



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 13, 2016 – 05:27 PM EST

PDB ID : 5GMK
EMDB ID: : EMD-9525
Title : Cryo-EM structure of the Catalytic Step I spliceosome (C complex) at 3.4 angstrom resolution
Authors : Wan, R.; Yan, C.; Bai, R.; Huang, G.; Shi, Y.
Deposited on : 2016-07-14
Resolution : 3.40 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

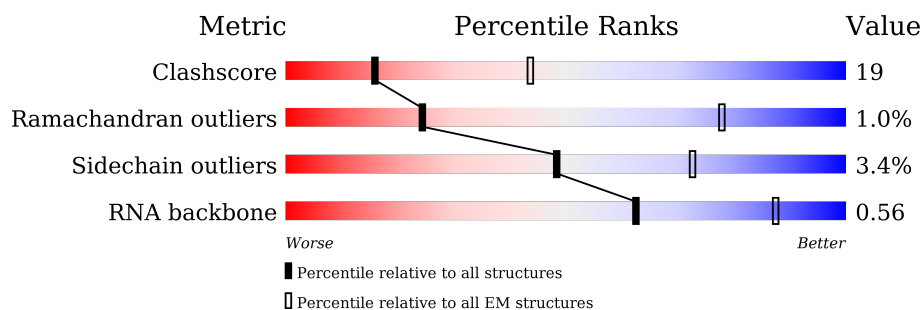
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.




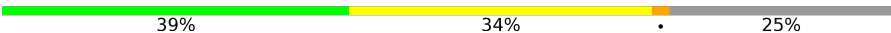
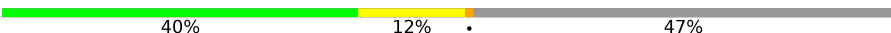






















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2413	49% 29% . 21%
2	C	1008	54% 32% . 13%
3	D	214	34% 11% 9% . 45%
4	E	112	32% 35% 25% 8%
5	L	1175	. . 5% 89%
6	M	29	38% 34% 28%
7	B	13	31% 31% 38%
8	N	15	40% 20% 33% 7%


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	135	
10	O	451	
11	P	379	
12	Q	364	
13	R	339	
14	S	175	
15	T	157	
16	Z	577	
17	c	587	
18	d	687	
19	F	278	
20	G	179	
21	H	235	
22	I	215	
23	v	859	
24	n	455	
25	o	503	
25	p	503	
25	q	503	
25	r	503	
26	t	175	
27	k	196	
27	s	196	
28	i	94	
28	u	94	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	h	86	 78% . 19%
29	w	86	 78% . 19%
30	j	77	 86% . . 10%
30	x	77	 86% . . 10%
31	l	101	 77% . 19%
31	y	101	 77% . 19%
32	m	146	 52% . 44%
32	z	146	 52% . 44%
33	e	110	 54% . . 41%
33	g	110	 79% 5% . 15%
34	a	111	 68% 5% 27%
35	b	238	 48% 7% . 43%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 75273 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1910	Total	C	N	O	S	0	0
			15775	10142	2709	2867	57		

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	878	Total	C	N	O	S	0	0
			7019	4529	1166	1295	29		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	117	Total	C	N	O	P	0	0
			2465	1104	414	830	117		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 5 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	127	Total	C	N	O	P	0	0
			2673	1197	445	904	127		

- Molecule 6 is a RNA chain called Intron_BPS.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	29	Total	C	N	O	P	0	0
			608	274	101	204	29		

- Molecule 7 is a RNA chain called 5'-Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	13	Total	C	N	O	P	0	0
			275	124	47	91	13		

- Molecule 8 is a RNA chain called 5'-Splicing Site.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	15	Total	C	N	O	P	0	0
			312	140	45	112	15		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 10 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	337	Total	C	N	O	S	0	0
			2646	1669	466	501	10		

- Molecule 11 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	201	Total	C	N	O	S	0	0
			1583	988	290	298	7		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	185	Total	C	N	O	S	0	0
			1472	930	256	271	15		

- Molecule 13 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	69	Total	C	N	O	S	0	0
			560	351	112	96	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	436	Total	C	N	O	S	0	0
			2971	1841	549	573	8		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	549	Total	C	N	O	S	0	0
			3590	2232	675	675	8		

- Molecule 19 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	115	Total	C	N	O	S	0	0
			937	592	167	169	9		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	41	Total	C	N	O	S	0	0
			342	215	63	63	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	95	Total	C	N	O	S	0	0
			810	506	152	151	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	673	Total	C	N	O	S	0	0
			3580	2190	683	706	1		

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	299	Total	C	N	O	S	0	0
			1890	1175	340	369	6		

- Molecule 25 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	o	126	Total	C	N	O	S	0	0
			830	525	134	169	2		
25	p	128	Total	C	N	O	S	0	0
			843	532	136	173	2		
25	q	387	Total	C	N	O	S	0	0
			2345	1471	402	464	8		
25	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	t	156	Total	C	N	O	S	0	0
			926	585	160	180	1		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
27	s	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	u	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
29	w	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
30	x	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	y	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
33	e	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

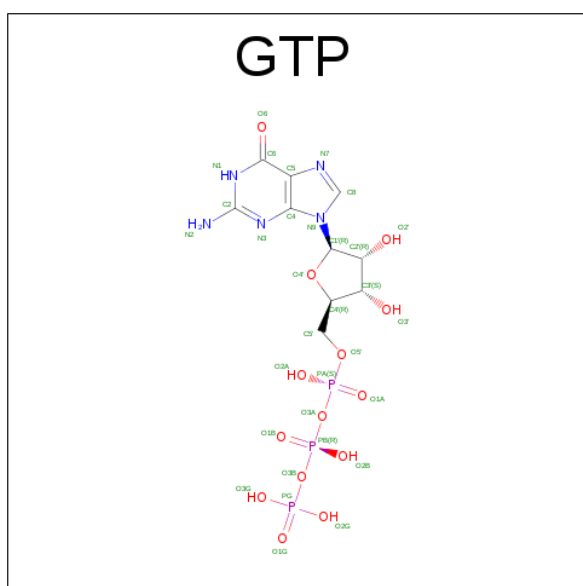
- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	a	81	Total	C	N	O	0	0
			513	332	89	92		

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	b	135	Total	C	N	O	0	0
			841	538	142	161		

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
36	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	E	5	Total	Mg	0
			5	5	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

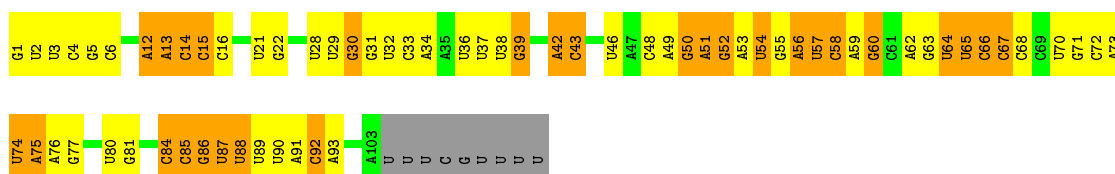
Mol	Chain	Residues	Atoms		AltConf
38	R	1	Total	Zn	0
			1	1	
38	Q	2	Total	Zn	0
			2	2	
38	T	3	Total	Zn	0
			3	3	
38	F	1	Total	Zn	0
			1	1	

[illegible]

- Molecule 2: Pre-mRNA-splicing factor SNU114

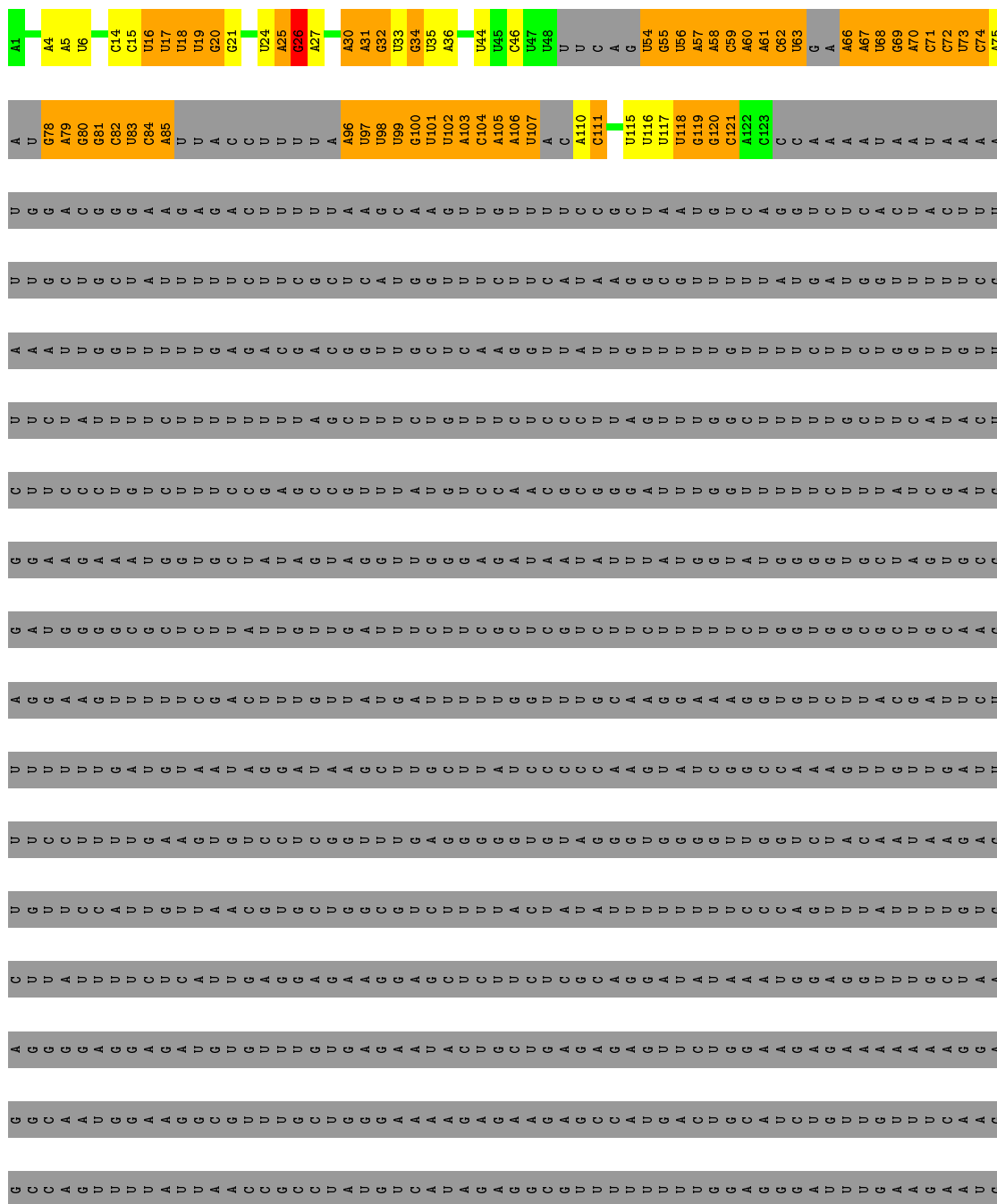
Chain C:  54% 32% 13%

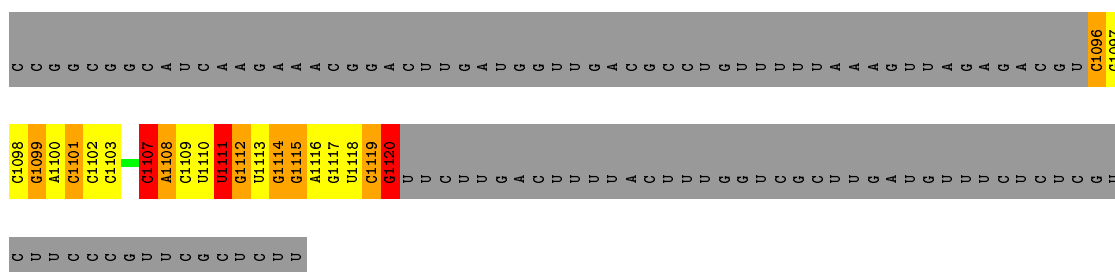
WET	GLU	GLY	ASP	ASP	LEU	PHE	ASP	GLU	PHE	GLY	ASN	LEU	ILE	GLY	VAL	ASP	PRO	PHE	ASP	SER	ASP	GLU	GLU	GLN	GLN	TYR	GLN	THR	ASN	THR	PHE	GLU	GLY	SER	GLY	ASN	ASN	ASN	GLU	ILE	GLU	SER	ARG	GLN	LEU	THR	SER	LEU	GLY	LYS	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
GLU	LEU	GLY	ILE	SER	SER	E87	H86	P89	G71	E75	V76	L77	M78	E79	T80	K81	N82	P89	K99	I100	Q101	E102	H103	LEU	T104	ASP	GLU	GLN	GLU	Q108	L109	K110	T116	R117	Y118	M119	R120	M123	M126	E131	R132	I133	I134	N135	V136	G137	V138	I139	L142	H143	S144	L152																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L153	V154	S157	H158	I161	P162	D163	K166	N167	L170	G171	R176	Y177	L178	D179	Q183	N194	L199	C200	H201	I202	D203	L204	K206	S207	R208	N209	I210	R211	F212	D213	D214	A215	H218	V219	N220	F221	I222	K223	A231	S232	D233	L234	V235	L236	I237	V238	I341	D342	D240	D343																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V245	T246	V247	V248	Q251	L252	Q255	F265	N268	K269	L270	R272	L275	L286	N289	E290	I291	I292	A293	N294	I295	N296	F304	S305	I307	I311	A314	S315	T316	G319	F320	T321	I324	K325	E326	S329	S335	S336	S339	K340	I341	D342	D343	D344	D345	D346	D347	D348	D349																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
T346	L347	L348	W349	Y353	R360	T361	K362	P363	E365	N366	P371	T372	P373	F376	I377	L378	L379	P380	I384	F385	S386	Y387	K391	E392	K393	K397	W407	L408	A412	Y415	D416	F417	Q418	P419	F420	L425	L435	V436	D437	A438	L439	T440	D441	D442	D443	D444	D445	D446	D447	D448																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
R441	P445	F446	E447	N451	K452	H455	L458	K461	S462	T463	E465	L468	H471	V472	L473	D477	L485	F486	R487	G491	L492	L493	V499	R500	I501	L502	D503	Q506	R510	GLN	LYS	ARG	GLN	LEU	ASP	ILE	SER	LYS	THR	GLU	THR	SER	ASN	GLU	D553																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
ASP	GLU	ASP	E530	E533	T534	P535	S536	V539	I542	E543	L544	L545	S546	P552	V553	H557	O560	I561	V562	L563	I564	I567	P571	A575	T576	L577	V578	F592	V602	L607	R613	E614	L615	S616	V617	V618	V619	V620	V621	V622	V623	V624	V625	V626	V627	V628	V629	V630	V631	V632	V633	V634	V635	V636	V637	V638	V639	V640	V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V663	V664	V665	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681	V682	V683	V684	V685	V686	V687	V688	V689	V690	V691	V692	V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V708	V709	V710	V711	V712	V713	V714	V715	V716	V717	V718	V719	V720	V721	V722	V723	V724	V725	V726	V727	V728	V729	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V1503	V1504	V1505	V1506	V1507	V1508	V1509	V1510	V1511	V1512	V1513	V1514	V1515	V1516	V1517	V1518	V1519	V1520	V1521	V1522	V1523	V1524	V1525	V1526	V1527	V1528	V1529	V1530	V1531	V1532	V1533	V1534	V1535	V1536	V1537	V1538	V1539	V1540	V1541	V1542	V1543	V1544	V1545	V1546	V1547	V1548	V1549	V1550	V1551	V1552	V1553	V1554	V1555	V1556	V1557	V1558	V1559	V1560	V1561	V1562	V1563	V1564	V1565	V1566	V1567	V1568	V1569	V1570	V1571	V1572	V1573	V1574	V1575	V1576	V1577	V1578	V1579	V1580	V1581	V1582	V1583	V1584	V1585	V1586	V1587	V1588	V1589	V1590	V1591	V1592	V1593	V1594	V1595	V1596	V1597	V1598	V1599	V1600	V1601	V1602	V1603	V1604	V1605	V1606	V1607	V1608	V1609	V1610	V1611	V1612	V1613	V1614	V1615	V1616	V1617	V1618	V1619	V1620	V1621	V1622	V1623	V1624	V1625	V1626	V1627	V1628	V1629	V1630	V1631	V1632	V1633	V1634	V1635	V1636	V1637	V1638	V1639	V1640	V1641	V1642	V1643	V1644	V1645	V1646	V1647	V1648	V1649	V1650	V1651	V1652	V1653	V1654	V1655	V1656	V1657	V1658	V1659	V1660	V1661	V1662	V1663	V1664	V1665	V1666	V1667	V1668	V1669	V1670	V1671	V1672	V1673	V1674	V1675	V1676	V1677	V1678	V1679	V1680	V1681	V1682	V1683	V1684	V1685	V1686	V1687	V1688	V1689	V1690	V1691	V1692	V1693	V1694	V1695	V1696	V1697	V1698	V1699	V1700	V1701	V1702	V1703	V1704	V1705	V1706	V1707	V1708	V1709	V1710	V1711	V1712	V1713	V1714	V1715	V1716	V1717	V1718	V1719	V



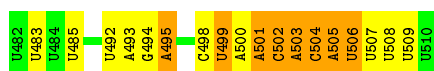
• Molecule 5: U2 snRNA

Chain L: . . 5% 89%





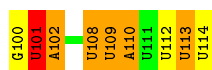
- Molecule 6: Intron_BPS



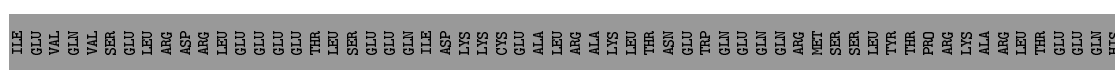
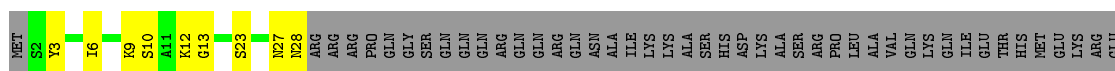
- Molecule 7: 5'-Exon



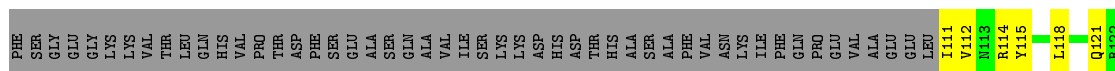
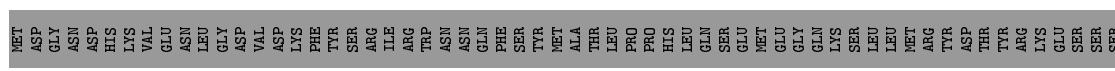
- Molecule 8: 5'-Splicing Site

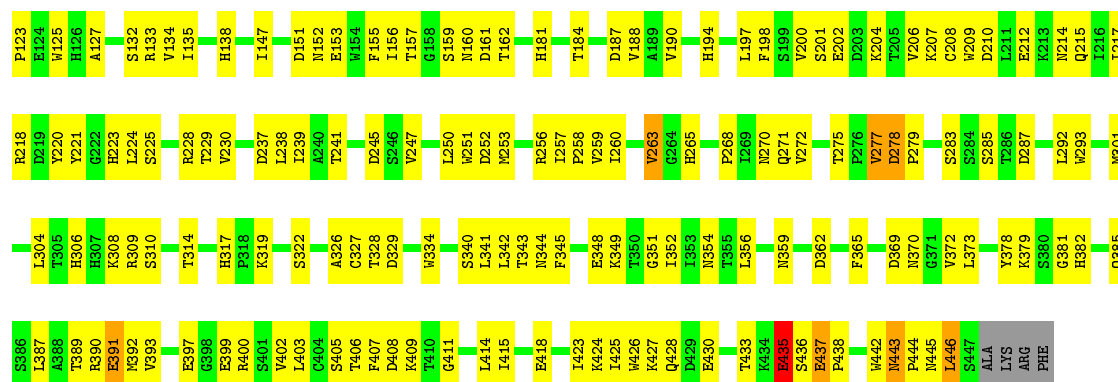


- Molecule 9: Pre-mRNA-splicing factor CWC21



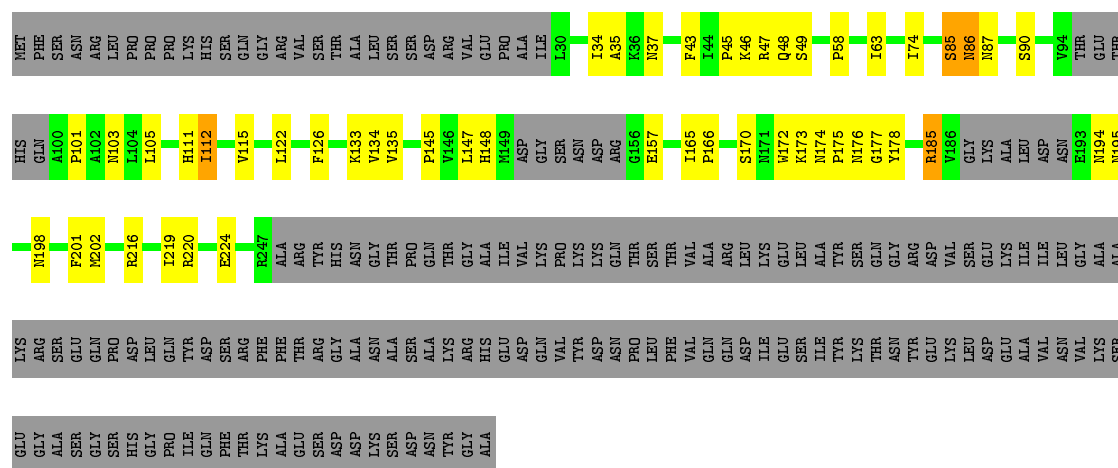
- Molecule 10: Pre-mRNA-splicing factor PRP46





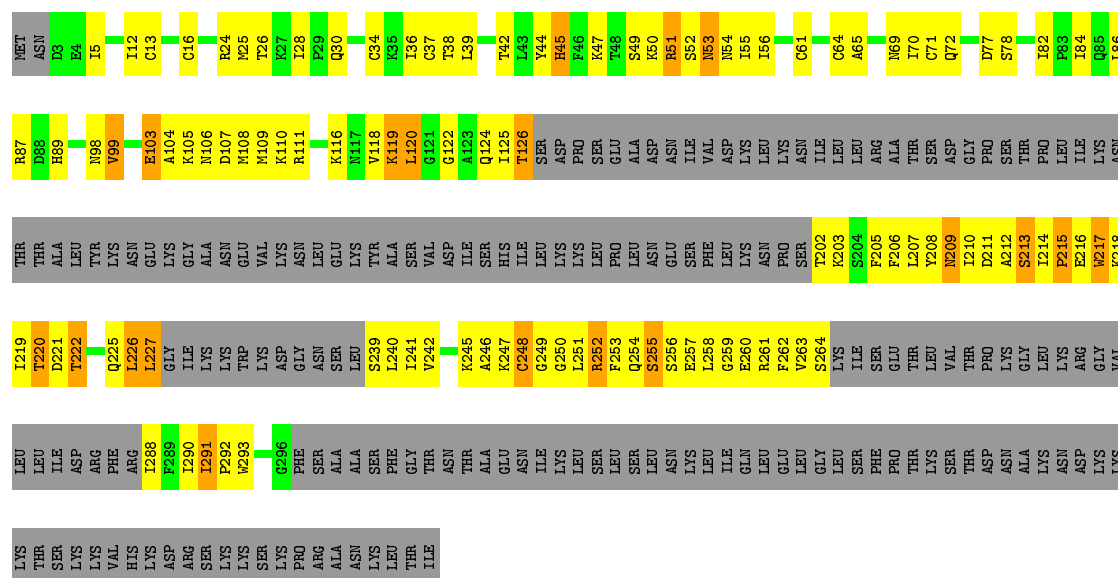
• Molecule 11: Pre-mRNA-processing protein 45

Chain P: 40% 12% 47%

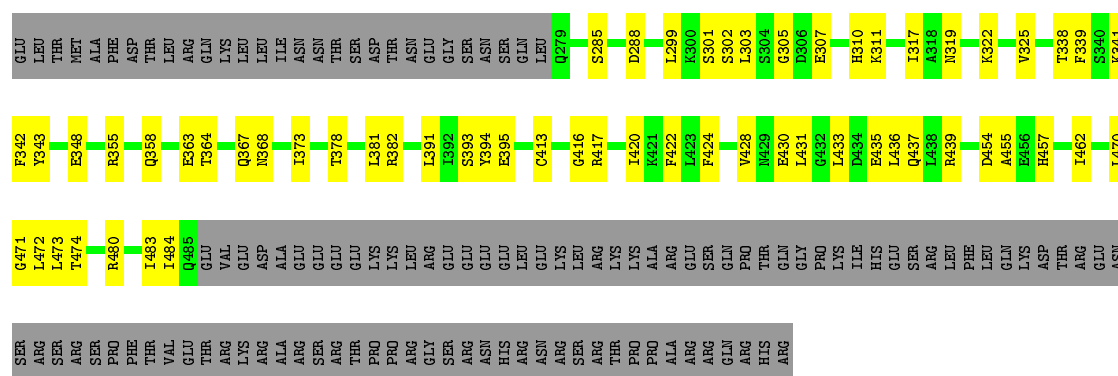


• Molecule 12: Pre-mRNA-splicing factor SLT11

Chain Q: 20% 25% 5% 49%

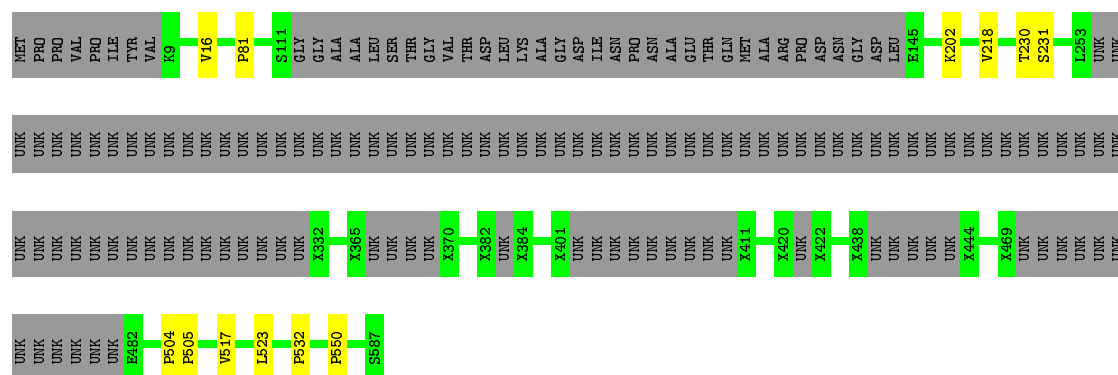


	W174	L177	R178	Y179	L180	L181	Q182	T183	Q184	E185	L186	S187	S188	T189	R190	R191	S192	S193	L194	E195	T196	L197	F198	E199	I200	R201	Q202	K203	D204	Y205	K206	S207	G211	I214	L215	D216	S219	Y227	I228	V229	E232	D233	E234	A235	I241	F242	E243	K244	C245	E246	PHE						
MET		THR	ALA	THR	ILE	GLN	DE	K12		E16		R22		M34		R42		R53		D62		R67	Q68	N69		L94		R108		L118		E132	T133	V134		I138		L143	E144	K145	N146	S147	L148	R149	L150	V151	I152	A153	V154		L162		K167	K168	T169	H170	D171



