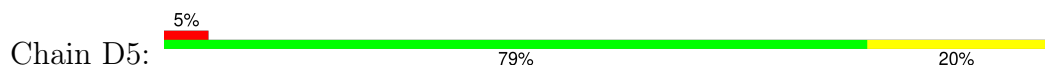




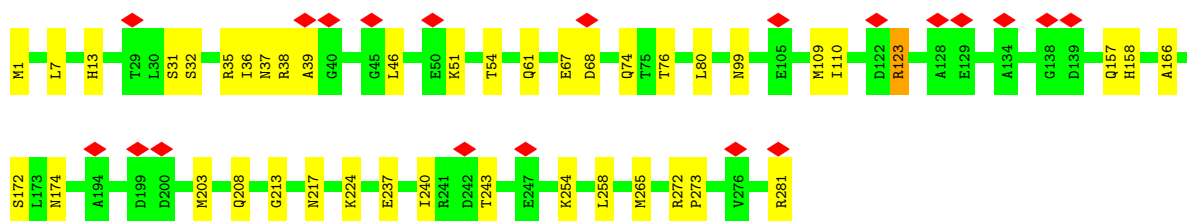
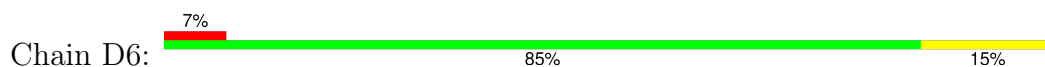
• Molecule 1: Flagellin



• Molecule 1: Flagellin

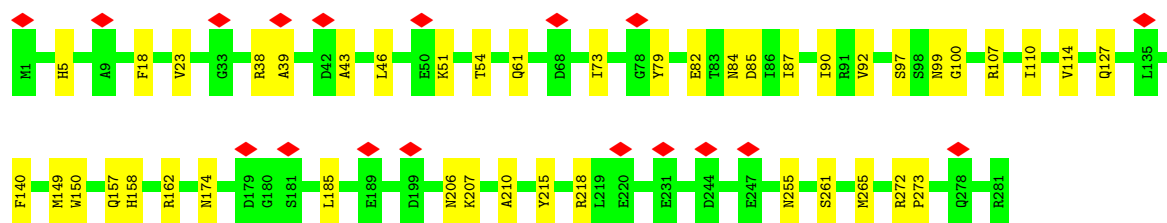


• Molecule 1: Flagellin

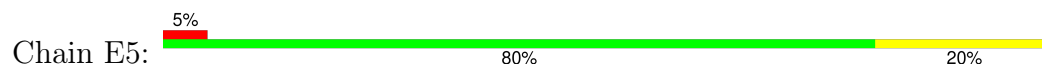


• Molecule 1: Flagellin

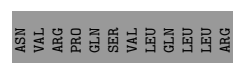
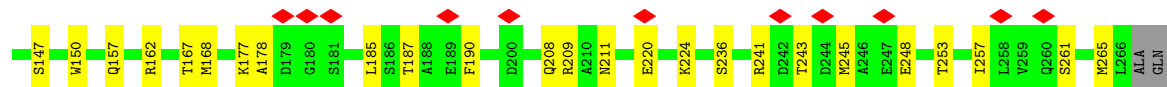
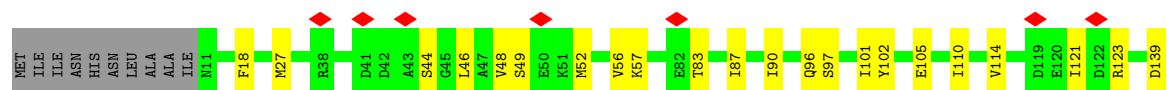
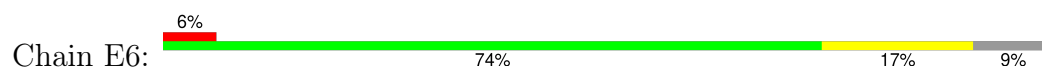




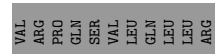
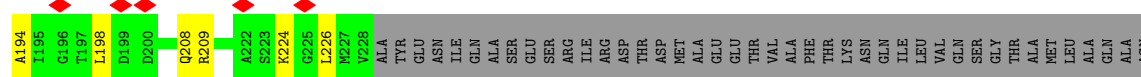
• Molecule 1: Flagellin



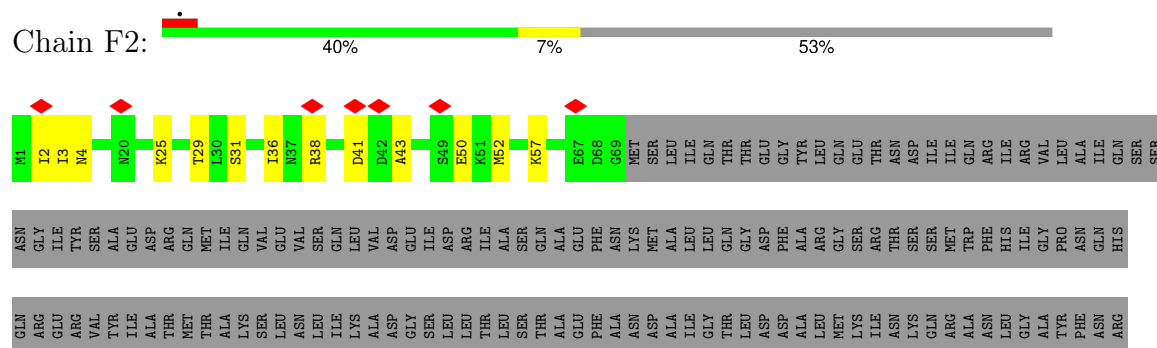
• Molecule 1: Flagellin



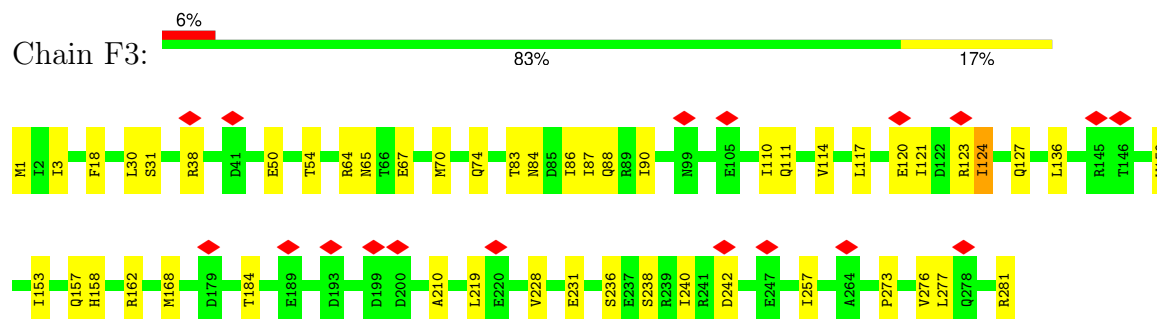
• Molecule 1: Flagellin



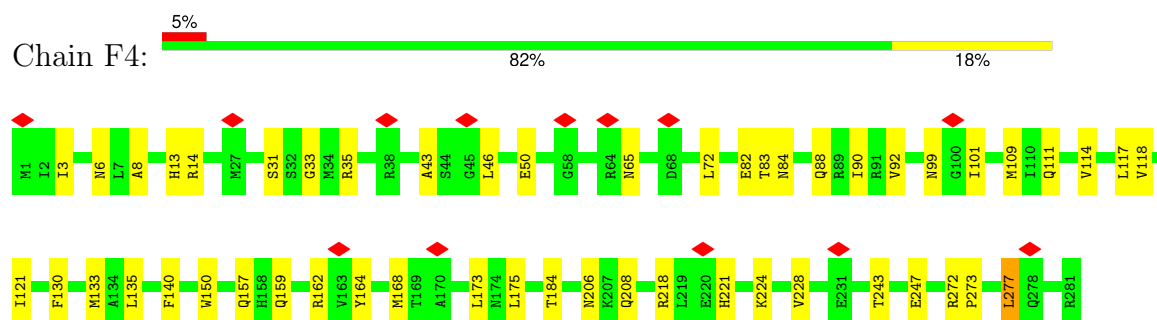
• Molecule 1: Flagellin



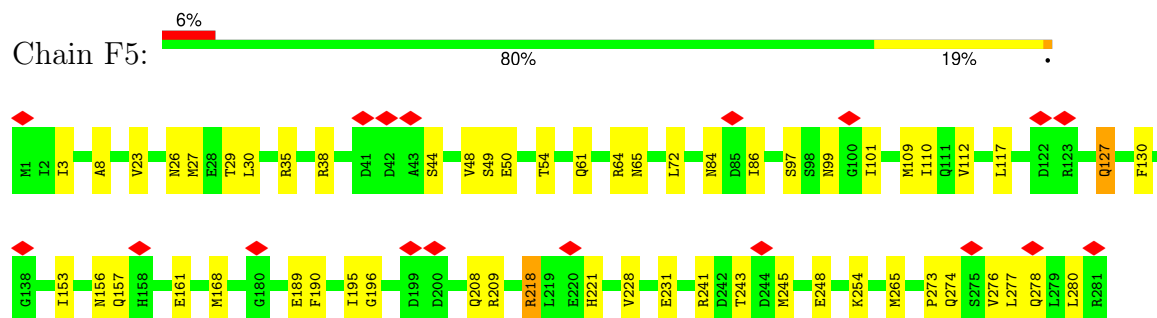
• Molecule 1: Flagellin



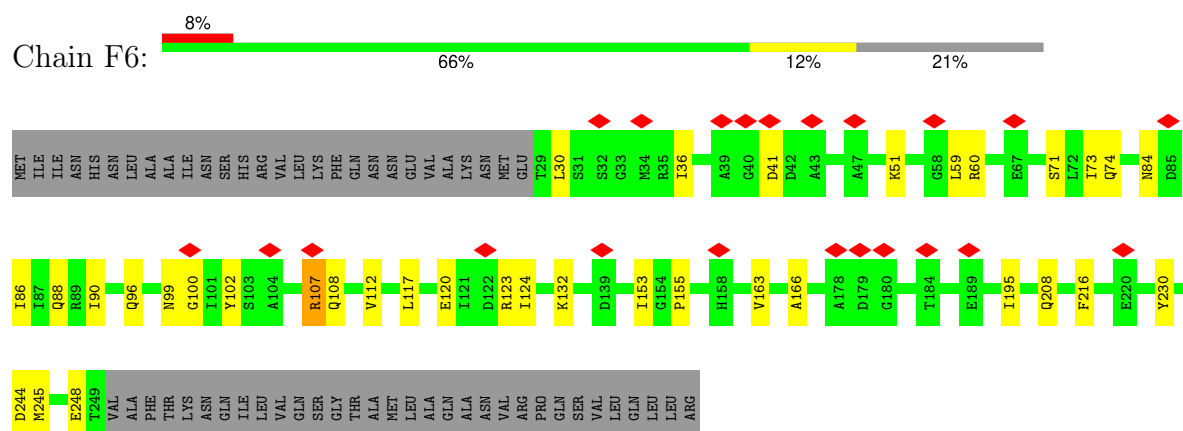
• Molecule 1: Flagellin



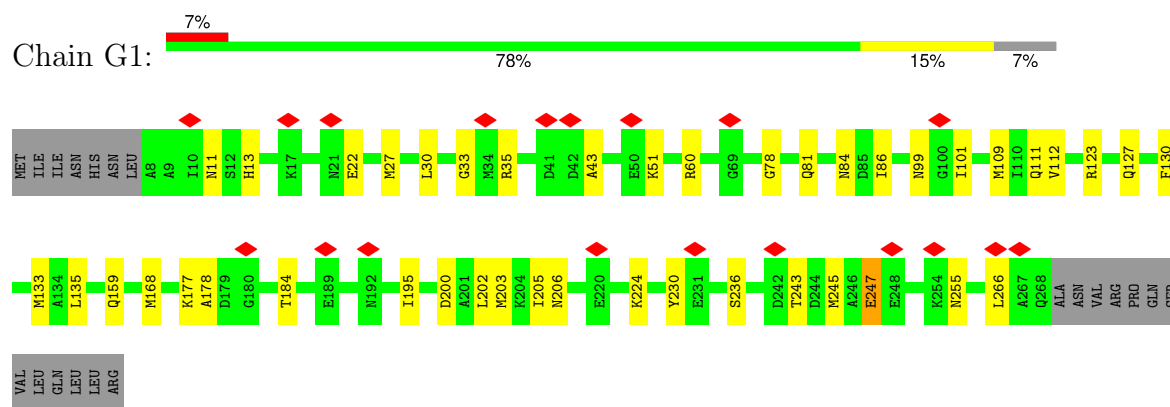
• Molecule 1: Flagellin



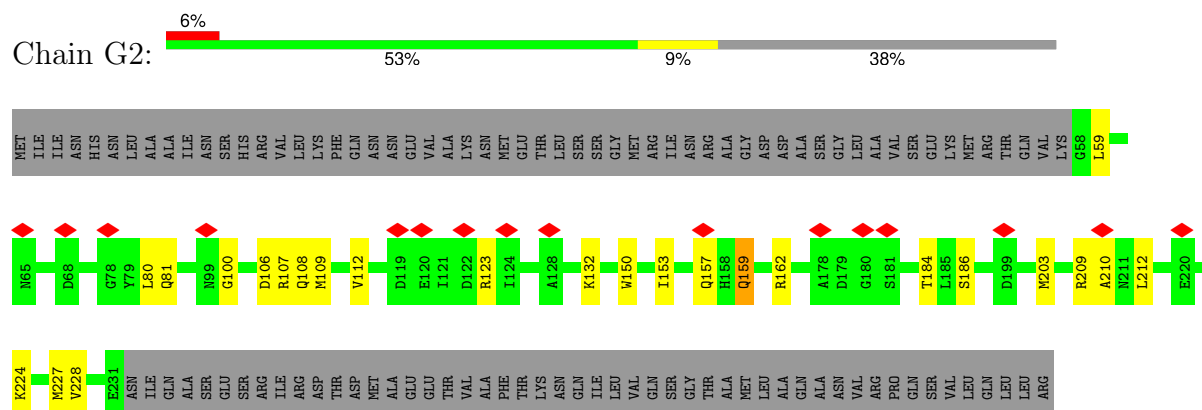
• Molecule 1: Flagellin



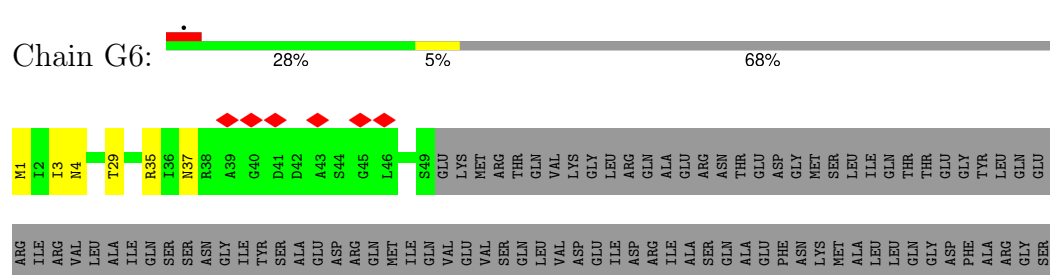
- Molecule 1: Flagellin

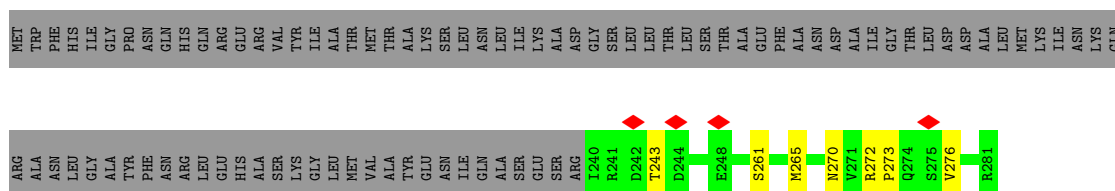


- Molecule 1: Flagellin

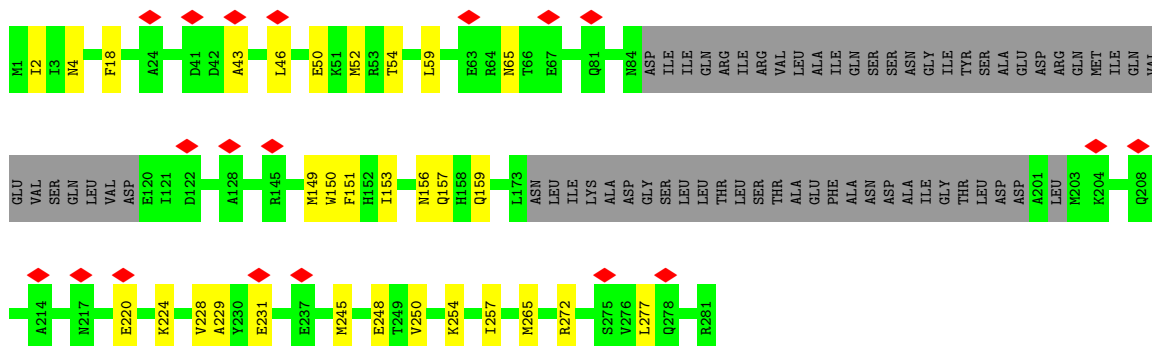


- Molecule 1: Flagellin

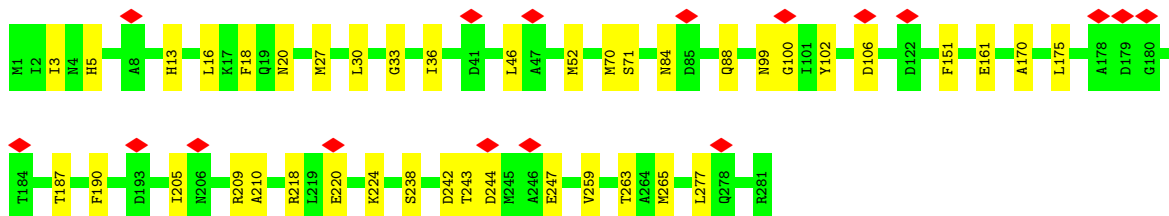
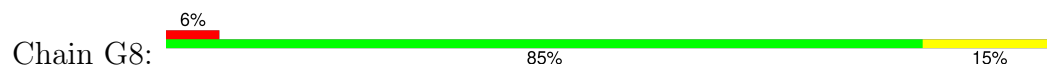




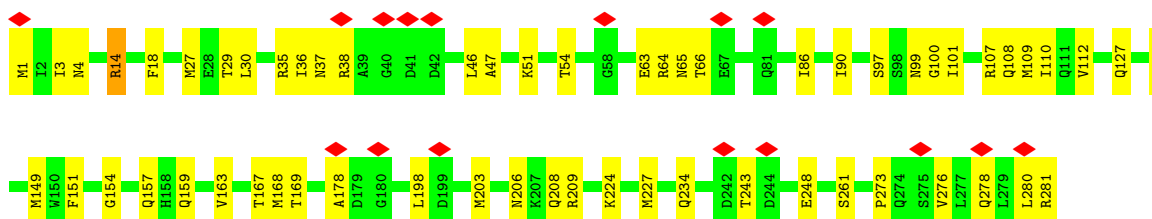
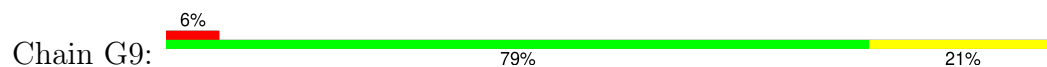
- Molecule 1: Flagellin



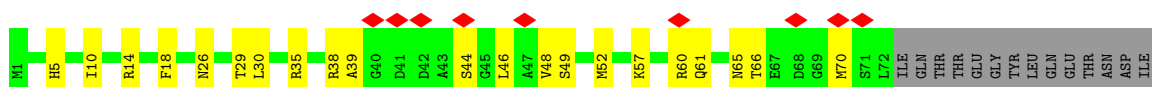
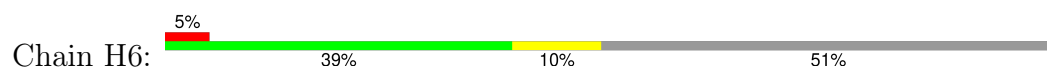
- Molecule 1: Flagellin



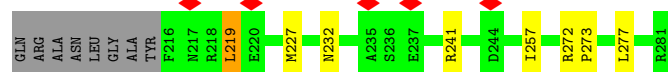
- Molecule 1: Flagellin



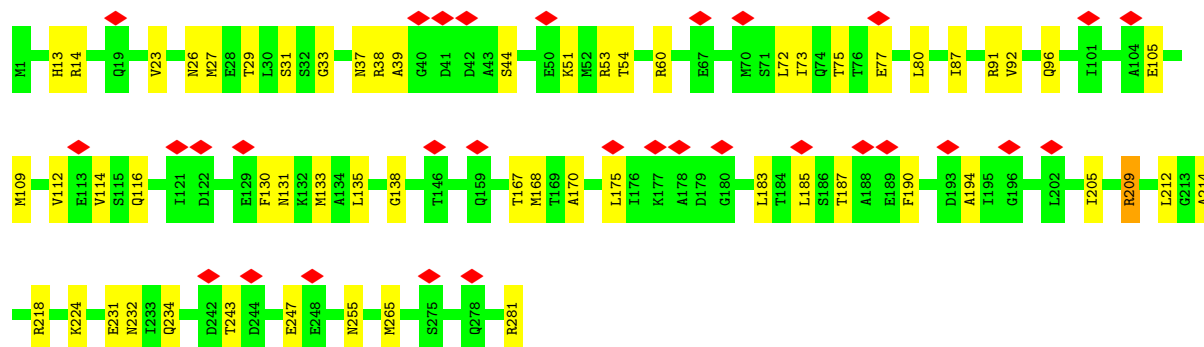
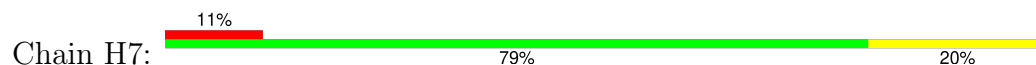
- Molecule 1: Flagellin



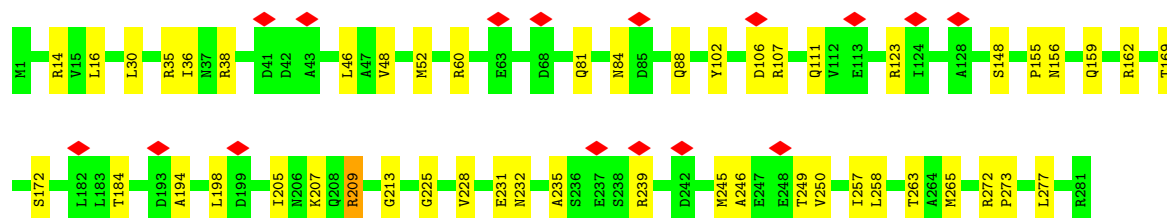
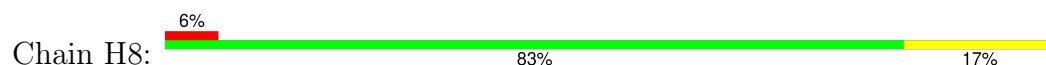
GLN	ARG	ILE	ALA	ASN	VAL	LEU	GLY	ALA	ILE	GLN	SER	SER	GLN	ASN	GLY	ILE	TYR	VAL	ILE	GLU	ASP	ARG	GLN	MET	THR	ALA	ILE	GLN	VAL	GLU	VAL	LEU	ASN	LEU	ILE	LYS	VAL	GLU	VAL	LEU	GLN	ILE	VAL	ASP	GLY	ASP	ILE	SER	LEU	ASP	ARG	ILE	ALA	SER	GLN	GLU	ALA	GLU	PHE	ALA	ASN	LYS	ASP	ASP	ALA	ALA	ILE	LEU	LEU	GLY	THR	GLN	GLY	ASP	PHE	ALA	ALA	ARG	GLY	ARG	SER	LYS	ILE	ARG	ASN	THR	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



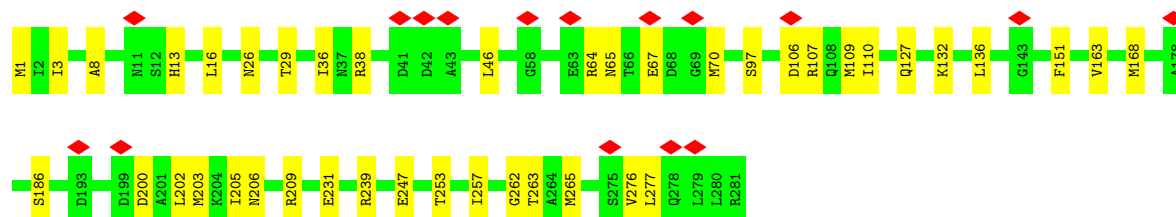
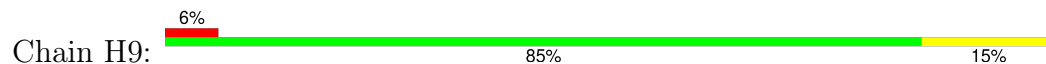
• Molecule 1: Flagellin



• Molecule 1: Flagellin

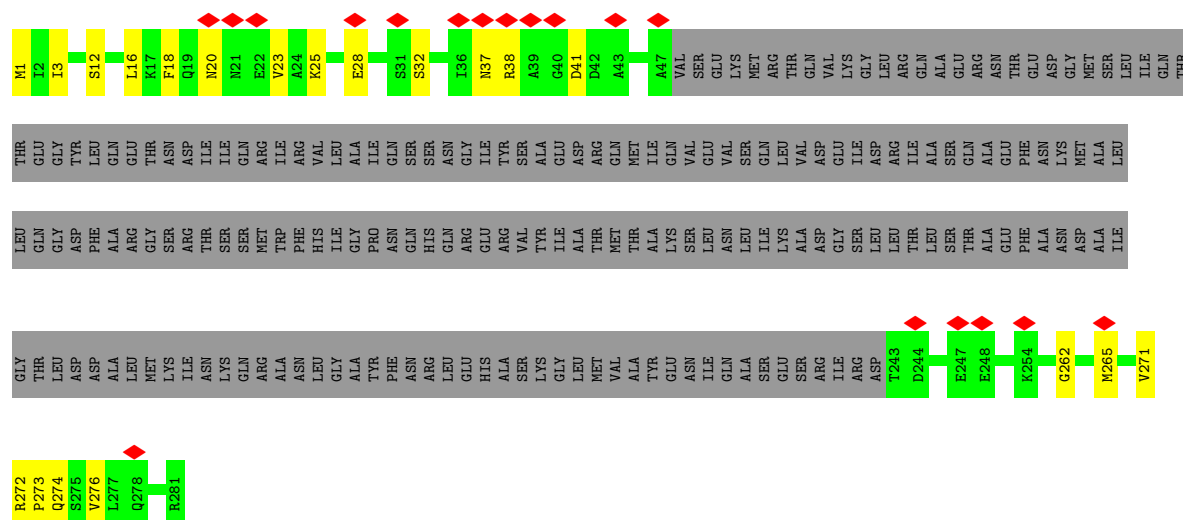


• Molecule 1: Flagellin

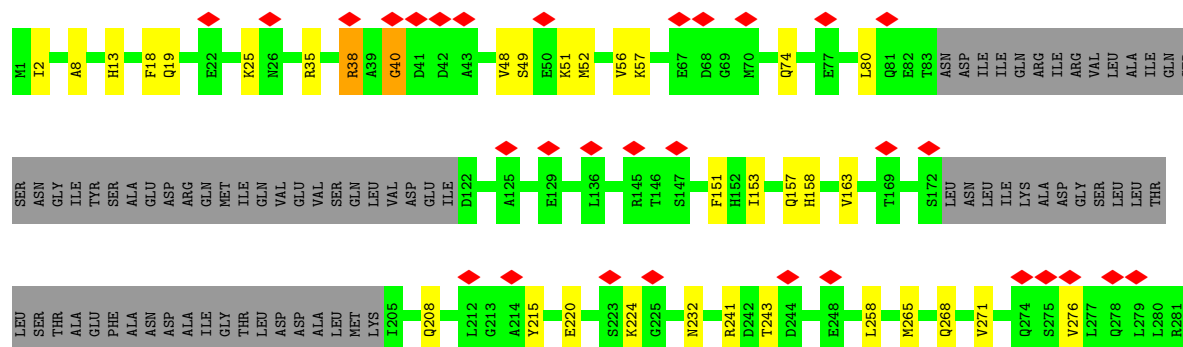


• Molecule 1: Flagellin

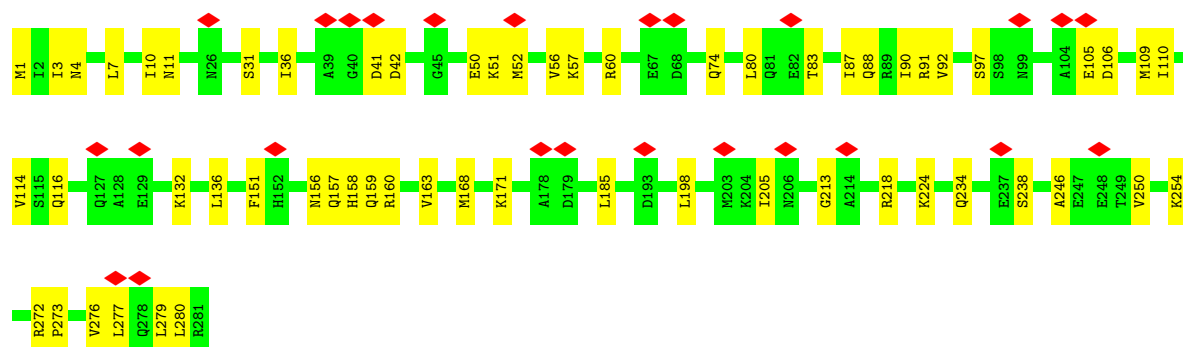
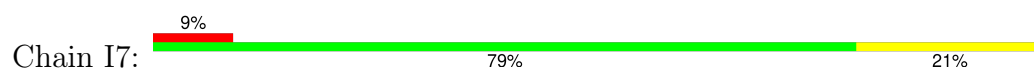




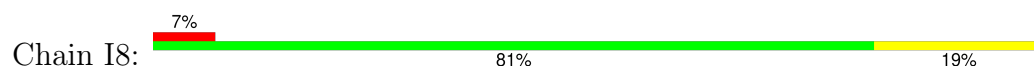
• Molecule 1: Flagellin



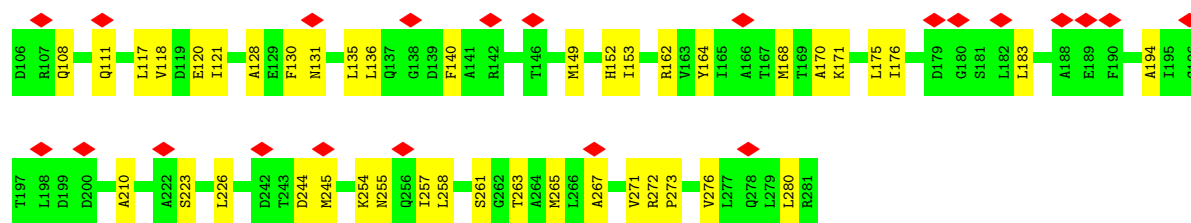
• Molecule 1: Flagellin



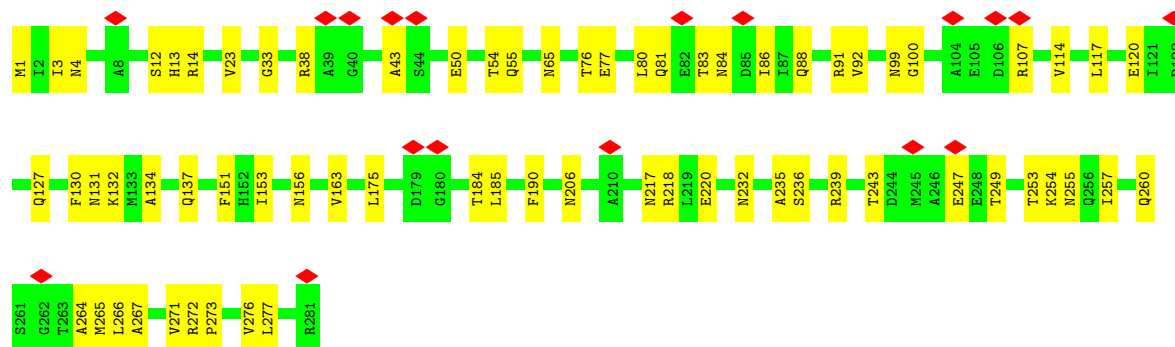
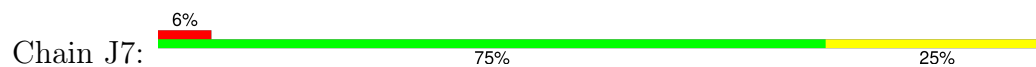
• Molecule 1: Flagellin



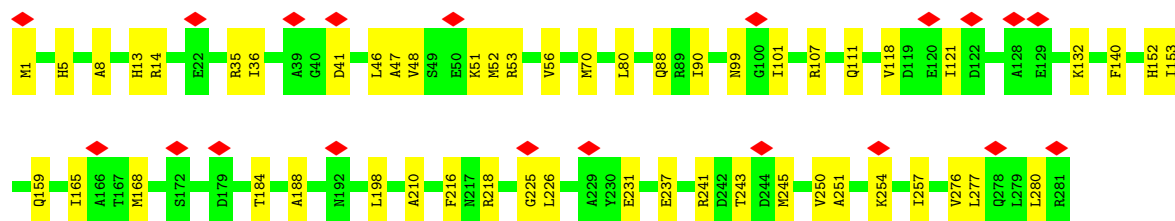
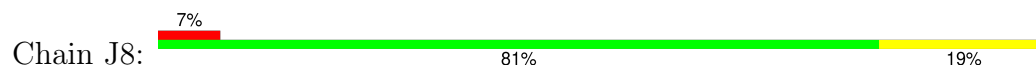




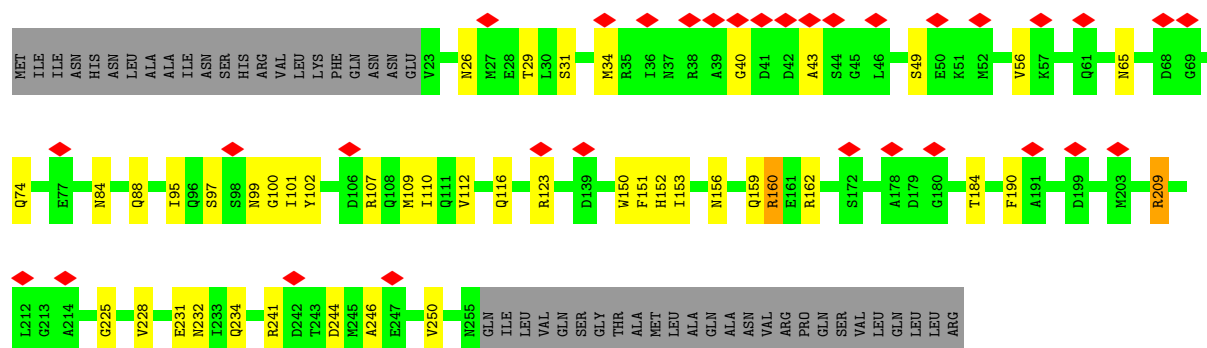
• Molecule 1: Flagellin



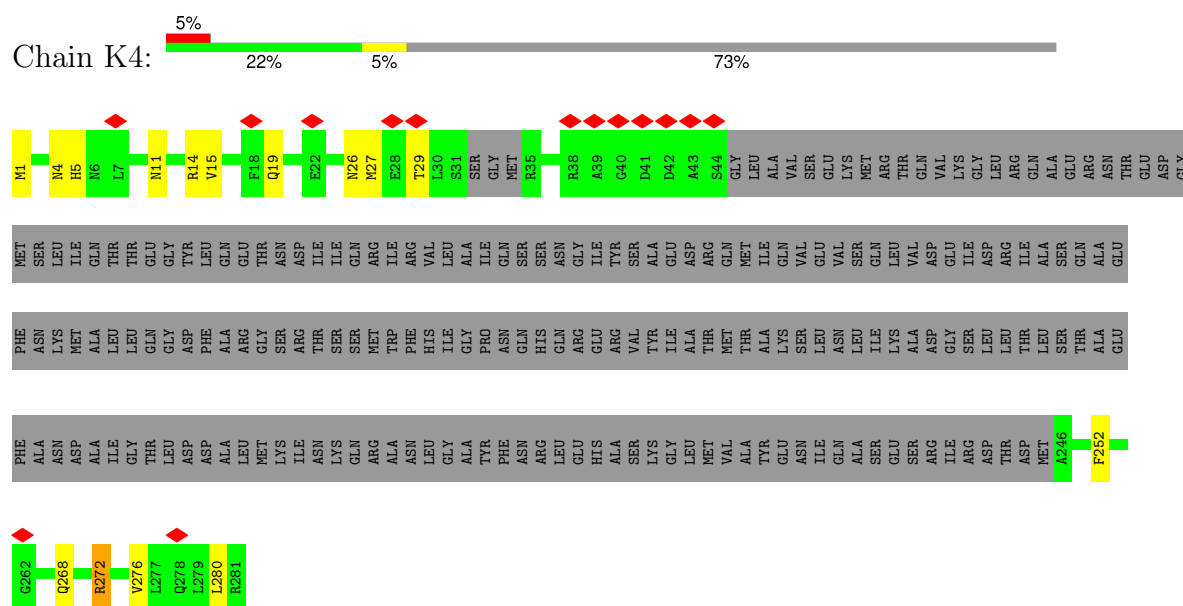
• Molecule 1: Flagellin



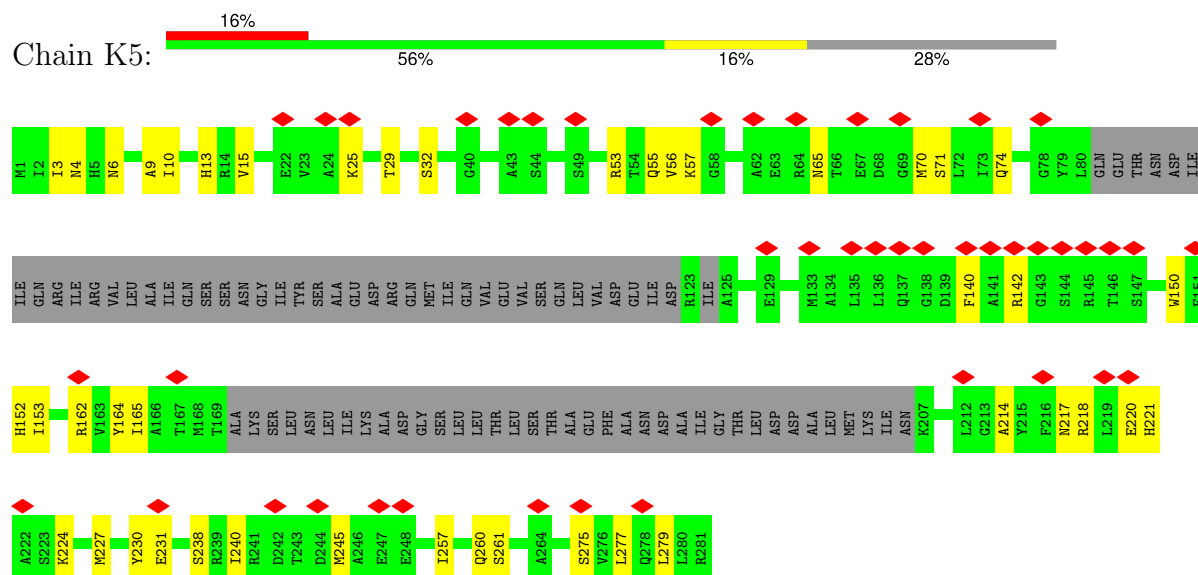
• Molecule 1: Flagellin



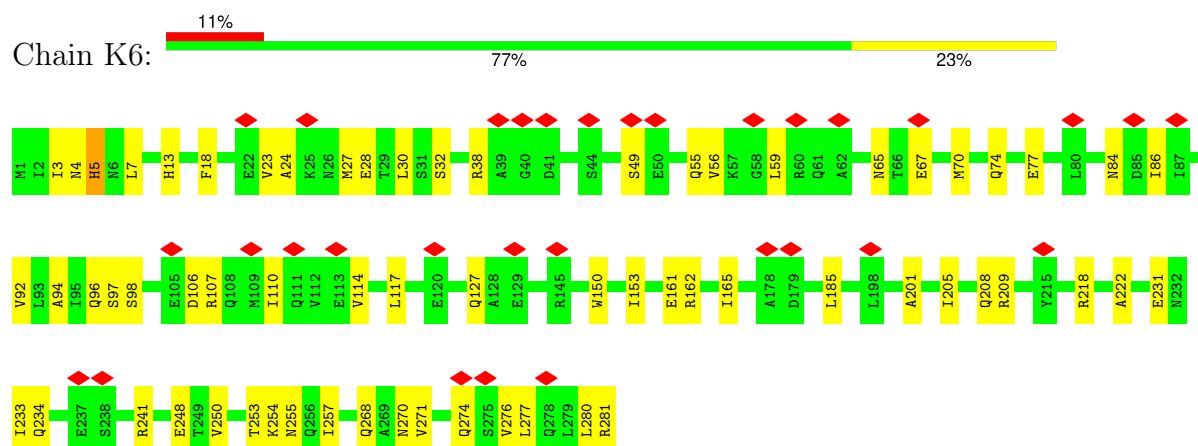
• Molecule 1: Flagellin



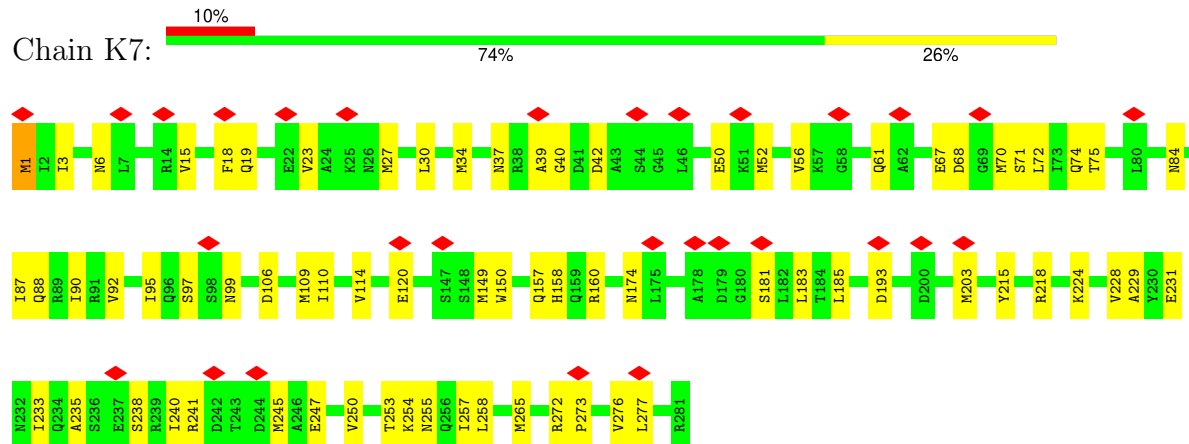
- Molecule 1: Flagellin



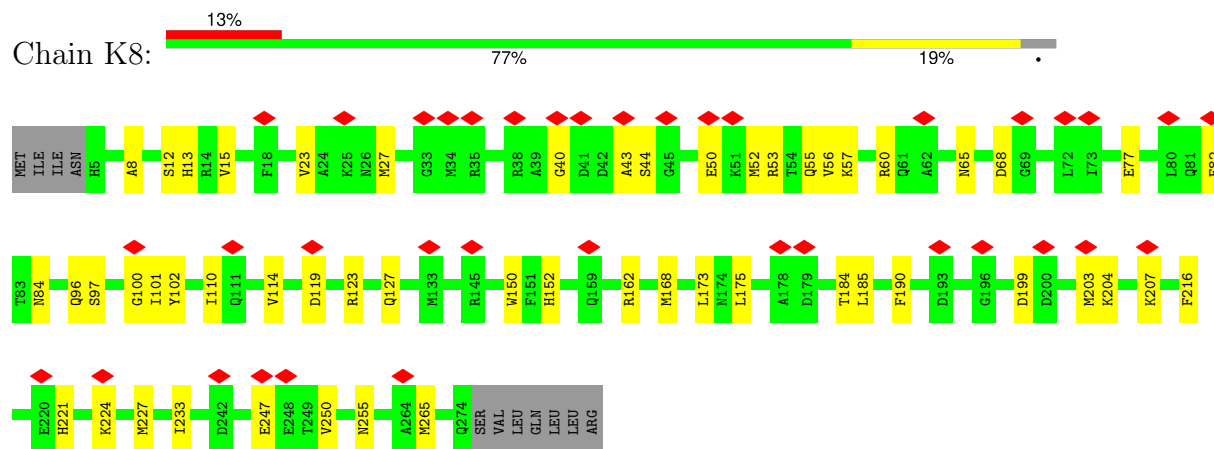
- Molecule 1: Flagellin



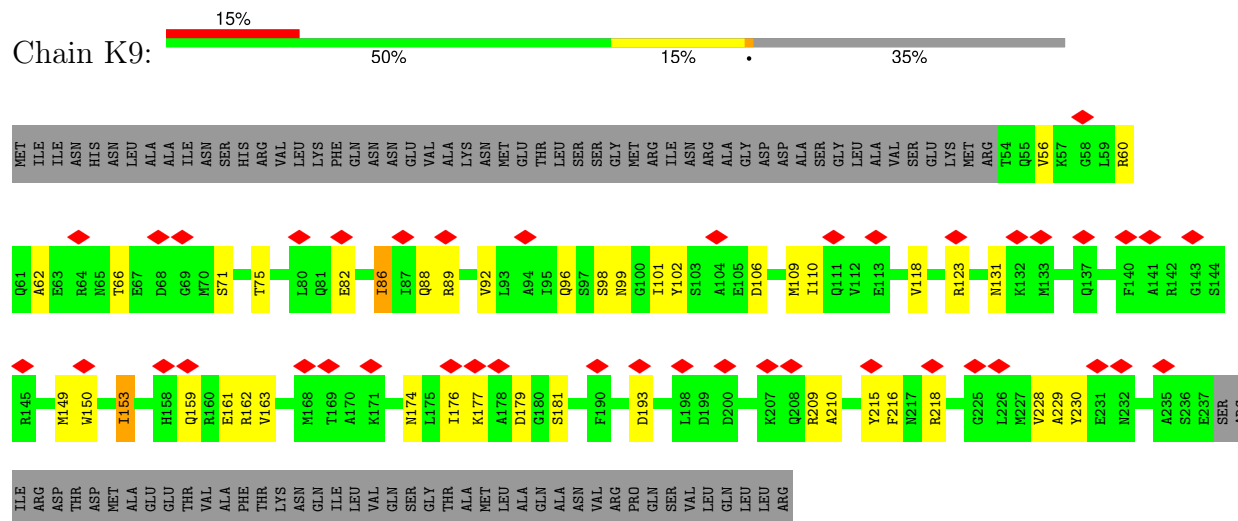
- Molecule 1: Flagellin



- Molecule 1: Flagellin

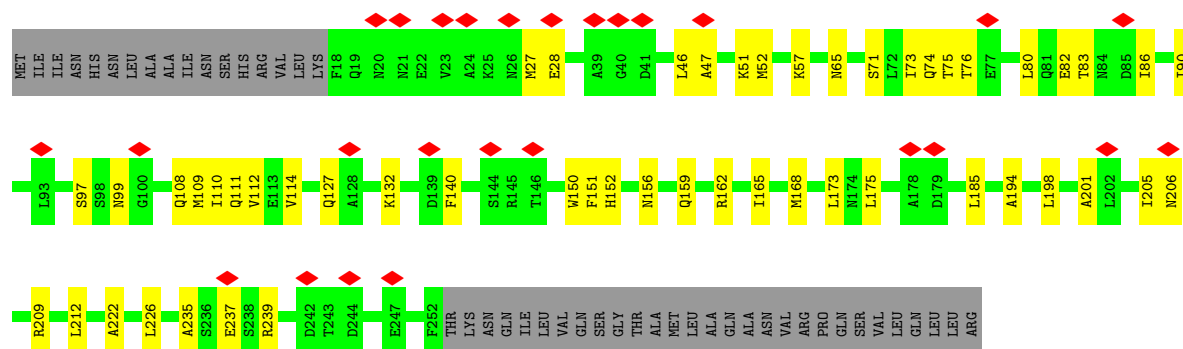


- Molecule 1: Flagellin



- Molecule 1: Flagellin



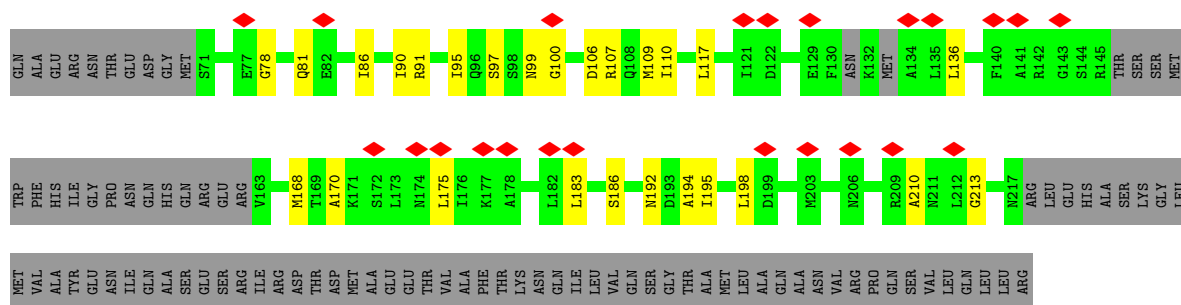


• Molecule 1: Flagellin

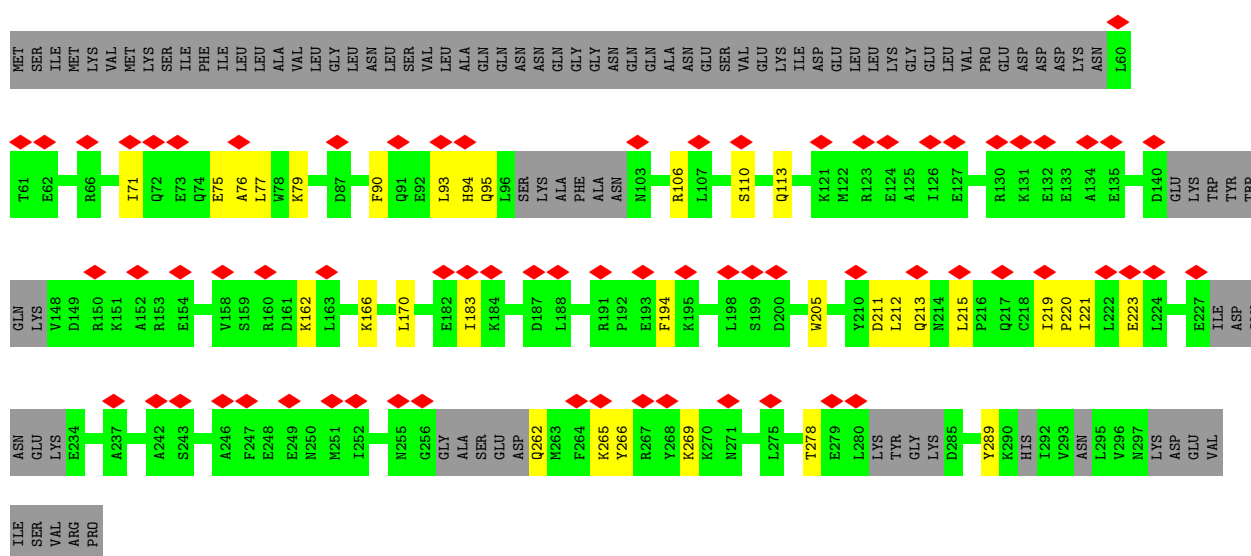


• Molecule 1: Flagellin

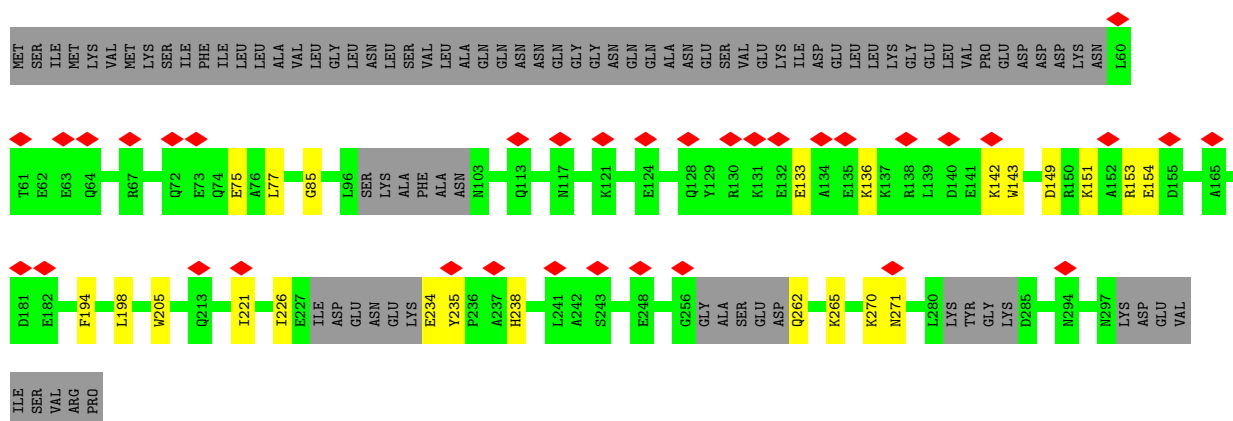




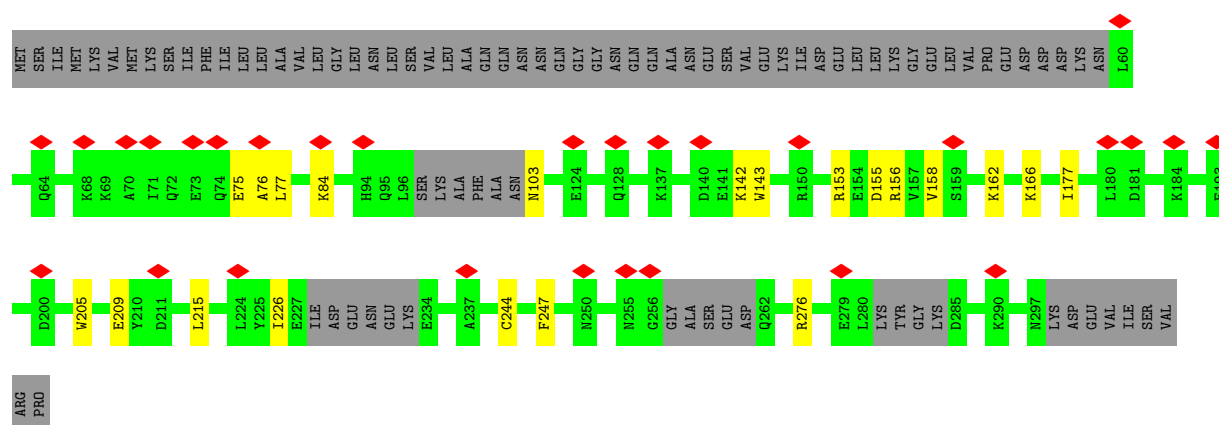
• Molecule 2: Flagellar Coiling Protein A (FcpA)



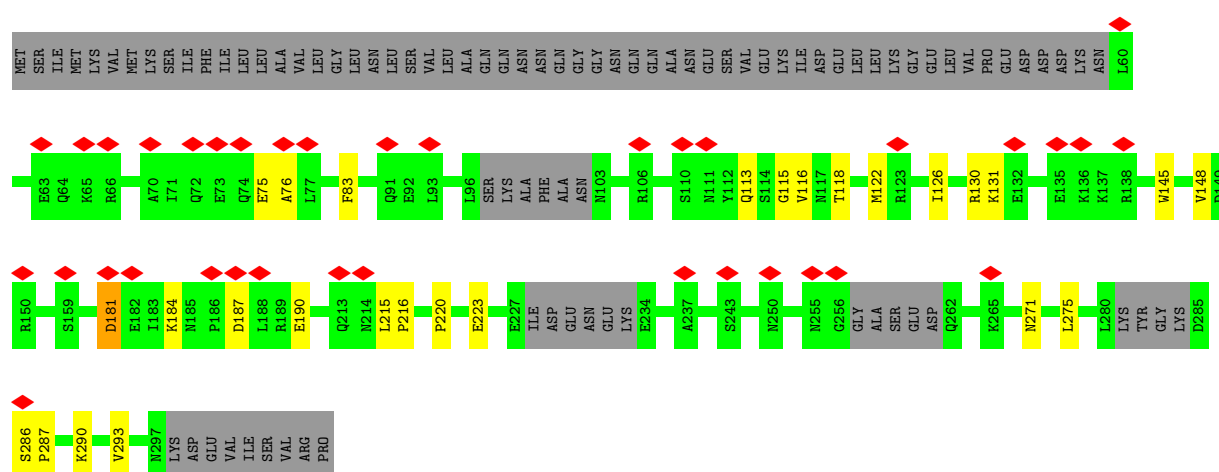
• Molecule 2: Flagellar Coiling Protein A (FcpA)



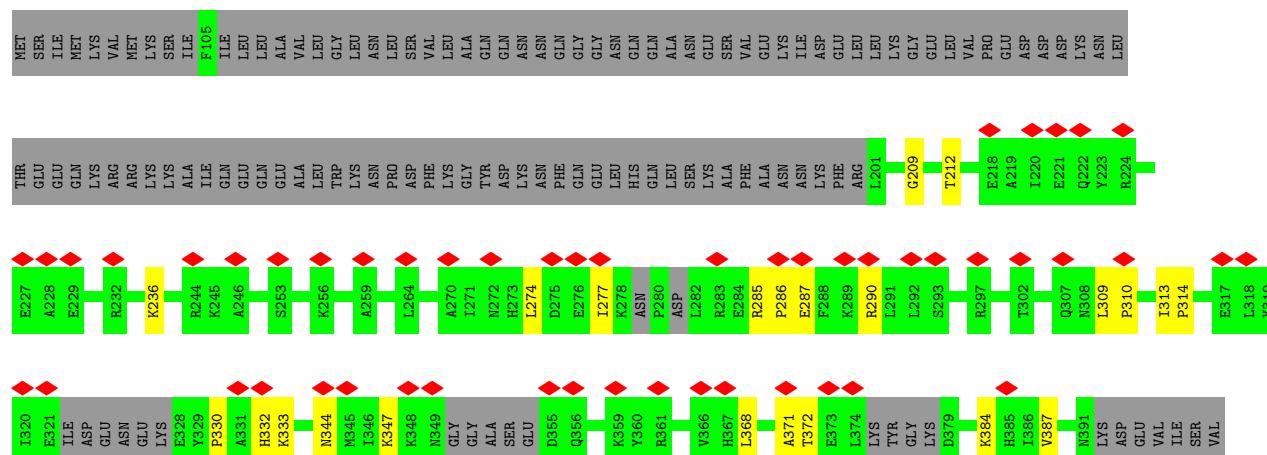
• Molecule 2: Flagellar Coiling Protein A (FcpA)

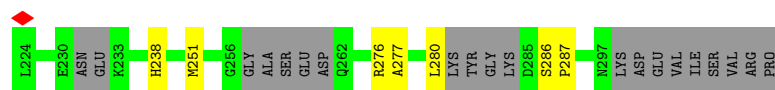


• Molecule 2: Flagellar Coiling Protein A (FcpA)

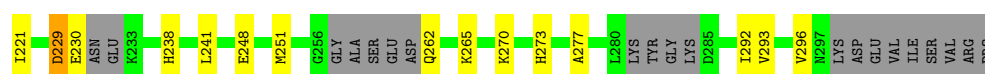
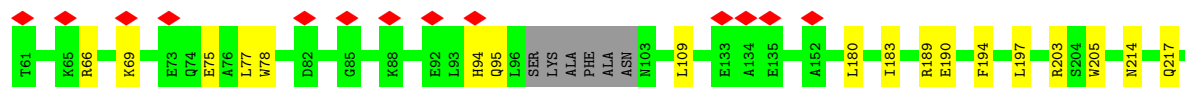
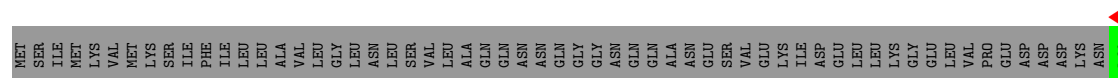


• Molecule 2: Flagellar Coiling Protein A (FcpA)

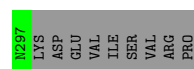
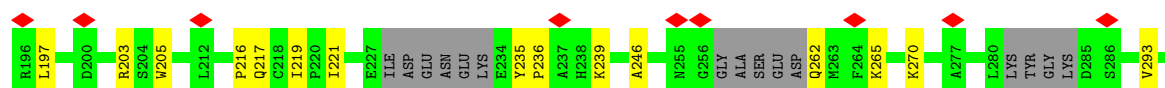
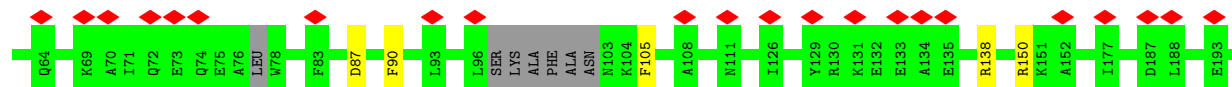




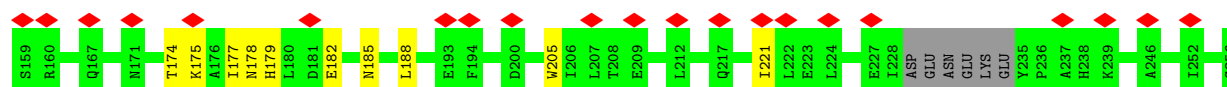
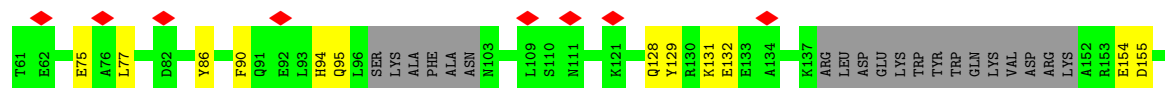
• Molecule 2: Flagellar Coiling Protein A (FcpA)



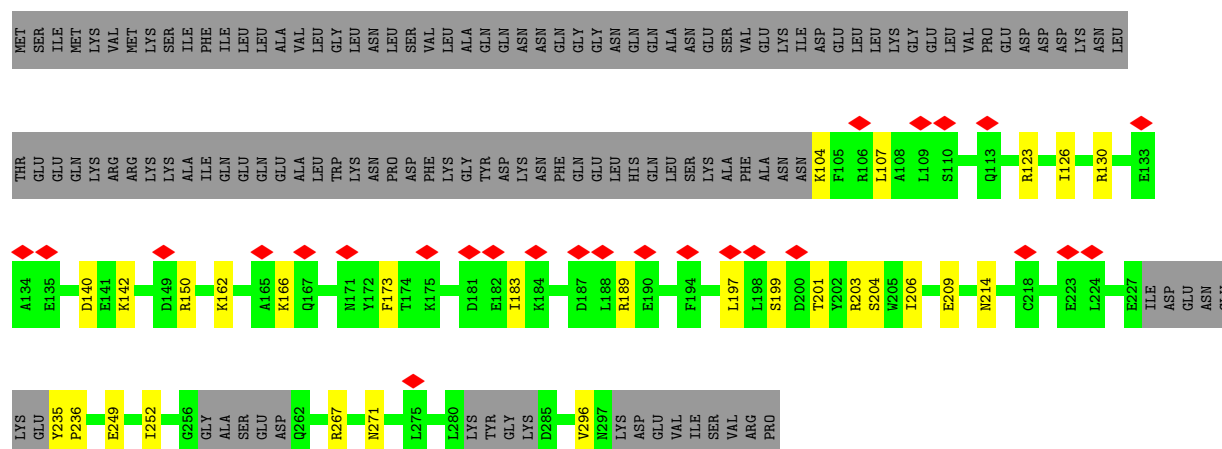
• Molecule 2: Flagellar Coiling Protein A (FcpA)



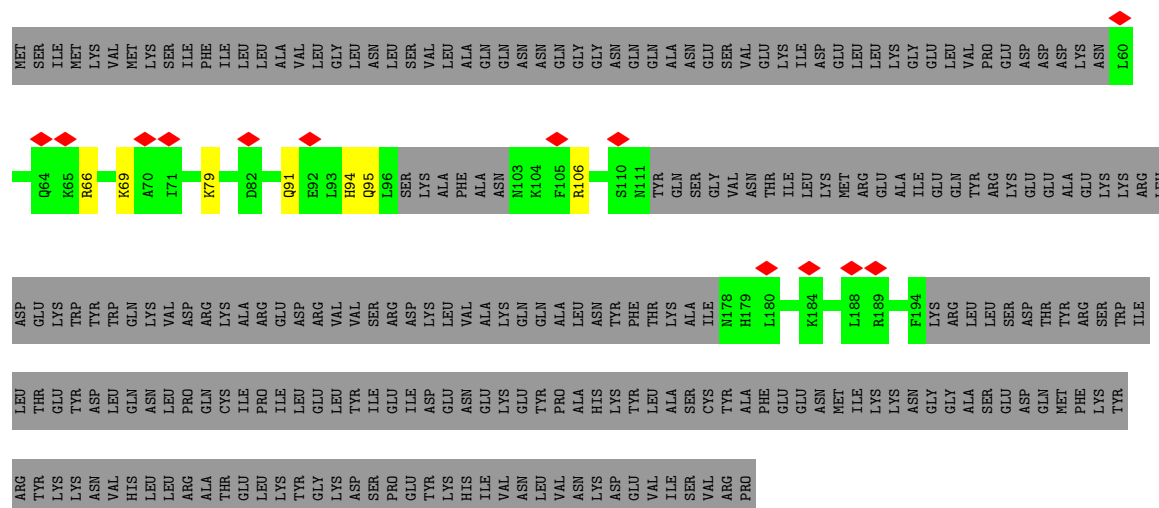
• Molecule 2: Flagellar Coiling Protein A (FcpA)



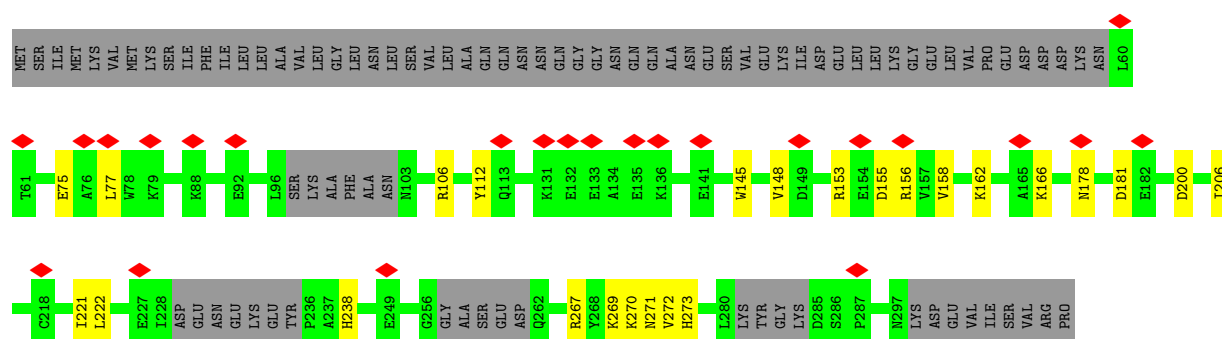




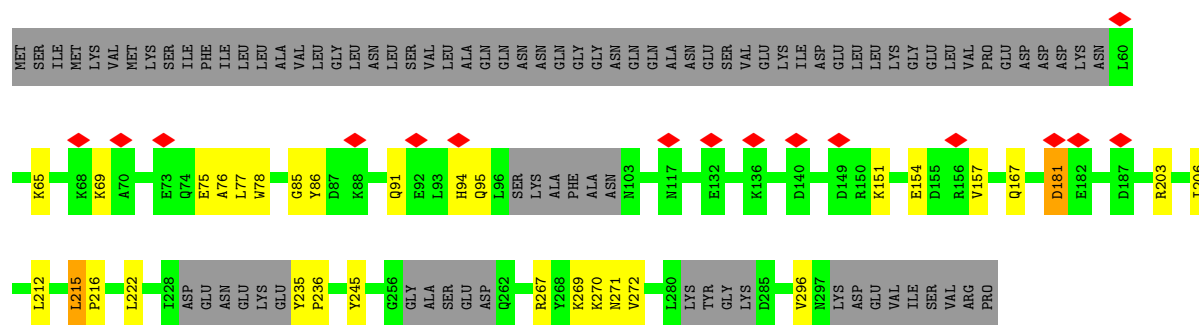
• Molecule 2: Flagellar Coiling Protein A (FcpA)



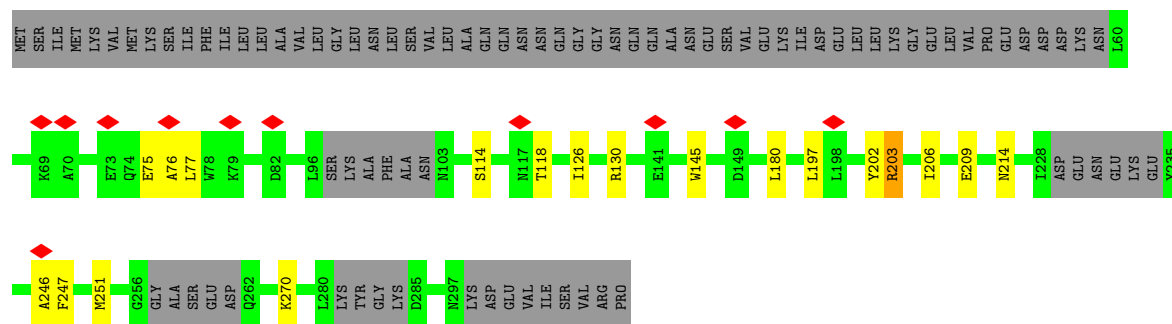
• Molecule 2: Flagellar Coiling Protein A (FcpA)



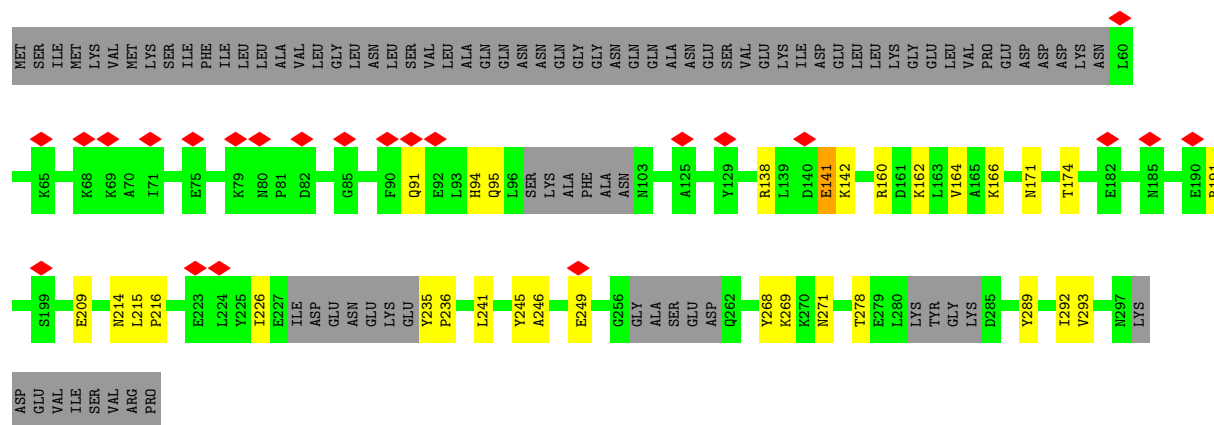
• Molecule 2: Flagellar Coiling Protein A (FcpA)



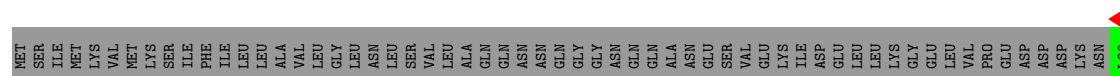
• Molecule 2: Flagellar Coiling Protein A (FcpA)

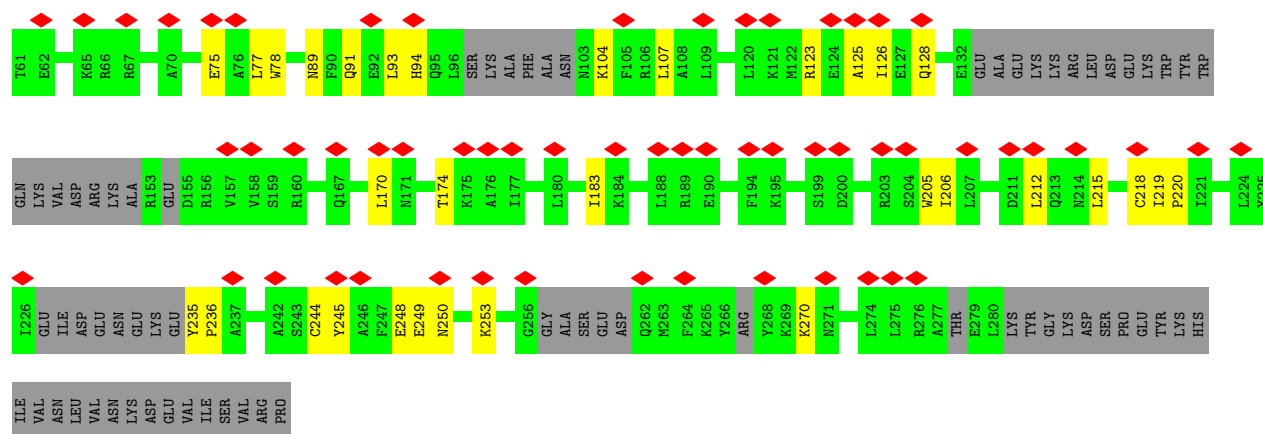


• Molecule 2: Flagellar Coiling Protein A (FcpA)

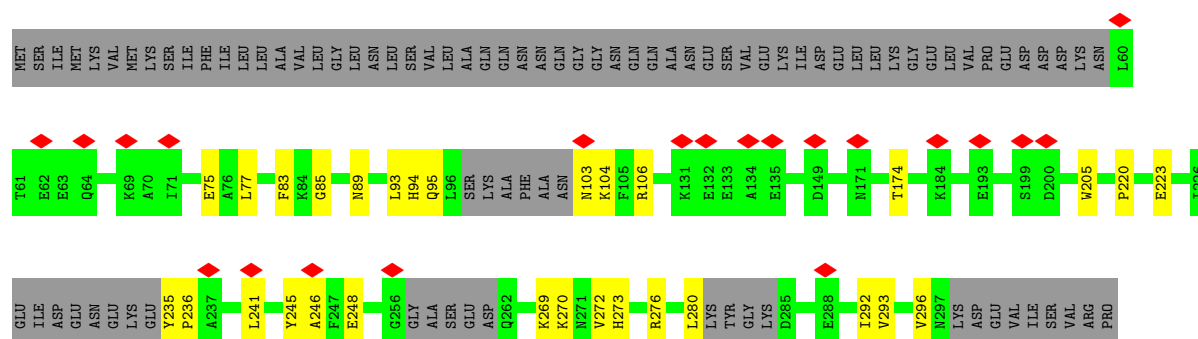


• Molecule 2: Flagellar Coiling Protein A (FcpA)

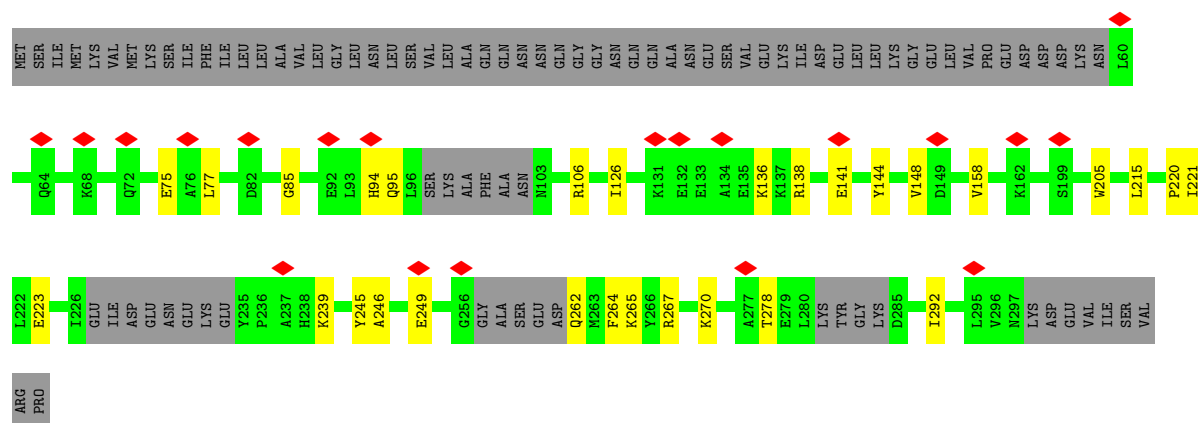




• Molecule 2: Flagellar Coiling Protein A (FcpA)

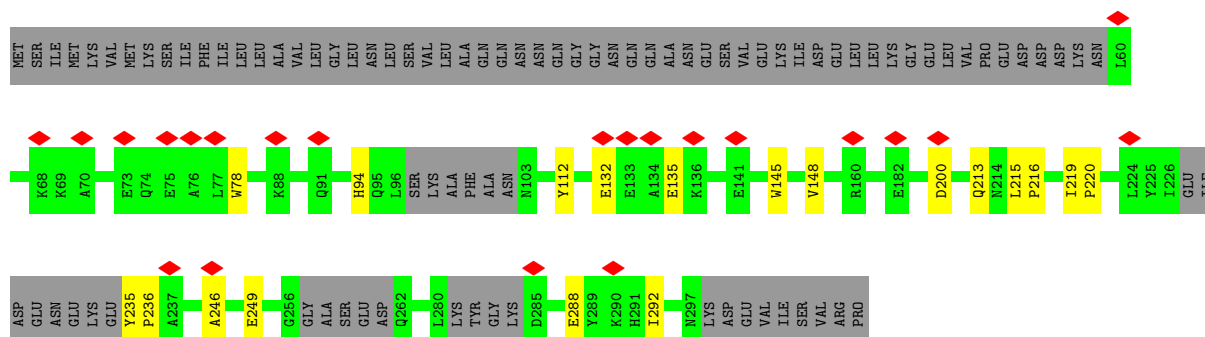


• Molecule 2: Flagellar Coiling Protein A (FcpA)

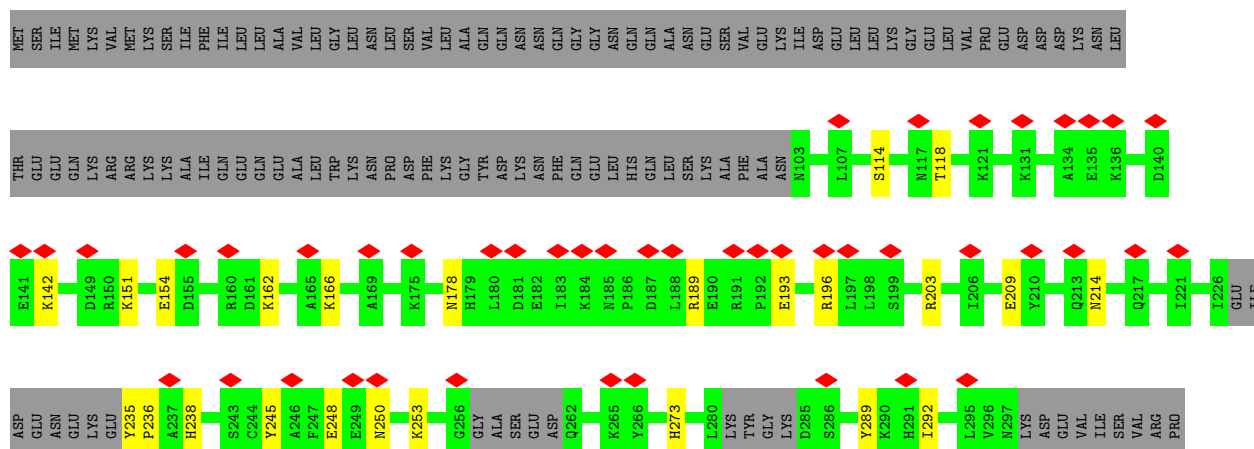


• Molecule 2: Flagellar Coiling Protein A (FcpA)

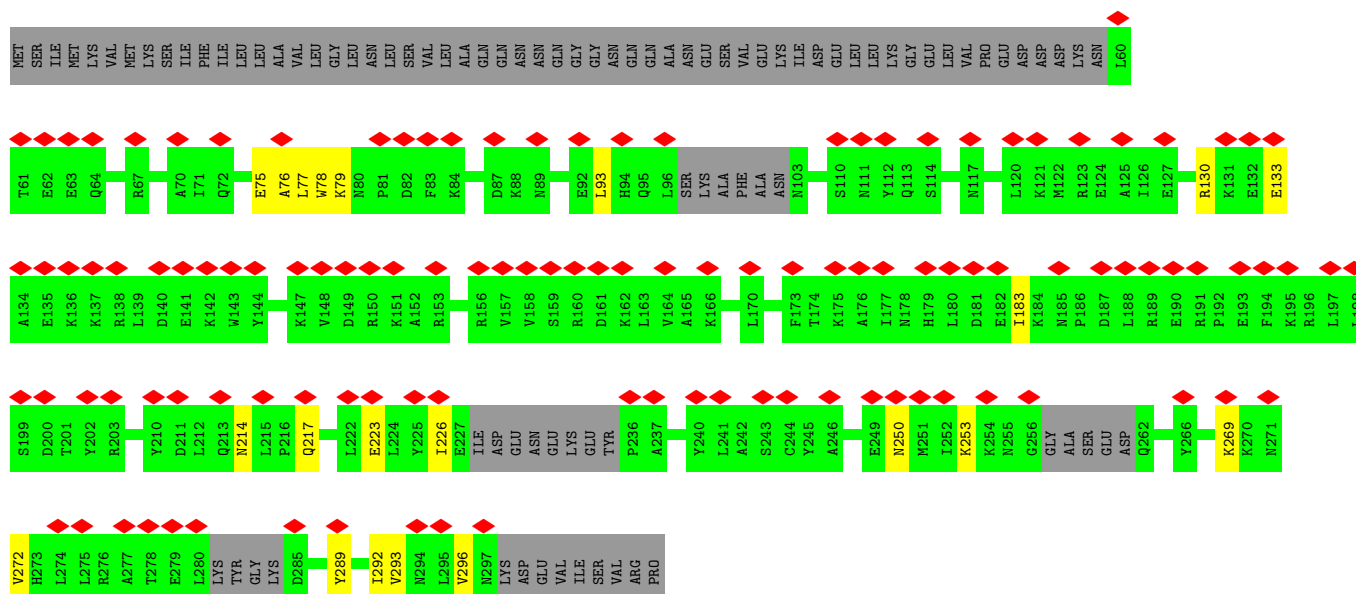
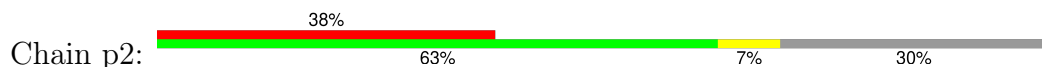




• Molecule 2: Flagellar Coiling Protein A (FcpA)

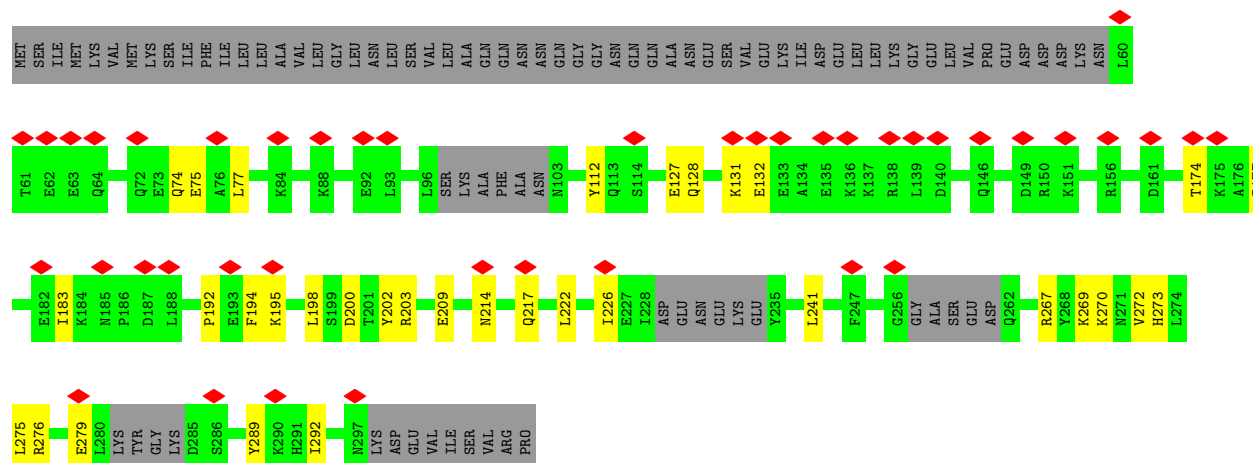


• Molecule 2: Flagellar Coiling Protein A (FcpA)



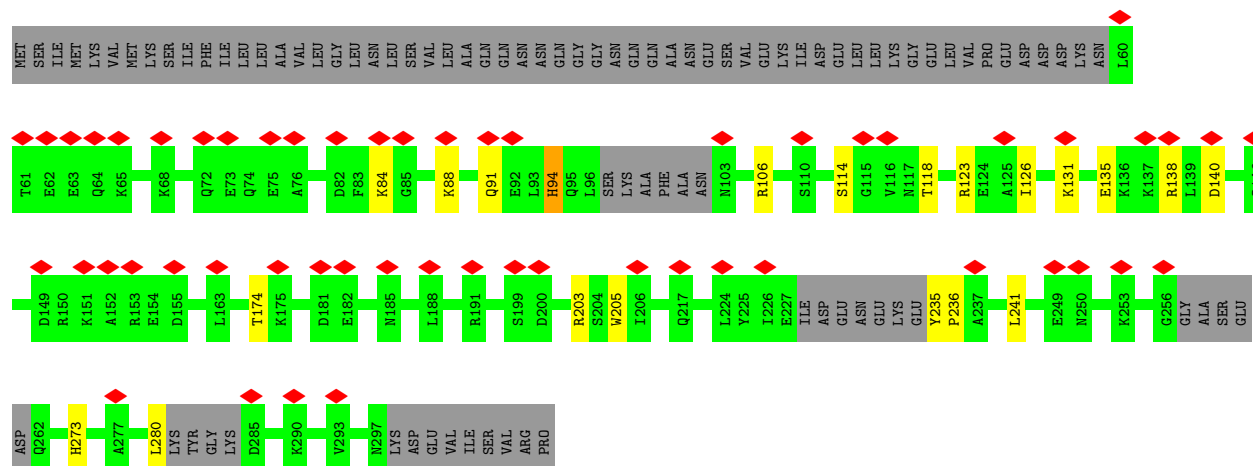
- Molecule 2: Flagellar Coiling Protein A (FcpA)

Chain p3: 



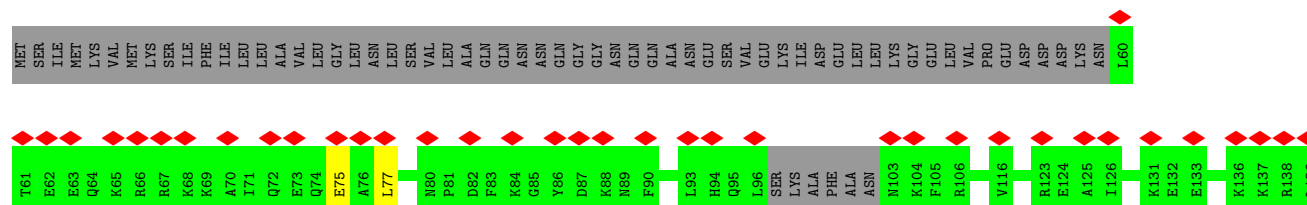
- Molecule 2: Flagellar Coiling Protein A (FcpA)

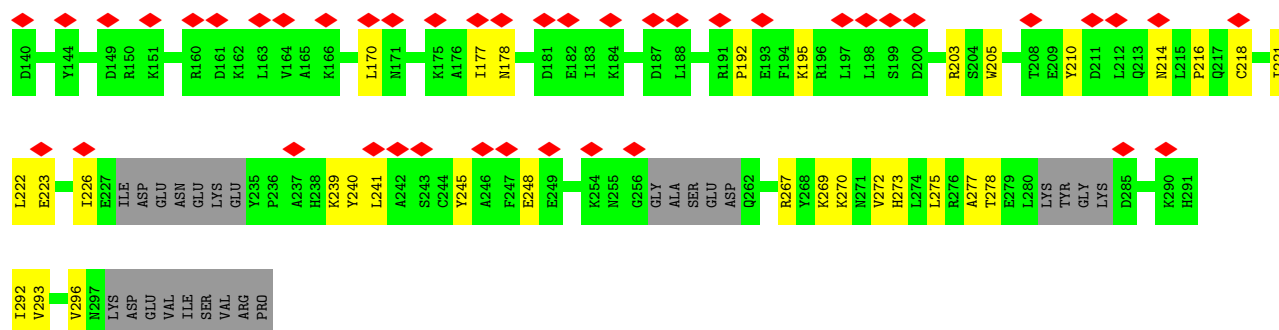
Chain p4: 



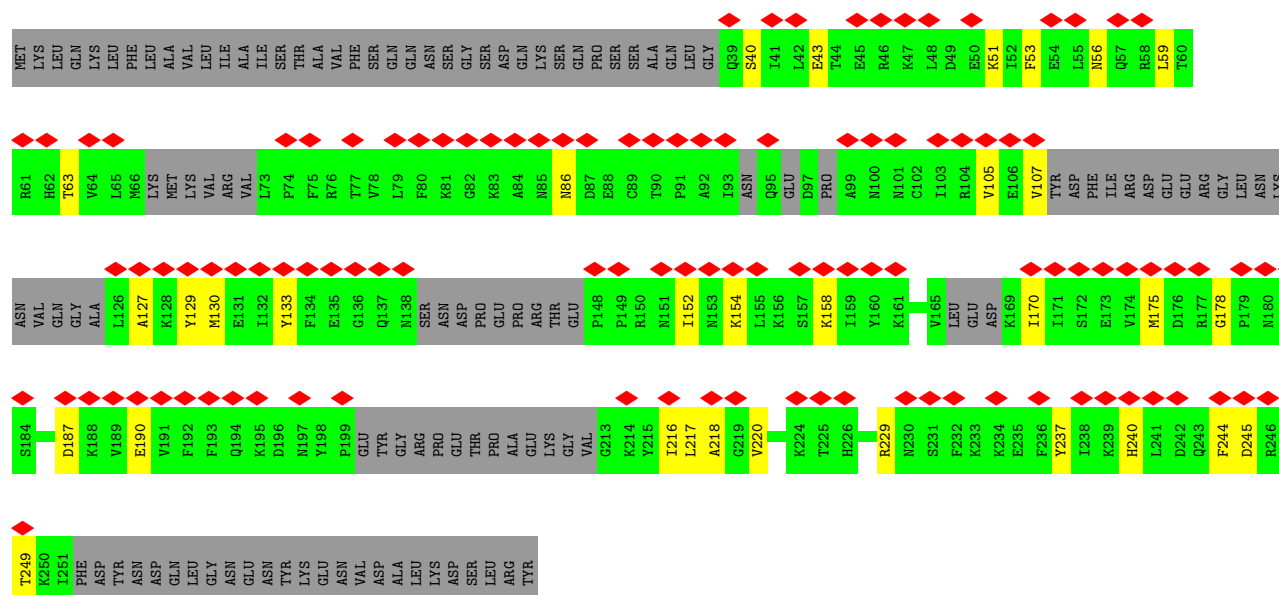
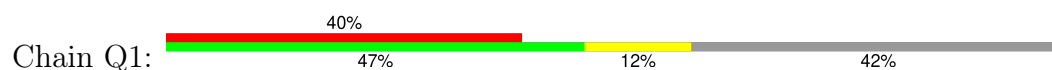
- Molecule 2: Flagellar Coiling Protein A (FcpA)

Chain p5: 

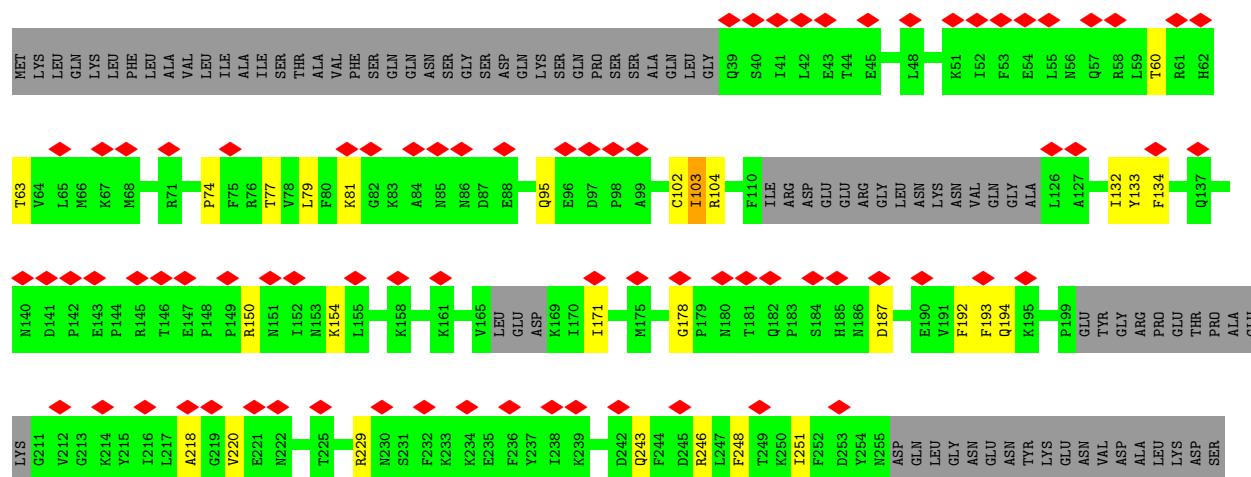




• Molecule 3: Flagellar Coiling Protein B (FcpB)



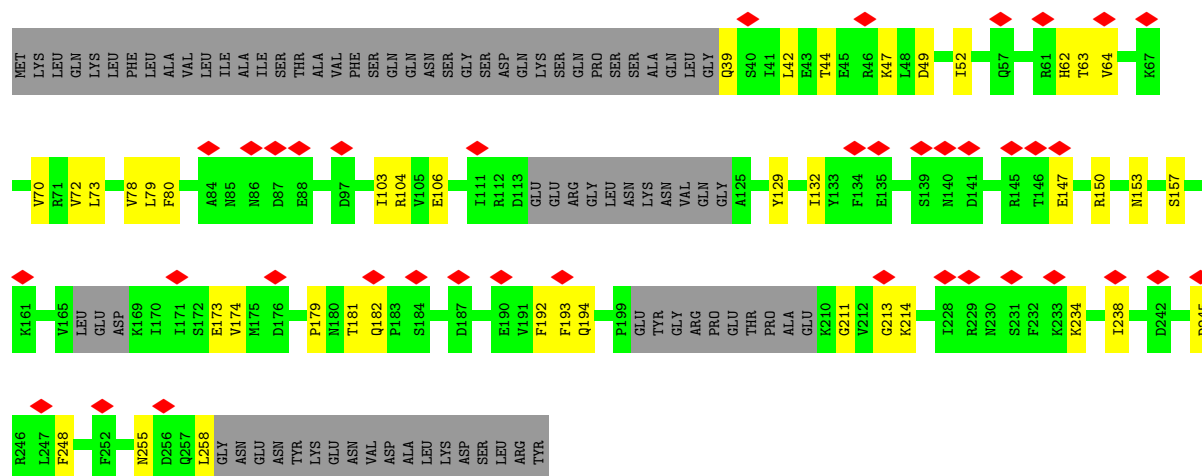
• Molecule 3: Flagellar Coiling Protein B (FcpB)



LEU
ARG
TYR

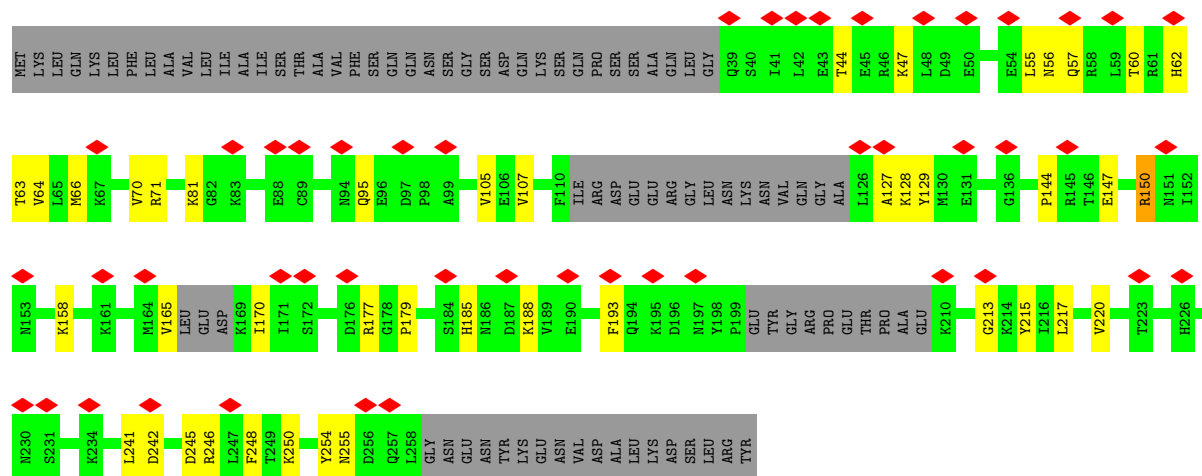
• Molecule 3: Flagellar Coiling Protein B (FcpB)

Chain Q3: 



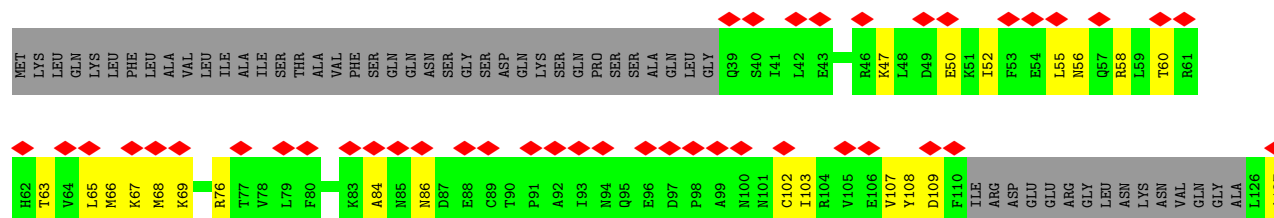
• Molecule 3: Flagellar Coiling Protein B (FcpB)

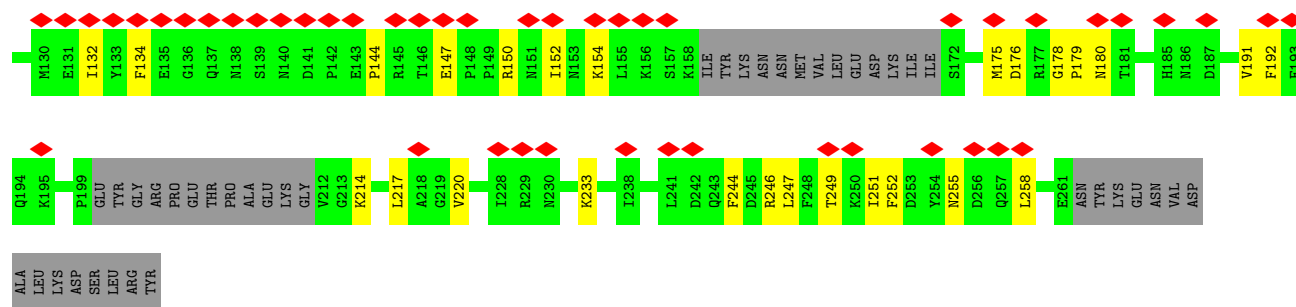
Chain Q4: 



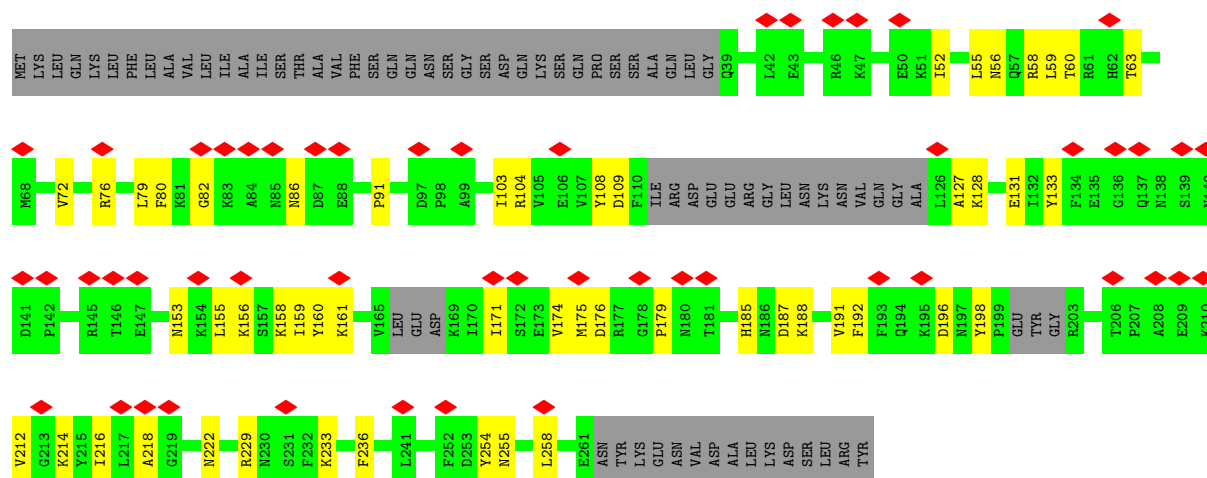
• Molecule 3: Flagellar Coiling Protein B (FcpB)

Chain R2: 

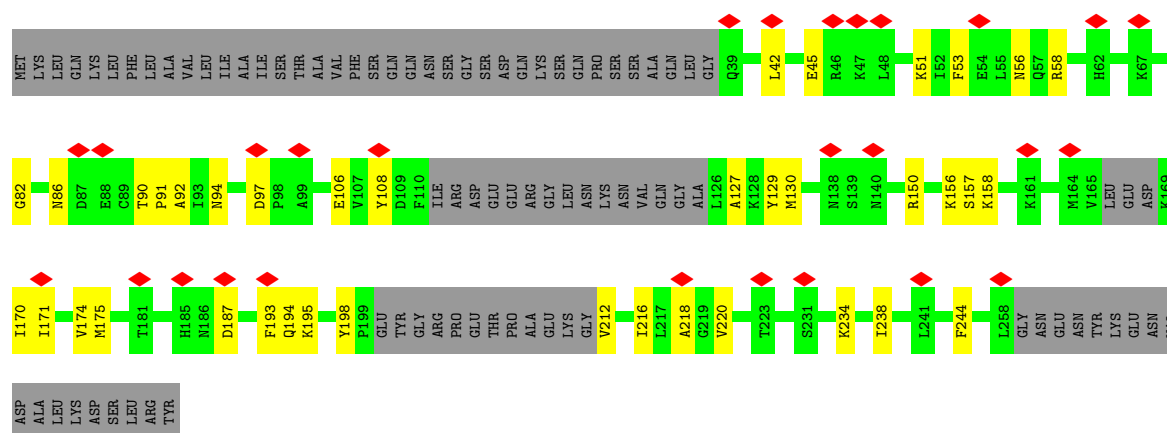




• Molecule 3: Flagellar Coiling Protein B (FcpB)

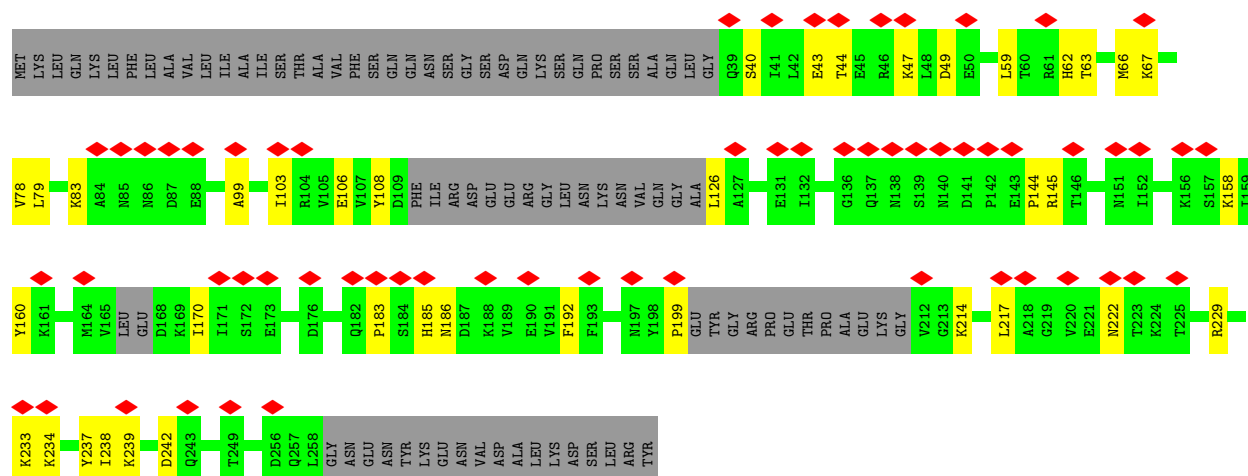


• Molecule 3: Flagellar Coiling Protein B (FcpB)

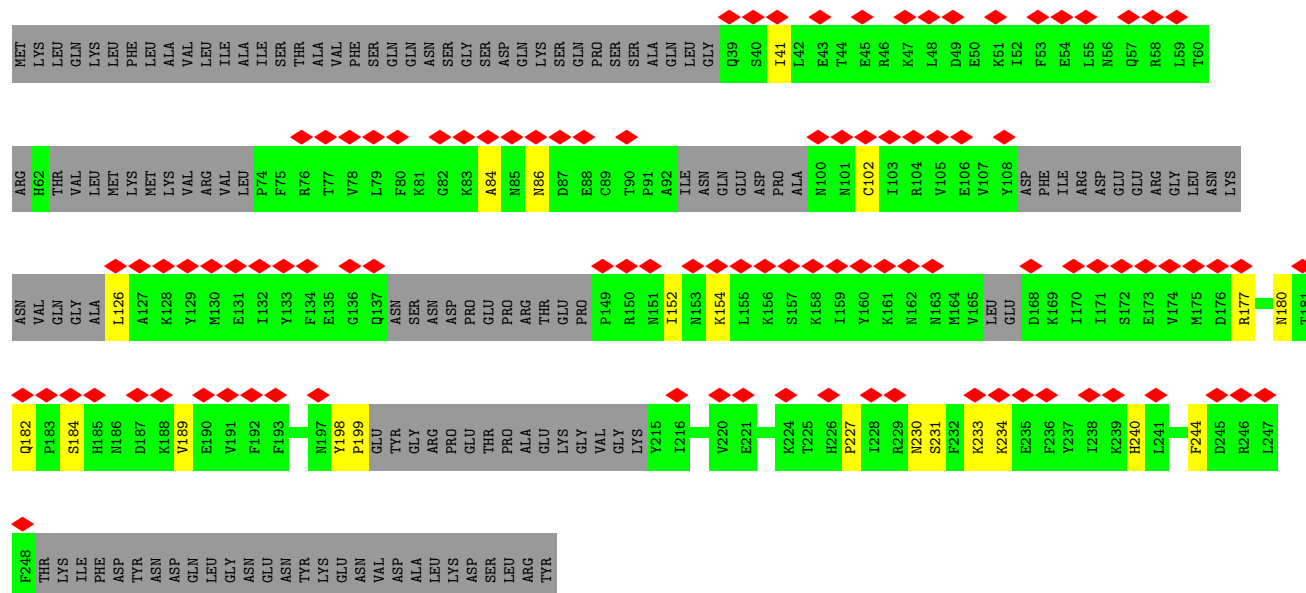


• Molecule 3: Flagellar Coiling Protein B (FcpB)

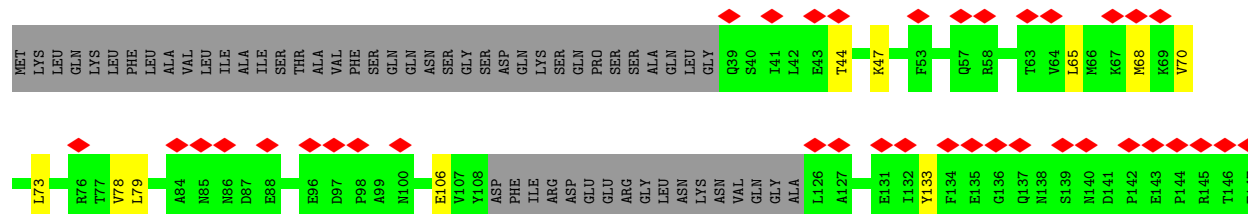


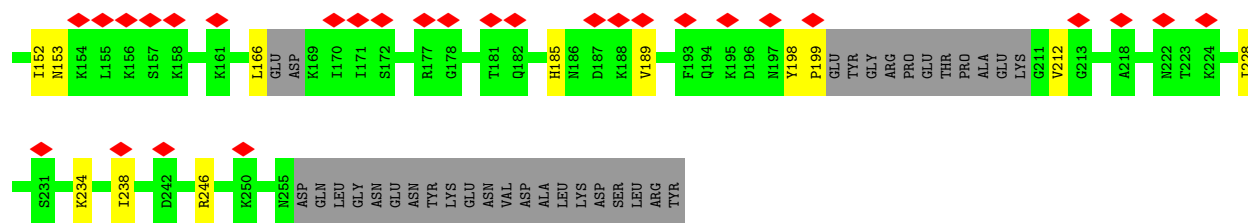


• Molecule 3: Flagellar Coiling Protein B (FcpB)

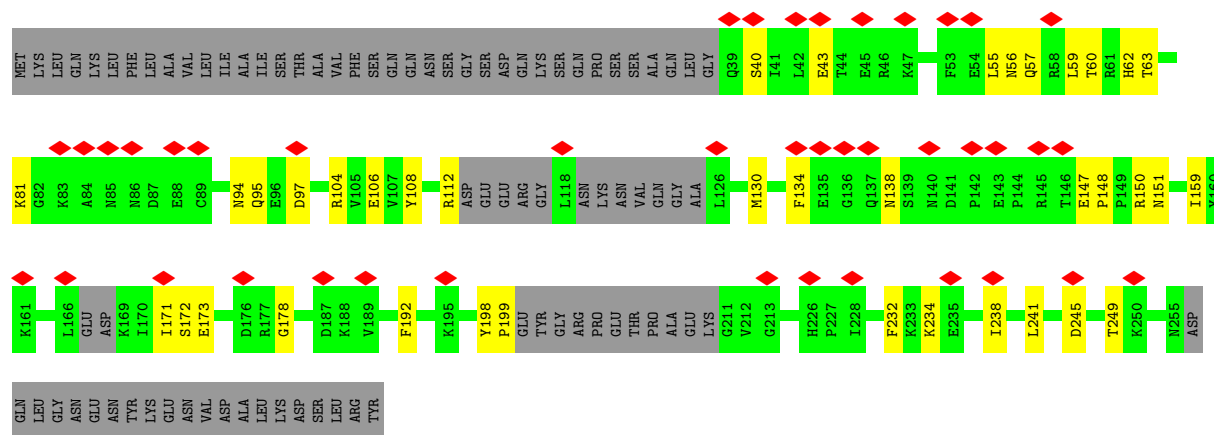


• Molecule 3: Flagellar Coiling Protein B (FcpB)

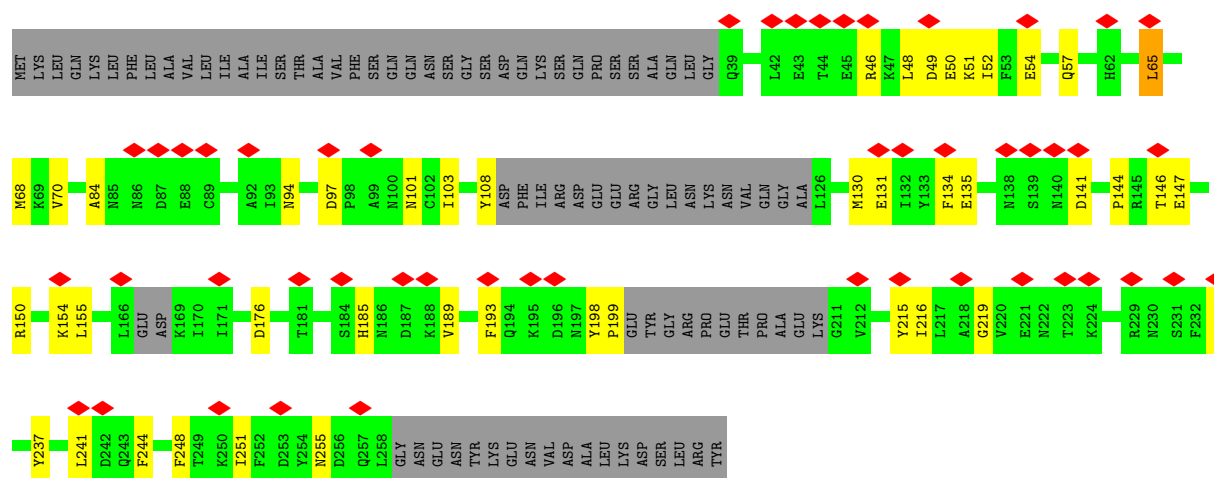




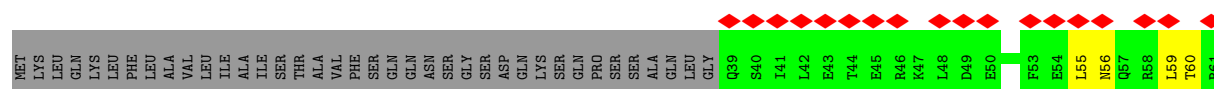
• Molecule 3: Flagellar Coiling Protein B (FcpB)

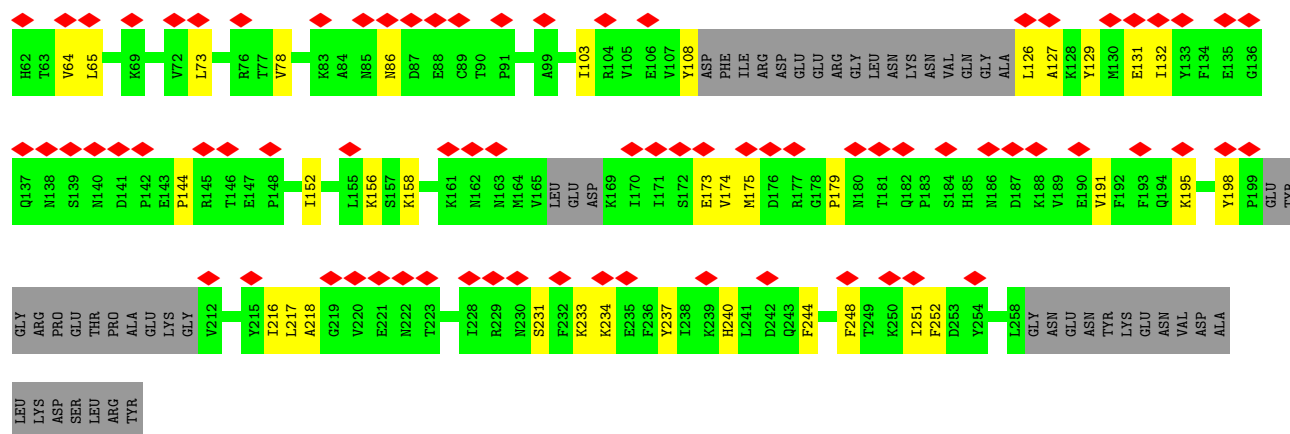


• Molecule 3: Flagellar Coiling Protein B (FcpB)



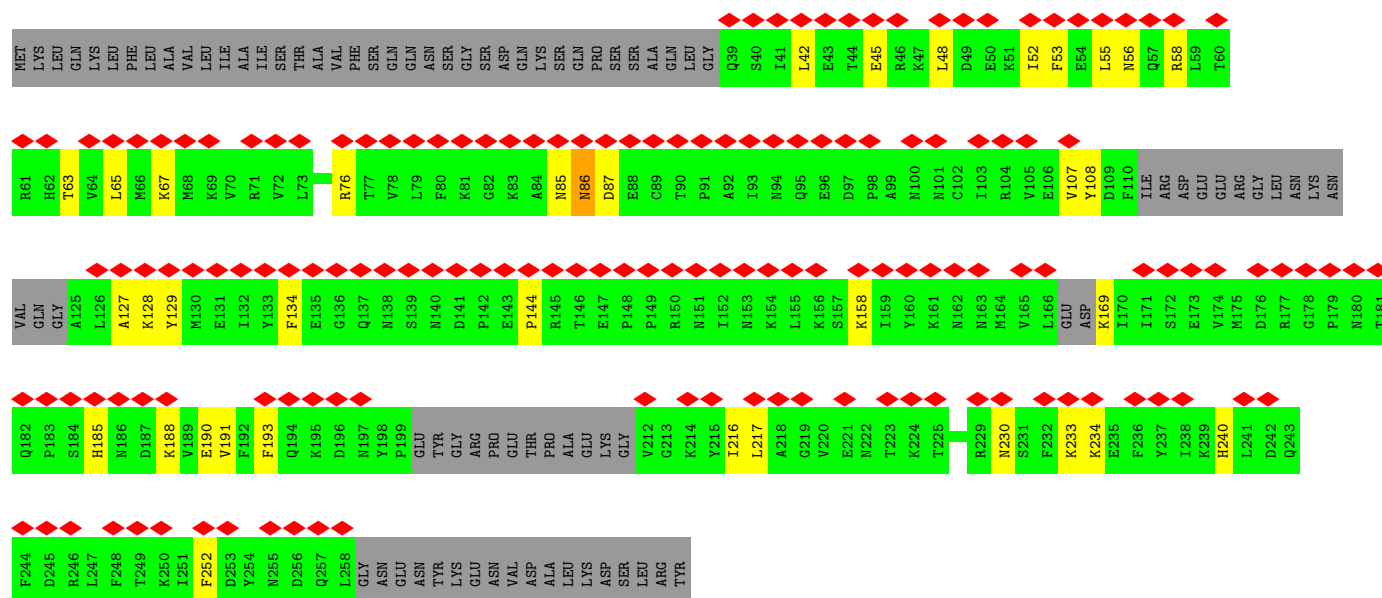
• Molecule 3: Flagellar Coiling Protein B (FcpB)





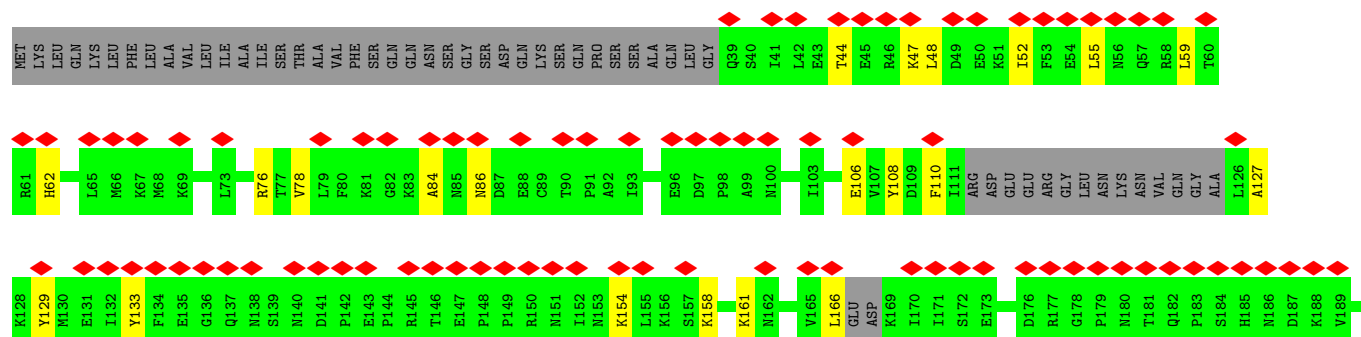
• Molecule 3: Flagellar Coiling Protein B (FcpB)

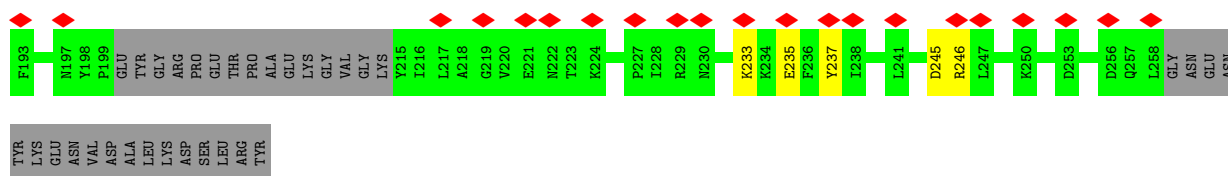
Chain s3:



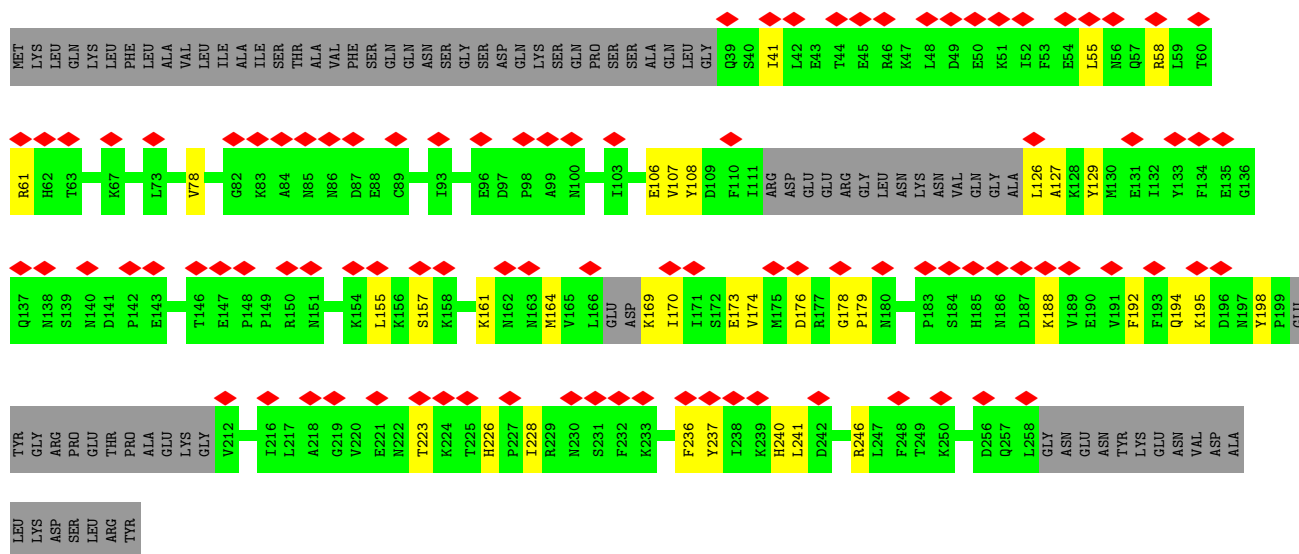
• Molecule 3: Flagellar Coiling Protein B (FcpB)

Chain s4:

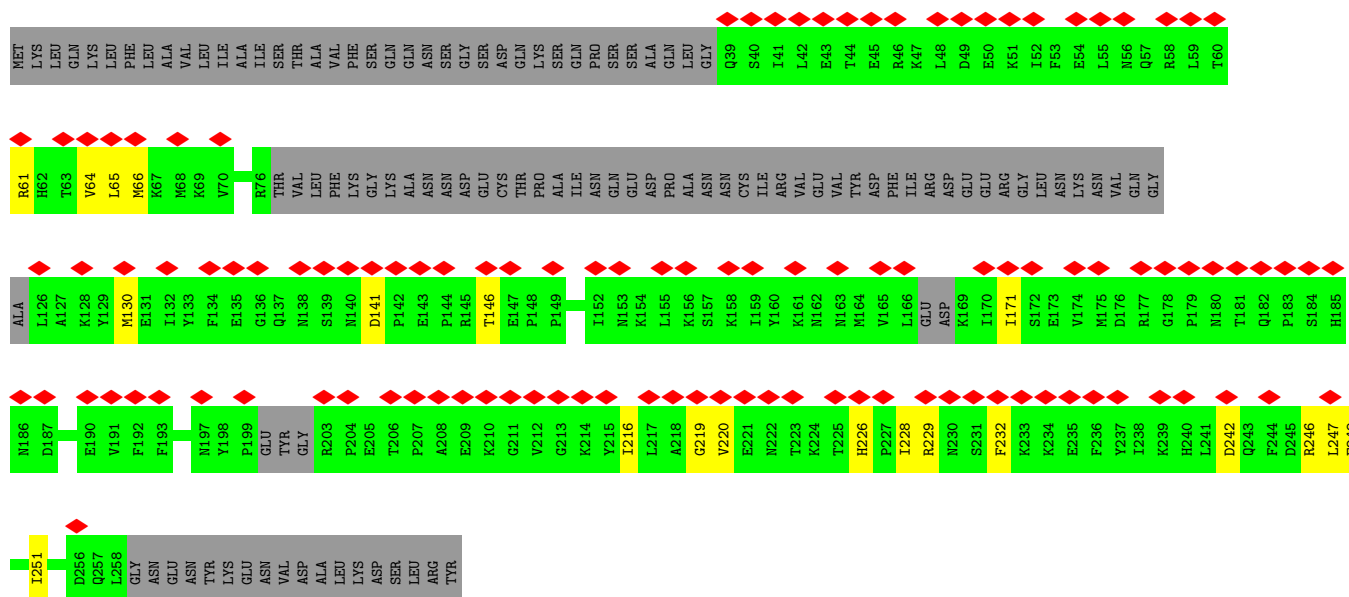
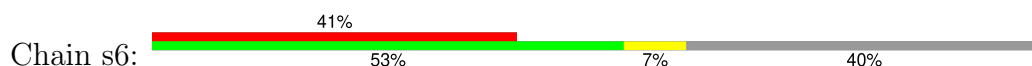




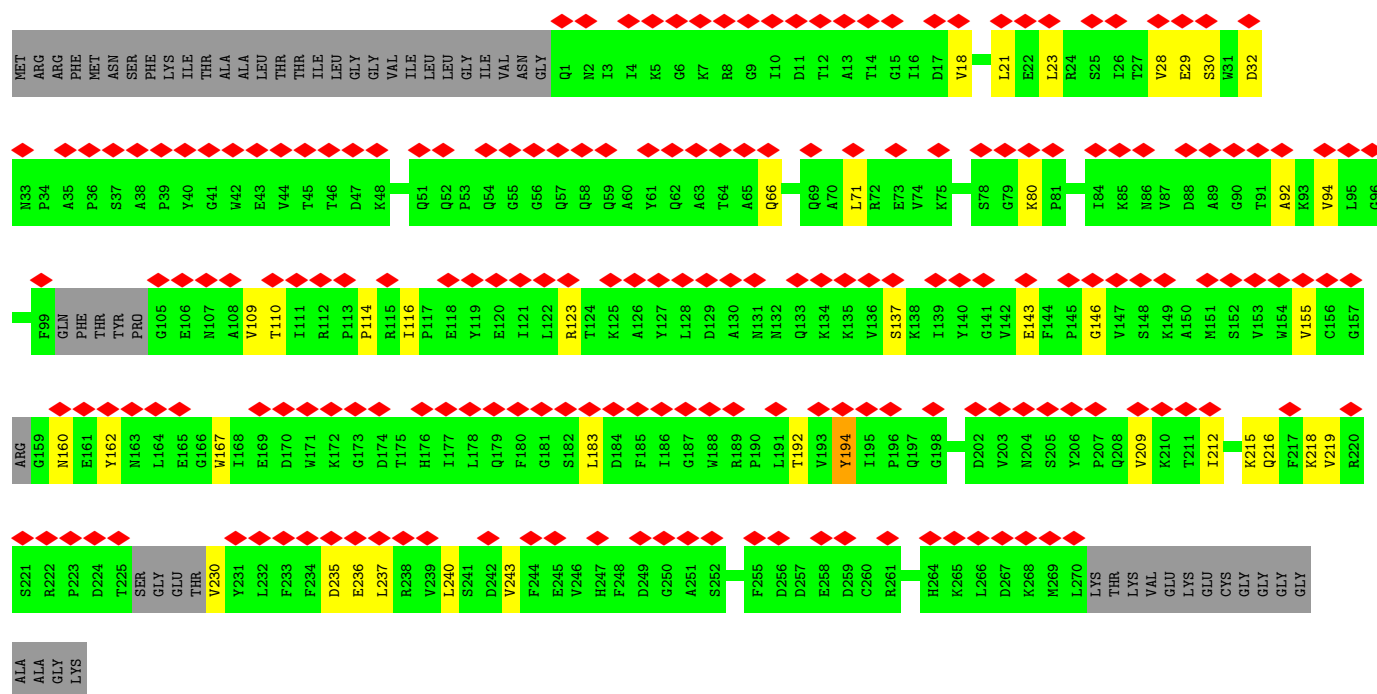
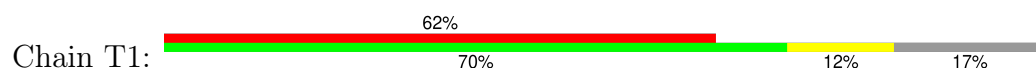
• Molecule 3: Flagellar Coiling Protein B (FcpB)



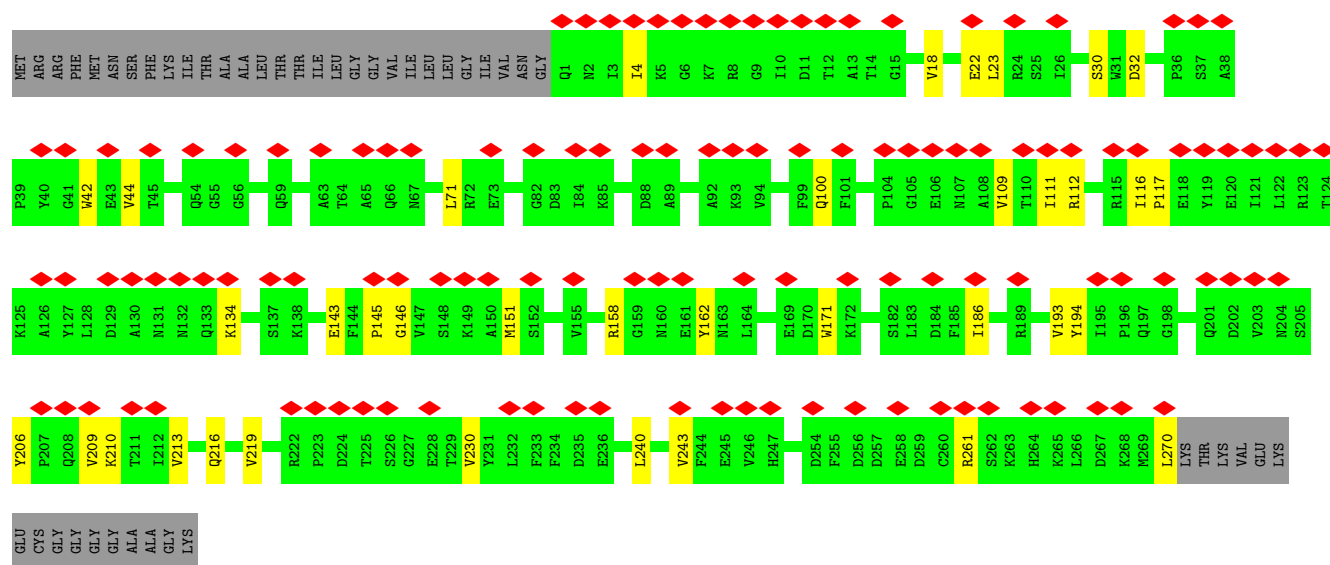
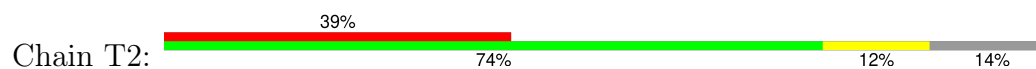
• Molecule 3: Flagellar Coiling Protein B (FcpB)



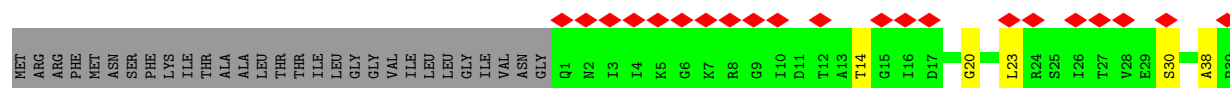
• Molecule 4: Flagellar filament sheath protein

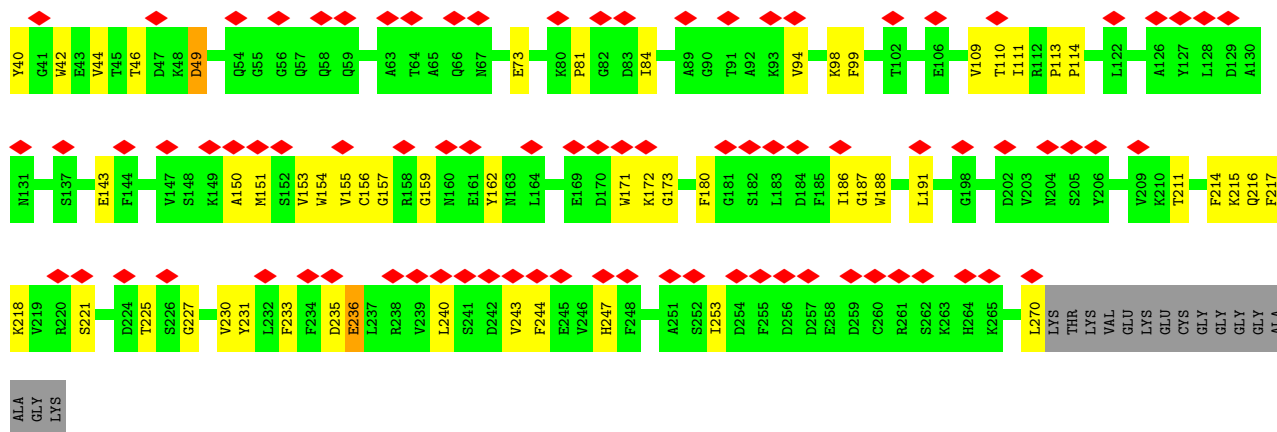


• Molecule 4: Flagellar filament sheath protein

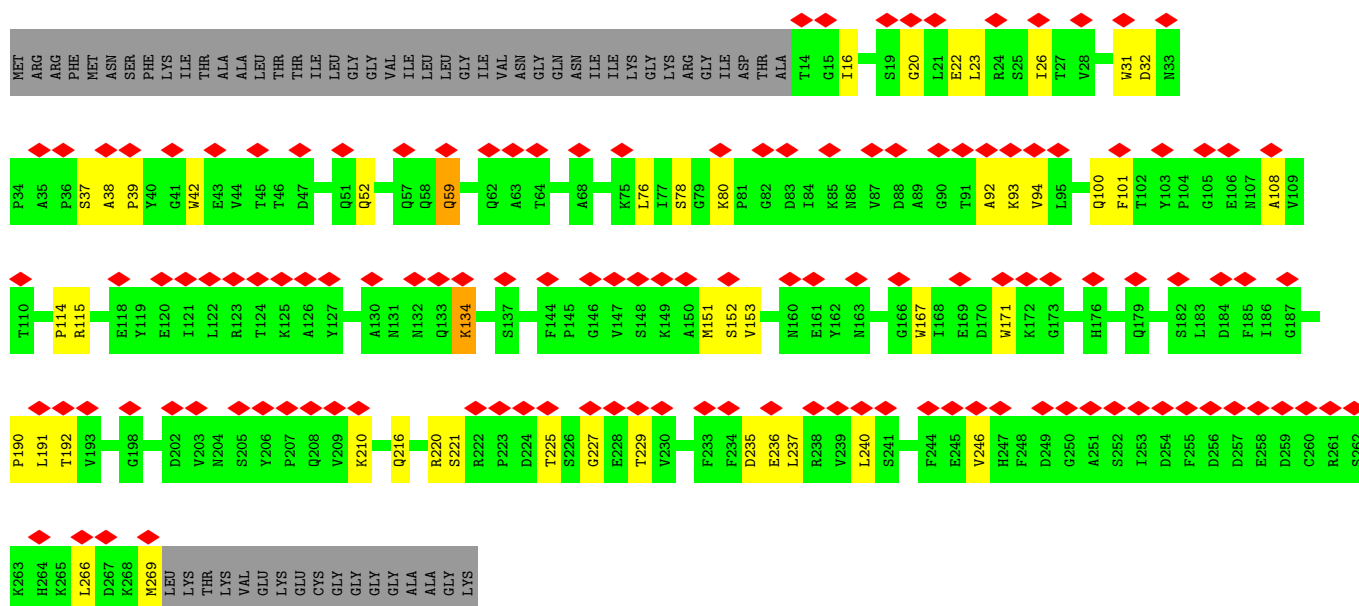
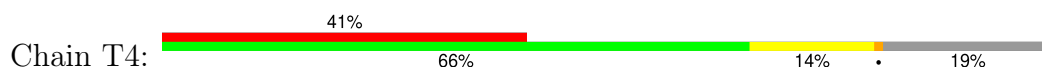


• Molecule 4: Flagellar filament sheath protein

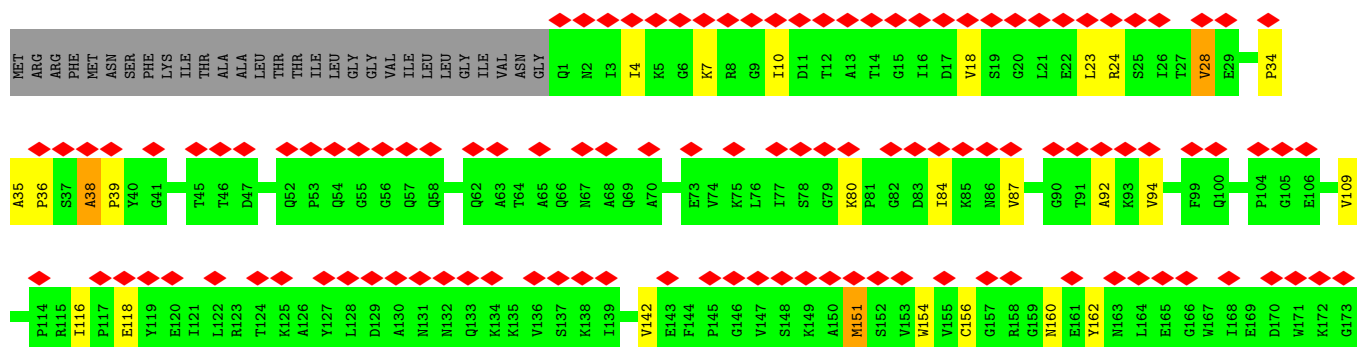


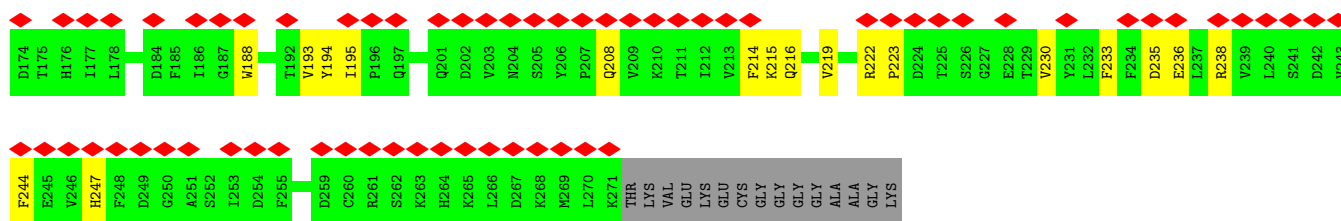


• Molecule 4: Flagellar filament sheath protein

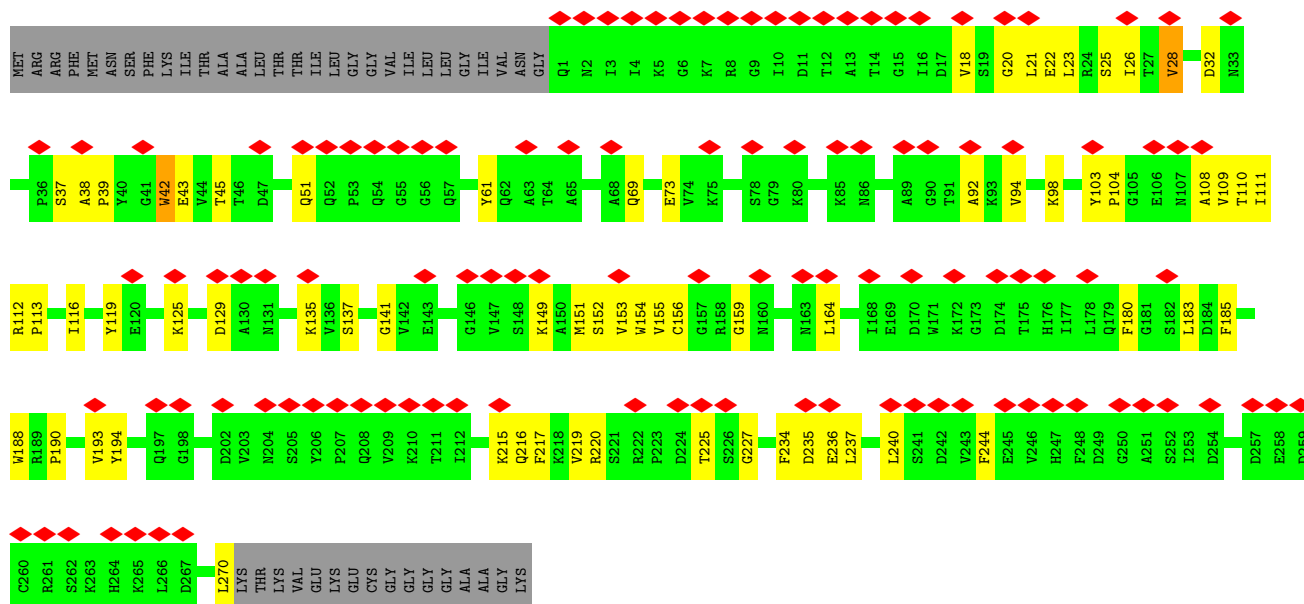


• Molecule 4: Flagellar filament sheath protein

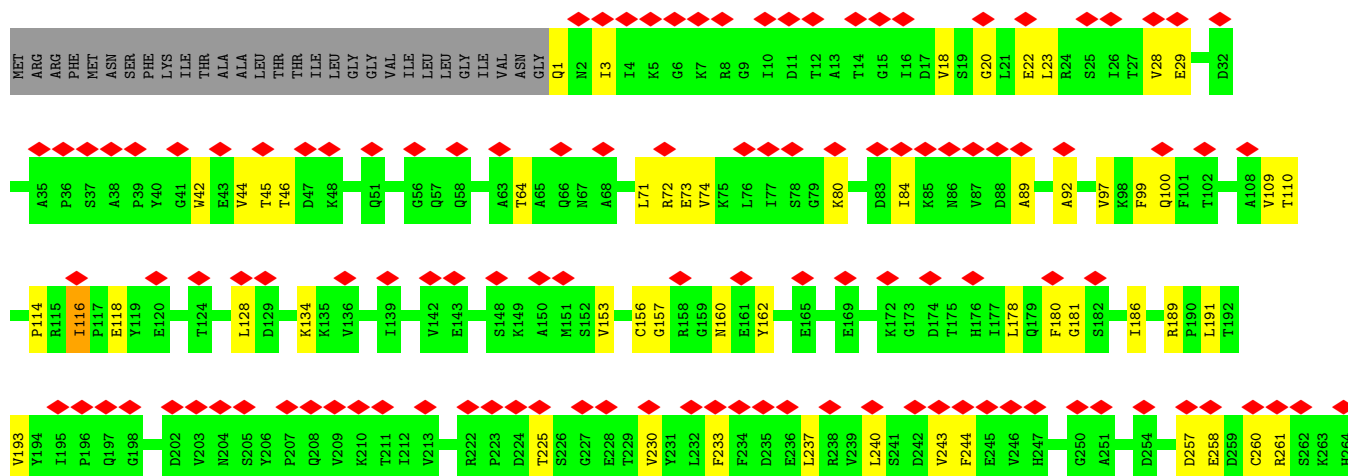
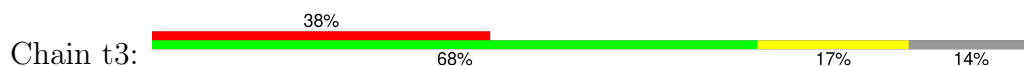