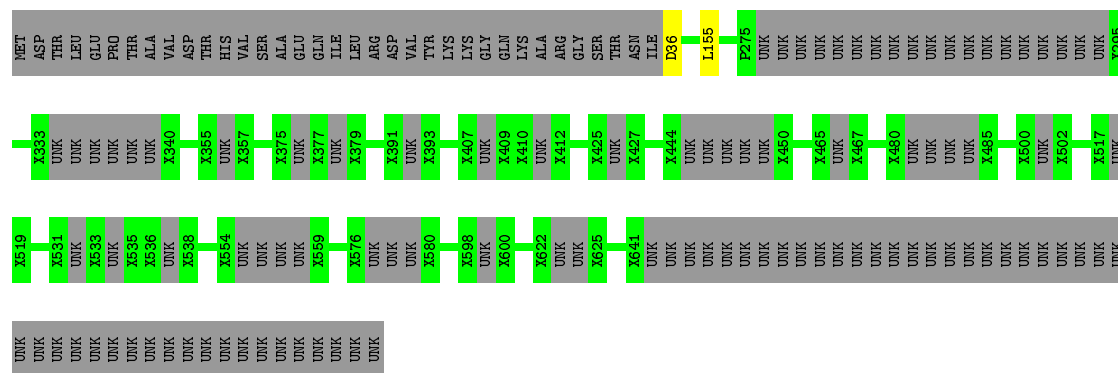
• Molecule 17: Pre-mRNA-splicing factor CEF1

Chain c: 72% 26%



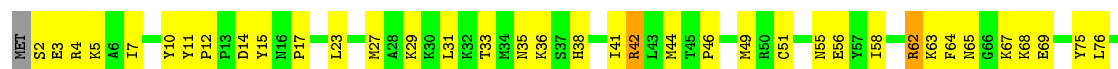
• Molecule 18: Pre-mRNA-splicing factor CLF1

Chain d: 80% 20%



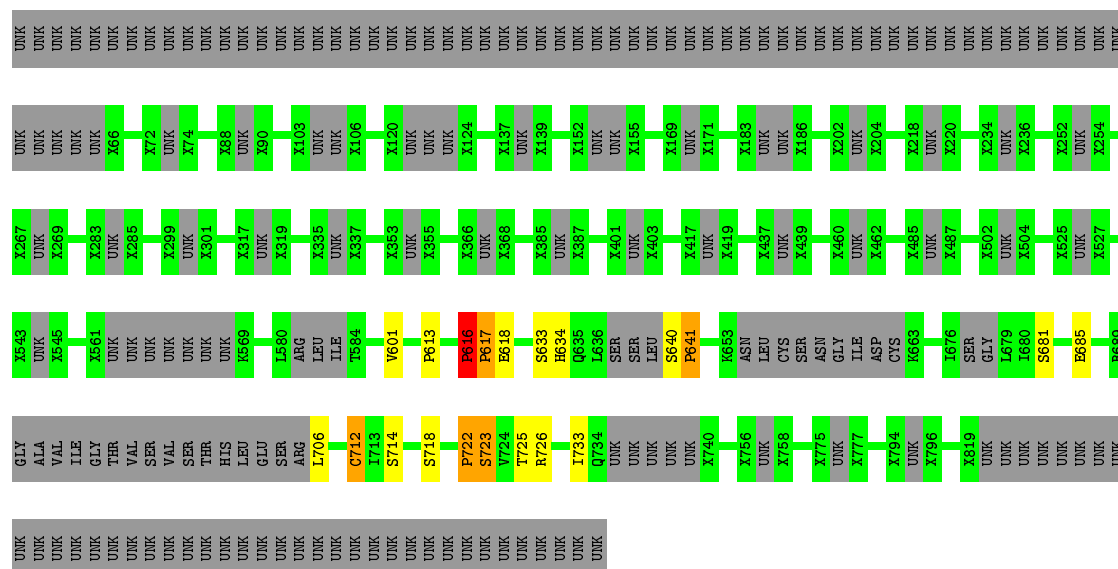
• Molecule 19: Protein CWC16

Chain F: 22% 18% 59%



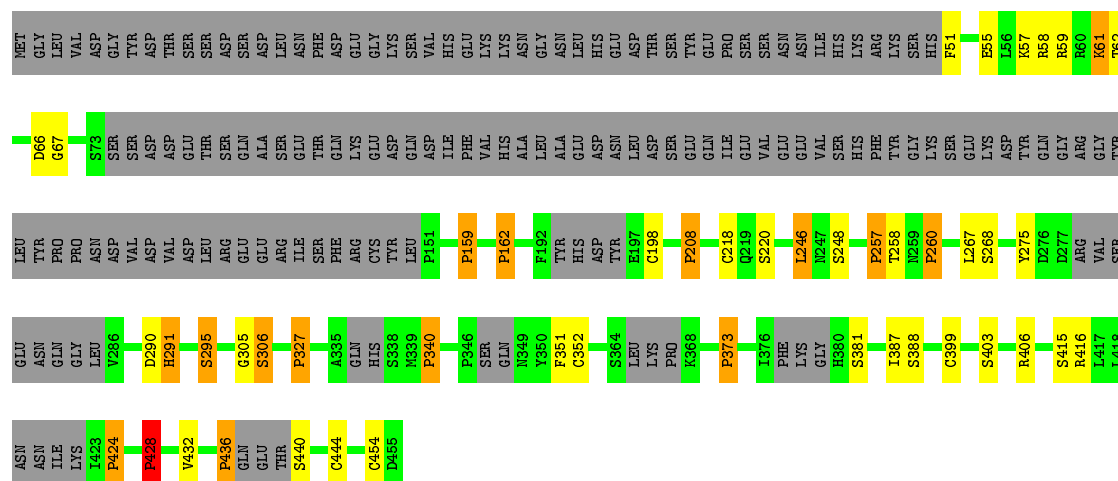
- Molecule 23: Pre-mRNA-splicing factor SYF1

Chain v:  76% .. 22%



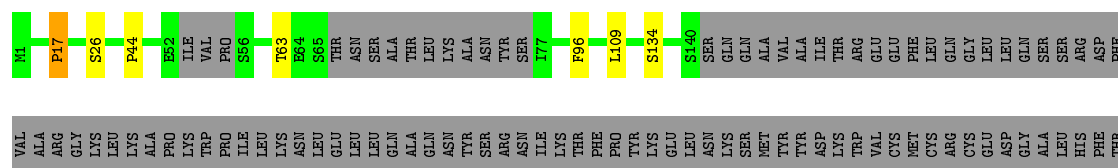
- Molecule 24: Pre-mRNA-processing factor 17

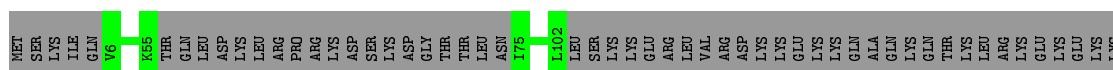
Chain n:  55% 7% • 34%



- Molecule 25: Pre-mRNA-processing factor 19

Chain o:  24% 75%





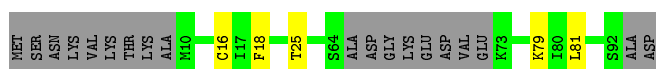
- Molecule 28: Small nuclear ribonucleoprotein E

Chain i:  74% 5% 20%




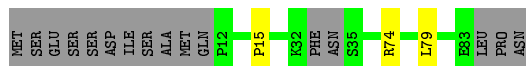
- Molecule 28: Small nuclear ribonucleoprotein E

Chain u:  74% 5% 20%




- Molecule 29: Small nuclear ribonucleoprotein F

Chain h:  78% 19%




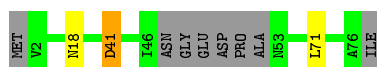
- Molecule 29: Small nuclear ribonucleoprotein F

Chain w:  78% 19%



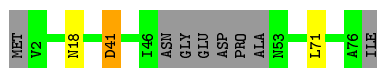
- Molecule 30: Small nuclear ribonucleoprotein G

Chain j:  86% 10%




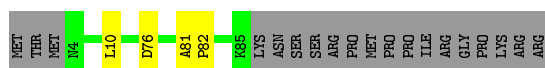
- Molecule 30: Small nuclear ribonucleoprotein G

Chain x:  86% 10%




- Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain l:  77% 19%



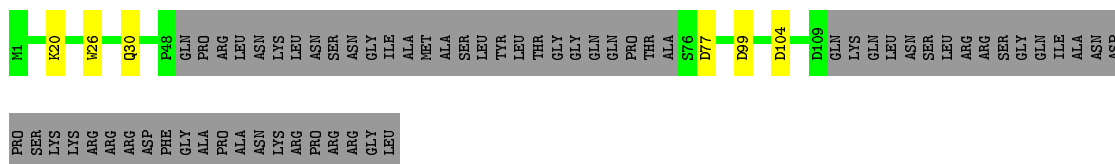
- Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain y:  77% 19%



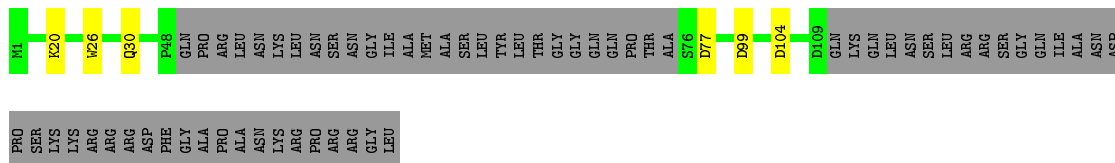
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain m:  52% 44%




- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain z:  52% 44%



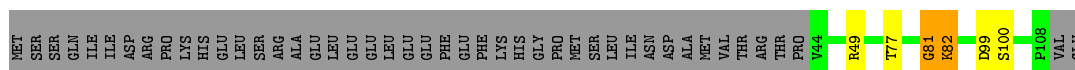
- Molecule 33: Small nuclear ribonucleoprotein Sm D2

Chain g:  79% 5% 15%



- Molecule 33: Small nuclear ribonucleoprotein Sm D2

Chain e:  54% 41%



- Molecule 34: U2 small nuclear ribonucleoprotein B"

Chain a:  68% 5% 27%

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	161066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, MG

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.48	3/16178 (0.0%)	0.60	6/21929 (0.0%)
10	O	0.57	0/2704	0.63	1/3676 (0.0%)
11	P	0.42	2/1604 (0.1%)	0.52	0/2160
12	Q	0.47	1/1496 (0.1%)	0.62	0/2014
13	R	0.44	0/2135	0.56	0/2871
14	S	0.46	1/574 (0.2%)	0.56	0/766
15	T	0.51	1/1315 (0.1%)	0.61	0/1759
16	Z	0.50	0/3712	0.85	7/5004 (0.1%)
17	c	0.41	1/2405 (0.0%)	0.50	0/3218
18	d	0.49	0/2107	0.54	1/2852 (0.0%)
19	F	0.37	0/955	0.55	0/1277
2	C	0.47	1/7168 (0.0%)	0.57	3/9707 (0.0%)
20	G	0.27	0/346	0.51	0/462
21	H	0.33	0/826	0.54	0/1108
22	I	0.34	0/826	0.47	0/1097
23	v	1.04	8/905 (0.9%)	0.76	6/1214 (0.5%)
24	n	1.48	19/1900 (1.0%)	0.89	15/2537 (0.6%)
25	o	0.40	0/835	0.53	0/1126
25	p	0.40	0/848	0.55	0/1143
25	q	0.44	0/2342	0.65	0/3139
25	r	0.39	0/828	0.54	1/1117 (0.1%)
26	t	0.42	0/924	0.56	2/1244 (0.2%)
27	k	0.37	0/636	0.61	0/856
27	s	0.37	0/615	0.61	0/829
28	i	0.42	0/585	0.62	0/795
28	u	0.42	0/585	0.62	0/795
29	h	0.44	0/564	0.65	1/761 (0.1%)
29	w	0.44	0/564	0.65	1/761 (0.1%)
3	D	0.73	0/2747	0.93	2/4267 (0.0%)
30	j	0.37	0/532	0.60	0/715
30	x	0.37	0/532	0.60	0/715
31	l	0.40	0/634	0.70	0/859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
31	y	0.40	0/634	0.70	0/859
32	m	0.41	0/649	0.61	0/880
32	z	0.41	0/649	0.61	0/880
33	e	0.43	0/535	0.67	2/717 (0.3%)
33	g	0.45	0/753	0.69	2/1013 (0.2%)
34	a	0.82	4/514 (0.8%)	1.32	2/686 (0.3%)
35	b	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
4	E	0.76	1/2452 (0.0%)	0.96	3/3817 (0.1%)
5	L	0.94	33/2974 (1.1%)	1.51	88/4610 (1.9%)
6	M	0.73	2/678 (0.3%)	1.01	3/1051 (0.3%)
7	B	1.01	1/307 (0.3%)	0.95	0/475
8	N	1.27	5/346 (1.4%)	1.29	10/535 (1.9%)
9	J	0.41	0/191	0.57	0/254
All	All	0.59	92/72448 (0.1%)	0.75	167/99677 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
10	O	0	6
11	P	0	1
12	Q	0	3
16	Z	0	5
17	c	0	1
2	C	0	2
20	G	0	1
24	n	0	4
30	j	0	1
30	x	0	1
31	l	0	2
31	y	0	2
33	e	0	2
33	g	0	2
All	All	0	41

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	399	CYS	CB-SG	-24.10	1.41	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	444	CYS	CB-SG	-22.82	1.43	1.82
24	n	454	CYS	CB-SG	-19.98	1.48	1.82
24	n	218	CYS	CB-SG	-19.56	1.49	1.82
24	n	352	CYS	CB-SG	-18.84	1.50	1.82
24	n	198	CYS	CB-SG	-17.69	1.52	1.82
23	v	712	CYS	CB-SG	-17.09	1.53	1.82
7	B	98	A	O3'-P	-11.86	1.47	1.61
5	L	1096	C	O3'-P	-9.98	1.49	1.61
8	N	102	A	O3'-P	-9.15	1.50	1.61
23	v	718	SER	CB-OG	8.60	1.53	1.42
23	v	723	SER	CB-OG	8.51	1.53	1.42
4	E	84	C	O3'-P	-8.03	1.51	1.61
23	v	714	SER	CB-OG	7.93	1.52	1.42
24	n	440	SER	CB-OG	7.88	1.52	1.42
23	v	681	SER	CB-OG	7.79	1.52	1.42
24	n	248	SER	CB-OG	7.58	1.52	1.42
5	L	59	C	C1'-N1	7.51	1.60	1.48
5	L	1096	C	C1'-N1	7.50	1.59	1.48
5	L	71	C	C1'-N1	7.47	1.59	1.48
35	b	46	SER	CB-OG	7.43	1.51	1.42
5	L	82	C	C1'-N1	7.43	1.59	1.48
5	L	84	C	C1'-N1	7.38	1.59	1.48
24	n	381	SER	CB-OG	7.37	1.51	1.42
5	L	1118	U	C1'-N1	7.36	1.59	1.48
5	L	1120	G	C1'-N9	-7.30	1.36	1.46
35	b	45	SER	CB-OG	7.29	1.51	1.42
8	N	101	U	C2-N3	-7.20	1.32	1.37
24	n	246	LEU	CA-CB	-7.09	1.37	1.53
34	a	33	SER	CB-OG	7.03	1.51	1.42
35	b	6	SER	CB-OG	7.00	1.51	1.42
35	b	69	ASP	CA-CB	-6.97	1.38	1.53
5	L	63	U	C1'-N1	6.95	1.59	1.48
5	L	97	U	C1'-N1	6.92	1.59	1.48
5	L	99	U	C1'-N1	6.91	1.59	1.48
23	v	633	SER	CB-OG	6.89	1.51	1.42
5	L	98	U	C1'-N1	6.88	1.59	1.48
5	L	107	U	C1'-N1	6.87	1.59	1.48
5	L	101	U	C1'-N1	6.86	1.59	1.48
5	L	54	U	C1'-N1	6.85	1.59	1.48
5	L	56	U	C1'-N1	6.85	1.59	1.48
5	L	26	G	O3'-P	-6.84	1.52	1.61
5	L	102	U	C1'-N1	6.80	1.58	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	68	U	C1'-N1	6.80	1.58	1.48
5	L	73	U	C1'-N1	6.79	1.58	1.48
5	L	1111	U	C1'-N1	6.79	1.58	1.48
5	L	1119	C	C1'-N1	6.78	1.58	1.48
5	L	83	U	C1'-N1	6.77	1.58	1.48
5	L	1101	C	C1'-N1	6.77	1.58	1.48
24	n	415	SER	CB-OG	6.66	1.50	1.42
17	c	202	LYS	C-N	-6.63	1.21	1.34
24	n	268	SER	CB-OG	6.58	1.50	1.42
5	L	1115	G	C1'-N9	-6.54	1.37	1.46
6	M	501	A	C6-N1	-6.41	1.31	1.35
6	M	502	C	O3'-P	6.34	1.68	1.61
5	L	62	C	C1'-N1	6.33	1.58	1.48
5	L	104	C	C1'-N1	6.29	1.58	1.48
5	L	72	C	C1'-N1	6.25	1.58	1.48
5	L	74	C	C1'-N1	6.24	1.58	1.48
8	N	102	A	N3-C4	-6.16	1.31	1.34
15	T	148	CYS	CB-SG	-6.15	1.71	1.82
5	L	1109	C	C1'-N1	6.05	1.57	1.48
24	n	220	SER	CB-OG	5.98	1.50	1.42
35	b	42	SER	CB-OG	5.94	1.50	1.42
24	n	388	SER	CB-OG	5.88	1.49	1.42
24	n	403	SER	CB-OG	5.85	1.49	1.42
35	b	102	THR	CB-OG1	5.78	1.54	1.43
23	v	640	SER	CB-OG	5.73	1.49	1.42
24	n	351	PHE	CB-CG	-5.70	1.41	1.51
5	L	121	C	C1'-N1	5.67	1.57	1.48
35	b	15	TYR	CB-CG	-5.64	1.43	1.51
5	L	1112	G	C1'-N9	-5.58	1.39	1.46
35	b	51	THR	CB-OG1	5.57	1.54	1.43
8	N	102	A	C6-N1	-5.57	1.31	1.35
5	L	34	G	O3'-P	-5.50	1.54	1.61
24	n	275	TYR	CB-CG	-5.47	1.43	1.51
1	A	1206	CYS	C-N	-5.45	1.21	1.34
24	n	432	VAL	CB-CG1	-5.41	1.41	1.52
1	A	902	PRO	N-CD	5.36	1.55	1.47
12	Q	215	PRO	N-CD	5.35	1.55	1.47
1	A	899	PRO	N-CD	5.33	1.55	1.47
8	N	102	A	C5-C4	-5.32	1.35	1.38
23	v	685	GLU	CB-CG	-5.32	1.42	1.52
34	a	75	THR	CB-OG1	5.21	1.53	1.43
34	a	110	THR	CB-OG1	5.17	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	175	PRO	N-CD	5.17	1.55	1.47
11	P	135	VAL	C-N	-5.16	1.22	1.34
14	S	7	PRO	N-CD	5.11	1.55	1.47
24	n	291	HIS	CA-CB	-5.07	1.42	1.53
34	a	65	PHE	CB-CG	-5.07	1.42	1.51
2	C	464	PRO	N-CD	5.06	1.54	1.47
35	b	153	THR	CB-OG1	5.05	1.53	1.43

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	PRO	O-C-N	-28.27	77.47	122.70
6	M	502	C	O3'-P-O5'	-12.66	79.95	104.00
5	L	1110	U	C5-C4-O4	12.01	133.11	125.90
6	M	502	C	P-O3'-C3'	11.50	133.50	119.70
5	L	1107	C	N1-C2-O2	-10.12	112.83	118.90
16	Z	42	ARG	NE-CZ-NH2	9.67	125.14	120.30
6	M	502	C	OP1-P-O3'	9.22	125.49	105.20
1	A	483	PRO	CA-C-N	8.96	136.92	117.20
16	Z	22	ARG	NE-CZ-NH2	8.95	124.77	120.30
5	L	1109	C	O4'-C1'-N1	8.86	115.29	108.20
35	b	44	PRO	N-CA-CB	8.83	113.89	103.30
8	N	101	U	C5-C6-N1	-8.48	118.46	122.70
5	L	1112	G	P-O3'-C3'	8.30	129.66	119.70
5	L	1107	C	C5'-C4'-O4'	-8.27	99.18	109.10
8	N	101	U	N1-C2-N3	8.16	119.80	114.90
5	L	1110	U	N3-C4-O4	-8.13	113.71	119.40
5	L	1107	C	N3-C2-O2	7.56	127.19	121.90
5	L	1107	C	P-O3'-C3'	7.54	128.75	119.70
5	L	1110	U	N1-C2-O2	7.44	128.01	122.80
24	n	428	PRO	N-CA-CB	7.35	112.12	103.30
35	b	5	PRO	N-CA-CB	7.27	112.03	103.30
35	b	42	SER	N-CA-CB	-7.24	99.64	110.50
5	L	68	U	OP2-P-O3'	7.23	121.10	105.20
5	L	99	U	OP2-P-O3'	7.23	121.10	105.20
5	L	59	C	OP2-P-O3'	7.22	121.09	105.20
5	L	97	U	OP2-P-O3'	7.22	121.09	105.20
5	L	102	U	OP2-P-O3'	7.22	121.09	105.20
5	L	74	C	OP2-P-O3'	7.22	121.09	105.20
5	L	56	U	OP2-P-O3'	7.22	121.08	105.20
5	L	69	G	OP2-P-O3'	7.22	121.08	105.20
5	L	70	A	OP2-P-O3'	7.22	121.08	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	55	G	OP2-P-O3'	7.22	121.08	105.20
5	L	54	U	OP2-P-O3'	7.22	121.08	105.20
5	L	78	G	OP2-P-O3'	7.22	121.08	105.20
5	L	81	G	OP2-P-O3'	7.22	121.08	105.20
5	L	103	A	OP2-P-O3'	7.22	121.08	105.20
5	L	104	C	OP2-P-O3'	7.22	121.08	105.20
5	L	67	A	OP2-P-O3'	7.21	121.07	105.20
5	L	100	G	OP2-P-O3'	7.21	121.07	105.20
5	L	82	C	OP2-P-O3'	7.21	121.07	105.20
5	L	101	U	OP2-P-O3'	7.21	121.06	105.20
5	L	105	A	OP2-P-O3'	7.21	121.07	105.20
5	L	66	A	OP2-P-O3'	7.21	121.06	105.20
5	L	71	C	OP2-P-O3'	7.21	121.06	105.20
5	L	57	A	OP2-P-O3'	7.21	121.06	105.20
5	L	83	U	OP2-P-O3'	7.21	121.06	105.20
5	L	96	A	OP2-P-O3'	7.21	121.06	105.20
5	L	62	C	OP2-P-O3'	7.21	121.05	105.20
5	L	73	U	OP2-P-O3'	7.21	121.05	105.20
5	L	80	G	OP2-P-O3'	7.21	121.06	105.20
5	L	98	U	OP2-P-O3'	7.21	121.05	105.20
5	L	79	A	OP2-P-O3'	7.20	121.05	105.20
5	L	61	A	OP2-P-O3'	7.20	121.05	105.20
5	L	106	A	OP2-P-O3'	7.20	121.04	105.20
5	L	58	A	OP2-P-O3'	7.20	121.04	105.20
5	L	60	A	OP2-P-O3'	7.19	121.01	105.20
5	L	72	C	OP2-P-O3'	7.19	121.01	105.20
8	N	101	U	C2-N1-C1'	-7.12	109.16	117.70
5	L	1111	U	P-O5'-C5'	-7.11	109.53	120.90
8	N	101	U	C2-N3-C4	-7.08	122.75	127.00
16	Z	108	ARG	NE-CZ-NH2	7.03	123.81	120.30
5	L	1110	U	N3-C2-O2	-6.95	117.33	122.20
5	L	1108	A	O4'-C1'-N9	-6.94	102.65	108.20
5	L	71	C	O3'-P-O5'	-6.80	91.08	104.00
5	L	104	C	O3'-P-O5'	-6.80	91.08	104.00
5	L	70	A	O3'-P-O5'	-6.80	91.08	104.00
5	L	54	U	O3'-P-O5'	-6.79	91.10	104.00
5	L	73	U	O3'-P-O5'	-6.79	91.10	104.00
5	L	78	G	O3'-P-O5'	-6.79	91.10	104.00
5	L	80	G	O3'-P-O5'	-6.79	91.10	104.00
5	L	106	A	O3'-P-O5'	-6.79	91.10	104.00
5	L	79	A	O3'-P-O5'	-6.79	91.10	104.00
5	L	81	G	O3'-P-O5'	-6.79	91.10	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	U	N3-C2-O2	-6.79	117.45	122.20
5	L	82	C	O3'-P-O5'	-6.78	91.11	104.00
5	L	83	U	O3'-P-O5'	-6.78	91.11	104.00
5	L	57	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	102	U	O3'-P-O5'	-6.78	91.12	104.00
5	L	58	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	67	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	74	C	O3'-P-O5'	-6.78	91.12	104.00
5	L	56	U	O3'-P-O5'	-6.78	91.12	104.00
5	L	66	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	99	U	O3'-P-O5'	-6.78	91.13	104.00
5	L	103	A	O3'-P-O5'	-6.78	91.13	104.00
5	L	105	A	O3'-P-O5'	-6.78	91.13	104.00
5	L	72	C	O3'-P-O5'	-6.77	91.13	104.00
5	L	59	C	O3'-P-O5'	-6.77	91.13	104.00
5	L	96	A	O3'-P-O5'	-6.77	91.13	104.00
5	L	98	U	O3'-P-O5'	-6.77	91.13	104.00
5	L	68	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	101	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	55	G	O3'-P-O5'	-6.77	91.14	104.00
5	L	97	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	100	G	O3'-P-O5'	-6.77	91.14	104.00
5	L	61	A	O3'-P-O5'	-6.76	91.15	104.00
5	L	62	C	O3'-P-O5'	-6.76	91.15	104.00
5	L	69	G	O3'-P-O5'	-6.76	91.15	104.00
5	L	60	A	O3'-P-O5'	-6.76	91.16	104.00
35	b	12	PRO	N-CA-CB	6.67	111.31	103.30
23	v	617	PRO	CA-CB-CG	6.62	117.37	104.80
23	v	613	PRO	N-CA-CB	6.53	111.13	103.30
23	v	722	PRO	N-CA-CB	6.49	111.09	103.30
35	b	4	THR	N-CA-CB	-6.31	98.31	110.30
35	b	57	LEU	N-CA-CB	6.31	123.01	110.40
10	O	443	ASN	C-N-CD	6.29	141.62	128.40
16	Z	149	ARG	NE-CZ-NH2	6.19	123.40	120.30
24	n	257	PRO	N-CA-CB	6.18	110.72	103.30
24	n	159	PRO	N-CA-CB	6.16	110.70	103.30
24	n	373	PRO	N-CA-CB	6.14	110.67	103.30
1	A	1882	LEU	C-N-CA	-6.13	106.38	121.70
24	n	208	PRO	N-CA-CB	6.12	110.64	103.30
3	D	79	C	C2-N1-C1'	6.02	125.42	118.80
24	n	424	PRO	N-CA-CB	6.02	110.52	103.30
23	v	641	PRO	CA-CB-CG	5.98	116.16	104.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	458	ILE	C-N-CD	5.97	140.95	128.40
23	v	616	PRO	N-CA-CB	5.96	110.45	103.30
35	b	7	ILE	CA-CB-CG1	5.95	122.31	111.00
35	b	141	ARG	CD-NE-CZ	5.93	131.90	123.60
8	N	101	U	N3-C4-O4	-5.91	115.26	119.40
5	L	1107	C	C5-C4-N4	-5.88	116.08	120.20
1	A	1419	ASP	CB-CG-OD1	5.84	123.55	118.30
5	L	1111	U	C5'-C4'-C3'	-5.83	106.67	116.00
5	L	1110	U	O3'-P-O5'	-5.80	92.99	104.00
24	n	162	PRO	N-CA-CB	5.79	110.25	103.30
24	n	373	PRO	CA-CB-CG	5.78	115.79	104.80
2	C	656	LEU	CA-CB-CG	-5.77	102.03	115.30
26	t	105	PRO	CA-CB-CG	5.77	115.76	104.80
2	C	463	THR	C-N-CD	5.75	140.48	128.40
16	Z	53	ARG	NE-CZ-NH2	5.75	123.18	120.30
24	n	327	PRO	N-CA-CB	5.70	110.14	103.30
24	n	436	PRO	N-CA-CB	5.69	110.13	103.30
24	n	436	PRO	CA-CB-CG	5.64	115.51	104.80
35	b	68	PRO	N-CA-CB	5.63	110.06	103.30
8	N	101	U	C6-N1-C1'	5.61	129.05	121.20
1	A	901	PRO	C-N-CD	5.60	140.16	128.40
8	N	101	U	C5-C4-O4	5.58	129.25	125.90
24	n	260	PRO	N-CA-CB	5.57	109.98	103.30
33	e	81	GLY	CA-C-N	-5.57	104.96	117.20
1	A	898	ILE	C-N-CD	5.55	140.05	128.40
24	n	306	SER	N-CA-CB	-5.54	102.19	110.50
33	g	81	GLY	CA-C-N	-5.53	105.03	117.20
4	E	77	G	C6-C5-N7	-5.49	127.11	130.40
26	t	77	PRO	CA-CB-CG	5.31	114.89	104.80
4	E	58	C	C2-N1-C1'	5.28	124.61	118.80
24	n	340	PRO	N-CA-CB	5.28	109.63	103.30
5	L	1113	U	O4'-C1'-C2'	-5.27	100.53	105.80
8	N	102	A	OP2-P-O3'	5.25	116.76	105.20
25	r	62	LEU	CA-CB-CG	-5.22	103.28	115.30
35	b	71	SER	N-CA-CB	-5.22	102.67	110.50
8	N	102	A	P-O3'-C3'	-5.21	113.45	119.70
18	d	36	ASP	CB-CG-OD2	5.19	122.97	118.30
29	h	74	ARG	NE-CZ-NH1	5.18	122.89	120.30
4	E	55	G	N3-C4-N9	5.17	129.10	126.00
16	Z	42	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
5	L	1119	C	OP1-P-OP2	-5.16	111.86	119.60
16	Z	62	ASP	CB-CG-OD1	5.16	122.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	295	SER	N-CA-CB	-5.14	102.79	110.50
23	v	617	PRO	N-CA-CB	5.11	109.44	103.30
33	e	82	LYS	N-CA-C	5.09	124.75	111.00
34	a	33	SER	N-CA-CB	5.08	118.12	110.50
33	g	82	LYS	N-CA-C	5.07	124.70	111.00
29	w	74	ARG	NE-CZ-NH1	5.07	122.84	120.30
34	a	46	VAL	CA-CB-CG2	5.07	118.51	110.90
35	b	107	SER	N-CA-CB	-5.04	102.93	110.50
3	D	90	C	C5-C6-N1	5.01	123.50	121.00
5	L	1096	C	OP2-P-O3'	5.01	116.22	105.20

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1346	PHE	Peptide
1	A	1375	LEU	Peptide
1	A	1377	SER	Peptide
1	A	257	ASN	Peptide
1	A	483	PRO	Mainchain
1	A	539	PRO	Peptide
1	A	773	SER	Peptide
2	C	170	LEU	Peptide
2	C	534	THR	Peptide
20	G	16	LEU	Peptide
10	O	123	PRO	Peptide
10	O	263	VAL	Peptide
10	O	278	ASP	Peptide
10	O	435	GLU	Peptide
10	O	436	SER	Peptide
10	O	437	GLU	Peptide
11	P	85	SER	Peptide
12	Q	103	GLU	Peptide
12	Q	291	ILE	Peptide
12	Q	45	HIS	Peptide
16	Z	211	GLY	Peptide
16	Z	219	SER	Peptide
16	Z	227	TYR	Sidechain
16	Z	232	GLU	Peptide
16	Z	241	ASN	Peptide
17	c	81	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
33	e	81	GLY	Mainchain,Peptide
33	g	81	GLY	Mainchain,Peptide
30	j	41	ASP	Peptide
31	l	81	ALA	Mainchain,Peptide
24	n	290	ASP	Peptide
24	n	305	GLY	Peptide
24	n	67	GLY	Mainchain,Peptide
30	x	41	ASP	Peptide
31	y	81	ALA	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15775	0	15756	707	0
2	C	7019	0	7201	312	0
3	D	2465	0	1251	53	0
4	E	2192	0	1106	112	0
5	L	2673	0	1360	281	0
6	M	608	0	307	44	0
7	B	275	0	137	20	0
8	N	312	0	156	18	0
9	J	190	0	186	15	0
10	O	2646	0	2639	131	0
11	P	1583	0	1608	79	0
12	Q	1472	0	1485	173	0
13	R	2089	0	2053	116	0
14	S	560	0	545	68	0
15	T	1291	0	1312	44	0
16	Z	3651	0	3707	180	0
17	c	2971	0	2336	0	0
18	d	3590	0	2359	0	0
19	F	937	0	962	54	0
20	G	342	0	360	16	0
21	H	810	0	799	37	0
22	I	822	0	845	62	0
23	v	3580	0	1298	0	0
24	n	1890	0	1407	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	o	830	0	663	0	0
25	p	843	0	675	0	0
25	q	2345	0	1636	0	0
25	r	823	0	654	0	0
26	t	926	0	606	0	0
27	k	631	0	670	0	0
27	s	610	0	640	0	0
28	i	575	0	597	0	0
28	u	575	0	597	0	0
29	h	554	0	556	0	0
29	w	554	0	556	0	0
30	j	529	0	557	0	0
30	x	529	0	557	0	0
31	l	625	0	647	0	0
31	y	625	0	647	0	0
32	m	644	0	686	0	0
32	z	644	0	686	0	0
33	e	528	0	573	0	0
33	g	741	0	778	0	0
34	a	513	0	402	0	0
35	b	841	0	614	0	0
36	C	32	0	12	1	0
37	C	1	0	0	0	0
37	E	5	0	0	0	0
38	F	1	0	0	0	0
38	Q	2	0	0	0	0
38	R	1	0	0	0	0
38	T	3	0	0	0	0
All	All	75273	0	65184	2096	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 19.