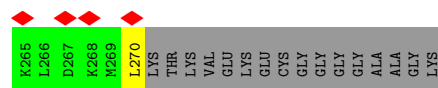


• Molecule 4: Flagellar filament sheath protein

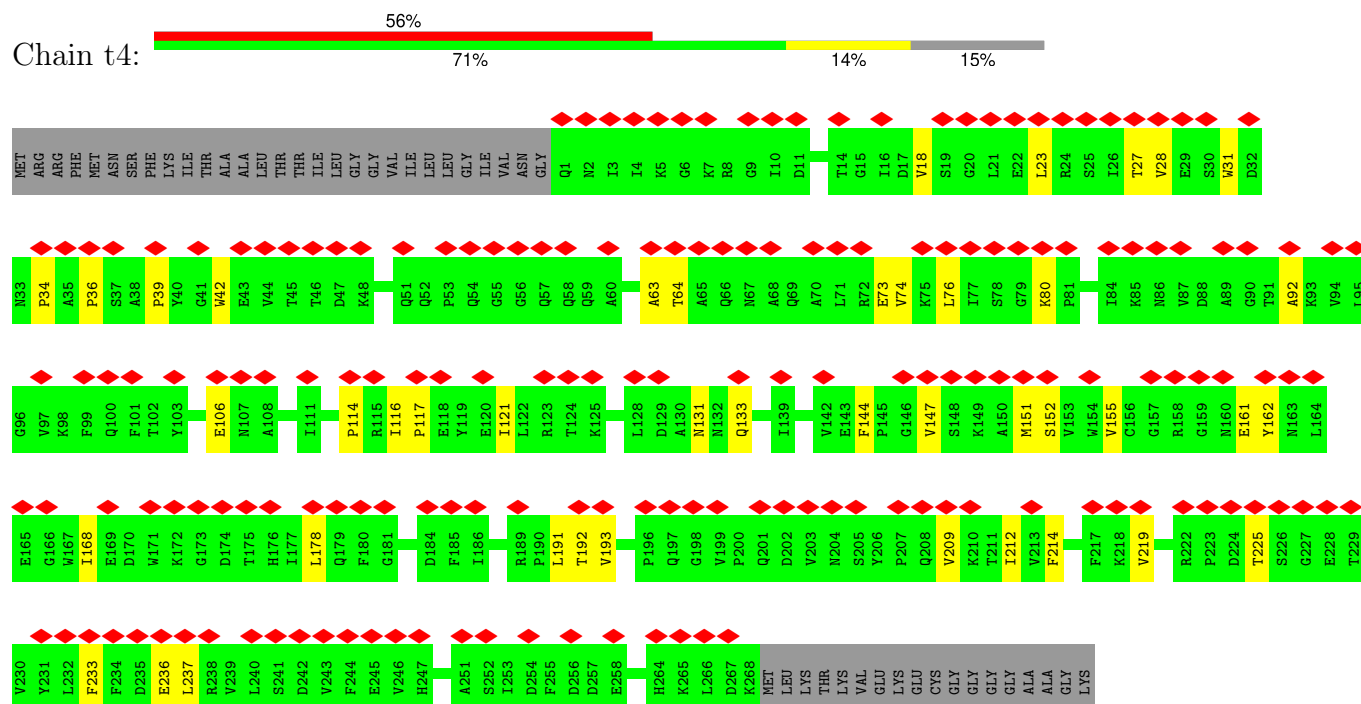


• Molecule 4: Flagellar filament sheath protein

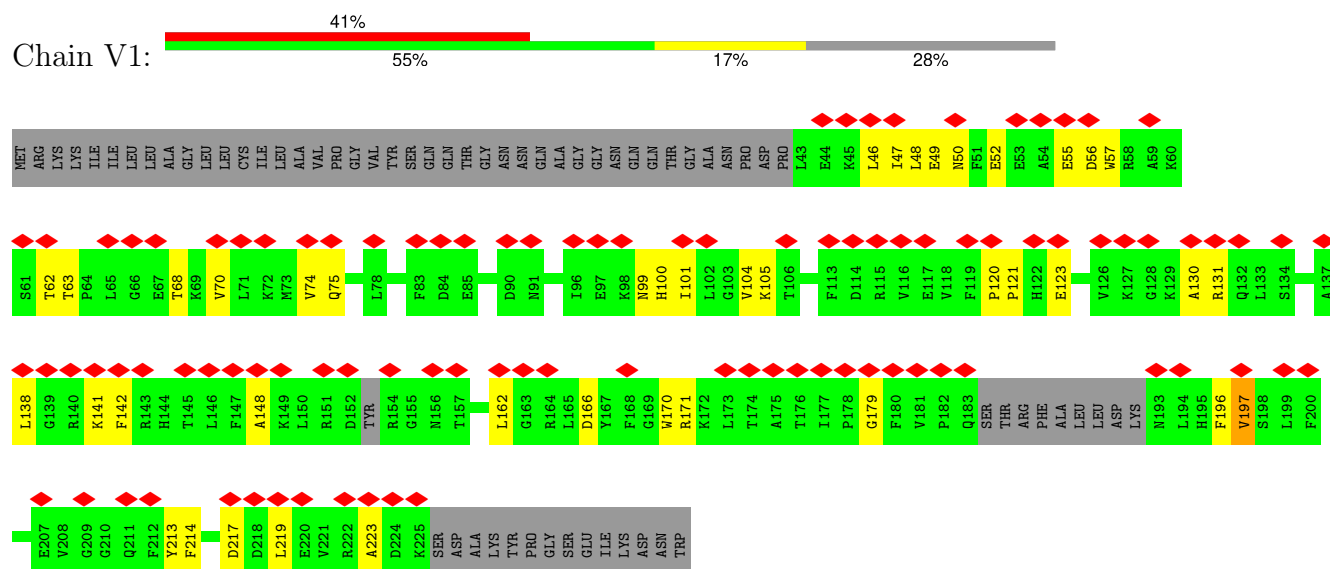




• Molecule 4: Flagellar filament sheath protein

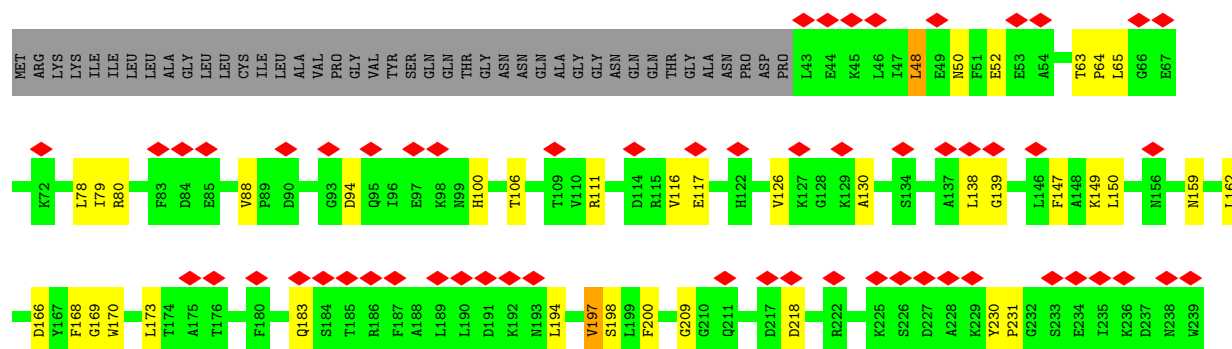


• Molecule 5: Flagellar filament sheath protein

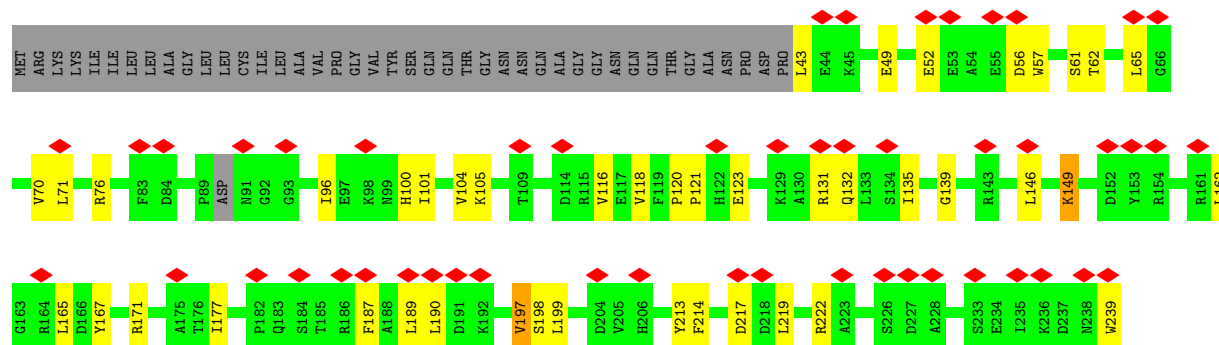


• Molecule 5: Flagellar filament sheath protein

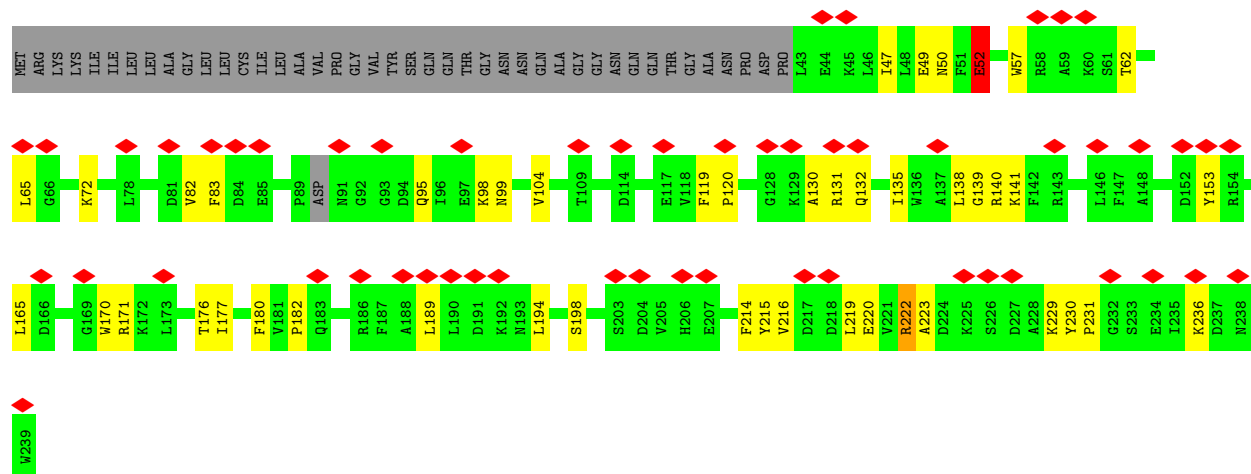




• Molecule 5: Flagellar filament sheath protein

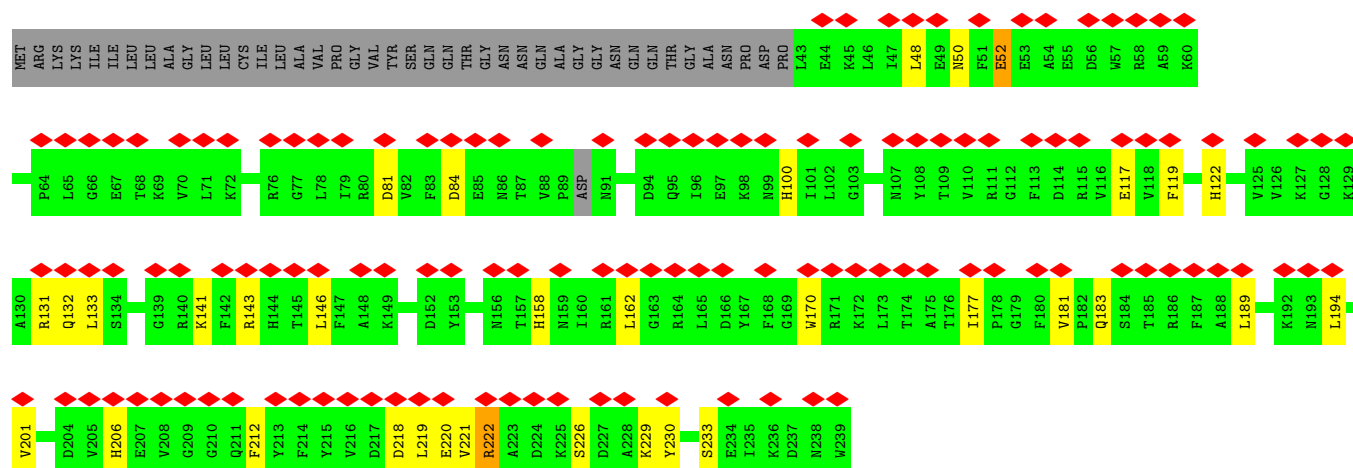


• Molecule 5: Flagellar filament sheath protein

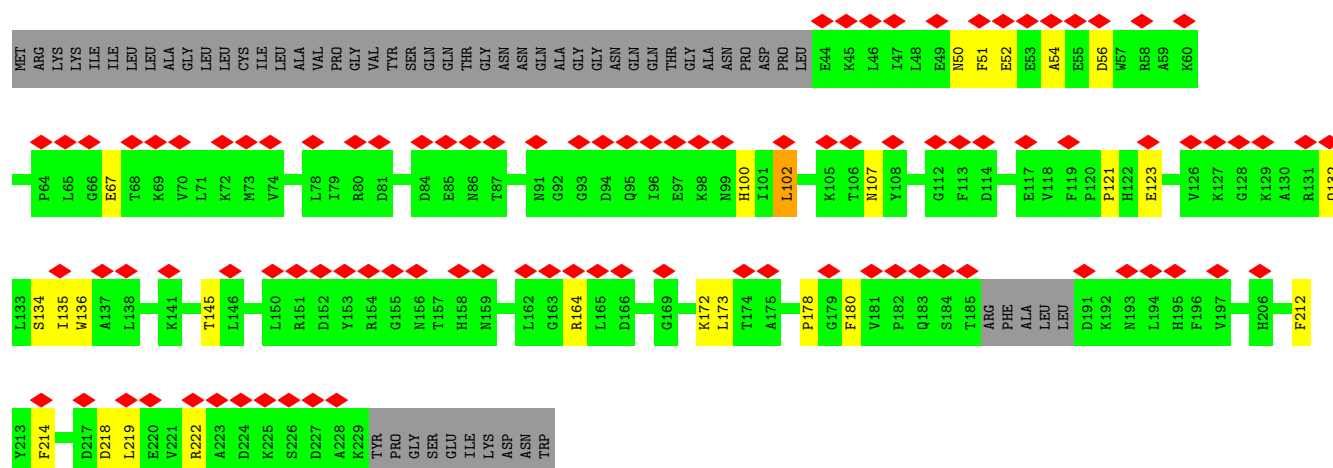
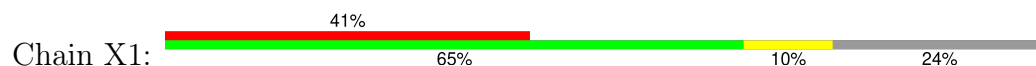


• Molecule 5: Flagellar filament sheath protein

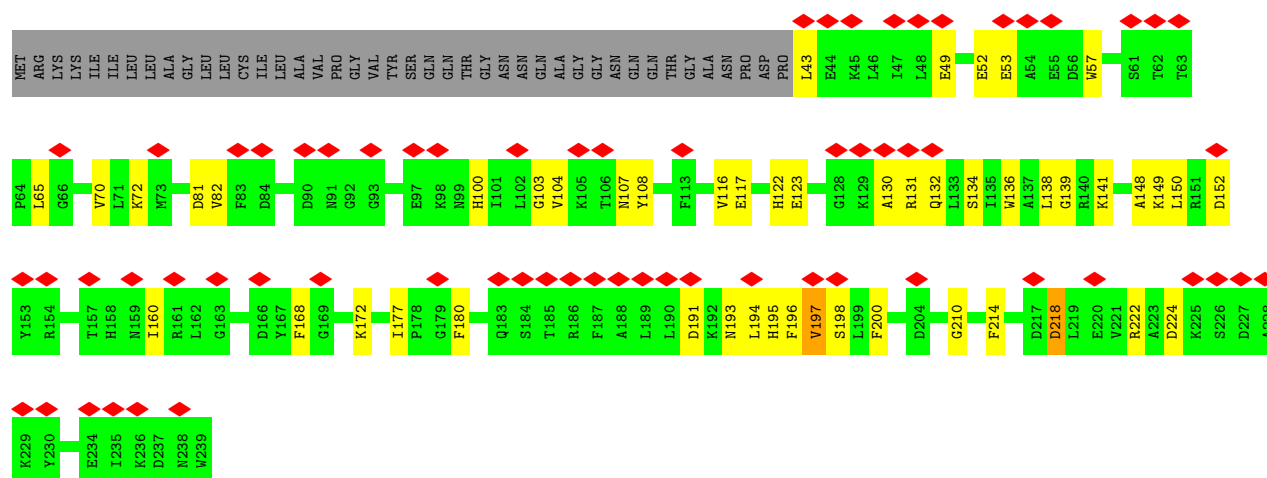




• Molecule 5: Flagellar filament sheath protein

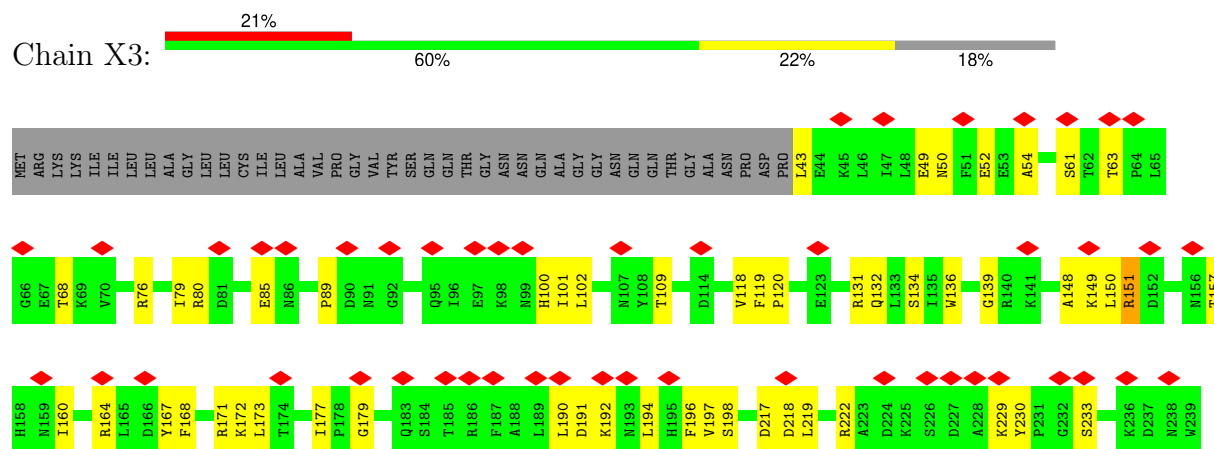


• Molecule 5: Flagellar filament sheath protein



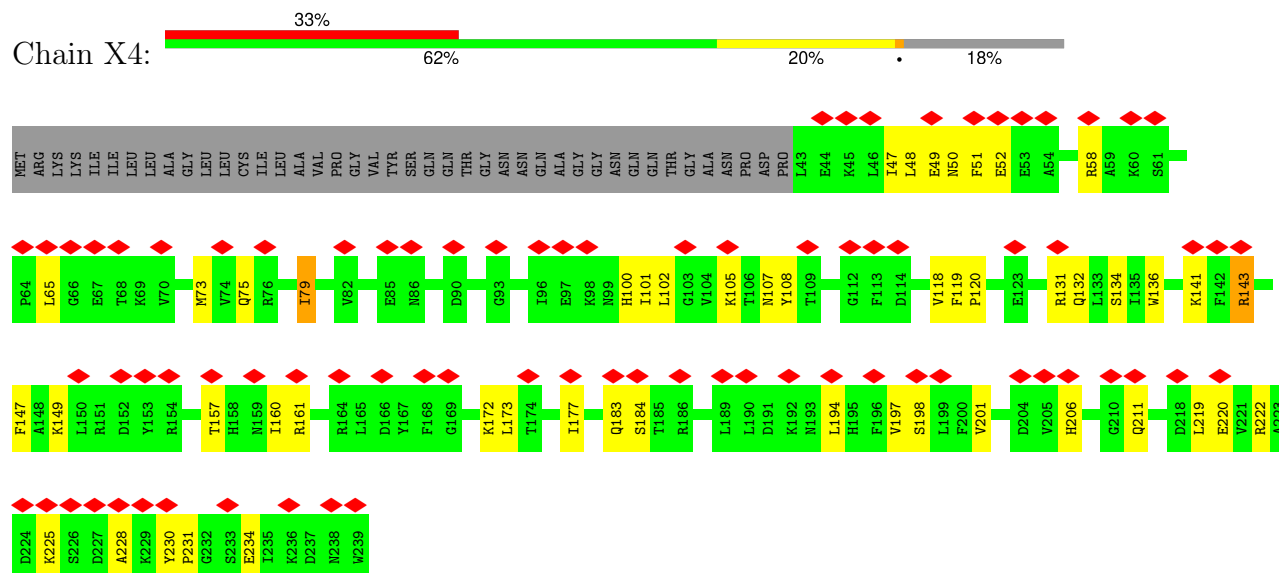
- Molecule 5: Flagellar filament sheath protein

Chain X3:



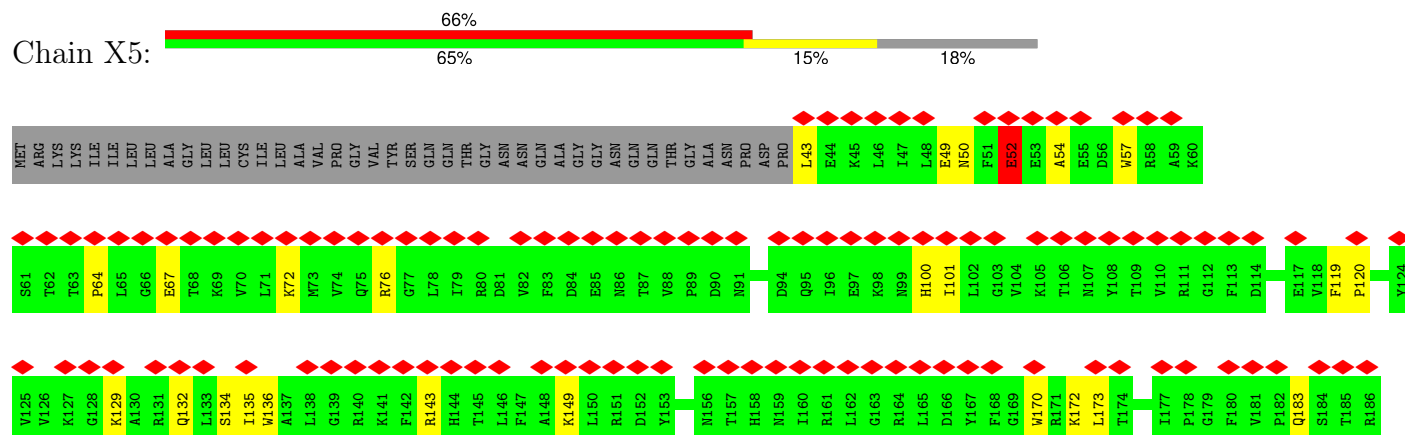
- Molecule 5: Flagellar filament sheath protein

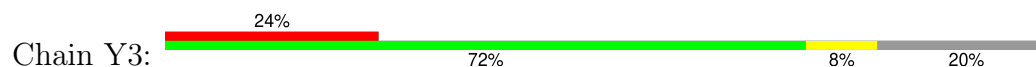
Chain X4:

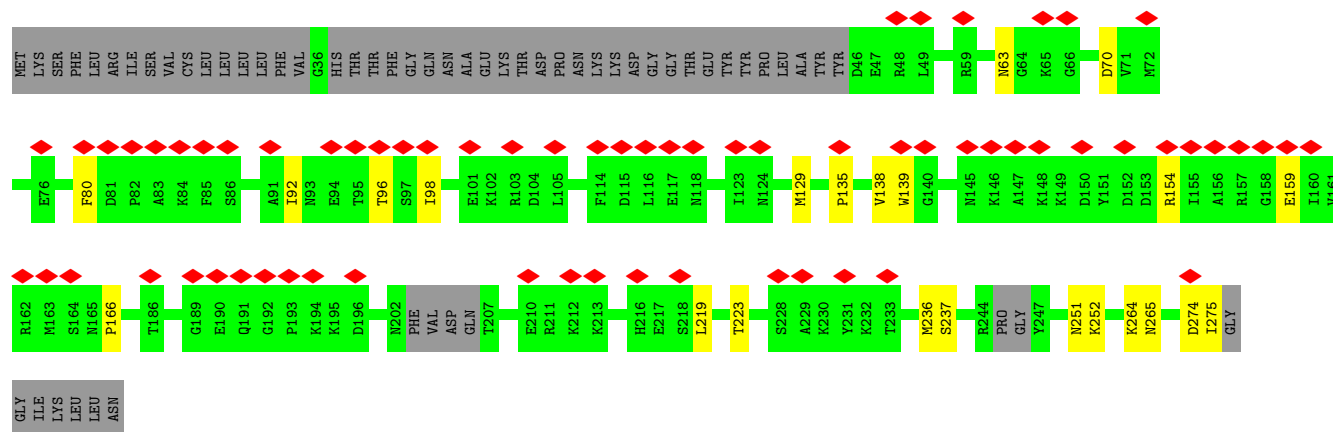


- Molecule 5: Flagellar filament sheath protein

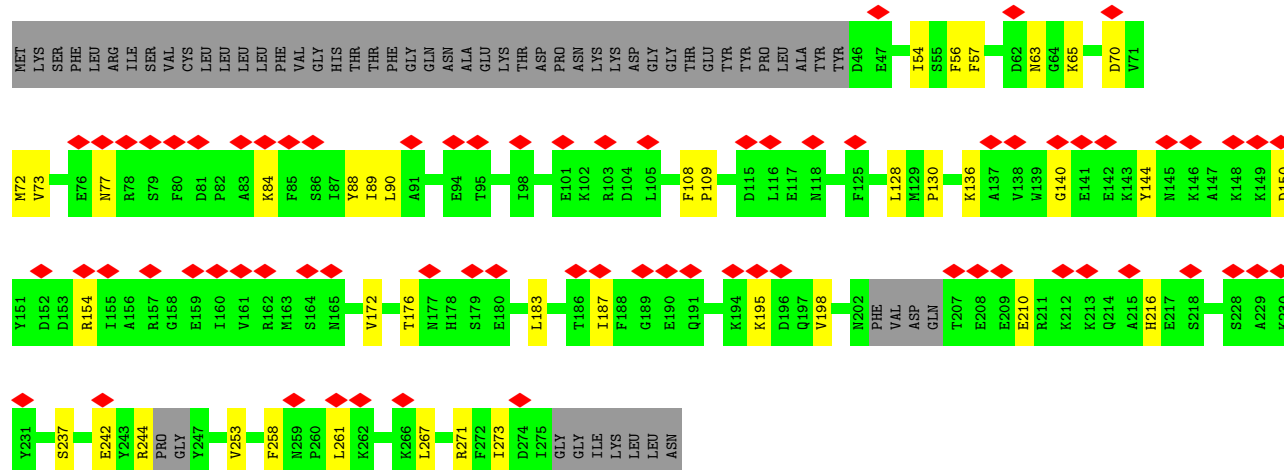
Chain X5:



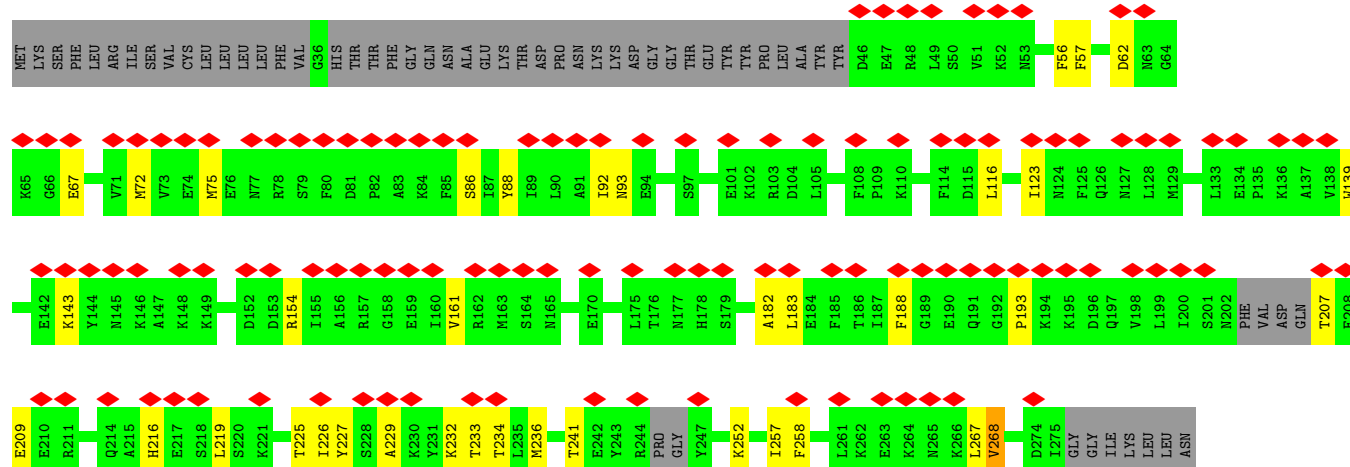
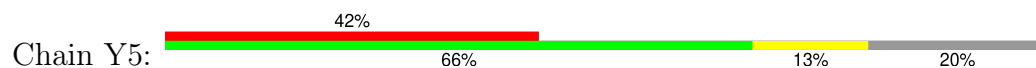


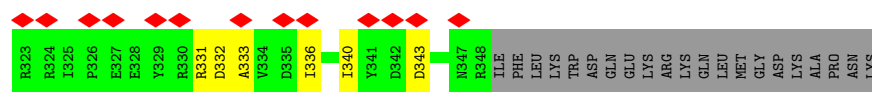


• Molecule 6: FlaA2 associated protein 2

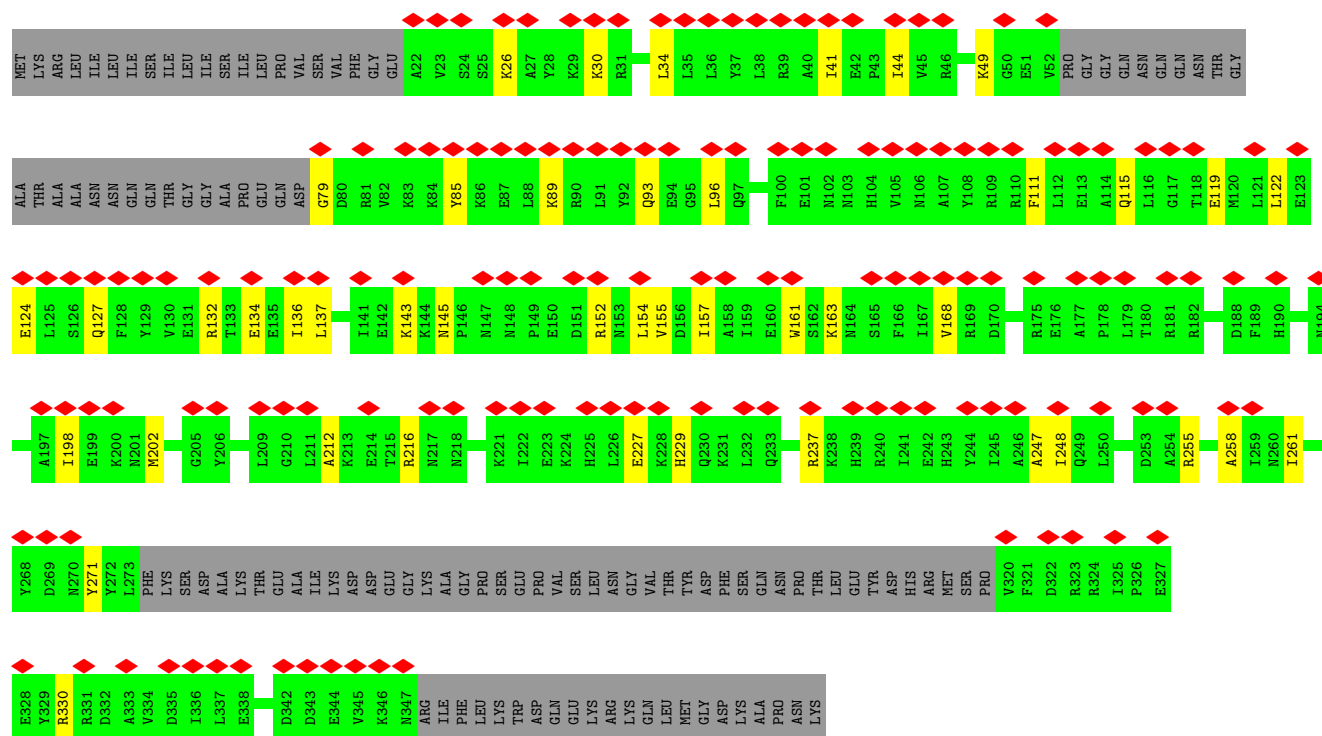
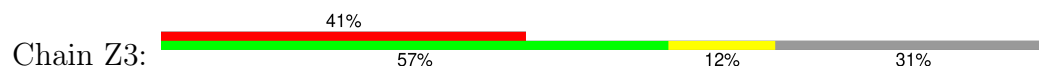


• Molecule 6: FlaA2 associated protein 2



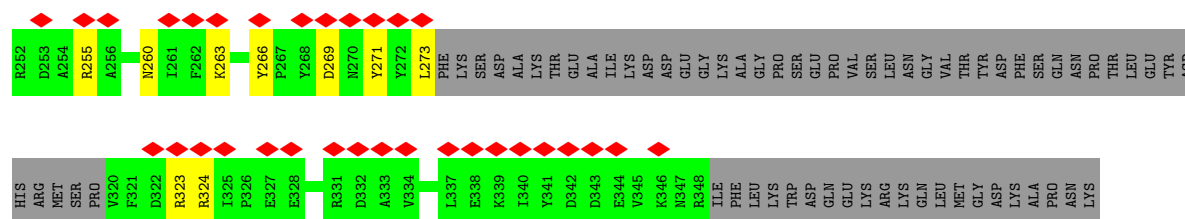


• Molecule 7: FlaA2-associated protein 1 (FlaAP)

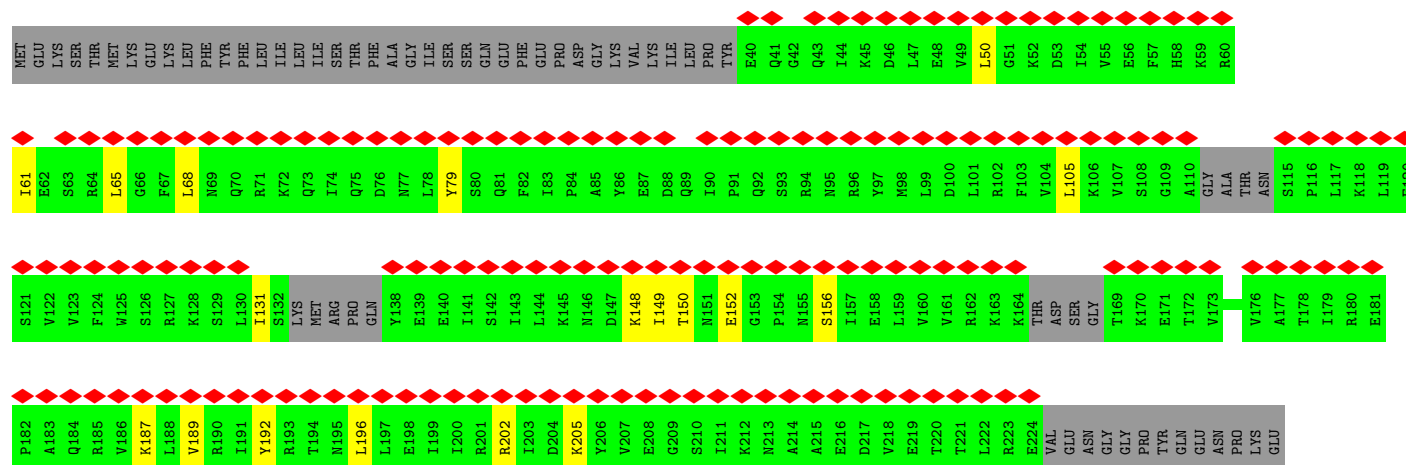


• Molecule 7: FlaA2-associated protein 1 (FlaAP)

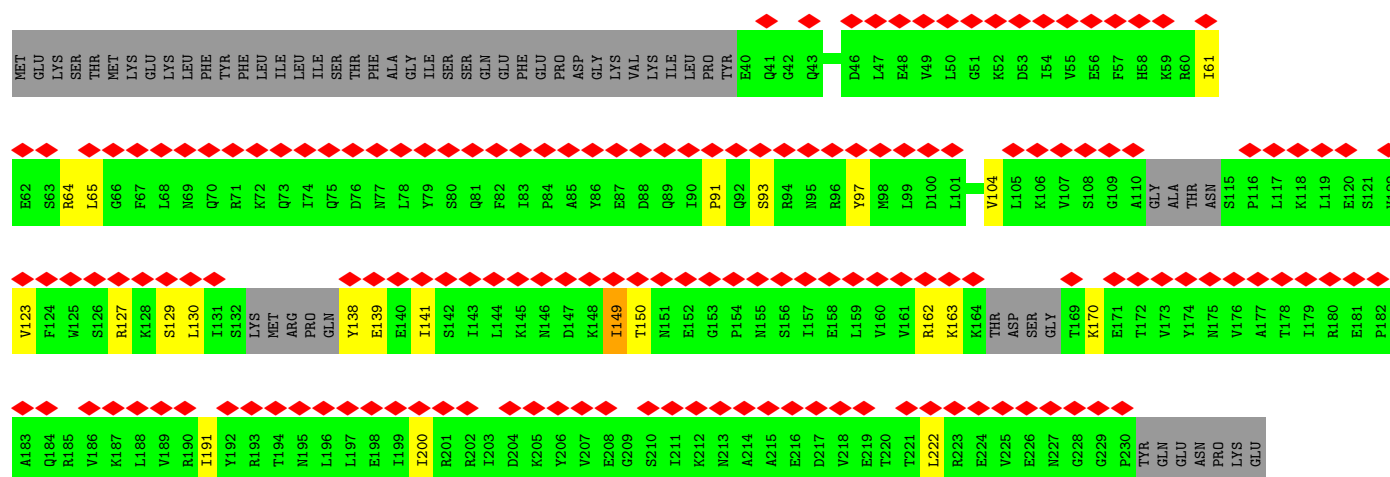




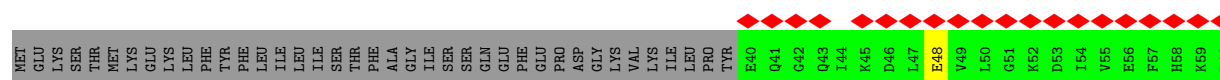
• Molecule 8: DUF4468 domain-containing protein

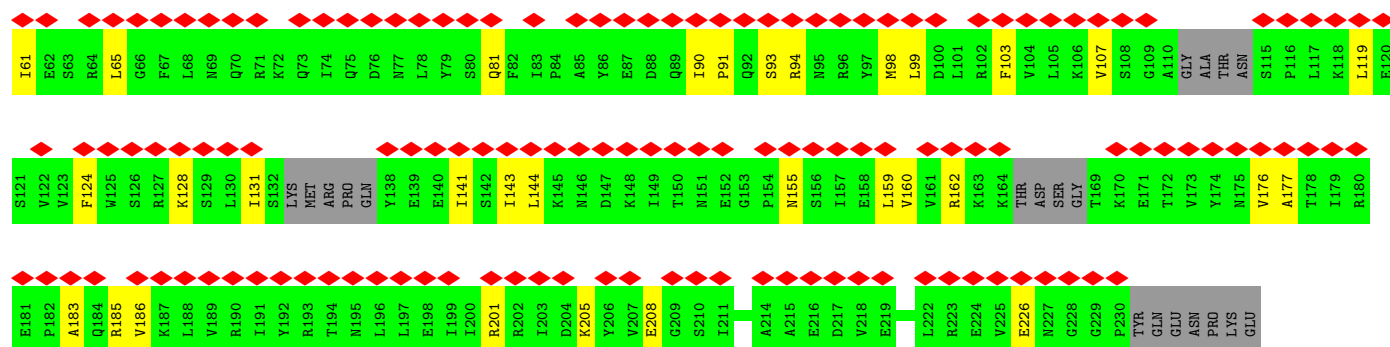


• Molecule 8: DUF4468 domain-containing protein

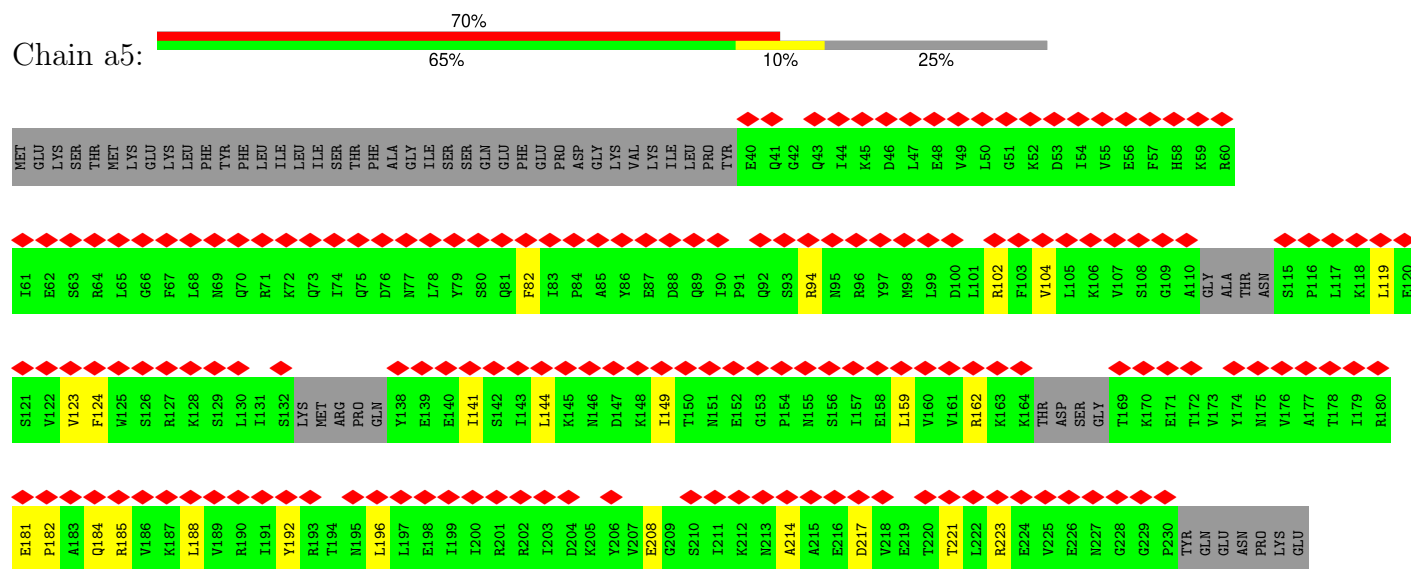


• Molecule 8: DUF4468 domain-containing protein

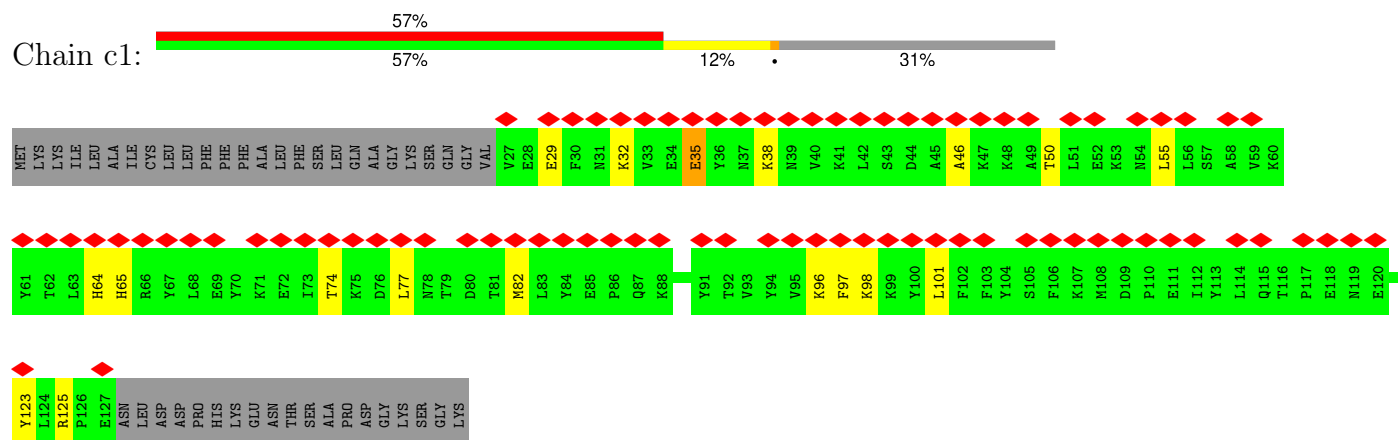


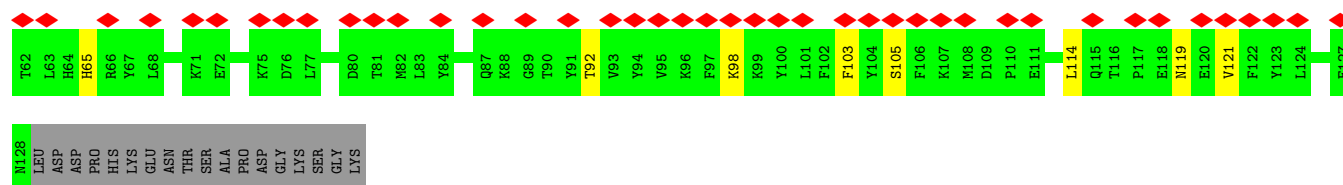


• Molecule 8: DUF4468 domain-containing protein

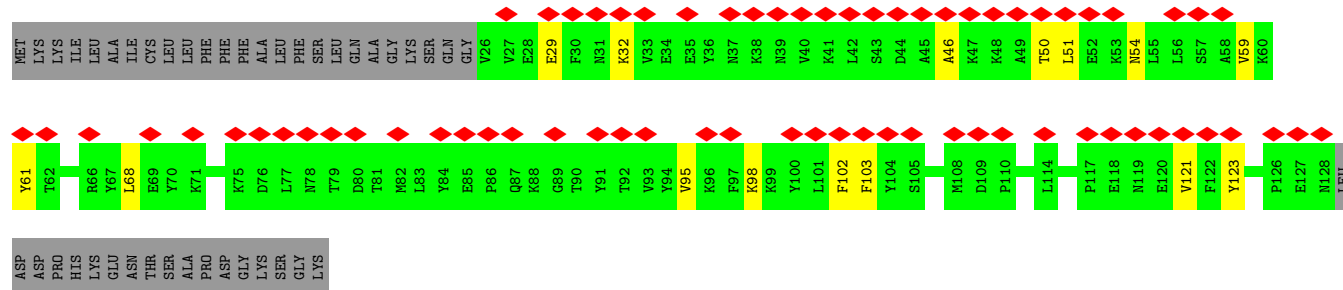


• Molecule 9: Lipoprotein

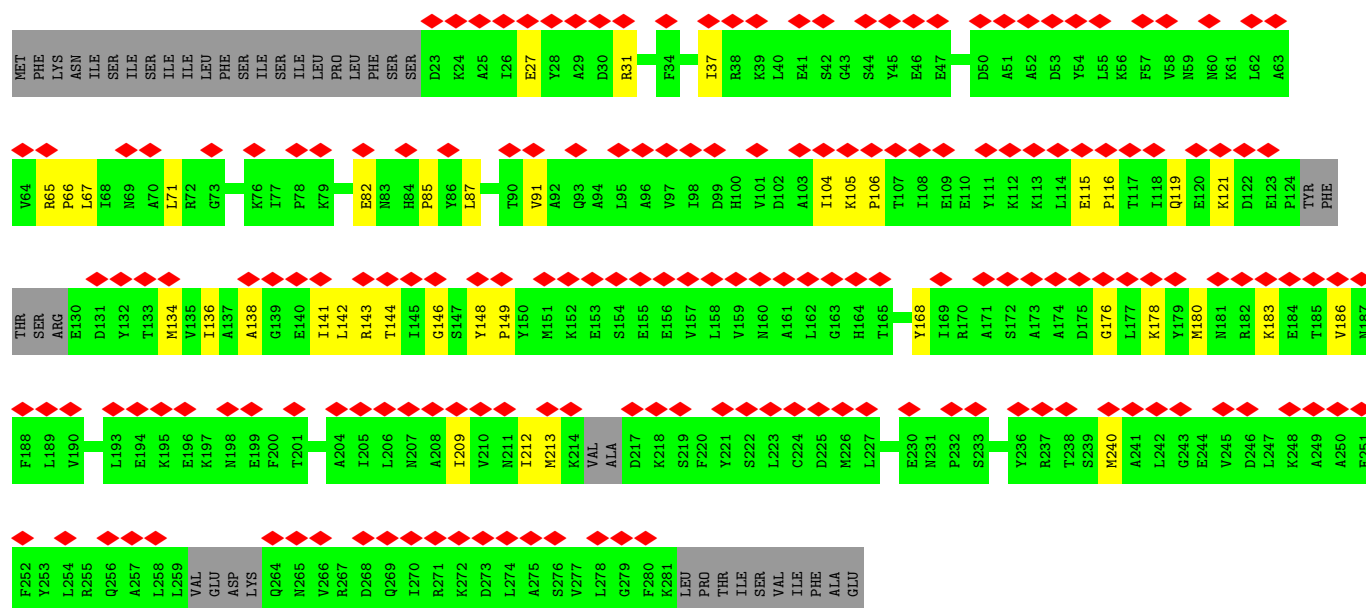




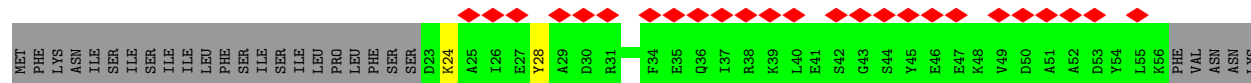
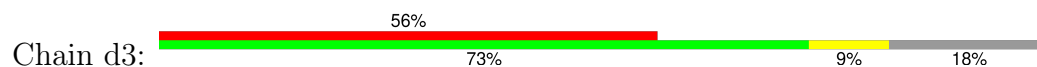
• Molecule 9: Lipoprotein

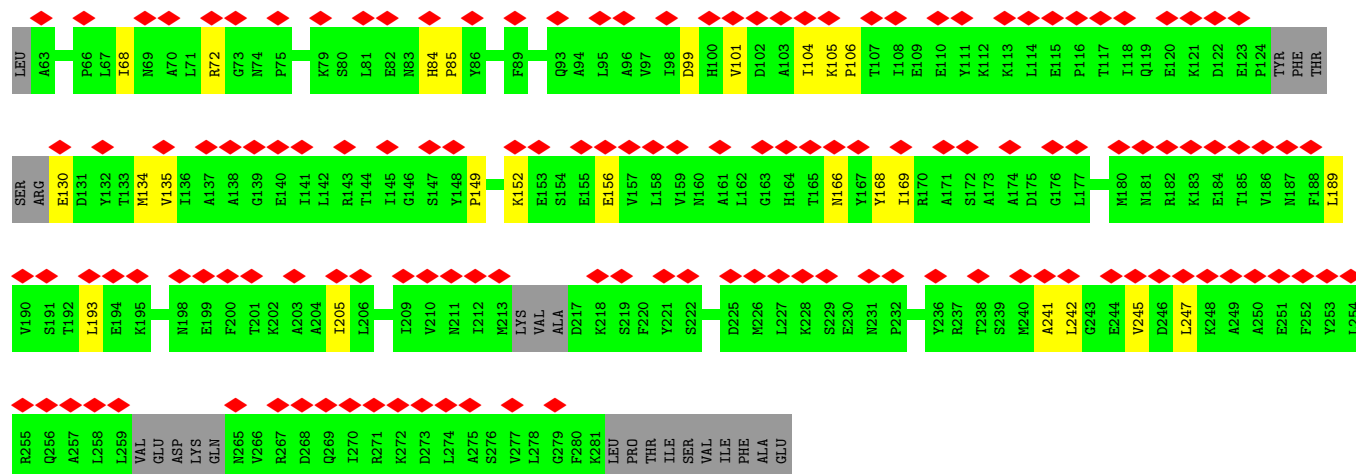


• Molecule 10: HEAT repeat domain-containing protein

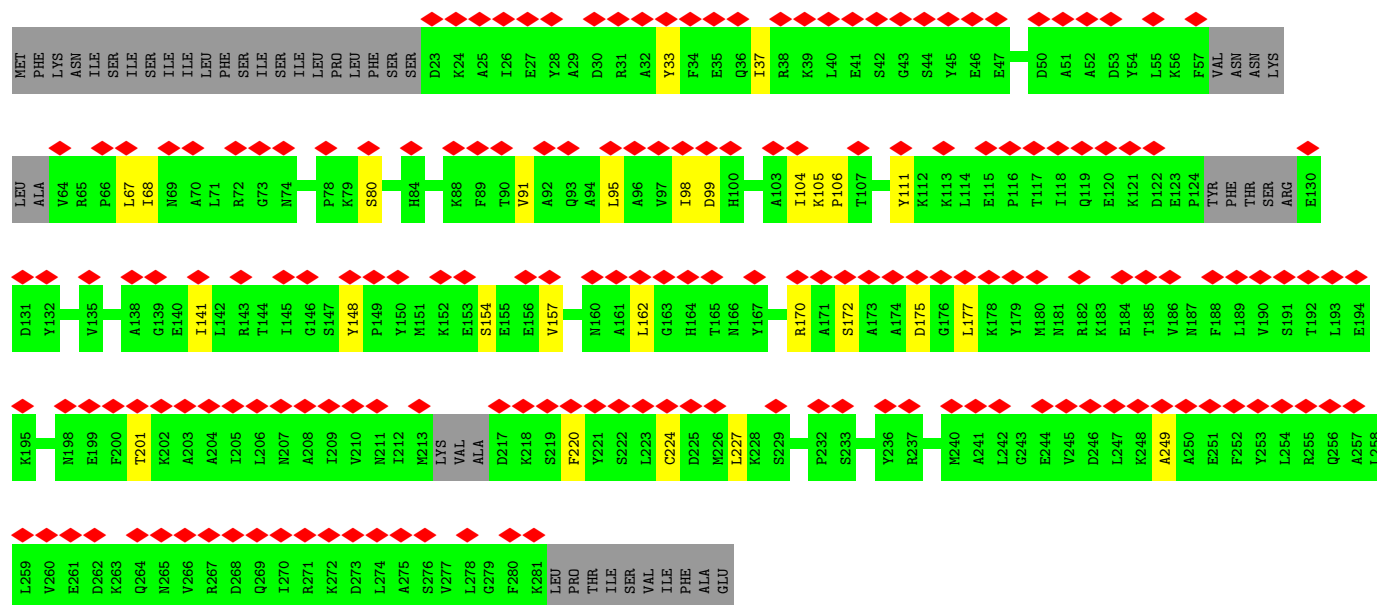
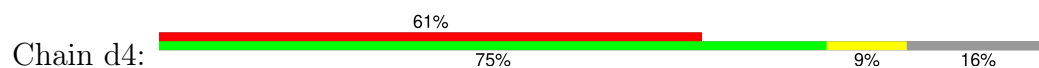


• Molecule 10: HEAT repeat domain-containing protein





- Molecule 10: HEAT repeat domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.240	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	273.408, 273.408, 273.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	A4	0.21	0/794	0.50	0/1064
1	A5	0.19	0/2071	0.53	0/2782
1	A6	0.21	0/2210	0.55	0/2972
1	A7	0.19	0/2210	0.49	0/2972
1	A8	0.21	0/1962	0.54	0/2638
1	A9	0.17	0/1160	0.50	0/1561
1	B3	0.19	0/503	0.54	0/675
1	B4	0.19	0/1145	0.50	0/1535
1	B5	0.20	0/2210	0.54	0/2972
1	B6	0.20	0/2210	0.53	0/2972
1	B7	0.20	0/2182	0.51	0/2936
1	B8	0.18	0/1556	0.49	0/2091
1	C3	0.21	0/794	0.50	0/1064
1	C4	0.19	0/1938	0.54	0/2600
1	C5	0.21	0/2210	0.51	0/2972
1	C6	0.20	0/2210	0.51	0/2972
1	C7	0.20	0/1961	0.52	0/2636
1	C8	0.17	0/1252	0.52	0/1680
1	D3	0.20	0/1273	0.56	0/1700
1	D4	0.20	0/2210	0.49	0/2972
1	D5	0.21	0/2210	0.51	0/2972
1	D6	0.21	0/2210	0.55	0/2972
1	D7	0.21	0/1652	0.58	0/2217
1	E2	0.19	0/760	0.55	0/1017
1	E3	0.21	0/1847	0.54	0/2476
1	E4	0.20	0/2210	0.52	0/2972
1	E5	0.22	0/2210	0.54	0/2972
1	E6	0.21	0/2013	0.55	0/2705
1	E7	0.19	0/1304	0.54	0/1752
1	F2	0.19	0/1013	0.52	0/1355
1	F3	0.21	0/2210	0.52	0/2972
1	F4	0.21	0/2210	0.52	0/2972

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F5	0.21	0/2210	0.55	0/2972
1	F6	0.19	0/1734	0.50	0/2330
1	G1	0.21	0/2045	0.54	1/2749 (0.0%)
1	G2	0.18	0/1376	0.48	0/1852
1	G6	0.18	0/697	0.45	0/936
1	G7	0.19	0/1725	0.52	0/2309
1	G8	0.20	0/2210	0.52	0/2972
1	G9	0.21	0/2210	0.53	0/2972
1	H6	0.21	0/1073	0.51	0/1436
1	H7	0.20	0/2210	0.50	0/2972
1	H8	0.19	0/2210	0.52	0/2972
1	H9	0.21	0/2210	0.52	0/2972
1	I5	0.19	0/657	0.54	0/882
1	I6	0.19	0/1671	0.51	0/2239
1	I7	0.20	0/2210	0.50	0/2972
1	I8	0.21	0/2210	0.56	0/2972
1	I9	0.20	0/2081	0.54	0/2799
1	J5	0.22	0/939	0.54	0/1257
1	J6	0.20	0/2168	0.51	0/2912
1	J7	0.20	0/2210	0.50	0/2972
1	J8	0.19	0/2210	0.51	0/2972
1	J9	0.21	0/1828	0.55	0/2456
1	K4	0.18	0/598	0.48	0/802
1	K5	0.20	0/1593	0.54	0/2132
1	K6	0.20	0/2210	0.53	0/2972
1	K7	0.22	0/2210	0.57	0/2972
1	K8	0.19	0/2120	0.53	0/2852
1	K9	0.19	0/1457	0.55	0/1961
1	h0	0.20	0/1843	0.55	0/2477
1	h1	0.16	0/818	0.47	0/1099
1	i0	0.17	0/1412	0.51	0/1900
1	j0	0.19	0/993	0.51	0/1334
2	L2	0.16	0/1705	0.44	0/2286
2	L3	0.17	0/1804	0.51	0/2427
2	L4	0.17	0/1804	0.44	0/2427
2	L5	0.17	0/1804	0.44	0/2427
2	L6	0.15	0/1471	0.45	0/1974
2	M1	0.16	0/735	0.52	0/986
2	M2	0.16	0/1835	0.44	0/2468
2	M3	0.17	0/1835	0.50	0/2468
2	M4	0.18	0/1835	0.52	0/2468
2	M5	0.17	0/1795	0.44	0/2413
2	N2	0.17	0/1573	0.46	0/2111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	N3	0.17	0/1803	0.47	0/2426
2	N4	0.18	0/1803	0.48	0/2426
2	N5	0.17	0/1803	0.49	0/2426
2	N6	0.17	0/1494	0.47	0/2010
2	O1	0.16	0/516	0.52	0/692
2	O2	0.16	0/1790	0.44	0/2407
2	O3	0.18	0/1803	0.48	0/2426
2	O4	0.18	0/1803	0.49	0/2426
2	O5	0.17	0/1795	0.45	0/2415
2	P2	0.15	0/1484	0.43	0/1987
2	P3	0.18	0/1786	0.50	0/2403
2	P4	0.16	0/1786	0.49	0/2403
2	P5	0.18	0/1786	0.45	0/2403
2	P6	0.18	0/1493	0.47	0/2009
2	p2	0.16	0/1782	0.42	0/2396
2	p3	0.17	0/1803	0.46	0/2426
2	p4	0.17	0/1795	0.48	0/2415
2	p5	0.18	0/1795	0.48	0/2415
3	Q1	0.15	0/1358	0.50	0/1812
3	Q2	0.17	0/1598	0.53	0/2147
3	Q3	0.19	0/1664	0.61	0/2235
3	Q4	0.18	0/1632	0.54	0/2192
3	R2	0.16	0/1554	0.50	0/2089
3	R3	0.19	0/1710	0.55	0/2299
3	R4	0.18	0/1619	0.56	0/2176
3	R5	0.16	0/1615	0.53	0/2171
3	S2	0.15	0/1248	0.45	0/1665
3	S3	0.17	0/1586	0.57	0/2131
3	S4	0.15	0/1632	0.54	0/2191
3	S5	0.17	0/1611	0.52	0/2165
3	S6	0.15	0/1599	0.49	0/2149
3	s3	0.16	0/1625	0.52	2/2185 (0.1%)
3	s4	0.16	0/1615	0.53	0/2172
3	s5	0.16	0/1635	0.49	0/2198
3	s6	0.16	0/1425	0.53	0/1911
4	T1	0.15	0/2103	0.51	0/2848
4	T2	0.15	0/2192	0.56	0/2974
4	T3	0.19	0/2192	0.59	0/2974
4	T4	0.19	0/2086	0.62	1/2833 (0.0%)
4	t1	0.16	0/2201	0.60	0/2985
4	t2	0.17	0/2192	0.56	0/2974
4	t3	0.16	0/2192	0.52	0/2974
4	t4	0.14	0/2176	0.49	0/2953

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	V1	0.16	0/1454	0.55	0/1961
5	V2	0.16	0/1661	0.58	0/2243
5	V3	0.17	0/1652	0.59	0/2229
5	V4	0.16	0/1652	0.60	1/2229 (0.0%)
5	V5	0.14	0/1652	0.55	0/2229
5	X1	0.16	0/1518	0.58	0/2048
5	X2	0.16	0/1661	0.59	0/2243
5	X3	0.18	0/1661	0.57	0/2243
5	X4	0.17	0/1661	0.60	0/2243
5	X5	0.15	0/1649	0.57	1/2225 (0.0%)
6	Y1	0.13	0/845	0.51	0/1129
6	Y2	0.15	0/1884	0.52	0/2537
6	Y3	0.14	0/1916	0.48	0/2578
6	Y4	0.15	0/1913	0.54	0/2576
6	Y5	0.14	0/1916	0.50	0/2578
7	Z1	0.17	0/2215	0.50	0/2972
7	Z2	0.18	0/2215	0.49	0/2972
7	Z3	0.16	0/2204	0.48	0/2958
7	Z4	0.14	0/2215	0.41	0/2972
8	a2	0.14	0/1437	0.47	0/1928
8	a3	0.15	0/1477	0.47	0/1983
8	a4	0.14	0/1477	0.48	0/1983
8	a5	0.14	0/1477	0.44	0/1983
9	c1	0.13	0/889	0.46	0/1199
9	c2	0.14	0/904	0.47	0/1220
9	c3	0.15	0/904	0.45	0/1220
10	d2	0.16	0/2024	0.46	0/2725
10	d3	0.17	0/1953	0.48	0/2629
10	d4	0.16	0/2003	0.45	0/2697
All	All	0.18	0/251723	0.52	6/338599 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A5	0	2
1	A6	0	3
1	A7	0	1
1	A8	0	2
1	B5	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B6	0	2
1	C3	0	2
1	C4	0	2
1	C5	0	2
1	C6	0	3
1	C7	0	1
1	D7	0	2
1	E2	0	1
1	E4	0	1
1	E5	0	1
1	E6	0	1
1	F4	0	1
1	F5	0	1
1	F6	0	1
1	G8	0	1
1	G9	0	1
1	H6	0	1
1	H7	0	5
1	H8	0	4
1	I6	0	1
1	I8	0	1
1	I9	0	3
1	J7	0	1
1	J9	0	2
1	K4	0	1
1	K5	0	1
1	K8	0	1
2	L2	0	1
2	L4	0	1
2	M3	0	1
2	N3	0	1
2	N6	0	1
2	O4	0	1
2	O5	0	1
2	P6	0	1
2	p5	0	1
3	Q4	0	2
3	R4	0	2
3	R5	0	1
3	S3	0	1
3	S4	0	1
5	V1	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	V4	0	2
5	V5	0	1
5	X3	0	1
5	X4	0	2
7	Z4	0	1
All	All	0	77

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X5	52	GLU	CA-CB-CG	5.87	125.85	114.10
4	T4	38	ALA	N-CA-C	5.15	121.19	109.81
5	V4	52	GLU	CA-CB-CG	5.11	124.33	114.10
3	s3	85	ASN	CA-C-N	5.10	131.28	121.54
3	s3	85	ASN	C-N-CA	5.10	131.28	121.54
1	G1	247	GLU	CA-CB-CG	5.08	124.27	114.10

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A5	239	ARG	Sidechain
1	A5	281	ARG	Sidechain
1	A6	123	ARG	Sidechain
1	A6	53	ARG	Sidechain
1	A6	64	ARG	Sidechain
1	A7	35	ARG	Sidechain
1	A8	14	ARG	Sidechain
1	A8	209	ARG	Sidechain
1	B5	64	ARG	Sidechain
1	B6	14	ARG	Sidechain
1	B6	218	ARG	Sidechain
1	C3	14	ARG	Sidechain
1	C3	38	ARG	Sidechain
1	C4	38	ARG	Sidechain
1	C4	64	ARG	Sidechain
1	C5	209	ARG	Sidechain
1	C5	281	ARG	Sidechain
1	C6	123	ARG	Sidechain
1	C6	14	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C6	218	ARG	Sidechain
1	C7	64	ARG	Sidechain
1	D7	209	ARG	Sidechain
1	D7	53	ARG	Sidechain
1	E2	281	ARG	Sidechain
1	E4	218	ARG	Sidechain
1	E5	218	ARG	Sidechain
1	E6	123	ARG	Sidechain
1	F4	218	ARG	Sidechain
1	F5	218	ARG	Sidechain
1	F6	107	ARG	Sidechain
1	G8	218	ARG	Sidechain
1	G9	14	ARG	Sidechain
1	H6	14	ARG	Sidechain
1	H7	209	ARG	Sidechain
1	H7	218	ARG	Sidechain
1	H7	53	ARG	Sidechain
1	H7	60	ARG	Sidechain
1	H7	91	ARG	Sidechain
1	H8	107	ARG	Sidechain
1	H8	209	ARG	Sidechain
1	H8	38	ARG	Sidechain
1	H8	60	ARG	Sidechain
1	I6	38	ARG	Sidechain
1	I8	239	ARG	Sidechain
1	I9	218	ARG	Sidechain
1	I9	241	ARG	Sidechain
1	I9	60	ARG	Sidechain
1	J7	91	ARG	Sidechain
1	J9	160	ARG	Sidechain
1	J9	209	ARG	Sidechain
1	K4	272	ARG	Sidechain
1	K5	53	ARG	Sidechain
1	K8	53	ARG	Sidechain
2	L2	106	ARG	Sidechain
2	L4	276	ARG	Sidechain
2	M3	160	ARG	Sidechain
2	N3	267	ARG	Sidechain
2	N6	150	ARG	Sidechain
2	O4	203	ARG	Sidechain
2	O5	191	ARG	Sidechain
2	P6	189	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	Q4	150	ARG	Sidechain
3	Q4	177	ARG	Sidechain
3	R4	150	ARG	Sidechain
3	R4	58	ARG	Sidechain
3	R5	145	ARG	Sidechain
3	S3	246	ARG	Sidechain
3	S4	112	ARG	Sidechain
5	V1	171	ARG	Sidechain
5	V4	171	ARG	Sidechain
5	V4	222	ARG	Sidechain
5	V5	222	ARG	Sidechain
5	X3	151	ARG	Sidechain
5	X4	143	ARG	Sidechain
5	X4	58	ARG	Sidechain
7	Z4	110	ARG	Sidechain
2	p5	203	ARG	Sidechain

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	A4	791	0	808	22	0
1	A5	2054	0	2079	43	0
1	A6	2190	0	2201	60	0
1	A7	2190	0	2201	44	0
1	A8	1945	0	1929	53	0
1	A9	1151	0	1143	19	0
1	B3	500	0	522	10	0
1	B4	1138	0	1150	33	0
1	B5	2190	0	2201	44	0
1	B6	2190	0	2201	65	0
1	B7	2162	0	2166	58	0
1	B8	1541	0	1537	35	0
1	C3	791	0	808	15	0
1	C4	1922	0	1938	36	0
1	C5	2190	0	2201	33	0
1	C6	2190	0	2201	34	0
1	C7	1944	0	1936	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C8	1243	0	1241	23	0
1	D3	1263	0	1267	27	0
1	D4	2190	0	2201	41	0
1	D5	2190	0	2201	49	0
1	D6	2190	0	2201	41	0
1	D7	1638	0	1632	34	0
1	E2	757	0	774	17	0
1	E3	1832	0	1834	46	0
1	E4	2190	0	2201	38	0
1	E5	2190	0	2201	51	0
1	E6	1995	0	1987	31	0
1	E7	1292	0	1284	20	0
1	F2	1009	0	1023	16	0
1	F3	2190	0	2201	39	0
1	F4	2190	0	2201	48	0
1	F5	2190	0	2201	50	0
1	F6	1719	0	1704	29	0
1	G1	2027	0	2021	42	0
1	G2	1361	0	1347	15	0
1	G6	694	0	709	11	0
1	G7	1710	0	1713	25	0
1	G8	2190	0	2201	35	0
1	G9	2190	0	2201	51	0
1	H6	1067	0	1079	29	0
1	H7	2190	0	2201	44	0
1	H8	2190	0	2201	36	0
1	H9	2190	0	2201	31	0
1	I5	654	0	667	17	0
1	I6	1655	0	1653	31	0
1	I7	2190	0	2201	49	0
1	I8	2190	0	2201	38	0
1	I9	2063	0	2058	40	0
1	J5	935	0	957	21	0
1	J6	2151	0	2165	52	0
1	J7	2190	0	2201	56	0
1	J8	2190	0	2201	47	0
1	J9	1812	0	1801	38	0
1	K4	596	0	610	15	0
1	K5	1578	0	1576	36	0
1	K6	2190	0	2201	50	0
1	K7	2190	0	2201	61	0
1	K8	2100	0	2093	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K9	1442	0	1431	41	0
1	h0	1827	0	1803	38	0
1	h1	819	0	825	12	0
1	i0	1397	0	1392	15	0
1	j0	989	0	995	18	0
2	L2	1678	0	1607	22	0
2	L3	1768	0	1681	13	0
2	L4	1768	0	1681	14	0
2	L5	1768	0	1681	16	0
2	L6	1444	0	1395	15	0
2	M1	724	0	695	11	0
2	M2	1799	0	1713	15	0
2	M3	1799	0	1713	22	0
2	M4	1799	0	1713	22	0
2	M5	1760	0	1669	14	0
2	N2	1545	0	1493	15	0
2	N3	1767	0	1686	20	0
2	N4	1767	0	1686	14	0
2	N5	1767	0	1686	16	0
2	N6	1464	0	1417	17	0
2	O1	507	0	460	6	0
2	O2	1755	0	1678	15	0
2	O3	1767	0	1686	21	0
2	O4	1767	0	1686	13	0
2	O5	1759	0	1675	18	0
2	P2	1459	0	1410	20	0
2	P3	1750	0	1669	19	0
2	P4	1750	0	1669	18	0
2	P5	1750	0	1669	11	0
2	P6	1463	0	1417	15	0
2	p2	1747	0	1667	13	0
2	p3	1767	0	1686	24	0
2	p4	1759	0	1675	13	0
2	p5	1759	0	1675	23	0
3	Q1	1339	0	1349	19	0
3	Q2	1567	0	1561	16	0
3	Q3	1633	0	1630	26	0
3	Q4	1601	0	1597	26	0
3	R2	1524	0	1498	28	0
3	R3	1677	0	1663	34	0
3	R4	1588	0	1581	25	0
3	R5	1585	0	1576	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S2	1228	0	1216	11	0
3	S3	1556	0	1559	12	0
3	S4	1602	0	1606	21	0
3	S5	1581	0	1582	26	0
3	S6	1569	0	1568	23	0
3	s3	1595	0	1590	22	0
3	s4	1584	0	1578	17	0
3	s5	1604	0	1603	26	0
3	s6	1397	0	1411	9	0
4	T1	2058	0	2024	25	0
4	T2	2141	0	2101	26	0
4	T3	2141	0	2100	45	0
4	T4	2035	0	1979	36	0
4	t1	2150	0	2114	31	0
4	t2	2141	0	2101	46	0
4	t3	2141	0	2101	37	0
4	t4	2125	0	2081	23	0
5	V1	1422	0	1412	24	0
5	V2	1621	0	1602	22	0
5	V3	1613	0	1597	33	0
5	V4	1613	0	1597	26	0
5	V5	1613	0	1597	24	0
5	X1	1484	0	1467	19	0
5	X2	1621	0	1602	35	0
5	X3	1621	0	1602	42	0
5	X4	1621	0	1602	30	0
5	X5	1610	0	1589	27	0
6	Y1	834	0	837	6	0
6	Y2	1844	0	1826	25	0
6	Y3	1876	0	1853	14	0
6	Y4	1872	0	1851	22	0
6	Y5	1876	0	1853	22	0
7	Z1	2173	0	2184	20	0
7	Z2	2173	0	2184	33	0
7	Z3	2162	0	2171	32	0
7	Z4	2173	0	2184	25	0
8	a2	1421	0	1472	12	0
8	a3	1460	0	1506	12	0
8	a4	1460	0	1506	18	0
8	a5	1460	0	1506	16	0
9	c1	867	0	860	9	0
9	c2	882	0	875	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	c3	882	0	875	9	0
10	d2	1993	0	2019	24	0
10	d3	1924	0	1943	16	0
10	d4	1972	0	1988	16	0
11	T1	1	0	0	0	0
11	T2	1	0	0	0	0
11	T3	1	0	0	0	0
11	T4	1	0	0	0	0
11	V1	1	0	0	0	0
11	V2	1	0	0	0	0
11	V3	1	0	0	0	0
11	V4	1	0	0	0	0
11	V5	1	0	0	0	0
11	X1	1	0	0	0	0
11	X2	1	0	0	0	0
11	X3	1	0	0	0	0
11	X4	1	0	0	0	0
11	X5	1	0	0	0	0
11	t1	1	0	0	0	0
11	t2	1	0	0	0	0
11	t3	1	0	0	0	0
11	t4	1	0	0	0	0
12	T1	2	0	0	0	0
12	T2	2	0	0	0	0
12	T3	2	0	0	1	0
12	T4	2	0	0	0	0
12	V1	2	0	0	0	0
12	V2	2	0	0	0	0
12	V3	2	0	0	0	0
12	V4	2	0	0	0	0
12	V5	2	0	0	1	0
12	X1	2	0	0	1	0
12	X2	2	0	0	1	0
12	X3	2	0	0	1	0
12	X4	2	0	0	1	0
12	X5	2	0	0	0	0
12	t1	2	0	0	0	0
12	t2	2	0	0	0	0
12	t3	2	0	0	0	0
12	t4	2	0	0	0	0
All	All	248049	0	245849	3312	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 7.