All (2096) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:HB3	16:Z:201:ARG:CG	1.38	1.50
1:A:1327:THR:CG2	5:L:35:U:H5'	1.41	1.48
1:A:1327:THR:HG22	5:L:35:U:C5'	1.47	1.44
5:L:15:C:H1'	5:L:16:U:C5	1.50	1.42
16:Z:192:GLU:CA	16:Z:195:GLU:OE2	1.70	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:170:HIS:CE1	16:Z:174:TRP:CZ3	2.20	1.30
12:Q:215:PRO:HB3	13:R:171:ASP:OD1	1.28	1.29
2:C:468:LEU:CD1	2:C:492:LEU:N	1.98	1.27
1:A:1904:ARG:HA	6:M:492:U:OP1	1.35	1.25
16:Z:192:GLU:HA	16:Z:195:GLU:OE2	1.08	1.25
1:A:426:PRO:CB	16:Z:201:ARG:HG3	1.66	1.22
12:Q:212:ALA:O	13:R:237:ARG:NH2	1.71	1.22
1:A:512:GLU:OE1	7:B:89:A:N1	1.73	1.21
16:Z:170:HIS:CE1	16:Z:174:TRP:HZ3	1.59	1.20
2:C:462:SER:O	2:C:464:PRO:HD3	1.39	1.19
5:L:14:C:C2'	5:L:15:C:H5'	1.75	1.17
16:Z:177:LEU:CD2	16:Z:194:LEU:HD21	1.76	1.15
5:L:5:A:C5'	22:I:114:THR:HG21	1.76	1.14
5:L:15:C:H41	22:I:209:ARG:CG	1.60	1.14
1:A:899:PRO:HD3	1:A:1006:ARG:HH22	1.03	1.14
5:L:1111:U:C6	5:L:1111:U:H5''	1.86	1.11
2:C:468:LEU:HD12	2:C:491:GLY:CA	1.80	1.11
1:A:928:ARG:NH2	5:L:32:G:C8	2.18	1.10
5:L:5:A:H5'	22:I:114:THR:CG2	1.80	1.09
16:Z:170:HIS:CE1	16:Z:174:TRP:CE3	2.41	1.08
12:Q:49:SER:OG	12:Q:52:SER:CB	2.00	1.08
16:Z:178:ARG:HG3	16:Z:198:PHE:CE2	1.87	1.08
2:C:126:MET:CE	2:C:132:ARG:NH1	2.17	1.07
16:Z:178:ARG:CB	16:Z:198:PHE:HZ	1.68	1.07
16:Z:181:LEU:HG	16:Z:194:LEU:HD13	1.37	1.06
2:C:468:LEU:HD12	2:C:491:GLY:HA3	1.27	1.06
5:L:1102:C:H2'	5:L:1103:C:C6	1.91	1.05
16:Z:177:LEU:HD22	16:Z:194:LEU:HD21	1.35	1.04
14:S:134:GLY:O	14:S:135:ARG:HB2	1.54	1.04
1:A:899:PRO:HD3	1:A:1006:ARG:NH2	1.73	1.04
5:L:20:G:H21	14:S:6:ARG:CB	1.70	1.04
5:L:1116:A:H2'	5:L:1117:G:H8	1.18	1.04
1:A:512:GLU:OE2	7:B:89:A:N6	1.90	1.03
15:T:120:CYS:HB2	15:T:122:CYS:HB3	1.37	1.03
5:L:14:C:H2'	5:L:15:C:C5'	1.89	1.03
4:E:29:U:H2'	4:E:30:G:H5'	1.41	1.03
1:A:426:PRO:CB	16:Z:201:ARG:CG	2.29	1.03
2:C:286:LEU:HD21	16:Z:183:THR:HG22	1.39	1.02
16:Z:174:TRP:CZ2	16:Z:197:LEU:HD11	1.93	1.02
1:A:431:ILE:HG23	16:Z:182:GLN:HG2	1.41	1.02
3:D:165:A:H4'	3:D:166:U:C5'	1.89	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:149:ARG:HH11	16:Z:193:SER:HB3	1.25	1.02
1:A:905:TYR:HE2	1:A:907:ASN:HB2	1.23	1.01
5:L:33:U:OP1	20:G:17:MET:HG3	1.60	1.01
16:Z:149:ARG:HH11	16:Z:193:SER:CB	1.73	1.01
1:A:1904:ARG:CA	6:M:492:U:OP1	2.08	1.01
4:E:52:G:H21	14:S:5:HIS:CE1	1.77	1.00
5:L:110:A:C4'	5:L:111:C:H5'	1.92	1.00
5:L:110:A:H4'	5:L:111:C:C5'	1.89	1.00
16:Z:149:ARG:NH1	16:Z:193:SER:HB3	1.77	1.00
3:D:165:A:C4'	3:D:166:U:H5'	1.92	1.00
5:L:1116:A:H2'	5:L:1117:G:C8	1.95	1.00
1:A:899:PRO:CD	1:A:1006:ARG:HH22	1.74	1.00
2:C:177:TYR:CE1	2:C:548:ARG:HG3	1.97	1.00
12:Q:226:LEU:CD1	12:Q:227:LEU:HD23	1.91	0.99
5:L:1097:G:N2	5:L:1119:C:O2	1.96	0.99
16:Z:181:LEU:HD21	16:Z:191:ARG:HG3	1.44	0.99
11:P:174:ASN:HD21	11:P:177:GLY:CA	1.76	0.98
14:S:4:SER:O	14:S:6:ARG:HD3	1.63	0.98
16:Z:178:ARG:CG	16:Z:198:PHE:CZ	2.46	0.98
12:Q:215:PRO:CB	13:R:171:ASP:OD1	2.11	0.98
16:Z:170:HIS:HE1	16:Z:174:TRP:CZ3	1.70	0.98
2:C:126:MET:SD	2:C:132:ARG:NH1	2.37	0.97
5:L:15:C:C1'	5:L:16:U:C5	2.47	0.97
12:Q:226:LEU:HD21	12:Q:262:PHE:CD1	2.00	0.97
4:E:65:U:O2'	4:E:67:C:OP2	1.81	0.97
1:A:512:GLU:CD	7:B:89:A:H61	1.67	0.97
1:A:426:PRO:HB3	16:Z:201:ARG:HG2	1.45	0.97
11:P:174:ASN:HD21	11:P:177:GLY:HA2	1.27	0.97
5:L:33:U:OP1	20:G:17:MET:CG	2.13	0.96
2:C:468:LEU:HD11	2:C:492:LEU:N	1.78	0.96
5:L:15:C:N4	22:I:209:ARG:HB2	1.80	0.96
12:Q:212:ALA:HB1	13:R:237:ARG:HH12	1.30	0.96
12:Q:216:GLU:OE2	12:Q:240:LEU:HG	1.64	0.96
5:L:1116:A:C2	5:L:1117:G:C4	2.54	0.95
5:L:15:C:H1'	5:L:16:U:H5	1.28	0.95
1:A:899:PRO:CD	1:A:1006:ARG:NH2	2.28	0.95
12:Q:226:LEU:HD11	12:Q:227:LEU:HD23	1.49	0.95
12:Q:226:LEU:CG	12:Q:227:LEU:HD23	1.97	0.94
16:Z:199:GLU:O	16:Z:202:GLN:HG2	1.67	0.94
2:C:468:LEU:HD12	2:C:492:LEU:N	1.79	0.94
2:C:734:CYS:HG	2:C:755:TYR:HH	0.95	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1111:U:H6	5:L:1111:U:H5''	1.25	0.94
3:D:96:U:H3	7:B:99:G:H22	1.05	0.93
5:L:1102:C:H2'	5:L:1103:C:C5	2.03	0.93
6:M:498:C:O2'	21:H:2:SER:HA	1.67	0.93
1:A:902:PRO:HD2	1:A:905:TYR:HD1	1.34	0.93
1:A:972:MET:HE1	6:M:505:A:C2	2.03	0.93
5:L:14:C:H2'	5:L:15:C:H5'	0.93	0.93
5:L:1116:A:C6	5:L:1117:G:C6	2.57	0.93
5:L:15:C:H41	22:I:209:ARG:HG2	1.32	0.92
1:A:1327:THR:HG22	5:L:35:U:H5''	1.50	0.92
4:E:31:G:O6	12:Q:47:LYS:NZ	2.02	0.92
5:L:5:A:H5'	22:I:114:THR:CB	2.00	0.92
12:Q:49:SER:OG	12:Q:52:SER:HB2	1.68	0.92
12:Q:214:ILE:HD11	12:Q:218:LYS:CG	1.99	0.91
5:L:1099:G:C5	5:L:1100:A:C8	2.58	0.91
1:A:972:MET:HE1	6:M:505:A:H2	1.35	0.91
6:M:498:C:OP1	19:F:41:ILE:HD11	1.70	0.91
1:A:140:ARG:O	1:A:144:ASN:HB2	1.71	0.90
5:L:15:C:O2'	5:L:16:U:H5''	1.71	0.90
4:E:89:U:H5'	5:L:17:U:OP2	1.71	0.90
5:L:20:G:H21	14:S:6:ARG:HB2	1.37	0.90
1:A:312:TYR:O	1:A:319:ARG:NH2	2.05	0.90
5:L:110:A:H4'	5:L:111:C:H5'	0.95	0.89
5:L:15:C:O2'	5:L:16:U:C6	2.23	0.89
12:Q:255:SER:OG	12:Q:257:GLU:HG2	1.70	0.89
2:C:468:LEU:CD1	2:C:492:LEU:H	1.79	0.89
16:Z:178:ARG:HG3	16:Z:198:PHE:HE2	1.33	0.89
4:E:63:G:O2'	14:S:8:GLN:HG3	1.72	0.89
1:A:900:PHE:CD2	1:A:901:PRO:HD2	2.06	0.89
5:L:15:C:N4	22:I:209:ARG:CG	2.35	0.89
1:A:1327:THR:HG22	5:L:35:U:H5'	0.90	0.89
5:L:5:A:H5'	22:I:114:THR:HG21	1.37	0.89
12:Q:242:VAL:O	13:R:161:ARG:NH2	2.05	0.89
16:Z:192:GLU:HA	16:Z:195:GLU:CD	1.91	0.89
1:A:928:ARG:HG2	5:L:30:A:N3	1.89	0.88
4:E:88:U:H5''	5:L:17:U:H5	1.37	0.88
10:O:152:ASN:HD21	10:O:409:LYS:HB3	1.39	0.88
5:L:1099:G:C6	5:L:1100:A:N7	2.41	0.88
1:A:905:TYR:HB3	1:A:908:ASP:HB2	1.56	0.88
11:P:174:ASN:ND2	11:P:177:GLY:HA2	1.89	0.87
5:L:5:A:P	22:I:114:THR:HG21	2.14	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LEU:HD11	14:S:8:GLN:NE2	1.89	0.87
2:C:468:LEU:HD12	2:C:491:GLY:C	1.94	0.87
12:Q:212:ALA:HB1	13:R:237:ARG:NH1	1.90	0.87
2:C:206:LYS:HD3	2:C:208:ARG:HE	1.40	0.86
1:A:737:ARG:HH11	1:A:737:ARG:HG2	1.37	0.86
5:L:1099:G:N7	5:L:1100:A:C8	2.43	0.86
2:C:126:MET:HE3	2:C:132:ARG:NH1	1.87	0.86
4:E:63:G:N2	14:S:6:ARG:HG2	1.90	0.85
4:E:84:C:O2'	4:E:85:C:OP1	1.94	0.85
4:E:50:G:N3	19:F:65:ASN:ND2	2.24	0.85
1:A:972:MET:CE	6:M:505:A:C2	2.57	0.85
3:D:165:A:H4'	3:D:166:U:H5'	0.95	0.85
16:Z:178:ARG:CB	16:Z:198:PHE:CZ	2.58	0.85
5:L:1099:G:C5	5:L:1100:A:N7	2.44	0.85
10:O:223:HIS:ND1	10:O:245:ASP:OD2	2.10	0.84
16:Z:178:ARG:HA	16:Z:198:PHE:CZ	2.12	0.84
5:L:15:C:N4	22:I:209:ARG:CB	2.39	0.84
12:Q:37:CYS:HB3	12:Q:64:CYS:SG	2.16	0.84
16:Z:170:HIS:NE2	16:Z:174:TRP:CZ3	2.45	0.84
5:L:18:U:O2'	5:L:19:U:OP2	1.95	0.84
5:L:20:G:N2	14:S:6:ARG:CB	2.38	0.84
4:E:31:G:O6	12:Q:47:LYS:CE	2.25	0.84
12:Q:226:LEU:HG	12:Q:227:LEU:HD23	1.59	0.84
16:Z:181:LEU:HG	16:Z:194:LEU:CD1	2.07	0.84
16:Z:192:GLU:N	16:Z:192:GLU:OE1	2.11	0.84
16:Z:152:ILE:HD13	16:Z:194:LEU:HA	1.60	0.84
1:A:1870:VAL:HB	5:L:46:C:H4'	1.59	0.83
16:Z:197:LEU:O	16:Z:197:LEU:HD12	1.77	0.83
4:E:63:G:HO2'	14:S:8:GLN:HG3	1.43	0.83
1:A:1323:SER:O	1:A:1370:ARG:NH2	2.11	0.83
2:C:697:ARG:NH1	2:C:852:THR:OG1	2.12	0.83
19:F:4:ARG:HH12	19:F:5:LYS:HZ2	1.23	0.83
1:A:1851:PHE:O	1:A:1881:THR:HA	1.77	0.83
1:A:972:MET:CE	6:M:505:A:N1	2.42	0.83
1:A:426:PRO:HG2	16:Z:201:ARG:NE	1.94	0.83
8:N:113:U:C6	13:R:183:PHE:CE2	2.67	0.83
5:L:18:U:OP1	22:I:199:LYS:NZ	2.11	0.83
5:L:15:C:H1'	5:L:16:U:C6	2.13	0.83
1:A:1642:LYS:HE3	19:F:7:ILE:HA	1.58	0.82
16:Z:178:ARG:HG3	16:Z:198:PHE:CZ	2.11	0.82
1:A:936:GLU:HG2	1:A:986:PRO:HB3	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:57:U:OP1	19:F:62:ARG:HA	1.79	0.82
15:T:27:GLU:OE2	15:T:31:ARG:NH1	2.12	0.82
2:C:286:LEU:HD23	16:Z:182:GLN:HB3	1.60	0.82
5:L:20:G:H21	14:S:6:ARG:HB3	1.45	0.82
16:Z:180:ILE:HG22	16:Z:186:LEU:HD21	1.61	0.82
5:L:15:C:N4	22:I:209:ARG:HG2	1.93	0.82
16:Z:152:ILE:CD1	16:Z:194:LEU:HA	2.09	0.82
3:D:43:G:O2'	3:D:45:A:H5'	1.78	0.82
2:C:462:SER:O	2:C:464:PRO:CD	2.26	0.82
19:F:4:ARG:HH12	19:F:5:LYS:NZ	1.77	0.82
12:Q:53:ASN:HD22	12:Q:54:ASN:H	1.26	0.82
1:A:426:PRO:CG	16:Z:201:ARG:NE	2.43	0.81
1:A:1485:ASP:O	1:A:1490:ARG:NH2	2.11	0.81
1:A:716:ARG:HD2	3:D:112:C:H1'	1.61	0.81
12:Q:209:ASN:ND2	12:Q:288:ILE:O	2.12	0.81
12:Q:49:SER:OG	12:Q:52:SER:N	2.13	0.81
15:T:31:ARG:HG3	15:T:31:ARG:HH11	1.44	0.81
16:Z:177:LEU:HD21	16:Z:194:LEU:HD21	1.61	0.81
1:A:1327:THR:CG2	5:L:35:U:C5'	2.26	0.81
4:E:88:U:H5''	5:L:17:U:C5	2.15	0.81
12:Q:207:LEU:HB2	12:Q:249:GLY:O	1.81	0.81
16:Z:178:ARG:CG	16:Z:198:PHE:CE2	2.61	0.81
16:Z:192:GLU:C	16:Z:195:GLU:OE2	2.19	0.81
12:Q:209:ASN:ND2	12:Q:288:ILE:HG22	1.95	0.81
16:Z:168:LYS:NZ	16:Z:171:ASP:HB2	1.96	0.81
4:E:63:G:O2'	14:S:8:GLN:CG	2.28	0.80
1:A:728:ASN:ND2	4:E:72:C:O2'	2.14	0.80
1:A:898:ILE:HA	1:A:1006:ARG:NH1	1.95	0.80
5:L:20:G:N2	14:S:6:ARG:HB3	1.96	0.80
6:M:498:C:C2'	6:M:499:U:H5'	2.11	0.80
2:C:126:MET:CE	2:C:132:ARG:HH12	1.94	0.80
4:E:29:U:C2'	4:E:30:G:H5'	2.11	0.80
1:A:518:VAL:HG12	1:A:685:HIS:HB3	1.62	0.80
2:C:468:LEU:CD1	2:C:491:GLY:C	2.47	0.80
12:Q:215:PRO:HG3	12:Q:217:TRP:CZ3	2.16	0.80
12:Q:56:ILE:HD12	13:R:105:ARG:NH2	1.97	0.80
12:Q:256:SER:O	12:Q:259:GLY:N	2.14	0.80
13:R:161:ARG:O	13:R:165:SER:HB3	1.82	0.80
10:O:433:THR:OG1	10:O:435:GLU:OE1	2.00	0.80
5:L:19:U:O2	11:P:176:ASN:HB2	1.82	0.80
1:A:911:ILE:HG23	1:A:997:GLN:CG	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1111:U:C6	5:L:1111:U:C5'	2.65	0.80
12:Q:222:THR:HA	12:Q:225:GLN:NE2	1.96	0.80
1:A:1696:SER:HA	1:A:1759:TYR:HE1	1.45	0.79
2:C:468:LEU:CD2	2:C:493:LEU:HD23	2.12	0.79
16:Z:178:ARG:CA	16:Z:198:PHE:HZ	1.94	0.79
5:L:1099:G:H5''	5:L:1099:G:N3	1.97	0.79
12:Q:209:ASN:O	12:Q:209:ASN:ND2	2.15	0.79
5:L:17:U:H4'	5:L:18:U:OP2	1.83	0.79
1:A:326:ASN:ND2	2:C:924:GLY:O	2.15	0.79
16:Z:180:ILE:O	16:Z:184:GLN:HB2	1.82	0.79
1:A:899:PRO:O	1:A:998:TYR:OH	2.01	0.79
5:L:18:U:H5'	5:L:18:U:H6	1.47	0.79
1:A:1044:GLY:HA3	1:A:1176:GLU:HG3	1.64	0.79
8:N:110:A:C2	13:R:46:ARG:NH1	2.47	0.78
12:Q:214:ILE:HD11	12:Q:218:LYS:HG2	1.62	0.78
5:L:15:C:H41	22:I:209:ARG:CD	1.96	0.78
1:A:928:ARG:NH2	5:L:32:G:H8	1.79	0.78
16:Z:174:TRP:CZ2	16:Z:197:LEU:CD1	2.67	0.78
13:R:25:GLN:HG3	21:H:24:GLY:HA3	1.65	0.78
12:Q:39:LEU:HD11	12:Q:111:ARG:HG3	1.65	0.78
13:R:96:GLU:OE2	13:R:187:LYS:NZ	2.17	0.78
1:A:796:ASN:ND2	1:A:861:GLN:OE1	2.17	0.78
1:A:905:TYR:HE2	1:A:907:ASN:CB	1.94	0.78
12:Q:217:TRP:CD1	13:R:187:LYS:HE2	2.18	0.78
5:L:5:A:H5'	22:I:114:THR:HB	1.66	0.78
16:Z:192:GLU:CB	16:Z:195:GLU:OE2	2.30	0.78
1:A:487:ASN:OD1	1:A:488:ARG:HG2	1.84	0.78
1:A:905:TYR:CE2	1:A:907:ASN:HB2	2.14	0.77
5:L:1100:A:H61	5:L:1116:A:H61	1.30	0.77
15:T:31:ARG:NH1	15:T:31:ARG:HG3	1.99	0.77
1:A:426:PRO:HB3	16:Z:201:ARG:HG3	0.79	0.77
1:A:1879:ILE:O	1:A:1891:LEU:HA	1.84	0.77
2:C:462:SER:C	2:C:464:PRO:HD3	2.05	0.77
5:L:1102:C:H2'	5:L:1103:C:H6	1.42	0.77
12:Q:226:LEU:HD21	12:Q:262:PHE:CE1	2.18	0.77
4:E:31:G:O6	12:Q:47:LYS:HE2	1.85	0.77
12:Q:104:ALA:HB1	12:Q:110:LYS:HB3	1.66	0.77
1:A:431:ILE:CG2	16:Z:182:GLN:HG2	2.13	0.77
4:E:29:U:OP2	12:Q:51:ARG:NH2	2.18	0.77
12:Q:56:ILE:CD1	13:R:105:ARG:NH2	2.47	0.77
1:A:1365:THR:O	1:A:1369:ASN:ND2	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:ILE:HD13	2:C:567:ILE:HG23	1.65	0.76
5:L:1100:A:N1	5:L:1116:A:N1	2.33	0.76
1:A:1906:SER:OG	6:M:493:A:OP1	2.02	0.76
6:M:498:C:H2'	6:M:499:U:H5'	1.67	0.76
1:A:900:PHE:CE2	1:A:901:PRO:HD2	2.20	0.76
2:C:365:GLU:HG3	2:C:366:ASN:H	1.49	0.76
1:A:227:GLU:OE2	1:A:231:ARG:NH1	2.18	0.76
1:A:771:PRO:O	10:O:309:ARG:NH2	2.18	0.76
1:A:484:PHE:CE1	3:D:81:A:N6	2.53	0.76
19:F:46:PRO:HG2	19:F:106:TYR:HE2	1.51	0.76
1:A:1650:ARG:NH2	6:M:495:A:C8	2.54	0.76
16:Z:178:ARG:CA	16:Z:198:PHE:CZ	2.69	0.76
1:A:900:PHE:CD2	1:A:901:PRO:CD	2.67	0.76
13:R:96:GLU:HG2	13:R:188:TYR:HE2	1.50	0.76
1:A:1403:SER:OG	1:A:1429:MET:SD	2.44	0.76
12:Q:209:ASN:HD22	12:Q:288:ILE:HG22	1.48	0.76
1:A:1889:LEU:HB2	1:A:1989:PHE:HB2	1.66	0.76
12:Q:34:CYS:HB3	12:Q:36:ILE:H	1.51	0.76
19:F:12:PRO:HG2	19:F:15:TYR:HB2	1.65	0.75
1:A:791:ARG:NH2	11:P:173:LYS:HE2	2.00	0.75
12:Q:202:THR:HA	12:Q:252:ARG:HG3	1.68	0.75
1:A:1405:ILE:HG22	1:A:1406:LEU:H	1.51	0.75
1:A:1379:MET:HE1	1:A:1620:TYR:H	1.52	0.75
12:Q:70:ILE:HD13	12:Q:84:ILE:HD11	1.69	0.75
16:Z:178:ARG:CG	16:Z:198:PHE:HZ	1.92	0.75
1:A:1051:GLU:OE1	1:A:1204:ARG:NH2	2.20	0.75
12:Q:217:TRP:CZ3	13:R:171:ASP:OD1	2.40	0.75
12:Q:34:CYS:SG	12:Q:61:CYS:N	2.60	0.75
1:A:185:GLN:HE21	1:A:263:PRO:HD3	1.52	0.75
1:A:756:LEU:HD11	14:S:8:GLN:HE22	1.52	0.75
12:Q:215:PRO:HG3	12:Q:217:TRP:CH2	2.21	0.74
5:L:15:C:HO2'	5:L:16:U:H6	1.32	0.74
2:C:234:LEU:HD21	2:C:439:ILE:HG23	1.67	0.74
5:L:15:C:H42	22:I:209:ARG:HB2	1.53	0.74
1:A:1870:VAL:HG21	5:L:46:C:H5''	1.69	0.74
1:A:1860:VAL:HA	1:A:1873:LYS:O	1.88	0.74
2:C:831:ILE:HG13	2:C:832:ASP:H	1.51	0.74
1:A:1379:MET:HG2	7:B:94:U:H1'	1.68	0.74
16:Z:174:TRP:CH2	16:Z:197:LEU:HD11	2.22	0.74
16:Z:191:ARG:NH1	16:Z:192:GLU:OE2	2.21	0.74
2:C:126:MET:CE	2:C:132:ARG:HH11	1.93	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:230:VAL:HG22	10:O:241:THR:HG22	1.70	0.74
2:C:236:LEU:HD21	2:C:435:LEU:HD11	1.70	0.73
16:Z:186:LEU:HD12	16:Z:186:LEU:N	2.03	0.73
1:A:928:ARG:HG2	5:L:30:A:C2	2.24	0.73
2:C:133:ILE:HG22	2:C:209:MET:HB3	1.70	0.73
2:C:177:TYR:CE1	2:C:548:ARG:CG	2.69	0.73
4:E:64:U:O2'	4:E:65:U:OP1	2.06	0.73
10:O:382:HIS:CE1	10:O:442:TRP:H	2.06	0.73
14:S:134:GLY:O	14:S:135:ARG:CB	2.32	0.73
2:C:468:LEU:HD21	2:C:493:LEU:HG	1.70	0.73
1:A:737:ARG:HG2	1:A:737:ARG:NH1	2.00	0.73
1:A:426:PRO:HG2	16:Z:201:ARG:CZ	2.18	0.73
1:A:426:PRO:O	16:Z:202:GLN:HB3	1.88	0.73
1:A:512:GLU:OE1	7:B:89:A:C6	2.42	0.73
2:C:340:LYS:O	2:C:343:ASP:HB3	1.89	0.73
8:N:109:U:OP2	8:N:109:U:C6	2.42	0.73
5:L:18:U:O2	22:I:206:LYS:HD2	1.88	0.73
2:C:385:PHE:HE1	2:C:425:LEU:HD11	1.54	0.72
2:C:468:LEU:CD2	2:C:493:LEU:CD2	2.67	0.72
1:A:238:ARG:NH2	1:A:1762:ASP:OD2	2.22	0.72
16:Z:167:LYS:NZ	16:Z:171:ASP:OD2	2.19	0.72
15:T:122:CYS:HB2	15:T:145:CYS:HB2	1.70	0.72
10:O:285:SER:OG	10:O:287:ASP:OD1	2.07	0.72
1:A:452:PHE:HZ	2:C:347:ARG:HG3	1.55	0.72
6:M:485:U:H5'	21:H:36:ARG:HE	1.55	0.72
4:E:66:C:H5'	4:E:66:C:C6	2.24	0.72
12:Q:259:GLY:O	12:Q:263:VAL:HG23	1.90	0.72
1:A:1650:ARG:NH2	6:M:495:A:N7	2.38	0.72
1:A:1050:LEU:O	1:A:1169:TYR:HA	1.90	0.71
1:A:607:THR:OG1	8:N:101:U:H3'	1.90	0.71
1:A:1850:LEU:HD13	1:A:1930:PRO:HB3	1.71	0.71
3:D:174:G:H4'	3:D:174:G:OP1	1.90	0.71
1:A:713:ASN:ND2	3:D:83:C:H4'	2.04	0.71
5:L:119:G:OP1	5:L:119:G:H4'	1.90	0.71
1:A:1048:VAL:HG22	1:A:1250:VAL:HG22	1.71	0.71
1:A:681:LYS:O	1:A:684:LYS:HB3	1.89	0.71
16:Z:190:LEU:HD23	16:Z:191:ARG:N	2.06	0.71
1:A:1211:SER:O	1:A:1257:ASN:ND2	2.23	0.71
1:A:416:GLU:HB3	1:A:419:THR:HG23	1.73	0.71
10:O:354:ASN:ND2	10:O:369:ASP:OD1	2.24	0.71
12:Q:212:ALA:C	13:R:237:ARG:NH2	2.43	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:655:LEU:O	2:C:658:ASP:N	2.24	0.71
6:M:495:A:OP2	6:M:495:A:O4'	2.08	0.71
12:Q:118:VAL:HG23	12:Q:119:LYS:O	1.90	0.71
8:N:110:A:H2	13:R:46:ARG:CD	2.04	0.71
4:E:63:G:O2'	14:S:8:GLN:CB	2.39	0.71
15:T:3:ARG:NH2	15:T:85:LYS:O	2.24	0.71
1:A:905:TYR:HB3	1:A:908:ASP:CB	2.20	0.70
5:L:33:U:OP1	20:G:17:MET:CB	2.39	0.70
3:D:43:G:N3	3:D:43:G:H2'	2.06	0.70
5:L:25:A:H2'	5:L:27:A:OP2	1.92	0.70
1:A:1362:LYS:NZ	9:J:13:GLY:O	2.24	0.70
1:A:1488:ILE:HG23	1:A:1489:PRO:HD3	1.72	0.70
12:Q:207:LEU:O	12:Q:248:CYS:HA	1.89	0.70
14:S:167:GLN:O	14:S:171:HIS:HB2	1.90	0.70
1:A:427:SER:HA	16:Z:202:GLN:HB2	1.73	0.70
3:D:173:U:H4'	3:D:174:G:OP1	1.91	0.70
5:L:19:U:C4	11:P:174:ASN:OD1	2.44	0.70
1:A:1431:HIS:CD2	1:A:1434:GLU:HA	2.26	0.70
1:A:911:ILE:HG23	1:A:997:GLN:HG3	1.73	0.70
5:L:15:C:H41	22:I:209:ARG:CB	2.01	0.70
12:Q:221:ASP:C	12:Q:225:GLN:HE21	1.93	0.70
12:Q:226:LEU:HD21	12:Q:262:PHE:HD1	1.57	0.70
12:Q:226:LEU:CD2	12:Q:262:PHE:CE1	2.75	0.70
12:Q:16:CYS:SG	13:R:105:ARG:NH2	2.64	0.70
4:E:84:C:O2'	14:S:4:SER:OG	2.09	0.70
5:L:1116:A:C6	5:L:1117:G:C5	2.79	0.70
5:L:69:G:H1	5:L:83:U:H3	1.40	0.70
8:N:110:A:H2	13:R:46:ARG:HH11	1.36	0.70
8:N:110:A:N3	13:R:46:ARG:NH1	2.37	0.70
1:A:140:ARG:HD2	1:A:566:GLU:OE2	1.92	0.70
22:I:195:PHE:HE1	22:I:204:ASN:HD22	1.37	0.70
12:Q:49:SER:OG	12:Q:52:SER:HB3	1.89	0.70
1:A:610:ARG:NH1	8:N:101:U:OP2	2.22	0.69
1:A:372:ARG:O	2:C:973:ARG:NH2	2.25	0.69
10:O:317:HIS:NE2	10:O:362:ASP:OD1	2.20	0.69
15:T:120:CYS:CB	15:T:122:CYS:HB3	2.18	0.69
10:O:111:ILE:HB	10:O:114:ARG:HH21	1.57	0.69
16:Z:170:HIS:CE1	16:Z:174:TRP:HE3	2.05	0.69
16:Z:194:LEU:HD22	16:Z:194:LEU:O	1.93	0.69
2:C:320:PHE:HB2	2:C:429:PHE:HD2	1.57	0.69
1:A:1161:TYR:HD1	1:A:1170:MET:HG2	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:HE1	1:A:198:ALA:HA	1.57	0.69
12:Q:209:ASN:ND2	12:Q:288:ILE:CG2	2.56	0.69
5:L:1102:C:O2	5:L:1114:G:N2	2.24	0.69
5:L:1116:A:C2	5:L:1117:G:C5	2.80	0.69
12:Q:210:ILE:HG22	12:Q:211:ASP:O	1.93	0.69
12:Q:49:SER:OG	12:Q:52:SER:CA	2.40	0.69
4:E:63:G:O2'	14:S:8:GLN:HB2	1.93	0.69
1:A:1048:VAL:HA	1:A:1249:SER:O	1.92	0.68
1:A:1043:ARG:HG3	1:A:1044:GLY:H	1.58	0.68
1:A:751:ASP:OD1	1:A:752:ALA:N	2.26	0.68
5:L:1116:A:C4	5:L:1117:G:C8	2.81	0.68
16:Z:454:ASP:HB3	16:Z:457:HIS:HD2	1.58	0.68
1:A:946:ASN:HB3	1:A:949:ASP:HB3	1.75	0.68
12:Q:53:ASN:HD22	12:Q:54:ASN:N	1.91	0.68
16:Z:170:HIS:HE1	16:Z:174:TRP:HZ3	1.14	0.68
1:A:1618:ASN:N	1:A:1744:ASP:OD2	2.26	0.68
19:F:109:GLU:HG3	19:F:110:VAL:HG12	1.74	0.68
1:A:1627:LEU:HD11	1:A:1634:LEU:HG	1.74	0.68
5:L:18:U:C5	22:I:202:GLN:CG	2.76	0.68
5:L:19:U:N3	11:P:174:ASN:OD1	2.27	0.68
1:A:1710:GLU:HG2	1:A:1728:ILE:HG12	1.75	0.68
1:A:1859:ARG:NH2	1:A:1876:ASN:O	2.26	0.68
21:H:34:ARG:HH12	21:H:36:ARG:HH11	1.41	0.68
5:L:118:U:H4'	5:L:119:G:OP1	1.91	0.68
15:T:128:GLN:O	15:T:131:GLU:N	2.26	0.68
2:C:701:GLU:HB2	2:C:841:LEU:HD22	1.76	0.68
14:S:9:LEU:O	14:S:10:GLU:HB2	1.93	0.68
1:A:1755:LYS:HE3	1:A:1759:TYR:HE2	1.58	0.68
1:A:621:LEU:HD23	1:A:722:LEU:HD21	1.76	0.68
2:C:829:VAL:HG12	2:C:830:ASN:H	1.59	0.68
2:C:662:SER:O	2:C:665:LYS:NZ	2.24	0.67
13:R:206:LEU:HD12	13:R:207:PRO:HD2	1.76	0.67
15:T:61:ARG:NH1	15:T:101:GLU:O	2.22	0.67
1:A:1049:LEU:HA	1:A:1170:MET:O	1.94	0.67
2:C:915:GLU:OE2	2:C:919:ARG:NE	2.21	0.67
10:O:275:THR:OG1	10:O:279:PRO:O	2.13	0.67
5:L:18:U:H5'	5:L:18:U:C6	2.29	0.67
5:L:20:G:C2	14:S:6:ARG:HB3	2.30	0.67
19:F:69:GLU:OE1	19:F:83:ARG:NH2	2.27	0.67
22:I:196:ILE:HB	22:I:200:ASN:ND2	2.09	0.67
5:L:1116:A:C4	5:L:1117:G:N7	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:G:O6	13:R:127:ILE:O	2.13	0.67
1:A:487:ASN:OD1	1:A:488:ARG:N	2.28	0.67
11:P:174:ASN:ND2	11:P:177:GLY:CA	2.52	0.67
16:Z:191:ARG:HE	16:Z:192:GLU:CD	1.98	0.67
1:A:1253:LYS:O	1:A:1274:ARG:NH2	2.27	0.67
1:A:972:MET:HE2	6:M:505:A:N1	2.08	0.67
10:O:391:GLU:HG3	10:O:392:MET:H	1.60	0.67
12:Q:125:ILE:C	12:Q:125:ILE:HD12	2.15	0.67
1:A:791:ARG:NH2	11:P:173:LYS:CE	2.58	0.67
1:A:992:ASP:OD2	1:A:1085:LYS:NZ	2.28	0.67
10:O:217:ILE:HG22	10:O:218:ARG:HG3	1.77	0.67
1:A:759:ARG:HH12	14:S:7:PRO:HB2	1.58	0.67
1:A:177:GLU:HB3	1:A:712:LEU:HD11	1.76	0.67
1:A:902:PRO:HD2	1:A:905:TYR:CD1	2.25	0.67
5:L:18:U:C5	22:I:202:GLN:HG2	2.29	0.67
5:L:1102:C:O5'	5:L:1102:C:H6	1.76	0.67
12:Q:82:ILE:HD11	13:R:253:LEU:HD11	1.77	0.67
1:A:1815:LEU:O	1:A:1818:ARG:N	2.28	0.67
1:A:705:GLN:HE21	1:A:709:ARG:HG3	1.60	0.67
1:A:391:TYR:OH	2:C:912:ALA:O	2.10	0.67
3:D:78:A:O2'	3:D:79:C:O5'	2.12	0.67
16:Z:462:ILE:HG12	16:Z:474:THR:HB	1.77	0.67
8:N:110:A:H2	13:R:46:ARG:HD2	1.58	0.67
10:O:362:ASP:OD2	10:O:379:LYS:NZ	2.27	0.66
12:Q:226:LEU:C	12:Q:226:LEU:HD12	2.15	0.66
16:Z:190:LEU:HD23	16:Z:190:LEU:C	2.15	0.66
1:A:213:TYR:CZ	1:A:217:TRP:CD1	2.83	0.66
2:C:292:ILE:O	2:C:296:ASN:ND2	2.29	0.66
12:Q:125:ILE:HD12	12:Q:126:THR:N	2.11	0.66
1:A:791:ARG:HH22	11:P:173:LYS:HD2	1.58	0.66
2:C:461:LYS:O	2:C:461:LYS:HD3	1.96	0.66
6:M:500:A:N3	6:M:502:C:N4	2.43	0.66
2:C:101:GLN:HE21	3:D:75:A:H61	1.42	0.66
2:C:780:PRO:HA	2:C:783:ILE:HB	1.78	0.66
16:Z:192:GLU:O	16:Z:195:GLU:OE2	2.13	0.66
1:A:1445:THR:OG1	1:A:1450:GLU:OE2	2.14	0.66
1:A:803:GLY:O	11:P:166:PRO:HG2	1.96	0.66
1:A:854:ARG:NH2	5:L:25:A:H5"	2.11	0.66
1:A:911:ILE:HG23	1:A:997:GLN:HG2	1.75	0.66
2:C:807:PRO:HG3	2:C:850:LEU:HD23	1.77	0.66
12:Q:214:ILE:CD1	12:Q:218:LYS:HG2	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:245:GLU:HA	13:R:248:ASN:HD22	1.59	0.66
16:Z:200:ILE:O	16:Z:204:ASP:N	2.27	0.66
1:A:914:LEU:HD13	1:A:1505:ASP:HB2	1.78	0.65
2:C:468:LEU:HD11	2:C:492:LEU:CA	2.26	0.65
16:Z:177:LEU:CD2	16:Z:194:LEU:CD2	2.65	0.65
1:A:1067:ASN:O	1:A:1071:ARG:HG2	1.96	0.65
1:A:416:GLU:HG2	1:A:418:ASP:H	1.60	0.65
2:C:922:THR:OG1	2:C:925:LEU:O	2.06	0.65
4:E:64:U:O2'	4:E:65:U:P	2.55	0.65
2:C:607:LEU:HD22	2:C:668:ILE:HD12	1.78	0.65
11:P:111:HIS:O	11:P:112:ILE:HG13	1.96	0.65
15:T:32:ASP:HA	15:T:35:LYS:HD3	1.77	0.65
1:A:1372:LYS:HG2	1:A:1383:PHE:CD2	2.30	0.65
1:A:1882:LEU:HD22	1:A:1991:ILE:HD11	1.78	0.65
2:C:183:GLN:HE22	2:C:654:CYS:HA	1.60	0.65
16:Z:184:GLN:HE21	16:Z:184:GLN:CA	2.09	0.65
16:Z:184:GLN:HE21	16:Z:185:GLU:H	1.43	0.65
1:A:1896:THR:HA	1:A:1899:TRP:HD1	1.62	0.65
2:C:830:ASN:HB2	2:C:834:MET:HG2	1.79	0.65
1:A:737:ARG:NH2	4:E:71:G:N7	2.45	0.65
13:R:253:LEU:O	13:R:257:ASN:HB2	1.97	0.65
19:F:14:ASP:OD1	19:F:15:TYR:N	2.30	0.65
1:A:1195:PHE:HB3	1:A:1217:ARG:HE	1.61	0.64
1:A:766:ILE:HG21	1:A:782:ILE:HG12	1.79	0.64
2:C:218:HIS:HB3	2:C:221:PHE:HD2	1.62	0.64
1:A:1051:GLU:OE2	1:A:1261:SER:N	2.24	0.64
2:C:761:ALA:HA	2:C:764:ASN:HB2	1.80	0.64
10:O:206:VAL:HG21	10:O:241:THR:HG21	1.78	0.64
4:E:63:G:H22	14:S:6:ARG:HG2	1.60	0.64
1:A:366:GLU:HG3	1:A:372:ARG:HH11	1.62	0.64
7:B:89:A:OP2	7:B:89:A:O4'	2.15	0.64
2:C:296:ASN:OD1	2:C:304:PHE:N	2.30	0.64
2:C:468:LEU:HD22	2:C:493:LEU:HD23	1.78	0.64
16:Z:188:SER:O	16:Z:192:GLU:HG2	1.96	0.64
1:A:1309:ILE:HG12	1:A:1356:LEU:HD12	1.79	0.64
4:E:63:G:N2	14:S:6:ARG:CG	2.60	0.64
16:Z:299:LEU:HD21	16:Z:343:TYR:HE1	1.61	0.64
1:A:1842:GLU:OE1	1:A:1845:ASN:ND2	2.31	0.64
1:A:907:ASN:ND2	1:A:1504:TYR:CE1	2.66	0.64
2:C:765:VAL:HG22	2:C:775:ILE:HG12	1.78	0.64
4:E:46:U:OP1	19:F:33:THR:OG1	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:5:A:OP1	22:I:114:THR:HG21	1.97	0.64
5:L:5:A:C5'	22:I:114:THR:CB	2.73	0.64
12:Q:87:ARG:NH2	12:Q:122:GLY:O	2.30	0.64
1:A:1087:ASN:ND2	1:A:1099:ASN:O	2.28	0.64
1:A:1991:ILE:HG21	1:A:2008:LEU:HD22	1.80	0.64
5:L:70:A:H61	5:L:82:C:H42	1.44	0.64
13:R:15:GLU:OE1	15:T:44:LYS:NZ	2.30	0.64
14:S:8:GLN:HG2	14:S:10:GLU:O	1.96	0.64
1:A:1338:SER:O	1:A:1341:SER:OG	2.10	0.64
5:L:20:G:N3	14:S:6:ARG:HB3	2.13	0.64
21:H:21:GLU:HG2	21:H:27:LYS:HB3	1.78	0.64
5:L:5:A:C5'	22:I:114:THR:CG2	2.50	0.64
14:S:6:ARG:HG3	14:S:6:ARG:NH1	2.13	0.63
1:A:928:ARG:CZ	5:L:32:G:C8	2.81	0.63
1:A:1535:LYS:NZ	6:M:509:U:O2'	2.20	0.63
5:L:19:U:O4	11:P:174:ASN:OD1	2.17	0.63
16:Z:177:LEU:HD21	16:Z:194:LEU:CD2	2.25	0.63
1:A:899:PRO:HD2	1:A:1006:ARG:NH2	2.12	0.63
3:D:83:C:O2'	3:D:84:A:O5'	2.15	0.63
16:Z:168:LYS:HZ3	16:Z:171:ASP:HB2	1.60	0.63
1:A:1458:TRP:HE1	1:A:1489:PRO:HD2	1.62	0.63
12:Q:226:LEU:HG	12:Q:227:LEU:CD2	2.29	0.63
15:T:121:ILE:HD11	15:T:129:LEU:HD21	1.80	0.63
1:A:645:ASP:OD1	1:A:646:ALA:N	2.32	0.63
2:C:105:ILE:HD11	3:D:44:A:N7	2.12	0.63
4:E:50:G:C4	19:F:65:ASN:ND2	2.66	0.63
5:L:33:U:OP1	20:G:17:MET:HB2	1.99	0.63
2:C:412:ALA:HA	2:C:415:TYR:CE2	2.34	0.63
1:A:512:GLU:CD	7:B:89:A:N6	2.46	0.63
1:A:581:LEU:O	1:A:585:ARG:HB2	1.99	0.63
16:Z:178:ARG:HD3	16:Z:182:GLN:HE22	1.62	0.63
16:Z:178:ARG:HB2	16:Z:198:PHE:HZ	1.58	0.63
2:C:468:LEU:CD1	2:C:491:GLY:HA3	2.16	0.63
16:Z:195:GLU:HG2	16:Z:196:THR:N	2.13	0.63
1:A:1122:ASP:OD1	1:A:1161:TYR:OH	2.16	0.63
1:A:407:VAL:O	2:C:272:ARG:NH2	2.32	0.63
12:Q:49:SER:HG	12:Q:52:SER:CB	2.12	0.63
1:A:1185:GLU:OE1	14:S:128:ARG:NH1	2.18	0.62
1:A:1696:SER:HA	1:A:1759:TYR:CE1	2.32	0.62
4:E:53:A:H5'	4:E:54:U:OP2	1.99	0.62
2:C:919:ARG:NH2	2:C:927:MET:SD	2.70	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:LEU:HD21	16:Z:183:THR:CG2	2.22	0.62
4:E:56:A:O2'	4:E:57:U:O5'	2.17	0.62
15:T:107:ARG:HH21	15:T:147:HIS:CE1	2.17	0.62
13:R:157:GLU:OE2	13:R:161:ARG:NE	2.32	0.62
4:E:66:C:H3'	4:E:66:C:H6	1.63	0.62
1:A:1073:ILE:HG23	1:A:1074:VAL:HG23	1.82	0.62
1:A:364:TYR:OH	1:A:1205:LYS:NZ	2.31	0.62
1:A:1377:SER:HA	7:B:95:U:OP1	1.98	0.62
21:H:29:TYR:O	21:H:53:GLN:NE2	2.32	0.62
5:L:19:U:N1	11:P:178:TYR:HD2	1.97	0.62
12:Q:108:MET:HA	12:Q:111:ARG:HB3	1.81	0.62
5:L:1099:G:C8	5:L:1100:A:C8	2.87	0.62
5:L:1120:G:H8	5:L:1120:G:H5''	1.65	0.62
13:R:170:ILE:HD13	13:R:173:ILE:HD11	1.81	0.62
1:A:1411:ASP:H	9:J:6:ILE:HG22	1.64	0.62
1:A:209:ILE:HB	1:A:212:VAL:HB	1.81	0.62
1:A:701:CYS:SG	1:A:702:GLY:N	2.72	0.62
3:D:31:G:H2'	3:D:32:G:H5'	1.81	0.62
12:Q:207:LEU:N	12:Q:249:GLY:O	2.31	0.62
1:A:467:GLU:O	2:C:387:TYR:OH	2.10	0.62
2:C:307:ILE:HA	2:C:324:ILE:HD11	1.82	0.62
4:E:57:U:OP1	19:F:62:ARG:HG2	1.99	0.62
13:R:161:ARG:O	13:R:165:SER:CB	2.47	0.62
5:L:1107:C:H6	5:L:1107:C:H5'	1.63	0.62
10:O:259:VAL:HG12	10:O:260:ILE:HG13	1.82	0.62
2:C:727:THR:H	2:C:736:ASP:HB2	1.64	0.61
1:A:484:PHE:CE1	3:D:81:A:C6	2.88	0.61
12:Q:61:CYS:O	12:Q:72:GLN:NE2	2.32	0.61
13:R:121:ARG:HD3	13:R:125:GLY:HA3	1.82	0.61
1:A:1563:LYS:O	1:A:1782:ASN:ND2	2.33	0.61
2:C:801:TRP:CD1	2:C:843:LYS:HD2	2.36	0.61
6:M:505:A:C3'	6:M:506:U:H4'	2.30	0.61
12:Q:215:PRO:HB2	12:Q:217:TRP:CE3	2.36	0.61
1:A:1811:ALA:O	1:A:1814:VAL:N	2.33	0.61
13:R:23:PRO:O	13:R:37:TRP:NE1	2.28	0.61
1:A:1733:TRP:CE2	1:A:1772:GLY:HA3	2.35	0.61
1:A:794:LYS:HB3	1:A:854:ARG:NH1	2.15	0.61
4:E:32:U:C4	12:Q:28:ILE:HD13	2.36	0.61
1:A:1856:ASN:ND2	1:A:1966:SER:O	2.34	0.61
22:I:196:ILE:HB	22:I:200:ASN:HD21	1.64	0.61
5:L:1116:A:N1	5:L:1117:G:C6	2.68	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:19:U:C1'	11:P:178:TYR:CE2	2.83	0.61
5:L:1098:C:H6	5:L:1098:C:O5'	1.83	0.61
13:R:255:ASN:O	13:R:259:ASN:ND2	2.34	0.61
16:Z:187:SER:OG	16:Z:190:LEU:HB3	2.00	0.61
16:Z:200:ILE:HA	16:Z:203:LYS:HB2	1.83	0.61
1:A:1447:TRP:HB3	1:A:1451:PHE:HE2	1.65	0.61
1:A:1935:VAL:HG11	1:A:1940:MET:HB2	1.83	0.61
1:A:972:MET:HE2	6:M:505:A:C2	2.36	0.61
16:Z:168:LYS:HZ2	16:Z:171:ASP:HB2	1.65	0.61
13:R:244:LEU:O	13:R:248:ASN:ND2	2.34	0.61
1:A:1624:LEU:HD21	1:A:1635:HIS:CE1	2.36	0.61
22:I:180:LYS:O	22:I:183:MET:HB2	2.01	0.61
2:C:265:PHE:HD2	2:C:295:ILE:HD12	1.66	0.60
5:L:4:A:O3'	22:I:114:THR:CG2	2.49	0.60
14:S:6:ARG:CG	14:S:6:ARG:HH11	2.14	0.60
16:Z:170:HIS:NE2	16:Z:174:TRP:CE3	2.66	0.60
2:C:472:VAL:HB	2:C:575:ALA:O	2.00	0.60
11:P:34:ILE:HG23	11:P:35:ALA:H	1.67	0.60
16:Z:364:THR:O	16:Z:368:ASN:ND2	2.32	0.60
1:A:1270:LEU:HD12	1:A:1301:TYR:HE2	1.66	0.60
2:C:108:GLN:O	2:C:109:LEU:HD12	2.01	0.60
22:I:92:ARG:N	22:I:93:GLY:HA3	2.17	0.60
16:Z:181:LEU:CD2	16:Z:191:ARG:HG3	2.26	0.60
1:A:1488:ILE:CG2	1:A:1489:PRO:HD3	2.31	0.60
2:C:177:TYR:HE1	2:C:548:ARG:HG3	1.63	0.60
2:C:794:GLN:NE2	2:C:835:LYS:HD2	2.17	0.60
3:D:96:U:H3	7:B:99:G:N2	1.89	0.60
16:Z:184:GLN:HE21	16:Z:184:GLN:HA	1.66	0.60
2:C:703:LEU:O	2:C:705:GLY:N	2.33	0.60
5:L:14:C:C2'	5:L:15:C:C5'	2.64	0.60
5:L:15:C:H41	22:I:209:ARG:HD3	1.67	0.60
11:P:134:VAL:HG22	12:Q:111:ARG:HD3	1.83	0.60
1:A:817:LYS:NZ	14:S:159:ASP:OD1	2.33	0.60
21:H:41:VAL:HG12	21:H:42:LYS:H	1.66	0.60
2:C:468:LEU:HD13	2:C:492:LEU:H	1.61	0.60
4:E:88:U:H2'	5:L:17:U:H6	1.67	0.60
5:L:4:A:O3'	22:I:114:THR:HG22	2.02	0.60
10:O:212:GLU:OE1	14:S:38:LYS:NZ	2.29	0.60
10:O:373:LEU:HD21	10:O:402:VAL:HG21	1.84	0.60
12:Q:212:ALA:CB	13:R:237:ARG:NH1	2.64	0.60
1:A:1377:SER:HB3	1:A:1379:MET:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLN:HA	1:A:1622:GLY:O	2.02	0.60
1:A:744:THR:O	1:A:749:ARG:NH2	2.34	0.60
13:R:76:PHE:HB2	13:R:91:HIS:CD2	2.36	0.60
16:Z:148:LEU:HD12	16:Z:190:LEU:HD11	1.82	0.60
16:Z:455:ALA:HB2	16:Z:484:ILE:HG21	1.84	0.60
1:A:1852:VAL:HG22	1:A:1881:THR:HG22	1.84	0.60
10:O:229:THR:HG21	10:O:272:VAL:H	1.66	0.60
13:R:10:LYS:NZ	13:R:57:LEU:O	2.27	0.60
1:A:1275:MET:O	1:A:1276:GLU:HG2	2.01	0.60
2:C:468:LEU:HD21	2:C:493:LEU:CG	2.31	0.60
2:C:660:ARG:HH22	2:C:670:ILE:HD12	1.66	0.60
1:A:737:ARG:NH1	4:E:70:U:OP2	2.34	0.60
4:E:50:G:O2'	19:F:65:ASN:ND2	2.34	0.60
20:G:11:SER:O	20:G:19:ASN:ND2	2.35	0.60
15:T:123:ARG:HH11	15:T:153:CYS:HB3	1.66	0.60
1:A:1637:LYS:NZ	19:F:3:GLU:OE1	2.32	0.59
5:L:19:U:C1'	11:P:178:TYR:HE2	2.15	0.59
5:L:75:A:O3'	12:Q:252:ARG:NH1	2.34	0.59
1:A:1125:LEU:O	1:A:1233:ARG:NH1	2.34	0.59
1:A:1195:PHE:HB3	1:A:1217:ARG:NE	2.17	0.59
2:C:307:ILE:HG12	2:C:346:THR:HA	1.83	0.59
10:O:156:ILE:HD13	10:O:197:LEU:HD22	1.83	0.59
1:A:1326:THR:O	1:A:1327:THR:OG1	2.15	0.59
4:E:2:U:H2'	4:E:3:U:H6	1.68	0.59
4:E:89:U:C5	22:I:176:TYR:CD1	2.89	0.59
7:B:90:A:N1	9:J:6:ILE:HD11	2.17	0.59
10:O:392:MET:HG2	14:S:158:ASN:HD22	1.66	0.59
16:Z:152:ILE:HD11	16:Z:194:LEU:HA	1.84	0.59
1:A:161:PHE:CE1	1:A:198:ALA:HA	2.37	0.59
2:C:99:LYS:NZ	3:D:43:G:OP2	2.34	0.59
4:E:66:C:C3'	4:E:66:C:C6	2.85	0.59
4:E:89:U:C4	22:I:176:TYR:CE1	2.91	0.59
1:A:1378:LYS:HB2	7:B:94:U:H4'	1.85	0.59
1:A:1904:ARG:N	6:M:492:U:OP1	2.35	0.59
1:A:341:ALA:HA	1:A:355:LEU:HD23	1.85	0.59
2:C:161:ILE:HG22	2:C:163:ASP:H	1.67	0.59
12:Q:13:CYS:SG	12:Q:16:CYS:N	2.71	0.59
16:Z:317:ILE:HD13	16:Z:325:VAL:HG21	1.84	0.59
1:A:1286:TRP:NE1	1:A:1348:GLU:OE1	2.24	0.59
1:A:1512:ARG:NH2	1:A:1525:PHE:O	2.36	0.59
4:E:56:A:O2'	4:E:57:U:P	2.61	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:27:ASN:OD1	9:J:28:ASN:N	2.30	0.59
1:A:1870:VAL:CB	5:L:46:C:H4'	2.30	0.59
2:C:683:ASN:HD22	2:C:713:GLU:HG2	1.68	0.59
3:D:78:A:O2'	3:D:79:C:P	2.61	0.59
11:P:85:SER:O	11:P:87:ASN:N	2.36	0.59
1:A:1862:VAL:HG13	1:A:1870:VAL:HG13	1.83	0.59
1:A:514:TYR:HB3	1:A:518:VAL:CG2	2.32	0.59
1:A:794:LYS:HB3	1:A:854:ARG:HH12	1.66	0.59
19:F:105:ASP:OD1	20:G:15:LYS:NZ	2.34	0.59
5:L:1116:A:N1	5:L:1117:G:C5	2.71	0.59
16:Z:184:GLN:NE2	16:Z:184:GLN:HA	2.18	0.59
1:A:191:VAL:HA	1:A:201:PHE:O	2.02	0.59
1:A:297:SER:HB3	3:D:32:G:OP1	2.02	0.59
2:C:749:LYS:O	2:C:753:THR:OG1	2.14	0.59
19:F:75:TYR:HB3	19:F:79:ILE:HB	1.83	0.59
10:O:277:VAL:HG13	11:P:63:ILE:HG22	1.83	0.59
12:Q:49:SER:HG	12:Q:52:SER:CA	2.15	0.59
1:A:1268:ARG:HE	1:A:1301:TYR:HD2	1.50	0.59
4:E:88:U:H2'	5:L:17:U:C6	2.37	0.59
1:A:1327:THR:HG21	5:L:35:U:H5'	1.67	0.59
13:R:253:LEU:O	13:R:257:ASN:CB	2.51	0.59
1:A:1458:TRP:CZ2	1:A:1489:PRO:HB2	2.38	0.58
1:A:484:PHE:CZ	3:D:81:A:C5	2.91	0.58
1:A:905:TYR:HD2	1:A:908:ASP:N	2.01	0.58
2:C:468:LEU:O	2:C:578:TYR:HA	2.04	0.58
1:A:2025:ILE:HD12	1:A:2058:LEU:HD11	1.84	0.58
1:A:620:HIS:HB3	1:A:669:TYR:CE2	2.38	0.58
1:A:899:PRO:HD3	1:A:1006:ARG:CZ	2.34	0.58
1:A:757:GLU:OE1	10:O:202:GLU:HG3	2.04	0.58
1:A:388:PRO:HB2	1:A:398:VAL:HG11	1.86	0.58
1:A:532:ASN:ND2	3:D:84:A:OP2	2.35	0.58
1:A:905:TYR:HB3	1:A:908:ASP:CG	2.23	0.58
1:A:912:LEU:HD21	1:A:916:LEU:HD11	1.85	0.58
1:A:791:ARG:NH2	11:P:173:LYS:HD2	2.18	0.58
5:L:21:G:N7	14:S:5:HIS:HB2	2.17	0.58
14:S:6:ARG:HG3	14:S:6:ARG:HH11	1.68	0.58