All (3312) 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)
4:T2:23:LEU:HB3	4:T2:240:LEU:HD11	1.49	0.94
1:H8:257:ILE:HG23	1:I7:277:LEU:HD11	1.50	0.92
5:V2:130:ALA:H	5:V2:183:GLN:HG2	1.37	0.90
1:I6:57:LYS:HE3	1:I7:92:VAL:HG21	1.54	0.90
4:T4:32:ASP:HB3	4:T4:93:LYS:HG2	1.54	0.89
1:B6:14:ARG:HH21	1:B7:231:GLU:HG3	1.37	0.89
1:E2:3:ILE:HD13	1:E3:245:MET:HG2	1.54	0.87
1:A7:105:GLU:HG3	1:K7:203:MET:HE3	1.58	0.86
1:A7:1:MET:HG2	1:A8:245:MET:HE2	1.56	0.86
5:V1:52:GLU:HA	5:V1:100:HIS:HB2	1.57	0.86
1:H7:265:MET:HE3	1:I7:31:SER:HA	1.58	0.85
1:G9:35:ARG:HB3	1:G9:243:THR:HB	1.57	0.85
1:G1:245:MET:HE1	1:G9:280:LEU:HD11	1.57	0.85
1:I7:50:GLU:HG3	1:I8:209:ARG:HH22	1.41	0.85
1:J9:65:ASN:HD21	1:j0:99:ASN:HD21	1.23	0.84
1:D6:38:ARG:HE	1:D7:74:GLN:HE22	1.26	0.83
1:F5:265:MET:HE3	1:G1:30:LEU:HB3	1.61	0.83
1:D3:14:ARG:NH1	1:D4:228:VAL:HA	1.95	0.81
6:Y4:242:GLU:HB3	6:Y4:244:ARG:HH21	1.46	0.81
1:D7:135:LEU:HD12	1:D7:136:LEU:HD22	1.61	0.81
2:p3:74:GLN:HE22	2:p4:236:PRO:HD2	1.47	0.80
1:A5:123:ARG:HH22	1:K5:153:ILE:HG13	1.47	0.80
7:Z1:138:LYS:HE3	9:c1:65:HIS:HA	1.63	0.79
1:D4:65:ASN:HD21	1:D5:99:ASN:HB2	1.47	0.79
4:T4:23:LEU:HD12	4:T4:240:LEU:HD21	1.65	0.79
1:E5:3:ILE:HD12	1:E6:245:MET:HE3	1.63	0.79
1:B7:133:MET:HE2	1:B8:103:SER:HA	1.65	0.79
1:D3:276:VAL:HG13	1:E3:263:THR:HG21	1.64	0.79
1:K9:149:MET:HE1	1:K9:163:VAL:HB	1.65	0.79
5:X3:52:GLU:HG3	5:X3:100:HIS:HB2	1.64	0.79
1:C4:170:ALA:HB1	1:C4:175:LEU:HB2	1.65	0.79
5:V5:52:GLU:HA	5:V5:100:HIS:HB2	1.66	0.78
1:E2:47:ALA:HA	1:E3:206:ASN:HD21	1.48	0.78
1:D7:235:ALA:HB1	1:D7:239:ARG:HH21	1.48	0.77
1:C3:3:ILE:HG21	1:C3:277:LEU:HD21	1.65	0.77
1:D5:38:ARG:HD3	1:D6:74:GLN:HE22	1.49	0.77
5:X3:61:SER:HB2	5:X3:68:THR:HG21	1.67	0.77
1:I9:19:GLN:HG3	1:I9:258:LEU:HD22	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X3:76:ARG:HD2	5:X4:234:GLU:HG3	1.67	0.76
1:B5:12:SER:HB2	1:B5:265:MET:HE1	1.68	0.76
4:t3:71:LEU:HB2	4:t3:100:GLN:HB3	1.67	0.76
8:a4:141:ILE:HB	8:a4:162:ARG:HB2	1.66	0.76
1:C7:16:LEU:HD12	1:C7:19:GLN:HE21	1.50	0.75
1:B7:83:THR:HG21	1:B7:168:MET:HE1	1.68	0.75
1:I6:35:ARG:HB3	1:I6:243:THR:HB	1.66	0.75
5:X2:149:LYS:HB3	5:X2:198:SER:HB3	1.66	0.75
1:B6:133:MET:HE3	1:B7:103:SER:HA	1.69	0.75
4:t1:151:MET:HE2	4:t1:193:VAL:HG13	1.69	0.74
1:H9:136:LEU:HD23	1:H9:168:MET:HE2	1.67	0.74
2:O5:162:LYS:HG2	2:O5:166:LYS:HE2	1.69	0.74
4:t2:45:THR:HG23	4:t2:110:THR:HG23	1.69	0.74
1:K8:57:LYS:HE3	1:K9:92:VAL:HG22	1.70	0.74
1:F4:90:ILE:HD11	1:F4:117:LEU:HB2	1.70	0.74
2:O1:91:GLN:HA	2:O1:94:HIS:CE1	2.22	0.74
3:Q4:64:VAL:HG23	3:Q4:147:GLU:HB3	1.69	0.74
1:I6:40:GLY:HA2	1:I7:213:GLY:HA2	1.69	0.73
1:F6:30:LEU:HD13	1:F6:248:GLU:HG2	1.69	0.73
1:J5:15:VAL:HG21	1:K5:32:SER:HA	1.70	0.73
1:E3:65:ASN:HD21	1:E4:99:ASN:HD21	1.34	0.73
1:A7:51:LYS:HE3	1:A8:206:ASN:HD22	1.54	0.73
5:X3:136:TRP:HD1	5:X3:218:ASP:HB2	1.54	0.72
7:Z2:97:GLN:HA	7:Z2:100:PHE:CZ	2.23	0.72
4:T3:243:VAL:HG12	4:T3:270:LEU:HD22	1.71	0.72
1:D4:257:ILE:HG23	1:E3:277:LEU:HD22	1.71	0.72
10:d4:170:ARG:HE	10:d4:201:THR:HG21	1.53	0.72
2:M2:193:GLU:HA	2:M2:196:ARG:HE	1.52	0.72
5:V3:52:GLU:HA	5:V3:100:HIS:HB2	1.72	0.72
1:B6:266:LEU:HD23	1:B6:270:ASN:HD21	1.54	0.72
1:B8:206:ASN:HA	1:B8:209:ARG:HG2	1.71	0.72
1:C6:44:SER:HA	1:D7:109:MET:HE1	1.72	0.72
1:C6:232:ASN:HD21	1:D6:74:GLN:HG3	1.55	0.72
1:F4:90:ILE:HD12	1:F4:114:VAL:HG23	1.72	0.71
2:L2:262:GLN:HA	2:L2:265:LYS:HE3	1.72	0.71
3:R2:109:ASP:HB2	3:R2:127:ALA:HB2	1.73	0.71
5:V4:176:THR:HG21	6:Y4:72:MET:HE1	1.72	0.71
1:C5:280:LEU:HD21	1:C6:249:THR:HG21	1.72	0.71
4:T4:31:TRP:HE1	4:T4:235:ASP:HA	1.55	0.71
2:M3:91:GLN:HA	2:M3:94:HIS:CE1	2.26	0.71
1:J9:232:ASN:HB3	1:K9:75:THR:HG22	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X3:136:TRP:CD1	5:X3:218:ASP:HB2	2.26	0.71
1:E3:27:MET:HA	1:E3:27:MET:HE2	1.72	0.71
3:s4:133:TYR:HB3	3:s4:154:LYS:HD2	1.71	0.71
5:V1:70:VAL:HG12	5:V1:104:VAL:HG22	1.72	0.71
5:X4:52:GLU:HB3	5:X4:100:HIS:HB2	1.73	0.71
1:K9:56:VAL:HG13	1:K9:230:TYR:HE1	1.56	0.71
1:H7:44:SER:HA	1:I8:109:MET:HE1	1.72	0.70
1:K6:97:SER:HB2	1:K6:110:ILE:HG21	1.73	0.70
1:F6:51:LYS:HE2	1:G2:132:LYS:HD3	1.73	0.70
4:T4:26:ILE:HG21	4:T4:269:MET:HG2	1.72	0.70
4:T2:18:VAL:HG23	4:t2:152:SER:HB3	1.73	0.70
1:B4:280:LEU:HD21	1:B5:249:THR:HG21	1.73	0.70
1:F3:90:ILE:HD11	1:F3:114:VAL:HG22	1.74	0.70
5:X2:148:ALA:HB1	5:X2:196:PHE:HE2	1.55	0.70
1:G8:5:HIS:CG	1:G9:234:GLN:HE22	2.09	0.70
4:t3:258:GLU:HA	4:t3:261:ARG:HH11	1.55	0.70
1:I9:121:ILE:HD13	1:I9:175:LEU:HD13	1.74	0.70
4:t4:147:VAL:HG22	4:t4:209:VAL:HB	1.74	0.70
1:A6:265:MET:HE2	1:B6:31:SER:HB2	1.74	0.70
1:H9:8:ALA:HB1	1:I9:27:MET:HE2	1.74	0.69
5:V4:140:ARG:HB3	5:V5:189:LEU:HD13	1.74	0.69
1:B6:280:LEU:HD21	1:B7:245:MET:HE1	1.74	0.69
1:C4:120:GLU:HA	1:C4:123:ARG:HG2	1.73	0.69
1:I7:36:ILE:HG23	1:I7:41:ASP:HB2	1.74	0.69
1:F5:97:SER:HB2	1:F5:110:ILE:HG21	1.74	0.69
1:J7:65:ASN:HD21	1:J8:99:ASN:HB2	1.58	0.69
5:V3:190:LEU:HD21	5:V3:239:TRP:HE1	1.56	0.69
5:V4:47:ILE:HD13	5:V4:220:GLU:HG2	1.75	0.69
5:V4:95:GLN:HG2	5:V4:99:ASN:HB2	1.75	0.69
4:t3:156:CYS:HB3	4:t3:233:PHE:HB2	1.74	0.69
1:G7:265:MET:HG3	1:H7:31:SER:HA	1.74	0.69
1:I8:170:ALA:HB1	1:I8:175:LEU:HB2	1.75	0.69
4:T1:123:ARG:HB3	4:T1:137:SER:HB3	1.75	0.69
5:V1:50:ASN:HB2	5:V1:52:GLU:OE2	1.93	0.69
1:D5:41:ASP:HA	1:D6:217:ASN:HD21	1.57	0.68
1:I6:57:LYS:HD3	1:I7:88:GLN:HE22	1.58	0.68
1:J6:47:ALA:HB1	1:J7:206:ASN:HD21	1.58	0.68
1:K7:23:VAL:HG22	1:K7:255:ASN:HB3	1.73	0.68
1:K7:56:VAL:HG22	1:K7:233:ILE:HG23	1.73	0.68
1:G1:245:MET:HG3	1:G9:3:ILE:HD11	1.76	0.68
1:E5:250:VAL:HG13	1:F4:6:ASN:HD21	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I8:136:LEU:HB3	1:I8:168:MET:HB2	1.76	0.68
3:R4:187:ASP:HA	3:R4:218:ALA:HB2	1.73	0.68
4:t3:45:THR:HG23	4:t3:110:THR:HG23	1.76	0.68
1:D5:100:GLY:HA2	1:D5:107:ARG:HH22	1.59	0.68
6:Y4:84:LYS:HD2	6:Y4:261:LEU:HD21	1.75	0.68
1:A8:70:MET:HE2	1:A8:216:PHE:HE1	1.59	0.68
2:P4:106:ARG:HD3	3:s5:108:TYR:CD1	2.29	0.68
1:F6:123:ARG:HD3	1:F6:124:ILE:HD13	1.75	0.68
1:J8:46:LEU:HD21	1:J9:209:ARG:HH22	1.57	0.68
3:Q3:44:THR:HA	3:Q3:47:LYS:HE3	1.75	0.68
7:Z2:158:ALA:HA	7:Z2:195:LYS:HE2	1.76	0.68
1:B6:265:MET:SD	1:C6:31:SER:HB2	2.33	0.67
4:t4:80:LYS:HB3	4:t4:92:ALA:HB1	1.76	0.67
1:J6:1:MET:HE2	1:J6:276:VAL:HG11	1.75	0.67
1:J7:14:ARG:HH22	1:K7:37:ASN:HD21	1.42	0.67
1:A8:86:ILE:HD11	1:A8:117:LEU:HD22	1.75	0.67
1:F4:65:ASN:HD21	1:F5:99:ASN:HB2	1.58	0.67
5:X4:52:GLU:CB	5:X4:100:HIS:HB2	2.24	0.67
8:a5:141:ILE:HD11	8:a5:162:ARG:HD2	1.75	0.67
3:R2:56:ASN:ND2	3:R2:179:PRO:HG2	2.10	0.67
8:a2:187:LYS:HD2	8:a3:222:LEU:HB3	1.75	0.67
1:F4:3:ILE:HG13	1:F5:245:MET:HE2	1.76	0.67
2:L2:205:TRP:CD1	2:L2:221:ILE:HG21	2.29	0.67
1:D5:40:GLY:HA2	1:D6:213:GLY:HA2	1.76	0.67
1:K7:3:ILE:HG21	1:K7:277:LEU:HD23	1.77	0.67
5:V2:48:LEU:HD21	5:V2:126:VAL:HG22	1.75	0.67
1:A6:8:ALA:HB1	1:B6:27:MET:HG2	1.77	0.67
1:B8:239:ARG:HH22	1:C8:64:ARG:HA	1.60	0.67
5:V4:131:ARG:HA	5:V4:177:ILE:HB	1.76	0.67
5:V4:139:GLY:HA3	5:V4:165:LEU:HD23	1.77	0.67
5:V5:230:TYR:HB2	5:V5:233:SER:HB2	1.77	0.67
6:Y4:140:GLY:HA2	6:Y4:144:TYR:HB3	1.77	0.67
6:Y4:88:TYR:HB3	6:Y4:128:LEU:HD11	1.76	0.66
1:A6:54:THR:HG22	1:A7:88:GLN:HE22	1.61	0.66
1:A6:265:MET:SD	1:B6:27:MET:HE2	2.35	0.66
1:K4:26:ASN:HA	1:K4:29:THR:HG22	1.76	0.66
2:O5:138:ARG:HD3	2:O5:141:GLU:HG2	1.77	0.66
3:S4:57:GLN:O	3:S4:60:THR:HG22	1.95	0.66
1:C7:64:ARG:HH11	1:C7:64:ARG:HG3	1.61	0.66
1:F2:43:ALA:HB1	1:F3:210:ALA:HB1	1.76	0.66
1:G7:257:ILE:HG23	1:H6:277:LEU:HD22	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V5:131:ARG:HB2	5:V5:177:ILE:HB	1.78	0.66
4:t1:156:CYS:HG	4:t1:188:TRP:CD1	2.13	0.66
1:A8:67:GLU:HA	1:A8:70:MET:HG3	1.77	0.66
1:I7:114:VAL:HG21	1:I7:185:LEU:HD12	1.77	0.66
1:J7:232:ASN:ND2	1:K7:75:THR:HA	2.11	0.66
1:G9:273:PRO:HA	1:G9:276:VAL:HG12	1.76	0.66
1:A5:265:MET:HG3	1:B5:30:LEU:HD22	1.78	0.66
1:J7:12:SER:HB3	1:J7:265:MET:HE1	1.78	0.66
1:G9:97:SER:HB2	1:G9:110:ILE:HG21	1.78	0.66
1:H6:38:ARG:HH22	1:H7:212:LEU:HB3	1.60	0.66
6:Y4:130:PRO:HG3	6:Y4:183:LEU:HD23	1.76	0.66
1:D5:65:ASN:HD21	1:D6:99:ASN:ND2	1.94	0.65
1:D6:166:ALA:HB3	1:D6:208:GLN:HE22	1.61	0.65
1:H8:265:MET:HE1	1:I8:27:MET:HE3	1.78	0.65
5:V1:131:ARG:HH22	5:V1:179:GLY:HA2	1.61	0.65
2:P2:174:THR:HG22	2:P2:205:TRP:HE1	1.61	0.65
5:V5:183:GLN:HE22	5:V5:194:LEU:HB2	1.62	0.65
1:B6:43:ALA:HB1	1:B7:210:ALA:HA	1.78	0.65
2:N5:235:TYR:HB3	2:N5:236:PRO:HD3	1.78	0.65
2:P2:250:ASN:HA	2:P2:253:LYS:HE2	1.79	0.65
3:Q3:157:SER:HB2	3:Q3:174:VAL:HG22	1.78	0.65
2:p3:241:LEU:HD23	2:p3:273:HIS:HE1	1.61	0.65
10:d3:166:ASN:HD21	10:d3:169:ILE:HG12	1.61	0.65
2:p3:241:LEU:HD23	2:p3:273:HIS:CE1	2.32	0.65
3:R3:174:VAL:HG12	3:R3:191:VAL:HG13	1.77	0.65
1:A5:250:VAL:HG23	1:B4:6:ASN:HD21	1.60	0.65
1:C7:264:ALA:HB2	1:D6:281:ARG:HE	1.62	0.65
4:t1:156:CYS:HB2	4:t1:233:PHE:HB2	1.79	0.65
5:V5:230:TYR:HE1	6:Y5:62:ASP:HA	1.62	0.65
7:Z1:97:GLN:HE22	7:Z2:138:LYS:HE2	1.60	0.65
1:I5:12:SER:HB3	1:I5:265:MET:HE1	1.78	0.65
2:M3:185:ASN:HD21	2:M3:188:LEU:HD12	1.62	0.65
4:t1:215:LYS:HG3	4:t1:216:GLN:H	1.62	0.65
1:A5:253:THR:HG21	1:B4:270:ASN:HB2	1.79	0.65
1:H7:51:LYS:HE3	1:I7:132:LYS:HE3	1.79	0.65
1:H7:170:ALA:HB1	1:H7:175:LEU:HB2	1.79	0.65
1:J9:65:ASN:ND2	1:j0:99:ASN:HD21	1.93	0.65
1:I5:1:MET:HG3	1:I5:276:VAL:HG11	1.77	0.65
2:O5:94:HIS:ND1	2:O5:95:GLN:HG2	2.12	0.65
1:A4:15:VAL:HG11	1:B4:32:SER:HA	1.77	0.64
1:D5:1:MET:HG3	1:D5:276:VAL:HG11	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a4:176:VAL:HG13	8:a4:185:ARG:HD2	1.79	0.64
1:D5:97:SER:HB2	1:D5:110:ILE:HG21	1.78	0.64
1:K7:215:TYR:O	1:K7:218:ARG:HG2	1.97	0.64
4:T1:29:GLU:HB3	4:T1:237:LEU:HB3	1.79	0.64
1:E6:97:SER:HB2	1:E6:110:ILE:HG21	1.78	0.64
3:Q3:234:LYS:HD2	3:Q3:238:ILE:HD12	1.80	0.64
5:V3:135:ILE:HD12	5:V3:219:LEU:HD13	1.79	0.64
1:C7:23:VAL:HG22	1:C7:27:MET:HE3	1.79	0.64
4:T4:152:SER:HA	4:T4:191:LEU:O	1.97	0.64
1:K7:34:MET:HE3	1:K7:241:ARG:HE	1.62	0.64
3:S4:234:LYS:HA	3:S4:238:ILE:HD12	1.78	0.64
4:T4:152:SER:HB3	4:t4:18:VAL:HG13	1.79	0.64
1:B4:239:ARG:NH2	1:C4:68:ASP:HA	2.12	0.64
3:S5:70:VAL:HG13	3:S5:255:ASN:HD21	1.62	0.64
1:C5:218:ARG:HE	1:D5:120:GLU:HB2	1.63	0.64
4:T2:23:LEU:HD13	4:T2:240:LEU:HD21	1.79	0.64
5:V2:106:THR:HG21	5:V2:116:VAL:HG21	1.80	0.64
1:A8:160:ARG:HH22	1:A9:189:GLU:HG3	1.61	0.64
1:H9:97:SER:HB2	1:H9:110:ILE:HG21	1.78	0.64
5:X3:54:ALA:HB1	5:X3:102:LEU:HD13	1.79	0.64
1:j0:97:SER:HB2	1:j0:110:ILE:HG21	1.79	0.64
1:B7:157:GLN:HE22	1:B8:195:ILE:HG22	1.63	0.63
3:S5:216:ILE:HG23	3:S5:219:GLY:H	1.61	0.63
4:T4:32:ASP:HB3	4:T4:93:LYS:CG	2.28	0.63
1:B5:97:SER:HB2	1:B5:185:LEU:HD12	1.79	0.63
2:P6:238:HIS:HA	2:P6:273:HIS:HE1	1.63	0.63
3:Q3:64:VAL:HG23	3:Q3:147:GLU:HB3	1.80	0.63
1:B8:109:MET:O	1:B8:112:VAL:HG12	1.99	0.63
1:E7:118:VAL:HA	1:E7:121:ILE:HD12	1.81	0.63
5:X3:80:ARG:HD2	5:X3:85:GLU:HA	1.79	0.63
5:X4:75:GLN:HE22	5:X4:79:ILE:HD11	1.64	0.63
1:C4:19:GLN:HE22	1:C4:259:VAL:HG22	1.63	0.63
5:X5:119:PHE:CD1	5:X5:120:PRO:HD2	2.33	0.63
8:a2:50:LEU:HB2	8:a2:189:VAL:HG11	1.79	0.63
1:K5:140:PHE:HD2	1:K5:165:ILE:HD12	1.64	0.63
3:S3:133:TYR:HB2	3:S3:153:ASN:HB3	1.80	0.63
1:J7:33:GLY:O	1:J7:243:THR:HG23	1.99	0.63
1:K9:62:ALA:O	1:K9:66:THR:HG23	1.99	0.63
5:V2:80:ARG:HG2	5:V2:88:VAL:HG12	1.81	0.63
2:N3:162:LYS:HG2	2:N3:166:LYS:NZ	2.14	0.63
9:c1:82:MET:HE1	9:c1:97:PHE:HB2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:277:LEU:HD22	1:K6:257:ILE:HG23	1.80	0.62
1:A7:114:VAL:HG21	1:A7:185:LEU:HD12	1.80	0.62
1:C7:170:ALA:HB1	1:C7:175:LEU:HB2	1.81	0.62
1:I9:247:GLU:HB2	1:J8:13:HIS:CE1	2.34	0.62
10:d2:136:ILE:HG12	10:d2:168:TYR:HE2	1.64	0.62
1:j0:136:LEU:HB3	1:j0:168:MET:HB3	1.81	0.62
1:D5:38:ARG:HD3	1:D6:74:GLN:NE2	2.14	0.62
1:H9:253:THR:O	1:H9:257:ILE:HD12	1.99	0.62
1:I7:87:ILE:O	1:I7:90:ILE:HG22	1.99	0.62
1:J6:257:ILE:HG12	1:K5:277:LEU:HD23	1.80	0.62
1:K6:55:GLN:HE22	1:K6:233:ILE:HG21	1.63	0.62
5:V1:130:ALA:HB2	5:V1:223:ALA:HB2	1.80	0.62
4:t3:44:VAL:HG21	4:t3:72:ARG:CZ	2.28	0.62
1:B4:268:GLN:HE22	1:C4:27:MET:HE1	1.64	0.62
1:K7:27:MET:HE1	1:K7:30:LEU:HD23	1.82	0.62
5:V5:132:GLN:HB3	5:V5:222:ARG:HB3	1.81	0.62
2:O2:162:LYS:HE3	2:O2:166:LYS:HD2	1.81	0.62
3:R3:128:LYS:HB3	3:R3:159:ILE:HD12	1.79	0.62
7:Z3:89:LYS:HZ2	7:Z4:159:ILE:HD12	1.64	0.62
1:A7:107:ARG:HA	1:A7:110:ILE:HG22	1.82	0.62
1:B8:97:SER:HB2	1:B8:110:ILE:HG21	1.82	0.62
1:C4:276:VAL:HG13	1:D4:263:THR:HG21	1.82	0.62
1:D7:53:ARG:HG3	1:D7:53:ARG:HH11	1.64	0.62
7:Z2:129:TYR:O	7:Z2:133:THR:HG23	2.00	0.62
1:E3:157:GLN:HG3	1:E3:158:HIS:CD2	2.34	0.62
5:V4:132:GLN:HB3	5:V4:222:ARG:HB3	1.81	0.62
1:E3:56:VAL:HG22	1:E3:233:ILE:HG23	1.80	0.62
2:O1:94:HIS:HD2	2:O1:95:GLN:HG3	1.64	0.62
1:K7:27:MET:HA	1:K7:27:MET:HE3	1.82	0.62
1:D4:50:GLU:CD	1:D5:84:ASN:HD21	2.08	0.62
1:K7:87:ILE:HA	1:K7:90:ILE:HG22	1.79	0.62
5:X5:129:LYS:HE2	5:X5:188:ALA:HB1	1.82	0.62
1:D6:7:LEU:HD11	1:D7:235:ALA:HA	1.82	0.61
1:F4:14:ARG:HD2	1:F5:228:VAL:HG22	1.82	0.61
1:G1:43:ALA:HB1	1:G2:210:ALA:HA	1.81	0.61
1:K5:56:VAL:HG13	1:K5:230:TYR:HE1	1.64	0.61
3:R5:59:LEU:HA	3:R5:62:HIS:CD2	2.35	0.61
5:V3:70:VAL:HG22	5:V3:104:VAL:HA	1.82	0.61
1:B5:67:GLU:HA	1:B5:70:MET:HG2	1.81	0.61
1:h0:168:MET:O	1:h0:168:MET:HG2	2.00	0.61
1:C7:179:ASP:HA	5:V4:180:PHE:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G9:227:MET:HE2	1:G9:227:MET:HA	1.80	0.61
2:P2:245:TYR:HB3	2:P2:270:LYS:HD3	1.80	0.61
3:Q4:55:LEU:HD21	3:Q4:241:LEU:HB3	1.81	0.61
3:Q4:63:THR:HG21	3:Q4:150:ARG:HG2	1.81	0.61
3:R3:104:ARG:HE	3:R3:131:GLU:HG2	1.64	0.61
5:X3:118:VAL:O	5:X3:198:SER:HB2	2.00	0.61
1:A9:120:GLU:HG3	1:K9:218:ARG:HG2	1.82	0.61
1:B7:100:GLY:HA2	1:B7:107:ARG:HH22	1.66	0.61
1:D7:159:GLN:HB2	1:E7:127:GLN:HE21	1.64	0.61
1:H6:257:ILE:HD13	1:I5:273:PRO:HB2	1.82	0.61
1:B5:218:ARG:HG3	1:C5:120:GLU:CD	2.26	0.61
1:J7:3:ILE:HD11	1:J7:277:LEU:HD21	1.81	0.61
1:A5:35:ARG:HG3	1:A5:36:ILE:HG13	1.82	0.61
1:D4:65:ASN:ND2	1:D5:99:ASN:HB2	2.15	0.61
1:E3:63:GLU:HG2	1:E3:227:MET:HE3	1.83	0.61
1:J7:43:ALA:HB1	1:J8:210:ALA:HA	1.83	0.61
1:I9:156:ASN:H	1:I9:159:GLN:NE2	1.97	0.61
1:j0:100:GLY:HA2	1:j0:107:ARG:HH21	1.66	0.61
4:t4:178:LEU:HD13	4:t4:193:VAL:HG11	1.83	0.61
1:H7:54:THR:HA	1:H8:88:GLN:HE22	1.65	0.61
1:J8:159:GLN:HG2	1:K8:127:GLN:HB3	1.83	0.61
4:T3:23:LEU:HD13	4:T3:240:LEU:HD11	1.83	0.61
5:V1:62:THR:HG23	5:V1:63:THR:HG22	1.81	0.61
7:Z3:89:LYS:HB3	7:Z4:155:VAL:HG11	1.82	0.61
1:C6:232:ASN:ND2	1:D6:74:GLN:HG3	2.16	0.60
1:E3:227:MET:HE2	1:E3:227:MET:HA	1.83	0.60
1:I9:177:LYS:HD3	1:I9:179:ASP:H	1.66	0.60
2:N5:91:GLN:HA	2:N5:94:HIS:CE1	2.36	0.60
1:A6:136:LEU:HB3	1:A6:168:MET:HB3	1.82	0.60
2:O5:278:THR:HG21	2:O5:292:ILE:HG13	1.84	0.60
3:Q2:134:PHE:CZ	3:Q2:150:ARG:HD2	2.37	0.60
1:B4:61:GLN:NE2	1:B5:96:GLN:HE21	1.99	0.60
1:D6:272:ARG:HB3	1:D6:273:PRO:HD3	1.82	0.60
1:H9:1:MET:HE3	1:H9:276:VAL:HG21	1.82	0.60
5:X4:147:PHE:HE1	5:X4:161:ARG:HG3	1.66	0.60
7:Z1:258:ALA:HA	7:Z1:261:ILE:HD12	1.82	0.60
1:B5:43:ALA:HB1	1:B6:210:ALA:HA	1.82	0.60
2:L5:215:LEU:HD23	2:L5:216:PRO:HD3	1.82	0.60
1:D5:65:ASN:HD21	1:D6:99:ASN:HD21	1.47	0.60
1:J6:280:LEU:HD12	1:J7:249:THR:HG21	1.83	0.60
5:X2:49:GLU:HG2	5:X2:57:TRP:HE1	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p4:84:LYS:H	2:p5:210:TYR:HE1	1.50	0.60
4:t2:23:LEU:HB3	4:t2:240:LEU:HD11	1.84	0.60
1:D4:59:LEU:HD22	1:D4:230:TYR:HB2	1.84	0.60
1:G6:3:ILE:HD11	1:G7:245:MET:HB2	1.83	0.60
1:G7:52:MET:HE1	1:H7:130:PHE:CE1	2.37	0.60
2:P3:83:PHE:CE2	2:P4:239:LYS:HE2	2.36	0.60
1:h1:97:SER:HB2	1:h1:110:ILE:HG21	1.84	0.60
1:G9:276:VAL:HG23	1:H9:263:THR:HG21	1.83	0.60
2:p2:76:ALA:HA	2:p2:79:LYS:HB2	1.83	0.60
1:C6:118:VAL:HA	1:C6:121:ILE:HD12	1.84	0.60
1:E2:16:LEU:HD11	1:E2:263:THR:HG22	1.84	0.60
1:J6:23:VAL:HG22	1:J6:255:ASN:HB3	1.84	0.60
3:R2:247:LEU:O	3:R2:251:ILE:HG12	2.02	0.60
4:T2:145:PRO:HG2	4:T2:270:LEU:HD21	1.83	0.60
2:p4:88:LYS:HA	2:p4:91:GLN:HG2	1.83	0.60
5:X1:52:GLU:HA	5:X1:100:HIS:HB2	1.84	0.60
1:B6:265:MET:CE	1:C6:27:MET:HG3	2.32	0.59
1:F4:130:PHE:HB2	1:F4:135:LEU:HD11	1.82	0.59
2:N3:235:TYR:HB3	2:N3:236:PRO:HD3	1.83	0.59
7:Z2:88:LEU:HD21	7:Z2:117:GLY:HA3	1.82	0.59
1:A5:3:ILE:O	1:K6:254:LYS:HD2	2.01	0.59
1:B7:154:GLY:HA3	1:B7:159:GLN:CD	2.27	0.59
1:F5:254:LYS:HE2	1:G9:4:ASN:O	2.01	0.59
1:G6:265:MET:HE2	1:H6:30:LEU:HD22	1.84	0.59
1:I7:97:SER:HB3	1:I7:110:ILE:HG21	1.84	0.59
6:Y2:154:ARG:HD2	6:Y2:161:VAL:HG21	1.84	0.59
3:s3:67:LYS:HB2	3:s3:144:PRO:HB3	1.82	0.59
1:B3:3:ILE:HG21	1:B4:245:MET:HE3	1.82	0.59
1:J9:97:SER:HB2	1:J9:110:ILE:HG21	1.85	0.59
1:C4:20:ASN:HA	1:C4:23:VAL:HG12	1.84	0.59
1:E4:157:GLN:HG3	1:E4:158:HIS:CD2	2.38	0.59
2:M5:205:TRP:HE1	2:M5:221:ILE:HG13	1.67	0.59
2:O5:91:GLN:HA	2:O5:94:HIS:CD2	2.38	0.59
4:T1:21:LEU:HD11	4:t1:194:TYR:HE1	1.66	0.59
4:t3:153:VAL:HG22	4:t3:237:LEU:HD13	1.83	0.59
4:t4:131:ASN:HB3	4:t4:133:GLN:OE1	2.03	0.59
1:J6:254:LYS:HG3	1:K5:4:ASN:HA	1.84	0.59
5:X2:123:GLU:HB2	5:X2:195:HIS:HB3	1.83	0.59
6:Y5:207:THR:HG23	6:Y5:209:GLU:H	1.67	0.59
1:B8:161:GLU:HB2	1:C8:123:ARG:HH12	1.67	0.59
1:I8:114:VAL:HG21	1:I8:185:LEU:HD22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S4:171:ILE:HG21	3:S4:232:PHE:HE2	1.67	0.59
6:Y2:88:TYR:CE1	6:Y2:182:ALA:HB2	2.38	0.59
7:Z3:49:LYS:HZ3	7:Z3:79:GLY:N	2.01	0.59
2:P6:162:LYS:HG2	2:P6:166:LYS:HE3	1.84	0.59
3:R3:52:ILE:HD12	3:R3:233:LYS:HE3	1.85	0.59
4:T1:155:VAL:HG11	4:T1:183:LEU:HD13	1.85	0.59
8:a5:124:PHE:HB2	8:a5:144:LEU:HB3	1.84	0.59
10:d2:186:VAL:HG23	10:d2:213:MET:HE3	1.83	0.59
1:A5:16:LEU:HD11	1:A5:263:THR:HG22	1.85	0.59
1:A6:203:MET:O	1:A6:207:LYS:HG2	2.03	0.59
1:B6:67:GLU:HG3	1:B6:70:MET:HE2	1.84	0.59
3:S6:108:TYR:HA	3:S6:127:ALA:HB3	1.83	0.59
1:i0:187:THR:HG23	1:i0:189:GLU:HG2	1.85	0.59
1:A6:257:ILE:HG21	1:B5:3:ILE:HG21	1.85	0.59
1:B7:48:VAL:HG22	1:B7:52:MET:HE1	1.85	0.59
1:B7:239:ARG:HH11	1:C7:64:ARG:HD2	1.67	0.59
1:C5:44:SER:HA	1:D6:109:MET:HE1	1.85	0.59
3:S6:174:VAL:HG22	3:S6:191:VAL:HG12	1.85	0.59
4:T3:20:GLY:HA2	4:T3:244:PHE:HB2	1.85	0.59
3:s5:236:PHE:O	3:s5:240:HIS:HB2	2.03	0.59
1:I7:1:MET:HE2	1:I7:276:VAL:HG21	1.85	0.59
1:A6:114:VAL:HG11	1:A6:185:LEU:HD23	1.85	0.58
1:F3:87:ILE:HA	1:F3:90:ILE:HG22	1.84	0.58
1:F4:8:ALA:HB1	1:G9:27:MET:HE2	1.83	0.58
1:F5:157:GLN:HE22	1:F6:195:ILE:HG22	1.69	0.58
3:Q2:192:PHE:HB3	3:Q2:194:GLN:HE22	1.68	0.58
5:V1:123:GLU:HA	5:V1:197:VAL:HG13	1.85	0.58
7:Z4:157:ILE:HA	7:Z4:161:TRP:CD1	2.38	0.58
1:A4:276:VAL:HG23	1:A4:277:LEU:HD22	1.85	0.58
1:A6:52:MET:HE2	1:A6:52:MET:HA	1.84	0.58
1:D4:244:ASP:HB3	1:D4:247:GLU:HG2	1.84	0.58
1:H9:16:LEU:HD13	1:H9:262:GLY:HA3	1.85	0.58
2:L3:205:TRP:CD1	2:L3:221:ILE:HG21	2.38	0.58
3:R4:156:LYS:HG3	3:R4:175:MET:HG2	1.85	0.58
5:X1:56:ASP:HB3	5:X1:121:PRO:HG3	1.84	0.58
1:h0:173:LEU:HD13	1:h0:205:ILE:HD11	1.85	0.58
2:p4:131:LYS:O	2:p4:135:GLU:HG2	2.03	0.58
1:D4:33:GLY:O	1:D4:243:THR:HG22	2.03	0.58
1:K6:5:HIS:NE2	1:K7:238:SER:HB3	2.19	0.58
2:P6:245:TYR:HA	2:P6:248:GLU:HG2	1.86	0.58
9:c2:92:THR:HG23	9:c2:103:PHE:HE1	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:51:LYS:HE3	1:A8:206:ASN:ND2	2.19	0.58
1:A8:245:MET:HG3	1:A8:246:ALA:N	2.17	0.58
1:B8:71:SER:HA	1:B8:74:GLN:HG2	1.85	0.58
1:C7:232:ASN:HD21	1:D7:74:GLN:C	2.11	0.58
1:J8:47:ALA:HB3	1:K9:109:MET:HE1	1.86	0.58
1:B4:265:MET:HG3	1:C4:30:LEU:HD11	1.86	0.58
5:X5:183:GLN:HE22	5:X5:194:LEU:HD13	1.69	0.58
4:t2:153:VAL:HG22	4:t2:237:LEU:HD23	1.85	0.58
4:t3:80:LYS:HB3	4:t3:92:ALA:HB1	1.85	0.58
1:A5:91:ARG:HA	1:A5:198:LEU:HD13	1.85	0.58
1:B7:100:GLY:HA2	1:B7:107:ARG:NH2	2.18	0.58
1:K7:50:GLU:HG3	1:K8:84:ASN:HD21	1.67	0.58
3:R4:108:TYR:HD1	3:R4:127:ALA:H	1.49	0.58
5:V5:226:SER:O	5:V5:229:LYS:HG2	2.04	0.58
4:t2:43:GLU:HG3	4:t2:61:TYR:CZ	2.39	0.58
1:J6:86:ILE:HG23	1:J6:117:LEU:HD12	1.85	0.58
2:P6:142:LYS:HE2	2:p5:214:ASN:HA	1.86	0.58
5:V4:50:ASN:CG	5:V4:52:GLU:HB2	2.29	0.58
5:X5:101:ILE:HD12	5:X5:215:TYR:HB3	1.84	0.58
10:d4:67:LEU:HD22	10:d4:91:VAL:HG13	1.84	0.58
1:A7:7:LEU:HD13	1:A8:235:ALA:HB2	1.84	0.58
1:D6:166:ALA:HB3	1:D6:208:GLN:NE2	2.17	0.58
1:G6:1:MET:HE1	1:G6:272:ARG:HH21	1.69	0.58
2:L4:103:ASN:HD21	8:a4:98:MET:HE2	1.69	0.58
2:L4:215:LEU:HG	2:L4:244:CYS:HA	1.85	0.58
1:h0:57:LYS:HE3	1:h1:88:GLN:HE22	1.68	0.58
3:s6:61:ARG:O	3:s6:64:VAL:HG22	2.04	0.58
4:t2:164:LEU:HD11	4:t2:217:PHE:HB3	1.86	0.58
1:B6:65:ASN:HD21	1:B7:99:ASN:HB2	1.68	0.58
1:I7:91:ARG:HD3	1:I7:198:LEU:HD11	1.85	0.58
2:N2:75:GLU:C	2:N2:77:LEU:H	2.10	0.58
4:T2:4:ILE:HD11	4:t2:194:TYR:HE1	1.69	0.58
1:B6:2:ILE:HD13	1:B7:238:SER:HB3	1.85	0.57
3:Q2:187:ASP:HA	3:Q2:218:ALA:HB2	1.84	0.57
5:X2:52:GLU:HA	5:X2:100:HIS:HB2	1.84	0.57
1:h0:47:ALA:O	1:h0:51:LYS:HG2	2.03	0.57
1:i0:228:VAL:O	1:i0:231:GLU:HG3	2.03	0.57
4:t3:46:THR:HB	4:t3:109:VAL:HG13	1.85	0.57
1:A9:115:SER:HB2	1:A9:182:LEU:HD13	1.85	0.57
1:B7:118:VAL:HA	1:B7:121:ILE:HG22	1.86	0.57
1:C6:12:SER:HB2	1:C6:265:MET:HE1	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F3:257:ILE:HG12	1:G7:277:LEU:HD12	1.85	0.57
1:J7:100:GLY:HA2	1:J7:107:ARG:NH2	2.18	0.57
1:K6:153:ILE:HD13	1:K6:161:GLU:HG3	1.87	0.57
2:L4:155:ASP:HA	2:L4:158:VAL:HG12	1.84	0.57
5:X5:52:GLU:HA	5:X5:100:HIS:HB3	1.85	0.57
1:h0:65:ASN:HD21	1:h1:99:ASN:HB2	1.69	0.57
1:A5:51:LYS:NZ	1:B5:132:LYS:HG3	2.20	0.57
1:I9:154:GLY:HA3	1:I9:159:GLN:HE21	1.69	0.57
1:B5:218:ARG:HG3	1:C5:120:GLU:OE1	2.05	0.57
1:K9:177:LYS:HG2	1:K9:179:ASP:H	1.69	0.57
2:N3:162:LYS:HG2	2:N3:166:LYS:HZ2	1.67	0.57
2:P2:215:LEU:HD21	2:P2:244:CYS:HA	1.86	0.57
5:X4:149:LYS:HB3	5:X4:197:VAL:HB	1.85	0.57
6:Y5:75:MET:HB2	6:Y5:233:THR:OG1	2.04	0.57
1:A5:133:MET:HE1	1:A5:149:MET:HE1	1.87	0.57
1:A6:4:ASN:O	1:K7:254:LYS:HD2	2.04	0.57
1:K8:173:LEU:HG	1:K8:175:LEU:HD13	1.85	0.57
3:Q4:250:LYS:HE3	3:Q4:254:TYR:CZ	2.39	0.57
3:R2:134:PHE:HB3	3:R2:150:ARG:HH21	1.69	0.57
5:X3:139:GLY:O	5:X3:168:PHE:HA	2.04	0.57
7:Z1:138:LYS:HD2	9:c1:64:HIS:CE1	2.40	0.57
1:K9:106:ASP:O	1:K9:110:ILE:HD12	2.04	0.57
3:S5:94:ASN:HB3	3:S5:97:ASP:HB2	1.86	0.57
4:T4:31:TRP:NE1	4:T4:235:ASP:HA	2.20	0.57
5:V2:78:LEU:HD21	5:V2:94:ASP:HB2	1.86	0.57
6:Y3:139:TRP:CE2	6:Y3:166:PRO:HD3	2.39	0.57
1:J7:1:MET:HG2	1:J7:276:VAL:HG11	1.87	0.57
1:J7:3:ILE:HD13	1:J8:245:MET:SD	2.44	0.57
3:R3:108:TYR:HA	3:R3:127:ALA:HB3	1.86	0.57
1:A7:4:ASN:HD21	1:A8:242:ASP:CG	2.12	0.57
1:C5:52:MET:HE3	1:C5:237:GLU:HA	1.85	0.57
1:C6:130:PHE:HB2	1:C6:135:LEU:HD11	1.85	0.57
1:E5:246:ALA:HB1	1:F4:13:HIS:HE1	1.69	0.57
1:K4:272:ARG:O	1:K4:276:VAL:HG23	2.05	0.57
7:Z3:115:GLN:O	7:Z3:119:GLU:HG3	2.05	0.57
1:D7:53:ARG:O	1:D7:56:VAL:HG12	2.04	0.57
1:F5:161:GLU:HG3	1:F5:218:ARG:NH2	2.20	0.57
1:H6:70:MET:HG2	1:H6:219:LEU:HB3	1.86	0.57
2:L2:220:PRO:HA	2:L2:223:GLU:HG2	1.87	0.57
1:D3:67:GLU:HA	1:D3:70:MET:HG2	1.87	0.57
1:E3:83:THR:HA	1:E3:86:ILE:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N2:179:HIS:O	2:N2:182:GLU:HG2	2.04	0.57
3:s6:141:ASP:HB3	3:s6:146:THR:HG21	1.87	0.57
1:F5:65:ASN:ND2	1:F6:99:ASN:HD21	2.03	0.56
1:G8:265:MET:HE3	1:H8:30:LEU:HD22	1.87	0.56
1:G9:51:LYS:HE2	1:H9:132:LYS:HD3	1.87	0.56
1:I9:207:LYS:HA	1:J9:109:MET:HE2	1.87	0.56
2:L2:166:LYS:HE2	2:L2:211:ASP:HB3	1.87	0.56
2:O4:75:GLU:HG2	2:O4:76:ALA:H	1.69	0.56
3:Q2:133:TYR:HB2	3:Q2:154:LYS:HG2	1.85	0.56
3:R4:106:GLU:HB3	3:R4:108:TYR:CE2	2.40	0.56
5:X3:150:LEU:HD13	5:X3:194:LEU:HD21	1.87	0.56
5:X4:230:TYR:HB3	5:X4:231:PRO:HD2	1.86	0.56
5:X5:149:LYS:O	5:X5:197:VAL:HB	2.05	0.56
6:Y5:183:LEU:HD21	6:Y5:226:ILE:HD11	1.86	0.56
1:F4:206:ASN:HB3	1:G9:109:MET:HE1	1.87	0.56
1:F5:280:LEU:HD11	1:G1:266:LEU:HD22	1.87	0.56
2:M1:75:GLU:C	2:M1:77:LEU:H	2.13	0.56
5:X3:179:GLY:HA3	4:t2:104:PRO:HB2	1.86	0.56
1:A6:3:ILE:HG13	1:A6:4:ASN:H	1.70	0.56
1:A7:54:THR:HG22	1:A8:88:GLN:NE2	2.19	0.56
1:A7:277:LEU:HA	1:A7:280:LEU:HG	1.87	0.56
1:C7:36:ILE:HG21	1:C7:46:LEU:HD13	1.88	0.56
1:D4:117:LEU:O	1:D4:121:ILE:HD12	2.06	0.56
1:E7:87:ILE:HA	1:E7:90:ILE:HG22	1.86	0.56
1:G7:43:ALA:HB1	1:G8:210:ALA:HA	1.87	0.56
1:I6:40:GLY:HA2	1:I7:213:GLY:CA	2.34	0.56
3:S5:141:ASP:HB3	3:S5:146:THR:HG23	1.86	0.56
5:X5:149:LYS:HD2	5:X5:197:VAL:HG11	1.87	0.56
2:p3:276:ARG:O	2:p3:279:GLU:HG2	2.05	0.56
4:t2:112:ARG:HG2	4:t2:216:GLN:HB3	1.86	0.56
1:A6:48:VAL:HG13	1:B6:131:ASN:HD21	1.71	0.56
1:B4:49:SER:HB2	1:B4:241:ARG:HG2	1.87	0.56
1:C5:276:VAL:HG13	1:D5:263:THR:HG21	1.86	0.56
1:E3:39:ALA:HB2	1:E3:46:LEU:HD22	1.87	0.56
1:H9:247:GLU:HG2	1:I9:60:ARG:HH22	1.70	0.56
1:J5:254:LYS:HE3	1:K4:4:ASN:O	2.06	0.56
2:N6:199:SER:O	2:N6:203:ARG:HG2	2.06	0.56
1:A8:225:GLY:HA2	1:B8:82:GLU:HG3	1.88	0.56
2:O3:245:TYR:CE1	2:O3:269:LYS:HE3	2.39	0.56
5:X3:49:GLU:HG2	5:X3:219:LEU:HB3	1.88	0.56
1:B8:215:TYR:O	1:B8:218:ARG:HG2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H9:36:ILE:HD12	1:H9:46:LEU:HA	1.87	0.56
2:N6:173:PHE:CZ	2:N6:204:SER:HB2	2.41	0.56
5:X3:136:TRP:NE1	5:X3:172:LYS:HD3	2.20	0.56
4:t1:34:PRO:HB2	4:t1:39:PRO:HA	1.88	0.56
1:F6:100:GLY:HA2	1:F6:107:ARG:NH2	2.21	0.56
1:I7:105:GLU:O	1:I7:109:MET:HG2	2.06	0.56
1:I8:3:ILE:HD12	1:I9:245:MET:HE2	1.88	0.56
5:V2:149:LYS:HB3	5:V2:198:SER:HB3	1.88	0.56
8:a4:159:LEU:HD21	8:a5:221:THR:HB	1.87	0.56
8:a5:104:VAL:HB	8:a5:123:VAL:HG22	1.88	0.56
1:B8:111:GLN:HG2	1:B8:185:LEU:HB2	1.88	0.56
1:B8:177:LYS:HE3	1:B8:179:ASP:HB3	1.88	0.56
1:C7:16:LEU:HD23	1:C7:20:ASN:HD21	1.71	0.56
1:E3:65:ASN:HD21	1:E4:99:ASN:ND2	2.00	0.56
1:F6:166:ALA:N	1:F6:208:GLN:HE22	2.04	0.56
1:H6:35:ARG:HD2	1:H6:35:ARG:O	2.05	0.56
1:J5:50:GLU:O	1:J5:54:THR:HG23	2.06	0.56
3:R3:79:LEU:HD21	3:R3:103:ILE:HD11	1.87	0.56
4:T1:23:LEU:HB3	4:T1:240:LEU:HG	1.88	0.56
1:H9:1:MET:HG2	1:H9:276:VAL:HG11	1.87	0.56
1:K9:82:GLU:O	1:K9:86:ILE:HD12	2.06	0.56
2:N4:75:GLU:C	2:N4:77:LEU:H	2.14	0.56
7:Z4:42:GLU:HB3	7:Z4:43:PRO:HD3	1.87	0.56
1:C7:110:ILE:HA	1:C7:113:GLU:OE2	2.05	0.55
1:I6:51:LYS:NZ	1:J6:131:ASN:HA	2.20	0.55
3:S4:55:LEU:O	3:S4:59:LEU:HG	2.06	0.55
3:S6:132:ILE:HG23	3:S6:152:ILE:HD11	1.87	0.55
5:X4:132:GLN:HE21	5:X4:222:ARG:HB2	1.71	0.55
1:F4:247:GLU:HG2	1:G8:13:HIS:NE2	2.21	0.55
1:J5:43:ALA:HB1	1:J6:210:ALA:HA	1.88	0.55
1:J6:15:VAL:HG21	1:K6:32:SER:HA	1.89	0.55
2:L2:75:GLU:C	2:L2:77:LEU:H	2.15	0.55
2:L2:183:ILE:HD11	2:L2:194:PHE:CE1	2.42	0.55
3:Q4:44:THR:HA	3:Q4:47:LYS:HG2	1.88	0.55
3:R2:76:ARG:HG2	3:R2:108:TYR:HB2	1.88	0.55
8:a3:64:ARG:HH12	8:a3:200:ILE:HG12	1.71	0.55
1:A5:192:ASN:HA	1:A5:195:ILE:HG12	1.86	0.55
1:A8:73:ILE:HG21	1:A8:216:PHE:HB2	1.88	0.55
1:C8:84:ASN:O	1:C8:88:GLN:HG3	2.05	0.55
1:E5:59:LEU:HD11	1:E5:233:ILE:HD12	1.88	0.55
1:I5:18:PHE:CZ	1:I6:224:LYS:HD2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I7:51:LYS:HE3	1:J7:132:LYS:HD3	1.88	0.55
2:L4:205:TRP:CZ3	2:L4:209:GLU:HG3	2.41	0.55
2:O2:267:ARG:O	2:O2:270:LYS:HG3	2.05	0.55
3:Q1:105:VAL:HB	3:Q1:130:MET:SD	2.47	0.55
5:X2:132:GLN:HB2	5:X2:222:ARG:HB2	1.89	0.55
5:X3:134:SER:HA	5:X3:173:LEU:O	2.07	0.55
1:j0:170:ALA:HB1	1:j0:175:LEU:HB2	1.89	0.55
1:A6:187:THR:HG23	1:A6:190:PHE:H	1.71	0.55
1:D4:114:VAL:HG21	1:D4:185:LEU:HD22	1.88	0.55
1:I6:80:LEU:HD13	1:I6:208:GLN:HE22	1.71	0.55
3:Q1:237:TYR:HA	3:Q1:240:HIS:CE1	2.42	0.55
3:s6:247:LEU:O	3:s6:251:ILE:HG23	2.06	0.55
1:E3:65:ASN:ND2	1:E4:99:ASN:HD21	2.04	0.55
1:H8:272:ARG:HB3	1:H8:273:PRO:HD3	1.89	0.55
2:L5:75:GLU:HG3	2:L5:76:ALA:H	1.70	0.55
5:X2:196:PHE:O	5:X2:197:VAL:HG13	2.07	0.55
5:X3:52:GLU:OE2	5:X3:100:HIS:N	2.38	0.55
7:Z2:233:GLN:HB3	7:Z2:236:HIS:CD2	2.41	0.55
3:s4:55:LEU:O	3:s4:59:LEU:HG	2.06	0.55
1:A7:265:MET:HE3	1:B7:30:LEU:HD22	1.89	0.55
1:K9:71:SER:O	1:K9:75:THR:HG23	2.07	0.55
2:N4:78:TRP:CG	2:N5:236:PRO:HG2	2.42	0.55
5:X3:132:GLN:NE2	5:X3:222:ARG:HH21	2.05	0.55
7:Z2:37:TYR:O	7:Z2:41:ILE:HG12	2.07	0.55
7:Z2:180:THR:HG23	7:Z2:181:ARG:H	1.70	0.55
3:s4:44:THR:HA	3:s4:47:LYS:HG2	1.87	0.55
4:t2:156:CYS:HG	4:t2:188:TRP:CD1	2.24	0.55
1:A4:277:LEU:HB2	1:K5:257:ILE:HD11	1.88	0.55
1:B8:177:LYS:HG3	1:B8:179:ASP:H	1.72	0.55
1:C7:48:VAL:O	1:C7:52:MET:HG2	2.06	0.55
1:D7:107:ARG:HA	1:D7:110:ILE:HG12	1.88	0.55
1:K9:96:GLN:HG3	1:K9:102:TYR:HE2	1.72	0.55
4:t1:109:VAL:HB	4:t1:219:VAL:HG22	1.89	0.55
1:K8:56:VAL:HG22	1:K8:233:ILE:HG13	1.87	0.55
2:M4:293:VAL:O	2:M4:296:VAL:HG12	2.07	0.55
5:X4:47:ILE:HB	5:X4:220:GLU:HG3	1.89	0.55
2:p3:183:ILE:HD12	2:p3:194:PHE:HE2	1.72	0.55
1:J6:51:LYS:O	1:J6:54:THR:HG22	2.06	0.55
3:R3:185:HIS:HB2	3:R3:188:LYS:HE3	1.89	0.55
8:a4:107:VAL:HA	8:a4:119:LEU:HG	1.89	0.55
1:J9:49:SER:OG	1:J9:241:ARG:HD3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K7:39:ALA:H	1:K8:77:GLU:CD	2.14	0.55
2:L6:330:PRO:HA	2:L6:333:LYS:HG2	1.88	0.55
3:Q4:81:LYS:HE2	3:Q4:95:GLN:O	2.07	0.55
4:T1:21:LEU:HD11	4:t1:194:TYR:CE1	2.42	0.55
4:T1:194:TYR:H	4:T1:194:TYR:HD1	1.55	0.55
5:V2:52:GLU:HA	5:V2:100:HIS:HB2	1.88	0.55
1:D3:153:ILE:HD11	1:E3:123:ARG:HD2	1.89	0.54
1:D4:36:ILE:HD11	1:D4:241:ARG:HG3	1.88	0.54
1:D4:115:SER:HA	1:D4:182:LEU:HD21	1.88	0.54
1:G8:161:GLU:HG3	1:H8:123:ARG:HH12	1.71	0.54
3:S2:154:LYS:HB2	3:S2:177:ARG:HA	1.89	0.54
5:V3:43:LEU:HD21	5:V3:222:ARG:NH1	2.22	0.54
5:X5:54:ALA:HA	5:X5:57:TRP:HE3	1.70	0.54
1:A6:272:ARG:HB3	1:A6:273:PRO:HD3	1.88	0.54
1:A8:40:GLY:HA3	1:A9:216:PHE:CD1	2.41	0.54
1:G2:80:LEU:HD21	1:G2:212:LEU:HD12	1.87	0.54
1:K5:65:ASN:HD21	1:K6:96:GLN:HA	1.71	0.54
3:S6:103:ILE:HB	3:S6:132:ILE:HB	1.90	0.54
1:A5:57:LYS:HE2	1:A6:92:VAL:HG21	1.88	0.54
1:G7:65:ASN:HB3	1:G8:99:ASN:HD21	1.72	0.54
2:L6:330:PRO:O	2:L6:333:LYS:HG2	2.06	0.54
2:N4:197:LEU:O	2:N4:201:THR:HG23	2.07	0.54
4:T3:156:CYS:SG	4:T3:233:PHE:HB2	2.48	0.54
2:p5:278:THR:HG21	2:p5:292:ILE:HG21	1.88	0.54
4:t4:152:SER:HA	4:t4:191:LEU:O	2.07	0.54
1:D3:1:MET:HE3	1:D3:276:VAL:HG11	1.90	0.54
1:E2:262:GLY:HA2	1:E2:265:MET:SD	2.47	0.54
1:G1:22:GLU:HG2	1:G1:255:ASN:ND2	2.22	0.54
1:I8:155:PRO:HD2	1:I8:159:GLN:HE22	1.72	0.54
2:L2:162:LYS:HB3	2:L2:166:LYS:HE3	1.90	0.54
2:P3:106:ARG:HD2	3:s4:108:TYR:CD2	2.42	0.54
5:X1:67:GLU:HB3	5:X1:107:ASN:HD22	1.73	0.54
10:d4:220:PHE:HE2	10:d4:249:ALA:HB3	1.71	0.54
1:A8:109:MET:HE1	1:K8:207:LYS:HG2	1.90	0.54
1:B4:254:LYS:HE2	1:C3:4:ASN:HB2	1.89	0.54
1:C4:14:ARG:HH21	1:C5:228:VAL:HG12	1.71	0.54
1:E4:18:PHE:CE2	1:E5:224:LYS:HD2	2.42	0.54
1:G9:159:GLN:CD	1:H9:127:GLN:HG2	2.33	0.54
2:M4:238:HIS:HB2	2:M4:277:ALA:HB2	1.90	0.54
2:O2:75:GLU:C	2:O2:77:LEU:H	2.16	0.54
2:p3:209:GLU:HG3	2:p3:214:ASN:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s5:170:ILE:HD12	3:s5:195:LYS:HA	1.89	0.54
1:B5:240:ILE:HG23	1:C5:64:ARG:NH2	2.21	0.54
1:E5:90:ILE:HD11	1:E5:114:VAL:HG13	1.90	0.54
1:G8:244:ASP:CG	1:H7:13:HIS:HE1	2.16	0.54
1:H9:16:LEU:HD21	1:H9:263:THR:HG22	1.90	0.54
2:M3:205:TRP:HE1	2:M3:221:ILE:HG13	1.73	0.54
3:R5:79:LEU:HD21	3:R5:103:ILE:HD11	1.90	0.54
3:s5:169:LYS:HE2	3:s5:228:ILE:HG21	1.88	0.54
3:s6:171:ILE:HD13	3:s6:232:PHE:CE1	2.43	0.54
4:t3:44:VAL:HG21	4:t3:72:ARG:NE	2.21	0.54
1:A4:278:GLN:HE22	1:K5:260:GLN:HG2	1.72	0.54
1:E5:218:ARG:HG2	1:E5:218:ARG:HH11	1.73	0.54
6:Y4:56:PHE:CE1	6:Y4:253:VAL:HG21	2.42	0.54
10:d2:178:LYS:HA	10:d2:212:ILE:HD11	1.90	0.54
1:G7:46:LEU:HD21	1:G8:209:ARG:NH2	2.22	0.54
1:K4:27:MET:HE1	1:K4:252:PHE:CE2	2.43	0.54
2:M2:148:VAL:HG23	2:M2:151:LYS:HE2	1.90	0.54
2:P4:94:HIS:CD2	2:P4:95:GLN:HG3	2.42	0.54
3:R5:222:ASN:HB2	3:R5:229:ARG:HD3	1.88	0.54
4:T3:214:PHE:CZ	4:T3:217:PHE:HE1	2.25	0.54
5:V1:104:VAL:HB	5:V1:214:PHE:CE1	2.43	0.54
2:p5:222:LEU:HB3	2:p5:241:LEU:HD22	1.89	0.54
1:A4:274:GLN:O	1:A4:278:GLN:HG2	2.08	0.54
1:B6:72:LEU:O	1:B6:75:THR:HG22	2.07	0.54
1:C5:87:ILE:HD12	1:C5:205:ILE:HD13	1.90	0.54
1:C7:232:ASN:HD22	1:D7:75:THR:HA	1.72	0.54
1:G9:278:GLN:HA	1:G9:281:ARG:HG3	1.89	0.54
2:N6:271:ASN:HD22	2:N6:296:VAL:HG13	1.72	0.54
2:O1:94:HIS:CD2	2:O1:95:GLN:HG3	2.43	0.54
3:Q3:153:ASN:HA	3:Q3:179:PRO:HD2	1.90	0.54
3:S4:81:LYS:HD2	3:S4:95:GLN:HG3	1.89	0.54
4:T4:167:TRP:HB2	4:T4:216:GLN:H	1.73	0.54
5:V2:230:TYR:CD1	5:V2:231:PRO:HD2	2.42	0.54
1:B4:49:SER:HB2	1:B4:241:ARG:CG	2.38	0.54
1:F2:25:LYS:O	1:F2:29:THR:HG23	2.08	0.54
1:H8:111:GLN:HE22	1:H8:184:THR:HA	1.71	0.54
1:H8:265:MET:SD	1:I8:27:MET:HG3	2.47	0.54
1:K6:201:ALA:O	1:K6:205:ILE:HG12	2.08	0.54
2:N2:270:LYS:HA	2:N2:273:HIS:CE1	2.43	0.54
1:A7:20:ASN:HD22	1:K7:1:MET:HE2	1.73	0.53
1:B5:82:GLU:O	1:B5:86:ILE:HG12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E3:265:MET:SD	1:F3:31:SER:HA	2.47	0.53
1:I8:39:ALA:H	1:I9:77:GLU:HG2	1.72	0.53
2:P3:220:PRO:HA	2:P3:223:GLU:HG2	1.90	0.53
2:p5:170:LEU:HG	2:p5:205:TRP:HZ3	1.73	0.53
4:t4:116:ILE:HG13	4:t4:117:PRO:HD2	1.90	0.53
1:A6:54:THR:HG22	1:A7:88:GLN:NE2	2.23	0.53
1:B6:18:PHE:HE2	1:B7:227:MET:HG2	1.73	0.53
1:C6:194:ALA:O	1:C6:198:LEU:HD23	2.08	0.53
1:D5:87:ILE:HA	1:D5:90:ILE:HG22	1.89	0.53
1:E3:168:MET:HA	1:E3:173:LEU:HD21	1.90	0.53
1:F4:83:THR:HG23	1:F4:121:ILE:HD13	1.89	0.53
1:F6:73:ILE:HG21	1:F6:216:PHE:HB2	1.89	0.53
1:H6:272:ARG:HB3	1:H6:273:PRO:HD3	1.90	0.53
1:I9:59:LEU:HD11	1:I9:233:ILE:HD12	1.90	0.53
1:K4:1:MET:HG2	1:K4:276:VAL:HG11	1.91	0.53
4:T1:30:SER:C	4:T1:32:ASP:H	2.16	0.53
4:T1:80:LYS:HE2	4:T1:92:ALA:HB2	1.90	0.53
5:X2:117:GLU:HG2	5:X2:200:PHE:HB2	1.89	0.53
1:I8:51:LYS:HE3	1:J8:132:LYS:HE3	1.89	0.53
1:K5:56:VAL:HG13	1:K5:230:TYR:CE1	2.43	0.53
2:N3:75:GLU:C	2:N3:77:LEU:H	2.16	0.53
2:N3:271:ASN:HB2	2:N3:296:VAL:HG23	1.88	0.53
3:Q2:248:PHE:HA	3:Q2:251:ILE:HG22	1.89	0.53
5:X4:48:LEU:HD21	7:Z4:179:LEU:HA	1.90	0.53
1:A7:123:ARG:NH2	1:A7:127:GLN:HG2	2.24	0.53
1:A7:152:HIS:C	1:A7:154:GLY:H	2.16	0.53
1:D4:166:ALA:HB3	1:D4:208:GLN:NE2	2.24	0.53
1:J6:86:ILE:HD13	1:J6:120:GLU:HB3	1.91	0.53
1:J6:117:LEU:O	1:J6:120:GLU:HB2	2.08	0.53
1:K6:30:LEU:HD21	1:K6:248:GLU:HB3	1.90	0.53
2:M4:241:LEU:HD23	2:M4:273:HIS:CD2	2.44	0.53
3:R4:82:GLY:HA2	3:R4:92:ALA:H	1.72	0.53
4:T4:246:VAL:HG21	4:T4:266:LEU:HB3	1.91	0.53
3:s5:173:GLU:HB3	3:s5:192:PHE:HB2	1.91	0.53
4:t2:154:TRP:HB2	4:t2:236:GLU:HB2	1.88	0.53
1:G2:184:THR:HG22	1:G2:186:SER:H	1.72	0.53
1:I7:156:ASN:H	1:I7:159:GLN:NE2	2.05	0.53
1:K7:272:ARG:HB3	1:K7:273:PRO:HD3	1.90	0.53
2:P4:220:PRO:HA	2:P4:223:GLU:HG2	1.90	0.53
4:T4:31:TRP:HZ3	4:T4:42:TRP:CG	2.26	0.53
1:D3:11:ASN:O	1:D3:14:ARG:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D6:61:GLN:HE21	1:D7:96:GLN:CD	2.16	0.53
1:E3:150:TRP:CZ3	1:E3:162:ARG:HB2	2.44	0.53
1:E4:114:VAL:HG21	1:E4:185:LEU:HD23	1.90	0.53
1:F3:83:THR:HG23	1:F3:121:ILE:HD12	1.91	0.53
1:I7:106:ASP:O	1:I7:110:ILE:HG13	2.09	0.53
3:Q4:62:HIS:CD2	3:Q4:248:PHE:HB3	2.44	0.53
3:R4:106:GLU:HB3	3:R4:108:TYR:HE2	1.73	0.53
7:Z3:198:ILE:HG23	7:Z3:261:ILE:HD11	1.90	0.53
1:h0:76:THR:HG23	1:h0:212:LEU:HD13	1.90	0.53
1:A5:254:LYS:HD2	1:B4:4:ASN:O	2.08	0.53
1:E4:140:PHE:CD1	1:E4:149:MET:HB2	2.43	0.53
1:H6:232:ASN:ND2	1:I6:74:GLN:HG2	2.24	0.53
1:J6:19:GLN:NE2	1:J6:258:LEU:HD13	2.24	0.53
2:L6:332:HIS:HB2	2:L6:371:ALA:HB2	1.90	0.53
2:M3:78:TRP:CE2	2:M4:203:ARG:HG3	2.44	0.53
2:M4:180:LEU:HD21	2:M4:197:LEU:HD23	1.90	0.53
2:P3:269:LYS:HA	2:P3:272:VAL:HG12	1.90	0.53
3:R2:217:LEU:O	3:R2:220:VAL:HG22	2.08	0.53
5:X1:54:ALA:HB1	5:X1:102:LEU:HD21	1.91	0.53
8:a3:130:LEU:HB3	8:a3:138:TYR:HB3	1.90	0.53
1:B5:133:MET:HE2	1:B6:103:SER:HA	1.91	0.53
1:H7:23:VAL:HG22	1:H7:255:ASN:HB3	1.91	0.53
2:L5:131:LYS:HE3	8:a5:223:ARG:NE	2.24	0.53
2:M3:75:GLU:CD	2:M3:76:ALA:H	2.16	0.53
3:S4:173:GLU:HB3	3:S4:192:PHE:HB2	1.90	0.53
5:X2:148:ALA:HB1	5:X2:196:PHE:CE2	2.40	0.53
7:Z4:161:TRP:HB3	7:Z4:192:VAL:HG22	1.91	0.53
3:s6:216:ILE:HG23	3:s6:219:GLY:HA3	1.90	0.53
1:C6:277:LEU:HD13	1:C7:245:MET:HE3	1.91	0.53
1:E3:163:VAL:HG23	1:E3:215:TYR:CZ	2.44	0.53
1:I5:20:ASN:HA	1:I5:23:VAL:HG12	1.91	0.53
1:I8:14:ARG:HG3	1:I9:227:MET:SD	2.48	0.53
1:K7:265:MET:HA	1:K7:265:MET:HE3	1.91	0.53
2:L2:71:ILE:HD13	2:L3:235:TYR:OH	2.09	0.53
2:P5:235:TYR:HB3	2:P5:236:PRO:HD3	1.91	0.53
1:h0:73:ILE:HD11	1:h0:151:PHE:HE2	1.74	0.53
2:p2:214:ASN:HB3	2:p2:217:GLN:HB2	1.91	0.53
4:t1:23:LEU:HD23	4:t1:23:LEU:H	1.74	0.53
1:C4:1:MET:HE1	1:C4:276:VAL:HG11	1.91	0.53
1:C7:72:LEU:HD12	1:C7:130:PHE:HD2	1.74	0.53
1:D4:59:LEU:HD21	1:D4:226:LEU:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H6:46:LEU:HD21	1:H7:209:ARG:HE	1.73	0.53
1:I9:232:ASN:OD1	1:J9:74:GLN:HG3	2.09	0.53
3:Q3:63:THR:HG21	3:Q3:150:ARG:HG2	1.90	0.53
3:Q4:250:LYS:HG3	3:Q4:254:TYR:CE2	2.44	0.53
5:V2:139:GLY:O	5:V2:168:PHE:HA	2.09	0.53
5:X4:105:LYS:HE3	5:X5:239:TRP:HZ2	1.74	0.53
10:d2:209:ILE:HG23	10:d2:213:MET:HE2	1.89	0.53
3:s5:176:ASP:HB3	3:s5:188:LYS:NZ	2.24	0.53
1:B6:74:GLN:HA	1:B6:77:GLU:HG2	1.91	0.52
1:E5:86:ILE:HD13	1:E5:120:GLU:OE1	2.09	0.52
1:F3:18:PHE:CZ	1:F4:224:LYS:HA	2.44	0.52
1:F3:150:TRP:CZ3	1:F3:162:ARG:HB2	2.44	0.52
1:F4:99:ASN:HD21	1:F4:101:ILE:HG23	1.73	0.52
1:I7:57:LYS:HD2	1:I8:92:VAL:HG21	1.92	0.52
1:J9:65:ASN:HD21	1:j0:99:ASN:ND2	2.00	0.52
1:K8:50:GLU:HG3	1:K9:209:ARG:NH2	2.25	0.52
3:S6:55:LEU:O	3:S6:59:LEU:HG	2.08	0.52
4:T3:46:THR:OG1	4:T3:49:ASP:HB3	2.09	0.52
5:X3:79:ILE:HD11	5:X3:89:PRO:HG3	1.91	0.52
5:X5:135:ILE:HG23	5:X5:173:LEU:HB2	1.91	0.52
1:j0:78:GLY:O	1:j0:81:GLN:HG3	2.10	0.52
4:t2:18:VAL:O	4:t2:22:GLU:HG3	2.08	0.52
1:C5:1:MET:HE1	1:C5:276:VAL:HG11	1.90	0.52
1:F4:118:VAL:HA	1:F4:121:ILE:HG22	1.91	0.52
1:G9:29:THR:HG22	1:G9:37:ASN:HD22	1.74	0.52
2:N5:130:ARG:O	2:N5:133:GLU:HG2	2.09	0.52
2:O2:238:HIS:CD2	2:O2:273:HIS:HD2	2.28	0.52
2:O4:209:GLU:HG3	2:O4:214:ASN:HB3	1.91	0.52
5:X4:50:ASN:HB2	12:X4:402:HOH:O	2.08	0.52
1:A9:120:GLU:CG	1:K9:218:ARG:HG2	2.38	0.52
1:I8:91:ARG:HG3	1:I8:198:LEU:HD11	1.91	0.52
1:K8:50:GLU:HG3	1:K9:209:ARG:HH21	1.73	0.52
1:K8:97:SER:HB3	1:K8:110:ILE:HG21	1.89	0.52
1:K8:199:ASP:O	1:K8:203:MET:HG2	2.10	0.52
3:R2:55:LEU:HA	3:R2:58:ARG:HD3	1.90	0.52
3:R4:156:LYS:HD2	3:R4:175:MET:HE3	1.91	0.52
5:V2:162:LEU:HB3	5:V2:173:LEU:HD13	1.90	0.52
5:V4:49:GLU:HB3	5:V4:219:LEU:HB3	1.91	0.52
5:X3:167:TYR:CZ	5:X3:171:ARG:HD3	2.44	0.52
2:p5:210:TYR:HB2	2:p5:240:TYR:OH	2.09	0.52
1:D5:36:ILE:HG23	1:D5:42:ASP:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D5:40:GLY:HA2	1:D6:213:GLY:CA	2.40	0.52
1:D6:32:SER:HB3	1:D6:37:ASN:HD21	1.75	0.52
2:O5:215:LEU:HB2	2:O5:216:PRO:HD3	1.90	0.52
2:O5:268:TYR:HA	2:O5:271:ASN:ND2	2.23	0.52
3:R5:78:VAL:CG1	3:R5:106:GLU:HB2	2.39	0.52
4:T1:110:THR:HG23	4:T1:216:GLN:OE1	2.10	0.52
4:T2:194:TYR:OH	4:t2:21:LEU:HD13	2.10	0.52
4:T3:151:MET:SD	4:T3:151:MET:C	2.93	0.52
4:t2:42:TRP:CE3	4:t2:111:ILE:HG22	2.44	0.52
1:A8:202:LEU:HA	1:A8:205:ILE:HG22	1.90	0.52
1:C3:46:LEU:HD21	1:C4:209:ARG:HH12	1.74	0.52
1:C7:218:ARG:HH11	1:D7:116:GLN:NE2	2.08	0.52
1:F5:30:LEU:HD13	1:F5:248:GLU:HB3	1.91	0.52
1:G1:101:ILE:HG22	1:G9:149:MET:HE1	1.91	0.52
1:G7:228:VAL:HA	1:G7:231:GLU:HG2	1.91	0.52
1:K9:215:TYR:O	1:K9:218:ARG:HB2	2.10	0.52
2:N3:166:LYS:HD2	2:N3:211:ASP:OD1	2.09	0.52
2:O4:75:GLU:C	2:O4:77:LEU:H	2.16	0.52
2:P5:145:TRP:HA	2:P5:148:VAL:HG22	1.91	0.52
3:Q1:63:THR:HG21	3:Q1:152:ILE:HD11	1.90	0.52
1:D4:35:ARG:HG3	1:D4:36:ILE:HG23	1.90	0.52
1:E6:57:LYS:HE2	1:E7:92:VAL:HG21	1.91	0.52
1:F3:120:GLU:O	1:F3:124:ILE:HD12	2.09	0.52
1:F4:272:ARG:HG2	1:F4:273:PRO:HD3	1.91	0.52
1:H8:232:ASN:HD21	1:I8:74:GLN:HG2	1.75	0.52
3:Q1:133:TYR:HB2	3:Q1:154:LYS:H	1.74	0.52
5:V1:46:LEU:O	5:V1:47:ILE:HD13	2.09	0.52
1:i0:162:ARG:HG2	1:i0:164:TYR:CZ	2.45	0.52
4:t1:4:ILE:HG21	4:t1:7:LYS:HE3	1.91	0.52
1:A9:75:THR:HG22	1:K9:229:ALA:HA	1.91	0.52
1:B3:5:HIS:HB2	1:B4:238:SER:HB3	1.92	0.52
1:D3:157:GLN:HG3	1:D3:158:HIS:CD2	2.43	0.52
1:E2:18:PHE:CZ	1:E3:224:LYS:HA	2.45	0.52
1:K7:157:GLN:HE21	1:K7:158:HIS:CD2	2.28	0.52
4:T4:23:LEU:HD23	4:T4:23:LEU:H	1.74	0.52
5:V3:123:GLU:HA	5:V3:197:VAL:HG11	1.91	0.52
1:B6:88:GLN:O	1:B6:92:VAL:HG23	2.10	0.52
1:B7:160:ARG:HG2	1:B7:160:ARG:HH11	1.75	0.52
1:E5:117:LEU:O	1:E5:121:ILE:HD12	2.10	0.52
1:J5:272:ARG:HB3	1:J5:273:PRO:HD3	1.91	0.52
2:O3:235:TYR:CD1	2:O3:236:PRO:HD3	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S3:185:HIS:O	3:S3:189:VAL:HG13	2.09	0.52
4:T2:30:SER:C	4:T2:32:ASP:H	2.18	0.52
2:p5:218:CYS:O	2:p5:221:ILE:HG12	2.10	0.52
3:s4:166:LEU:HD22	3:s4:235:GLU:HB2	1.91	0.52
1:E7:153:ILE:HD13	1:E7:226:LEU:HD11	1.91	0.52
1:F3:236:SER:OG	1:G8:71:SER:HB2	2.10	0.52
1:H6:38:ARG:HH21	1:H7:73:ILE:HG22	1.74	0.52
1:H7:80:LEU:HD21	1:H7:168:MET:HE1	1.91	0.52
1:I9:65:ASN:HD22	1:I9:65:ASN:C	2.17	0.52
1:J5:61:GLN:HB3	1:J6:95:ILE:HD11	1.92	0.52
1:K5:10:ILE:HG23	1:K6:231:GLU:HG3	1.91	0.52
1:K7:67:GLU:O	1:K7:70:MET:HG2	2.10	0.52
1:K7:114:VAL:HG21	1:K7:185:LEU:HD12	1.92	0.52
1:K8:40:GLY:HA3	1:K9:216:PHE:CD1	2.44	0.52
2:P2:93:LEU:HD21	2:P3:292:ILE:HD11	1.92	0.52
3:Q1:187:ASP:HA	3:Q1:216:ILE:HD11	1.92	0.52
3:Q4:71:ARG:H	3:Q4:255:ASN:ND2	2.07	0.52
5:X2:117:GLU:HG2	5:X2:200:PHE:CB	2.40	0.52
5:X4:160:ILE:HG12	5:X4:177:ILE:HD12	1.92	0.52
10:d4:162:LEU:HD11	10:d4:177:LEU:HD11	1.92	0.52
3:s4:48:LEU:O	3:s4:52:ILE:HG12	2.10	0.52
1:C6:265:MET:HE2	1:D6:31:SER:HB3	1.92	0.52
1:D7:170:ALA:HB1	1:D7:175:LEU:HD11	1.92	0.52
1:G7:2:ILE:HG21	1:G8:238:SER:HB2	1.92	0.52
5:X2:131:ARG:HA	5:X2:177:ILE:HD13	1.90	0.52
5:X5:212:PHE:CZ	5:X5:214:PHE:HB3	2.45	0.52
7:Z4:106:ASN:O	7:Z4:110:ARG:HG2	2.10	0.52
2:p2:93:LEU:HD22	2:p3:292:ILE:HD13	1.92	0.52
2:p3:192:PRO:HA	2:p3:195:LYS:HG2	1.91	0.52
1:E7:120:GLU:O	1:E7:124:ILE:HG12	2.09	0.51
1:F3:54:THR:HA	1:F4:88:GLN:HE22	1.75	0.51
1:F3:273:PRO:O	1:F3:276:VAL:HG12	2.10	0.51
1:J6:265:MET:SD	1:K6:27:MET:HG3	2.51	0.51
2:N6:249:GLU:HA	2:N6:252:ILE:HG22	1.92	0.51
2:P3:293:VAL:O	2:P3:296:VAL:HG22	2.10	0.51
4:T1:146:GLY:H	4:T1:209:VAL:HG23	1.75	0.51
5:V3:131:ARG:HA	5:V3:177:ILE:HB	1.92	0.51
5:X2:136:TRP:CE2	5:X2:172:LYS:HD3	2.46	0.51
7:Z2:227:GLU:HB3	7:Z2:230:GLN:OE1	2.10	0.51
1:A6:1:MET:HE1	1:B6:20:ASN:ND2	2.24	0.51
1:B7:114:VAL:HG21	1:B7:185:LEU:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F6:30:LEU:HD11	1:F6:245:MET:SD	2.51	0.51
1:J6:57:LYS:HE2	1:J7:92:VAL:HG21	1.92	0.51
1:K6:55:GLN:HE22	1:K6:233:ILE:CG2	2.24	0.51
2:M4:109:LEU:HD22	2:M4:197:LEU:HD22	1.92	0.51
3:R4:51:LYS:HE3	3:R4:238:ILE:HD13	1.92	0.51
6:Y2:53:ASN:HB3	6:Y2:74:GLU:HB2	1.91	0.51
1:C7:52:MET:HE3	1:C7:233:ILE:HG23	1.93	0.51
1:D7:86:ILE:HG23	1:D7:117:LEU:HD12	1.92	0.51
1:G8:205:ILE:O	1:G8:209:ARG:HG2	2.11	0.51
1:J8:53:ARG:HA	1:J8:56:VAL:HG12	1.91	0.51
1:K8:96:GLN:HG3	1:K8:102:TYR:HE2	1.75	0.51
2:L6:310:PRO:O	2:L6:313:ILE:HG12	2.11	0.51
2:M3:206:ILE:HG23	2:M3:218:CYS:SG	2.50	0.51
2:O2:106:ARG:HG3	2:O2:106:ARG:HH11	1.76	0.51
4:T4:152:SER:CB	4:t4:18:VAL:HG13	2.40	0.51
10:d3:101:VAL:HG12	10:d3:149:PRO:HG3	1.92	0.51
1:j0:192:ASN:HA	1:j0:195:ILE:HD12	1.91	0.51
4:t2:149:LYS:HE3	4:t2:240:LEU:HD23	1.91	0.51
1:B7:193:ASP:HA	5:V3:65:LEU:HD13	1.93	0.51
1:C5:51:LYS:HZ1	1:D5:132:LYS:HE2	1.75	0.51
1:C8:138:GLY:HA3	1:C8:167:THR:HG22	1.93	0.51
1:I6:49:SER:OG	1:I6:241:ARG:HB3	2.10	0.51
1:K6:18:PHE:CE1	1:K7:224:LYS:HD3	2.45	0.51
3:R3:55:LEU:O	3:R3:58:ARG:HG2	2.11	0.51
3:R5:170:ILE:HD12	3:R5:170:ILE:H	1.75	0.51
3:S5:185:HIS:O	3:S5:189:VAL:HG23	2.11	0.51
4:T4:31:TRP:O	4:T4:76:LEU:HD11	2.11	0.51
5:V1:131:ARG:HH21	6:Y1:55:SER:HB3	1.76	0.51
7:Z1:215:THR:HA	7:Z1:218:ASN:ND2	2.26	0.51
10:d4:111:TYR:HB2	10:d4:141:ILE:HG21	1.92	0.51
2:p3:75:GLU:C	2:p3:77:LEU:H	2.18	0.51
4:t2:225:THR:HG22	4:t2:227:GLY:H	1.75	0.51
1:A7:34:MET:HA	1:A7:242:ASP:HA	1.91	0.51
1:B6:218:ARG:HG3	1:C6:120:GLU:CD	2.36	0.51
1:C5:20:ASN:HA	1:C5:23:VAL:HG12	1.91	0.51
1:E6:46:LEU:HD21	1:E7:209:ARG:CZ	2.41	0.51
1:E7:166:ALA:N	1:E7:208:GLN:HE22	2.08	0.51
1:H8:46:LEU:HD21	1:H9:209:ARG:HD3	1.92	0.51
1:I5:265:MET:SD	1:J5:27:MET:HE3	2.51	0.51
1:I6:265:MET:SD	1:J6:30:LEU:HD22	2.50	0.51
1:J8:153:ILE:HD11	1:K8:123:ARG:NE	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K7:72:LEU:O	1:K7:75:THR:HG22	2.11	0.51
1:K7:106:ASP:O	1:K7:109:MET:HG3	2.11	0.51
4:T3:98:LYS:HD3	4:T3:231:TYR:HA	1.93	0.51
4:T3:150:ALA:HB3	4:T3:240:LEU:HB3	1.92	0.51
4:T3:244:PHE:HA	4:T3:247:HIS:HD2	1.75	0.51
7:Z3:26:LYS:O	7:Z3:30:LYS:HG2	2.11	0.51
4:t3:116:ILE:HD12	4:t3:118:GLU:H	1.74	0.51
1:E4:43:ALA:HB1	1:E5:210:ALA:HB1	1.93	0.51
1:I6:163:VAL:HG13	1:I6:215:TYR:CD2	2.45	0.51
1:I9:118:VAL:HA	1:I9:121:ILE:HD12	1.91	0.51
3:S6:231:SER:O	3:S6:234:LYS:HG3	2.11	0.51
4:T3:157:GLY:O	4:T3:186:ILE:HA	2.11	0.51
5:V2:147:PHE:HB3	5:V2:159:ASN:OD1	2.11	0.51
1:h0:80:LEU:HA	1:h0:83:THR:HG22	1.92	0.51
1:A5:76:THR:HG23	1:A5:136:LEU:HD21	1.92	0.51
1:A7:35:ARG:HB2	1:A7:243:THR:HA	1.92	0.51
1:D3:56:VAL:HG22	1:D3:233:ILE:HG22	1.93	0.51
1:F2:38:ARG:HG2	1:F2:38:ARG:HH11	1.74	0.51
1:I9:91:ARG:HG3	1:I9:198:LEU:HD11	1.91	0.51
5:X5:54:ALA:HA	5:X5:57:TRP:CE3	2.45	0.51
9:c2:54:ASN:HD21	9:c2:114:LEU:HA	1.74	0.51
1:h0:90:ILE:HG22	1:h0:198:LEU:HD21	1.92	0.51
1:H6:257:ILE:HG21	1:I5:3:ILE:HD11	1.93	0.51
1:I9:46:LEU:HD21	1:i0:209:ARG:CZ	2.41	0.51
1:J6:79:TYR:CZ	1:J6:128:ALA:HA	2.46	0.51
1:C4:130:PHE:HB2	1:C4:135:LEU:HD11	1.93	0.51
1:D6:203:MET:HE2	1:E6:105:GLU:CD	2.35	0.51
1:E4:39:ALA:HB3	1:E5:213:GLY:HA3	1.93	0.51
1:F3:65:ASN:HD21	1:F4:99:ASN:CG	2.19	0.51
1:F5:157:GLN:HE22	1:F6:195:ILE:C	2.19	0.51
1:F5:221:HIS:HB3	1:G1:86:ILE:HD11	1.92	0.51
1:I7:279:LEU:HG	1:J7:264:ALA:HA	1.93	0.51
2:P2:219:ILE:HD12	2:P2:245:TYR:CE1	2.46	0.51
5:V5:48:LEU:HB2	5:V5:219:LEU:O	2.10	0.51
5:X3:222:ARG:HH22	4:t3:128:LEU:HB2	1.76	0.51
7:Z3:157:ILE:HA	7:Z3:161:TRP:CD1	2.46	0.51
3:s4:129:TYR:CE2	3:s4:158:LYS:HB2	2.46	0.51
1:A5:64:ARG:NH1	1:K5:240:ILE:HA	2.25	0.51
1:A6:3:ILE:HG13	1:A6:4:ASN:N	2.26	0.51
1:E5:30:LEU:HD13	1:E5:248:GLU:HB3	1.93	0.51
1:F3:120:GLU:HA	1:F3:123:ARG:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I9:257:ILE:HG23	1:J8:277:LEU:HD11	1.93	0.51
2:M2:123:ARG:NH1	2:M2:126:ILE:HD11	2.26	0.51
3:R4:53:PHE:HA	3:R4:56:ASN:ND2	2.25	0.51
3:S3:73:LEU:HD21	3:S3:78:VAL:HA	1.93	0.51
3:S6:233:LYS:HA	3:S6:237:TYR:HD2	1.76	0.51
5:X5:136:TRP:HE1	5:X5:170:TRP:HB3	1.76	0.51
6:Y4:140:GLY:HA2	6:Y4:144:TYR:CB	2.40	0.51
10:d3:105:LYS:HB3	10:d3:106:PRO:HD3	1.93	0.51
10:d3:135:VAL:HG22	10:d3:168:TYR:CD1	2.46	0.51
10:d3:189:LEU:HG	10:d3:205:ILE:HG23	1.93	0.51
1:i0:114:VAL:HG21	1:i0:185:LEU:HD22	1.93	0.51
1:A6:154:GLY:HA3	1:A6:159:GLN:HG2	1.93	0.50
1:C3:20:ASN:HA	1:C3:23:VAL:HG12	1.92	0.50
1:E2:44:SER:O	1:E2:48:VAL:HG12	2.11	0.50
1:E3:16:LEU:HD11	1:E3:263:THR:HG22	1.93	0.50
1:E3:239:ARG:HD3	1:F3:67:GLU:HG3	1.92	0.50
1:G1:159:GLN:NE2	1:h0:127:GLN:HG3	2.25	0.50
1:I7:7:LEU:HA	1:I7:10:ILE:HG22	1.93	0.50
1:J6:272:ARG:HB3	1:J6:273:PRO:HD3	1.92	0.50
1:J7:247:GLU:HB2	1:K6:13:HIS:CE1	2.46	0.50
2:P2:107:LEU:HA	3:s3:76:ARG:HH12	1.77	0.50
2:P6:114:SER:O	2:P6:118:THR:HG23	2.11	0.50
3:Q4:107:VAL:HG13	3:Q4:127:ALA:HB3	1.92	0.50
3:R3:156:LYS:HG3	3:R3:175:MET:HE1	1.92	0.50
3:R3:216:ILE:HG22	3:R3:218:ALA:H	1.74	0.50
3:S6:65:LEU:HD21	3:S6:252:PHE:HA	1.93	0.50
5:X4:118:VAL:O	5:X4:198:SER:HB2	2.11	0.50
7:Z4:137:LEU:HD13	7:Z4:206:TYR:CE1	2.45	0.50
2:p5:192:PRO:O	2:p5:195:LYS:HG2	2.12	0.50
1:C6:247:GLU:HG2	1:D5:13:HIS:NE2	2.26	0.50
1:D4:281:ARG:C	1:D4:281:ARG:HD2	2.36	0.50
1:E4:207:LYS:O	1:E4:207:LYS:HD3	2.11	0.50
1:G1:99:ASN:HB2	1:G9:65:ASN:HD21	1.76	0.50
1:K6:276:VAL:HG12	1:K6:280:LEU:HD23	1.93	0.50
1:K7:193:ASP:CG	5:X2:65:LEU:HG	2.37	0.50
2:P3:241:LEU:HD23	2:P3:273:HIS:CE1	2.46	0.50
3:S6:216:ILE:HG22	3:S6:218:ALA:H	1.76	0.50
5:X4:149:LYS:HD2	5:X4:157:THR:HB	1.94	0.50
6:Y1:86:SER:OG	6:Y1:258:PHE:HB2	2.11	0.50
6:Y1:258:PHE:CE2	6:Y1:267:LEU:HD13	2.45	0.50
10:d3:242:LEU:HA	10:d3:245:VAL:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t3:18:VAL:O	4:t3:22:GLU:HB2	2.10	0.50
1:A8:25:LYS:O	1:A8:29:THR:HG23	2.11	0.50
1:B6:14:ARG:NH2	1:B7:231:GLU:HG3	2.18	0.50
1:G9:159:GLN:NE2	1:H9:127:GLN:HG2	2.27	0.50
1:I5:32:SER:HB2	1:I5:37:ASN:HD21	1.77	0.50
1:I7:160:ARG:NH2	1:I8:188:ALA:HB1	2.26	0.50
1:I9:83:THR:O	1:I9:87:ILE:HG12	2.11	0.50
2:L5:184:LYS:HE3	6:Y5:116:LEU:HD12	1.93	0.50
3:R2:47:LYS:O	3:R2:50:GLU:HG3	2.12	0.50
4:T2:116:ILE:HG23	4:T2:117:PRO:HD2	1.94	0.50
5:V4:189:LEU:HD22	5:V4:236:LYS:HA	1.93	0.50
5:X2:122:HIS:ND1	7:Z2:171:MET:HG3	2.26	0.50
4:t3:243:VAL:HG11	4:t3:270:LEU:HD21	1.93	0.50
1:A8:89:ARG:HH22	1:K7:42:ASP:CG	2.19	0.50
1:A9:118:VAL:HA	1:A9:121:ILE:HD12	1.92	0.50
1:G7:52:MET:HE1	1:H7:130:PHE:HE1	1.75	0.50
1:I6:51:LYS:HZ3	1:J6:131:ASN:HA	1.76	0.50
1:J8:36:ILE:HG22	1:J8:46:LEU:HD22	1.92	0.50
2:O1:66:ARG:HA	2:O1:69:LYS:HE2	1.93	0.50
2:O4:202:TYR:O	2:O4:206:ILE:HG12	2.12	0.50
3:Q4:246:ARG:HG3	3:Q4:246:ARG:HH11	1.75	0.50
3:S3:152:ILE:HG22	3:S3:153:ASN:O	2.11	0.50
4:T2:22:GLU:OE1	4:t2:25:SER:HB2	2.11	0.50
7:Z3:44:ILE:HD13	7:Z3:248:ILE:HD13	1.93	0.50
1:C4:90:ILE:HB	1:C4:198:LEU:HD22	1.93	0.50
1:C8:136:LEU:HD22	1:C8:168:MET:HG3	1.94	0.50
1:F3:277:LEU:O	1:F3:281:ARG:HB3	2.11	0.50
1:F4:35:ARG:NH2	1:G9:64:ARG:HH12	2.10	0.50
1:G9:151:PHE:CE2	1:G9:163:VAL:HG11	2.45	0.50
1:I8:254:LYS:HE3	1:J7:4:ASN:HA	1.93	0.50
1:J7:14:ARG:HD3	1:J8:231:GLU:OE1	2.12	0.50
1:J7:50:GLU:O	1:J7:54:THR:HG23	2.11	0.50
2:N4:118:THR:O	2:N4:121:LYS:HG3	2.10	0.50
3:R4:90:THR:HG23	3:R4:91:PRO:HD2	1.94	0.50
3:S5:46:ARG:HH12	3:S5:50:GLU:HB3	1.77	0.50
5:X1:132:GLN:NE2	5:X1:222:ARG:HB2	2.26	0.50
5:X1:134:SER:HA	5:X1:173:LEU:O	2.11	0.50
7:Z1:98:TYR:HE2	7:Z1:110:ARG:HE	1.59	0.50
1:B6:53:ARG:HB2	1:B6:241:ARG:HH22	1.76	0.50
1:B6:265:MET:HE1	1:C6:27:MET:HG3	1.93	0.50
1:F4:159:GLN:HB3	1:G9:127:GLN:NE2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J7:23:VAL:HG22	1:J7:255:ASN:HB3	1.94	0.50
2:L5:145:TRP:HA	2:L5:148:VAL:HG12	1.93	0.50
2:M5:105:PHE:CE1	2:M5:197:LEU:HD13	2.47	0.50
5:X3:119:PHE:HD1	5:X3:198:SER:HB3	1.76	0.50
7:Z3:41:ILE:HG12	7:Z3:122:LEU:HD21	1.94	0.50
7:Z3:216:ARG:HA	7:Z3:216:ARG:CZ	2.41	0.50
7:Z3:258:ALA:O	7:Z3:261:ILE:HG22	2.11	0.50
7:Z4:133:THR:HA	7:Z4:136:ILE:HG12	1.94	0.50
8:a4:124:PHE:HD2	8:a4:144:LEU:HB3	1.77	0.50
1:i0:67:GLU:O	1:i0:70:MET:HG3	2.12	0.50
4:t3:64:THR:HG22	4:t3:73:GLU:HG3	1.93	0.50
1:A6:157:GLN:HG3	1:A6:158:HIS:CD2	2.47	0.50
2:L4:162:LYS:HG2	2:L4:166:LYS:HE2	1.94	0.50
2:N5:78:TRP:CD1	2:N6:236:PRO:HB2	2.46	0.50
3:Q3:192:PHE:CE2	3:Q3:194:GLN:HB2	2.47	0.50
3:S4:63:THR:HG22	3:S4:134:PHE:CE1	2.47	0.50
4:T4:94:VAL:HG12	4:T4:235:ASP:OD2	2.12	0.50
5:X3:63:THR:HG22	5:X3:109:THR:HG21	1.94	0.50
6:Y4:54:ILE:HD13	6:Y4:73:VAL:HA	1.94	0.50
6:Y5:225:THR:HB	6:Y5:236:MET:HB2	1.94	0.50
9:c3:29:GLU:HA	9:c3:32:LYS:HG2	1.93	0.50
10:d4:172:SER:HA	10:d4:175:ASP:OD2	2.12	0.50
1:A7:277:LEU:HD13	1:A7:280:LEU:HD11	1.93	0.50
1:H7:26:ASN:HA	1:H7:29:THR:HG22	1.92	0.50
1:H7:114:VAL:HG21	1:H7:185:LEU:HD12	1.94	0.50
1:J6:33:GLY:C	1:J6:34:MET:HE2	2.37	0.50
1:J6:152:HIS:H	1:J7:99:ASN:ND2	2.09	0.50
2:L2:76:ALA:HA	2:L2:79:LYS:HB2	1.94	0.50
2:M4:66:ARG:O	2:M4:69:LYS:HG3	2.12	0.50
2:O4:246:ALA:HB2	2:O4:270:LYS:HE3	1.94	0.50
3:R3:185:HIS:CG	3:R3:188:LYS:HE3	2.47	0.50
5:V2:138:LEU:HA	5:V2:169:GLY:O	2.12	0.50
5:V5:50:ASN:HB2	12:V5:402:HOH:O	2.11	0.50
5:X3:119:PHE:CD1	5:X3:120:PRO:HD2	2.47	0.50
7:Z3:85:TYR:CZ	7:Z3:89:LYS:HE3	2.46	0.50
2:p3:222:LEU:O	2:p3:226:ILE:HG23	2.11	0.50
4:t3:181:GLY:H	4:t3:191:LEU:HD11	1.75	0.50
1:B4:16:LEU:HD11	1:B4:263:THR:HG22	1.93	0.50
1:B5:105:GLU:O	1:B5:109:MET:HG2	2.12	0.50
1:B6:158:HIS:CE1	5:V3:62:THR:HG22	2.47	0.50
1:D5:228:VAL:O	1:D5:231:GLU:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F4:43:ALA:HB1	1:G1:109:MET:HE3	1.93	0.50
1:K5:150:TRP:CE2	1:K5:162:ARG:HD3	2.47	0.50
2:P3:276:ARG:NH1	2:P3:280:LEU:HD11	2.27	0.50
10:d4:80:SER:HA	2:p4:106:ARG:HE	1.76	0.50
3:s3:129:TYR:CZ	3:s3:158:LYS:HB3	2.46	0.50
4:t2:116:ILE:HD11	4:t2:119:TYR:CD2	2.47	0.50
4:t4:144:PHE:CE2	4:t4:214:PHE:HB2	2.47	0.50
1:A8:162:ARG:HG3	1:A8:162:ARG:HH11	1.77	0.49
1:B6:272:ARG:HB3	1:B6:273:PRO:HD3	1.93	0.49
1:B7:11:ASN:HD21	1:C7:28:GLU:CD	2.20	0.49
1:C5:44:SER:HB3	1:D6:110:ILE:HD13	1.94	0.49
1:C8:174:ASN:OD1	1:C8:197:THR:HB	2.12	0.49
1:D5:217:ASN:O	1:D5:220:GLU:HG3	2.11	0.49
1:F5:99:ASN:ND2	1:F5:101:ILE:HG12	2.26	0.49
1:F5:168:MET:HE1	1:F5:208:GLN:HG3	1.93	0.49
1:H6:66:THR:O	1:H6:70:MET:HG3	2.12	0.49
1:H9:38:ARG:HH11	1:h0:74:GLN:CD	2.20	0.49
1:J7:55:GLN:HE22	1:J7:156:ASN:HD21	1.59	0.49
1:J8:250:VAL:HG13	1:K7:6:ASN:HD22	1.77	0.49
3:Q2:103:ILE:HG22	3:Q2:132:ILE:HG22	1.94	0.49
3:R4:106:GLU:HG2	3:R4:129:TYR:HB2	1.94	0.49
4:T1:109:VAL:HG12	4:T1:219:VAL:HB	1.94	0.49
4:T2:158:ARG:HG3	4:T2:186:ILE:HG22	1.94	0.49
7:Z1:125:LEU:HB3	7:Z1:129:TYR:CE2	2.46	0.49
7:Z4:49:LYS:HD2	7:Z4:82:VAL:HG21	1.93	0.49
9:c2:105:SER:HB3	9:c2:119:ASN:HD21	1.76	0.49
9:c3:51:LEU:HA	9:c3:54:ASN:ND2	2.27	0.49
2:p3:128:GLN:O	2:p3:132:GLU:HG2	2.12	0.49
1:B5:265:MET:CE	1:C5:31:SER:HB2	2.42	0.49
1:B7:24:ALA:HA	1:B7:27:MET:HE3	1.94	0.49
1:G1:35:ARG:HB2	1:G1:243:THR:HA	1.94	0.49
1:J6:130:PHE:HB3	1:J6:135:LEU:HD21	1.94	0.49
1:J8:8:ALA:HB1	1:K8:27:MET:SD	2.52	0.49
1:J8:52:MET:HE3	1:J8:237:GLU:HA	1.94	0.49
2:M3:94:HIS:CD2	2:M3:95:GLN:HG2	2.47	0.49
2:P3:246:ALA:HB2	2:P3:270:LYS:HE3	1.92	0.49
4:T3:111:ILE:HD11	4:T3:217:PHE:HD2	1.78	0.49
6:Y2:258:PHE:CE2	6:Y2:267:LEU:HD13	2.48	0.49
8:a3:191:ILE:HG21	8:a4:226:GLU:HG2	1.93	0.49
10:d2:104:ILE:HD11	10:d2:149:PRO:HD2	1.94	0.49
4:t2:108:ALA:HB2	4:t2:220:ARG:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t2:151:MET:HE3	4:t2:193:VAL:HG12	1.94	0.49
1:B8:232:ASN:HD21	1:C8:71:SER:HA	1.78	0.49
1:C6:66:THR:HG23	1:C6:219:LEU:HD22	1.93	0.49
1:D5:114:VAL:HG21	1:D5:185:LEU:HD23	1.94	0.49
1:E4:265:MET:HG2	1:F4:31:SER:HB2	1.93	0.49
1:F4:168:MET:SD	1:F4:208:GLN:HG3	2.52	0.49
1:F5:38:ARG:HD3	1:F6:74:GLN:HE22	1.76	0.49
1:G7:50:GLU:CD	1:G8:84:ASN:HD21	2.20	0.49
1:H9:3:ILE:HG21	1:H9:277:LEU:HD21	1.94	0.49
1:J8:46:LEU:CD2	1:J9:209:ARG:HH22	2.22	0.49
2:P4:141:GLU:HG2	2:p3:217:GLN:HG3	1.94	0.49
3:Q3:73:LEU:HD13	3:Q3:78:VAL:HA	1.94	0.49
3:Q4:62:HIS:HE1	3:Q4:245:ASP:OD1	1.95	0.49
3:R3:80:PHE:CE1	3:R3:91:PRO:HG3	2.47	0.49
4:T3:225:THR:HG22	4:T3:227:GLY:H	1.76	0.49
6:Y5:154:ARG:HD2	6:Y5:161:VAL:HG21	1.94	0.49
1:C4:11:ASN:O	1:C4:14:ARG:HG2	2.12	0.49
1:D3:34:MET:HE1	1:D3:37:ASN:HA	1.94	0.49
1:E3:232:ASN:HD21	1:F3:74:GLN:HG2	1.77	0.49
1:F6:244:ASP:OD2	1:G1:13:HIS:HE1	1.95	0.49
1:H8:209:ARG:HG2	1:H8:209:ARG:HH11	1.77	0.49
1:I6:35:ARG:HG2	1:I6:241:ARG:O	2.12	0.49
2:N2:175:LYS:HA	2:N2:178:ASN:ND2	2.27	0.49
2:O3:215:LEU:HB2	2:O3:216:PRO:HD3	1.94	0.49
2:P4:246:ALA:HB2	2:P4:270:LYS:HE3	1.94	0.49
3:R3:171:ILE:HD12	3:R3:236:PHE:CD2	2.48	0.49
3:S2:240:HIS:CE1	3:S2:244:PHE:HE2	2.31	0.49
9:c1:74:THR:HG23	9:c1:77:LEU:HD12	1.94	0.49
1:A7:225:GLY:HA3	1:B7:82:GLU:OE1	2.12	0.49
1:C8:200:ASP:O	1:C8:203:MET:HG3	2.11	0.49
1:F3:236:SER:O	1:F3:240:ILE:HG12	2.12	0.49
1:I8:12:SER:HB3	1:I8:266:LEU:HD23	1.95	0.49
1:J8:70:MET:HE3	1:J8:216:PHE:CE2	2.47	0.49
1:J8:251:ALA:HA	1:J8:254:LYS:HG2	1.95	0.49
1:K7:92:VAL:HA	1:K7:95:ILE:HG22	1.95	0.49
2:N3:76:ALA:HA	2:N3:79:LYS:HB2	1.94	0.49
3:S6:195:LYS:HB3	3:S6:198:TYR:HB2	1.93	0.49
5:V1:75:GLN:NE2	5:V1:99:ASN:HD21	2.09	0.49
9:c2:35:GLU:HG2	9:c3:123:TYR:CE1	2.47	0.49
1:A6:51:LYS:HA	1:A6:54:THR:HG23	1.94	0.49
1:A7:15:VAL:HG11	1:B7:32:SER:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:89:ARG:HG2	1:A7:89:ARG:HH11	1.78	0.49
1:A8:138:GLY:HA3	1:A8:167:THR:HG23	1.94	0.49
1:D4:276:VAL:HG12	1:D4:280:LEU:HD23	1.95	0.49
1:E6:253:THR:O	1:E6:257:ILE:HG12	2.12	0.49
1:H9:26:ASN:HA	1:H9:29:THR:HG22	1.95	0.49
1:K9:60:ARG:HD3	1:K9:230:TYR:CZ	2.47	0.49
2:M4:214:ASN:HB3	2:M4:217:GLN:NE2	2.28	0.49
2:O3:94:HIS:CD2	2:O3:95:GLN:HG2	2.47	0.49
3:Q1:175:MET:HE2	3:Q1:190:GLU:HB2	1.93	0.49
3:S6:233:LYS:HA	3:S6:237:TYR:CD2	2.48	0.49
4:T2:162:TYR:CE2	4:T2:230:VAL:HG11	2.48	0.49
4:T3:73:GLU:CD	4:T3:98:LYS:HB2	2.37	0.49
1:C4:268:GLN:HA	1:C4:271:VAL:HG12	1.94	0.49
1:E5:246:ALA:CB	1:F4:13:HIS:HE1	2.26	0.49
1:G6:261:SER:O	1:G6:265:MET:HG2	2.12	0.49
1:G6:273:PRO:HA	1:G6:276:VAL:HG22	1.95	0.49
1:J7:100:GLY:HA2	1:J7:107:ARG:HH21	1.76	0.49
1:J7:253:THR:HG21	1:K6:270:ASN:HB3	1.95	0.49
1:K7:1:MET:HE1	1:K7:276:VAL:HG21	1.94	0.49
1:K8:65:ASN:HB3	1:K9:99:ASN:HD22	1.77	0.49
2:N4:262:GLN:HA	2:N4:265:LYS:HE2	1.93	0.49
3:Q2:74:PRO:HD3	3:Q2:251:ILE:HD12	1.95	0.49
4:T3:111:ILE:HD11	4:T3:217:PHE:CD2	2.47	0.49
5:V3:118:VAL:HG22	5:V3:199:LEU:HB3	1.95	0.49
5:V4:57:TRP:CZ2	5:V4:120:PRO:HG3	2.48	0.49
5:X3:131:ARG:HA	5:X3:177:ILE:HD13	1.93	0.49
5:X3:230:TYR:CZ	5:X3:233:SER:HA	2.48	0.49
1:A6:111:GLN:HA	1:A6:114:VAL:HG12	1.94	0.49
1:B6:3:ILE:HG22	1:B6:277:LEU:HD21	1.95	0.49
1:B8:239:ARG:NH2	1:C8:64:ARG:HA	2.26	0.49
1:C3:280:LEU:HD21	1:C4:246:ALA:HA	1.94	0.49
1:J5:52:MET:HE1	1:J5:237:GLU:HA	1.94	0.49
1:J6:171:LYS:HE2	1:J6:176:ILE:HD13	1.95	0.49
1:K5:3:ILE:HG21	1:K5:277:LEU:HD22	1.95	0.49
1:K8:184:THR:HG23	1:K8:190:PHE:HB3	1.94	0.49
2:M5:205:TRP:CD1	2:M5:221:ILE:HG21	2.48	0.49
2:O5:235:TYR:CD2	2:O5:236:PRO:HD3	2.47	0.49
5:V4:135:ILE:HD11	5:V4:216:VAL:HB	1.95	0.49
8:a4:61:ILE:O	8:a4:65:LEU:HG	2.13	0.49
3:s5:127:ALA:HA	3:s5:161:LYS:HB2	1.94	0.49
1:B7:184:THR:HB	1:B7:190:PHE:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:19:GLN:NE2	1:D3:258:LEU:HD13	2.28	0.49
1:D5:66:THR:HG21	1:D5:223:SER:HB2	1.95	0.49
1:F4:50:GLU:CD	1:F5:84:ASN:HD21	2.21	0.49
1:F5:65:ASN:CG	1:F6:99:ASN:HD21	2.21	0.49
1:J8:46:LEU:HG	1:J9:209:ARG:HH12	1.76	0.49
2:N5:269:LYS:HA	2:N5:272:VAL:HG12	1.93	0.49
3:R3:222:ASN:HB2	3:R3:229:ARG:HD3	1.94	0.49
4:T1:18:VAL:HG21	4:t1:238:ARG:HG3	1.95	0.49
5:X3:150:LEU:HD23	5:X3:196:PHE:HA	1.95	0.49
6:Y5:57:PHE:CD1	6:Y5:72:MET:HE1	2.48	0.49
10:d3:68:ILE:O	10:d3:72:ARG:HG3	2.12	0.49
1:D4:23:VAL:HG22	1:D4:255:ASN:HB3	1.94	0.49
1:D4:268:GLN:HA	1:D4:271:VAL:HG22	1.95	0.49
1:E6:52:MET:O	1:E6:56:VAL:HG23	2.13	0.49
1:F4:173:LEU:HB3	1:F4:175:LEU:HD23	1.94	0.49
1:F5:26:ASN:HA	1:F5:29:THR:HG22	1.95	0.49
1:G9:167:THR:HG22	1:G9:169:THR:HG22	1.94	0.49
1:H7:112:VAL:O	1:H7:116:GLN:HG2	2.13	0.49
1:I7:56:VAL:HG11	1:I7:234:GLN:HG2	1.95	0.49
1:J8:14:ARG:CZ	1:J9:228:VAL:HG22	2.43	0.49
2:L2:94:HIS:CD2	2:L2:95:GLN:HG3	2.48	0.49
2:L4:75:GLU:HG2	2:L4:76:ALA:H	1.77	0.49
2:M5:246:ALA:HB2	2:M5:270:LYS:HE3	1.94	0.49
2:O4:126:ILE:O	2:O4:130:ARG:HG2	2.12	0.49
2:P5:112:TYR:CZ	2:P5:200:ASP:HB3	2.48	0.49
4:T4:153:VAL:O	4:T4:190:PRO:HA	2.12	0.49
5:X5:190:LEU:HD23	5:X5:192:LYS:HE2	1.94	0.49
8:a4:183:ALA:HA	8:a4:186:VAL:HG12	1.94	0.49
1:j0:86:ILE:HG23	1:j0:117:LEU:HD12	1.94	0.49
1:A4:36:ILE:HG23	1:A4:41:ASP:HB2	1.94	0.48
1:A4:281:ARG:NH2	1:K5:261:SER:HB2	2.28	0.48
1:B5:34:MET:HB2	1:B5:37:ASN:HB3	1.95	0.48
1:B6:151:PHE:HA	1:B7:99:ASN:OD1	2.13	0.48
1:D5:18:PHE:CD2	1:D6:224:LYS:HE3	2.47	0.48
1:E5:259:VAL:O	1:E5:263:THR:HG23	2.13	0.48
1:E7:107:ARG:HD3	1:E7:186:SER:O	2.13	0.48
1:F2:52:MET:HE2	1:F2:52:MET:HA	1.93	0.48
1:F4:88:GLN:O	1:F4:92:VAL:HG23	2.13	0.48
1:G1:200:ASP:O	1:G1:203:MET:HG3	2.13	0.48
1:G9:163:VAL:O	1:G9:163:VAL:HG13	2.13	0.48
1:G9:261:SER:HB3	1:H8:277:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q1:245:ASP:O	3:Q1:249:THR:HG23	2.12	0.48
3:S3:78:VAL:HG12	3:S3:106:GLU:HG2	1.95	0.48
5:X1:136:TRP:CE2	5:X1:172:LYS:HD3	2.48	0.48
5:X5:143:ARG:HB2	5:X5:207:GLU:HG2	1.95	0.48
8:a5:82:PHE:CE2	8:a5:102:ARG:HD2	2.48	0.48
4:t3:257:ASP:HA	4:t3:260:CYS:SG	2.53	0.48
1:A4:252:PHE:HZ	1:K4:268:GLN:HG3	1.77	0.48
1:E2:265:MET:SD	1:F2:31:SER:HA	2.54	0.48
1:F3:236:SER:CB	1:G8:71:SER:HB2	2.42	0.48
1:G8:70:MET:HE2	1:G8:220:GLU:HA	1.95	0.48
1:I5:38:ARG:HH12	1:I5:41:ASP:CG	2.21	0.48
1:I8:80:LEU:HD11	1:I8:168:MET:HE3	1.95	0.48
1:J6:162:ARG:HG2	1:J6:164:TYR:CZ	2.48	0.48
1:K7:106:ASP:O	1:K7:110:ILE:HG13	2.12	0.48
1:K9:150:TRP:CH2	1:K9:162:ARG:HB2	2.48	0.48
2:O3:78:TRP:HA	2:O4:203:ARG:NH2	2.27	0.48
2:O3:267:ARG:O	2:O3:270:LYS:HG2	2.12	0.48
3:R3:76:ARG:NH1	3:R3:76:ARG:HA	2.28	0.48
3:R5:63:THR:O	3:R5:66:MET:HG2	2.13	0.48
4:T1:216:GLN:HE22	4:T1:218:LYS:HB2	1.78	0.48
5:X2:104:VAL:HB	5:X2:214:PHE:CZ	2.48	0.48
8:a4:99:LEU:HD21	8:a4:128:LYS:HE3	1.95	0.48
9:c2:30:PHE:O	9:c2:34:GLU:HG2	2.13	0.48
3:s3:53:PHE:HA	3:s3:56:ASN:ND2	2.28	0.48
1:B8:104:ALA:O	1:B8:108:GLN:HG2	2.13	0.48
1:B8:193:ASP:HB3	5:V4:65:LEU:HG	1.95	0.48
1:C3:18:PHE:CZ	1:C4:224:LYS:HA	2.48	0.48
1:E2:23:VAL:HG22	1:E2:255:ASN:HB3	1.95	0.48
1:I8:130:PHE:O	1:I8:133:MET:HG2	2.13	0.48
1:J9:150:TRP:CZ3	1:J9:162:ARG:HB2	2.48	0.48
2:M1:87:ASP:HB2	2:M2:243:SER:HA	1.94	0.48
2:M2:148:VAL:HA	2:M2:151:LYS:HG2	1.95	0.48
2:N3:268:TYR:HA	2:N3:271:ASN:ND2	2.28	0.48
3:R3:56:ASN:O	3:R3:60:THR:HG23	2.13	0.48
3:S6:56:ASN:O	3:S6:60:THR:HG23	2.13	0.48
4:T3:154:TRP:HB2	4:T3:235:ASP:O	2.13	0.48
4:T3:156:CYS:HB3	4:T3:188:TRP:CD2	2.48	0.48
5:X2:191:ASP:C	5:X2:193:ASN:H	2.22	0.48
8:a2:148:LYS:HB3	8:a2:152:GLU:HB2	1.95	0.48
10:d4:95:LEU:HA	10:d4:98:ILE:HG22	1.94	0.48
4:t1:160:ASN:CG	4:t1:230:VAL:HG13	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B4:14:ARG:NH1	1:B5:228:VAL:HG22	2.29	0.48
1:C4:16:LEU:HD11	1:C4:263:THR:HG22	1.94	0.48
1:E4:261:SER:HB2	1:F3:277:LEU:HD13	1.94	0.48
1:E5:61:GLN:HE21	1:E6:96:GLN:CD	2.22	0.48
1:G1:130:PHE:HB2	1:G1:135:LEU:HD11	1.95	0.48
1:K8:57:LYS:CE	1:K9:92:VAL:HG22	2.43	0.48
3:R2:152:ILE:HB	3:R2:180:ASN:HD22	1.77	0.48
3:S4:62:HIS:HE1	3:S4:245:ASP:OD1	1.95	0.48
3:S5:237:TYR:CZ	3:S5:241:LEU:HD11	2.49	0.48
4:T4:31:TRP:HZ3	4:T4:42:TRP:CD1	2.31	0.48
5:V1:138:LEU:HD12	5:V1:170:TRP:CZ2	2.48	0.48
5:V3:56:ASP:HB3	5:V3:121:PRO:HG3	1.95	0.48
5:X3:50:ASN:HB2	12:X3:401:HOH:O	2.14	0.48
4:t2:109:VAL:HB	4:t2:219:VAL:HG22	1.95	0.48
1:A6:239:ARG:HH22	1:B6:68:ASP:N	2.11	0.48
1:E5:90:ILE:HD11	1:E5:114:VAL:HA	1.95	0.48
1:E5:163:VAL:HG23	1:E5:215:TYR:CZ	2.49	0.48
1:I7:151:PHE:CE2	1:I7:163:VAL:HG21	2.49	0.48
1:J7:86:ILE:HG23	1:J7:117:LEU:HD12	1.94	0.48
1:K5:214:ALA:O	1:K5:218:ARG:HG3	2.14	0.48
2:M4:262:GLN:HA	2:M4:265:LYS:HE2	1.95	0.48
2:P5:246:ALA:O	2:P5:249:GLU:HG3	2.13	0.48
3:S2:198:TYR:CG	3:S2:199:PRO:HD2	2.48	0.48
4:T3:14:THR:HB	4:t3:189:ARG:HD2	1.94	0.48
5:V1:50:ASN:CG	5:V1:52:GLU:HG2	2.39	0.48
5:X5:134:SER:OG	5:X5:172:LYS:HE3	2.14	0.48
7:Z1:97:GLN:NE2	7:Z2:138:LYS:HE2	2.29	0.48
7:Z2:333:ALA:HA	7:Z2:336:ILE:HD12	1.96	0.48
8:a2:149:ILE:HG13	8:a2:150:THR:N	2.29	0.48
9:c1:46:ALA:O	9:c1:50:THR:HG23	2.14	0.48
10:d4:104:ILE:HG12	10:d4:148:TYR:CG	2.48	0.48
1:j0:106:ASP:HA	1:j0:109:MET:HE3	1.95	0.48
2:p4:174:THR:HG1	2:p4:205:TRP:HZ3	1.61	0.48
4:t1:10:ILE:HD11	4:t1:208:GLN:HG2	1.96	0.48
1:C8:86:ILE:O	1:C8:90:ILE:HG13	2.14	0.48
1:F3:110:ILE:O	1:F3:114:VAL:HG23	2.13	0.48
1:K8:150:TRP:CE2	1:K8:162:ARG:HD3	2.47	0.48
2:M1:186:PRO:HA	2:M1:189:ARG:HG3	1.94	0.48
2:M4:229:ASP:CG	2:M4:230:GLU:H	2.22	0.48
6:Y5:257:ILE:O	6:Y5:267:LEU:HD12	2.13	0.48
7:Z3:143:LYS:HE2	7:Z3:145:ASN:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z3:163:LYS:HA	7:Z3:168:VAL:HG21	1.96	0.48
10:d4:105:LYS:HB2	10:d4:106:PRO:HD3	1.96	0.48
1:h1:111:GLN:HA	1:h1:114:VAL:HG12	1.94	0.48
1:j0:183:LEU:HD21	1:j0:194:ALA:HB1	1.96	0.48
3:s5:223:THR:HG23	3:s5:226:HIS:H	1.77	0.48
1:A7:52:MET:HE2	1:A7:233:ILE:HG23	1.94	0.48
1:A8:218:ARG:HH22	1:B8:119:ASP:CG	2.22	0.48
1:C4:82:GLU:HA	1:C4:85:ASP:OD2	2.13	0.48
1:D6:36:ILE:HD12	1:D6:46:LEU:HA	1.96	0.48
1:E5:211:ASN:OD1	1:F5:112:VAL:HG11	2.14	0.48
1:F3:3:ILE:HG21	1:F3:277:LEU:HD11	1.96	0.48
1:G8:18:PHE:CZ	1:G9:224:LYS:HA	2.49	0.48
1:H9:106:ASP:O	1:H9:109:MET:HG2	2.13	0.48
2:P5:213:GLN:HG3	2:P5:213:GLN:O	2.13	0.48
3:Q4:217:LEU:O	3:Q4:220:VAL:HG22	2.13	0.48
4:T4:151:MET:O	4:T4:192:THR:HA	2.13	0.48
5:V5:201:VAL:HG11	5:V5:212:PHE:CE2	2.49	0.48
7:Z1:218:ASN:O	7:Z1:222:ILE:HG12	2.14	0.48
10:d2:37:ILE:HD12	10:d2:66:PRO:HG2	1.95	0.48
3:s3:48:LEU:HD11	3:s3:234:LYS:HG2	1.94	0.48
1:B6:91:ARG:O	1:B6:95:ILE:HD12	2.13	0.48
1:B7:84:ASN:O	1:B7:87:ILE:HG22	2.14	0.48
1:C7:23:VAL:O	1:C7:27:MET:HG2	2.14	0.48
1:D4:118:VAL:HG11	1:D4:182:LEU:HD11	1.96	0.48
1:D5:107:ARG:HG2	1:D5:186:SER:O	2.14	0.48
1:D6:237:GLU:HA	1:D6:240:ILE:HG22	1.95	0.48
1:E2:18:PHE:CE2	1:E3:224:LYS:HG3	2.48	0.48
1:H7:130:PHE:HB2	1:H7:135:LEU:HD11	1.96	0.48
2:N2:128:GLN:HA	2:N2:131:LYS:HG2	1.95	0.48
3:Q3:62:HIS:CD2	3:Q3:248:PHE:HB3	2.49	0.48
3:Q3:106:GLU:CD	3:Q3:129:TYR:HE1	2.21	0.48
3:R4:42:LEU:HA	3:R4:45:GLU:HG2	1.94	0.48
4:T3:214:PHE:HZ	4:T3:217:PHE:HE1	1.62	0.48
4:T4:78:SER:HA	4:T4:93:LYS:HB3	1.96	0.48
3:s3:65:LEU:HD12	3:s3:252:PHE:HB2	1.96	0.48
4:t1:142:VAL:HB	4:t1:214:PHE:HB3	1.95	0.48
4:t2:113:PRO:HG3	4:t2:141:GLY:HA2	1.95	0.48
1:B6:24:ALA:O	1:B6:27:MET:HB3	2.13	0.48
1:C3:5:HIS:CE1	1:C4:234:GLN:HE22	2.32	0.48
1:D6:265:MET:HE2	1:E6:27:MET:HE3	1.96	0.48
1:E4:51:LYS:HA	1:E4:54:THR:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E5:261:SER:OG	1:F4:277:LEU:HD11	2.14	0.48
1:E6:236:SER:OG	1:F6:71:SER:HB3	2.14	0.48
1:F4:65:ASN:HD21	1:F5:99:ASN:CB	2.25	0.48
1:F4:157:GLN:NE2	1:F5:195:ILE:HG22	2.29	0.48
1:F4:157:GLN:NE2	1:F5:196:GLY:HA2	2.29	0.48
1:F5:157:GLN:NE2	1:F6:195:ILE:HG22	2.28	0.48
1:H7:87:ILE:HD12	1:H7:205:ILE:HD13	1.96	0.48
1:I7:36:ILE:HG12	1:I7:42:ASP:HB3	1.96	0.48
1:K9:56:VAL:HG13	1:K9:230:TYR:CE1	2.44	0.48
1:K9:66:THR:HG22	1:K9:153:ILE:HG23	1.96	0.48
2:N6:183:ILE:HG23	2:N6:189:ARG:HH22	1.77	0.48
2:O3:206:ILE:HG12	2:O3:222:LEU:HD21	1.95	0.48
3:Q1:59:LEU:O	3:Q1:63:THR:HG23	2.13	0.48
3:R2:84:ALA:HB2	3:R2:102:CYS:HB3	1.96	0.48
3:S5:48:LEU:HD12	3:S5:51:LYS:HD2	1.94	0.48
5:X2:43:LEU:HD23	5:X2:224:ASP:OD1	2.13	0.48
5:X2:53:GLU:HB2	7:Z2:182:ARG:HH22	1.79	0.48
5:X2:130:ALA:HB1	5:X2:222:ARG:O	2.13	0.48
5:X3:49:GLU:CG	5:X3:219:LEU:HB3	2.43	0.48
6:Y2:268:VAL:O	6:Y2:268:VAL:HG13	2.14	0.48
7:Z2:128:PHE:HB3	7:Z2:132:ARG:HH21	1.79	0.48
2:p2:130:ARG:O	2:p2:133:GLU:HG3	2.14	0.48
4:t1:244:PHE:HA	4:t1:247:HIS:CE1	2.48	0.48
4:t2:94:VAL:HA	4:t2:235:ASP:OD1	2.14	0.48
1:A5:66:THR:HG23	1:A5:219:LEU:HD12	1.96	0.48
1:B6:111:GLN:HG2	1:B6:185:LEU:HD12	1.96	0.48
1:E6:261:SER:O	1:E6:265:MET:HG2	2.14	0.48
1:H7:138:GLY:HA2	1:H7:167:THR:HG22	1.96	0.48
1:I9:85:ASP:O	1:I9:88:GLN:HG3	2.14	0.48
1:K6:277:LEU:HA	1:K6:280:LEU:HG	1.96	0.48
2:N2:269:LYS:O	2:N2:272:VAL:HG12	2.14	0.48
2:P2:78:TRP:CE3	2:P3:236:PRO:HB3	2.49	0.48
3:S4:245:ASP:O	3:S4:249:THR:HG23	2.14	0.48
3:S6:73:LEU:HD13	3:S6:78:VAL:HA	1.94	0.48
4:T3:99:PHE:CE2	4:T3:230:VAL:HG21	2.49	0.48
8:a3:127:ARG:HE	8:a3:139:GLU:CD	2.22	0.48
1:h0:111:GLN:OE1	1:h0:185:LEU:HB2	2.14	0.48
1:B8:167:THR:HG22	1:B8:172:SER:HB3	1.95	0.47
1:C7:247:GLU:CD	1:D6:13:HIS:CE1	2.92	0.47
1:K7:229:ALA:O	1:K7:233:ILE:HG22	2.14	0.47
2:N4:214:ASN:OD1	2:N4:217:GLN:HB2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P4:126:ILE:HD12	2:P4:158:VAL:HG13	1.95	0.47
3:Q3:173:GLU:HB3	3:Q3:192:PHE:HB3	1.95	0.47
7:Z4:94:GLU:HA	7:Z4:97:GLN:HG2	1.96	0.47
4:t3:20:GLY:HA2	4:t3:244:PHE:CB	2.44	0.47
4:t3:180:PHE:HB3	4:t3:191:LEU:HD11	1.95	0.47
1:A5:218:ARG:CD	1:B5:120:GLU:HB2	2.44	0.47
1:A6:179:ASP:HA	5:X2:180:PHE:HB2	1.96	0.47
1:B6:114:VAL:HG21	1:B6:185:LEU:HD21	1.96	0.47
1:E5:168:MET:HE1	1:E5:205:ILE:HA	1.96	0.47
1:F5:23:VAL:O	1:F5:27:MET:HG2	2.13	0.47
1:G8:187:THR:HG23	1:G8:190:PHE:H	1.80	0.47
1:G8:265:MET:HE3	1:H8:30:LEU:CD2	2.43	0.47
1:H7:23:VAL:CG2	1:H7:255:ASN:HB3	2.44	0.47
1:K6:3:ILE:HD12	1:K7:245:MET:HE3	1.96	0.47
2:P2:219:ILE:HB	2:P2:220:PRO:HD3	1.97	0.47
3:Q3:78:VAL:HG22	3:Q3:106:GLU:HB2	1.96	0.47
3:S5:103:ILE:O	3:S5:131:GLU:HA	2.13	0.47
4:T3:81:PRO:HG2	4:T3:84:ILE:HB	1.97	0.47
5:V3:187:PHE:CD2	5:V3:189:LEU:HB2	2.49	0.47
1:i0:60:ARG:O	1:i0:63:GLU:HG3	2.14	0.47
3:s3:52:ILE:HA	3:s3:55:LEU:HG	1.95	0.47
4:t4:36:PRO:HA	4:t4:39:PRO:HG3	1.95	0.47
1:B6:150:TRP:CZ3	1:B6:162:ARG:HB2	2.49	0.47
1:C5:150:TRP:CZ3	1:C5:162:ARG:HB2	2.49	0.47
1:E4:272:ARG:HB3	1:E4:273:PRO:HD3	1.95	0.47
1:F2:3:ILE:HD11	1:F2:276:VAL:HG11	1.97	0.47
1:F2:36:ILE:HD12	1:F2:41:ASP:HB2	1.96	0.47
1:G2:203:MET:HE3	1:h1:105:GLU:HG2	1.95	0.47
1:H7:187:THR:HG23	1:H7:190:PHE:H	1.80	0.47
1:H9:200:ASP:HA	1:H9:203:MET:HG2	1.95	0.47
1:I6:18:PHE:CD2	1:I7:224:LYS:HD3	2.49	0.47
1:I6:157:GLN:HG2	1:I6:158:HIS:CD2	2.50	0.47
1:J8:152:HIS:HE1	1:J9:99:ASN:ND2	2.13	0.47
1:K7:61:GLN:NE2	1:K8:96:GLN:HB2	2.28	0.47
2:P2:235:TYR:CG	2:P2:236:PRO:HD3	2.48	0.47
3:S3:44:THR:O	3:S3:47:LYS:HG3	2.14	0.47
3:S6:103:ILE:O	3:S6:131:GLU:HA	2.14	0.47
4:T1:192:THR:HG22	4:t1:18:VAL:HG13	1.95	0.47
3:s5:58:ARG:O	3:s5:61:ARG:HG2	2.14	0.47
4:t4:155:VAL:HA	4:t4:233:PHE:O	2.14	0.47
1:A5:132:LYS:H	1:K5:55:GLN:NE2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:203:MET:HE3	1:A5:207:LYS:HB2	1.96	0.47
1:A7:25:LYS:O	1:A7:29:THR:HG23	2.14	0.47
1:E3:47:ALA:HA	1:E4:206:ASN:HD21	1.78	0.47
1:F5:99:ASN:HD22	1:F5:101:ILE:HG12	1.78	0.47
1:I6:151:PHE:HB3	1:I6:153:ILE:HD11	1.95	0.47
2:N6:123:ARG:HD3	2:N6:126:ILE:HD11	1.95	0.47
2:O3:75:GLU:C	2:O3:77:LEU:H	2.23	0.47
3:S5:70:VAL:HG22	3:S5:255:ASN:ND2	2.29	0.47
4:T2:243:VAL:HG12	4:T2:243:VAL:O	2.14	0.47
10:d2:85:PRO:HG3	10:d2:134:MET:HG2	1.96	0.47
4:t3:160:ASN:ND2	4:t3:230:VAL:HG22	2.30	0.47
1:A6:246:ALA:HB3	1:B5:13:HIS:CE1	2.49	0.47
1:A7:27:MET:O	1:A7:27:MET:HE3	2.14	0.47
1:A8:28:GLU:HG2	1:A8:37:ASN:HD22	1.79	0.47
1:C8:105:GLU:O	1:C8:109:MET:HG2	2.15	0.47
1:D6:51:LYS:HA	1:D6:54:THR:HG22	1.97	0.47
1:E4:157:GLN:HG3	1:E4:158:HIS:CG	2.49	0.47
1:F4:224:LYS:O	1:F4:228:VAL:HG23	2.14	0.47
1:I7:254:LYS:HD2	1:J6:4:ASN:O	2.14	0.47
1:J9:26:ASN:HA	1:J9:29:THR:HG22	1.97	0.47
3:R2:65:LEU:HD12	3:R2:252:PHE:HB2	1.96	0.47
4:T4:37:SER:C	4:T4:39:PRO:HD3	2.39	0.47
5:V1:57:TRP:CZ2	5:V1:120:PRO:HG3	2.50	0.47
5:V5:81:ASP:HA	5:V5:170:TRP:O	2.15	0.47
6:Y3:96:THR:HG23	6:Y3:98:ILE:HG12	1.96	0.47
7:Z1:223:GLU:CD	7:Z1:240:ARG:HH21	2.21	0.47
1:h0:235:ALA:O	1:h0:239:ARG:HG2	2.15	0.47
3:s5:41:ILE:H	3:s5:41:ILE:HD12	1.80	0.47
4:t1:35:ALA:HB1	4:t1:36:PRO:HD2	1.96	0.47
1:A5:72:LEU:HD12	1:A5:130:PHE:CD1	2.50	0.47
1:C5:22:GLU:O	1:C5:25:LYS:HG3	2.15	0.47
1:E6:44:SER:O	1:E6:48:VAL:HG12	2.14	0.47
1:G2:81:GLN:NE2	1:G2:209:ARG:HH11	2.12	0.47
1:J5:19:GLN:O	1:J5:23:VAL:HG23	2.15	0.47
2:L3:151:LYS:O	2:L3:154:GLU:HG3	2.13	0.47
2:N4:179:HIS:O	2:N4:182:GLU:HG2	2.15	0.47
2:O1:79:LYS:HG3	2:O1:79:LYS:O	2.14	0.47
2:P2:170:LEU:HD22	2:P2:212:LEU:HD22	1.95	0.47
3:S6:131:GLU:HB2	3:S6:156:LYS:HB3	1.95	0.47
4:T4:80:LYS:HD3	4:T4:92:ALA:HB1	1.97	0.47
5:V5:146:LEU:HG	5:V5:162:LEU:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z3:216:ARG:NH1	7:Z3:247:ALA:HB2	2.30	0.47
1:h0:46:LEU:HD21	1:h1:209:ARG:NH2	2.29	0.47
3:s3:185:HIS:HB2	3:s3:188:LYS:HG2	1.95	0.47
3:s4:62:HIS:CE1	3:s4:245:ASP:HA	2.49	0.47
3:s4:76:ARG:HD3	3:s4:110:PHE:CE1	2.50	0.47
1:A5:232:ASN:HD21	1:B5:74:GLN:C	2.23	0.47
1:A8:22:GLU:HG2	1:A8:25:LYS:HE3	1.97	0.47
1:A8:82:GLU:OE2	1:K8:221:HIS:HB3	2.15	0.47
1:B7:136:LEU:HB3	1:B7:168:MET:HB2	1.97	0.47
1:D7:85:ASP:O	1:D7:88:GLN:HG3	2.14	0.47
1:E4:97:SER:OG	1:E4:185:LEU:HB3	2.15	0.47
1:E6:18:PHE:CE1	1:E7:224:LYS:HD2	2.50	0.47
1:G1:130:PHE:O	1:G1:133:MET:HG2	2.15	0.47
1:H8:84:ASN:HD22	1:H8:205:ILE:HD11	1.80	0.47
1:I5:16:LEU:HD13	1:I5:262:GLY:HA3	1.96	0.47
1:I5:25:LYS:O	1:I5:28:GLU:HG3	2.15	0.47
1:I7:136:LEU:HD13	1:I7:168:MET:HE2	1.96	0.47
1:I8:217:ASN:HA	1:I8:220:GLU:HG2	1.97	0.47
1:J8:35:ARG:HB2	1:J8:243:THR:HB	1.96	0.47
1:K8:150:TRP:CZ2	1:K8:162:ARG:HD3	2.49	0.47
2:L5:290:LYS:HA	2:L5:293:VAL:HG12	1.97	0.47
2:M3:128:GLN:HA	2:M3:131:LYS:HG2	1.95	0.47
3:Q2:171:ILE:HG12	3:Q2:193:PHE:CE1	2.50	0.47
3:R5:186:ASN:HB3	3:R5:217:LEU:HD23	1.96	0.47
3:S5:46:ARG:NH1	3:S5:50:GLU:HB3	2.30	0.47
3:S6:64:VAL:HB	3:S6:144:PRO:HB3	1.97	0.47
4:T2:44:VAL:HG12	4:T2:111:ILE:HG12	1.96	0.47
4:T3:23:LEU:HB2	4:T3:240:LEU:HD21	1.97	0.47
4:T3:151:MET:HE3	4:T3:153:VAL:HB	1.39	0.47
4:T3:244:PHE:HA	4:T3:247:HIS:CD2	2.49	0.47
4:T4:52:GLN:HG2	4:T4:59:GLN:HE22	1.78	0.47
4:T4:100:GLN:HG3	4:T4:229:THR:HA	1.96	0.47
5:V4:82:VAL:HG13	5:V4:83:PHE:CD2	2.50	0.47
5:X1:54:ALA:CB	5:X1:102:LEU:HD21	2.44	0.47
5:X1:123:GLU:HG3	7:Z1:174:ASN:OD1	2.14	0.47
5:X3:132:GLN:HE22	5:X3:222:ARG:HH21	1.60	0.47
6:Y2:68:PHE:HZ	6:Y2:219:LEU:HD21	1.79	0.47
6:Y3:129:MET:SD	6:Y3:223:THR:HB	2.54	0.47
6:Y4:195:LYS:O	6:Y4:198:VAL:HG22	2.15	0.47
7:Z1:204:MET:HG3	7:Z1:207:LYS:HE3	1.97	0.47
8:a2:192:TYR:CE2	8:a2:196:LEU:HD11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c1:96:LYS:HE3	9:c1:125:ARG:HH12	1.79	0.47
10:d3:84:HIS:CE1	10:d3:130:GLU:HA	2.49	0.47
2:p3:267:ARG:O	2:p3:270:LYS:HG2	2.15	0.47
3:s3:76:ARG:NE	3:s3:108:TYR:HB2	2.29	0.47
1:C5:255:ASN:O	1:C5:259:VAL:HG23	2.15	0.47
1:C5:257:ILE:HG21	1:D4:3:ILE:HD11	1.95	0.47
1:C7:97:SER:HB2	1:C7:110:ILE:HG21	1.95	0.47
1:D7:145:ARG:HH21	8:a5:94:ARG:HA	1.80	0.47
1:F5:50:GLU:CD	1:F6:84:ASN:HD21	2.23	0.47
1:H6:61:GLN:HG2	1:H7:96:GLN:HB2	1.97	0.47
1:K4:5:HIS:HB2	1:K5:238:SER:HB3	1.97	0.47
1:K6:7:LEU:HD13	1:K7:235:ALA:HB2	1.97	0.47
1:K6:65:ASN:HD21	1:K7:99:ASN:HB2	1.80	0.47
3:Q3:70:VAL:HA	3:Q3:255:ASN:HD21	1.80	0.47
4:T2:146:GLY:C	4:T2:209:VAL:HG11	2.40	0.47
5:X1:51:PHE:HB3	5:X1:102:LEU:HD23	1.97	0.47
6:Y2:108:PHE:CG	6:Y2:109:PRO:HD2	2.50	0.47
6:Y3:139:TRP:CD2	6:Y3:166:PRO:HD3	2.50	0.47
8:a3:163:LYS:HB2	8:a3:170:LYS:HG2	1.97	0.47
4:t2:37:SER:C	4:t2:39:PRO:HD3	2.38	0.47
1:A4:245:MET:O	1:A4:249:THR:HG23	2.15	0.47
1:A8:91:ARG:HE	1:A8:95:ILE:HD11	1.80	0.47
1:B5:3:ILE:HD13	1:B5:277:LEU:HD22	1.96	0.47
1:C4:151:PHE:CE2	1:C4:163:VAL:HG21	2.50	0.47
1:C8:99:ASN:ND2	1:C8:101:ILE:HG12	2.30	0.47
1:E3:157:GLN:HG3	1:E3:158:HIS:CG	2.50	0.47
1:E4:100:GLY:HA2	1:E4:107:ARG:NH2	2.29	0.47
1:G2:224:LYS:O	1:G2:228:VAL:HG23	2.15	0.47
1:H6:38:ARG:NH1	1:H7:77:GLU:HB2	2.30	0.47
1:J5:35:ARG:HH12	1:J5:42:ASP:HB2	1.80	0.47
2:L4:205:TRP:CH2	2:L4:209:GLU:HG3	2.50	0.47
2:L5:220:PRO:HA	2:L5:223:GLU:HG2	1.95	0.47
2:M3:205:TRP:NE1	2:M3:221:ILE:HG13	2.29	0.47
2:N4:205:TRP:NE1	2:N4:221:ILE:HG13	2.30	0.47
2:N5:91:GLN:OE1	2:N5:94:HIS:HE1	1.97	0.47
2:O2:145:TRP:HA	2:O2:148:VAL:HG22	1.96	0.47
3:R5:108:TYR:HD2	3:R5:126:LEU:N	2.13	0.47
3:S3:198:TYR:CE2	3:S3:212:VAL:HG21	2.50	0.47
5:V2:197:VAL:O	5:V2:198:SER:HB2	2.15	0.47
6:Y3:92:ILE:HG13	6:Y3:252:LYS:HB3	1.96	0.47
10:d4:170:ARG:NE	10:d4:201:THR:HG21	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p2:293:VAL:HA	2:p2:296:VAL:HG22	1.96	0.47
1:A6:207:LYS:HD3	1:B6:109:MET:HE1	1.96	0.47
1:B5:38:ARG:NH2	1:B6:74:GLN:HB2	2.29	0.47
1:C4:220:GLU:O	1:C4:224:LYS:HG2	2.15	0.47
1:D3:150:TRP:CZ2	1:D3:162:ARG:HD2	2.50	0.47
1:E5:187:THR:HG23	1:E5:189:GLU:HG2	1.97	0.47
1:E6:220:GLU:O	1:E6:224:LYS:HG2	2.15	0.47
1:F6:108:GLN:O	1:F6:112:VAL:HG23	2.15	0.47
1:G9:36:ILE:HD13	1:G9:46:LEU:HA	1.96	0.47
1:I6:18:PHE:CE2	1:I7:224:LYS:HD3	2.50	0.47
1:J6:66:THR:HG21	1:J6:223:SER:HB2	1.97	0.47
1:J6:257:ILE:HD11	1:K5:277:LEU:HB3	1.96	0.47
1:J7:218:ARG:HD2	1:K7:120:GLU:OE1	2.14	0.47
1:J9:246:ALA:O	1:J9:250:VAL:HG23	2.15	0.47
1:K6:107:ARG:HA	1:K6:110:ILE:HG12	1.97	0.47
1:K6:268:GLN:HA	1:K6:271:VAL:HG12	1.97	0.47
1:K7:52:MET:HE1	1:K7:240:ILE:HD12	1.96	0.47
2:M4:248:GLU:O	2:M4:251:MET:HG3	2.15	0.47
2:N3:238:HIS:HB3	2:N3:277:ALA:HB2	1.96	0.47
3:Q3:64:VAL:HA	3:Q3:147:GLU:HG2	1.97	0.47
10:d2:119:GLN:HE22	10:d2:121:LYS:HG3	1.80	0.47
1:A7:38:ARG:HE	1:A8:77:GLU:CD	2.23	0.46
1:B5:42:ASP:CG	1:C6:89:ARG:HH22	2.23	0.46
1:D5:130:PHE:O	1:D5:133:MET:HG3	2.15	0.46
1:F2:2:ILE:HG21	1:F3:238:SER:HB2	1.96	0.46
1:I8:23:VAL:HG22	1:I8:255:ASN:HB3	1.97	0.46
1:J7:272:ARG:HB3	1:J7:273:PRO:HD3	1.96	0.46
1:J8:14:ARG:HE	1:J9:231:GLU:CD	2.23	0.46
2:L2:215:LEU:O	2:L2:219:ILE:HG13	2.14	0.46
2:M4:94:HIS:CD2	2:M4:95:GLN:HG2	2.49	0.46
2:M4:205:TRP:HE1	2:M4:221:ILE:HG13	1.80	0.46
2:N4:94:HIS:C	2:N4:96:LEU:H	2.23	0.46
3:Q3:70:VAL:HA	3:Q3:255:ASN:ND2	2.29	0.46
4:T2:171:TRP:HD1	4:T2:210:LYS:HE2	1.79	0.46
5:V4:138:LEU:HD12	5:V4:170:TRP:CE2	2.51	0.46
7:Z3:34:LEU:HD13	7:Z3:111:PHE:CE2	2.50	0.46
8:a5:214:ALA:HA	8:a5:217:ASP:OD2	2.15	0.46
9:c2:103:PHE:HB3	9:c2:121:VAL:HB	1.96	0.46
4:t1:162:TYR:CE1	4:t1:230:VAL:HG21	2.51	0.46
1:B4:30:LEU:HB2	1:B4:248:GLU:HG2	1.97	0.46
1:B4:254:LYS:O	1:B4:258:LEU:HD23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:278:GLN:O	1:D3:281:ARG:HD2	2.14	0.46
1:E5:46:LEU:HD21	1:E6:209:ARG:HD3	1.96	0.46
1:F5:3:ILE:HD13	1:F5:277:LEU:HD21	1.98	0.46
1:G1:195:ILE:HG22	1:G9:157:GLN:NE2	2.30	0.46
1:G9:1:MET:HE1	1:G9:280:LEU:HD21	1.98	0.46
1:H8:169:THR:HG23	1:H8:172:SER:H	1.80	0.46
1:K7:68:ASP:HB3	1:K8:101:ILE:HD13	1.97	0.46
2:L6:285:ARG:HE	2:L6:286:PRO:HD2	1.79	0.46
2:P4:75:GLU:C	2:P4:77:LEU:H	2.23	0.46
2:P5:219:ILE:HB	2:P5:220:PRO:HD3	1.97	0.46
3:Q1:130:MET:HE2	3:Q1:244:PHE:CE1	2.50	0.46
3:R2:67:LYS:HB2	3:R2:144:PRO:HB3	1.96	0.46
3:R2:68:MET:HE3	3:R2:69:LYS:H	1.79	0.46
4:T1:94:VAL:HG12	4:T1:235:ASP:CG	2.39	0.46
1:h0:111:GLN:HA	1:h0:114:VAL:HG12	1.96	0.46
4:t3:80:LYS:HB2	4:t3:84:ILE:HD11	1.97	0.46
1:A7:160:ARG:HH21	1:A8:188:ALA:HB1	1.80	0.46
1:B5:20:ASN:HA	1:B5:23:VAL:HG12	1.97	0.46
1:C7:232:ASN:ND2	1:D7:75:THR:HA	2.30	0.46
1:E6:208:GLN:HA	1:E6:211:ASN:HD22	1.80	0.46
1:G1:168:MET:HA	1:G1:168:MET:HE2	1.97	0.46
1:J8:118:VAL:HA	1:J8:121:ILE:HG22	1.97	0.46
1:J9:65:ASN:ND2	1:J9:152:HIS:CE1	2.83	0.46
1:K5:275:SER:O	1:K5:279:LEU:HG	2.16	0.46
1:K6:74:GLN:O	1:K6:77:GLU:HG3	2.15	0.46
2:M4:189:ARG:HA	2:M4:194:PHE:CE2	2.50	0.46
3:Q3:49:ASP:O	3:Q3:52:ILE:HG22	2.16	0.46
3:R3:179:PRO:HA	3:R3:188:LYS:HZ1	1.81	0.46
5:X5:72:LYS:HB3	5:X5:100:HIS:NE2	2.30	0.46
5:X5:238:ASN:HD22	7:Z4:273:LEU:HB3	1.79	0.46
7:Z4:266:TYR:O	7:Z4:324:ARG:HG2	2.16	0.46
3:s5:176:ASP:HB3	3:s5:188:LYS:HZ2	1.80	0.46
3:s5:178:GLY:O	3:s5:188:LYS:HE2	2.16	0.46
1:C5:117:LEU:HA	1:C5:120:GLU:HG2	1.96	0.46
1:G8:46:LEU:HD21	1:G9:209:ARG:NH1	2.29	0.46
1:K5:217:ASN:HA	1:K5:220:GLU:HG2	1.98	0.46
1:K7:149:MET:HE1	1:K8:100:GLY:HA3	1.96	0.46
1:K9:193:ASP:OD1	5:X4:65:LEU:HD22	2.15	0.46
3:Q2:243:GLN:O	3:Q2:246:ARG:HG2	2.16	0.46
3:Q3:193:PHE:HB2	3:Q3:213:GLY:O	2.15	0.46
3:S5:54:GLU:O	3:S5:57:GLN:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T1:146:GLY:H	4:T1:209:VAL:CG2	2.28	0.46
4:T2:109:VAL:HG12	4:T2:219:VAL:HB	1.97	0.46
5:X2:141:LYS:HE2	5:X2:168:PHE:HB2	1.96	0.46
6:Y3:264:LYS:HD3	6:Y3:265:ASN:H	1.80	0.46
8:a2:68:LEU:HD21	8:a2:79:TYR:CE2	2.51	0.46
10:d3:85:PRO:HB3	10:d3:134:MET:HA	1.97	0.46
1:A6:99:ASN:OD1	1:A6:101:ILE:HG23	2.14	0.46
1:A8:236:SER:HB3	1:B8:71:SER:HB2	1.97	0.46
1:C8:177:LYS:HE3	1:C8:184:THR:HG23	1.97	0.46
1:E6:49:SER:HB2	1:E6:241:ARG:HD3	1.96	0.46
1:H8:35:ARG:HG3	1:H8:36:ILE:HG23	1.96	0.46
1:J9:84:ASN:O	1:J9:88:GLN:HG2	2.16	0.46
1:K5:140:PHE:HB2	1:K5:165:ILE:HB	1.98	0.46
1:K7:114:VAL:HG21	1:K7:185:LEU:CD1	2.45	0.46
1:K8:52:MET:O	1:K8:56:VAL:HG23	2.15	0.46
2:M3:143:TRP:HZ3	2:N3:251:MET:HG2	1.79	0.46
2:O3:269:LYS:O	2:O3:272:VAL:HG12	2.14	0.46
3:Q4:63:THR:HG23	3:Q4:66:MET:HE2	1.96	0.46
3:R3:196:ASP:C	3:R3:198:TYR:H	2.23	0.46
4:T3:30:SER:HB2	12:T3:402:HOH:O	2.15	0.46
5:X1:50:ASN:HB2	12:X1:401:HOH:O	2.14	0.46
5:X2:152:ASP:HA	5:X2:194:LEU:HD13	1.97	0.46
5:X4:131:ARG:HB3	5:X4:183:GLN:OE1	2.16	0.46
6:Y4:90:LEU:HD13	6:Y4:128:LEU:HB2	1.97	0.46
7:Z3:152:ARG:HG3	7:Z3:161:TRP:HZ2	1.80	0.46
4:t3:162:TYR:HE1	4:t3:225:THR:HG21	1.80	0.46
1:B3:276:VAL:HG12	1:B3:280:LEU:HD23	1.97	0.46
1:B8:55:GLN:OE1	1:C8:132:LYS:HE3	2.16	0.46
1:C3:16:LEU:HD11	1:C3:263:THR:HG22	1.98	0.46
1:C6:27:MET:HE1	1:C6:252:PHE:CD1	2.51	0.46
1:I9:46:LEU:HD21	1:i0:209:ARG:NH2	2.31	0.46
2:L5:122:MET:O	2:L5:126:ILE:HG12	2.15	0.46
2:O4:114:SER:O	2:O4:118:THR:HG23	2.16	0.46
2:O5:142:LYS:HG3	2:P5:216:PRO:HD2	1.98	0.46
2:P3:106:ARG:HD2	3:s4:108:TYR:CG	2.50	0.46
3:R2:255:ASN:HA	3:R2:258:LEU:HG	1.97	0.46
3:R4:129:TYR:CE2	3:R4:158:LYS:HB3	2.51	0.46
3:R4:234:LYS:HA	3:R4:238:ILE:HD12	1.97	0.46
6:Y5:227:TYR:HB3	6:Y5:234:THR:HB	1.97	0.46
7:Z3:154:LEU:HD21	7:Z3:202:MET:SD	2.55	0.46
1:h0:82:GLU:O	1:h0:86:ILE:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s3:107:VAL:O	3:s3:127:ALA:HB3	2.16	0.46
1:A5:261:SER:HB2	1:B4:277:LEU:HD11	1.97	0.46
1:A6:120:GLU:HG2	1:K6:218:ARG:HG3	1.97	0.46
1:B6:63:GLU:HG2	1:B6:227:MET:HE2	1.98	0.46
1:C7:123:ARG:HG3	1:C7:124:ILE:N	2.30	0.46
1:D5:222:ALA:O	1:D5:226:LEU:HG	2.16	0.46
1:E4:46:LEU:HD21	1:E5:209:ARG:HD3	1.97	0.46
1:E6:87:ILE:HA	1:E6:90:ILE:HG22	1.97	0.46
1:F4:157:GLN:HE22	1:F5:195:ILE:C	2.24	0.46
1:F5:35:ARG:HB3	1:F5:243:THR:HB	1.98	0.46
1:I5:32:SER:CB	1:I5:37:ASN:HD21	2.29	0.46
2:L4:142:LYS:HG3	2:L4:143:TRP:CD1	2.51	0.46
2:N2:205:TRP:NE1	2:N2:221:ILE:HG13	2.31	0.46
2:P3:103:ASN:CG	2:P3:104:LYS:H	2.22	0.46
3:Q1:218:ALA:HA	3:Q1:229:ARG:HH11	1.81	0.46
3:Q2:60:THR:HA	3:Q2:63:THR:HG23	1.97	0.46
3:S5:144:PRO:HA	3:S5:147:GLU:HB2	1.98	0.46
4:T1:143:GLU:HA	4:T1:212:ILE:O	2.16	0.46
5:V3:57:TRP:CD1	5:V3:121:PRO:HD3	2.51	0.46
10:d2:115:GLU:CG	10:d2:116:PRO:HD3	2.46	0.46
2:p2:289:TYR:HA	2:p2:292:ILE:HG22	1.97	0.46
2:p2:289:TYR:O	2:p2:292:ILE:HG22	2.16	0.46
3:s3:230:ASN:HA	3:s3:233:LYS:HG2	1.97	0.46
3:s5:192:PHE:HB3	3:s5:194:GLN:OE1	2.15	0.46
1:A6:23:VAL:HG22	1:A6:255:ASN:HB3	1.98	0.46
1:B5:7:LEU:HD21	1:B6:235:ALA:HA	1.96	0.46
1:B8:51:LYS:O	1:B8:55:GLN:HG2	2.16	0.46
1:D5:251:ALA:HA	1:D5:254:LYS:HG2	1.97	0.46
1:D7:117:LEU:O	1:D7:121:ILE:HG13	2.15	0.46
1:F2:273:PRO:O	1:F2:276:VAL:HG12	2.15	0.46
1:F5:127:GLN:OE1	1:F5:127:GLN:HA	2.16	0.46
1:F6:36:ILE:HG23	1:F6:41:ASP:HB2	1.96	0.46
1:H7:14:ARG:HD3	1:H8:231:GLU:HG2	1.98	0.46
1:J5:56:VAL:HG22	1:J5:233:ILE:HG22	1.98	0.46
1:J8:52:MET:HG2	1:J8:237:GLU:HB2	1.98	0.46
1:K7:97:SER:HB3	1:K7:110:ILE:HG21	1.98	0.46
1:K7:247:GLU:HA	1:K7:250:VAL:HG12	1.97	0.46
2:N5:180:LEU:HD21	2:N5:197:LEU:HD23	1.98	0.46
3:Q4:165:VAL:HG23	3:Q4:170:ILE:HG13	1.98	0.46
3:R2:66:MET:HE1	3:R2:150:ARG:HE	1.81	0.46
3:R3:158:LYS:HE3	3:R3:160:TYR:OH	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X3:150:LEU:O	5:X3:157:THR:HA	2.15	0.46
6:Y5:258:PHE:CE2	6:Y5:267:LEU:HB2	2.51	0.46
7:Z1:93:GLN:HE21	7:Z2:155:VAL:HG23	1.81	0.46
8:a3:61:ILE:O	8:a3:65:LEU:HG	2.15	0.46
10:d2:65:ARG:HB3	10:d2:66:PRO:HD3	1.96	0.46
10:d3:152:LYS:HG2	10:d3:156:GLU:OE2	2.16	0.46
1:i0:153:ILE:HG22	1:i0:226:LEU:HD11	1.98	0.46
4:t4:168:ILE:HD12	4:t4:212:ILE:HG21	1.98	0.46
1:A5:202:LEU:HA	1:A5:205:ILE:HG22	1.98	0.46
1:A7:99:ASN:OD1	1:A7:101:ILE:HG23	2.16	0.46
1:A9:123:ARG:NH1	1:K9:159:GLN:HA	2.30	0.46
1:C6:239:ARG:NH2	1:D6:68:ASP:HA	2.31	0.46
1:C8:109:MET:O	1:C8:112:VAL:HG22	2.16	0.46
1:E3:33:GLY:HA2	1:E3:245:MET:HE1	1.98	0.46
1:F3:50:GLU:CD	1:F4:84:ASN:HD21	2.24	0.46
1:I9:265:MET:HE1	1:J9:31:SER:N	2.31	0.46
1:J7:80:LEU:HA	1:J7:83:THR:HG22	1.97	0.46
1:K9:163:VAL:HG13	1:K9:215:TYR:CE2	2.51	0.46
2:M4:78:TRP:CE2	2:M5:203:ARG:HG3	2.50	0.46
2:M5:138:ARG:CZ	2:M5:150:ARG:HD2	2.46	0.46
2:O1:106:ARG:HH21	3:S2:126:LEU:N	2.12	0.46
2:O3:151:LYS:O	2:O3:154:GLU:HG3	2.16	0.46
3:S6:108:TYR:CE2	3:S6:126:LEU:HA	2.51	0.46
5:V3:101:ILE:HG22	5:V3:217:ASP:HB2	1.98	0.46
5:X1:178:PRO:HB2	5:X1:180:PHE:CD2	2.50	0.46
6:Y3:70:ASP:OD1	6:Y3:236:MET:HG3	2.16	0.46
8:a2:148:LYS:HB2	8:a2:156:SER:HB2	1.97	0.46
3:s4:84:ALA:HB2	3:s4:133:TYR:CE1	2.51	0.46
3:s5:157:SER:HB2	3:s5:174:VAL:HG12	1.97	0.46
3:s6:220:VAL:HG13	3:s6:229:ARG:HB3	1.97	0.46
1:A5:71:SER:O	1:A5:74:GLN:HG2	2.16	0.46
1:A8:254:LYS:HA	1:A8:257:ILE:HG22	1.98	0.46
1:C4:269:ALA:HB2	1:D4:27:MET:HE2	1.98	0.46
1:D7:161:GLU:OE2	1:E7:123:ARG:HD3	2.15	0.46
1:E3:34:MET:HG3	1:E3:242:ASP:HA	1.98	0.46
1:H6:49:SER:HB2	1:H6:241:ARG:HB2	1.97	0.46
2:N6:271:ASN:ND2	2:N6:296:VAL:HG13	2.30	0.46
3:R3:159:ILE:HG21	3:R3:236:PHE:CE2	2.51	0.46
3:R5:239:LYS:HA	3:R5:242:ASP:OD2	2.16	0.46
4:T1:162:TYR:HB3	4:T1:219:VAL:CG1	2.46	0.46
5:V2:50:ASN:HB2	5:V2:52:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p2:75:GLU:C	2:p2:77:LEU:H	2.24	0.46
4:t1:154:TRP:HB2	4:t1:235:ASP:O	2.15	0.46
4:t2:155:VAL:HG22	4:t2:234:PHE:CD2	2.51	0.46
1:A7:106:ASP:O	1:A7:109:MET:HG2	2.15	0.45
1:C4:44:SER:O	1:C4:48:VAL:HG12	2.16	0.45
1:E4:38:ARG:HE	1:E5:74:GLN:HG3	1.81	0.45
1:K4:4:ASN:O	1:K4:5:HIS:CD2	2.69	0.45
2:M1:187:ASP:O	2:M1:190:GLU:HG3	2.16	0.45
2:O2:271:ASN:OD1	2:O2:272:VAL:N	2.48	0.45
2:P3:235:TYR:CD2	2:P3:236:PRO:HD3	2.51	0.45
3:Q3:192:PHE:CD1	3:Q3:214:LYS:HB3	2.51	0.45
3:S4:138:ASN:HA	3:S4:150:ARG:HH21	1.82	0.45
4:T4:108:ALA:HB2	4:T4:220:ARG:HG2	1.98	0.45
5:V1:196:PHE:O	5:V1:197:VAL:HG13	2.15	0.45
5:V5:52:GLU:HB3	5:V5:100:HIS:HB2	1.98	0.45
6:Y3:251:ASN:HB2	6:Y3:275:ILE:HG12	1.97	0.45
1:h1:99:ASN:OD1	1:h1:101:ILE:HG23	2.17	0.45
1:i0:84:ASN:HA	1:i0:87:ILE:HG22	1.97	0.45
3:s5:107:VAL:O	3:s5:127:ALA:HB3	2.15	0.45
4:t2:94:VAL:HG12	4:t2:235:ASP:CG	2.41	0.45
1:A4:3:ILE:HD12	1:A4:3:ILE:N	2.30	0.45
1:A4:46:LEU:HD21	1:A5:209:ARG:CZ	2.46	0.45
1:F5:38:ARG:HG2	1:F5:38:ARG:HH11	1.80	0.45
1:G2:80:LEU:CD1	1:G2:209:ARG:HD3	2.46	0.45
1:K6:268:GLN:O	1:K6:271:VAL:HG12	2.16	0.45
2:M3:91:GLN:HA	2:M3:94:HIS:HE1	1.77	0.45
2:N5:94:HIS:CD2	2:N5:95:GLN:HG3	2.51	0.45
2:P5:132:GLU:HA	2:P5:135:GLU:HG2	1.97	0.45
3:R3:52:ILE:CD1	3:R3:233:LYS:HE3	2.46	0.45
4:T1:109:VAL:CG1	4:T1:219:VAL:HB	2.46	0.45
5:X2:134:SER:HB2	5:X2:172:LYS:HE2	1.98	0.45
5:X5:136:TRP:NE1	5:X5:170:TRP:HB3	2.31	0.45
7:Z3:136:ILE:HD13	7:Z3:255:ARG:HH11	1.80	0.45
8:a2:65:LEU:HD21	8:a2:105:LEU:HD22	1.99	0.45
9:c3:103:PHE:HB3	9:c3:121:VAL:HB	1.97	0.45
1:h0:97:SER:HB2	1:h0:110:ILE:HG21	1.97	0.45
1:h0:150:TRP:CZ2	1:h0:162:ARG:HD2	2.51	0.45
2:p3:127:GLU:O	2:p3:131:LYS:HG2	2.16	0.45
1:A5:23:VAL:O	1:A5:27:MET:HG2	2.17	0.45
1:A8:57:LYS:HE3	1:A9:92:VAL:HG21	1.97	0.45
1:A9:113:GLU:O	1:A9:117:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:57:LYS:HA	1:B5:60:ARG:HE	1.80	0.45
1:D6:203:MET:HE2	1:E6:105:GLU:OE1	2.17	0.45
1:D7:173:LEU:HD23	1:D7:201:ALA:HB1	1.97	0.45
1:E5:86:ILE:HG23	1:E5:117:LEU:HD12	1.99	0.45
1:E6:177:LYS:HG2	1:E6:178:ALA:N	2.32	0.45
1:F6:153:ILE:HG23	1:G2:123:ARG:HE	1.81	0.45
1:J7:265:MET:SD	1:K7:27:MET:HE2	2.57	0.45
2:P4:205:TRP:CD1	2:P4:205:TRP:C	2.94	0.45
2:P6:209:GLU:HG3	2:P6:214:ASN:HB2	1.98	0.45
3:R2:103:ILE:HG22	3:R2:132:ILE:HB	1.98	0.45
3:S3:234:LYS:HD2	3:S3:238:ILE:HD12	1.98	0.45
5:V5:230:TYR:CE1	6:Y5:62:ASP:HA	2.47	0.45
5:X4:51:PHE:HB3	5:X4:102:LEU:HB2	1.98	0.45
7:Z3:136:ILE:HG13	7:Z3:137:LEU:N	2.31	0.45
2:p2:269:LYS:HA	2:p2:272:VAL:HG12	1.99	0.45
1:A8:194:ALA:HA	1:A8:197:THR:HG22	1.98	0.45
1:C7:202:LEU:HA	1:C7:205:ILE:HG22	1.99	0.45
1:E3:35:ARG:N	1:E3:243:THR:HB	2.32	0.45
1:F4:133:MET:HE2	1:F4:140:PHE:HZ	1.82	0.45
1:F6:86:ILE:O	1:F6:90:ILE:HG12	2.17	0.45
1:G6:35:ARG:HB2	1:G6:243:THR:HA	1.98	0.45
1:H7:72:LEU:O	1:H7:75:THR:HG22	2.16	0.45
2:M1:183:ILE:HD11	2:M1:188:LEU:HD23	1.98	0.45
2:M2:293:VAL:O	2:M2:296:VAL:HG12	2.17	0.45
2:O2:178:ASN:HA	2:O2:181:ASP:OD2	2.17	0.45
3:Q4:57:GLN:O	3:Q4:60:THR:HG22	2.15	0.45
3:R3:187:ASP:HA	3:R3:218:ALA:HB2	1.99	0.45
3:S2:233:LYS:HG3	3:S2:234:LYS:N	2.31	0.45
5:V5:117:GLU:HG2	5:V5:119:PHE:CE1	2.52	0.45
5:X2:72:LYS:HE2	5:X2:100:HIS:CG	2.52	0.45
5:X2:218:ASP:HB3	12:X2:401:HOH:O	2.16	0.45
6:Y2:86:SER:OG	6:Y2:258:PHE:HB2	2.16	0.45
8:a4:81:GLN:HB2	8:a4:103:PHE:CE2	2.50	0.45
10:d4:154:SER:HA	10:d4:157:VAL:HG22	1.99	0.45
1:h0:156:ASN:O	1:h0:159:GLN:HG2	2.16	0.45
1:A6:53:ARG:O	1:A6:57:LYS:HG2	2.17	0.45
1:A7:278:GLN:HG2	1:A7:281:ARG:NH2	2.31	0.45
1:A8:236:SER:O	1:A8:240:ILE:HG22	2.16	0.45
1:B6:72:LEU:HD13	1:B7:101:ILE:HB	1.97	0.45
1:E4:84:ASN:OD1	1:E4:85:ASP:N	2.50	0.45
1:F4:72:LEU:HD12	1:F4:130:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F5:273:PRO:HA	1:F5:276:VAL:HG22	1.99	0.45
1:G9:154:GLY:HA3	1:G9:159:GLN:CD	2.42	0.45
1:I6:232:ASN:HD21	1:J6:74:GLN:C	2.25	0.45
1:J7:217:ASN:O	1:J7:220:GLU:HG2	2.16	0.45
2:L3:142:LYS:HE2	2:L3:143:TRP:CE2	2.52	0.45
2:P2:75:GLU:C	2:P2:77:LEU:H	2.24	0.45
2:P3:292:ILE:O	2:P3:296:VAL:HG13	2.17	0.45
3:R3:222:ASN:HB2	3:R3:229:ARG:CD	2.47	0.45
3:R4:194:GLN:HG2	3:R4:212:VAL:HG23	1.98	0.45
5:V2:111:ARG:HH11	5:V2:209:GLY:HA2	1.82	0.45
6:Y4:210:GLU:HB3	6:Y4:216:HIS:NE2	2.32	0.45
6:Y5:67:GLU:HG2	6:Y5:241:THR:OG1	2.17	0.45
7:Z2:85:TYR:CE2	7:Z2:89:LYS:HD2	2.51	0.45
7:Z2:340:ILE:HG23	7:Z2:343:ASP:HB2	1.98	0.45
1:A5:3:ILE:HD13	1:A6:245:MET:HB2	1.98	0.45
1:A5:246:ALA:HB3	1:B4:13:HIS:CE1	2.52	0.45
1:B3:265:MET:HE2	1:C3:30:LEU:HB3	1.99	0.45
1:B7:43:ALA:HB1	1:B8:210:ALA:HA	1.98	0.45
1:B7:265:MET:SD	1:C7:30:LEU:HD22	2.57	0.45
1:C4:202:LEU:HD23	1:C4:205:ILE:HD11	1.98	0.45
1:F3:70:MET:HG2	1:F3:219:LEU:HB2	1.98	0.45
1:F4:150:TRP:CH2	1:F4:162:ARG:HD3	2.52	0.45
1:G1:84:ASN:HA	1:G1:205:ILE:HD12	1.99	0.45
1:G7:46:LEU:HD21	1:G8:209:ARG:CZ	2.47	0.45
1:G9:63:GLU:O	1:G9:66:THR:HG22	2.16	0.45
1:I6:2:ILE:HD12	1:I7:238:SER:OG	2.16	0.45
1:K5:152:HIS:CE1	1:K6:98:SER:HB3	2.52	0.45
1:K6:67:GLU:O	1:K6:70:MET:HG2	2.17	0.45
1:K8:60:ARG:HE	1:K8:227:MET:HE1	1.80	0.45
1:K9:88:GLN:O	1:K9:92:VAL:HG23	2.17	0.45
1:K9:89:ARG:O	1:K9:92:VAL:HB	2.17	0.45
2:M3:166:LYS:HD3	2:M3:211:ASP:HB2	1.98	0.45
3:Q4:242:ASP:CG	3:Q4:246:ARG:HH12	2.25	0.45
3:R4:216:ILE:O	3:R4:220:VAL:HG23	2.17	0.45
3:S5:48:LEU:HD23	3:S5:233:LYS:HE2	1.99	0.45
4:T4:42:TRP:CD1	4:T4:114:PRO:HD3	2.52	0.45
6:Y1:267:LEU:O	6:Y1:268:VAL:HG13	2.16	0.45
6:Y3:135:PRO:HA	6:Y3:138:VAL:HG22	1.98	0.45
7:Z2:171:MET:HE1	7:Z2:184:TYR:CD2	2.51	0.45
9:c1:101:LEU:HB3	9:c1:123:TYR:HB2	1.99	0.45
10:d2:119:GLN:HE22	10:d2:121:LYS:CG	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D5:36:ILE:HG21	1:D5:46:LEU:HD13	1.99	0.45
1:D7:209:ARG:HH11	1:D7:209:ARG:HG3	1.82	0.45
1:E3:272:ARG:HH11	1:E3:272:ARG:HG3	1.80	0.45
1:E5:48:VAL:HG21	1:F6:102:TYR:CE2	2.51	0.45
1:E6:150:TRP:CZ3	1:E6:162:ARG:HB2	2.52	0.45
1:G8:18:PHE:CE2	1:G9:224:LYS:HG3	2.52	0.45
1:H6:257:ILE:HG12	1:I5:274:GLN:HG3	1.97	0.45
1:H8:225:GLY:HA3	1:I8:82:GLU:CD	2.42	0.45
1:I9:76:THR:HG23	1:I9:136:LEU:HD21	1.98	0.45
1:J5:254:LYS:HE2	1:J5:258:LEU:HD11	1.99	0.45
1:J6:79:TYR:CE1	1:J6:128:ALA:HA	2.52	0.45
1:J8:53:ARG:HH22	1:J8:241:ARG:CD	2.29	0.45
1:J8:153:ILE:HB	1:J8:226:LEU:HD11	1.98	0.45
1:J8:276:VAL:HG12	1:J8:280:LEU:HD23	1.99	0.45
1:K7:50:GLU:CG	1:K8:84:ASN:HD21	2.30	0.45
2:L6:368:LEU:O	2:L6:372:THR:HG23	2.17	0.45
2:M1:66:ARG:O	2:M1:69:LYS:HG2	2.16	0.45
5:X3:229:LYS:HB3	4:t2:51:GLN:HE21	1.82	0.45
3:s5:106:GLU:HG2	3:s5:129:TYR:CB	2.47	0.45
4:t2:20:GLY:HA2	4:t2:244:PHE:HB3	1.99	0.45
1:A5:86:ILE:HD13	1:A5:124:ILE:HD12	1.98	0.45
1:B5:273:PRO:HA	1:B5:276:VAL:HG22	1.98	0.45
1:B7:71:SER:HA	1:B7:74:GLN:HG2	1.98	0.45
1:D5:38:ARG:HH11	1:D5:38:ARG:HG3	1.80	0.45
1:D5:218:ARG:HH21	1:E5:123:ARG:HD3	1.82	0.45
1:D7:121:ILE:O	1:D7:124:ILE:HG22	2.17	0.45
1:G1:224:LYS:HA	1:G9:18:PHE:CZ	2.51	0.45
1:H7:247:GLU:HG2	1:I6:13:HIS:CE1	2.52	0.45
1:I6:19:GLN:HG3	1:I6:258:LEU:HD22	1.98	0.45
1:J8:80:LEU:HD11	1:J8:168:MET:SD	2.57	0.45
1:J8:225:GLY:HA3	1:K8:82:GLU:CD	2.41	0.45
1:K7:181:SER:HA	7:Z2:204:MET:HE3	1.98	0.45
1:K8:168:MET:HE1	1:K8:204:LYS:HG2	1.99	0.45
2:M2:235:TYR:HB3	2:M2:236:PRO:HD3	1.98	0.45
2:O3:86:TYR:HE2	2:O4:247:PHE:HA	1.81	0.45
2:O4:180:LEU:HD11	2:O4:197:LEU:HD11	1.97	0.45
3:R4:94:ASN:HB3	3:R4:97:ASP:HB2	1.98	0.45
4:T4:151:MET:SD	4:T4:237:LEU:HD11	2.57	0.45
5:V4:138:LEU:HD22	5:V4:215:TYR:HD2	1.82	0.45
5:X1:145:THR:HG23	5:X1:164:ARG:HG2	1.99	0.45
1:A6:50:GLU:O	1:A6:54:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B4:265:MET:SD	1:C4:27:MET:SD	3.15	0.45
1:C5:53:ARG:O	1:C5:56:VAL:HG12	2.17	0.45
1:E7:90:ILE:HD11	1:E7:114:VAL:HG22	1.98	0.45
1:F5:8:ALA:HB1	1:G1:27:MET:CE	2.46	0.45
1:I9:19:GLN:HG3	1:I9:258:LEU:CD2	2.44	0.45
1:J7:249:THR:HG23	1:K6:270:ASN:HD21	1.82	0.45
1:K9:118:VAL:HG11	1:K9:176:ILE:HD11	1.99	0.45
1:K9:150:TRP:CZ3	1:K9:162:ARG:HB2	2.52	0.45
2:L6:384:LYS:HA	2:L6:387:VAL:HG22	1.99	0.45
2:M2:90:PHE:HA	2:M2:93:LEU:HD23	1.98	0.45
2:M2:192:PRO:O	2:M2:196:ARG:HG2	2.17	0.45
2:O5:289:TYR:O	2:O5:293:VAL:HG23	2.17	0.45
2:P4:144:TYR:O	2:P4:148:VAL:HG13	2.17	0.45
3:Q1:51:LYS:HE2	3:Q1:51:LYS:HA	1.99	0.45
5:V5:143:ARG:HD3	5:V5:206:HIS:HB2	1.99	0.45
5:X4:183:GLN:O	5:X4:194:LEU:HD11	2.17	0.45
5:X5:49:GLU:HB3	5:X5:57:TRP:HH2	1.81	0.45
6:Y2:49:LEU:HD13	6:Y2:85:PHE:CE2	2.52	0.45
6:Y2:108:PHE:CD1	6:Y2:109:PRO:HD2	2.52	0.45
8:a3:149:ILE:HG13	8:a3:150:THR:N	2.31	0.45
1:A4:3:ILE:HD11	1:A5:245:MET:HB2	1.99	0.45
1:A8:22:GLU:O	1:A8:25:LYS:HG2	2.17	0.45
1:A9:70:MET:O	1:A9:74:GLN:HG2	2.16	0.45
1:B4:281:ARG:HD2	1:B4:281:ARG:C	2.41	0.45
1:C5:229:ALA:HB2	1:D5:79:TYR:HE1	1.82	0.45
1:D3:272:ARG:HB3	1:D3:273:PRO:HD3	1.99	0.45
1:E4:23:VAL:HG22	1:E4:255:ASN:HB3	1.99	0.45
1:G1:99:ASN:HB2	1:G9:65:ASN:ND2	2.32	0.45
1:G1:236:SER:HB2	1:h0:71:SER:OG	2.17	0.45
1:G9:47:ALA:HB3	1:h0:109:MET:HE1	1.99	0.45
1:H6:39:ALA:HA	1:H6:46:LEU:HD13	1.99	0.45
1:I8:18:PHE:O	1:I8:22:GLU:HG2	2.17	0.45
1:K6:49:SER:CB	1:K6:241:ARG:HG3	2.46	0.45
1:K8:114:VAL:HG11	1:K8:185:LEU:HD12	1.99	0.45
2:L5:286:SER:HB2	2:L5:287:PRO:HD2	1.98	0.45
2:M1:183:ILE:HG21	2:M1:189:ARG:HB3	1.99	0.45
2:M3:286:SER:HB2	2:M3:287:PRO:HD2	1.98	0.45
3:R4:130:MET:HE3	3:R4:130:MET:HB3	1.73	0.45
3:S2:198:TYR:CD1	3:S2:199:PRO:HD2	2.52	0.45
5:V1:142:PHE:O	5:V1:166:ASP:HA	2.17	0.45
6:Y5:216:HIS:NE2	6:Y5:219:LEU:HB2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p5:241:LEU:HD23	2:p5:273:HIS:CE1	2.51	0.45
3:s3:191:VAL:HB	3:s3:217:LEU:HB2	1.98	0.45
3:s4:78:VAL:HG12	3:s4:106:GLU:HG2	1.97	0.45
4:t2:73:GLU:HB2	4:t2:98:LYS:HB2	1.98	0.45
4:t2:108:ALA:HA	4:t2:219:VAL:O	2.17	0.45
1:A7:231:GLU:HG3	1:A7:232:ASN:N	2.31	0.44
1:C5:280:LEU:CD2	1:C6:249:THR:HG21	2.43	0.44
1:C7:158:HIS:C	1:C7:160:ARG:H	2.25	0.44
1:D3:14:ARG:HH22	1:D4:228:VAL:HG13	1.80	0.44
1:D7:218:ARG:HG3	1:E7:116:GLN:HE21	1.82	0.44
1:E3:237:GLU:HA	1:E3:240:ILE:HG22	1.98	0.44
1:F5:228:VAL:O	1:F5:231:GLU:HG3	2.16	0.44
1:H7:183:LEU:HD21	1:H7:194:ALA:HB1	1.99	0.44
1:H8:48:VAL:O	1:H8:52:MET:HG2	2.17	0.44
1:I8:100:GLY:HA2	1:I8:107:ARG:NH2	2.33	0.44
1:J8:277:LEU:HA	1:J8:280:LEU:HG	2.00	0.44
2:L4:215:LEU:HD23	2:L4:247:PHE:HB2	1.98	0.44
2:P3:89:ASN:O	2:P3:93:LEU:HD23	2.17	0.44
2:P6:151:LYS:O	2:P6:154:GLU:HG3	2.16	0.44
3:Q4:107:VAL:HG12	3:Q4:128:LYS:HG2	1.99	0.44
4:T3:111:ILE:O	4:T3:216:GLN:HB2	2.17	0.44
6:Y3:63:ASN:HB2	6:Y3:219:LEU:HD12	1.99	0.44
7:Z4:234:PRO:O	7:Z4:238:LYS:HG3	2.16	0.44
1:h0:71:SER:O	1:h0:75:THR:HG23	2.17	0.44
2:p5:275:LEU:HA	2:p5:278:THR:HG22	1.98	0.44
4:t3:42:TRP:HA	4:t3:114:PRO:HD3	1.99	0.44
4:t3:162:TYR:CE1	4:t3:225:THR:HG21	2.52	0.44
4:t4:151:MET:O	4:t4:192:THR:HA	2.17	0.44
1:A5:130:PHE:HB3	1:A5:135:LEU:HD11	1.99	0.44
1:A6:4:ASN:C	1:K7:254:LYS:HD2	2.42	0.44
1:A8:36:ILE:HG21	1:A8:46:LEU:HB3	1.99	0.44
1:B7:240:ILE:HD11	1:C7:64:ARG:NH2	2.32	0.44
1:C4:232:ASN:ND2	1:D4:75:THR:HA	2.32	0.44
1:D7:34:MET:HG3	1:D7:36:ILE:H	1.82	0.44
1:E4:51:LYS:O	1:E4:54:THR:HG22	2.17	0.44
1:J7:84:ASN:O	1:J7:88:GLN:HG2	2.18	0.44
1:J7:267:ALA:O	1:J7:271:VAL:HG23	2.18	0.44
2:L3:235:TYR:HA	2:L3:238:HIS:HD1	1.81	0.44
2:L6:309:LEU:HB2	2:L6:310:PRO:HD3	1.99	0.44
2:P4:246:ALA:HA	2:P4:249:GLU:HG2	1.98	0.44
3:S3:65:LEU:O	3:S3:68:MET:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S3:70:VAL:HG21	3:S3:79:LEU:HD22	1.99	0.44
5:X1:56:ASP:HB3	5:X1:121:PRO:CG	2.45	0.44
5:X2:81:ASP:OD1	5:X2:82:VAL:N	2.50	0.44
5:X2:116:VAL:O	5:X2:200:PHE:HA	2.17	0.44
5:X3:101:ILE:HG22	5:X3:217:ASP:CG	2.42	0.44
3:s6:130:MET:HB2	3:s6:248:PHE:CZ	2.51	0.44
1:A6:46:LEU:HD11	1:A7:209:ARG:NH2	2.31	0.44
1:B7:158:HIS:CE1	5:V4:62:THR:HB	2.52	0.44
1:D3:35:ARG:HB2	1:D3:243:THR:HB	1.99	0.44
1:D4:107:ARG:O	1:D4:110:ILE:HG22	2.17	0.44
1:D4:117:LEU:O	1:D4:120:GLU:HB3	2.17	0.44
1:D5:65:ASN:HD21	1:D6:99:ASN:CG	2.25	0.44
1:E6:83:THR:HG23	1:E6:121:ILE:HD12	1.99	0.44
1:F4:50:GLU:HG2	1:F5:84:ASN:HD21	1.82	0.44
1:F4:157:GLN:HE22	1:F5:195:ILE:HG22	1.82	0.44
1:H8:232:ASN:HD21	1:I8:74:GLN:C	2.25	0.44
2:L2:110:SER:O	2:L2:113:GLN:HG3	2.17	0.44
2:M2:152:ALA:O	2:M2:156:ARG:HG3	2.17	0.44
2:P4:245:TYR:HB3	2:P4:270:LYS:HB2	1.99	0.44
4:T2:171:TRP:CD1	4:T2:210:LYS:HE2	2.52	0.44
4:T3:173:GLY:O	5:V3:71:LEU:HD11	2.18	0.44
4:T3:215:LYS:HG3	4:T3:216:GLN:H	1.82	0.44
4:T3:253:ILE:H	4:T3:253:ILE:HD12	1.81	0.44
5:V1:141:LYS:HE3	6:Y2:60:HIS:CE1	2.52	0.44
5:V4:230:TYR:CG	5:V4:231:PRO:HD2	2.52	0.44
5:X3:222:ARG:NH2	4:t3:128:LEU:HB2	2.33	0.44
6:Y5:86:SER:OG	6:Y5:258:PHE:HB2	2.16	0.44
8:a2:148:LYS:CB	8:a2:152:GLU:HB2	2.48	0.44
2:p5:216:PRO:HB3	2:p5:248:GLU:HG3	1.98	0.44
3:s3:48:LEU:O	3:s3:52:ILE:HG12	2.18	0.44
4:t2:26:ILE:HD13	4:t2:270:LEU:HG	1.98	0.44
1:A4:16:LEU:HD11	1:A4:263:THR:HG22	2.00	0.44
1:A7:250:VAL:HG13	1:B6:6:ASN:HD21	1.82	0.44
1:B4:20:ASN:HA	1:B4:23:VAL:HG12	1.98	0.44
1:B6:123:ARG:HG3	1:B6:127:GLN:HG3	1.99	0.44
1:D3:19:GLN:HG2	1:D3:258:LEU:HD22	2.00	0.44
1:E4:5:HIS:CD2	1:E5:234:GLN:HE21	2.35	0.44
1:G8:170:ALA:HB1	1:G8:175:LEU:HB2	2.00	0.44
1:G9:203:MET:HA	1:G9:206:ASN:ND2	2.33	0.44
1:K8:265:MET:SD	1:K8:265:MET:C	3.00	0.44
2:M3:67:ARG:O	2:M3:71:ILE:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O5:91:GLN:HA	2:O5:94:HIS:NE2	2.32	0.44
3:S4:94:ASN:ND2	3:S4:97:ASP:HB2	2.32	0.44
3:S5:248:PHE:HA	3:S5:251:ILE:HG22	1.99	0.44
5:X4:143:ARG:HH21	5:X4:206:HIS:HB2	1.81	0.44
6:Y5:92:ILE:HG13	6:Y5:252:LYS:HB3	2.00	0.44
10:d3:193:LEU:HD13	10:d3:205:ILE:HG21	2.00	0.44
2:p4:94:HIS:C	2:p4:94:HIS:CD2	2.96	0.44
3:s3:128:LYS:HD2	3:s3:240:HIS:HE1	1.82	0.44
4:t2:164:LEU:O	4:t2:180:PHE:HB2	2.18	0.44
4:t3:29:GLU:HG3	4:t3:237:LEU:HD23	1.99	0.44
1:A9:187:THR:HG23	1:A9:190:PHE:H	1.82	0.44
1:B4:25:LYS:O	1:B4:29:THR:HG23	2.18	0.44
1:B6:266:LEU:HD23	1:B6:270:ASN:ND2	2.27	0.44
1:C3:52:MET:HE3	1:C3:237:GLU:HA	2.00	0.44
1:C4:133:MET:HE3	1:C4:133:MET:HB3	1.92	0.44
1:C7:260:GLN:O	1:C7:263:THR:HG22	2.17	0.44
1:D6:35:ARG:HB2	1:D6:243:THR:HB	1.99	0.44
1:E5:246:ALA:HB1	1:F4:13:HIS:CE1	2.49	0.44
1:G1:109:MET:O	1:G1:112:VAL:HG12	2.17	0.44
1:G1:111:GLN:HE22	1:G1:184:THR:HG22	1.81	0.44
1:H8:14:ARG:HD3	1:H9:231:GLU:OE1	2.18	0.44
1:I7:280:LEU:HD11	1:J7:266:LEU:HD22	1.99	0.44
1:J5:3:ILE:HD12	1:J6:245:MET:SD	2.57	0.44
1:J6:261:SER:HB3	1:K5:277:LEU:HD21	1.98	0.44
1:K6:59:LEU:HD11	1:K6:233:ILE:HD12	1.99	0.44
2:L3:270:LYS:HE3	2:L3:271:ASN:OD1	2.17	0.44
2:M4:205:TRP:CD1	2:M4:221:ILE:HG21	2.52	0.44
2:P5:215:LEU:HB2	2:P5:216:PRO:HD3	2.00	0.44
3:Q4:56:ASN:OD1	3:Q4:179:PRO:HG2	2.17	0.44
3:S5:216:ILE:HG23	3:S5:219:GLY:N	2.31	0.44
5:X2:150:LEU:HG	5:X2:196:PHE:HB2	1.97	0.44
10:d4:68:ILE:HD12	10:d4:106:PRO:HB2	1.98	0.44
2:p3:198:LEU:HG	2:p3:202:TYR:CE2	2.53	0.44
3:s3:55:LEU:HA	3:s3:58:ARG:CD	2.47	0.44
1:A4:35:ARG:HG3	1:A4:36:ILE:HD12	1.98	0.44
1:B7:49:SER:C	1:B7:241:ARG:HH22	2.26	0.44
1:E3:56:VAL:HG11	1:E3:234:GLN:OE1	2.18	0.44
1:F2:253:THR:O	1:F2:257:ILE:HG12	2.17	0.44
1:F4:111:GLN:HA	1:F4:114:VAL:HG12	2.00	0.44
1:G7:54:THR:HG22	1:G8:88:GLN:OE1	2.17	0.44
1:I7:51:LYS:HZ3	1:J7:131:ASN:HB3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I9:32:SER:CB	1:I9:37:ASN:HD21	2.31	0.44
1:J6:226:LEU:HD21	1:K6:127:GLN:NE2	2.33	0.44
1:J8:5:HIS:CE1	1:J9:34:MET:HE1	2.53	0.44
1:J9:40:GLY:HA2	1:j0:213:GLY:O	2.17	0.44
1:K5:57:LYS:HG3	1:K6:92:VAL:CG2	2.48	0.44
1:K7:255:ASN:HA	1:K7:258:LEU:HD12	2.00	0.44
2:L2:205:TRP:HE1	2:L2:221:ILE:HG13	1.83	0.44
2:M1:94:HIS:CG	2:M1:95:GLN:N	2.86	0.44
2:N3:205:TRP:HE1	2:N3:221:ILE:HD13	1.83	0.44
3:R5:192:PHE:CE1	3:R5:214:LYS:HG2	2.53	0.44
4:T3:153:VAL:HG13	4:T3:155:VAL:HG23	1.99	0.44
5:V3:76:ARG:HD2	5:V3:76:ARG:O	2.17	0.44
6:Y2:68:PHE:CE1	6:Y2:240:TYR:HB2	2.52	0.44
6:Y3:251:ASN:O	6:Y3:274:ASP:HA	2.17	0.44
7:Z4:263:LYS:HB2	7:Z4:324:ARG:CZ	2.48	0.44
10:d2:71:LEU:HB2	10:d2:91:VAL:HG11	2.00	0.44
10:d3:104:ILE:HD11	10:d3:149:PRO:HD2	1.99	0.44
1:B7:157:GLN:NE2	1:B8:195:ILE:HG22	2.30	0.44
1:E4:87:ILE:HA	1:E4:90:ILE:HG22	2.00	0.44
1:E5:73:ILE:HG23	1:E5:212:LEU:HD12	2.00	0.44
1:E7:108:GLN:O	1:E7:111:GLN:HB3	2.18	0.44
1:F3:157:GLN:HE21	1:F3:158:HIS:CE1	2.36	0.44
1:G1:60:ARG:HD3	1:G1:230:TYR:CZ	2.52	0.44
1:G8:102:TYR:HB3	1:G8:106:ASP:HB2	2.00	0.44
1:I7:83:THR:HG21	1:I7:168:MET:SD	2.57	0.44
1:K7:228:VAL:O	1:K7:231:GLU:HG2	2.17	0.44
1:K8:23:VAL:HG12	1:K8:255:ASN:HB3	1.99	0.44
2:N3:269:LYS:HA	2:N3:272:VAL:HG12	2.00	0.44
2:P2:104:LYS:HB3	2:P2:183:ILE:HD11	2.00	0.44
2:P2:206:ILE:HG23	2:P2:218:CYS:SG	2.57	0.44
3:Q2:79:LEU:HA	3:Q2:104:ARG:O	2.17	0.44
5:V2:149:LYS:HB3	5:V2:198:SER:CB	2.48	0.44
5:V3:132:GLN:HG2	5:V3:222:ARG:CZ	2.47	0.44
5:X3:120:PRO:HD2	5:X3:198:SER:HB3	1.98	0.44
1:h0:52:MET:SD	1:h0:237:GLU:HA	2.57	0.44
1:i0:166:ALA:HB2	1:i0:208:GLN:HG3	1.99	0.44
2:p3:112:TYR:OH	2:p3:200:ASP:HB3	2.18	0.44
1:D3:236:SER:O	1:D3:240:ILE:HG22	2.18	0.44
1:E7:115:SER:HA	1:E7:118:VAL:HG12	2.00	0.44
1:F2:50:GLU:HG3	1:F3:84:ASN:HD21	1.82	0.44
1:F5:72:LEU:HD12	1:F5:130:PHE:CD1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F6:59:LEU:HD12	1:F6:155:PRO:HB3	2.00	0.44
1:I5:272:ARG:HB3	1:I5:273:PRO:HD3	1.99	0.44
1:J8:140:PHE:CD2	1:J8:165:ILE:HD13	2.53	0.44
1:K6:150:TRP:CZ3	1:K6:162:ARG:HB2	2.53	0.44
2:M3:238:HIS:HB2	2:M3:277:ALA:HB2	1.99	0.44
2:N3:262:GLN:HA	2:N3:265:LYS:HG2	2.00	0.44
2:N5:197:LEU:O	2:N5:201:THR:HG23	2.18	0.44
2:O3:86:TYR:CE2	2:O4:247:PHE:HA	2.53	0.44
3:Q2:133:TYR:HB2	3:Q2:154:LYS:CG	2.48	0.44
5:X3:172:LYS:HE2	5:X3:172:LYS:HB3	1.78	0.44
6:Y2:264:LYS:O	6:Y2:265:ASN:HB2	2.18	0.44
7:Z4:260:ASN:HA	7:Z4:263:LYS:HG2	2.00	0.44
1:h0:173:LEU:HD12	1:h0:201:ALA:HB1	2.00	0.44
2:p4:114:SER:O	2:p4:118:THR:HG23	2.17	0.44
3:s3:63:THR:HG22	3:s3:134:PHE:CD1	2.53	0.44
3:s6:242:ASP:O	3:s6:246:ARG:HG2	2.18	0.44
4:t2:154:TRP:CE2	4:t2:190:PRO:HB3	2.53	0.44
1:A6:201:ALA:O	1:A6:205:ILE:HG12	2.18	0.44
1:A7:272:ARG:HB3	1:A7:273:PRO:HD3	2.00	0.44
1:B5:228:VAL:O	1:B5:231:GLU:HG2	2.18	0.44
1:B6:39:ALA:HB3	1:B7:77:GLU:HG2	2.00	0.44
1:B7:221:HIS:HA	1:B7:224:LYS:HG2	2.00	0.44
1:C3:273:PRO:HA	1:C3:276:VAL:HG12	1.99	0.44
1:C7:53:ARG:NH2	1:C8:88:GLN:HE22	2.15	0.44
1:I8:76:THR:HG23	1:I8:212:LEU:HD13	1.99	0.44
1:J6:8:ALA:HB1	1:K6:27:MET:HE3	1.98	0.44
1:K6:56:VAL:HG11	1:K6:234:GLN:OE1	2.18	0.44
1:K8:52:MET:HA	1:K8:55:GLN:NE2	2.33	0.44
2:M5:87:ASP:HB3	2:M5:90:PHE:HB3	2.00	0.44
2:N6:162:LYS:O	2:N6:166:LYS:HG2	2.17	0.44
2:O3:65:LYS:O	2:O3:69:LYS:HE2	2.17	0.44
2:P2:245:TYR:HA	2:P2:248:GLU:HG2	1.99	0.44
2:P3:245:TYR:HA	2:P3:248:GLU:HG2	1.99	0.44
4:T3:46:THR:HG22	4:T3:109:VAL:HG23	2.00	0.44
7:Z1:325:ILE:HB	7:Z1:330:ARG:HG2	1.99	0.44
7:Z2:138:LYS:HE3	9:c2:65:HIS:HA	1.99	0.44
8:a3:104:VAL:CG1	8:a3:123:VAL:HB	2.48	0.44
9:c2:36:TYR:CE2	9:c2:40:VAL:HG21	2.52	0.44
10:d2:138:ALA:HA	10:d2:141:ILE:HG12	2.00	0.44
3:s5:236:PHE:O	3:s5:240:HIS:CB	2.66	0.44
4:t1:116:ILE:HG23	4:t1:118:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:35:ARG:HB3	1:A6:243:THR:HB	1.99	0.43
1:A6:91:ARG:HA	1:A6:198:LEU:HD13	2.00	0.43
1:A7:38:ARG:HG3	1:A7:40:GLY:H	1.83	0.43
1:B7:229:ALA:O	1:B7:233:ILE:HG12	2.18	0.43
1:B8:202:LEU:HA	1:B8:205:ILE:HG22	1.98	0.43
1:C3:276:VAL:HG13	1:C3:277:LEU:HD23	2.00	0.43
1:C5:202:LEU:HA	1:C5:205:ILE:HG12	2.00	0.43
1:E4:61:GLN:CD	1:E5:96:GLN:HE21	2.26	0.43
1:F5:61:GLN:NE2	1:F6:96:GLN:HE21	2.16	0.43
1:G1:111:GLN:NE2	1:G1:184:THR:HG22	2.33	0.43
1:H8:207:LYS:HE3	1:I8:112:VAL:HG21	2.00	0.43
1:J6:121:ILE:HD13	1:J6:175:LEU:HD13	2.00	0.43
1:J7:260:GLN:NE2	1:K6:281:ARG:HH11	2.16	0.43
1:K6:86:ILE:HD11	1:K6:117:LEU:HD22	2.00	0.43
2:L5:271:ASN:O	2:L5:275:LEU:HG	2.17	0.43
2:O3:91:GLN:OE1	2:O3:94:HIS:HE1	2.01	0.43
3:R5:49:ASP:HB3	3:R5:183:PRO:HB3	2.00	0.43
3:S4:159:ILE:O	3:S4:172:SER:HB2	2.18	0.43
3:S5:84:ALA:HB3	3:S5:101:ASN:HD21	1.83	0.43
4:T4:134:LYS:HD2	4:T4:134:LYS:N	2.33	0.43
5:V1:49:GLU:HB3	5:V1:219:LEU:HB3	2.00	0.43
5:V3:139:GLY:HA3	5:V3:165:LEU:HD23	2.00	0.43
6:Y3:70:ASP:HA	6:Y3:237:SER:O	2.18	0.43
7:Z2:233:GLN:CD	7:Z2:234:PRO:HD2	2.43	0.43
7:Z3:216:ARG:HG2	7:Z3:216:ARG:HH11	1.83	0.43
7:Z3:227:GLU:HG3	7:Z3:229:HIS:H	1.82	0.43
2:p3:269:LYS:HA	2:p3:272:VAL:HG12	1.99	0.43
2:p5:275:LEU:O	2:p5:278:THR:HG22	2.18	0.43
1:B3:19:GLN:HE21	1:B3:255:ASN:HB3	1.84	0.43
1:B6:19:GLN:O	1:B6:23:VAL:HG23	2.18	0.43
1:C4:277:LEU:HD22	1:C4:280:LEU:HD21	1.99	0.43
1:C6:4:ASN:HD21	1:C7:242:ASP:CG	2.25	0.43
1:C6:94:ALA:HA	1:C6:185:LEU:HD13	2.00	0.43
1:D6:39:ALA:HB2	1:D7:209:ARG:HH12	1.83	0.43
1:E2:3:ILE:CD1	1:E3:245:MET:HG2	2.37	0.43
1:E3:204:LYS:O	1:E3:208:GLN:HG2	2.18	0.43
1:G1:101:ILE:O	1:G9:133:MET:HE1	2.18	0.43
1:G1:247:GLU:OE2	1:H9:13:HIS:CE1	2.72	0.43
1:G2:106:ASP:HA	1:G2:109:MET:HE3	2.00	0.43
1:G9:35:ARG:NH1	1:H9:64:ARG:HH12	2.16	0.43
1:H8:102:TYR:HB3	1:H8:106:ASP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H8:155:PRO:HG2	1:H8:156:ASN:OD1	2.18	0.43
1:H8:228:VAL:O	1:H8:231:GLU:HG3	2.18	0.43
1:J6:118:VAL:HA	1:J6:121:ILE:HD12	2.00	0.43
2:L2:75:GLU:HG2	2:L2:76:ALA:H	1.83	0.43
2:L5:130:ARG:HH11	2:L5:130:ARG:HG3	1.81	0.43
2:M5:235:TYR:CG	2:M5:236:PRO:HD3	2.53	0.43
2:N3:249:GLU:O	2:N3:252:ILE:HG22	2.18	0.43
3:Q4:105:VAL:O	3:Q4:129:TYR:HA	2.17	0.43
3:R4:108:TYR:HA	3:R4:127:ALA:HB3	2.00	0.43
4:T3:84:ILE:HG21	4:T3:236:GLU:OE2	2.19	0.43
5:V4:153:TYR:HE2	5:V4:182:PRO:HB2	1.83	0.43
5:X1:136:TRP:NE1	5:X1:172:LYS:HD3	2.33	0.43
5:X3:52:GLU:HG3	5:X3:100:HIS:CB	2.44	0.43
6:Y4:108:PHE:CD1	6:Y4:109:PRO:HD2	2.53	0.43
7:Z1:113:GLU:O	7:Z1:116:LEU:HG	2.18	0.43
8:a5:192:TYR:CZ	8:a5:196:LEU:HD11	2.53	0.43
10:d2:146:GLY:HA3	10:d2:176:GLY:HA2	2.00	0.43
1:j0:90:ILE:HG22	1:j0:198:LEU:HD21	2.00	0.43
3:s3:76:ARG:HE	3:s3:108:TYR:HB2	1.83	0.43
1:A7:251:ALA:O	1:A7:254:LYS:HG3	2.17	0.43
1:A8:27:MET:CE	1:K8:8:ALA:HB1	2.48	0.43
1:A9:178:ALA:C	1:A9:180:GLY:H	2.25	0.43
1:B3:5:HIS:HB2	1:B4:238:SER:CB	2.48	0.43
1:B3:6:ASN:HD21	1:B3:9:ALA:HB2	1.83	0.43
1:B8:105:GLU:O	1:B8:109:MET:HG2	2.19	0.43
1:D3:3:ILE:HG21	1:D4:245:MET:HE3	2.00	0.43
1:F2:4:ASN:HD21	1:F3:242:ASP:CG	2.26	0.43
1:G2:108:GLN:O	1:G2:112:VAL:HG23	2.18	0.43
1:H9:65:ASN:HD21	1:h0:99:ASN:HB2	1.82	0.43
1:I6:232:ASN:HD22	1:J6:75:THR:HA	1.84	0.43
1:I7:3:ILE:HG21	1:I7:277:LEU:HD21	2.00	0.43
1:I9:18:PHE:CE1	1:i0:227:MET:HE3	2.54	0.43
2:L5:187:ASP:HA	2:L5:190:GLU:HG2	1.99	0.43
2:N6:104:LYS:O	2:N6:107:LEU:HG	2.17	0.43
2:N6:140:ASP:C	2:N6:142:LYS:H	2.27	0.43
2:N6:249:GLU:CD	2:N6:267:ARG:HH11	2.26	0.43
2:P2:123:ARG:HE	2:P2:126:ILE:HD11	1.83	0.43
3:Q4:185:HIS:CD2	3:Q4:188:LYS:HB2	2.53	0.43
4:T3:38:ALA:HB1	4:T3:40:TYR:CE1	2.52	0.43
4:T3:156:CYS:HA	4:T3:187:GLY:O	2.18	0.43
5:V2:79:ILE:HG23	5:V2:170:TRP:CG	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X5:76:ARG:HD3	5:X5:76:ARG:H	1.83	0.43
8:a3:141:ILE:HB	8:a3:162:ARG:HB2	2.00	0.43
1:h0:206:ASN:HA	1:h0:209:ARG:HG2	2.00	0.43
2:p3:174:THR:HA	2:p3:177:ILE:HG22	1.99	0.43
2:p4:235:TYR:HB3	2:p4:280:LEU:HB2	2.00	0.43
2:p5:177:ILE:HG13	2:p5:178:ASN:N	2.32	0.43
4:t4:64:THR:HG22	4:t4:73:GLU:HG3	2.00	0.43
1:A4:257:ILE:HG23	1:B3:277:LEU:HD22	2.01	0.43
1:A8:130:PHE:HB2	1:A8:135:LEU:HD11	2.00	0.43
1:B7:118:VAL:O	1:B7:121:ILE:HG22	2.19	0.43
1:C5:6:ASN:O	1:C5:10:ILE:HG13	2.19	0.43
1:D5:118:VAL:HA	1:D5:121:ILE:HG22	2.01	0.43
1:E3:11:ASN:HD21	1:F3:38:ARG:NH2	2.16	0.43
1:F5:156:ASN:HB2	1:G1:127:GLN:HE22	1.84	0.43
1:G9:30:LEU:HD12	1:G9:248:GLU:HB3	1.99	0.43
1:I6:8:ALA:HB1	1:J6:27:MET:SD	2.58	0.43
1:J7:184:THR:HG23	1:J7:190:PHE:HB3	2.01	0.43
1:K4:15:VAL:O	1:K4:19:GLN:HG2	2.18	0.43
1:K5:6:ASN:HB3	1:K5:9:ALA:HB3	1.99	0.43
2:L2:183:ILE:O	2:L2:183:ILE:HG13	2.19	0.43
2:M4:183:ILE:HD11	2:M4:194:PHE:CE1	2.54	0.43
2:P6:238:HIS:HA	2:P6:273:HIS:CE1	2.49	0.43
3:Q4:185:HIS:NE2	3:Q4:188:LYS:HB2	2.34	0.43
3:S4:106:GLU:HG2	3:S4:108:TYR:HE1	1.84	0.43
3:S5:193:PHE:CE1	3:S5:215:TYR:HB2	2.53	0.43
4:T2:151:MET:HB2	4:T2:193:VAL:CG1	2.48	0.43
4:T3:42:TRP:HA	4:T3:114:PRO:HG3	1.99	0.43
4:T4:225:THR:HG22	4:T4:227:GLY:H	1.82	0.43
5:V4:104:VAL:HB	5:V4:214:PHE:CE1	2.53	0.43
6:Y5:56:PHE:O	6:Y5:57:PHE:HD1	2.00	0.43
7:Z2:100:PHE:CE2	7:Z3:202:MET:HE3	2.53	0.43
9:c3:95:VAL:CG1	9:c3:102:PHE:HB2	2.48	0.43
1:h1:91:ARG:HA	1:h1:198:LEU:HD13	2.01	0.43
2:p3:275:LEU:HD22	3:s4:246:ARG:HD2	2.01	0.43
2:p4:123:ARG:HA	2:p4:126:ILE:HG22	2.00	0.43
3:s6:226:HIS:C	3:s6:228:ILE:H	2.26	0.43
1:B7:165:ILE:HG23	1:B7:208:GLN:NE2	2.34	0.43
1:D3:253:THR:O	1:D3:257:ILE:HG12	2.19	0.43
1:E5:105:GLU:HG3	1:E5:106:ASP:N	2.33	0.43
1:F5:44:SER:O	1:F5:48:VAL:HG12	2.19	0.43
1:G9:168:MET:SD	1:G9:208:GLN:HG3	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I7:159:GLN:OE1	1:J7:127:GLN:HB3	2.18	0.43
1:J5:276:VAL:HG12	1:J5:280:LEU:HD23	2.01	0.43
1:J7:76:THR:O	1:J7:80:LEU:HD23	2.18	0.43
1:J9:153:ILE:HD11	1:K9:123:ARG:HG2	2.01	0.43
1:K5:142:ARG:HG2	1:K5:164:TYR:CD2	2.54	0.43
1:K6:84:ASN:HB2	1:K6:209:ARG:HH21	1.82	0.43
2:M3:75:GLU:C	2:M3:77:LEU:H	2.26	0.43
3:Q2:81:LYS:HE2	3:Q2:95:GLN:OE1	2.18	0.43
3:R2:154:LYS:HA	3:R2:176:ASP:O	2.19	0.43
3:R3:185:HIS:HB2	3:R3:188:LYS:CE	2.48	0.43
3:S5:135:GLU:O	3:S5:150:ARG:HD3	2.18	0.43
4:T3:44:VAL:HG22	4:T3:111:ILE:HG22	2.00	0.43
5:V2:111:ARG:NH1	5:V2:209:GLY:HA2	2.33	0.43
5:V2:150:LEU:HD13	5:V2:194:LEU:HD21	2.01	0.43
5:V3:57:TRP:CH2	5:V3:120:PRO:HG3	2.53	0.43
5:X1:135:ILE:HG13	5:X1:136:TRP:N	2.33	0.43
5:X3:43:LEU:HG	4:t2:69:GLN:HE21	1.82	0.43
4:t2:215:LYS:HB3	4:t2:216:GLN:OE1	2.18	0.43
1:A6:129:GLU:HB2	1:A6:133:MET:O	2.18	0.43
1:A7:240:ILE:HD13	1:B7:64:ARG:HH22	1.83	0.43
1:A8:111:GLN:HA	1:A8:114:VAL:HG12	2.00	0.43
1:B7:136:LEU:HD22	1:B7:168:MET:HG3	1.99	0.43
1:D7:154:GLY:HA3	1:D7:159:GLN:HE21	1.84	0.43
1:D7:209:ARG:HH11	1:D7:209:ARG:CG	2.30	0.43
1:E2:51:LYS:HG2	1:E3:203:MET:HE1	2.01	0.43
1:E5:61:GLN:NE2	1:E6:96:GLN:HA	2.33	0.43
1:J7:254:LYS:HG3	1:K6:4:ASN:O	2.19	0.43
1:J8:90:ILE:HG22	1:J8:198:LEU:HD11	2.00	0.43
1:J9:244:ASP:OD2	1:K8:13:HIS:HE1	2.02	0.43
1:K8:68:ASP:HB3	1:K9:101:ILE:HD13	2.01	0.43
2:L2:278:THR:HG21	2:L2:289:TYR:CD1	2.54	0.43
2:L4:143:TRP:CZ3	2:M3:251:MET:HE1	2.53	0.43
2:M2:246:ALA:HB2	2:M2:270:LYS:HD2	2.01	0.43
2:O2:155:ASP:HA	2:O2:158:VAL:HG12	1.99	0.43
2:O3:181:ASP:C	2:O3:181:ASP:OD1	2.62	0.43
2:P4:106:ARG:HG3	2:P4:106:ARG:HH11	1.83	0.43
3:Q1:130:MET:HE2	3:Q1:244:PHE:CZ	2.54	0.43
3:R2:246:ARG:HA	3:R2:249:THR:HG22	2.00	0.43
3:S2:152:ILE:HB	3:S2:180:ASN:HB3	2.00	0.43
3:S6:240:HIS:NE2	3:S6:244:PHE:HE2	2.16	0.43
5:X3:164:ARG:H	5:X3:164:ARG:HD3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y2:267:LEU:HD11	6:Y2:269:TYR:O	2.18	0.43
6:Y5:229:ALA:HB3	6:Y5:232:LYS:HB3	2.00	0.43
7:Z1:83:LYS:O	7:Z1:86:LYS:HG2	2.19	0.43
1:j0:107:ARG:HD2	1:j0:186:SER:O	2.18	0.43
2:p2:250:ASN:HA	2:p2:253:LYS:HG2	2.00	0.43
4:t2:32:ASP:OD1	4:t2:92:ALA:HA	2.19	0.43
4:t3:128:LEU:HD23	4:t3:134:LYS:HA	2.00	0.43
1:A4:256:GLN:NE2	1:K4:268:GLN:HE22	2.17	0.43
1:D6:224:LYS:HD3	1:D6:224:LYS:HA	1.78	0.43
1:E3:47:ALA:HB2	1:F4:109:MET:HE1	2.00	0.43
1:E4:38:ARG:HE	1:E5:74:GLN:CG	2.32	0.43
1:E5:56:VAL:HG11	1:E5:234:GLN:OE1	2.18	0.43
1:G7:18:PHE:CZ	1:G8:224:LYS:HA	2.53	0.43
1:G8:247:GLU:HB2	1:H7:13:HIS:NE2	2.33	0.43
1:H6:38:ARG:NH2	1:H7:73:ILE:HG22	2.33	0.43
1:I6:48:VAL:O	1:I6:51:LYS:HG3	2.19	0.43
1:I9:46:LEU:O	1:I9:50:GLU:HG2	2.18	0.43
1:I9:65:ASN:C	1:I9:65:ASN:ND2	2.74	0.43
1:J6:170:ALA:HB1	1:J6:175:LEU:HB2	2.00	0.43
1:J7:14:ARG:HH22	1:K7:37:ASN:ND2	2.14	0.43
2:L3:194:PHE:CE2	2:L3:198:LEU:HD22	2.53	0.43
3:Q3:79:LEU:HD21	3:Q3:103:ILE:HD11	2.00	0.43
3:R4:130:MET:HE1	3:R4:244:PHE:CZ	2.54	0.43
3:S5:49:ASP:HA	3:S5:52:ILE:HG12	1.99	0.43
1:j0:90:ILE:HD11	1:j0:117:LEU:HB3	2.01	0.43
3:s3:169:LYS:HD3	3:s3:193:PHE:CE2	2.54	0.43
3:s5:237:TYR:CZ	3:s5:241:LEU:HD11	2.54	0.43
4:t1:94:VAL:HG12	4:t1:235:ASP:CG	2.44	0.43
1:A6:54:THR:HG22	1:A7:88:GLN:OE1	2.19	0.43
1:A6:168:MET:HG3	1:A6:168:MET:O	2.19	0.43
1:C5:19:GLN:HG2	1:C5:258:LEU:HD22	2.00	0.43
1:C7:133:MET:HE1	1:C7:135:LEU:HD23	1.99	0.43
1:E5:207:LYS:HD2	1:F5:109:MET:HE1	2.00	0.43
1:F2:258:LEU:HD21	1:G6:4:ASN:OD1	2.18	0.43
1:G8:3:ILE:HG21	1:G8:277:LEU:HD11	2.01	0.43
1:I7:171:LYS:HA	1:I7:171:LYS:HD2	1.82	0.43
1:J9:101:ILE:HG13	1:J9:102:TYR:CD1	2.53	0.43
1:K7:181:SER:HA	7:Z2:204:MET:CE	2.49	0.43
2:L6:274:LEU:HA	2:L6:277:ILE:HG22	2.01	0.43
3:Q3:39:GLN:O	3:Q3:42:LEU:HG	2.18	0.43
4:T1:66:GLN:HB3	4:T1:71:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T2:4:ILE:HD11	4:t2:194:TYR:CE1	2.53	0.43
4:T3:180:PHE:HB3	4:T3:191:LEU:HD13	2.01	0.43
5:V2:117:GLU:HA	5:V2:200:PHE:CB	2.48	0.43
7:Z3:119:GLU:OE2	7:Z3:237:ARG:HD3	2.18	0.43
8:a4:201:ARG:HA	8:a4:201:ARG:HD3	1.92	0.43
1:h1:118:VAL:HA	1:h1:121:ILE:HD12	2.00	0.43
2:p5:269:LYS:HA	2:p5:272:VAL:HG22	2.01	0.43
4:t3:80:LYS:HE2	4:t3:89:ALA:HB2	2.00	0.43
1:A6:84:ASN:O	1:A6:88:GLN:HG2	2.18	0.43
1:A8:80:LEU:HD22	1:A8:205:ILE:HD11	2.00	0.43
1:B4:265:MET:SD	1:B4:265:MET:C	3.02	0.43
1:B8:67:GLU:HA	1:B8:70:MET:HE3	2.01	0.43
1:C4:2:ILE:HD12	1:C5:242:ASP:HB2	2.01	0.43
1:C4:255:ASN:O	1:C4:259:VAL:HG23	2.18	0.43
1:F3:228:VAL:HA	1:F3:231:GLU:OE2	2.19	0.43
1:H7:39:ALA:HB3	1:H8:213:GLY:HA3	2.00	0.43
1:I7:218:ARG:CD	1:J7:120:GLU:HB2	2.49	0.43
1:K6:24:ALA:O	1:K6:28:GLU:HG2	2.19	0.43
2:O2:206:ILE:HD11	2:O2:221:ILE:HB	2.01	0.43
2:P6:289:TYR:HA	2:P6:292:ILE:HG22	2.01	0.43
3:R2:132:ILE:HD11	3:R2:244:PHE:CZ	2.54	0.43
3:R2:154:LYS:HD2	3:R2:175:MET:HE3	2.00	0.43
3:R3:76:ARG:HA	3:R3:76:ARG:CZ	2.49	0.43
3:R3:109:ASP:HB2	3:R3:161:LYS:HD3	1.99	0.43
3:S2:84:ALA:HB2	3:S2:102:CYS:SG	2.58	0.43
6:Y2:68:PHE:CZ	6:Y2:219:LEU:HD11	2.54	0.43
6:Y4:89:ILE:HD12	6:Y4:237:SER:HB2	2.01	0.43
4:t1:222:ARG:HG3	4:t1:223:PRO:HD2	2.01	0.43
4:t2:42:TRP:NE1	4:t2:113:PRO:HA	2.34	0.43
4:t2:129:ASP:HB3	4:t2:135:LYS:HD3	2.01	0.43
1:A4:35:ARG:NH1	1:A4:36:ILE:HD11	2.34	0.43
1:B4:70:MET:HA	1:B4:73:ILE:HG22	2.00	0.43
1:B5:14:ARG:HE	1:B5:18:PHE:HE2	1.66	0.43
1:E2:247:GLU:O	1:E2:250:VAL:HG22	2.18	0.43
1:F6:90:ILE:HD11	1:F6:117:LEU:CB	2.49	0.43
1:G7:50:GLU:O	1:G7:54:THR:HG23	2.19	0.43
1:G9:90:ILE:HG22	1:G9:198:LEU:HD11	2.00	0.43
1:H9:205:ILE:HG13	1:H9:206:ASN:N	2.33	0.43
1:I5:262:GLY:O	1:I5:265:MET:HE3	2.18	0.43
1:I9:36:ILE:HG21	1:I9:46:LEU:HB2	2.00	0.43
1:J6:108:GLN:HA	1:J6:111:GLN:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J7:257:ILE:HD12	1:K6:274:GLN:HA	2.01	0.43
1:K9:181:SER:HA	7:Z4:204:MET:HE1	2.01	0.43
2:L6:236:LYS:HB2	2:M5:217:GLN:HE22	1.83	0.43
2:M3:78:TRP:CZ2	2:M4:203:ARG:HG3	2.54	0.43
2:N2:174:THR:O	2:N2:177:ILE:HG22	2.19	0.43
3:R2:52:ILE:HD13	3:R2:233:LYS:HE3	2.00	0.43
3:R5:67:LYS:HD3	3:R5:144:PRO:HA	2.01	0.43
3:S5:155:LEU:HB3	3:S5:176:ASP:HB2	2.00	0.43
4:T2:143:GLU:HG2	4:T2:213:VAL:HG22	2.01	0.43
5:V1:105:LYS:HE2	5:V1:213:TYR:CD1	2.54	0.43
5:V5:48:LEU:HD11	5:V5:221:VAL:HG23	2.00	0.43
5:V5:133:LEU:HD11	5:V5:219:LEU:HD11	2.01	0.43
5:X2:138:LEU:HD23	5:X2:139:GLY:N	2.34	0.43
7:Z2:154:LEU:HA	7:Z2:157:ILE:HG12	2.00	0.43
8:a3:97:TYR:HA	8:a3:129:SER:O	2.19	0.43
9:c2:33:VAL:HG22	9:c2:37:ASN:HD21	1.84	0.43
2:p5:245:TYR:CD1	2:p5:269:LYS:HE3	2.54	0.43
3:s3:86:ASN:OD1	3:s3:87:ASP:N	2.52	0.43
3:s5:155:LEU:HB3	3:s5:176:ASP:HB2	2.00	0.43
4:t3:74:VAL:HG12	4:t3:97:VAL:HG12	2.00	0.43
1:A6:108:GLN:O	1:A6:112:VAL:HG23	2.19	0.42
1:A8:153:ILE:HD12	1:B8:123:ARG:NH1	2.34	0.42
1:A9:109:MET:HE3	1:A9:109:MET:HB2	1.80	0.42
1:C5:168:MET:HG3	1:C5:168:MET:O	2.19	0.42
1:D4:272:ARG:HB3	1:D4:273:PRO:HD3	2.00	0.42
1:F3:1:MET:HG2	1:G8:20:ASN:ND2	2.34	0.42
1:F4:162:ARG:HG2	1:F4:164:TYR:CZ	2.54	0.42
1:G1:33:GLY:O	1:G1:243:THR:HG22	2.19	0.42
1:G1:51:LYS:HD3	1:h0:132:LYS:HG2	2.01	0.42
1:G7:59:LEU:HD21	1:G7:229:ALA:HB3	2.01	0.42
1:G9:99:ASN:HD22	1:G9:101:ILE:HG12	1.83	0.42
1:H7:232:ASN:OD1	1:I7:74:GLN:HG2	2.19	0.42
1:H8:148:SER:HA	1:H8:162:ARG:HH12	1.83	0.42
1:I9:137:GLN:HE21	1:I9:139:ASP:HB2	1.83	0.42
1:J8:51:LYS:HB3	1:J8:51:LYS:HE3	1.81	0.42
1:K4:14:ARG:HG3	1:K5:227:MET:HE1	2.01	0.42
1:K7:23:VAL:CG2	1:K7:255:ASN:HB3	2.46	0.42
1:K7:40:GLY:HA3	1:K8:216:PHE:CD1	2.54	0.42
1:K9:60:ARG:HD3	1:K9:230:TYR:CE1	2.54	0.42
2:L6:344:ASN:O	2:L6:347:LYS:HG2	2.18	0.42
2:M3:112:TYR:CZ	2:M3:200:ASP:HB3	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N2:129:TYR:HA	2:N2:132:GLU:HG2	2.01	0.42
2:N4:209:GLU:HG2	2:N4:214:ASN:HB3	2.01	0.42
2:N5:72:GLN:HB3	3:R5:199:PRO:HB2	2.01	0.42
2:O3:269:LYS:HA	2:O3:272:VAL:HG12	2.01	0.42
2:P4:205:TRP:NE1	2:P4:221:ILE:HG13	2.33	0.42
4:T1:160:ASN:HD21	4:T1:230:VAL:HG12	1.84	0.42
4:T4:101:PHE:CZ	4:T4:227:GLY:HA2	2.54	0.42
5:V4:95:GLN:HB2	5:V4:98:LYS:HG2	2.01	0.42
5:V4:130:ALA:HB2	5:V4:223:ALA:HB2	2.01	0.42
6:Y4:271:ARG:HG2	6:Y4:273:ILE:HD11	2.00	0.42
7:Z2:156:ASP:O	7:Z2:160:GLU:HB2	2.19	0.42
7:Z3:124:GLU:O	7:Z3:127:GLN:HG3	2.19	0.42
8:a2:202:ARG:HA	8:a2:205:LYS:HE3	2.00	0.42
9:c2:54:ASN:ND2	9:c2:114:LEU:HA	2.34	0.42
1:A6:207:LYS:HD3	1:B6:109:MET:CE	2.50	0.42
1:B6:18:PHE:CE2	1:B7:227:MET:HG2	2.53	0.42
1:B6:84:ASN:O	1:B6:87:ILE:HG22	2.19	0.42
1:B8:218:ARG:HB3	1:C8:116:GLN:NE2	2.34	0.42
1:C4:23:VAL:HB	1:C4:255:ASN:HB3	2.01	0.42
1:C7:33:GLY:O	1:C7:243:THR:HG22	2.19	0.42
1:D3:14:ARG:HA	1:D4:227:MET:HE1	2.01	0.42
1:D5:276:VAL:HG22	1:E5:263:THR:HG21	2.01	0.42
1:E4:18:PHE:CE1	1:E5:227:MET:HG3	2.54	0.42
1:H6:57:LYS:HG2	1:H7:92:VAL:HG21	2.01	0.42
1:H7:37:ASN:OD1	1:H7:38:ARG:HG3	2.19	0.42
1:K7:150:TRP:CG	1:K7:160:ARG:HH21	2.37	0.42
1:K8:12:SER:HA	1:K8:15:VAL:HG12	2.01	0.42
2:N5:159:SER:HA	2:N5:162:LYS:HG2	2.01	0.42
2:O2:206:ILE:HG21	2:O2:222:LEU:HD21	2.00	0.42
2:P2:91:GLN:HA	2:P2:94:HIS:NE2	2.34	0.42
3:R4:195:LYS:O	3:R4:198:TYR:HD1	2.02	0.42
3:S4:198:TYR:CG	3:S4:199:PRO:HD2	2.54	0.42
3:S5:130:MET:HE3	3:S5:244:PHE:CD2	2.54	0.42
3:S5:154:LYS:H	3:S5:154:LYS:HD2	1.85	0.42
4:T2:112:ARG:HA	4:T2:216:GLN:HE22	1.84	0.42
4:T3:94:VAL:HG11	4:T3:188:TRP:HH2	1.84	0.42
5:X2:122:HIS:CE1	7:Z2:171:MET:HG3	2.54	0.42
6:Y4:172:VAL:O	6:Y4:176:THR:HG23	2.18	0.42
1:h0:152:HIS:H	1:h1:99:ASN:ND2	2.17	0.42
2:p4:241:LEU:HD23	2:p4:273:HIS:CE1	2.54	0.42
4:t1:151:MET:HE1	4:t1:195:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t3:178:LEU:HD12	4:t3:193:VAL:HB	2.01	0.42
1:A5:265:MET:CE	1:B5:31:SER:HB3	2.49	0.42
1:A9:129:GLU:OE2	1:A9:132:LYS:HA	2.19	0.42
1:C6:80:LEU:HD23	1:C6:80:LEU:HA	1.86	0.42
1:D6:76:THR:O	1:D6:80:LEU:HD23	2.19	0.42
1:D6:123:ARG:HD2	1:D6:123:ARG:C	2.44	0.42
1:F2:57:LYS:HE3	1:F3:88:GLN:HE21	1.84	0.42
1:G1:109:MET:HE2	1:G1:109:MET:HB3	1.93	0.42
1:H8:232:ASN:ND2	1:I8:74:GLN:HG2	2.34	0.42
1:I9:156:ASN:HB2	1:I9:159:GLN:OE1	2.18	0.42
1:J6:136:LEU:HB3	1:J6:168:MET:HB3	2.01	0.42
1:J7:54:THR:HG22	1:J8:88:GLN:HG2	2.00	0.42
1:J7:77:GLU:O	1:J7:81:GLN:HG2	2.19	0.42
1:J7:151:PHE:CE2	1:J7:163:VAL:HG21	2.55	0.42
1:K7:15:VAL:O	1:K7:19:GLN:HG2	2.20	0.42
2:M5:235:TYR:CD2	2:M5:236:PRO:HD3	2.54	0.42
2:O2:153:ARG:HD3	2:O2:156:ARG:NH2	2.35	0.42
3:R2:192:PHE:CE1	3:R2:214:LYS:HG3	2.54	0.42
4:T2:206:TYR:HB2	4:T3:186:ILE:HD12	2.01	0.42
5:V1:68:THR:HA	5:V1:105:LYS:O	2.19	0.42
5:V3:146:LEU:HG	5:V3:162:LEU:HD12	2.00	0.42
5:X1:135:ILE:HD13	5:X1:219:LEU:HD13	2.00	0.42
7:Z3:132:ARG:HG3	7:Z3:255:ARG:HH12	1.82	0.42
8:a2:148:LYS:HB2	8:a2:156:SER:CB	2.49	0.42
8:a4:90:ILE:HB	8:a4:93:SER:HB3	2.01	0.42
8:a5:181:GLU:OE1	8:a5:184:GLN:HB3	2.19	0.42
1:h0:173:LEU:HG	1:h0:175:LEU:HG	2.01	0.42
2:p5:223:GLU:HA	2:p5:226:ILE:HG12	2.02	0.42
3:s5:78:VAL:HG23	3:s5:108:TYR:HE2	1.83	0.42
3:s5:106:GLU:HG2	3:s5:129:TYR:HB2	2.01	0.42
1:A6:254:LYS:HG2	1:B5:4:ASN:HA	2.02	0.42
1:A9:78:GLY:HA3	1:K9:228:VAL:HG11	2.00	0.42
1:B6:67:GLU:O	1:B6:70:MET:HG2	2.18	0.42
1:B7:5:HIS:CE1	1:B8:234:GLN:HE22	2.38	0.42
1:B7:71:SER:HA	1:B7:74:GLN:HE21	1.84	0.42
1:B7:254:LYS:CG	1:C6:4:ASN:HA	2.49	0.42
1:C3:48:VAL:O	1:C3:52:MET:HG3	2.20	0.42
1:C6:239:ARG:HD3	1:D6:67:GLU:HB3	2.01	0.42
1:D5:276:VAL:HG13	1:E5:263:THR:HG22	2.01	0.42
1:D7:79:TYR:CD2	1:D7:128:ALA:HB1	2.54	0.42
1:E2:1:MET:HG2	1:E2:276:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E5:37:ASN:O	1:E5:38:ARG:HD2	2.19	0.42
1:E6:167:THR:O	1:E6:168:MET:HE2	2.20	0.42
1:E7:130:PHE:HB2	1:E7:135:LEU:HD11	2.01	0.42
1:G9:108:GLN:O	1:G9:112:VAL:HG23	2.19	0.42
1:I5:271:VAL:HA	1:I5:274:GLN:OE1	2.19	0.42
2:N3:87:ASP:HB2	2:N4:243:SER:HA	2.02	0.42
2:N5:251:MET:HE2	2:N5:251:MET:HB3	1.84	0.42
2:P3:75:GLU:C	2:P3:77:LEU:H	2.27	0.42
2:P4:136:LYS:HE3	2:P4:138:ARG:NH2	2.34	0.42
2:P5:78:TRP:CZ2	2:P6:203:ARG:HG2	2.55	0.42
3:Q3:78:VAL:CG2	3:Q3:106:GLU:HB2	2.49	0.42
3:S4:171:ILE:HG21	3:S4:232:PHE:CE2	2.50	0.42
5:X4:108:TYR:OH	5:X4:201:VAL:HG13	2.19	0.42
6:Y3:80:PHE:HD1	6:Y4:244:ARG:HD2	1.84	0.42
10:d3:241:ALA:O	10:d3:245:VAL:HG23	2.19	0.42
1:i0:73:ILE:HD13	1:i0:215:TYR:HB3	2.01	0.42
4:t4:42:TRP:HA	4:t4:114:PRO:HD3	2.01	0.42
1:A8:35:ARG:H	1:A8:242:ASP:HA	1.84	0.42
1:B3:272:ARG:HB3	1:B3:273:PRO:HD3	2.00	0.42
1:B4:23:VAL:HB	1:B4:255:ASN:HB3	2.01	0.42
1:B5:150:TRP:CZ2	1:B5:162:ARG:HD3	2.55	0.42
1:C8:108:GLN:O	1:C8:112:VAL:HG13	2.20	0.42
1:F5:274:GLN:HE22	1:F5:278:GLN:CD	2.27	0.42
1:H8:246:ALA:O	1:H8:250:VAL:HG23	2.19	0.42
1:I9:218:ARG:HH21	1:J9:123:ARG:HD2	1.84	0.42
1:J6:183:LEU:HD11	1:J6:194:ALA:CB	2.50	0.42
1:K4:14:ARG:HE	1:K5:231:GLU:CD	2.27	0.42
2:M2:247:PHE:CZ	2:M2:251:MET:HE3	2.54	0.42
2:M4:262:GLN:HA	2:M4:265:LYS:HG2	2.02	0.42
2:O2:269:LYS:HA	2:O2:272:VAL:HG12	2.01	0.42
2:O4:75:GLU:C	2:O4:77:LEU:N	2.78	0.42
2:P6:142:LYS:HD2	2:p5:216:PRO:HG2	2.00	0.42
3:Q4:213:GLY:HA3	3:Q4:215:TYR:CZ	2.55	0.42
3:R2:144:PRO:O	3:R2:147:GLU:HG2	2.20	0.42
3:S6:129:TYR:CE2	3:S6:158:LYS:HD3	2.54	0.42
4:T4:134:LYS:HD2	4:T4:134:LYS:H	1.84	0.42
5:V1:148:ALA:HB2	5:V1:162:LEU:HD11	2.02	0.42
5:X2:70:VAL:HA	5:X2:103:GLY:O	2.20	0.42
5:X2:107:ASN:HA	5:X2:210:GLY:O	2.20	0.42
7:Z4:171:MET:HE1	7:Z4:184:TYR:CZ	2.54	0.42
7:Z4:222:ILE:HD11	7:Z4:240:ARG:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p5:293:VAL:HA	2:p5:296:VAL:HG22	2.00	0.42
3:s5:246:ARG:NE	3:s5:246:ARG:HA	2.34	0.42
4:t1:80:LYS:HE3	4:t1:87:VAL:HB	2.00	0.42
1:A6:214:ALA:HB1	1:B6:116:GLN:HG3	2.02	0.42
1:A8:105:GLU:HG3	1:A8:109:MET:HE3	2.00	0.42
1:A8:131:ASN:O	1:A8:132:LYS:HG2	2.19	0.42
1:B6:76:THR:HG23	1:B6:135:LEU:HD13	2.01	0.42
1:B6:239:ARG:HD2	1:C6:67:GLU:OE2	2.19	0.42
1:B7:106:ASP:HA	1:B7:109:MET:HE3	2.01	0.42
1:D4:176:ILE:HD12	1:D4:182:LEU:HA	2.01	0.42
1:D5:251:ALA:HA	1:D5:254:LYS:HD3	2.01	0.42
1:E5:12:SER:HA	1:E5:15:VAL:HG12	2.02	0.42
1:E6:243:THR:HG21	1:E6:248:GLU:HG3	2.01	0.42
1:H7:33:GLY:O	1:H7:243:THR:HG22	2.19	0.42
1:I8:103:SER:OG	1:I8:105:GLU:HG3	2.19	0.42
1:I9:6:ASN:O	1:I9:10:ILE:HG13	2.19	0.42
1:J5:35:ARG:HH12	1:J5:42:ASP:CB	2.33	0.42
1:J8:5:HIS:HE1	1:J9:34:MET:HE1	1.85	0.42
1:J9:156:ASN:HB2	1:J9:159:GLN:NE2	2.35	0.42
1:K6:94:ALA:HA	1:K6:185:LEU:HD13	2.01	0.42
2:P5:288:GLU:O	2:P5:292:ILE:HG12	2.20	0.42
3:Q1:129:TYR:CE1	3:Q1:158:LYS:HB3	2.54	0.42
3:Q2:102:CYS:HA	3:Q2:132:ILE:O	2.19	0.42
3:Q3:103:ILE:CG2	3:Q3:132:ILE:HB	2.50	0.42
3:R4:157:SER:OG	3:R4:174:VAL:HG22	2.20	0.42
3:R5:44:THR:HA	3:R5:47:LYS:HG2	2.00	0.42
3:S5:65:LEU:HA	3:S5:68:MET:SD	2.60	0.42
3:S6:152:ILE:HG23	3:S6:179:PRO:HG2	2.01	0.42
4:T3:215:LYS:HG3	4:T3:216:GLN:N	2.34	0.42
5:V4:52:GLU:O	5:V4:72:LYS:HE3	2.19	0.42
5:X2:70:VAL:HG23	5:X2:104:VAL:HG22	2.01	0.42
7:Z2:133:THR:HG21	7:Z2:251:CYS:HB3	2.01	0.42
7:Z4:129:TYR:HD1	7:Z4:255:ARG:HH12	1.65	0.42
8:a4:155:ASN:HD21	8:a4:177:ALA:HB2	1.84	0.42
1:h0:194:ALA:O	1:h0:198:LEU:HD13	2.20	0.42
3:s3:190:GLU:HG2	3:s3:216:ILE:HG12	2.01	0.42
1:A4:27:MET:CE	1:K4:272:ARG:HH22	2.33	0.42
1:A7:149:MET:HE1	1:A7:151:PHE:CZ	2.55	0.42
1:A8:27:MET:HG2	1:K8:265:MET:SD	2.60	0.42
1:B4:48:VAL:O	1:B4:52:MET:HG2	2.20	0.42
1:C6:23:VAL:O	1:C6:27:MET:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:12:SER:HB3	1:D3:266:LEU:HD13	2.01	0.42
1:E4:150:TRP:CZ3	1:E4:162:ARG:HB2	2.55	0.42
1:E6:101:ILE:HG13	1:E6:102:TYR:N	2.35	0.42
1:E6:187:THR:HG22	1:E6:190:PHE:CD1	2.54	0.42
1:H6:18:PHE:CZ	1:H7:224:LYS:HA	2.55	0.42
1:H6:232:ASN:HD21	1:I6:74:GLN:HG2	1.84	0.42
1:H7:281:ARG:HD2	1:H7:281:ARG:C	2.45	0.42
1:H8:258:LEU:HD21	1:I7:4:ASN:HB3	2.02	0.42
1:I9:34:MET:HE1	1:I9:241:ARG:HB2	2.02	0.42
2:P4:264:PHE:HA	2:P4:267:ARG:HG2	2.01	0.42
3:Q3:62:HIS:HE1	3:Q3:245:ASP:OD1	2.03	0.42
3:R4:195:LYS:HB3	3:R4:198:TYR:CD1	2.54	0.42
3:S3:166:LEU:HD11	3:S3:228:ILE:HG23	2.02	0.42
4:T4:115:ARG:N	4:T4:115:ARG:HD2	2.34	0.42
6:Y3:154:ARG:HG2	6:Y3:159:GLU:HB2	2.01	0.42
7:Z2:256:ALA:HB2	7:Z2:336:ILE:HG21	2.02	0.42
7:Z3:330:ARG:HG3	7:Z3:330:ARG:HH11	1.85	0.42
9:c3:46:ALA:O	9:c3:50:THR:HG23	2.19	0.42
10:d2:67:LEU:HG	10:d2:91:VAL:HG13	2.02	0.42
10:d2:176:GLY:O	10:d2:180:MET:HG2	2.20	0.42
4:t1:215:LYS:CG	4:t1:216:GLN:H	2.29	0.42
1:A6:239:ARG:CZ	1:A6:239:ARG:HB3	2.48	0.42
1:C6:131:ASN:C	1:C6:133:MET:H	2.28	0.42
1:D3:25:LYS:O	1:D3:29:THR:HG23	2.20	0.42
1:E2:5:HIS:CG	1:E3:234:GLN:HE21	2.38	0.42
1:F4:33:GLY:O	1:F4:243:THR:HG22	2.20	0.42
1:F4:46:LEU:HD11	1:F5:209:ARG:NH2	2.35	0.42
1:F4:221:HIS:HB3	1:G9:86:ILE:HD11	2.02	0.42
1:G1:78:GLY:O	1:G1:81:GLN:HG2	2.19	0.42
1:I6:268:GLN:HA	1:I6:271:VAL:HG22	2.02	0.42
1:I8:29:THR:HG23	1:I8:35:ARG:HA	2.00	0.42
1:I8:48:VAL:O	1:I8:52:MET:HG2	2.19	0.42
1:J6:23:VAL:CG2	1:J6:255:ASN:HB3	2.49	0.42
1:J7:114:VAL:HG21	1:J7:185:LEU:HD11	2.01	0.42
1:K7:84:ASN:O	1:K7:88:GLN:HG2	2.20	0.42
2:L6:313:ILE:HG13	2:L6:314:PRO:HD3	2.01	0.42
2:M1:71:ILE:O	2:M1:75:GLU:HG2	2.19	0.42
2:N2:154:GLU:HG2	2:N2:155:ASP:N	2.35	0.42
2:N6:203:ARG:NH1	2:N6:206:ILE:HG21	2.34	0.42
3:Q2:74:PRO:HG2	3:Q2:77:THR:HB	2.02	0.42
4:T4:23:LEU:HD21	4:t4:23:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X2:107:ASN:OD1	5:X2:108:TYR:N	2.52	0.42
6:Y4:77:ASN:HB2	6:Y4:187:ILE:HG13	2.01	0.42
7:Z3:134:GLU:HG3	9:c3:61:TYR:CE2	2.55	0.42
9:c1:35:GLU:O	9:c1:38:LYS:HG2	2.19	0.42
2:p5:205:TRP:CD1	2:p5:221:ILE:HD12	2.55	0.42
4:t4:63:ALA:HB1	4:t4:74:VAL:HG12	2.02	0.42
1:A4:28:GLU:CD	1:K4:11:ASN:HD21	2.28	0.42
1:A6:63:GLU:HA	1:A6:66:THR:HG22	2.01	0.42
1:B5:156:ASN:HA	1:B6:195:ILE:HG21	2.02	0.42
1:B6:157:GLN:HG3	1:B6:158:HIS:ND1	2.34	0.42
1:B7:55:GLN:NE2	1:C7:132:LYS:HE3	2.35	0.42
1:D6:157:GLN:HG3	1:D6:158:HIS:CD2	2.54	0.42
1:E5:194:ALA:O	1:E5:198:LEU:HG	2.20	0.42
1:F4:111:GLN:OE1	1:F4:184:THR:HA	2.19	0.42
1:F5:54:THR:HG23	1:F6:88:GLN:OE1	2.19	0.42
1:G1:11:ASN:ND2	1:h0:28:GLU:HG3	2.35	0.42
1:H9:107:ARG:HD2	1:H9:186:SER:C	2.44	0.42
1:I7:11:ASN:HD21	1:J7:38:ARG:HH22	1.68	0.42
1:I8:16:LEU:HD11	1:I8:263:THR:HG22	2.02	0.42
1:J7:134:ALA:HB1	1:J7:137:GLN:HB2	2.02	0.42
1:K7:18:PHE:CE2	1:K8:224:LYS:HG3	2.55	0.42
2:L2:266:TYR:HA	2:L2:269:LYS:HE2	2.02	0.42
2:L3:149:ASP:O	2:L3:153:ARG:HG2	2.19	0.42
2:L4:84:LYS:HD2	8:a4:94:ARG:HD2	2.02	0.42
2:N6:235:TYR:N	2:N6:236:PRO:CD	2.82	0.42
2:P6:235:TYR:N	2:P6:236:PRO:HD2	2.34	0.42
3:Q3:181:THR:HG23	3:Q3:182:GLN:H	1.84	0.42
3:S2:182:GLN:HG2	3:S2:184:SER:H	1.85	0.42
4:T4:171:TRP:CD1	4:T4:210:LYS:HZ2	2.38	0.42
4:T4:221:SER:HB2	4:T4:225:THR:OG1	2.20	0.42
5:V4:119:PHE:CD1	5:V4:198:SER:HB2	2.55	0.42
6:Y2:154:ARG:HD3	6:Y2:161:VAL:HG11	2.01	0.42
6:Y5:93:ASN:O	6:Y5:123:ILE:HA	2.19	0.42
7:Z1:33:GLU:OE1	7:Z1:238:LYS:HE3	2.20	0.42
7:Z1:115:GLN:HG3	7:Z1:237:ARG:HG2	2.01	0.42
7:Z2:93:GLN:HB2	7:Z3:155:VAL:HG21	2.01	0.42
8:a5:159:LEU:HD21	8:a5:188:LEU:HD11	2.02	0.42
10:d4:224:CYS:HA	10:d4:227:LEU:HD12	2.02	0.42
2:p2:78:TRP:CH2	2:p3:203:ARG:HG2	2.55	0.42
3:s3:129:TYR:CE1	3:s3:158:LYS:HB3	2.55	0.42
3:s4:62:HIS:HE1	3:s4:245:ASP:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s5:194:GLN:HB3	3:s5:198:TYR:HB2	2.01	0.42
4:t4:27:THR:HG23	4:t4:237:LEU:O	2.20	0.42
4:t4:161:GLU:HB2	4:t4:225:THR:HG23	2.02	0.42
1:A6:185:LEU:HD13	1:A6:191:ALA:HA	2.01	0.42
1:A8:20:ASN:HA	1:A8:23:VAL:HG12	2.01	0.42
1:A8:245:MET:O	1:A8:249:THR:HG23	2.20	0.42
1:B5:129:GLU:CD	1:B5:132:LYS:HA	2.45	0.42
1:B6:215:TYR:O	1:B6:218:ARG:HB3	2.19	0.42
1:B8:153:ILE:HD11	1:C8:123:ARG:HD2	2.01	0.42
1:C5:2:ILE:HD13	1:C6:239:ARG:HA	2.02	0.42
1:D3:44:SER:HB3	1:E4:110:ILE:HG13	2.02	0.42
1:D4:194:ALA:O	1:D4:198:LEU:HG	2.19	0.42
1:E5:35:ARG:NH2	1:F5:64:ARG:HD2	2.35	0.42
1:E5:250:VAL:HG13	1:F4:6:ASN:ND2	2.32	0.42
1:F3:111:GLN:OE1	1:F3:184:THR:HA	2.20	0.42
1:F5:86:ILE:HG23	1:F5:117:LEU:HD12	2.01	0.42
1:G6:29:THR:HA	1:G6:37:ASN:ND2	2.35	0.42
1:G7:250:VAL:O	1:G7:254:LYS:HG2	2.20	0.42
1:I8:247:GLU:HG3	1:J7:13:HIS:NE2	2.35	0.42
1:J5:277:LEU:HA	1:J5:280:LEU:HG	2.01	0.42
1:J8:107:ARG:NH2	1:J8:188:ALA:HB2	2.35	0.42
1:K8:96:GLN:HG3	1:K8:102:TYR:CE2	2.54	0.42
1:K9:181:SER:HA	7:Z4:204:MET:SD	2.60	0.42
2:L2:90:PHE:HA	2:L2:93:LEU:CD2	2.50	0.42
2:L5:83:PHE:CE2	2:L6:333:LYS:HE2	2.55	0.42
2:P2:249:GLU:O	2:P2:253:LYS:HG2	2.19	0.42
3:Q1:218:ALA:HA	3:Q1:229:ARG:NH1	2.34	0.42
3:R3:192:PHE:HD1	3:R3:214:LYS:HG2	1.85	0.42
3:S6:248:PHE:HA	3:S6:251:ILE:HG22	2.01	0.42
4:T2:145:PRO:HB2	4:T2:270:LEU:HD11	2.01	0.42
4:T3:171:TRP:CZ2	4:T3:172:LYS:HE3	2.55	0.42
4:T4:78:SER:HA	4:T4:93:LYS:CB	2.49	0.42
5:X4:184:SER:HA	5:X4:194:LEU:HD21	2.01	0.42
5:X4:225:LYS:HB3	5:X4:228:ALA:HB3	2.02	0.42
5:X5:119:PHE:HB2	5:X5:198:SER:HB2	2.01	0.42
6:Y2:162:ARG:HD3	6:Y2:163:MET:N	2.35	0.42
7:Z2:204:MET:HE2	7:Z2:204:MET:HB2	1.72	0.42
10:d2:105:LYS:HB2	10:d2:106:PRO:HD3	2.02	0.42
4:t1:151:MET:HE2	4:t1:193:VAL:CG1	2.46	0.42
1:A6:247:GLU:OE2	1:B5:13:HIS:CD2	2.73	0.41
1:A8:251:ALA:O	1:A8:254:LYS:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B6:55:GLN:NE2	1:C6:131:ASN:HA	2.34	0.41
1:B7:87:ILE:HD11	1:B7:201:ALA:HB1	2.01	0.41
1:B7:182:LEU:H	1:B7:182:LEU:HD23	1.84	0.41
1:D3:43:ALA:HB1	1:D4:210:ALA:HB1	2.02	0.41
1:E3:43:ALA:HB1	1:E4:210:ALA:HA	2.02	0.41
1:F6:60:ARG:HD3	1:F6:230:TYR:CZ	2.54	0.41
1:F6:132:LYS:HG3	1:F6:132:LYS:O	2.20	0.41
1:G8:259:VAL:O	1:G8:263:THR:HG23	2.19	0.41
1:H6:44:SER:OG	1:I7:110:ILE:HG12	2.20	0.41
1:I6:52:MET:O	1:I6:56:VAL:HG23	2.20	0.41
1:J9:184:THR:HG23	1:J9:190:PHE:HB3	2.02	0.41
2:N2:185:ASN:HB3	2:N2:188:LEU:HB2	2.02	0.41
3:Q1:217:LEU:O	3:Q1:220:VAL:HG12	2.20	0.41
3:R3:104:ARG:HE	3:R3:131:GLU:CG	2.31	0.41
3:S4:59:LEU:HD11	3:S4:241:LEU:HD21	2.02	0.41
4:T1:114:PRO:HB2	4:T1:116:ILE:HD12	2.02	0.41
4:T4:16:ILE:HG23	4:T4:20:GLY:HA3	2.02	0.41
6:Y4:63:ASN:C	6:Y4:65:LYS:H	2.27	0.41
6:Y5:139:TRP:CD1	6:Y5:143:LYS:HD2	2.54	0.41
7:Z1:85:TYR:CE2	7:Z1:89:LYS:HE3	2.55	0.41
10:d2:27:GLU:O	10:d2:31:ARG:HG2	2.20	0.41
10:d3:24:LYS:O	10:d3:28:TYR:HB2	2.20	0.41
4:t3:20:GLY:HA2	4:t3:244:PHE:HB2	2.02	0.41
4:t4:31:TRP:HE1	4:t4:42:TRP:CD1	2.38	0.41
1:A5:25:LYS:O	1:A5:29:THR:HG23	2.20	0.41
1:A5:276:VAL:HG12	1:A5:280:LEU:HD23	2.01	0.41
1:A6:52:MET:HB3	1:A6:237:GLU:HB2	2.01	0.41
1:A8:150:TRP:CZ2	1:A8:162:ARG:HD2	2.55	0.41
1:C5:261:SER:HB3	1:D4:277:LEU:HD21	2.01	0.41
1:E3:159:GLN:CB	1:F3:127:GLN:HE22	2.33	0.41
1:E3:265:MET:SD	1:F3:30:LEU:HD23	2.60	0.41
1:E4:39:ALA:CB	1:E5:210:ALA:HA	2.51	0.41
1:E4:73:ILE:HD13	1:E4:215:TYR:HB3	2.02	0.41
1:E6:114:VAL:HG21	1:E6:185:LEU:HD12	2.01	0.41
1:F6:163:VAL:O	1:F6:163:VAL:HG13	2.20	0.41
1:G1:203:MET:HA	1:G1:206:ASN:ND2	2.35	0.41
1:G9:100:GLY:HA2	1:G9:107:ARG:NH2	2.35	0.41
1:H6:10:ILE:HG22	1:H7:231:GLU:OE2	2.20	0.41
1:H6:46:LEU:HD21	1:H7:209:ARG:NE	2.33	0.41
1:H6:60:ARG:HH11	1:H6:227:MET:HE1	1.85	0.41
1:H7:105:GLU:O	1:H7:109:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H9:265:MET:HE1	1:I9:30:LEU:C	2.45	0.41
1:J8:36:ILE:HG23	1:J8:41:ASP:HB2	2.01	0.41
1:K4:280:LEU:HG	1:K5:245:MET:HE1	2.02	0.41
1:K5:71:SER:HA	1:K5:74:GLN:OE1	2.20	0.41
2:O3:167:GLN:HE22	2:O3:212:LEU:HD21	1.85	0.41
2:O3:203:ARG:O	2:O3:206:ILE:HG22	2.20	0.41
2:O5:160:ARG:NH1	2:O5:164:VAL:HG11	2.35	0.41
3:Q4:70:VAL:HG13	3:Q4:255:ASN:OD1	2.20	0.41
3:Q4:128:LYS:HA	3:Q4:158:LYS:O	2.20	0.41
5:V2:63:THR:OG1	5:V2:64:PRO:HA	2.20	0.41
5:V3:105:LYS:HG3	5:V3:213:TYR:CD1	2.54	0.41
5:V3:105:LYS:HG3	5:V3:213:TYR:CE1	2.55	0.41
5:V3:167:TYR:CZ	5:V3:171:ARG:HB2	2.55	0.41
5:V4:138:LEU:HD22	5:V4:215:TYR:CD2	2.55	0.41
5:V5:158:HIS:CG	5:V5:181:VAL:HG22	2.55	0.41
5:X2:148:ALA:O	5:X2:160:ILE:HG22	2.20	0.41
5:X5:132:GLN:HB2	5:X5:222:ARG:HB3	2.02	0.41
5:X5:238:ASN:HD22	7:Z4:273:LEU:CB	2.33	0.41
6:Y2:260:PRO:HA	6:Y2:266:LYS:HE3	2.02	0.41
7:Z4:269:ASP:HB3	7:Z4:323:ARG:HB3	2.02	0.41
2:p3:289:TYR:O	2:p3:292:ILE:HG22	2.20	0.41
2:p4:138:ARG:HG3	2:p4:140:ASP:H	1.85	0.41
1:A5:27:MET:HE2	1:A5:27:MET:HA	2.03	0.41
1:A6:100:GLY:HA2	1:A6:107:ARG:HH22	1.84	0.41
1:A6:140:PHE:HD2	1:A6:165:ILE:HD11	1.85	0.41
1:B7:194:ALA:O	1:B7:198:LEU:HD23	2.20	0.41
1:D5:63:GLU:HG3	1:D5:227:MET:HG2	2.02	0.41
1:D6:1:MET:H3	1:D7:244:ASP:CG	2.28	0.41
1:F2:253:THR:HG21	1:G6:270:ASN:HD21	1.85	0.41
1:G7:272:ARG:HD2	1:H7:27:MET:HE1	2.01	0.41
1:H6:5:HIS:CD2	1:H7:234:GLN:HE22	2.39	0.41
1:I5:265:MET:SD	1:I5:265:MET:C	3.03	0.41
1:I8:259:VAL:O	1:I8:263:THR:HG23	2.20	0.41
1:I9:38:ARG:HA	1:I9:38:ARG:HE	1.85	0.41
1:I9:113:GLU:O	1:I9:116:GLN:HG3	2.20	0.41
1:I9:222:ALA:O	1:I9:226:LEU:HD23	2.20	0.41
1:J6:140:PHE:CZ	1:J6:149:MET:HG3	2.55	0.41
1:J7:236:SER:HB3	1:K7:71:SER:HB3	2.02	0.41
1:J8:111:GLN:HE21	1:J8:184:THR:HG22	1.86	0.41
2:L5:181:ASP:OD1	2:L5:181:ASP:C	2.63	0.41
2:L6:287:GLU:O	2:L6:290:ARG:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O3:75:GLU:CD	2:O3:76:ALA:H	2.29	0.41
2:O3:271:ASN:ND2	2:O3:296:VAL:HG22	2.36	0.41
3:Q1:237:TYR:HA	3:Q1:240:HIS:ND1	2.34	0.41
3:R3:133:TYR:C	3:R3:153:ASN:HB2	2.45	0.41
3:R5:83:LYS:HE3	3:R5:99:ALA:C	2.44	0.41
3:S5:101:ASN:HA	3:S5:134:PHE:CZ	2.55	0.41
3:S5:198:TYR:CG	3:S5:199:PRO:HD2	2.55	0.41
4:T2:71:LEU:HG	4:T2:100:GLN:HB2	2.01	0.41
4:T3:143:GLU:HB3	4:T3:211:THR:HB	2.02	0.41
4:T3:162:TYR:CE2	4:T3:221:SER:HB3	2.55	0.41
5:X4:134:SER:HA	5:X4:173:LEU:O	2.20	0.41
5:X5:50:ASN:HB2	5:X5:218:ASP:HA	2.02	0.41
10:d3:245:VAL:HG12	10:d3:247:LEU:H	1.86	0.41
10:d4:67:LEU:CD2	10:d4:91:VAL:HG13	2.49	0.41
2:p2:183:ILE:H	2:p2:183:ILE:HD12	1.84	0.41
3:s4:127:ALA:HA	3:s4:161:LYS:HG3	2.02	0.41
4:t1:24:ARG:HA	4:t1:24:ARG:HD2	1.92	0.41
4:t2:125:LYS:HE2	4:t2:137:SER:HB3	2.01	0.41
1:A5:31:SER:C	1:K5:15:VAL:HG11	2.45	0.41
1:B4:3:ILE:HD13	1:B5:245:MET:SD	2.61	0.41
1:B5:217:ASN:HA	1:B5:220:GLU:HG2	2.02	0.41
1:C6:254:LYS:O	1:C6:258:LEU:HD23	2.21	0.41
1:C7:25:LYS:O	1:C7:29:THR:HG22	2.21	0.41
1:D4:159:GLN:CD	1:E4:127:GLN:HB2	2.45	0.41
1:E2:249:THR:O	1:E2:253:THR:HG23	2.21	0.41
1:E2:272:ARG:HB3	1:E2:273:PRO:HD3	2.02	0.41
1:E3:27:MET:HE3	1:E3:252:PHE:CD1	2.55	0.41
1:G2:157:GLN:C	1:G2:159:GLN:N	2.78	0.41
1:G9:14:ARG:HD2	1:G9:14:ARG:C	2.45	0.41
1:G9:86:ILE:O	1:G9:90:ILE:HD12	2.20	0.41
1:J7:265:MET:SD	1:J7:265:MET:C	3.04	0.41
1:J9:150:TRP:O	1:J9:151:PHE:HD1	2.04	0.41
1:K6:153:ILE:HG21	1:K6:222:ALA:HB1	2.02	0.41
1:K6:250:VAL:O	1:K6:253:THR:HG22	2.20	0.41
1:K7:253:THR:O	1:K7:257:ILE:HG12	2.21	0.41
2:L3:265:LYS:HE2	2:L3:265:LYS:HB3	1.95	0.41
2:L4:153:ARG:O	2:L4:156:ARG:HG2	2.19	0.41
2:M5:293:VAL:HG13	8:a5:208:GLU:HG2	2.01	0.41
2:N4:106:ARG:HH22	3:R4:108:TYR:HD2	1.66	0.41
2:N5:286:SER:HB3	2:N5:289:TYR:CG	2.55	0.41
2:N6:209:GLU:CG	2:N6:214:ASN:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P6:193:GLU:HA	2:P6:196:ARG:HG2	2.02	0.41
3:R2:152:ILE:HB	3:R2:180:ASN:ND2	2.35	0.41
3:S4:106:GLU:HG2	3:S4:108:TYR:CE1	2.55	0.41
5:V3:132:GLN:HG2	5:V3:222:ARG:NH2	2.35	0.41
6:Y2:257:ILE:H	6:Y2:269:TYR:HB3	1.86	0.41
6:Y2:260:PRO:HA	6:Y2:266:LYS:CE	2.50	0.41
4:t3:1:GLN:HE21	4:t3:3:ILE:HD12	1.84	0.41
1:A7:277:LEU:HD13	1:A7:280:LEU:HD21	2.02	0.41
1:C4:57:LYS:HG2	1:C5:92:VAL:HG21	2.03	0.41
1:D5:29:THR:HG22	1:D5:37:ASN:HD21	1.84	0.41
1:D5:224:LYS:HD3	1:D5:224:LYS:HA	1.80	0.41
1:E2:272:ARG:O	1:E2:276:VAL:HG22	2.20	0.41
1:E4:174:ASN:OD1	1:E4:174:ASN:C	2.64	0.41
1:E5:33:GLY:C	1:E5:34:MET:HE2	2.46	0.41
1:G7:149:MET:HE1	1:G8:100:GLY:C	2.46	0.41
1:G8:16:LEU:HD11	1:G8:263:THR:HG22	2.01	0.41
1:I7:157:GLN:NE2	1:I7:158:HIS:HB2	2.34	0.41
1:J6:80:LEU:HD23	1:J6:80:LEU:HA	1.86	0.41
1:K6:106:ASP:O	1:K6:110:ILE:HG12	2.20	0.41
1:K7:183:LEU:HD23	1:K7:183:LEU:HA	1.91	0.41
2:L2:75:GLU:C	2:L2:77:LEU:N	2.79	0.41
2:M3:276:ARG:NH1	2:M3:280:LEU:HD23	2.35	0.41
2:N3:112:TYR:OH	2:N3:200:ASP:HB3	2.21	0.41
2:O5:160:ARG:HH11	2:O5:160:ARG:HG3	1.86	0.41
2:O5:209:GLU:HG3	2:O5:214:ASN:HB2	2.03	0.41
3:S4:104:ARG:HA	3:S4:130:MET:O	2.20	0.41
5:V5:117:GLU:HG2	5:V5:119:PHE:HE1	1.85	0.41
5:X3:148:ALA:HB3	5:X3:160:ILE:HD11	2.01	0.41
5:X3:149:LYS:HB3	5:X3:197:VAL:HB	2.03	0.41
5:X4:107:ASN:HA	5:X4:211:GLN:HA	2.03	0.41
6:Y2:72:MET:HG3	6:Y2:236:MET:HG2	2.01	0.41
10:d2:144:THR:HG22	10:d2:148:TYR:CZ	2.54	0.41
2:p5:239:LYS:HB2	2:p5:277:ALA:HB1	2.02	0.41
4:t2:155:VAL:HG22	4:t2:234:PHE:CE2	2.55	0.41
4:t4:80:LYS:HB3	4:t4:92:ALA:CB	2.48	0.41
1:A5:123:ARG:HD2	1:A5:127:GLN:OE1	2.21	0.41
1:A6:73:ILE:HG21	1:A6:216:PHE:HB2	2.03	0.41
1:A6:97:SER:HB2	1:A6:110:ILE:HG21	2.02	0.41
1:A8:211:ASN:OD1	1:B8:112:VAL:HG21	2.20	0.41
1:B4:72:LEU:HD13	1:B5:101:ILE:HG22	2.02	0.41
1:C6:150:TRP:CZ3	1:C6:162:ARG:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D5:207:LYS:HA	1:E5:109:MET:SD	2.60	0.41
1:E6:139:ASP:OD1	1:E6:147:SER:HB2	2.20	0.41
1:G1:177:LYS:HG2	1:G1:178:ALA:H	1.86	0.41
1:G7:220:GLU:O	1:G7:224:LYS:HG2	2.20	0.41
1:H6:48:VAL:O	1:H6:52:MET:HG2	2.20	0.41
1:H7:131:ASN:C	1:H7:133:MET:H	2.29	0.41
1:H9:239:ARG:HD2	1:I9:67:GLU:OE2	2.21	0.41
1:I7:272:ARG:HG2	1:I7:273:PRO:HD3	2.01	0.41
1:I7:280:LEU:HD13	1:I7:280:LEU:HA	1.95	0.41
1:I8:154:GLY:HA3	1:I8:159:GLN:CD	2.45	0.41
1:K8:247:GLU:HA	1:K8:250:VAL:HG22	2.01	0.41
1:K9:153:ILE:HD13	1:K9:161:GLU:HG2	2.03	0.41
2:L3:75:GLU:C	2:L3:77:LEU:H	2.29	0.41
2:L3:133:GLU:OE1	2:L3:136:LYS:HE2	2.20	0.41
2:L6:209:GLY:O	2:L6:212:THR:HG22	2.20	0.41
2:M1:189:ARG:HA	2:M1:194:PHE:CG	2.55	0.41
2:M3:93:LEU:HD12	2:M4:292:ILE:HD13	2.03	0.41
2:M4:183:ILE:O	2:M4:183:ILE:HG13	2.21	0.41
2:P3:174:THR:HG22	2:P3:205:TRP:HE1	1.86	0.41
3:R2:65:LEU:O	3:R2:65:LEU:HD23	2.20	0.41
3:R2:107:VAL:O	3:R2:127:ALA:HB3	2.20	0.41
3:R2:191:VAL:HB	3:R2:217:LEU:HD21	2.02	0.41
3:R5:40:SER:HA	3:R5:43:GLU:HG2	2.01	0.41
5:V1:56:ASP:HB3	5:V1:121:PRO:HB3	2.02	0.41
5:X4:48:LEU:HD11	7:Z4:179:LEU:HA	2.01	0.41
8:a2:61:ILE:CD1	8:a2:196:LEU:HD22	2.50	0.41
8:a4:143:ILE:HB	8:a4:160:VAL:HB	2.02	0.41
4:t1:35:ALA:H	4:t1:38:ALA:HB3	1.86	0.41
4:t1:80:LYS:HE2	4:t1:92:ALA:HB1	2.03	0.41
4:t2:109:VAL:HB	4:t2:219:VAL:CG2	2.51	0.41
1:A6:52:MET:O	1:A6:56:VAL:HG23	2.21	0.41
1:A8:222:ALA:HB1	1:B8:123:ARG:HH22	1.86	0.41
1:B3:281:ARG:HH11	1:B3:281:ARG:HG2	1.86	0.41
1:B6:197:THR:HG23	5:V2:65:LEU:HD12	2.02	0.41
1:B7:53:ARG:HG3	1:B7:241:ARG:NH1	2.36	0.41
1:B7:245:MET:HE3	1:B7:245:MET:HB3	1.89	0.41
1:C8:90:ILE:HG22	1:C8:198:LEU:HD11	2.02	0.41
1:D5:23:VAL:HG22	1:D5:255:ASN:HB3	2.03	0.41
1:D5:79:TYR:HA	1:D5:82:GLU:HG2	2.01	0.41
1:F3:86:ILE:HG23	1:F3:117:LEU:HD12	2.03	0.41
1:G1:202:LEU:HD11	1:G9:54:THR:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J6:40:GLY:HA2	1:J7:217:ASN:ND2	2.36	0.41
1:J8:218:ARG:NH2	1:K8:119:ASP:HB3	2.36	0.41
2:M3:206:ILE:HD13	2:M3:222:LEU:HD23	2.02	0.41
2:N2:75:GLU:C	2:N2:77:LEU:N	2.78	0.41
2:N2:90:PHE:CD2	2:N3:239:LYS:HE2	2.56	0.41
2:N3:206:ILE:HD11	2:N3:221:ILE:HB	2.03	0.41
2:O2:238:HIS:HD2	2:O2:273:HIS:HD2	1.67	0.41
2:O5:226:ILE:HD11	2:O5:241:LEU:HD22	2.03	0.41
3:R3:72:VAL:HG11	3:R3:254:TYR:HB3	2.02	0.41
5:V3:123:GLU:HA	5:V3:197:VAL:CG1	2.51	0.41
5:X3:151:ARG:HG3	5:X3:157:THR:HG22	2.02	0.41
5:X4:119:PHE:CD1	5:X4:120:PRO:HD2	2.56	0.41
7:Z2:331:ARG:HG3	7:Z2:332:ASP:N	2.36	0.41
8:a5:181:GLU:HB3	8:a5:184:GLN:HG2	2.03	0.41
10:d3:189:LEU:HD11	10:d3:205:ILE:HG12	2.02	0.41
2:p5:205:TRP:HE1	2:p5:221:ILE:HG21	1.86	0.41
2:p5:267:ARG:HA	2:p5:270:LYS:HG2	2.03	0.41
3:s3:42:LEU:O	3:s3:45:GLU:HG3	2.21	0.41
1:A5:86:ILE:O	1:A5:90:ILE:HG13	2.21	0.41
1:A5:232:ASN:HD21	1:B5:74:GLN:HG3	1.84	0.41
1:A6:15:VAL:O	1:A6:19:GLN:HG2	2.21	0.41
1:A6:124:ILE:O	1:A6:128:ALA:HB3	2.21	0.41
1:A6:218:ARG:HG3	1:B6:120:GLU:HG2	2.02	0.41
1:A7:6:ASN:HD21	1:K8:250:VAL:HB	1.86	0.41
1:B5:35:ARG:H	1:B5:242:ASP:HA	1.84	0.41
1:B5:46:LEU:HD21	1:B6:209:ARG:CZ	2.51	0.41
1:C4:48:VAL:O	1:C4:52:MET:HG2	2.20	0.41
1:C4:218:ARG:HD2	1:D4:120:GLU:HB2	2.03	0.41
1:C8:97:SER:HB2	1:C8:110:ILE:HG21	2.03	0.41
1:D7:87:ILE:HD12	1:D7:205:ILE:HD12	2.02	0.41
1:E7:194:ALA:O	1:E7:198:LEU:HD13	2.21	0.41
1:G6:270:ASN:OD1	1:G6:270:ASN:C	2.64	0.41
1:G8:33:GLY:O	1:G8:243:THR:HG22	2.21	0.41
1:G8:36:ILE:HG21	1:G8:46:LEU:HB2	2.03	0.41
1:G8:151:PHE:HA	1:G9:99:ASN:OD1	2.21	0.41
1:H6:26:ASN:HA	1:H6:29:THR:HG22	2.02	0.41
1:H9:67:GLU:O	1:H9:70:MET:HG2	2.20	0.41
1:H9:151:PHE:CD2	1:H9:163:VAL:HG21	2.55	0.41
1:J9:100:GLY:HA2	1:J9:107:ARG:NH2	2.35	0.41
1:K5:25:LYS:O	1:K5:29:THR:HG23	2.21	0.41
2:L2:166:LYS:CE	2:L2:211:ASP:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L3:262:GLN:O	2:L3:265:LYS:HG2	2.21	0.41
2:M2:75:GLU:C	2:M2:77:LEU:H	2.28	0.41
2:M4:75:GLU:C	2:M4:77:LEU:H	2.29	0.41
2:M5:262:GLN:HA	2:M5:265:LYS:HE3	2.02	0.41
2:O4:251:MET:HE3	2:O4:251:MET:HB2	1.89	0.41
2:P2:89:ASN:O	2:P2:93:LEU:HG	2.21	0.41
4:T2:30:SER:HB3	4:T2:32:ASP:CG	2.46	0.41
5:X1:212:PHE:CE2	5:X1:214:PHE:HB3	2.56	0.41
5:X4:73:MET:SD	5:X4:101:ILE:HB	2.60	0.41
6:Y5:188:PHE:CE2	6:Y5:193:PRO:HB3	2.56	0.41
7:Z2:180:THR:HG23	7:Z2:181:ARG:N	2.33	0.41
10:d2:82:GLU:O	10:d2:87:LEU:HD13	2.21	0.41
10:d2:240:MET:HE1	2:p3:132:GLU:OE1	2.21	0.41
4:t1:28:VAL:O	4:t1:28:VAL:HG13	2.21	0.41
4:t1:80:LYS:HD2	4:t1:84:ILE:HB	2.03	0.41
4:t3:72:ARG:HH11	4:t3:72:ARG:HG3	1.85	0.41
1:A4:269:ALA:O	1:A4:272:ARG:HG2	2.21	0.41
1:A5:39:ALA:HB2	1:A5:46:LEU:HD13	2.02	0.41
1:A7:100:GLY:HA2	1:A7:107:ARG:NH2	2.36	0.41
1:A8:70:MET:HE2	1:A8:216:PHE:CE1	2.48	0.41
1:A8:72:LEU:HD13	1:A9:101:ILE:HG22	2.02	0.41
1:B6:72:LEU:HA	1:B6:75:THR:HG22	2.02	0.41
1:C6:115:SER:HB2	1:C6:182:LEU:HD12	2.02	0.41
1:C6:158:HIS:C	1:C6:160:ARG:H	2.29	0.41
1:C8:220:GLU:HG3	1:C8:224:LYS:HE3	2.02	0.41
1:D4:38:ARG:HG3	1:D4:40:GLY:H	1.86	0.41
1:D5:15:VAL:HG11	1:E5:32:SER:HA	2.02	0.41
1:D5:67:GLU:HA	1:D5:70:MET:HG2	2.03	0.41
1:D5:168:MET:HE3	1:D5:168:MET:HB3	2.01	0.41
1:D6:172:SER:C	1:D6:174:ASN:H	2.29	0.41
1:E6:187:THR:HG22	1:E6:190:PHE:HD1	1.85	0.41
1:E7:131:ASN:C	1:E7:133:MET:H	2.29	0.41
1:F2:270:ASN:O	1:F2:273:PRO:HD2	2.21	0.41
1:G7:4:ASN:HB3	1:G8:242:ASP:CG	2.46	0.41
1:G9:154:GLY:HA3	1:G9:159:GLN:NE2	2.35	0.41
1:I6:276:VAL:HG13	1:J6:263:THR:HG21	2.03	0.41
1:J5:54:THR:HG22	1:J6:88:GLN:HE22	1.86	0.41
1:J6:19:GLN:HG3	1:J6:258:LEU:HD22	2.02	0.41
1:J6:244:ASP:OD2	1:K5:13:HIS:HE1	2.04	0.41
1:J7:235:ALA:O	1:J7:239:ARG:HG2	2.21	0.41
1:J8:99:ASN:OD1	1:J8:101:ILE:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K5:221:HIS:HA	1:K5:224:LYS:HG2	2.01	0.41
1:K6:23:VAL:HG22	1:K6:255:ASN:HB3	2.02	0.41
1:K8:43:ALA:HB1	1:K9:210:ALA:HB1	2.02	0.41
1:K8:52:MET:HA	1:K8:55:GLN:CD	2.45	0.41
2:L2:212:LEU:O	2:L2:213:GLN:HG3	2.21	0.41
2:L5:113:GLN:HA	2:L5:116:VAL:HG12	2.01	0.41
2:M2:143:TRP:HB2	2:M2:146:GLN:OE1	2.20	0.41
2:M5:236:PRO:HA	2:M5:239:LYS:HG2	2.03	0.41
2:N4:93:LEU:HD13	2:N5:292:ILE:HD11	2.02	0.41
2:N4:269:LYS:HA	2:N4:272:VAL:HG12	2.03	0.41
2:N6:130:ARG:HG2	2:N6:130:ARG:HH11	1.85	0.41
2:O5:171:ASN:O	2:O5:174:THR:HG22	2.21	0.41
2:P3:94:HIS:CE1	2:P3:95:GLN:HG3	2.56	0.41
3:Q1:107:VAL:O	3:Q1:127:ALA:HB3	2.21	0.41
3:R3:82:GLY:HA3	3:R3:91:PRO:HA	2.03	0.41
3:R3:155:LEU:CD2	3:R3:176:ASP:HB3	2.51	0.41
3:R5:233:LYS:HG2	3:R5:237:TYR:CE2	2.56	0.41
3:R5:234:LYS:HD3	3:R5:238:ILE:HD12	2.02	0.41
3:S2:230:ASN:OD1	3:S2:231:SER:N	2.53	0.41
4:T1:167:TRP:HE3	4:T1:215:LYS:HB2	1.86	0.41
4:T2:42:TRP:HE3	4:T2:111:ILE:HG22	1.85	0.41
5:V1:74:VAL:HA	5:V1:99:ASN:O	2.20	0.41
5:V3:49:GLU:HB3	5:V3:219:LEU:HB3	2.03	0.41
5:V3:149:LYS:HB3	5:V3:198:SER:HB2	2.02	0.41
5:V5:52:GLU:CA	5:V5:100:HIS:HB2	2.42	0.41
5:V5:84:ASP:OD1	5:V5:84:ASP:N	2.53	0.41
6:Y2:57:PHE:CD2	6:Y2:72:MET:HE3	2.56	0.41
6:Y2:68:PHE:CZ	6:Y2:219:LEU:HD21	2.56	0.41
6:Y2:256:LEU:HD23	6:Y2:270:ARG:HA	2.02	0.41
6:Y4:258:PHE:CE2	6:Y4:267:LEU:HD13	2.55	0.41
7:Z1:26:LYS:O	7:Z1:30:LYS:HG2	2.21	0.41
7:Z3:93:GLN:HE22	7:Z3:96:LEU:HD11	1.86	0.41
7:Z3:212:ALA:O	7:Z3:216:ARG:HG2	2.20	0.41
9:c3:68:LEU:HD23	9:c3:68:LEU:H	1.85	0.41
10:d4:33:TYR:O	10:d4:37:ILE:HG12	2.21	0.41
1:h0:165:ILE:O	1:h0:165:ILE:HG13	2.21	0.41
1:h0:222:ALA:O	1:h0:226:LEU:HD23	2.21	0.41
1:h1:105:GLU:O	1:h1:109:MET:HG2	2.21	0.41
3:s5:157:SER:HB2	3:s5:174:VAL:CG1	2.51	0.41
4:t2:28:VAL:O	4:t2:28:VAL:HG13	2.21	0.41
4:t3:23:LEU:HD11	4:t3:240:LEU:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:39:ALA:HB3	1:A5:77:GLU:HG3	2.02	0.41
1:A8:105:GLU:O	1:A8:109:MET:HG2	2.21	0.41
1:A8:202:LEU:O	1:A8:205:ILE:HG22	2.21	0.41
1:A9:110:ILE:HG12	1:K8:44:SER:HB3	2.03	0.41
1:C3:265:MET:HE1	1:D3:27:MET:O	2.21	0.41
1:C7:80:LEU:HD11	1:C7:168:MET:HE3	2.03	0.41
1:D3:7:LEU:HD13	1:D3:7:LEU:HA	1.88	0.41
1:D6:254:LYS:HE2	1:D6:258:LEU:HD11	2.03	0.41
1:F5:153:ILE:HG13	1:G1:123:ARG:NH2	2.37	0.41
1:F6:120:GLU:O	1:F6:124:ILE:HG12	2.20	0.41
1:G8:52:MET:HE2	1:G8:52:MET:HA	2.03	0.41
1:H8:235:ALA:O	1:H8:239:ARG:HG2	2.21	0.41
1:I7:51:LYS:CE	1:J7:132:LYS:HD3	2.51	0.41
1:I7:80:LEU:HD12	1:I7:205:ILE:HG23	2.03	0.41
1:J5:23:VAL:HG22	1:J5:255:ASN:HB3	2.03	0.41
1:J8:152:HIS:NE2	1:J9:95:ILE:HG23	2.35	0.41
1:J9:56:VAL:HG21	1:J9:234:GLN:HG2	2.02	0.41
1:K5:70:MET:HG2	1:K5:74:GLN:HE22	1.86	0.41
1:K6:38:ARG:HD2	1:K7:74:GLN:CG	2.51	0.41
1:K6:114:VAL:HG21	1:K6:185:LEU:HD12	2.02	0.41
2:N3:189:ARG:HD3	2:N3:194:PHE:CE2	2.56	0.41
2:O3:154:GLU:O	2:O3:157:VAL:HG12	2.21	0.41
3:Q1:40:SER:HA	3:Q1:43:GLU:HG2	2.02	0.41
3:Q1:53:PHE:HA	3:Q1:56:ASN:ND2	2.36	0.41
3:Q2:220:VAL:HB	3:Q2:229:ARG:HD3	2.03	0.41
3:R2:60:THR:HA	3:R2:63:THR:HG23	2.02	0.41
3:R3:255:ASN:HA	3:R3:258:LEU:HG	2.02	0.41
3:S4:40:SER:HA	3:S4:43:GLU:HG2	2.03	0.41
5:V3:187:PHE:HD2	5:V3:189:LEU:HB2	1.85	0.41
6:Y4:150:ASP:O	6:Y4:154:ARG:HG3	2.21	0.41
6:Y5:88:TYR:CZ	6:Y5:182:ALA:HB2	2.56	0.41
10:d2:209:ILE:HG23	10:d2:213:MET:CE	2.50	0.41
2:p5:75:GLU:C	2:p5:77:LEU:H	2.28	0.41
4:t2:183:LEU:HA	4:t2:185:PHE:CE2	2.55	0.41
1:A6:1:MET:HE1	1:B6:20:ASN:CG	2.46	0.40
1:A6:150:TRP:CZ3	1:A6:162:ARG:HG2	2.57	0.40
1:A7:229:ALA:O	1:A7:233:ILE:HG13	2.21	0.40
1:B4:44:SER:OG	1:C5:110:ILE:HA	2.20	0.40
1:B7:108:GLN:O	1:B7:112:VAL:HG23	2.21	0.40
1:B7:239:ARG:CZ	1:C7:67:GLU:HB3	2.51	0.40
1:B8:191:ALA:O	1:B8:195:ILE:HG12	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:14:ARG:CZ	1:D4:228:VAL:HG22	2.51	0.40
1:D4:215:TYR:O	1:D4:219:LEU:HD23	2.20	0.40
1:D5:280:LEU:HD11	1:E5:266:LEU:HD12	2.02	0.40
1:E3:36:ILE:HD11	1:F3:64:ARG:HH22	1.86	0.40
1:E3:168:MET:HE3	1:E3:205:ILE:HG22	2.03	0.40
1:F3:228:VAL:HA	1:F3:231:GLU:CD	2.46	0.40
1:F5:49:SER:OG	1:F5:241:ARG:HB2	2.21	0.40
1:G2:227:MET:HE2	1:G2:227:MET:HA	2.03	0.40
1:I6:151:PHE:CE2	1:I6:163:VAL:HG21	2.56	0.40
1:I7:246:ALA:O	1:I7:250:VAL:HG23	2.20	0.40
1:I8:261:SER:O	1:I8:265:MET:HG2	2.21	0.40
1:J9:152:HIS:HA	1:J9:160:ARG:HA	2.03	0.40
1:J9:225:GLY:HA3	1:K9:82:GLU:OE1	2.21	0.40
2:L4:177:ILE:HD12	2:L4:177:ILE:HA	1.94	0.40
2:M1:175:LYS:HE3	2:M1:179:HIS:CE1	2.56	0.40
2:N5:241:LEU:HD23	2:N5:273:HIS:CD2	2.56	0.40
2:P2:125:ALA:O	2:P2:128:GLN:HG3	2.21	0.40
2:P4:262:GLN:O	2:P4:265:LYS:HG3	2.21	0.40
2:P4:278:THR:OG1	2:P4:292:ILE:HD13	2.22	0.40
3:R5:158:LYS:HE3	3:R5:160:TYR:CE1	2.55	0.40
3:S2:41:ILE:HD12	3:S2:227:PRO:HB3	2.03	0.40
3:S3:198:TYR:CD1	3:S3:199:PRO:HD2	2.56	0.40
4:T3:113:PRO:HA	4:T3:114:PRO:HD3	1.87	0.40
5:V5:48:LEU:HD12	5:V5:220:GLU:HA	2.02	0.40
5:X3:49:GLU:HG2	5:X3:49:GLU:O	2.20	0.40
5:X5:43:LEU:HG	5:X5:222:ARG:HD3	2.03	0.40
7:Z3:136:ILE:CD1	7:Z3:255:ARG:HH11	2.34	0.40
8:a4:91:PRO:C	8:a4:93:SER:H	2.29	0.40
8:a5:182:PRO:HG3	8:a5:185:ARG:NH2	2.37	0.40
9:c3:59:VAL:HG13	9:c3:102:PHE:CE2	2.56	0.40
1:h0:226:LEU:HD21	1:i0:123:ARG:HH22	1.85	0.40
1:j0:91:ARG:O	1:j0:95:ILE:HG22	2.21	0.40
2:p3:267:ARG:HA	2:p3:270:LYS:HG2	2.03	0.40
1:A4:265:MET:HG2	1:B4:31:SER:HB2	2.03	0.40
1:A5:191:ALA:O	1:A5:195:ILE:HG23	2.22	0.40
1:B6:266:LEU:CD2	1:B6:270:ASN:HD21	2.29	0.40
1:B8:239:ARG:CZ	1:C8:67:GLU:HB3	2.52	0.40
1:C4:117:LEU:O	1:C4:120:GLU:HG2	2.20	0.40
1:D7:157:GLN:HG3	1:D7:158:HIS:CD2	2.56	0.40
1:E4:18:PHE:HE1	1:E5:227:MET:HG3	1.87	0.40
1:E4:79:TYR:O	1:E4:82:GLU:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F3:136:LEU:HB3	1:F3:168:MET:HB2	2.02	0.40
1:G1:111:GLN:HE22	1:G1:184:THR:HA	1.85	0.40
1:G2:100:GLY:HA2	1:G2:107:ARG:HH22	1.86	0.40
1:G7:149:MET:HE3	1:G7:150:TRP:H	1.85	0.40
1:G9:51:LYS:HE2	1:H9:132:LYS:CD	2.50	0.40
1:H7:214:ALA:HB1	1:I7:116:GLN:HG2	2.02	0.40
1:I7:52:MET:HE1	1:J7:130:PHE:CE2	2.56	0.40
1:J5:253:THR:O	1:J5:257:ILE:HG12	2.21	0.40
1:J6:267:ALA:O	1:J6:271:VAL:HG23	2.21	0.40
2:L3:142:LYS:HG3	2:L3:143:TRP:CD1	2.56	0.40
2:L5:115:GLY:O	2:L5:118:THR:HG22	2.20	0.40
2:N2:94:HIS:ND1	2:N2:95:GLN:HG2	2.37	0.40
2:O5:246:ALA:O	2:O5:249:GLU:HG3	2.22	0.40
3:Q3:80:PHE:CZ	3:Q3:104:ARG:HD3	2.55	0.40
5:X1:172:LYS:HB3	5:X1:172:LYS:HE2	1.80	0.40
5:X3:190:LEU:C	5:X3:192:LYS:H	2.30	0.40
5:X4:136:TRP:CZ2	5:X4:172:LYS:HD3	2.57	0.40
8:a5:181:GLU:O	8:a5:184:GLN:HG2	2.21	0.40
9:c1:29:GLU:HA	9:c1:32:LYS:HE2	2.03	0.40
2:p2:223:GLU:O	2:p2:226:ILE:HG22	2.21	0.40
4:t3:42:TRP:CD1	4:t3:114:PRO:HD3	2.56	0.40
4:t3:157:GLY:O	4:t3:186:ILE:HA	2.22	0.40
1:A9:141:ALA:HA	1:A9:166:ALA:HA	2.04	0.40
1:C5:281:ARG:OXT	1:C5:281:ARG:HD2	2.22	0.40
1:C7:93:LEU:HD13	1:C7:93:LEU:HA	1.89	0.40
1:D6:39:ALA:HB2	1:D7:209:ARG:NH1	2.36	0.40
1:E3:57:LYS:HE3	1:E4:92:VAL:HG21	2.02	0.40
1:E6:157:GLN:HG2	1:E7:192:ASN:OD1	2.21	0.40
1:F5:189:GLU:HG2	1:F5:190:PHE:N	2.36	0.40
1:G1:51:LYS:HD3	1:h0:132:LYS:CG	2.51	0.40
1:G1:99:ASN:OD1	1:G1:101:ILE:HG23	2.21	0.40
1:H8:159:GLN:HG3	1:I8:127:GLN:HG3	2.02	0.40
1:J8:48:VAL:HA	1:J8:51:LYS:HG2	2.02	0.40
1:K6:165:ILE:HA	1:K6:208:GLN:NE2	2.36	0.40
1:K9:174:ASN:OD1	1:K9:174:ASN:C	2.65	0.40
2:L4:75:GLU:C	2:L4:77:LEU:H	2.29	0.40
2:N2:205:TRP:CD1	2:N2:205:TRP:C	2.98	0.40
2:N3:212:LEU:HD23	2:N3:212:LEU:HA	1.90	0.40
2:N6:197:LEU:O	2:N6:201:THR:HG23	2.21	0.40
2:O2:112:TYR:CZ	2:O2:200:ASP:HB3	2.57	0.40
2:P6:235:TYR:N	2:P6:236:PRO:CD	2.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S4:147:GLU:OE1	3:S4:148:PRO:HD2	2.21	0.40
3:S6:191:VAL:HG11	3:S6:217:LEU:HD21	2.03	0.40
4:T3:110:THR:HB	4:T3:218:LYS:HD2	2.02	0.40
5:V3:149:LYS:CB	5:V3:198:SER:HB2	2.51	0.40
7:Z2:143:LYS:HE2	7:Z2:145:ASN:O	2.22	0.40
8:a3:91:PRO:C	8:a3:93:SER:H	2.29	0.40
10:d2:143:ARG:HH22	10:d2:168:TYR:HE1	1.68	0.40
1:h0:57:LYS:HE3	1:h1:88:GLN:NE2	2.36	0.40
1:h0:140:PHE:HD2	1:h0:165:ILE:HD11	1.86	0.40
2:p3:77:LEU:HD21	2:p4:203:ARG:NH1	2.37	0.40
4:t3:20:GLY:HA2	4:t3:244:PHE:CG	2.56	0.40
4:t4:34:PRO:HG3	4:t4:76:LEU:HD11	2.02	0.40
4:t4:162:TYR:HB3	4:t4:219:VAL:CG2	2.51	0.40
1:A7:151:PHE:HE2	1:A7:163:VAL:HG21	1.86	0.40
1:B5:38:ARG:HH22	1:B6:74:GLN:C	2.29	0.40
1:B5:38:ARG:HH22	1:B6:74:GLN:HB2	1.86	0.40
1:C3:265:MET:HB2	1:C3:265:MET:HE3	1.88	0.40
1:E7:121:ILE:HD13	1:E7:175:LEU:HD13	2.04	0.40
1:H8:194:ALA:O	1:H8:198:LEU:HD23	2.21	0.40
1:J5:2:ILE:HD12	1:J5:2:ILE:H	1.87	0.40
1:J5:52:MET:O	1:J5:56:VAL:HG23	2.22	0.40
1:J9:43:ALA:HB1	1:j0:210:ALA:HA	2.04	0.40
1:J9:112:VAL:O	1:J9:116:GLN:HG2	2.21	0.40
1:K8:150:TRP:CZ3	1:K8:162:ARG:HG2	2.56	0.40
3:R4:171:ILE:HA	3:R4:193:PHE:CE1	2.56	0.40
3:S6:173:GLU:HG2	3:S6:175:MET:SD	2.61	0.40
5:V3:65:LEU:HD23	5:V3:65:LEU:HA	1.88	0.40
5:X4:49:GLU:HB3	5:X4:219:LEU:O	2.21	0.40
6:Y1:253:VAL:HB	6:Y1:273:ILE:HB	2.04	0.40
6:Y2:77:ASN:HB3	6:Y2:187:ILE:HG12	2.03	0.40
6:Y4:57:PHE:HB2	6:Y4:70:ASP:HB2	2.02	0.40
7:Z4:260:ASN:O	7:Z4:263:LYS:HG2	2.21	0.40
8:a5:119:LEU:HD11	8:a5:149:ILE:HG21	2.04	0.40
10:d2:183:LYS:O	10:d2:186:VAL:HG12	2.22	0.40
1:h0:108:GLN:O	1:h0:112:VAL:HG23	2.21	0.40
3:s5:55:LEU:HA	3:s5:58:ARG:HG2	2.02	0.40
1:B6:84:ASN:HA	1:B6:87:ILE:HG22	2.03	0.40
1:B7:35:ARG:HD2	1:B7:36:ILE:HG13	2.02	0.40
1:D4:68:ASP:OD2	1:D5:101:ILE:HD11	2.21	0.40
1:D4:179:ASP:HA	2:L2:170:LEU:HD21	2.03	0.40
1:D5:34:MET:HE2	1:D5:36:ILE:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D7:34:MET:SD	1:D7:241:ARG:HB3	2.62	0.40
1:E3:21:ASN:O	1:E3:25:LYS:HG3	2.22	0.40
1:E5:140:PHE:CD1	1:E5:140:PHE:N	2.87	0.40
1:G2:150:TRP:CZ3	1:G2:162:ARG:HB2	2.56	0.40
1:G6:265:MET:CE	1:H6:30:LEU:HD22	2.49	0.40
1:G7:149:MET:HE2	1:G7:151:PHE:CE1	2.57	0.40
1:G7:156:ASN:HD21	1:G7:159:GLN:HE22	1.68	0.40
1:H8:16:LEU:HD11	1:H8:263:THR:HG22	2.04	0.40
1:H8:111:GLN:NE2	1:H8:184:THR:HA	2.35	0.40
1:H8:245:MET:O	1:H8:249:THR:HG23	2.21	0.40
1:I6:25:LYS:HG2	1:I6:38:ARG:NH2	2.36	0.40
1:J8:14:ARG:NH1	1:J9:228:VAL:HG22	2.36	0.40
1:J8:257:ILE:HG22	1:K7:277:LEU:HD21	2.03	0.40
2:M2:144:TYR:O	2:M2:148:VAL:HG12	2.21	0.40
2:M5:216:PRO:HA	2:M5:219:ILE:HG13	2.04	0.40
2:O5:245:TYR:CE2	2:O5:269:LYS:HD3	2.57	0.40
2:P6:250:ASN:HA	2:P6:253:LYS:HE2	2.02	0.40
3:Q3:72:VAL:HG21	3:Q3:258:LEU:HD12	2.04	0.40
3:Q4:193:PHE:CE1	3:Q4:215:TYR:HB2	2.57	0.40
3:R3:59:LEU:O	3:R3:63:THR:HG23	2.21	0.40
3:S4:56:ASN:HA	3:S4:59:LEU:HD12	2.04	0.40
4:T1:243:VAL:HG12	4:T1:243:VAL:O	2.22	0.40
5:V1:101:ILE:HG22	5:V1:217:ASP:CG	2.46	0.40
5:V3:61:SER:HB2	5:V3:116:VAL:HG23	2.02	0.40
5:V3:104:VAL:HB	5:V3:214:PHE:CE1	2.56	0.40
5:V3:162:LEU:HD23	5:V3:162:LEU:HA	1.93	0.40
5:X5:64:PRO:HG2	5:X5:67:GLU:HG2	2.03	0.40
6:Y1:84:LYS:HB3	6:Y1:84:LYS:HE2	1.93	0.40
8:a4:205:LYS:O	8:a4:208:GLU:HG3	2.21	0.40
1:i0:166:ALA:CB	1:i0:208:GLN:HG3	2.51	0.40
3:s4:233:LYS:O	3:s4:237:TYR:HB3	2.21	0.40
3:s4:246:ARG:HA	3:s4:246:ARG:NE	2.37	0.40
3:s5:108:TYR:CD1	3:s5:126:LEU:HA	2.56	0.40
4:t2:103:TYR:HA	4:t2:104:PRO:HD3	1.87	0.40
4:t2:151:MET:HE1	4:t2:180:PHE:CE2	2.57	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	A4	99/281 (35%)	96 (97%)	3 (3%)	0	100	100
1	A5	257/281 (92%)	244 (95%)	13 (5%)	0	100	100
1	A6	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	A7	279/281 (99%)	268 (96%)	10 (4%)	1 (0%)	30	66
1	A8	248/281 (88%)	240 (97%)	8 (3%)	0	100	100
1	A9	144/281 (51%)	141 (98%)	3 (2%)	0	100	100
1	B3	60/281 (21%)	60 (100%)	0	0	100	100
1	B4	143/281 (51%)	140 (98%)	3 (2%)	0	100	100
1	B5	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	B6	279/281 (99%)	274 (98%)	5 (2%)	0	100	100
1	B7	276/281 (98%)	265 (96%)	11 (4%)	0	100	100
1	B8	194/281 (69%)	185 (95%)	9 (5%)	0	100	100
1	C3	99/281 (35%)	96 (97%)	3 (3%)	0	100	100
1	C4	240/281 (85%)	233 (97%)	7 (3%)	0	100	100
1	C5	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
1	C6	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	C7	248/281 (88%)	240 (97%)	8 (3%)	0	100	100
1	C8	154/281 (55%)	148 (96%)	6 (4%)	0	100	100
1	D3	153/281 (54%)	144 (94%)	9 (6%)	0	100	100
1	D4	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	30	66
1	D5	279/281 (99%)	269 (96%)	8 (3%)	2 (1%)	18	55
1	D6	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	D7	206/281 (73%)	199 (97%)	6 (3%)	1 (0%)	24	62
1	E2	94/281 (34%)	91 (97%)	3 (3%)	0	100	100
1	E3	226/281 (80%)	220 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E4	279/281 (99%)	273 (98%)	6 (2%)	0	100	100
1	E5	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	E6	254/281 (90%)	245 (96%)	9 (4%)	0	100	100
1	E7	161/281 (57%)	156 (97%)	5 (3%)	0	100	100
1	F2	126/281 (45%)	122 (97%)	4 (3%)	0	100	100
1	F3	279/281 (99%)	272 (98%)	6 (2%)	1 (0%)	30	66
1	F4	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
1	F5	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
1	F6	219/281 (78%)	206 (94%)	13 (6%)	0	100	100
1	G1	259/281 (92%)	251 (97%)	8 (3%)	0	100	100
1	G2	172/281 (61%)	166 (96%)	6 (4%)	0	100	100
1	G6	87/281 (31%)	83 (95%)	4 (5%)	0	100	100
1	G7	211/281 (75%)	202 (96%)	8 (4%)	1 (0%)	24	62
1	G8	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	G9	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	30	66
1	H6	134/281 (48%)	130 (97%)	4 (3%)	0	100	100
1	H7	279/281 (99%)	269 (96%)	10 (4%)	0	100	100
1	H8	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
1	H9	279/281 (99%)	265 (95%)	14 (5%)	0	100	100
1	I5	82/281 (29%)	79 (96%)	3 (4%)	0	100	100
1	I6	205/281 (73%)	198 (97%)	6 (3%)	1 (0%)	24	62
1	I7	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	I8	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	I9	264/281 (94%)	256 (97%)	8 (3%)	0	100	100
1	J5	117/281 (42%)	113 (97%)	4 (3%)	0	100	100
1	J6	271/281 (96%)	264 (97%)	6 (2%)	1 (0%)	30	66
1	J7	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	30	66
1	J8	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	J9	231/281 (82%)	224 (97%)	7 (3%)	0	100	100
1	K4	71/281 (25%)	68 (96%)	3 (4%)	0	100	100
1	K5	194/281 (69%)	187 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K6	279/281 (99%)	268 (96%)	10 (4%)	1 (0%)	30	66
1	K7	279/281 (99%)	268 (96%)	10 (4%)	1 (0%)	30	66
1	K8	268/281 (95%)	264 (98%)	4 (2%)	0	100	100
1	K9	182/281 (65%)	170 (93%)	9 (5%)	3 (2%)	7	36
1	h0	233/281 (83%)	221 (95%)	12 (5%)	0	100	100
1	h1	102/281 (36%)	101 (99%)	1 (1%)	0	100	100
1	i0	176/281 (63%)	168 (96%)	8 (4%)	0	100	100
1	j0	121/281 (43%)	119 (98%)	2 (2%)	0	100	100
2	L2	192/306 (63%)	186 (97%)	6 (3%)	0	100	100
2	L3	207/306 (68%)	197 (95%)	8 (4%)	2 (1%)	12	47
2	L4	207/306 (68%)	198 (96%)	8 (4%)	1 (0%)	24	62
2	L5	207/306 (68%)	200 (97%)	7 (3%)	0	100	100
2	L6	163/306 (53%)	161 (99%)	2 (1%)	0	100	100
2	M1	82/306 (27%)	77 (94%)	4 (5%)	1 (1%)	10	42
2	M2	211/306 (69%)	202 (96%)	9 (4%)	0	100	100
2	M3	211/306 (69%)	201 (95%)	10 (5%)	0	100	100
2	M4	211/306 (69%)	204 (97%)	6 (3%)	1 (0%)	24	62
2	M5	204/306 (67%)	200 (98%)	4 (2%)	0	100	100
2	N2	180/306 (59%)	177 (98%)	2 (1%)	1 (1%)	21	58
2	N3	207/306 (68%)	201 (97%)	5 (2%)	1 (0%)	24	62
2	N4	207/306 (68%)	197 (95%)	10 (5%)	0	100	100
2	N5	207/306 (68%)	199 (96%)	8 (4%)	0	100	100
2	N6	170/306 (56%)	165 (97%)	5 (3%)	0	100	100
2	O1	57/306 (19%)	51 (90%)	6 (10%)	0	100	100
2	O2	206/306 (67%)	199 (97%)	7 (3%)	0	100	100
2	O3	207/306 (68%)	201 (97%)	4 (2%)	2 (1%)	12	47
2	O4	207/306 (68%)	199 (96%)	8 (4%)	0	100	100
2	O5	206/306 (67%)	199 (97%)	7 (3%)	0	100	100
2	P2	164/306 (54%)	158 (96%)	6 (4%)	0	100	100
2	P3	205/306 (67%)	200 (98%)	4 (2%)	1 (0%)	24	62
2	P4	205/306 (67%)	198 (97%)	5 (2%)	2 (1%)	12	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P5	205/306 (67%)	199 (97%)	6 (3%)	0	100	100
2	P6	170/306 (56%)	165 (97%)	5 (3%)	0	100	100
2	p2	205/306 (67%)	198 (97%)	7 (3%)	0	100	100
2	p3	207/306 (68%)	198 (96%)	9 (4%)	0	100	100
2	p4	206/306 (67%)	200 (97%)	6 (3%)	0	100	100
2	p5	206/306 (67%)	198 (96%)	8 (4%)	0	100	100
3	Q1	145/276 (52%)	133 (92%)	9 (6%)	3 (2%)	5	29
3	Q2	180/276 (65%)	165 (92%)	14 (8%)	1 (1%)	21	58
3	Q3	188/276 (68%)	174 (93%)	13 (7%)	1 (0%)	24	62
3	Q4	184/276 (67%)	166 (90%)	17 (9%)	1 (0%)	24	62
3	R2	175/276 (63%)	167 (95%)	6 (3%)	2 (1%)	11	45
3	R3	194/276 (70%)	175 (90%)	16 (8%)	3 (2%)	8	38
3	R4	182/276 (66%)	164 (90%)	16 (9%)	2 (1%)	11	45
3	R5	182/276 (66%)	167 (92%)	14 (8%)	1 (0%)	24	62
3	S2	131/276 (48%)	116 (88%)	14 (11%)	1 (1%)	16	52
3	S3	179/276 (65%)	165 (92%)	14 (8%)	0	100	100
3	S4	183/276 (66%)	168 (92%)	13 (7%)	2 (1%)	11	45
3	S5	182/276 (66%)	163 (90%)	19 (10%)	0	100	100
3	S6	180/276 (65%)	165 (92%)	14 (8%)	1 (1%)	21	58
3	s3	184/276 (67%)	174 (95%)	9 (5%)	1 (0%)	24	62
3	s4	181/276 (66%)	163 (90%)	17 (9%)	1 (1%)	21	58
3	s5	184/276 (67%)	166 (90%)	17 (9%)	1 (0%)	24	62
3	s6	158/276 (57%)	145 (92%)	12 (8%)	1 (1%)	21	58
4	T1	252/315 (80%)	229 (91%)	21 (8%)	2 (1%)	16	52
4	T2	268/315 (85%)	242 (90%)	26 (10%)	0	100	100
4	T3	268/315 (85%)	248 (92%)	18 (7%)	2 (1%)	18	55
4	T4	254/315 (81%)	234 (92%)	18 (7%)	2 (1%)	16	52
4	t1	269/315 (85%)	249 (93%)	17 (6%)	3 (1%)	11	45
4	t2	268/315 (85%)	239 (89%)	26 (10%)	3 (1%)	11	45
4	t3	268/315 (85%)	245 (91%)	22 (8%)	1 (0%)	30	66
4	t4	266/315 (84%)	244 (92%)	20 (8%)	2 (1%)	16	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	V1	167/239 (70%)	145 (87%)	21 (13%)	1 (1%)	21	58
5	V2	195/239 (82%)	170 (87%)	22 (11%)	3 (2%)	8	38
5	V3	192/239 (80%)	170 (88%)	20 (10%)	2 (1%)	12	47
5	V4	192/239 (80%)	169 (88%)	22 (12%)	1 (0%)	24	62
5	V5	192/239 (80%)	174 (91%)	15 (8%)	3 (2%)	7	36
5	X1	177/239 (74%)	159 (90%)	17 (10%)	1 (1%)	21	58
5	X2	195/239 (82%)	173 (89%)	20 (10%)	2 (1%)	12	47
5	X3	195/239 (82%)	166 (85%)	28 (14%)	1 (0%)	24	62
5	X4	195/239 (82%)	174 (89%)	19 (10%)	2 (1%)	12	47
5	X5	191/239 (80%)	171 (90%)	19 (10%)	1 (0%)	24	62
6	Y1	88/282 (31%)	83 (94%)	4 (4%)	1 (1%)	11	45
6	Y2	216/282 (77%)	196 (91%)	19 (9%)	1 (0%)	24	62
6	Y3	218/282 (77%)	209 (96%)	9 (4%)	0	100	100
6	Y4	218/282 (77%)	207 (95%)	10 (5%)	1 (0%)	24	62
6	Y5	218/282 (77%)	209 (96%)	8 (4%)	1 (0%)	24	62
7	Z1	249/369 (68%)	247 (99%)	2 (1%)	0	100	100
7	Z2	249/369 (68%)	245 (98%)	4 (2%)	0	100	100
7	Z3	248/369 (67%)	245 (99%)	2 (1%)	1 (0%)	30	66
7	Z4	249/369 (68%)	243 (98%)	5 (2%)	1 (0%)	30	66
8	a2	164/237 (69%)	154 (94%)	9 (6%)	1 (1%)	21	58
8	a3	170/237 (72%)	163 (96%)	6 (4%)	1 (1%)	21	58
8	a4	170/237 (72%)	158 (93%)	11 (6%)	1 (1%)	21	58
8	a5	170/237 (72%)	165 (97%)	5 (3%)	0	100	100
9	c1	99/146 (68%)	95 (96%)	3 (3%)	1 (1%)	12	47
9	c2	101/146 (69%)	96 (95%)	4 (4%)	1 (1%)	12	47
9	c3	101/146 (69%)	99 (98%)	1 (1%)	1 (1%)	12	47
10	d2	240/291 (82%)	236 (98%)	4 (2%)	0	100	100
10	d3	230/291 (79%)	225 (98%)	4 (2%)	1 (0%)	30	66
10	d4	237/291 (81%)	229 (97%)	7 (3%)	1 (0%)	30	66
All	All	30109/41605 (72%)	28645 (95%)	1368 (4%)	96 (0%)	37	71