16:Z:197:LEU:C	16:Z:197:LEU:HD12	2.24	0.58
2:C:468:LEU:CD1	2:C:492:LEU:C	2.72	0.58
5:L:1102:C:C2'	5:L:1103:C:H6	2.15	0.58
1:A:1169:TYR:CE2	1:A:1262:MET:HG2	2.38	0.58
1:A:1047:ALA:HA	1:A:1172:PHE:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD21	1:A:626:LEU:HD21	1.86	0.58
4:E:42:A:O2'	4:E:43:C:OP1	2.19	0.58
19:F:29:LYS:O	19:F:35:ASN:ND2	2.36	0.58
11:P:101:PRO:O	11:P:103:ASN:N	2.36	0.58
13:R:121:ARG:HB3	13:R:125:GLY:H	1.69	0.58
2:C:407:ASN:OD1	2:C:408:LEU:N	2.36	0.58
2:C:868:VAL:HG11	2:C:876:VAL:HG21	1.86	0.58
1:A:900:PHE:CD2	1:A:901:PRO:N	2.72	0.58
12:Q:49:SER:HG	12:Q:52:SER:N	2.00	0.58
4:E:1:G:O2'	15:T:101:GLU:OE1	2.17	0.58
1:A:1711:VAL:HG11	1:A:1789:ASN:HB3	1.86	0.58
1:A:381:SER:O	1:A:384:LYS:N	2.37	0.58
2:C:775:ILE:HD12	2:C:817:GLN:HE21	1.69	0.58
4:E:85:C:OP1	4:E:85:C:O4'	2.21	0.58
5:L:5:A:H5''	22:I:114:THR:HG21	1.76	0.58
5:L:78:G:H5'	13:R:155:GLN:NE2	2.19	0.58
8:N:108:U:C4'	8:N:109:U:OP2	2.51	0.58
10:O:379:LYS:HA	11:P:47:ARG:HH21	1.68	0.58
15:T:31:ARG:HH11	15:T:31:ARG:CG	2.14	0.58
10:O:392:MET:HG3	10:O:393:VAL:H	1.69	0.58
12:Q:54:ASN:ND2	13:R:70:LEU:HD12	2.19	0.58
1:A:907:ASN:OD1	1:A:1504:TYR:CZ	2.57	0.57
1:A:672:LYS:NZ	3:D:86:G:OP2	2.37	0.57
1:A:1899:TRP:HE3	1:A:1905:LEU:HD22	1.68	0.57
1:A:133:GLU:HG3	1:A:560:THR:HA	1.85	0.57
4:E:89:U:C5'	5:L:17:U:OP2	2.50	0.57
16:Z:470:LEU:HD12	16:Z:471:GLY:H	1.69	0.57
2:C:220:ASN:O	2:C:647:ASN:ND2	2.29	0.57
4:E:92:C:O2'	4:E:93:A:O4'	2.22	0.57
11:P:37:ASN:ND2	11:P:145:PRO:HD3	2.19	0.57
13:R:159:ARG:HD3	13:R:205:LEU:H	1.69	0.57
14:S:8:GLN:OE1	14:S:10:GLU:O	2.21	0.57
1:A:1281:ASN:ND2	1:A:1285:VAL:HG21	2.18	0.57
1:A:1801:SER:O	1:A:1804:THR:OG1	2.19	0.57
1:A:488:ARG:C	1:A:489:THR:HG23	2.24	0.57
6:M:505:A:H3'	6:M:506:U:H4'	1.86	0.57
12:Q:49:SER:HG	12:Q:52:SER:HB2	1.69	0.57
1:A:1441:PHE:HB3	16:Z:303:LEU:HD11	1.86	0.57
1:A:1449:ASN:HB3	16:Z:338:THR:HG21	1.86	0.57
20:G:29:ASP:O	20:G:32:THR:OG1	2.19	0.57
12:Q:219:ILE:O	12:Q:222:THR:OG1	2.16	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:217:TRP:CD1	13:R:187:LYS:CE	2.88	0.57
1:A:217:TRP:O	1:A:220:THR:OG1	2.22	0.57
1:A:344:ASN:OD1	9:J:3:TYR:HD2	1.87	0.57
10:O:187:ASP:OD1	10:O:188:VAL:N	2.37	0.57
12:Q:217:TRP:HZ3	13:R:171:ASP:OD1	1.85	0.57
16:Z:192:GLU:HB3	16:Z:195:GLU:OE2	2.03	0.57
1:A:1376:ASN:O	1:A:1377:SER:OG	2.17	0.57
1:A:421:ALA:HB3	1:A:469:ILE:HD12	1.85	0.57
1:A:740:GLU:HG3	1:A:741:ILE:H	1.68	0.57
1:A:928:ARG:CG	5:L:30:A:N3	2.64	0.57
12:Q:215:PRO:CB	12:Q:217:TRP:CE3	2.88	0.57
2:C:126:MET:HE1	2:C:132:ARG:HH12	1.68	0.57
10:O:245:ASP:HB3	10:O:247:VAL:HG22	1.86	0.57
1:A:837:GLY:HA3	1:A:1317:ARG:HH22	1.70	0.57
1:A:174:LYS:O	1:A:178:ASN:ND2	2.35	0.57
1:A:376:ARG:HD2	2:C:910:GLU:OE2	2.05	0.57
21:H:72:GLU:HA	21:H:75:ILE:HG12	1.85	0.57
5:L:5:A:P	22:I:114:THR:CG2	2.89	0.57
1:A:591:LEU:HB3	1:A:599:LEU:HD11	1.86	0.56
1:A:805:PRO:HG2	1:A:808:ILE:HD12	1.86	0.56
2:C:510:ARG:NH1	2:C:533:GLU:OE1	2.37	0.56
2:C:794:GLN:HB3	2:C:838:ILE:HG21	1.87	0.56
19:F:36:LYS:HG3	19:F:38:HIS:H	1.70	0.56
6:M:498:C:OP1	19:F:41:ILE:CD1	2.47	0.56
5:L:67:A:H2'	5:L:68:U:H6	1.70	0.56
16:Z:307:GLU:OE2	16:Z:311:LYS:HE3	2.04	0.56
1:A:1748:ILE:O	1:A:1751:TYR:N	2.39	0.56
1:A:716:ARG:HD2	3:D:112:C:C1'	2.34	0.56
2:C:447:GLU:O	2:C:451:ASN:ND2	2.38	0.56
2:C:811:GLU:HB3	2:C:812:PRO:HD2	1.86	0.56
2:C:952:PRO:HB2	2:C:955:LYS:HB2	1.87	0.56
5:L:55:G:H2'	5:L:56:U:H6	1.71	0.56
5:L:73:U:H2'	5:L:74:C:H6	1.70	0.56
11:P:105:LEU:HD21	12:Q:12:ILE:HB	1.87	0.56
12:Q:103:GLU:OE1	13:R:131:ARG:NH1	2.37	0.56
16:Z:118:LEU:HB3	16:Z:154:VAL:HG22	1.88	0.56
1:A:1559:HIS:O	1:A:1612:PRO:HG2	2.05	0.56
5:L:14:C:OP2	22:I:209:ARG:NH2	2.37	0.56
5:L:24:U:H5"	5:L:25:A:OP2	2.05	0.56
10:O:118:LEU:HD21	11:P:48:GLN:HB3	1.87	0.56
10:O:121:GLN:NE2	11:P:49:SER:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:LYS:HG2	10:O:399:GLU:OE2	2.05	0.56
1:A:1144:PHE:CD2	1:A:1145:MET:HG2	2.41	0.56
1:A:1447:TRP:HB3	1:A:1451:PHE:CE2	2.40	0.56
1:A:165:LEU:HD13	1:A:578:MET:HB3	1.86	0.56
1:A:1731:LYS:O	1:A:1769:SER:OG	2.19	0.56
1:A:420:PRO:HG2	1:A:423:PHE:HB2	1.87	0.56
2:C:755:TYR:HB2	2:C:757:TRP:HB2	1.87	0.56
4:E:39:G:N1	13:R:120:TYR:O	2.38	0.56
5:L:100:G:H2'	5:L:101:U:H6	1.71	0.56
5:L:71:C:C2	5:L:72:C:C5	2.93	0.56
16:Z:174:TRP:HZ2	16:Z:197:LEU:CD1	2.16	0.56
1:A:1454:SER:HA	1:A:1487:GLY:HA2	1.86	0.56
1:A:1880:PHE:HD1	1:A:1891:LEU:HD21	1.69	0.56
21:H:79:ASN:HA	21:H:82:LEU:HD12	1.88	0.56
5:L:96:A:H2'	5:L:97:U:H6	1.71	0.56
12:Q:226:LEU:O	12:Q:226:LEU:HD12	2.05	0.56
4:E:38:U:H4'	13:R:121:ARG:HH12	1.71	0.56
13:R:63:ARG:HH21	15:T:143:HIS:CD2	2.22	0.56
1:A:1604:ARG:HA	1:A:1640:THR:HG21	1.86	0.56
1:A:318:LEU:HD13	1:A:501:LEU:HD23	1.88	0.56
2:C:265:PHE:CD2	2:C:295:ILE:HD12	2.40	0.56
20:G:16:LEU:O	20:G:18:LYS:N	2.38	0.56
5:L:101:U:H2'	5:L:102:U:H6	1.70	0.56
5:L:72:C:C2	5:L:73:U:C5	2.94	0.56
16:Z:470:LEU:HD12	16:Z:471:GLY:N	2.20	0.56
2:C:163:ASP:OD2	2:C:548:ARG:NH1	2.38	0.56
4:E:1:G:H2'	4:E:2:U:C6	2.41	0.56
19:F:4:ARG:NH1	19:F:5:LYS:NZ	2.51	0.56
5:L:106:A:H2'	5:L:107:U:H6	1.71	0.56
5:L:1116:A:N3	5:L:1117:G:C8	2.74	0.56
12:Q:86:LEU:O	12:Q:89:HIS:N	2.38	0.56
2:C:770:ASN:OD1	2:C:771:GLY:N	2.39	0.56
1:A:352:PHE:O	9:J:10:SER:OG	2.21	0.56
3:D:79:C:H3'	3:D:80:G:H5'	1.88	0.56
5:L:21:G:N7	14:S:5:HIS:CB	2.69	0.56
5:L:70:A:H2'	5:L:71:C:H6	1.71	0.56
1:A:856:TRP:CD1	14:S:174:VAL:HG21	2.41	0.56
1:A:1014:LYS:NZ	1:A:1016:SER:OG	2.32	0.56
2:C:200:CYS:SG	2:C:210:ILE:HD12	2.46	0.56
2:C:758:ASP:HB3	2:C:761:ALA:HB3	1.87	0.56
1:A:381:SER:HB3	9:J:3:TYR:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:103:A:H2'	5:L:104:C:H6	1.71	0.56
5:L:72:C:H2'	5:L:73:U:H6	1.70	0.56
5:L:98:U:C2	5:L:99:U:C5	2.94	0.56
12:Q:240:LEU:HD12	12:Q:241:ILE:N	2.20	0.56
1:A:905:TYR:CD2	1:A:908:ASP:N	2.73	0.56
2:C:806:GLY:H	2:C:810:GLU:HA	1.71	0.55
5:L:61:A:H2'	5:L:62:C:H6	1.71	0.55
5:L:73:U:C2	5:L:74:C:C5	2.94	0.55
10:O:326:ALA:HB2	10:O:356:LEU:HD11	1.88	0.55
16:Z:192:GLU:O	16:Z:195:GLU:HG2	2.05	0.55
2:C:360:ARG:CZ	2:C:362:LYS:HD3	2.36	0.55
2:C:110:LYS:HE2	2:C:552:PRO:HG2	1.88	0.55
2:C:863:GLU:OE2	2:C:934:HIS:ND1	2.40	0.55
5:L:83:U:C2	5:L:84:C:C5	2.94	0.55
14:S:167:GLN:O	14:S:171:HIS:CB	2.54	0.55
4:E:74:U:H5	14:S:27:HIS:CG	2.24	0.55
16:Z:178:ARG:HA	16:Z:198:PHE:CE1	2.41	0.55
1:A:1122:ASP:OD2	1:A:1163:ARG:NE	2.29	0.55
1:A:1172:PHE:HZ	1:A:1230:ILE:HD11	1.71	0.55
1:A:905:TYR:CD2	1:A:907:ASN:N	2.73	0.55
2:C:468:LEU:HD21	2:C:493:LEU:CD2	2.36	0.55
5:L:62:C:C2	5:L:63:U:C5	2.94	0.55
5:L:82:C:C2	5:L:83:U:C5	2.93	0.55
5:L:97:U:H2'	5:L:98:U:H6	1.71	0.55
10:O:147:ILE:HD13	10:O:408:ASP:HA	1.88	0.55
10:O:210:ASP:OD2	14:S:38:LYS:NZ	2.40	0.55
4:E:52:G:N2	14:S:5:HIS:CE1	2.62	0.55
1:A:1161:TYR:CD1	1:A:1170:MET:HG2	2.40	0.55
1:A:194:HIS:CD2	11:P:122:LEU:HD22	2.42	0.55
2:C:787:LEU:HD12	2:C:790:LYS:HD2	1.88	0.55
5:L:1100:A:C2	5:L:1101:C:C2	2.95	0.55
5:L:61:A:C4	5:L:62:C:C5	2.95	0.55
5:L:97:U:C2	5:L:98:U:C5	2.94	0.55
5:L:98:U:H2'	5:L:99:U:H6	1.71	0.55
1:A:614:ARG:NH2	7:B:98:A:O3'	2.39	0.55
2:C:613:ARG:NH1	2:C:614:GLU:OE2	2.39	0.55
21:H:34:ARG:HH12	21:H:36:ARG:NH1	2.04	0.55
5:L:100:G:C4	5:L:101:U:C5	2.95	0.55
5:L:82:C:H2'	5:L:83:U:H6	1.70	0.55
10:O:306:HIS:CD2	11:P:147:LEU:HD11	2.41	0.55
1:A:1279:VAL:O	1:A:1299:LYS:NZ	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:101:U:C2	5:L:102:U:C5	2.94	0.55
12:Q:53:ASN:ND2	12:Q:54:ASN:H	2.02	0.55
13:R:96:GLU:HG2	13:R:188:TYR:CE2	2.35	0.55
16:Z:170:HIS:NE2	16:Z:174:TRP:HZ3	1.90	0.55
16:Z:203:LYS:O	16:Z:204:ASP:CB	2.55	0.55
5:L:15:C:H2'	5:L:16:U:OP2	2.07	0.55
5:L:15:C:O2	5:L:16:U:H5	1.90	0.55
5:L:58:A:H2'	5:L:59:C:H6	1.71	0.55
5:L:67:A:C4	5:L:68:U:C5	2.95	0.55
5:L:67:A:H2	5:L:85:A:H61	1.51	0.55
11:P:174:ASN:HB2	11:P:185:ARG:HH12	1.70	0.55
5:L:19:U:O4'	11:P:178:TYR:CE2	2.59	0.55
14:S:4:SER:C	14:S:6:ARG:HD3	2.26	0.55
2:C:437:ASP:OD1	2:C:441:ARG:NH2	2.40	0.55
2:C:468:LEU:HD11	2:C:492:LEU:C	2.26	0.55
4:E:2:U:H2'	4:E:3:U:C6	2.41	0.55
21:H:51:LYS:HG2	21:H:89:TRP:CZ3	2.42	0.55
5:L:71:C:H2'	5:L:72:C:H6	1.71	0.55
12:Q:208:TYR:O	12:Q:209:ASN:HB3	2.07	0.55
12:Q:257:GLU:HG3	12:Q:258:LEU:N	2.21	0.55
2:C:326:GLU:O	2:C:329:SER:N	2.40	0.55
2:C:919:ARG:HH12	2:C:927:MET:HE1	1.71	0.55
5:L:55:G:C4	5:L:56:U:C5	2.95	0.55
5:L:81:G:C4	5:L:82:C:C5	2.94	0.55
5:L:81:G:H2'	5:L:82:C:H6	1.71	0.55
12:Q:226:LEU:HD11	12:Q:227:LEU:CD2	2.29	0.55
15:T:13:PRO:HG2	15:T:77:LEU:HA	1.87	0.55
1:A:1282:ASP:OD1	1:A:1283:GLU:N	2.34	0.55
2:C:869:HIS:HD2	2:C:925:LEU:HB3	1.71	0.55
5:L:70:A:C4	5:L:71:C:C5	2.95	0.55
12:Q:116:LYS:HD3	12:Q:118:VAL:CG1	2.37	0.55
1:A:1458:TRP:NE1	1:A:1489:PRO:HD2	2.22	0.54
1:A:411:ILE:HD11	2:C:898:PRO:HG3	1.89	0.54
5:L:1102:C:C2'	5:L:1103:C:C6	2.80	0.54
1:A:928:ARG:NH1	5:L:30:A:O3'	2.40	0.54
13:R:146:LEU:HD23	13:R:147:ASN:H	1.70	0.54
4:E:38:U:O4	13:R:222:LEU:HA	2.06	0.54
16:Z:184:GLN:HE21	16:Z:185:GLU:N	2.05	0.54
1:A:1046:SER:HA	1:A:1251:TYR:O	2.07	0.54
2:C:291:ILE:O	2:C:294:ASN:N	2.39	0.54
4:E:56:A:H2'	4:E:57:U:C6	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:125:TRP:HE1	10:O:437:GLU:HB3	1.72	0.54
4:E:38:U:H4'	13:R:121:ARG:NH1	2.23	0.54
1:A:1372:LYS:HG2	1:A:1383:PHE:HD2	1.72	0.54
1:A:570:GLN:O	1:A:574:GLN:HG2	2.07	0.54
2:C:183:GLN:NE2	2:C:654:CYS:HA	2.22	0.54
5:L:58:A:C4	5:L:59:C:C5	2.95	0.54
5:L:62:C:H2'	5:L:63:U:H6	1.71	0.54
5:L:96:A:C4	5:L:97:U:C5	2.95	0.54
1:A:1468:ALA:HA	1:A:1473:ARG:HG2	1.88	0.54
2:C:251:GLN:NE2	2:C:255:GLN:HE21	2.06	0.54
2:C:697:ARG:NH1	2:C:852:THR:HG1	2.05	0.54
16:Z:149:ARG:CZ	16:Z:193:SER:HB3	2.37	0.54
1:A:653:ILE:HD11	1:A:704:TRP:CE2	2.43	0.54
2:C:139:ILE:HD12	2:C:252:LEU:HD22	1.89	0.54
2:C:477:ASP:HB2	2:C:628:TYR:CE1	2.43	0.54
5:L:83:U:H2'	5:L:84:C:H6	1.71	0.54
1:A:2012:LEU:HD23	1:A:2015:LEU:HD12	1.89	0.54
1:A:413:ASN:ND2	1:A:419:THR:OG1	2.40	0.54
1:A:881:THR:O	1:A:884:SER:OG	2.20	0.54
1:A:908:ASP:OD1	1:A:994:TYR:OH	2.21	0.54
2:C:101:GLN:NE2	3:D:77:A:N6	2.55	0.54
6:M:503:A:H2'	6:M:504:C:O4'	2.06	0.54
1:A:1883:ASN:HD21	1:A:1886:THR:HG23	1.73	0.54
1:A:606:THR:OG1	1:A:609:GLU:HG2	2.08	0.54
2:C:501:ILE:HD11	2:C:567:ILE:HD12	1.89	0.54
4:E:66:C:H6	4:E:66:C:C3'	2.20	0.54
5:L:1114:G:H2'	5:L:1115:G:C8	2.43	0.54
12:Q:226:LEU:CD2	12:Q:262:PHE:HE1	2.20	0.54
1:A:1041:VAL:HG13	1:A:1253:LYS:HG2	1.90	0.54
1:A:1305:SER:OG	1:A:1307:GLU:OE1	2.24	0.54
2:C:231:ALA:HB2	2:C:473:LEU:HD11	1.89	0.54
10:O:379:LYS:HD3	11:P:47:ARG:NH2	2.23	0.54
1:A:756:LEU:CD1	14:S:8:GLN:NE2	2.65	0.54
1:A:168:LEU:O	1:A:171:ALA:N	2.41	0.54
1:A:1990:ASN:ND2	1:A:1993:ASP:O	2.40	0.54
1:A:874:ILE:O	1:A:875:THR:OG1	2.19	0.54
1:A:936:GLU:O	1:A:940:ILE:HD12	2.08	0.54
2:C:314:ALA:HB1	2:C:321:THR:HG22	1.89	0.54
2:C:468:LEU:CD1	2:C:491:GLY:CA	2.72	0.54
21:H:46:GLU:OE2	21:H:50:TRP:NE1	2.40	0.54
5:L:1114:G:O5'	5:L:1114:G:H8	1.91	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:15:C:C2'	5:L:16:U:OP2	2.56	0.54
14:S:7:PRO:O	14:S:8:GLN:HB2	2.08	0.54
1:A:756:LEU:CD1	14:S:8:GLN:HE22	2.19	0.54
1:A:1051:GLU:HB3	1:A:1167:ARG:HH21	1.73	0.54
1:A:364:TYR:CD1	1:A:1209:LYS:HE2	2.43	0.54
5:L:103:A:C4	5:L:104:C:C5	2.95	0.54
5:L:106:A:C4	5:L:107:U:C5	2.95	0.54
10:O:155:PHE:CZ	10:O:415:ILE:HG12	2.42	0.54
11:P:170:SER:O	11:P:185:ARG:NH2	2.41	0.54
1:A:1144:PHE:CZ	1:A:1162:THR:HG21	2.43	0.53
1:A:923:TYR:HD1	1:A:926:LYS:HD3	1.73	0.53
2:C:499:VAL:O	2:C:536:SER:HA	2.08	0.53
1:A:372:ARG:HH21	2:C:973:ARG:HG3	1.73	0.53
22:I:184:GLN:HA	22:I:187:LYS:HZ3	1.73	0.53
12:Q:215:PRO:CG	12:Q:217:TRP:CE3	2.91	0.53
12:Q:82:ILE:HG23	12:Q:86:LEU:HD23	1.90	0.53
13:R:72:PHE:CE2	13:R:94:PRO:HG3	2.43	0.53
16:Z:179:TYR:O	16:Z:179:TYR:HD1	1.91	0.53
1:A:810:LYS:NZ	10:O:397:GLU:HB3	2.23	0.53
1:A:902:PRO:HG2	1:A:904:THR:O	2.08	0.53
4:E:14:C:H4'	4:E:15:C:O5'	2.08	0.53
5:L:15:C:O2'	5:L:16:U:H6	1.77	0.53
10:O:127:ALA:HB3	10:O:428:GLN:HE21	1.73	0.53
12:Q:24:ARG:HD2	15:T:116:ASN:HD22	1.73	0.53
12:Q:253:PHE:HB3	12:Q:258:LEU:HD12	1.90	0.53
14:S:7:PRO:HG2	14:S:9:LEU:HD23	1.89	0.53
16:Z:181:LEU:HD21	16:Z:191:ARG:CG	2.29	0.53
2:C:766:TRP:CG	2:C:792:LYS:HE3	2.43	0.53
1:A:1047:ALA:O	1:A:1250:VAL:HA	2.09	0.53
1:A:1443:TYR:OH	1:A:1545:ASP:OD2	2.15	0.53
1:A:602:THR:HG22	19:F:10:TYR:HD2	1.73	0.53
1:A:886:MET:SD	1:A:1120:VAL:HG22	2.49	0.53
2:C:137:GLY:N	2:C:232:SER:OG	2.40	0.53
2:C:766:TRP:CE3	2:C:792:LYS:HG3	2.44	0.53
2:C:77:LEU:HD11	10:O:135:ILE:HG12	1.90	0.53
19:F:99:THR:O	19:F:101:PRO:HD3	2.08	0.53
13:R:4:TRP:HZ3	13:R:5:ARG:CZ	2.21	0.53
1:A:1963:LEU:HD13	1:A:1965:PHE:HE2	1.73	0.53
1:A:342:LEU:HD13	1:A:392:ASN:HD22	1.74	0.53
1:A:426:PRO:CB	16:Z:201:ARG:HG2	2.18	0.53
1:A:899:PRO:CD	1:A:1006:ARG:CZ	2.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:182:GLN:O	22:I:186:ALA:HB2	2.07	0.53
10:O:218:ARG:HB3	10:O:256:ARG:HD3	1.91	0.53
1:A:1652:HIS:CE1	19:F:17:PRO:HB2	2.43	0.53
1:A:259:GLU:HG3	1:A:260:PRO:HD2	1.91	0.53
1:A:905:TYR:HD2	1:A:908:ASP:H	1.54	0.53
1:A:928:ARG:NE	5:L:32:G:C8	2.77	0.53
10:O:190:VAL:HG22	10:O:197:LEU:HD13	1.89	0.53
12:Q:56:ILE:HD12	13:R:105:ARG:HH22	1.72	0.53
1:A:835:LYS:HD2	14:S:173:HIS:CE1	2.44	0.53
2:C:240:ASP:OD1	2:C:269:LYS:HD3	2.08	0.53
2:C:794:GLN:NE2	2:C:835:LYS:HA	2.24	0.53
4:E:49:A:C2'	4:E:50:G:H5'	2.39	0.53
5:L:1103:C:C6	5:L:1114:G:N2	2.76	0.53
5:L:19:U:O4'	11:P:178:TYR:HE2	1.91	0.53
13:R:73:CYS:HB2	13:R:89:TYR:HB2	1.90	0.53
16:Z:168:LYS:O	16:Z:168:LYS:NZ	2.37	0.53
1:A:1389:TYR:CE1	1:A:1401:SER:HB3	2.44	0.53
1:A:2007:ARG:HH12	1:A:2048:TRP:HB3	1.73	0.53
1:A:412:GLN:OE1	1:A:412:GLN:N	2.42	0.53
3:D:79:C:H3'	3:D:79:C:O2	2.08	0.53
1:A:488:ARG:CZ	3:D:81:A:N6	2.72	0.53
5:L:1097:G:N1	5:L:1119:C:N3	2.50	0.53
11:P:147:LEU:HD12	11:P:147:LEU:O	2.08	0.53
1:A:1184:ASP:O	1:A:1188:ALA:HB2	2.09	0.53
1:A:728:ASN:HD22	4:E:72:C:HO2'	1.50	0.53
1:A:861:GLN:NE2	1:A:1097:HIS:HB3	2.23	0.53
2:C:671:SER:OG	2:C:672:ASP:N	2.42	0.53
1:A:928:ARG:NH2	5:L:30:A:O2'	2.42	0.52
2:C:286:LEU:CD2	16:Z:182:GLN:HB3	2.34	0.52
2:C:539:VAL:HG13	2:C:564:ILE:HG23	1.91	0.52
5:L:25:A:H3'	5:L:26:G:H5''	1.91	0.52
8:N:110:A:C2	13:R:46:ARG:HD2	2.43	0.52
1:A:907:ASN:OD1	1:A:1504:TYR:CE2	2.62	0.52
3:D:78:A:H4'	3:D:79:C:OP1	2.09	0.52
1:A:732:ARG:NH2	4:E:71:G:OP2	2.43	0.52
1:A:861:GLN:HE21	1:A:1097:HIS:HB3	1.74	0.52
21:H:86:PHE:CE2	21:H:90:LYS:HE3	2.44	0.52
5:L:1116:A:N6	5:L:1117:G:C6	2.78	0.52
10:O:138:HIS:CE1	10:O:159:SER:HB2	2.43	0.52
12:Q:213:SER:HA	13:R:237:ARG:NH2	2.25	0.52
1:A:1145:MET:SD	1:A:1160:LEU:HD22	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:LEU:HB2	16:Z:307:GLU:HG3	1.91	0.52
1:A:1762:ASP:OD1	1:A:1763:ASN:N	2.41	0.52
1:A:291:LYS:HE2	1:A:292:LYS:HD3	1.90	0.52
1:A:426:PRO:CG	16:Z:201:ARG:CZ	2.83	0.52
2:C:316:THR:OG1	36:C:1500:GTP:N7	2.42	0.52
2:C:883:ARG:HH22	2:C:913:GLY:H	1.58	0.52
19:F:23:LEU:C	21:H:18:GLN:HE22	2.12	0.52
5:L:1107:C:C6	5:L:1107:C:H5'	2.44	0.52
1:A:1567:PHE:CE1	1:A:1827:GLN:HB2	2.44	0.52
1:A:1899:TRP:HH2	1:A:1909:ALA:HA	1.75	0.52
1:A:244:ASP:OD1	1:A:596:ASN:ND2	2.43	0.52
2:C:468:LEU:HD11	2:C:491:GLY:C	2.23	0.52
19:F:68:LYS:HA	19:F:84:LEU:HD23	1.91	0.52
10:O:365:PHE:HZ	10:O:373:LEU:HD22	1.75	0.52
10:O:397:GLU:HG3	10:O:400:ARG:HH12	1.74	0.52
12:Q:208:TYR:HB2	12:Q:290:ILE:HD12	1.92	0.52
12:Q:215:PRO:CG	12:Q:217:TRP:CZ3	2.91	0.52
12:Q:25:MET:HB2	12:Q:45:HIS:O	2.09	0.52
13:R:138:TYR:HD1	13:R:183:PHE:HE1	1.58	0.52
15:T:150:CYS:SG	15:T:151:ARG:N	2.82	0.52
1:A:1449:ASN:ND2	16:Z:339:PHE:O	2.42	0.52
2:C:656:LEU:HD13	2:C:670:ILE:HD13	1.91	0.52
10:O:112:VAL:O	10:O:115:TYR:N	2.43	0.52
10:O:446:LEU:N	10:O:446:LEU:CD1	2.73	0.52
1:A:1539:LEU:O	1:A:1542:TYR:N	2.39	0.52
19:F:84:LEU:O	19:F:96:ALA:HA	2.10	0.52
22:I:102:LYS:NZ	22:I:106:GLU:OE2	2.36	0.52
12:Q:116:LYS:HD3	12:Q:118:VAL:HG11	1.92	0.52
12:Q:87:ARG:HH22	12:Q:122:GLY:C	2.13	0.52
12:Q:207:LEU:HB3	12:Q:210:ILE:HD11	1.90	0.52
12:Q:214:ILE:HD11	12:Q:218:LYS:HG3	1.89	0.52
1:A:299:LYS:HA	1:A:493:MET:HG2	1.91	0.52
2:C:416:ASP:HB2	2:C:419:PRO:HD2	1.91	0.52
5:L:1116:A:C5	5:L:1117:G:C5	2.97	0.52
11:P:174:ASN:HD21	11:P:177:GLY:C	2.12	0.52
13:R:254:ILE:O	13:R:258:THR:OG1	2.14	0.52
2:C:246:THR:HG23	2:C:248:VAL:HG12	1.91	0.52
12:Q:13:CYS:N	12:Q:71:CYS:SG	2.80	0.52
14:S:8:GLN:CG	14:S:10:GLU:O	2.56	0.52
15:T:131:GLU:OE2	15:T:135:LYS:NZ	2.43	0.52
16:Z:305:GLY:HA2	16:Z:342:PHE:CE1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:480:ARG:HD3	16:Z:483:ILE:HD12	1.92	0.52
1:A:1902:GLN:HG2	1:A:1908:LEU:HD22	1.91	0.52
6:M:505:A:OP2	6:M:505:A:H4'	2.10	0.52
10:O:407:PHE:CE1	10:O:414:LEU:HD13	2.45	0.52
1:A:1661:ILE:HG13	1:A:1809:ASN:ND2	2.25	0.51
1:A:1711:VAL:HG12	1:A:1712:SER:H	1.76	0.51
1:A:426:PRO:CG	16:Z:201:ARG:CG	2.87	0.51
1:A:932:SER:O	1:A:936:GLU:HG3	2.10	0.51
2:C:315:SER:HB3	2:C:320:PHE:CE1	2.46	0.51
2:C:393:LYS:O	2:C:397:LYS:HB2	2.10	0.51
22:I:196:ILE:H	22:I:200:ASN:HD22	1.58	0.51
10:O:365:PHE:CZ	10:O:373:LEU:HD22	2.44	0.51
1:A:1813:TYR:OH	1:A:1817:GLU:OE2	2.17	0.51
1:A:2011:LEU:HB3	1:A:2040:TRP:CH2	2.44	0.51
5:L:1102:C:O2'	5:L:1103:C:H5'	2.10	0.51
12:Q:119:LYS:C	12:Q:120:LEU:HD23	2.31	0.51
1:A:134:MET:HE1	15:T:107:ARG:HH11	1.75	0.51
1:A:1843:LEU:HD22	1:A:1851:PHE:HZ	1.76	0.51
1:A:416:GLU:HG2	1:A:418:ASP:N	2.25	0.51
2:C:103:HIS:CD2	2:C:104:THR:HG23	2.46	0.51
2:C:768:PHE:HB3	2:C:773:VAL:HG23	1.91	0.51
21:H:58:ILE:O	21:H:62:SER:HB3	2.09	0.51
1:A:1283:GLU:HB3	16:Z:341:LYS:HB2	1.92	0.51
2:C:468:LEU:HD13	2:C:492:LEU:N	2.10	0.51
12:Q:291:ILE:HG23	12:Q:292:PRO:HA	1.92	0.51
2:C:829:VAL:O	2:C:830:ASN:ND2	2.43	0.51
2:C:885:GLY:HA3	2:C:906:VAL:HG23	1.91	0.51
5:L:18:U:C6	22:I:202:GLN:HG3	2.45	0.51
10:O:239:ILE:HB	10:O:251:TRP:HB2	1.93	0.51
1:A:138:HIS:CD2	15:T:49:LEU:HD22	2.45	0.51
1:A:1527:TRP:CE3	1:A:1528:THR:HG23	2.44	0.51
1:A:837:GLY:HA3	1:A:1317:ARG:NH2	2.26	0.51
2:C:289:ASN:O	2:C:293:ALA:CB	2.59	0.51
3:D:103:A:O2'	3:D:104:G:OP2	2.23	0.51
4:E:66:C:H3'	4:E:66:C:C6	2.43	0.51
22:I:190:TYR:HE2	22:I:195:PHE:HZ	1.57	0.51
10:O:221:TYR:O	10:O:251:TRP:HH2	1.93	0.51
1:A:867:ILE:HG21	1:A:1101:TYR:CD1	2.45	0.51
1:A:613:SER:O	19:F:2:SER:OG	2.28	0.51
2:C:341:ILE:HG13	2:C:342:ASP:N	2.26	0.51
5:L:18:U:C5	22:I:202:GLN:HG3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:209:ASN:HB3	12:Q:288:ILE:O	2.10	0.51
19:F:67:LYS:HB2	19:F:85:THR:OG1	2.10	0.51
22:I:111:ASN:O	22:I:114:THR:OG1	2.21	0.51
10:O:238:LEU:HD21	11:P:74:ILE:HD13	1.92	0.51
1:A:1540:ASN:O	1:A:1543:ARG:HB3	2.11	0.51
1:A:1687:HIS:CG	1:A:1688:PRO:HD2	2.46	0.51
1:A:1773:VAL:HA	1:A:1788:GLY:HA2	1.92	0.51
1:A:468:LEU:HD12	1:A:469:ILE:HG12	1.91	0.51
1:A:503:LYS:HA	1:A:506:PHE:CE2	2.46	0.51
1:A:984:VAL:HG12	1:A:985:ASP:H	1.76	0.51
6:M:502:C:O2'	6:M:503:A:O4'	2.28	0.51
2:C:79:GLU:OE1	11:P:202:MET:HA	48.75	0.51
12:Q:256:SER:O	12:Q:259:GLY:CA	2.58	0.51
2:C:101:GLN:NE2	3:D:75:A:H61	2.07	0.51
2:C:437:ASP:O	2:C:440:THR:N	2.43	0.51
16:Z:355:ARG:O	16:Z:358:GLN:HB2	2.10	0.51
1:A:1881:THR:OG1	1:A:1890:PHE:HB2	2.11	0.50
1:A:649:LEU:O	1:A:652:GLY:N	2.45	0.50
4:E:66:C:H4'	11:P:133:LYS:HD3	1.93	0.50
21:H:41:VAL:HG21	21:H:92:TRP:CZ3	2.46	0.50
1:A:1041:VAL:CG1	1:A:1253:LYS:HG2	2.40	0.50
1:A:933:GLU:OE1	1:A:933:GLU:N	2.36	0.50
10:O:152:ASN:ND2	10:O:409:LYS:HB3	2.18	0.50
10:O:308:LYS:HA	11:P:148:HIS:CE1	2.46	0.50
1:A:1658:HIS:NE2	1:A:1700:ASP:OD2	2.40	0.50
2:C:602:VAL:HG12	2:C:908:VAL:HG21	1.93	0.50
2:C:918:LEU:HD23	2:C:928:CYS:HB2	1.94	0.50
2:C:968:MET:O	2:C:972:ARG:NH1	2.44	0.50
3:D:31:G:C2'	3:D:32:G:H5'	2.41	0.50
1:A:488:ARG:CZ	3:D:81:A:H61	2.23	0.50
21:H:41:VAL:HG12	21:H:42:LYS:N	2.26	0.50
12:Q:205:PHE:CD2	12:Q:291:ILE:HD11	2.46	0.50
1:A:1111:SER:HA	1:A:1514:PHE:HE2	1.76	0.50
1:A:1870:VAL:HG21	5:L:46:C:C5'	2.38	0.50
1:A:2009:THR:O	1:A:2013:ARG:HG3	2.11	0.50
1:A:687:ILE:HD11	1:A:706:PRO:HG2	1.93	0.50
1:A:905:TYR:HB3	1:A:908:ASP:OD2	2.10	0.50
5:L:1116:A:C5	5:L:1117:G:N7	2.79	0.50
12:Q:119:LYS:O	12:Q:120:LEU:HD23	2.11	0.50
12:Q:205:PHE:O	12:Q:250:GLY:HA2	2.11	0.50
1:A:1907:GLN:O	1:A:1911:TRP:HD1	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:CG2	1:A:640:ARG:HG2	2.41	0.50
2:C:223:ASP:CG	2:C:647:ASN:HD21	2.15	0.50
4:E:87:U:C4'	4:E:87:U:OP1	2.60	0.50
10:O:414:LEU:HB3	10:O:426:TRP:HB2	1.93	0.50
12:Q:220:THR:HG23	12:Q:240:LEU:HD23	1.94	0.50
16:Z:178:ARG:HG2	16:Z:198:PHE:CZ	2.40	0.50
1:A:329:TYR:CE1	2:C:919:ARG:HD2	2.46	0.50
1:A:839:HIS:ND1	1:A:839:HIS:O	2.45	0.50
2:C:232:SER:OG	2:C:234:LEU:O	2.30	0.50
2:C:362:LYS:HE2	2:C:365:GLU:HB3	1.93	0.50
2:C:675:THR:OG1	2:C:676:VAL:N	2.44	0.50
2:C:683:ASN:ND2	2:C:713:GLU:HG2	2.26	0.50
2:C:752:ARG:HD3	2:C:759:SER:HA	1.92	0.50
22:I:184:GLN:HA	22:I:187:LYS:NZ	2.26	0.50
11:P:35:ALA:O	11:P:37:ASN:N	2.45	0.50
13:R:4:TRP:NE1	13:R:92:HIS:HB3	2.27	0.50
1:A:1755:LYS:HE3	1:A:1759:TYR:CE2	2.42	0.50
2:C:738:ASP:HA	2:C:768:PHE:CZ	2.47	0.50
2:C:738:ASP:HA	2:C:768:PHE:HZ	1.77	0.50
3:D:103:A:O2'	3:D:104:G:P	2.69	0.50
21:H:55:SER:HB3	21:H:89:TRP:CZ3	2.46	0.50
22:I:187:LYS:HA	22:I:201:LYS:NZ	2.27	0.50
4:E:88:U:O2'	5:L:17:U:OP2	2.14	0.50
16:Z:416:GLY:O	16:Z:420:ILE:HD12	2.12	0.50
1:A:1862:VAL:HA	1:A:1871:ALA:O	2.12	0.50
1:A:460:PRO:HG3	2:C:376:PHE:CD1	2.47	0.50
4:E:88:U:C6	5:L:17:U:C6	3.00	0.50
1:A:128:TYR:HA	15:T:112:ASN:HD21	1.76	0.50
16:Z:395:GLU:OE2	16:Z:439:ARG:NH2	2.30	0.50
1:A:1364:GLU:OE1	1:A:1403:SER:OG	2.29	0.50
1:A:1348:GLU:HG2	1:A:1446:THR:HB	1.93	0.50
1:A:790:TRP:NE1	1:A:794:LYS:HE3	2.26	0.50
2:C:758:ASP:OD1	2:C:759:SER:N	2.45	0.50
4:E:63:G:HO2'	14:S:8:GLN:CG	2.13	0.50
19:F:31:LEU:O	21:H:33:GLN:NE2	2.45	0.50
5:L:19:U:H1'	11:P:178:TYR:CE2	2.46	0.50
10:O:322:SER:OG	10:O:378:TYR:OH	2.26	0.50
11:P:43:PHE:CD1	11:P:147:LEU:HD13	2.47	0.50
10:O:277:VAL:HG11	11:P:58:PRO:HB2	1.94	0.50
13:R:9:ALA:HB2	13:R:60:GLY:O	2.11	0.50
16:Z:204:ASP:C	16:Z:205:TYR:CD2	2.86	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1915:GLU:O	1:A:1918:SER:OG	2.17	0.49
1:A:1849:LYS:HG2	1:A:1932:GLN:HB2	1.93	0.49
1:A:427:SER:HA	16:Z:202:GLN:CB	2.41	0.49
1:A:724:ARG:HH21	1:A:725:TYR:HE1	1.60	0.49
2:C:363:PRO:O	2:C:364:PHE:CD2	2.65	0.49
10:O:201:SER:OG	10:O:202:GLU:N	2.45	0.49
10:O:343:THR:HB	11:P:47:ARG:HD3	1.94	0.49
13:R:75:PHE:O	13:R:80:MET:N	2.46	0.49
1:A:1315:ARG:O	1:A:1319:ILE:HD12	2.12	0.49
1:A:143:ILE:HD12	1:A:573:ARG:NH2	2.27	0.49
1:A:514:TYR:HB3	1:A:518:VAL:HG21	1.93	0.49
6:M:492:U:H2'	6:M:493:A:C8	2.47	0.49
1:A:1906:SER:OG	6:M:493:A:P	2.70	0.49
6:M:493:A:H2'	6:M:494:G:O4'	2.12	0.49
13:R:22:ILE:HG13	13:R:22:ILE:O	2.13	0.49
1:A:1458:TRP:HZ2	1:A:1489:PRO:HB2	1.74	0.49
1:A:288:GLU:N	1:A:288:GLU:OE1	2.45	0.49
1:A:310:ASN:OD1	1:A:313:ARG:NH2	2.43	0.49
1:A:590:TYR:OH	1:A:609:GLU:OE1	2.21	0.49
4:E:58:C:OP1	19:F:63:LYS:NZ	2.45	0.49
11:P:157:GLU:HG2	22:I:95:ILE:HA	1.94	0.49
9:J:23:SER:HA	16:Z:310:HIS:HD2	1.76	0.49
12:Q:105:LYS:O	12:Q:109:MET:HB2	2.11	0.49
12:Q:209:ASN:HD21	12:Q:288:ILE:CG2	2.23	0.49
12:Q:215:PRO:HG3	12:Q:217:TRP:CE3	2.47	0.49
15:T:143:HIS:O	15:T:151:ARG:HG2	2.13	0.49
1:A:1348:GLU:OE2	1:A:1447:TRP:N	2.45	0.49
2:C:468:LEU:CD1	2:C:492:LEU:CA	2.82	0.49
5:L:1120:G:H8	5:L:1120:G:C5'	2.26	0.49
5:L:15:C:O2'	5:L:16:U:C5'	2.53	0.49
12:Q:53:ASN:N	12:Q:53:ASN:HD22	2.10	0.49
1:A:555:LYS:HA	15:T:113:GLU:OE1	2.12	0.49
16:Z:168:LYS:HZ3	16:Z:171:ASP:CB	2.25	0.49
1:A:512:GLU:OE1	7:B:89:A:N6	2.43	0.49
1:A:618:SER:OG	1:A:725:TYR:HB3	2.13	0.49
1:A:600:LYS:HB2	19:F:10:TYR:HB2	1.94	0.49
19:F:85:THR:HA	19:F:95:ILE:O	2.12	0.49
6:M:499:U:OP2	20:G:10:LYS:NZ	2.45	0.49
8:N:108:U:H4'	8:N:109:U:OP2	2.12	0.49
16:Z:179:TYR:CD1	16:Z:179:TYR:C	2.86	0.49
1:A:1602:PRO:HD2	1:A:1605:ARG:HH21	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:221:TRP:HB3	2.12	0.49
15:T:133:ALA:O	15:T:137:GLY:N	2.45	0.49
1:A:1156:HIS:CG	1:A:1157:PRO:HD2	2.48	0.49
2:C:607:LEU:HD23	2:C:670:ILE:HG12	1.95	0.49
5:L:19:U:N1	11:P:178:TYR:CD2	2.78	0.49
1:A:912:LEU:HD23	1:A:916:LEU:HD12	1.95	0.49
2:C:468:LEU:HA	2:C:491:GLY:HA3	1.94	0.49
2:C:69:PRO:HB3	10:O:390:ARG:HG2	1.94	0.49
10:O:348:GLU:CD	10:O:349:LYS:H	2.16	0.49
10:O:344:ASN:HD22	11:P:45:PRO:HG3	1.78	0.49
12:Q:220:THR:HG23	12:Q:240:LEU:CD2	2.43	0.49
16:Z:150:LEU:O	16:Z:154:VAL:HG23	2.12	0.49
1:A:1883:ASN:OD1	1:A:1886:THR:OG1	2.25	0.49
2:C:154:VAL:O	2:C:157:SER:N	2.46	0.49
2:C:461:LYS:N	2:C:461:LYS:CD	2.75	0.49
2:C:646:GLY:HA3	2:C:652:MET:HE3	1.95	0.49
2:C:89:PRO:HA	10:O:212:GLU:O	2.13	0.49
21:H:28:ASP:HB3	21:H:30:SER:H	1.78	0.49
21:H:32:TYR:HB2	21:H:50:TRP:HH2	1.78	0.49
14:S:7:PRO:O	14:S:8:GLN:CB	2.61	0.49
16:Z:168:LYS:NZ	16:Z:171:ASP:CB	2.73	0.49
1:A:1111:SER:HA	1:A:1514:PHE:CE2	2.48	0.49
1:A:344:ASN:OD1	9:J:3:TYR:CD2	2.66	0.49
1:A:1677:GLN:HB3	1:A:1706:VAL:HB	1.94	0.48
1:A:1812:LEU:HB3	1:A:1816:ARG:HH12	1.78	0.48
2:C:194:ASN:O	2:C:214:ASP:HB3	2.13	0.48
2:C:706:LEU:HD21	2:C:834:MET:HE1	1.95	0.48
13:R:64:GLY:O	13:R:68:GLY:N	2.45	0.48
16:Z:299:LEU:HD21	16:Z:343:TYR:CE1	2.47	0.48
16:Z:433:LEU:HD21	16:Z:472:LEU:HD12	1.94	0.48
1:A:1080:ASP:HB3	2:C:82:ASN:HD22	58.71	0.48
1:A:1695:ASN:O	1:A:1759:TYR:OH	2.13	0.48
1:A:1711:VAL:HG12	1:A:1712:SER:N	2.28	0.48
1:A:900:PHE:C	1:A:900:PHE:CD2	2.86	0.48
2:C:271:ASP:OD1	2:C:272:ARG:N	2.46	0.48
12:Q:214:ILE:HD11	12:Q:218:LYS:CB	2.43	0.48
13:R:150:HIS:HB3	13:R:155:GLN:HG3	1.94	0.48
16:Z:301:SER:O	16:Z:302:SER:OG	2.31	0.48
1:A:1286:TRP:CE2	1:A:1302:LEU:HD11	2.48	0.48
10:O:151:ASP:HB3	10:O:153:GLU:HG2	1.95	0.48
12:Q:209:ASN:HD21	12:Q:288:ILE:HG23	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:413:CYS:O	16:Z:417:ARG:N	2.38	0.48
1:A:898:ILE:HA	1:A:1006:ARG:HH12	1.77	0.48
1:A:925:SER:O	6:M:507:U:OP2	2.31	0.48
2:C:503:ASP:HB2	2:C:506:GLN:HG2	1.95	0.48
2:C:629:TYR:OH	2:C:658:ASP:OD2	2.18	0.48
4:E:42:A:O5'	4:E:42:A:H8	1.96	0.48
19:F:46:PRO:HG2	19:F:106:TYR:CE2	2.39	0.48
1:A:1422:ILE:HD13	1:A:1425:PHE:CZ	2.47	0.48
1:A:263:PRO:HG2	1:A:265:ASN:ND2	2.28	0.48
1:A:772:GLU:HG3	1:A:773:SER:H	1.78	0.48
1:A:984:VAL:HG12	1:A:985:ASP:N	2.28	0.48
10:O:327:CYS:SG	10:O:328:THR:N	2.87	0.48
16:Z:319:ASN:HA	16:Z:322:LYS:HD3	1.95	0.48
1:A:269:ASP:OD1	1:A:270:SER:N	2.47	0.48
1:A:930:ASN:HB3	1:A:933:GLU:OE1	2.13	0.48
2:C:136:VAL:O	2:C:212:PHE:HA	2.14	0.48
2:C:700:GLU:HG2	2:C:701:GLU:O	2.14	0.48
19:F:49:MET:HB2	19:F:58:ILE:HB	1.96	0.48
12:Q:53:ASN:N	12:Q:53:ASN:ND2	2.60	0.48
14:S:40:ARG:HG2	14:S:41:LYS:H	1.78	0.48
1:A:1863:HIS:CD2	1:A:1873:LYS:HD2	2.49	0.48
1:A:518:VAL:HG11	1:A:689:TYR:CD2	2.48	0.48
1:A:849:LEU:HD12	1:A:973:GLU:HB3	1.96	0.48
2:C:461:LYS:H	2:C:461:LYS:CD	2.27	0.48
2:C:471:HIS:HB2	2:C:592:PHE:CZ	2.49	0.48
2:C:737:ILE:HD12	2:C:747:LEU:HD11	1.95	0.48
10:O:160:ASN:HA	10:O:184:THR:OG1	2.13	0.48
10:O:194:HIS:NE2	10:O:237:ASP:OD1	2.44	0.48
11:P:220:ARG:O	11:P:224:GLU:HG2	2.14	0.48
1:A:1156:HIS:HD2	1:A:1158:ILE:HB	1.79	0.48
1:A:2060:LEU:HD11	1:A:2083:ILE:HD11	1.95	0.48
1:A:705:GLN:HE21	1:A:709:ARG:CG	2.26	0.48
1:A:775:ARG:O	1:A:779:ALA:N	2.42	0.48
3:D:43:G:N3	3:D:43:G:C2'	2.76	0.48
5:L:1116:A:N6	5:L:1117:G:O6	2.46	0.48
10:O:345:PHE:CD2	10:O:381:GLY:HA2	2.49	0.48
11:P:126:PHE:HA	12:Q:30:GLN:HB2	1.95	0.48
1:A:1208:PRO:HB2	1:A:1417:GLN:O	2.14	0.48
1:A:1661:ILE:HG13	1:A:1809:ASN:HD21	1.79	0.48
1:A:183:TRP:HE3	1:A:220:THR:HG21	1.79	0.48
1:A:333:LYS:O	1:A:336:PHE:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLN:HB3	1:A:706:PRO:HD3	1.96	0.48
1:A:905:TYR:HD2	1:A:907:ASN:N	2.11	0.48
1:A:926:LYS:HE3	1:A:929:LEU:HD23	1.95	0.48
10:O:250:LEU:HB2	10:O:260:ILE:HB	1.96	0.48
11:P:174:ASN:O	11:P:174:ASN:ND2	2.46	0.48
1:A:300:LYS:HA	1:A:492:LYS:HA	1.96	0.48
11:P:37:ASN:HD21	11:P:145:PRO:HD3	1.79	0.48
15:T:114:THR:OG1	15:T:118:SER:HA	2.14	0.48
4:E:28:U:H5"	15:T:118:SER:O	2.14	0.48
16:Z:179:TYR:C	16:Z:179:TYR:HD1	2.17	0.48
16:Z:148:LEU:HD12	16:Z:190:LEU:HD21	1.96	0.48
16:Z:363:GLU:O	16:Z:367:GLN:HG2	2.13	0.48
1:A:1368:GLN:O	1:A:1372:LYS:HG3	2.14	0.47
1:A:1368:GLN:NE2	1:A:1389:TYR:OH	2.47	0.47
1:A:1870:VAL:HB	5:L:46:C:C4'	2.36	0.47
1:A:480:TYR:CE2	2:C:275:LEU:HD23	2.49	0.47
1:A:484:PHE:CZ	3:D:81:A:C6	3.02	0.47
1:A:1014:LYS:HG3	1:A:1016:SER:OG	2.15	0.47
1:A:2043:PHE:HB3	1:A:2047:GLN:HB2	1.96	0.47
1:A:2071:ILE:HA	1:A:2074:LEU:HD12	1.96	0.47
1:A:376:ARG:CD	2:C:910:GLU:OE2	2.61	0.47
2:C:167:ASN:O	2:C:171:GLY:HA2	2.15	0.47
2:C:468:LEU:HD13	2:C:492:LEU:C	2.34	0.47
2:C:545:LEU:HD12	2:C:545:LEU:O	2.15	0.47
4:E:14:C:C4'	4:E:15:C:OP2	2.63	0.47
10:O:200:VAL:HG11	10:O:230:VAL:HG23	1.96	0.47
12:Q:291:ILE:HG23	12:Q:292:PRO:N	2.29	0.47
1:A:2018:ASN:HB3	1:A:2021:SER:OG	2.14	0.47
1:A:484:PHE:O	1:A:485:PRO:C	2.52	0.47
1:A:518:VAL:HG11	1:A:689:TYR:HD2	1.79	0.47
1:A:688:TYR:HE1	1:A:701:CYS:HG	1.61	0.47
1:A:653:ILE:HD11	1:A:704:TRP:NE1	2.30	0.47
2:C:418:GLN:HB3	2:C:419:PRO:HD3	1.94	0.47
2:C:707:SER:H	2:C:824:SER:HB3	1.80	0.47
4:E:12:A:H2'	4:E:12:A:N3	2.29	0.47
5:L:15:C:C5	22:I:209:ARG:HG2	2.49	0.47
1:A:872:PRO:HD3	11:P:201:PHE:CE1	2.48	0.47
16:Z:378:THR:HA	16:Z:381:LEU:HD12	1.96	0.47
1:A:1180:GLU:HA	1:A:1183:THR:HG22	1.96	0.47
1:A:1739:ARG:HD2	1:A:1751:TYR:CE2	2.49	0.47
1:A:183:TRP:CD1	1:A:184:GLU:HG3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:O	1:A:473:THR:HG22	2.15	0.47
1:A:617:ASN:O	1:A:621:LEU:HB3	2.15	0.47
21:H:68:PRO:O	21:H:70:LEU:N	2.48	0.47
12:Q:227:LEU:HD21	12:Q:262:PHE:HD1	1.78	0.47
12:Q:77:ASP:OD1	12:Q:78:SER:N	2.47	0.47
1:A:1650:ARG:CZ	6:M:495:A:N7	2.77	0.47
1:A:912:LEU:CD2	1:A:916:LEU:CD1	2.93	0.47
2:C:735:LEU:HG	2:C:736:ASP:O	2.15	0.47
4:E:49:A:H2'	4:E:50:G:H5'	1.96	0.47
13:R:146:LEU:HD23	13:R:147:ASN:N	2.30	0.47
1:A:854:ARG:HD2	1:A:1095:MET:HE3	1.96	0.47
1:A:1339:LEU:HD22	1:A:1440:ILE:HD12	1.97	0.47
1:A:1329:THR:HG21	1:A:1600:GLN:HA	1.94	0.47
1:A:1810:PRO:O	1:A:1814:VAL:HG23	2.15	0.47
1:A:320:ASP:HB3	1:A:483:PRO:HG2	1.96	0.47
2:C:251:GLN:HE21	2:C:255:GLN:HG2	1.79	0.47
2:C:362:LYS:O	2:C:364:PHE:N	2.47	0.47
21:H:35:PRO:HD2	21:H:92:TRP:HH2	1.79	0.47
5:L:71:C:H2'	5:L:72:C:C6	2.49	0.47
5:L:81:G:H2'	5:L:82:C:C6	2.50	0.47
10:O:229:THR:HG21	10:O:272:VAL:N	2.30	0.47
10:O:379:LYS:HD3	11:P:47:ARG:HH22	1.79	0.47
2:C:139:ILE:O	2:C:237:ILE:HA	2.15	0.47
2:C:206:LYS:CD	2:C:208:ARG:HE	2.18	0.47
5:L:101:U:H2'	5:L:102:U:C6	2.50	0.47
5:L:1115:G:H2'	5:L:1116:A:C8	2.50	0.47
4:E:28:U:H1'	15:T:121:ILE:HD13	1.96	0.47
3:D:30:A:H2'	3:D:31:G:O4'	2.15	0.47
12:Q:256:SER:O	12:Q:260:GLU:OE1	2.32	0.47
16:Z:436:LEU:HD21	16:Z:473:LEU:HD11	1.97	0.47
1:A:1880:PHE:HA	1:A:1891:LEU:HD23	1.97	0.47
2:C:914:PHE:HE2	2:C:928:CYS:HG	1.63	0.47
19:F:38:HIS:CE1	19:F:67:LYS:HB3	2.50	0.47
8:N:108:U:H1'	8:N:109:U:OP1	2.15	0.47
10:O:184:THR:O	10:O:201:SER:OG	2.21	0.47
16:Z:203:LYS:HD3	16:Z:203:LYS:HA	1.67	0.47
1:A:756:LEU:CG	14:S:8:GLN:HE22	2.26	0.47
4:E:15:C:H6	4:E:15:C:OP2	1.98	0.47
4:E:59:A:H3'	4:E:60:G:H5''	1.97	0.47