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M4	229	ASP
2	O3	215	LEU
4	T4	236	GLU
5	X2	197	VAL
7	Z3	271	TYR
7	Z4	271	TYR
3	s4	86	ASN
1	G9	178	ALA
1	I6	40	GLY
2	M1	85	GLY
3	Q1	86	ASN
3	S4	151	ASN
3	S6	86	ASN
4	T3	159	GLY
5	V1	197	VAL
5	V2	218	ASP
5	V4	229	LYS
5	X1	218	ASP
5	X2	218	ASP
6	Y1	268	VAL
6	Y4	136	LYS
3	s3	86	ASN
1	K6	5	HIS
1	K7	174	ASN
2	L3	226	ILE
3	Q2	178	GLY
3	R2	86	ASN
3	R4	86	ASN
3	S2	86	ASN
4	T3	236	GLU
5	X4	141	LYS
6	Y2	268	VAL
9	c1	98	LYS
9	c2	98	LYS
10	d3	99	ASP
3	s5	179	PRO
4	t1	236	GLU
4	t2	28	VAL
4	t2	159	GLY
4	t4	28	VAL
1	D5	37	ASN
2	N2	86	TYR
2	P4	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R5	185	HIS
4	T1	236	GLU
5	V2	166	ASP
5	V2	197	VAL
5	V5	122	HIS
5	V5	141	LYS
10	d4	99	ASP
1	K9	98	SER
1	K9	131	ASN
2	L4	226	ILE
3	Q1	170	ILE
3	R3	86	ASN
3	R3	211	GLY
4	T1	28	VAL
4	T4	22	GLU
5	V5	218	ASP
5	X3	191	ASP
5	X4	79	ILE
5	X5	218	ASP
8	a3	149	ILE
9	c3	98	LYS
4	t2	38	ALA
1	D7	177	LYS
1	F3	153	ILE
1	K9	153	ILE
2	O3	85	GLY
2	P3	85	GLY
3	Q1	178	GLY
3	Q4	144	PRO
3	s6	66	MET
4	t1	38	ALA
4	t4	236	GLU
1	D4	153	ILE
1	D5	40	GLY
2	P4	85	GLY
3	R2	178	GLY
5	V3	197	VAL
1	A7	153	ILE
2	L3	85	GLY
2	N3	85	GLY
3	Q3	211	GLY
6	Y5	268	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	t1	28	VAL
4	t3	28	VAL
3	R3	212	VAL
8	a2	131	ILE
1	J6	153	ILE
3	R4	170	ILE
3	S4	178	GLY
8	a4	131	ILE
1	G7	153	ILE
1	J7	153	ILE
5	V3	96	ILE

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	A4	87/236 (37%)	86 (99%)	1 (1%)	65	74
1	A5	221/236 (94%)	221 (100%)	0	100	100
1	A6	236/236 (100%)	234 (99%)	2 (1%)	73	77
1	A7	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	A8	209/236 (89%)	207 (99%)	2 (1%)	68	76
1	A9	124/236 (52%)	124 (100%)	0	100	100
1	B3	55/236 (23%)	55 (100%)	0	100	100
1	B4	123/236 (52%)	121 (98%)	2 (2%)	55	69
1	B5	236/236 (100%)	236 (100%)	0	100	100
1	B6	236/236 (100%)	234 (99%)	2 (1%)	73	77
1	B7	233/236 (99%)	233 (100%)	0	100	100
1	B8	165/236 (70%)	164 (99%)	1 (1%)	78	80
1	C3	87/236 (37%)	87 (100%)	0	100	100
1	C4	207/236 (88%)	206 (100%)	1 (0%)	81	81
1	C5	236/236 (100%)	236 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C6	236/236 (100%)	236 (100%)	0	100	100
1	C7	209/236 (89%)	208 (100%)	1 (0%)	81	81
1	C8	133/236 (56%)	133 (100%)	0	100	100
1	D3	137/236 (58%)	137 (100%)	0	100	100
1	D4	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	D5	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	D6	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	D7	176/236 (75%)	175 (99%)	1 (1%)	78	80
1	E2	83/236 (35%)	83 (100%)	0	100	100
1	E3	196/236 (83%)	196 (100%)	0	100	100
1	E4	236/236 (100%)	236 (100%)	0	100	100
1	E5	236/236 (100%)	234 (99%)	2 (1%)	73	77
1	E6	215/236 (91%)	215 (100%)	0	100	100
1	E7	138/236 (58%)	138 (100%)	0	100	100
1	F2	109/236 (46%)	109 (100%)	0	100	100
1	F3	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	F4	236/236 (100%)	234 (99%)	2 (1%)	73	77
1	F5	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	F6	184/236 (78%)	184 (100%)	0	100	100
1	G1	217/236 (92%)	217 (100%)	0	100	100
1	G2	144/236 (61%)	141 (98%)	3 (2%)	47	65
1	G6	76/236 (32%)	76 (100%)	0	100	100
1	G7	182/236 (77%)	180 (99%)	2 (1%)	65	74
1	G8	236/236 (100%)	234 (99%)	2 (1%)	73	77
1	G9	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	H6	115/236 (49%)	113 (98%)	2 (2%)	53	67
1	H7	236/236 (100%)	236 (100%)	0	100	100
1	H8	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	H9	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	I5	71/236 (30%)	71 (100%)	0	100	100
1	I6	176/236 (75%)	175 (99%)	1 (1%)	78	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I7	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	I8	236/236 (100%)	236 (100%)	0	100	100
1	I9	221/236 (94%)	219 (99%)	2 (1%)	70	76
1	J5	101/236 (43%)	101 (100%)	0	100	100
1	J6	232/236 (98%)	232 (100%)	0	100	100
1	J7	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	J8	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	J9	194/236 (82%)	194 (100%)	0	100	100
1	K4	65/236 (28%)	65 (100%)	0	100	100
1	K5	167/236 (71%)	167 (100%)	0	100	100
1	K6	236/236 (100%)	236 (100%)	0	100	100
1	K7	236/236 (100%)	235 (100%)	1 (0%)	84	82
1	K8	225/236 (95%)	224 (100%)	1 (0%)	84	82
1	K9	154/236 (65%)	153 (99%)	1 (1%)	78	80
1	h0	195/236 (83%)	194 (100%)	1 (0%)	81	81
1	h1	88/236 (37%)	88 (100%)	0	100	100
1	i0	149/236 (63%)	146 (98%)	3 (2%)	48	66
1	j0	106/236 (45%)	106 (100%)	0	100	100
2	L2	160/278 (58%)	160 (100%)	0	100	100
2	L3	168/278 (60%)	167 (99%)	1 (1%)	78	80
2	L4	168/278 (60%)	168 (100%)	0	100	100
2	L5	168/278 (60%)	167 (99%)	1 (1%)	78	80
2	L6	141/278 (51%)	141 (100%)	0	100	100
2	M1	71/278 (26%)	70 (99%)	1 (1%)	59	71
2	M2	171/278 (62%)	171 (100%)	0	100	100
2	M3	171/278 (62%)	171 (100%)	0	100	100
2	M4	171/278 (62%)	169 (99%)	2 (1%)	63	73
2	M5	167/278 (60%)	167 (100%)	0	100	100
2	N2	148/278 (53%)	148 (100%)	0	100	100
2	N3	168/278 (60%)	168 (100%)	0	100	100
2	N4	168/278 (60%)	167 (99%)	1 (1%)	78	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N5	168/278 (60%)	168 (100%)	0	100	100
2	N6	142/278 (51%)	142 (100%)	0	100	100
2	O1	48/278 (17%)	48 (100%)	0	100	100
2	O2	167/278 (60%)	167 (100%)	0	100	100
2	O3	168/278 (60%)	167 (99%)	1 (1%)	78	80
2	O4	168/278 (60%)	167 (99%)	1 (1%)	78	80
2	O5	167/278 (60%)	166 (99%)	1 (1%)	78	80
2	P2	140/278 (50%)	140 (100%)	0	100	100
2	P3	166/278 (60%)	166 (100%)	0	100	100
2	P4	166/278 (60%)	166 (100%)	0	100	100
2	P5	166/278 (60%)	165 (99%)	1 (1%)	78	80
2	P6	142/278 (51%)	141 (99%)	1 (1%)	76	79
2	p2	166/278 (60%)	166 (100%)	0	100	100
2	p3	168/278 (60%)	168 (100%)	0	100	100
2	p4	167/278 (60%)	166 (99%)	1 (1%)	78	80
2	p5	167/278 (60%)	167 (100%)	0	100	100
3	Q1	151/252 (60%)	151 (100%)	0	100	100
3	Q2	177/252 (70%)	176 (99%)	1 (1%)	78	80
3	Q3	184/252 (73%)	184 (100%)	0	100	100
3	Q4	181/252 (72%)	181 (100%)	0	100	100
3	R2	172/252 (68%)	172 (100%)	0	100	100
3	R3	189/252 (75%)	189 (100%)	0	100	100
3	R4	180/252 (71%)	180 (100%)	0	100	100
3	R5	180/252 (71%)	180 (100%)	0	100	100
3	S2	138/252 (55%)	137 (99%)	1 (1%)	76	79
3	S3	176/252 (70%)	176 (100%)	0	100	100
3	S4	181/252 (72%)	181 (100%)	0	100	100
3	S5	179/252 (71%)	177 (99%)	2 (1%)	65	74
3	S6	178/252 (71%)	178 (100%)	0	100	100
3	s3	180/252 (71%)	180 (100%)	0	100	100
3	s4	180/252 (71%)	180 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s5	182/252 (72%)	181 (100%)	1 (0%)	81	81
3	s6	158/252 (63%)	157 (99%)	1 (1%)	78	80
4	T1	223/264 (84%)	222 (100%)	1 (0%)	84	82
4	T2	232/264 (88%)	230 (99%)	2 (1%)	70	76
4	T3	232/264 (88%)	231 (100%)	1 (0%)	84	82
4	T4	221/264 (84%)	219 (99%)	2 (1%)	70	76
4	t1	233/264 (88%)	232 (100%)	1 (0%)	84	82
4	t2	232/264 (88%)	231 (100%)	1 (0%)	84	82
4	t3	232/264 (88%)	230 (99%)	2 (1%)	70	76
4	t4	230/264 (87%)	228 (99%)	2 (1%)	70	76
5	V1	152/205 (74%)	150 (99%)	2 (1%)	61	72
5	V2	173/205 (84%)	172 (99%)	1 (1%)	78	80
5	V3	172/205 (84%)	171 (99%)	1 (1%)	78	80
5	V4	172/205 (84%)	169 (98%)	3 (2%)	53	67
5	V5	172/205 (84%)	171 (99%)	1 (1%)	78	80
5	X1	159/205 (78%)	158 (99%)	1 (1%)	78	80
5	X2	173/205 (84%)	173 (100%)	0	100	100
5	X3	173/205 (84%)	173 (100%)	0	100	100
5	X4	173/205 (84%)	173 (100%)	0	100	100
5	X5	172/205 (84%)	171 (99%)	1 (1%)	78	80
6	Y1	96/258 (37%)	96 (100%)	0	100	100
6	Y2	206/258 (80%)	204 (99%)	2 (1%)	68	76
6	Y3	209/258 (81%)	209 (100%)	0	100	100
6	Y4	209/258 (81%)	209 (100%)	0	100	100
6	Y5	209/258 (81%)	208 (100%)	1 (0%)	81	81
7	Z1	231/327 (71%)	231 (100%)	0	100	100
7	Z2	231/327 (71%)	230 (100%)	1 (0%)	84	82
7	Z3	230/327 (70%)	230 (100%)	0	100	100
7	Z4	231/327 (71%)	231 (100%)	0	100	100
8	a2	160/217 (74%)	160 (100%)	0	100	100
8	a3	164/217 (76%)	164 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	a4	164/217 (76%)	163 (99%)	1 (1%)	78	80
8	a5	164/217 (76%)	164 (100%)	0	100	100
9	c1	96/133 (72%)	94 (98%)	2 (2%)	47	65
9	c2	98/133 (74%)	98 (100%)	0	100	100
9	c3	98/133 (74%)	98 (100%)	0	100	100
10	d2	215/256 (84%)	214 (100%)	1 (0%)	81	81
10	d3	207/256 (81%)	207 (100%)	0	100	100
10	d4	213/256 (83%)	213 (100%)	0	100	100
All	All	26308/36245 (73%)	26212 (100%)	96 (0%)	81	82

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A4	277	LEU
1	A6	30	LEU
1	A6	51	LYS
1	A7	22	GLU
1	A8	16	LEU
1	A8	239	ARG
1	B4	63	GLU
1	B4	72	LEU
1	B6	27	MET
1	B6	218	ARG
1	B8	137	GLN
1	C4	120	GLU
1	C7	123	ARG
1	D4	59	LEU
1	D5	277	LEU
1	D6	123	ARG
1	D7	135	LEU
1	E5	136	LEU
1	E5	280	LEU
1	F3	124	ILE
1	F4	82	GLU
1	F4	277	LEU
1	F5	127	GLN
1	G2	59	LEU
1	G2	153	ILE
1	G2	159	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G7	157	GLN
1	G7	248	GLU
1	G8	27	MET
1	G8	30	LEU
1	G9	38	ARG
1	H6	65	ASN
1	H6	219	LEU
1	H8	81	GLN
1	H9	202	LEU
1	I6	220	GLU
1	I7	60	ARG
1	I9	65	ASN
1	I9	159	GLN
1	J7	175	LEU
1	J8	1	MET
1	K7	1	MET
1	K8	152	HIS
1	K9	86	ILE
2	L3	234	GLU
2	L5	181	ASP
2	M1	111	ASN
2	M4	190	GLU
2	M4	270	LYS
2	N4	180	LEU
2	O3	181	ASP
2	O4	145	TRP
2	O5	141	GLU
2	P5	94	HIS
2	P6	178	ASN
3	Q2	103	ILE
3	S2	189	VAL
3	S5	65	LEU
3	S5	108	TYR
4	T1	194	TYR
4	T2	134	LYS
4	T2	261	ARG
4	T3	49	ASP
4	T4	59	GLN
4	T4	134	LYS
5	V1	48	LEU
5	V1	55	GLU
5	V2	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	V3	149	LYS
5	V4	52	GLU
5	V4	141	LYS
5	V4	194	LEU
5	V5	52	GLU
5	X1	102	LEU
5	X5	52	GLU
6	Y2	142	GLU
6	Y2	153	ASP
6	Y5	268	VAL
7	Z2	101	GLU
8	a4	48	GLU
9	c1	35	GLU
9	c1	55	LEU
10	d2	142	LEU
1	h0	27	MET
1	i0	82	GLU
1	i0	116	GLN
1	i0	159	GLN
2	p4	94	HIS
3	s5	164	MET
3	s6	65	LEU
4	t1	151	MET
4	t2	42	TRP
4	t3	99	PHE
4	t3	116	ILE
4	t4	106	GLU
4	t4	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (590) such sidechains are listed below:

Mol	Chain	Res	Type
1	A4	20	ASN
1	A4	270	ASN
1	A4	278	GLN
1	A5	26	ASN
1	A5	152	HIS
1	A5	159	GLN
1	A5	192	ASN
1	A5	232	ASN
1	A5	255	ASN
1	A6	5	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A6	13	HIS
1	A6	20	ASN
1	A6	21	ASN
1	A6	61	GLN
1	A6	74	GLN
1	A6	116	GLN
1	A6	192	ASN
1	A6	206	ASN
1	A7	4	ASN
1	A7	6	ASN
1	A7	13	HIS
1	A7	21	ASN
1	A7	55	GLN
1	A7	74	GLN
1	A7	96	GLN
1	A7	156	ASN
1	A7	208	GLN
1	A7	232	ASN
1	A8	26	ASN
1	A8	84	ASN
1	A8	152	HIS
1	A8	156	ASN
1	A8	208	GLN
1	A8	217	ASN
1	A9	74	GLN
1	A9	84	ASN
1	B3	5	HIS
1	B3	26	ASN
1	B3	270	ASN
1	B4	6	ASN
1	B4	217	ASN
1	B4	268	GLN
1	B5	13	HIS
1	B5	21	ASN
1	B5	55	GLN
1	B5	61	GLN
1	B5	74	GLN
1	B5	96	GLN
1	B5	111	GLN
1	B5	131	ASN
1	B5	137	GLN
1	B5	208	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B5	232	ASN
1	B5	234	GLN
1	B6	88	GLN
1	B6	158	HIS
1	B6	206	ASN
1	B6	208	GLN
1	B6	232	ASN
1	B6	234	GLN
1	B6	268	GLN
1	B6	270	ASN
1	B6	274	GLN
1	B6	278	GLN
1	B7	4	ASN
1	B7	37	ASN
1	B7	131	ASN
1	B7	137	GLN
1	B7	152	HIS
1	B7	157	GLN
1	B7	192	ASN
1	B7	206	ASN
1	B8	65	ASN
1	B8	111	GLN
1	B8	152	HIS
1	B8	232	ASN
1	B8	234	GLN
1	C4	4	ASN
1	C4	61	GLN
1	C4	234	GLN
1	C4	260	GLN
1	C5	21	ASN
1	C5	88	GLN
1	C5	96	GLN
1	C5	192	ASN
1	C5	255	ASN
1	C6	26	ASN
1	C6	37	ASN
1	C6	55	GLN
1	C6	88	GLN
1	C6	116	GLN
1	C6	137	GLN
1	C6	158	HIS
1	C6	234	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C7	19	GLN
1	C7	108	GLN
1	C7	116	GLN
1	C7	217	ASN
1	C7	232	ASN
1	C8	99	ASN
1	D3	4	ASN
1	D3	11	ASN
1	D3	20	ASN
1	D3	152	HIS
1	D3	156	ASN
1	D3	158	HIS
1	D4	20	ASN
1	D4	84	ASN
1	D4	116	GLN
1	D4	127	GLN
1	D4	156	ASN
1	D4	159	GLN
1	D4	206	ASN
1	D4	232	ASN
1	D4	234	GLN
1	D5	65	ASN
1	D5	84	ASN
1	D5	157	GLN
1	D5	158	HIS
1	D5	234	GLN
1	D5	256	GLN
1	D6	13	HIS
1	D6	20	ASN
1	D6	37	ASN
1	D6	88	GLN
1	D6	99	ASN
1	D6	127	GLN
1	D6	157	GLN
1	D6	217	ASN
1	D6	260	GLN
1	D7	74	GLN
1	D7	131	ASN
1	D7	158	HIS
1	D7	159	GLN
1	D7	211	ASN
1	D7	234	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E2	4	ASN
1	E2	37	ASN
1	E2	268	GLN
1	E2	270	ASN
1	E2	278	GLN
1	E3	5	HIS
1	E3	20	ASN
1	E3	61	GLN
1	E3	65	ASN
1	E3	158	HIS
1	E3	206	ASN
1	E3	217	ASN
1	E3	232	ASN
1	E3	234	GLN
1	E3	255	ASN
1	E4	13	HIS
1	E4	20	ASN
1	E4	99	ASN
1	E4	152	HIS
1	E4	270	ASN
1	E4	278	GLN
1	E5	21	ASN
1	E5	61	GLN
1	E5	96	GLN
1	E5	108	GLN
1	E5	192	ASN
1	E5	208	GLN
1	E5	278	GLN
1	E6	37	ASN
1	E6	61	GLN
1	E6	152	HIS
1	E6	211	ASN
1	E7	61	GLN
1	E7	116	GLN
1	F2	5	HIS
1	F2	61	GLN
1	F2	232	ASN
1	F2	270	ASN
1	F3	26	ASN
1	F3	55	GLN
1	F3	65	ASN
1	F3	157	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F3	232	ASN
1	F4	61	GLN
1	F4	84	ASN
1	F4	96	GLN
1	F4	99	ASN
1	F4	157	GLN
1	F4	158	HIS
1	F5	5	HIS
1	F5	11	ASN
1	F5	61	GLN
1	F5	65	ASN
1	F5	84	ASN
1	F5	131	ASN
1	F5	156	ASN
1	F5	206	ASN
1	F5	274	GLN
1	F5	278	GLN
1	F6	74	GLN
1	F6	81	GLN
1	F6	96	GLN
1	F6	99	ASN
1	F6	206	ASN
1	G1	13	HIS
1	G1	74	GLN
1	G1	96	GLN
1	G1	127	GLN
1	G1	159	GLN
1	G1	232	ASN
1	G1	234	GLN
1	G2	81	GLN
1	G2	84	ASN
1	G2	156	ASN
1	G2	221	HIS
1	G6	6	ASN
1	G7	5	HIS
1	G7	20	ASN
1	G7	61	GLN
1	G7	137	GLN
1	G7	156	ASN
1	G7	208	GLN
1	G7	221	HIS
1	G7	260	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G8	26	ASN
1	G8	55	GLN
1	G8	74	GLN
1	G8	84	ASN
1	G8	99	ASN
1	G8	152	HIS
1	G8	211	ASN
1	G8	234	GLN
1	G8	255	ASN
1	G9	5	HIS
1	G9	11	ASN
1	G9	37	ASN
1	G9	61	GLN
1	G9	208	GLN
1	G9	232	ASN
1	G9	234	GLN
1	H6	5	HIS
1	H6	232	ASN
1	H6	270	ASN
1	H7	13	HIS
1	H7	61	GLN
1	H7	84	ASN
1	H7	152	HIS
1	H7	211	ASN
1	H7	256	GLN
1	H7	274	GLN
1	H8	5	HIS
1	H8	13	HIS
1	H8	61	GLN
1	H8	84	ASN
1	H8	131	ASN
1	H8	232	ASN
1	H9	61	GLN
1	H9	88	GLN
1	H9	174	ASN
1	H9	208	GLN
1	H9	260	GLN
1	H9	274	GLN
1	H9	278	GLN
1	I5	37	ASN
1	I5	270	ASN
1	I5	278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I6	5	HIS
1	I6	61	GLN
1	I6	81	GLN
1	I6	152	HIS
1	I6	156	ASN
1	I6	158	HIS
1	I7	11	ASN
1	I7	74	GLN
1	I7	96	GLN
1	I7	108	GLN
1	I7	159	GLN
1	I7	206	ASN
1	I7	234	GLN
1	I8	37	ASN
1	I8	61	GLN
1	I8	159	GLN
1	I8	192	ASN
1	I8	208	GLN
1	I8	217	ASN
1	I8	234	GLN
1	I8	278	GLN
1	I9	37	ASN
1	I9	61	GLN
1	I9	65	ASN
1	I9	152	HIS
1	I9	159	GLN
1	J5	5	HIS
1	J6	13	HIS
1	J6	19	GLN
1	J6	65	ASN
1	J6	84	ASN
1	J6	158	HIS
1	J6	217	ASN
1	J6	232	ASN
1	J6	274	GLN
1	J7	19	GLN
1	J7	55	GLN
1	J7	99	ASN
1	J7	111	GLN
1	J7	158	HIS
1	J7	206	ASN
1	J7	211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J7	217	ASN
1	J7	234	GLN
1	J8	5	HIS
1	J8	6	ASN
1	J8	65	ASN
1	J8	74	GLN
1	J8	152	HIS
1	J8	157	GLN
1	J8	174	ASN
1	J8	208	GLN
1	J8	234	GLN
1	J9	61	GLN
1	J9	65	ASN
1	J9	156	ASN
1	J9	192	ASN
1	J9	208	GLN
1	K4	5	HIS
1	K4	268	GLN
1	K5	11	ASN
1	K5	13	HIS
1	K5	55	GLN
1	K5	152	HIS
1	K5	234	GLN
1	K6	13	HIS
1	K6	20	ASN
1	K6	61	GLN
1	K6	152	HIS
1	K7	6	ASN
1	K7	37	ASN
1	K7	108	GLN
1	K7	156	ASN
1	K7	157	GLN
1	K7	158	HIS
1	K7	192	ASN
1	K7	234	GLN
1	K8	5	HIS
1	K8	84	ASN
1	K8	127	GLN
1	K8	152	HIS
1	K8	192	ASN
1	K9	157	GLN
1	K9	158	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K9	159	GLN
1	K9	232	ASN
2	L2	95	GLN
2	L2	178	ASN
2	L3	167	GLN
2	L3	273	HIS
2	L4	94	HIS
2	L4	103	ASN
2	L4	128	GLN
2	L4	294	ASN
2	L5	74	GLN
2	L5	217	GLN
2	L5	273	HIS
2	L6	205	ASN
2	M1	74	GLN
2	M1	117	ASN
2	M1	179	HIS
2	M3	94	HIS
2	M3	111	ASN
2	M3	185	ASN
2	M3	273	HIS
2	M4	95	GLN
2	M4	111	ASN
2	M4	171	ASN
2	M4	291	HIS
2	M5	167	GLN
2	M5	179	HIS
2	N2	111	ASN
2	N2	167	GLN
2	N2	179	HIS
2	N3	74	GLN
2	N4	94	HIS
2	N4	103	ASN
2	N4	167	GLN
2	N4	171	ASN
2	N4	179	HIS
2	N5	94	HIS
2	N5	171	ASN
2	N5	179	HIS
2	N6	171	ASN
2	N6	178	ASN
2	N6	238	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O1	94	HIS
2	O2	111	ASN
2	O2	117	ASN
2	O2	214	ASN
2	O2	238	HIS
2	O2	273	HIS
2	O3	94	HIS
2	O3	167	GLN
2	O3	171	ASN
2	O3	271	ASN
2	O4	91	GLN
2	O4	111	ASN
2	O4	214	ASN
2	O4	273	HIS
2	O5	167	GLN
2	O5	179	HIS
2	O5	238	HIS
2	P2	179	HIS
2	P3	94	HIS
2	P3	271	ASN
2	P5	111	ASN
2	P5	128	GLN
2	P5	179	HIS
2	P5	291	HIS
2	P6	179	HIS
2	P6	213	GLN
2	P6	273	HIS
3	Q1	151	ASN
3	Q1	226	HIS
3	Q2	138	ASN
3	Q2	226	HIS
3	Q2	240	HIS
3	Q3	180	ASN
3	Q3	255	ASN
3	Q4	62	HIS
3	Q4	138	ASN
3	Q4	163	ASN
3	Q4	186	ASN
3	Q4	226	HIS
3	R2	56	ASN
3	R2	62	HIS
3	R2	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R2	255	ASN
3	R2	257	GLN
3	R3	100	ASN
3	R5	86	ASN
3	R5	240	HIS
3	S2	151	ASN
3	S3	100	ASN
3	S3	226	HIS
3	S3	230	ASN
3	S4	62	HIS
3	S4	162	ASN
3	S4	185	HIS
3	S5	153	ASN
3	S5	186	ASN
3	S5	197	ASN
3	S5	255	ASN
3	S6	140	ASN
3	S6	194	GLN
3	S6	222	ASN
3	S6	230	ASN
4	T1	69	GLN
4	T1	86	ASN
4	T1	160	ASN
4	T1	176	HIS
4	T2	160	ASN
4	T2	264	HIS
4	T3	1	GLN
4	T3	52	GLN
4	T3	54	GLN
4	T4	59	GLN
5	V1	99	ASN
5	V1	122	HIS
5	V1	211	GLN
5	V2	158	HIS
5	V2	211	GLN
5	V3	86	ASN
5	V3	91	ASN
5	V3	95	GLN
5	V3	156	ASN
5	V3	195	HIS
5	V4	158	HIS
5	V4	238	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	V5	91	ASN
5	V5	99	ASN
5	V5	144	HIS
5	V5	183	GLN
5	X1	100	HIS
5	X1	107	ASN
5	X1	132	GLN
5	X1	158	HIS
5	X1	211	GLN
5	X2	86	ASN
5	X2	100	HIS
5	X2	132	GLN
5	X2	193	ASN
5	X2	211	GLN
5	X3	156	ASN
5	X3	211	GLN
5	X4	75	GLN
5	X4	195	HIS
5	X5	156	ASN
6	Y1	53	ASN
6	Y1	191	GLN
6	Y1	202	ASN
6	Y2	191	GLN
6	Y2	259	ASN
6	Y3	178	HIS
6	Y3	181	ASN
6	Y3	216	HIS
6	Y3	238	HIS
6	Y3	239	HIS
6	Y4	53	ASN
6	Y4	119	ASN
6	Y4	177	ASN
6	Y4	181	ASN
6	Y5	127	ASN
7	Z1	93	GLN
7	Z2	103	ASN
7	Z2	104	HIS
7	Z2	218	ASN
7	Z2	229	HIS
7	Z2	236	HIS
7	Z2	239	HIS
7	Z2	257	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	Z3	174	ASN
7	Z3	217	ASN
7	Z4	102	ASN
7	Z4	103	ASN
7	Z4	104	HIS
7	Z4	115	GLN
8	a2	69	ASN
8	a2	77	ASN
8	a2	89	GLN
8	a2	184	GLN
8	a2	213	ASN
8	a3	81	GLN
8	a3	184	GLN
8	a4	58	HIS
8	a4	73	GLN
8	a4	89	GLN
8	a4	155	ASN
8	a5	73	GLN
8	a5	89	GLN
8	a5	95	ASN
9	c1	65	HIS
9	c1	115	GLN
9	c2	64	HIS
9	c2	87	GLN
9	c3	64	HIS
9	c3	87	GLN
10	d2	84	HIS
10	d2	100	HIS
10	d3	231	ASN
10	d3	269	GLN
10	d4	83	ASN
10	d4	84	HIS
10	d4	93	GLN
1	h0	65	ASN
1	h0	116	GLN
1	h0	159	GLN
1	h1	211	ASN
1	i0	127	GLN
1	i0	208	GLN
1	i0	221	HIS
1	j0	99	ASN
2	p2	273	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	p3	74	GLN
2	p3	214	ASN
2	p4	94	HIS
2	p4	179	HIS
2	p4	273	HIS
2	p4	297	ASN
2	p5	74	GLN
2	p5	94	HIS
2	p5	111	ASN
2	p5	273	HIS
3	s3	57	GLN
3	s3	62	HIS
3	s3	226	HIS
3	s3	240	HIS
3	s4	62	HIS
3	s4	100	ASN
3	s4	243	GLN
3	s5	56	ASN
3	s5	57	GLN
3	s5	185	HIS
3	s6	56	ASN
3	s6	243	GLN
4	t1	1	GLN
4	t2	1	GLN
4	t2	58	GLN
4	t2	100	GLN
4	t2	176	HIS
4	t3	54	GLN
4	t3	62	GLN
4	t4	1	GLN
4	t4	52	GLN
4	t4	86	ASN
4	t4	163	ASN
4	t4	179	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

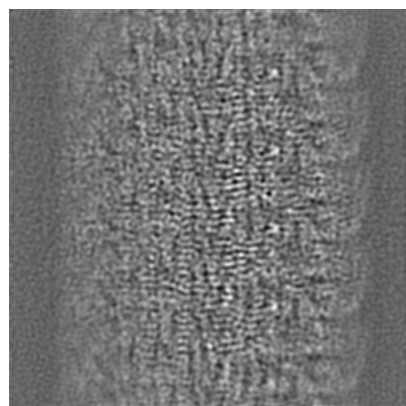
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75268. These allow visual inspection of the internal detail of the map and identification of artifacts.

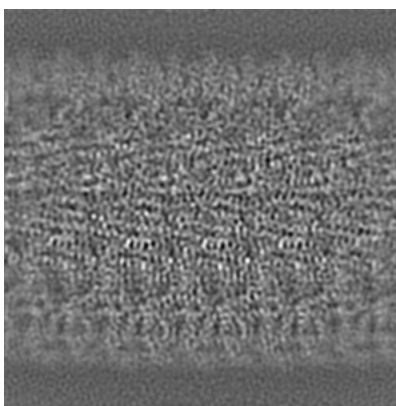
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

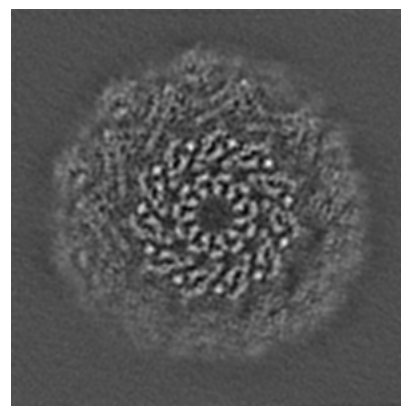
6.1.1 Primary map



X

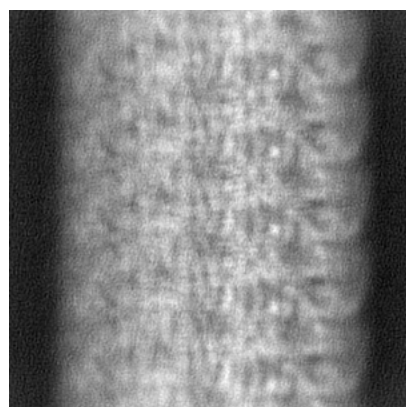


Y

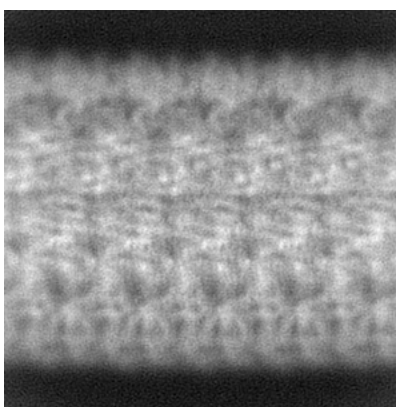


Z

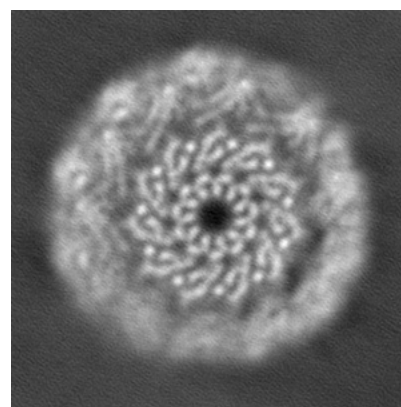
6.1.2 Raw map



X



Y

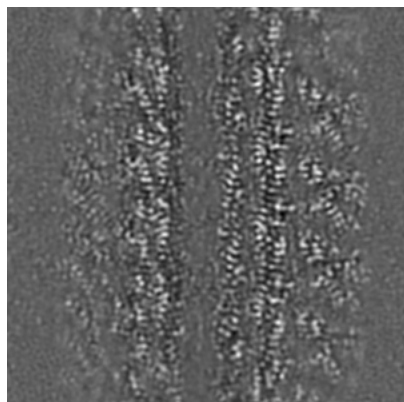


Z

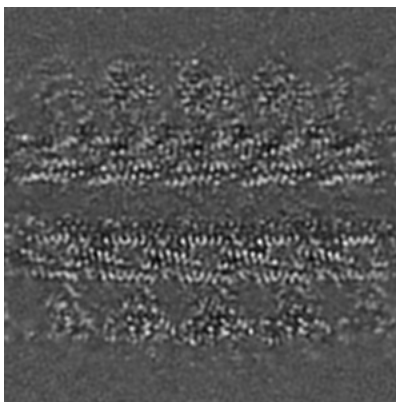
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

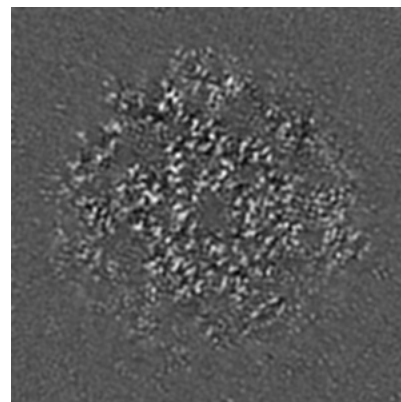
6.2.1 Primary map



X Index: 128

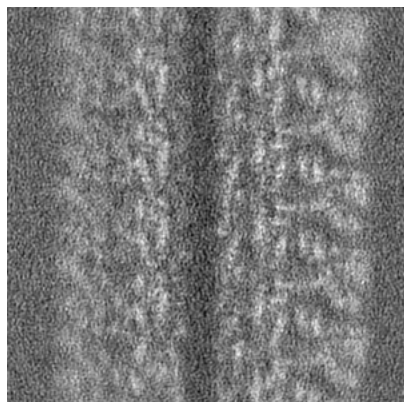


Y Index: 128

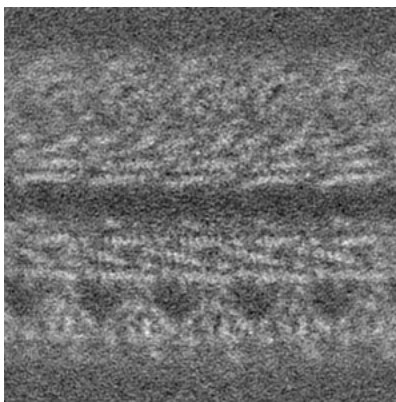


Z Index: 128

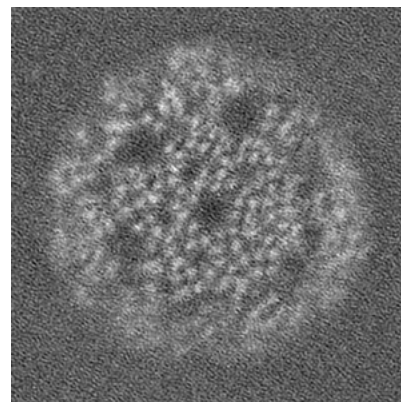
6.2.2 Raw map



X Index: 128



Y Index: 128

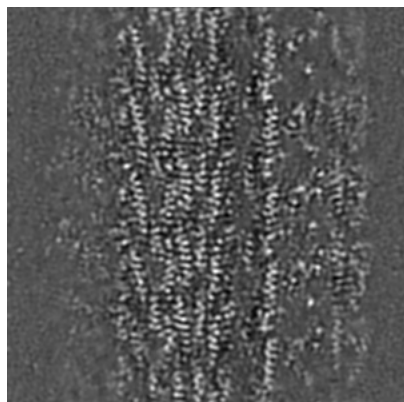


Z Index: 128

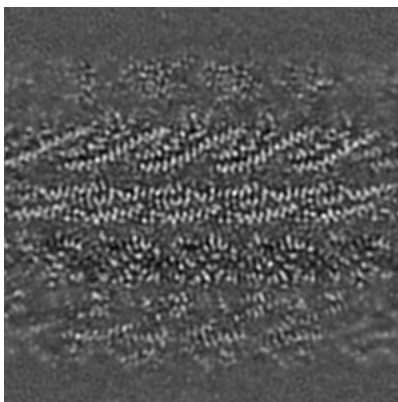
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

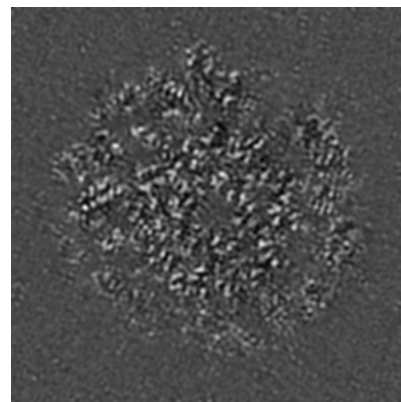
6.3.1 Primary map



X Index: 115

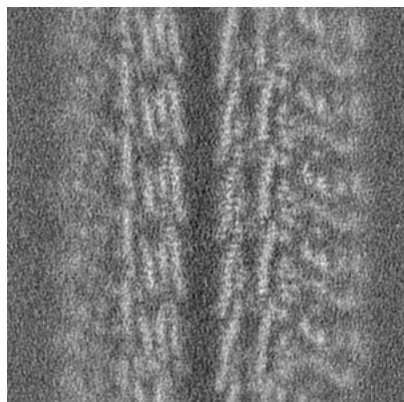


Y Index: 147

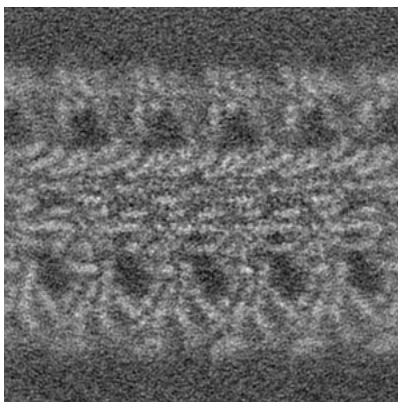


Z Index: 142

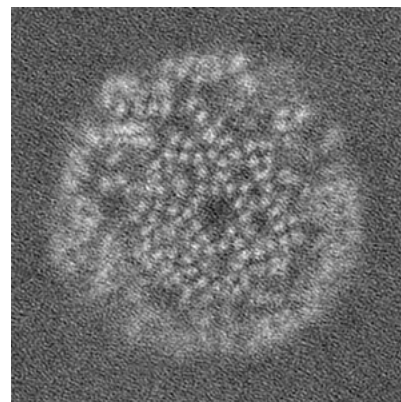
6.3.2 Raw map



X Index: 132



Y Index: 167

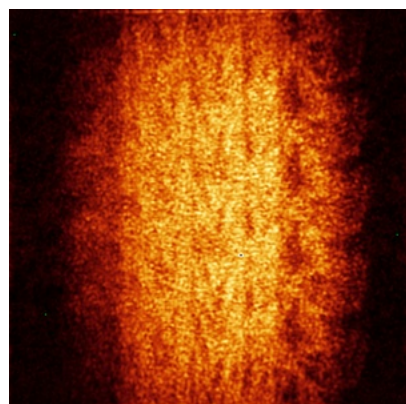


Z Index: 166

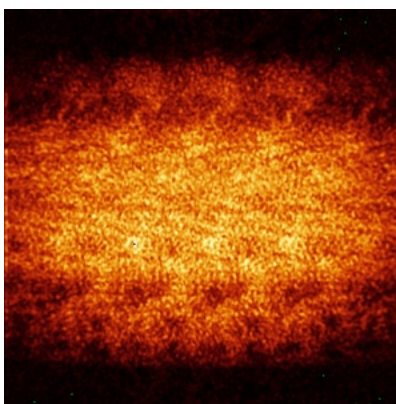
The images above show the largest variance slices of the map in three orthogonal directions.

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

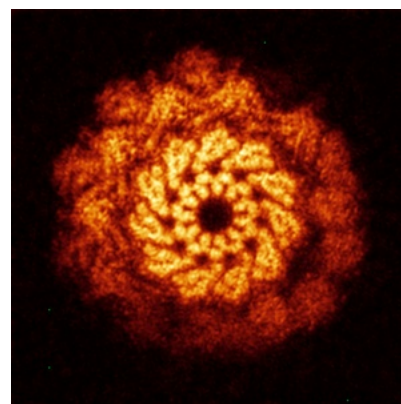
6.4.1 Primary map



X

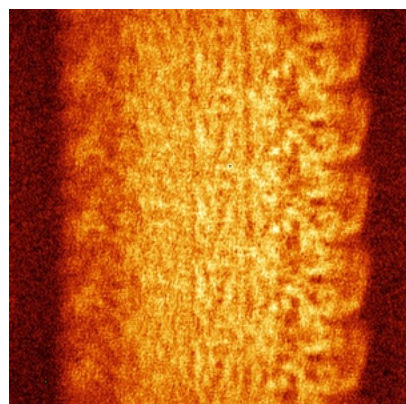


Y

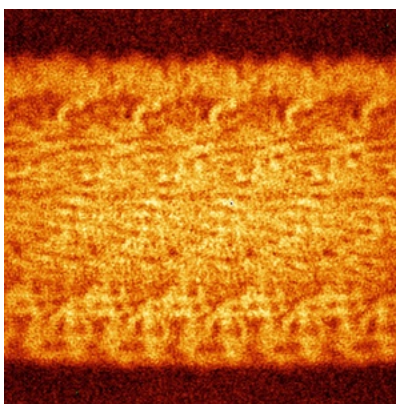


Z

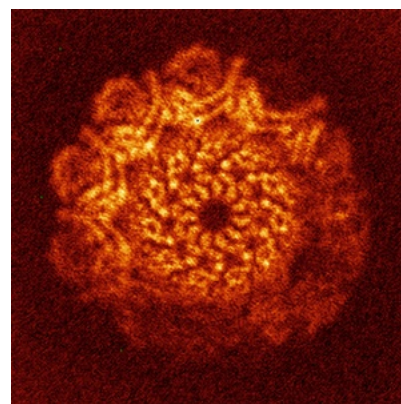
6.4.2 Raw map



X



Y

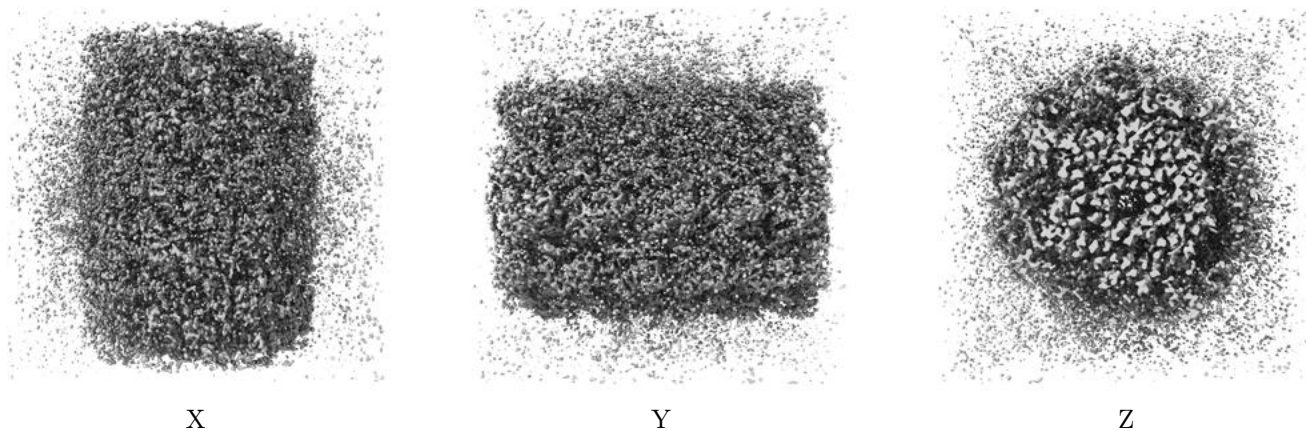


Z

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

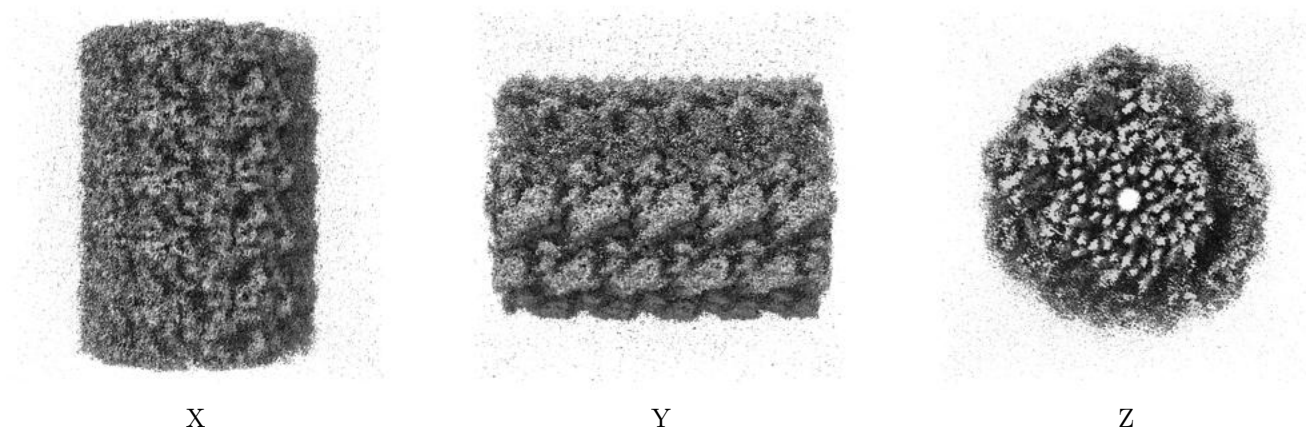
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

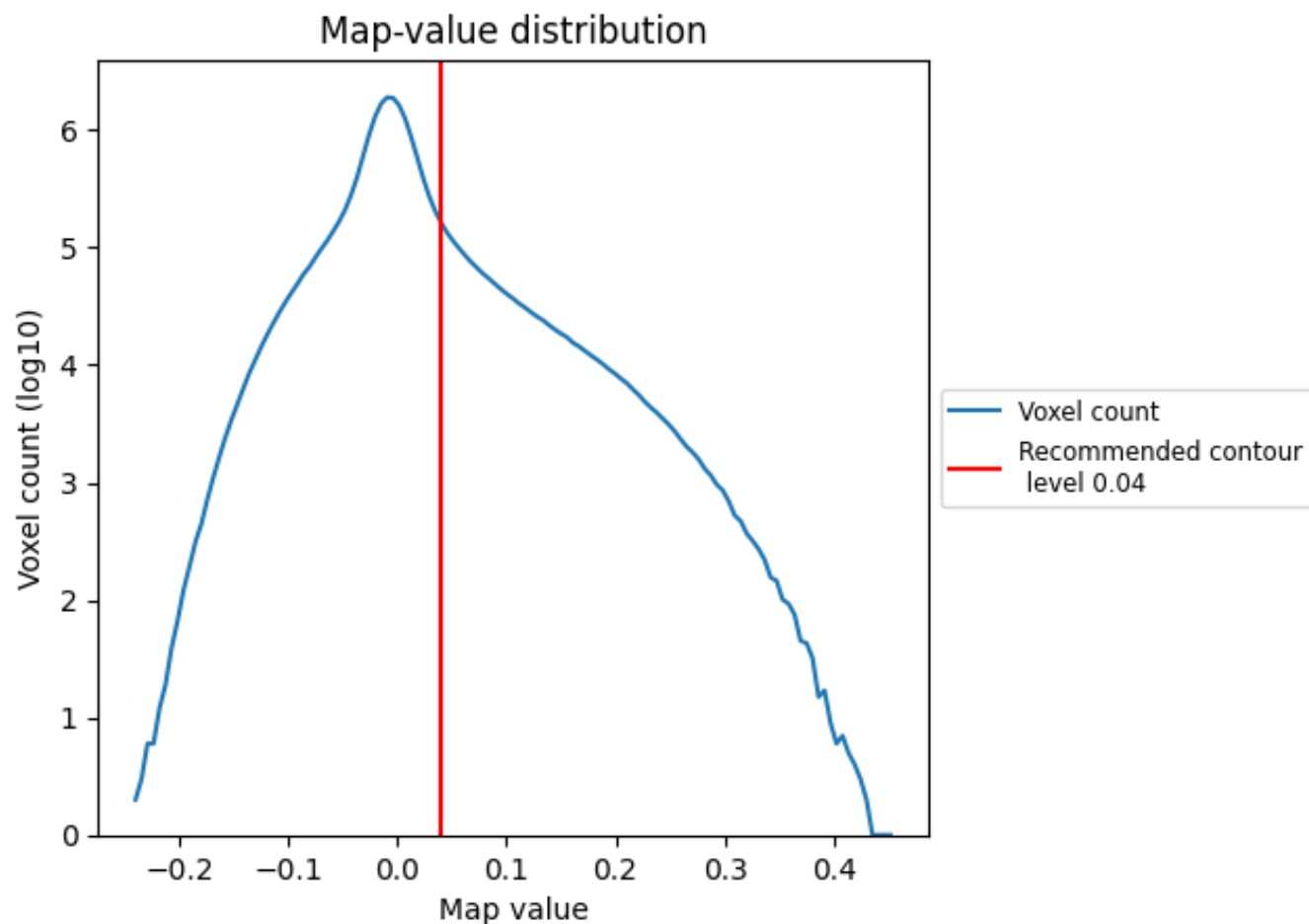
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

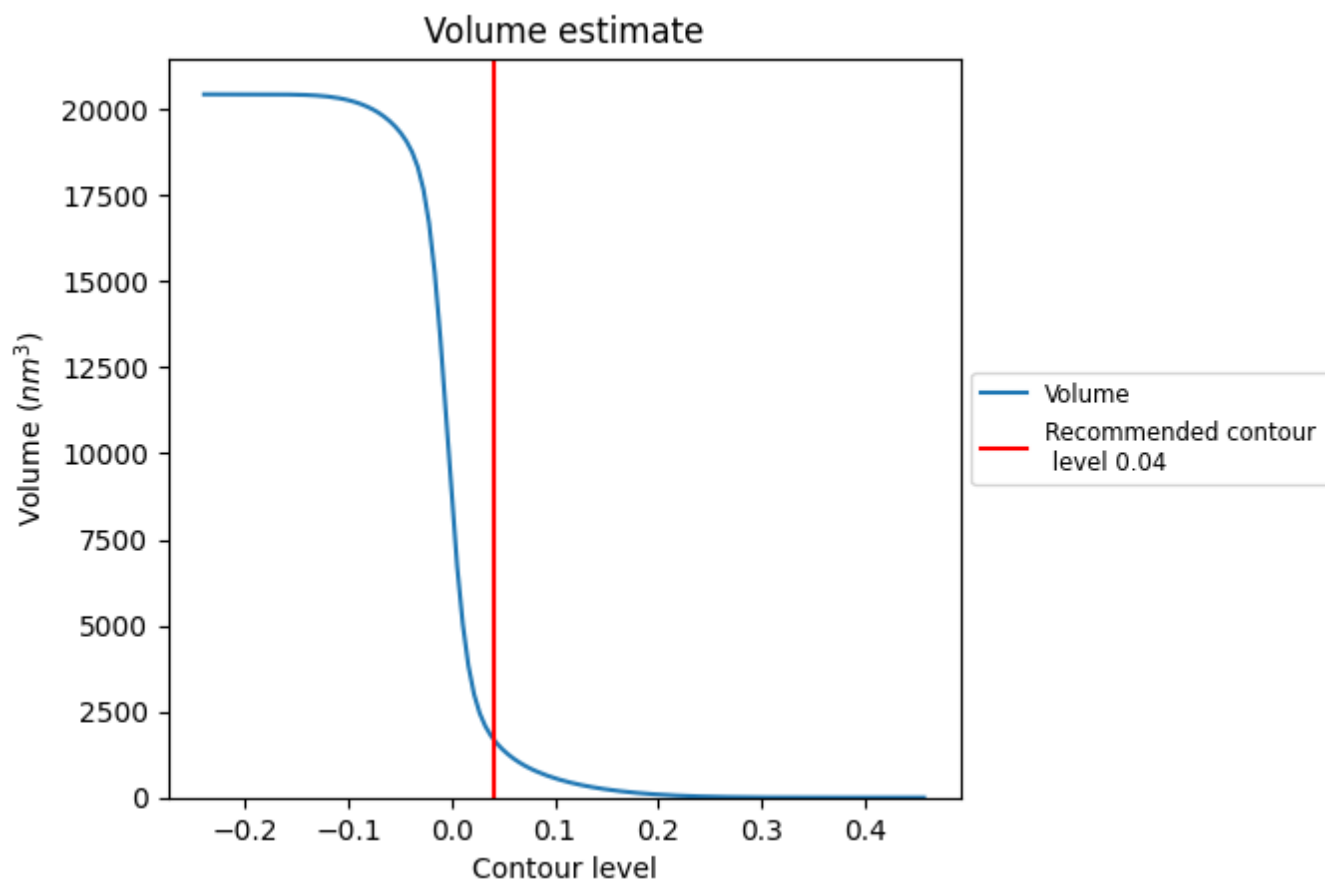
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

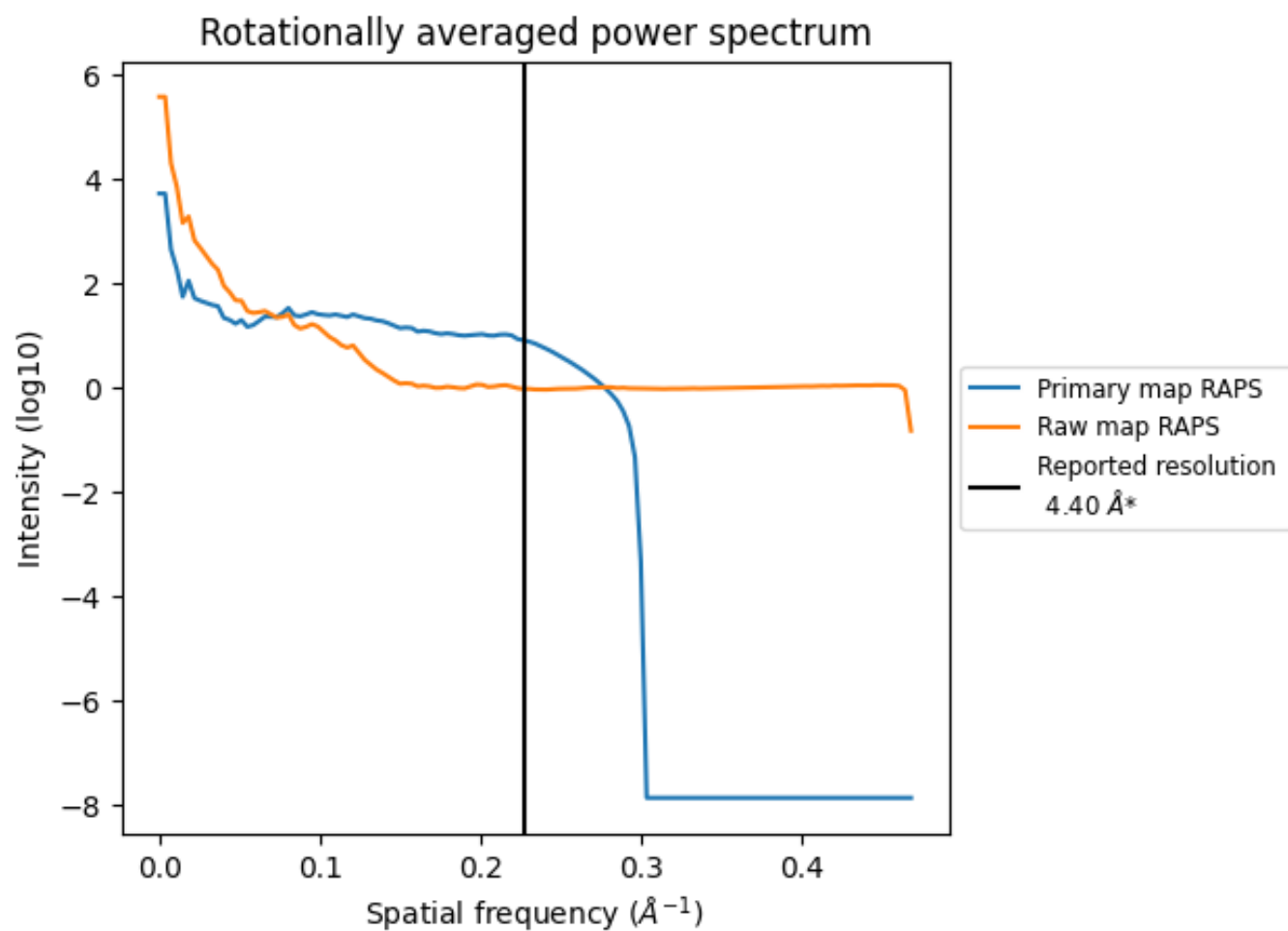
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1721 nm^3 ; this corresponds to an approximate mass of 1554 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 ⓘ

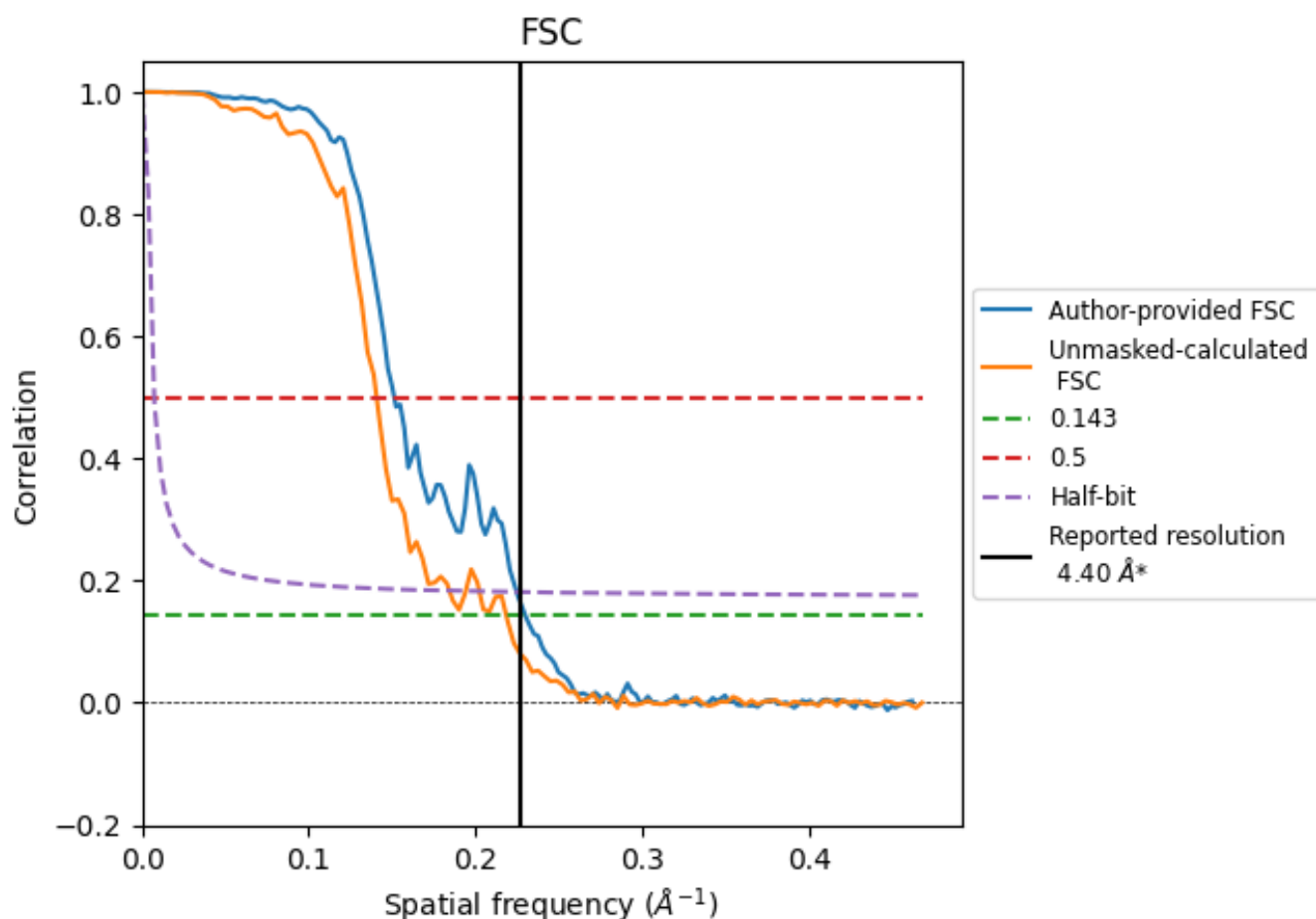


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

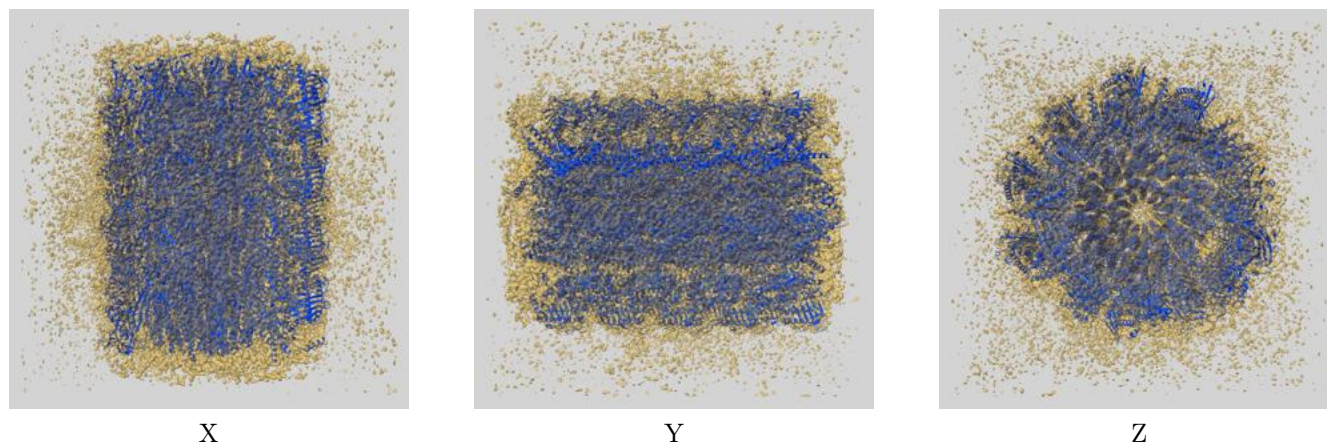
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.35	6.61	4.44
Unmasked-calculated*	4.58	7.11	5.42

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

9 Map-model fit [i](#)

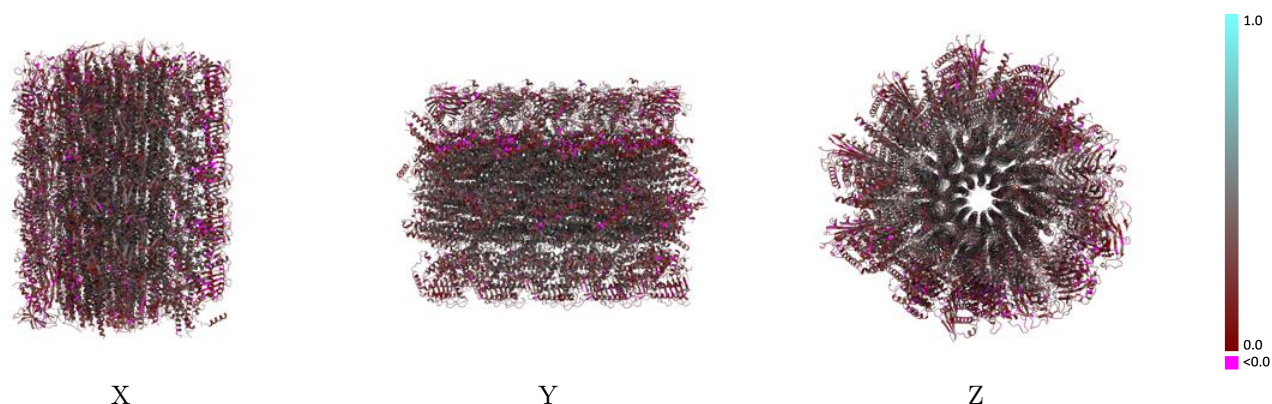
This section contains information regarding the fit between EMDB map EMD-75268 and PDB model 10LK. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



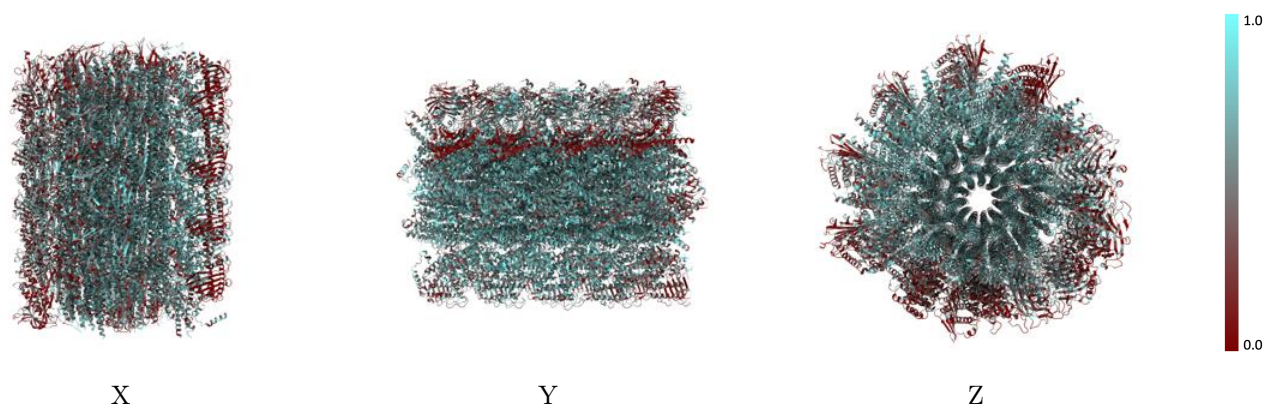
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



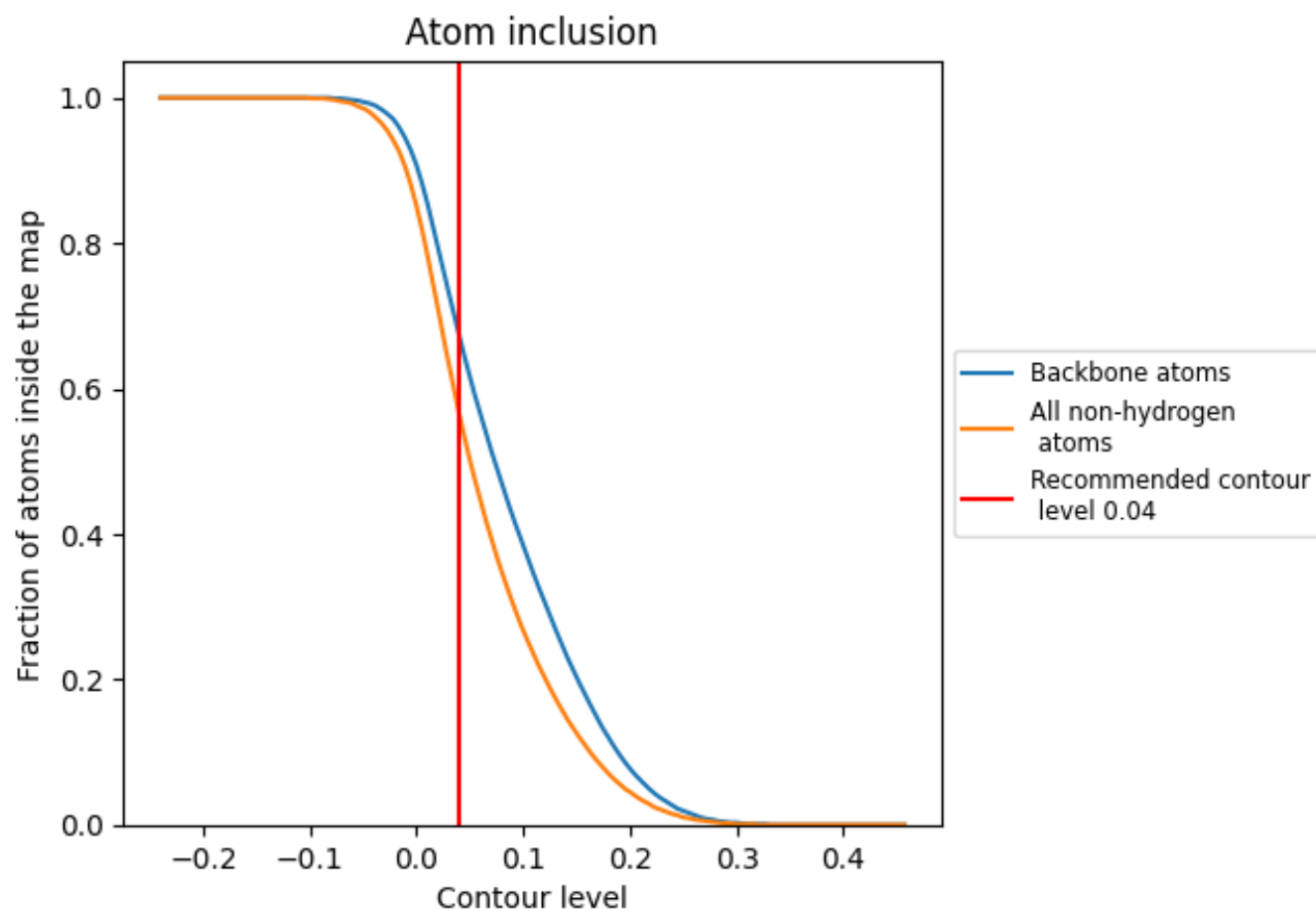
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5650	 0.3160
A4	 0.6570	 0.3340
A5	 0.6300	 0.3260
A6	 0.6900	 0.3700
A7	 0.6830	 0.3640
A8	 0.6360	 0.3260
A9	 0.5750	 0.2880
B3	 0.5950	 0.2770
B4	 0.6220	 0.3270
B5	 0.6470	 0.3380
B6	 0.6760	 0.3600
B7	 0.6810	 0.3620
B8	 0.6290	 0.3280
C3	 0.6700	 0.3550
C4	 0.6600	 0.3590
C5	 0.7020	 0.3890
C6	 0.7020	 0.3940
C7	 0.6770	 0.3770
C8	 0.6160	 0.3260
D3	 0.6840	 0.3810
D4	 0.6900	 0.3790
D5	 0.7220	 0.4040
D6	 0.7090	 0.3930
D7	 0.6810	 0.3640
E2	 0.6840	 0.3610
E3	 0.7000	 0.3800
E4	 0.7210	 0.4100
E5	 0.7360	 0.4150
E6	 0.7140	 0.3950
E7	 0.6770	 0.3570
F2	 0.6810	 0.3710
F3	 0.7110	 0.3900
F4	 0.7260	 0.4110
F5	 0.7080	 0.3960
F6	 0.6900	 0.3750



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
G1	 0.7080	 0.3980
G2	 0.6770	 0.3750
G6	 0.6360	 0.3670
G7	 0.7010	 0.3910
G8	 0.7110	 0.3940
G9	 0.7180	 0.3930
H6	 0.6660	 0.3580
H7	 0.6690	 0.3710
H8	 0.7070	 0.3990
H9	 0.7000	 0.3980
I5	 0.6170	 0.3120
I6	 0.6520	 0.3480
I7	 0.6810	 0.3820
I8	 0.6980	 0.4040
I9	 0.6830	 0.3830
J5	 0.6160	 0.3290
J6	 0.6480	 0.3530
J7	 0.6880	 0.3780
J8	 0.6750	 0.3700
J9	 0.6240	 0.3320
K4	 0.6060	 0.3450
K5	 0.6170	 0.3290
K6	 0.6520	 0.3530
K7	 0.6630	 0.3540
K8	 0.6380	 0.3350
K9	 0.5690	 0.2810
L2	 0.5150	 0.2440
L3	 0.6340	 0.3050
L4	 0.6780	 0.3420
L5	 0.6430	 0.3330
L6	 0.5480	 0.2800
M1	 0.5490	 0.2700
M2	 0.6780	 0.3390
M3	 0.7370	 0.3830
M4	 0.7300	 0.3780
M5	 0.6420	 0.3280
N2	 0.5980	 0.2970
N3	 0.7370	 0.3930
N4	 0.7470	 0.4000
N5	 0.7060	 0.3700
N6	 0.6130	 0.3180
O1	 0.6070	 0.3020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O2	 0.6620	 0.3380
O3	 0.7290	 0.3930
O4	 0.7480	 0.3880
O5	 0.6820	 0.3480
P2	 0.5290	 0.2830
P3	 0.6860	 0.3570
P4	 0.7010	 0.3780
P5	 0.6840	 0.3520
P6	 0.5820	 0.2930
Q1	 0.3120	 0.2050
Q2	 0.4680	 0.2350
Q3	 0.5900	 0.2890
Q4	 0.5700	 0.2860
R2	 0.4110	 0.2390
R3	 0.5700	 0.2950
R4	 0.6320	 0.3360
R5	 0.5340	 0.2850
S2	 0.3160	 0.2130
S3	 0.4940	 0.2590
S4	 0.5870	 0.3160
S5	 0.5590	 0.2800
S6	 0.4130	 0.2250
T1	 0.2610	 0.1790
T2	 0.4370	 0.2520
T3	 0.4840	 0.2690
T4	 0.4110	 0.2380
V1	 0.3750	 0.2420
V2	 0.5490	 0.3000
V3	 0.5860	 0.3150
V4	 0.5440	 0.3090
V5	 0.3210	 0.2150
X1	 0.3700	 0.2370
X2	 0.5280	 0.3090
X3	 0.5710	 0.3180
X4	 0.4590	 0.2540
X5	 0.2220	 0.1820
Y1	 0.2700	 0.2230
Y2	 0.4470	 0.2730
Y3	 0.5410	 0.3090
Y4	 0.5370	 0.2970
Y5	 0.3840	 0.2400
Z1	 0.2870	 0.2080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z2	 0.3690	 0.2400
Z3	 0.3650	 0.2350
Z4	 0.2460	 0.1820
a2	 0.0800	 0.1550
a3	 0.1310	 0.1470
a4	 0.1620	 0.1460
a5	 0.0840	 0.1490
c1	 0.1960	 0.1950
c2	 0.3320	 0.2460
c3	 0.3130	 0.2200
d2	 0.2720	 0.2180
d3	 0.3200	 0.2310
d4	 0.2600	 0.1950
h0	 0.6950	 0.3810
h1	 0.6100	 0.3260
i0	 0.6590	 0.3550
j0	 0.5650	 0.2910
p2	 0.4140	 0.2430
p3	 0.5770	 0.3110
p4	 0.6000	 0.3300
p5	 0.4800	 0.2780
s3	 0.2280	 0.1850
s4	 0.3840	 0.2410
s5	 0.4110	 0.2410
s6	 0.2980	 0.2070
t1	 0.2930	 0.2020
t2	 0.4750	 0.2660
t3	 0.4620	 0.2660
t4	 0.3270	 0.2110