5:L:1115:G:H2'	5:L:1116:A:H8	1.80	0.47
5:L:31:A:O2'	5:L:32:G:H5'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:GLU:HG2	1:A:1169:TYR:CD1	2.50	0.47
1:A:1275:MET:C	1:A:1277:GLU:H	2.18	0.47
1:A:1690:LYS:HD2	1:A:1698:ALA:H	1.79	0.47
1:A:266:LEU:HD23	1:A:268:LEU:H	1.79	0.47
2:C:746:LYS:O	2:C:750:ILE:HG12	2.15	0.47
1:A:1870:VAL:CG2	5:L:46:C:H5'	2.40	0.47
10:O:343:THR:HB	11:P:47:ARG:HB2	1.96	0.47
2:C:360:ARG:HG2	2:C:362:LYS:HB2	1.97	0.46
2:C:365:GLU:CG	2:C:366:ASN:H	2.25	0.46
3:D:103:A:O4'	9:J:12:LYS:NZ	2.48	0.46
1:A:488:ARG:NH1	3:D:81:A:H61	2.12	0.46
19:F:75:TYR:CE2	19:F:76:LEU:HG	2.50	0.46
5:L:61:A:H2'	5:L:62:C:C6	2.50	0.46
10:O:161:ASP:O	10:O:162:THR:OG1	2.26	0.46
13:R:33:TRP:HD1	13:R:34:TYR:CD1	2.33	0.46
1:A:165:LEU:O	1:A:622:MET:HE1	2.15	0.46
1:A:288:GLU:O	1:A:288:GLU:HG2	2.15	0.46
1:A:304:ASP:OD1	1:A:305:LEU:N	2.43	0.46
1:A:401:PRO:O	1:A:402:TRP:HB3	2.14	0.46
2:C:292:ILE:HG12	2:C:311:ILE:HD13	1.97	0.46
2:C:468:LEU:HD12	2:C:492:LEU:H	1.59	0.46
4:E:1:G:H2'	4:E:2:U:H6	1.81	0.46
5:L:73:U:H2'	5:L:74:C:C6	2.49	0.46
5:L:80:G:H2'	5:L:81:G:H8	1.81	0.46
13:R:206:LEU:HD23	13:R:208:SER:O	2.14	0.46
1:A:589:THR:OG1	13:R:38:SER:HB3	2.15	0.46
15:T:31:ARG:O	15:T:35:LYS:HG3	2.16	0.46
16:Z:382:ARG:HA	16:Z:422:PHE:CD2	2.50	0.46
1:A:1626:GLN:NE2	1:A:1692:TYR:O	2.47	0.46
1:A:2041:PRO:HG2	1:A:2043:PHE:HE2	1.80	0.46
1:A:610:ARG:O	1:A:614:ARG:HG3	2.16	0.46
1:A:757:GLU:HG3	1:A:758:LEU:N	2.29	0.46
1:A:791:ARG:NH2	11:P:173:LYS:CD	2.78	0.46
2:C:353:TYR:HD1	2:C:371:PRO:HA	1.80	0.46
2:C:945:LEU:O	2:C:945:LEU:HD12	2.15	0.46
5:L:25:A:C2'	5:L:27:A:OP2	2.63	0.46
5:L:98:U:H2'	5:L:99:U:C6	2.50	0.46
10:O:187:ASP:OD2	10:O:230:VAL:N	2.28	0.46
10:O:446:LEU:N	10:O:446:LEU:HD13	2.30	0.46
13:R:62:THR:HG21	13:R:89:TYR:O	2.15	0.46
16:Z:437:GLN:HG2	16:Z:473:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:LEU:HD23	1:A:1248:VAL:HG22	1.97	0.46
1:A:1882:LEU:HD21	1:A:1965:PHE:CE1	2.50	0.46
1:A:680:CYS:HG	1:A:711:TRP:HE1	1.62	0.46
1:A:756:LEU:HD21	14:S:8:GLN:HE22	1.79	0.46
2:C:567:ILE:HG22	2:C:571:TYR:HE2	1.81	0.46
4:E:64:U:HO2'	4:E:65:U:P	2.32	0.46
5:L:54:U:H2'	5:L:55:G:H8	1.81	0.46
10:O:279:PRO:HG2	10:O:292:LEU:HB3	1.97	0.46
10:O:329:ASP:OD2	10:O:349:LYS:HG3	2.16	0.46
13:R:170:ILE:HG12	13:R:186:PHE:CE1	2.51	0.46
1:A:2063:TYR:CD1	1:A:2067:TYR:HD2	2.34	0.46
1:A:2060:LEU:HD21	1:A:2079:ILE:HG23	1.97	0.46
1:A:354:PRO:O	1:A:355:LEU:HB3	2.16	0.46
1:A:177:GLU:CB	1:A:712:LEU:HD11	2.45	0.46
3:D:175:G:H4'	3:D:176:A:O4'	2.15	0.46
5:L:1099:G:N3	5:L:1099:G:C5'	2.73	0.46
5:L:120:G:H4'	5:L:121:C:O4'	2.15	0.46
14:S:159:ASP:OD1	14:S:160:MET:N	2.49	0.46
14:S:5:HIS:O	14:S:6:ARG:HD2	2.15	0.46
15:T:34:GLN:O	15:T:36:ASP:N	2.49	0.46
16:Z:152:ILE:HG23	16:Z:197:LEU:HB2	1.98	0.46
1:A:1476:ALA:C	1:A:1478:GLU:H	2.19	0.46
1:A:1773:VAL:HG22	1:A:1788:GLY:HA3	1.97	0.46
1:A:1805:ILE:HA	1:A:1808:ALA:HB3	1.97	0.46
1:A:133:GLU:OE2	1:A:561:THR:HG23	2.16	0.46
5:L:1100:A:C2	5:L:1101:C:N1	2.82	0.46
1:A:1327:THR:HG23	5:L:35:U:H5'	1.70	0.46
5:L:58:A:H2'	5:L:59:C:C6	2.50	0.46
12:Q:209:ASN:CG	12:Q:288:ILE:O	2.54	0.46
12:Q:98:ASN:O	12:Q:99:VAL:HG12	2.16	0.46
1:A:1019:GLU:OE2	1:A:1027:LYS:NZ	2.31	0.46
1:A:905:TYR:CE2	1:A:907:ASN:CB	2.86	0.46
2:C:144:SER:HA	2:C:240:ASP:OD1	2.14	0.46
2:C:306:PRO:HG2	2:C:349:TRP:CE3	2.51	0.46
2:C:544:LEU:HD23	2:C:562:VAL:HG12	1.97	0.46
10:O:317:HIS:CE1	10:O:319:LYS:HB2	2.51	0.46
10:O:317:HIS:HE1	10:O:319:LYS:HB2	1.81	0.46
15:T:61:ARG:HH22	15:T:101:GLU:HG2	1.81	0.46
1:A:1308:GLU:HG2	1:A:1311:LYS:HD2	1.98	0.46
1:A:2041:PRO:HG2	1:A:2043:PHE:CE2	2.51	0.46
1:A:617:ASN:O	1:A:621:LEU:CB	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:THR:O	1:A:913:VAL:HG23	2.14	0.46
2:C:268:ASN:HA	2:C:314:ALA:O	2.16	0.46
2:C:667:GLU:N	2:C:667:GLU:OE1	2.49	0.46
2:C:869:HIS:NE2	2:C:925:LEU:HD22	2.31	0.46
22:I:159:LYS:O	22:I:160:LEU:HB2	2.16	0.46
5:L:67:A:H2'	5:L:68:U:C6	2.50	0.46
10:O:427:LYS:HE2	10:O:430:GLU:OE2	2.16	0.46
16:Z:393:SER:OG	16:Z:430:GLU:OE1	2.19	0.46
1:A:1602:PRO:HD2	1:A:1605:ARG:NH2	2.31	0.46
1:A:426:PRO:O	16:Z:202:GLN:CB	2.61	0.46
1:A:997:GLN:OE1	1:A:1511:ARG:NH2	2.49	0.46
2:C:464:PRO:O	2:C:465:GLU:HG2	2.16	0.46
21:H:60:GLN:O	21:H:63:THR:OG1	2.30	0.46
5:L:15:C:C4	22:I:209:ARG:HG2	2.48	0.46
5:L:19:U:H1'	11:P:178:TYR:HE2	1.80	0.46
5:L:68:U:H2'	5:L:69:G:H8	1.81	0.46
5:L:79:A:H2'	5:L:80:G:H8	1.81	0.46
1:A:1033:ASN:HD22	1:A:1288:LEU:HB3	1.81	0.46
7:B:88:U:H2'	7:B:89:A:C4'	2.46	0.46
2:C:101:GLN:NE2	3:D:77:A:H61	2.14	0.46
2:C:348:LEU:HD21	2:C:377:ILE:HD11	1.97	0.46
2:C:680:SER:OG	2:C:681:CYS:N	2.49	0.46
1:A:484:PHE:CZ	3:D:81:A:N7	2.84	0.46
4:E:38:U:O2	13:R:196:LYS:NZ	2.40	0.46
5:L:25:A:H2'	5:L:27:A:P	2.55	0.46
10:O:218:ARG:NH1	10:O:253:MET:O	2.49	0.46
12:Q:222:THR:CA	12:Q:225:GLN:NE2	2.75	0.46
1:A:1434:GLU:HG2	1:A:1435:LYS:N	2.30	0.45
1:A:1716:LEU:HB2	1:A:1719:GLU:HG3	1.97	0.45
1:A:1964:PRO:HG3	1:A:2013:ARG:HG3	1.98	0.45
1:A:759:ARG:HH12	14:S:7:PRO:CB	2.26	0.45
1:A:772:GLU:HG3	1:A:773:SER:N	2.31	0.45
2:C:712:ALA:HA	2:C:817:GLN:O	2.16	0.45
2:C:927:MET:HB2	2:C:927:MET:HE2	1.82	0.45
20:G:18:LYS:O	20:G:22:LYS:HG2	2.16	0.45
7:B:90:A:H61	9:J:6:ILE:HD11	1.81	0.45
5:L:106:A:H2'	5:L:107:U:C6	2.50	0.45
5:L:69:G:H2'	5:L:70:A:H8	1.82	0.45
5:L:72:C:H2'	5:L:73:U:C6	2.50	0.45
5:L:78:G:H2'	5:L:79:A:H8	1.82	0.45
5:L:83:U:H2'	5:L:84:C:C6	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:265:HIS:NE2	10:O:283:SER:OG	2.43	0.45
12:Q:56:ILE:HD13	13:R:105:ARG:NH2	2.29	0.45
1:A:220:THR:O	1:A:224:MET:HG2	2.16	0.45
2:C:142:LEU:HB3	2:C:143:HIS:CD2	2.51	0.45
3:D:83:C:HO2'	3:D:84:A:P	2.38	0.45
4:E:63:G:HO2'	14:S:8:GLN:CB	2.29	0.45
19:F:99:THR:HG22	19:F:106:TYR:CE1	2.50	0.45
5:L:103:A:H2'	5:L:104:C:C6	2.50	0.45
5:L:1103:C:N1	5:L:1114:G:N2	2.64	0.45
5:L:19:U:C6	11:P:178:TYR:HD2	2.33	0.45
5:L:62:C:H2'	5:L:63:U:C6	2.50	0.45
1:A:742:VAL:HG12	10:O:224:LEU:HD23	1.97	0.45
16:Z:152:ILE:HD13	16:Z:194:LEU:CA	2.40	0.45
2:C:869:HIS:CD2	2:C:925:LEU:HD13	2.51	0.45
4:E:4:C:H2'	4:E:5:G:O4'	2.16	0.45
4:E:66:C:H5'	4:E:66:C:H6	1.79	0.45
19:F:42:ARG:O	20:G:10:LYS:HE3	2.16	0.45
12:Q:53:ASN:ND2	12:Q:54:ASN:N	2.60	0.45
13:R:170:ILE:HG21	13:R:173:ILE:HG13	1.98	0.45
2:C:485:LEU:HA	2:C:563:LEU:HD23	1.98	0.45
2:C:760:LEU:O	2:C:764:ASN:ND2	2.49	0.45
19:F:38:HIS:CE1	19:F:67:LYS:HD3	2.52	0.45
19:F:51:CYS:O	19:F:55:ASN:HA	2.17	0.45
5:L:100:G:H2'	5:L:101:U:C6	2.50	0.45
10:O:342:LEU:HB3	11:P:47:ARG:CD	2.47	0.45
12:Q:104:ALA:HB1	12:Q:110:LYS:CB	2.42	0.45
12:Q:206:PHE:HB3	12:Q:208:TYR:OH	2.17	0.45
1:A:1289:VAL:HG22	1:A:1296:ARG:HG2	1.97	0.45
1:A:1435:LYS:O	1:A:1436:LEU:HD12	2.16	0.45
1:A:1734:PHE:CD1	1:A:1773:VAL:HB	2.52	0.45
4:E:12:A:C2	4:E:13:A:O4'	2.70	0.45
10:O:252:ASP:HB2	10:O:259:VAL:CG2	2.47	0.45
10:O:372:VAL:HA	10:O:387:LEU:O	2.17	0.45
15:T:123:ARG:HD2	15:T:153:CYS:HB2	1.98	0.45
1:A:294:ASN:HB2	1:A:299:LYS:O	2.17	0.45
1:A:234:PHE:HE1	1:A:648:GLN:HG2	1.82	0.45
4:E:84:C:H3'	4:E:85:C:H5''	1.97	0.45
1:A:1508:HIS:HD2	1:A:1529:ASN:HD22	1.64	0.45
1:A:275:TYR:HB2	1:A:310:ASN:HD22	1.82	0.45
1:A:869:LYS:O	11:P:198:ASN:ND2	2.44	0.45
1:A:878:GLU:O	1:A:881:THR:OG1	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:LEU:HD11	1:A:1078:ILE:HG23	1.99	0.45
1:A:911:ILE:CG2	1:A:997:GLN:CG	2.88	0.45
2:C:131:GLU:OE2	2:C:445:PRO:HG3	2.17	0.45
2:C:135:ASN:O	2:C:233:ASP:N	2.47	0.45
1:A:371:ASP:HB3	2:C:972:ARG:HD3	1.99	0.45
3:D:107:C:O2'	14:S:34:HIS:HE1	1.99	0.45
5:L:56:U:H2'	5:L:57:A:H8	1.82	0.45
5:L:96:A:H2'	5:L:97:U:C6	2.50	0.45
10:O:214:ASN:O	10:O:215:GLN:NE2	2.50	0.45
1:A:1051:GLU:HG2	1:A:1169:TYR:CE1	2.52	0.45
1:A:299:LYS:HA	1:A:493:MET:CG	2.46	0.45
1:A:609:GLU:OE2	4:E:43:C:O2'	2.26	0.45
2:C:500:ARG:NH1	2:C:536:SER:OG	2.50	0.45
5:L:97:U:H2'	5:L:98:U:C6	2.50	0.45
10:O:304:LEU:HD13	10:O:334:TRP:CE3	2.52	0.45
13:R:145:ALA:HB2	13:R:204:LEU:HD12	1.99	0.45
15:T:156:THR:HG23	15:T:157:ASP:H	1.81	0.45
16:Z:203:LYS:O	16:Z:204:ASP:HB2	2.17	0.45
1:A:1275:MET:HE1	1:A:1299:LYS:HD2	1.98	0.45
1:A:1539:LEU:O	1:A:1541:ALA:N	2.50	0.45
1:A:1689:ARG:NH2	19:F:12:PRO:O	2.50	0.45
1:A:1880:PHE:CE1	1:A:1889:LEU:HD22	2.52	0.45
1:A:203:ASN:O	1:A:204:GLU:HG3	2.16	0.45
1:A:847:LYS:HG2	5:L:24:U:C6	2.51	0.45
1:A:852:LEU:HD23	1:A:852:LEU:HA	1.68	0.45
2:C:749:LYS:O	2:C:753:THR:CB	2.64	0.45
5:L:25:A:H3'	5:L:26:G:C5'	2.46	0.45
5:L:59:C:H2'	5:L:60:A:H8	1.82	0.45
5:L:99:U:H2'	5:L:100:G:H8	1.81	0.45
10:O:271:GLN:HG2	10:O:314:THR:H	1.82	0.45
12:Q:103:GLU:OE2	13:R:131:ARG:NH2	2.46	0.45
16:Z:174:TRP:CZ2	16:Z:201:ARG:HB2	2.52	0.45
16:Z:204:ASP:O	16:Z:205:TYR:CD2	2.70	0.45
1:A:867:ILE:HD13	1:A:1101:TYR:CE1	2.51	0.45
1:A:548:LEU:O	1:A:551:LEU:N	2.49	0.45
1:A:680:CYS:SG	1:A:711:TRP:NE1	2.89	0.45
2:C:245:VAL:HG11	2:C:295:ILE:HG22	1.98	0.45
5:L:19:U:H4'	5:L:19:U:OP1	2.17	0.45
1:A:1907:GLN:HG3	6:M:493:A:OP1	2.17	0.45
12:Q:107:ASP:O	12:Q:110:LYS:HG2	2.17	0.45
13:R:70:LEU:HB3	13:R:102:LEU:CD2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:4:TRP:CZ2	13:R:92:HIS:CD2	3.05	0.45
14:S:10:GLU:HG2	14:S:11:ALA:N	2.32	0.45
16:Z:179:TYR:CD1	16:Z:179:TYR:O	2.70	0.45
16:Z:186:LEU:N	16:Z:186:LEU:CD1	2.73	0.45
16:Z:191:ARG:NE	16:Z:192:GLU:OE2	2.50	0.45
1:A:1899:TRP:CE3	1:A:1905:LEU:HD22	2.52	0.44
1:A:213:TYR:OH	1:A:217:TRP:NE1	2.50	0.44
2:C:116:THR:HG22	2:C:158:HIS:CD2	2.51	0.44
2:C:780:PRO:O	2:C:784:SER:N	2.25	0.44
5:L:70:A:H2'	5:L:71:C:C6	2.50	0.44
1:A:1379:MET:HE1	1:A:1620:TYR:N	2.26	0.44
1:A:1716:LEU:HD11	1:A:1753:ARG:HH21	1.81	0.44
1:A:249:LEU:HD13	1:A:254:HIS:HB2	1.99	0.44
1:A:402:TRP:O	1:A:402:TRP:CG	2.69	0.44
2:C:126:MET:SD	2:C:132:ARG:HD2	2.57	0.44
2:C:154:VAL:HG11	2:C:177:TYR:CD2	2.52	0.44
19:F:27:MET:HE3	21:H:32:TYR:HE1	1.82	0.44
21:H:41:VAL:CG1	21:H:42:LYS:H	2.29	0.44
5:L:105:A:H2'	5:L:106:A:H8	1.82	0.44
6:M:498:C:O2	21:H:2:SER:HB3	2.18	0.44
10:O:220:TYR:CE1	10:O:256:ARG:HG2	2.53	0.44
12:Q:5:ILE:HG22	12:Q:42:THR:HG23	1.99	0.44
13:R:97:GLU:O	13:R:100:GLY:N	2.51	0.44
15:T:44:LYS:O	15:T:48:GLN:HG2	2.18	0.44
1:A:1617:ALA:N	1:A:1744:ASP:OD2	2.50	0.44
1:A:1799:GLN:O	1:A:1803:ARG:HG3	2.18	0.44
1:A:1993:ASP:CG	1:A:2038:HIS:HB3	2.38	0.44
1:A:484:PHE:HE1	1:A:488:ARG:CD	2.31	0.44
1:A:759:ARG:NH2	1:A:783:LEU:HD23	2.33	0.44
1:A:791:ARG:HH22	11:P:173:LYS:CD	2.27	0.44
5:L:1098:C:H2'	5:L:1099:G:H5"	1.98	0.44
6:M:493:A:H2'	6:M:494:G:C8	2.52	0.44
8:N:100:G:OP2	8:N:100:G:N2	2.45	0.44
10:O:121:GLN:OE1	10:O:121:GLN:N	2.51	0.44
12:Q:26:THR:O	12:Q:44:TYR:HA	2.17	0.44
1:A:1711:VAL:CG1	1:A:1789:ASN:HB3	2.47	0.44
7:B:88:U:H2'	7:B:89:A:H4'	2.00	0.44
2:C:67:GLU:O	2:C:71:GLY:N	2.51	0.44
5:L:5:A:C5'	22:I:114:THR:HB	2.42	0.44
5:L:1116:A:C4	5:L:1117:G:C5	3.05	0.44
5:L:55:G:H2'	5:L:56:U:C6	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:57:A:H2'	5:L:58:A:H8	1.82	0.44
5:L:5:A:H2'	5:L:6:U:C6	2.52	0.44
13:R:46:ARG:NH2	13:R:220:GLY:O	2.50	0.44
1:A:1647:GLN:O	1:A:1650:ARG:NH1	2.51	0.44
1:A:234:PHE:HD1	1:A:235:LYS:N	2.16	0.44
1:A:928:ARG:HH12	5:L:31:A:P	2.40	0.44
2:C:867:THR:O	2:C:926:GLY:HA2	2.17	0.44
4:E:42:A:HO2'	4:E:43:C:P	2.40	0.44
4:E:51:A:C1'	4:E:52:G:P	3.06	0.44
4:E:67:C:OP1	4:E:67:C:H6	2.00	0.44
6:M:485:U:C5'	21:H:36:ARG:HE	2.29	0.44
9:J:9:LYS:O	9:J:10:SER:OG	2.36	0.44
5:L:102:U:H2'	5:L:103:A:H8	1.82	0.44
10:O:251:TRP:CZ3	10:O:258:PRO:HB3	2.53	0.44
10:O:392:MET:HG3	10:O:393:VAL:N	2.32	0.44
10:O:437:GLU:N	10:O:438:PRO:HD3	2.32	0.44
13:R:117:PHE:O	13:R:129:SER:HA	2.17	0.44
13:R:154:ALA:O	13:R:158:SER:CB	2.64	0.44
16:Z:191:ARG:NE	16:Z:192:GLU:OE1	2.45	0.44
16:Z:285:SER:O	16:Z:288:ASP:N	2.51	0.44
1:A:1160:LEU:H	1:A:1171:LEU:HB3	1.83	0.44
1:A:1282:ASP:CG	1:A:1283:GLU:H	2.20	0.44
1:A:1893:ILE:O	1:A:1984:PRO:HA	2.17	0.44
1:A:2081:ASP:O	1:A:2085:GLY:N	2.51	0.44
2:C:233:ASP:OD1	2:C:487:ARG:NH1	2.43	0.44
4:E:67:C:OP1	4:E:67:C:C6	2.70	0.44
19:F:63:LYS:HE2	20:G:6:LEU:HD22	2.00	0.44
5:L:1120:G:C8	5:L:1120:G:C5'	3.00	0.44
5:L:74:C:H2'	5:L:75:A:H8	1.81	0.44
5:L:82:C:H2'	5:L:83:U:C6	2.50	0.44
11:P:216:ARG:HA	11:P:219:ILE:HD12	1.99	0.44
5:L:21:G:N7	14:S:5:HIS:HB3	2.33	0.44
1:A:1449:ASN:HB3	16:Z:338:THR:CG2	2.48	0.44
1:A:1350:ILE:HG23	1:A:1356:LEU:HD22	2.00	0.44
4:E:48:C:H2'	4:E:49:A:O4'	2.17	0.44
6:M:494:G:H2'	6:M:495:A:OP2	2.18	0.44
6:M:507:U:H2'	6:M:508:U:O4'	2.18	0.44
12:Q:246:ALA:O	12:Q:247:LYS:HB2	2.18	0.44
12:Q:51:ARG:HG3	12:Q:51:ARG:O	2.18	0.44
13:R:46:ARG:HH22	13:R:222:LEU:HG	1.83	0.44
1:A:1209:LYS:HD2	1:A:1417:GLN:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:TRP:CZ2	1:A:1491:ILE:HD13	2.53	0.44
2:C:362:LYS:HG3	2:C:363:PRO:HD2	1.98	0.44
2:C:378:LEU:HA	2:C:378:LEU:HD23	1.82	0.44
2:C:831:ILE:HG13	2:C:832:ASP:N	2.26	0.44
1:A:484:PHE:CE2	3:D:81:A:C5	3.06	0.44
4:E:5:G:H2'	4:E:6:C:C6	2.52	0.44
5:L:66:A:H2'	5:L:67:A:H8	1.82	0.44
2:C:75:GLU:HB2	10:O:133:ARG:HG3	2.00	0.44
13:R:221:LEU:O	13:R:221:LEU:HD12	2.18	0.44
1:A:1080:ASP:HB3	2:C:82:ASN:ND2	58.51	0.44
1:A:1129:GLU:O	1:A:1132:THR:OG1	2.23	0.44
1:A:1211:SER:OG	1:A:1268:ARG:NH1	2.51	0.44
1:A:1280:SER:HB3	16:Z:394:TYR:CD2	2.53	0.44
1:A:1703:MET:N	1:A:1732:MET:O	2.50	0.44
1:A:640:ARG:HH11	1:A:640:ARG:CG	2.31	0.44
1:A:912:LEU:HD12	1:A:951:LEU:HD21	2.00	0.44
2:C:202:ASP:OD1	2:C:206:LYS:O	2.36	0.44
10:O:204:LYS:HG2	10:O:225:SER:HA	2.00	0.44
10:O:446:LEU:H	10:O:446:LEU:HD13	1.83	0.44
12:Q:205:PHE:HB3	12:Q:291:ILE:O	2.17	0.44
12:Q:239:SER:O	12:Q:251:LEU:HD12	2.18	0.44
13:R:54:GLN:H	13:R:58:HIS:HD2	1.66	0.44
16:Z:191:ARG:HB3	16:Z:192:GLU:OE1	2.18	0.44
1:A:1214:ARG:HB2	1:A:1255:ASN:OD1	2.17	0.43
2:C:237:ILE:HD12	2:C:265:PHE:HE1	1.82	0.43
1:A:428:LEU:HD22	2:C:896:GLY:O	2.18	0.43
21:H:86:PHE:HE2	21:H:90:LYS:HE3	1.83	0.43
5:L:104:C:H2'	5:L:105:A:H8	1.82	0.43
10:O:208:CYS:SG	10:O:209:TRP:N	2.91	0.43
1:A:645:ASP:HB3	1:A:648:GLN:HB2	1.99	0.43
2:C:767:SER:OG	2:C:796:ILE:HD13	2.18	0.43
3:D:43:G:H4'	3:D:44:A:OP1	2.18	0.43
19:F:83:ARG:HG3	19:F:97:PHE:O	2.17	0.43
5:L:5:A:OP1	22:I:114:THR:CG2	2.64	0.43
5:L:60:A:H2'	5:L:61:A:H8	1.82	0.43
5:L:78:G:OP2	13:R:151:LEU:HD13	2.18	0.43
10:O:229:THR:OG1	10:O:270:ASN:O	2.34	0.43
10:O:351:GLY:HA2	10:O:352:ILE:HA	1.65	0.43
10:O:391:GLU:O	10:O:392:MET:HB2	2.18	0.43
11:P:101:PRO:C	11:P:103:ASN:H	2.20	0.43
1:A:1094:ASP:CG	11:P:172:TRP:HE1	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:194:LEU:C	16:Z:194:LEU:HD22	2.38	0.43
1:A:1280:SER:OG	16:Z:348:GLU:OE1	2.22	0.43
1:A:466:GLU:HG2	1:A:467:GLU:N	2.33	0.43
1:A:676:GLN:OE1	1:A:676:GLN:N	2.44	0.43
1:A:911:ILE:CG2	1:A:997:GLN:HG2	2.46	0.43
12:Q:16:CYS:HB2	13:R:104:LEU:HD21	1.99	0.43
16:Z:168:LYS:HA	16:Z:168:LYS:HD2	1.75	0.43
1:A:1045:GLN:HG2	1:A:1175:GLU:HG2	2.00	0.43
1:A:1714:PRO:HB2	1:A:1787:TYR:CZ	2.53	0.43
1:A:2013:ARG:CZ	1:A:2085:GLY:HA2	2.48	0.43
1:A:2013:ARG:NH2	1:A:2084:LEU:O	2.52	0.43
1:A:902:PRO:CG	1:A:904:THR:O	2.66	0.43
2:C:380:PRO:O	2:C:384:ILE:HG13	2.19	0.43
2:C:166:LYS:HE2	4:E:85:C:N4	79.46	0.43
10:O:359:ASN:OD1	10:O:411:GLY:HA3	2.19	0.43
12:Q:205:PHE:CD1	12:Q:205:PHE:N	2.85	0.43
12:Q:37:CYS:SG	12:Q:39:LEU:HB2	2.57	0.43
12:Q:241:ILE:HG12	13:R:161:ARG:HD3	1.98	0.43
1:A:1286:TRP:HA	1:A:1448:GLU:OE2	2.19	0.43
1:A:342:LEU:HD22	1:A:392:ASN:ND2	2.32	0.43
1:A:484:PHE:CD1	1:A:484:PHE:C	2.91	0.43
1:A:768:GLU:OE2	10:O:310:SER:HB3	2.18	0.43
2:C:458:ILE:HG12	2:C:458:ILE:H	1.57	0.43
2:C:576:THR:HG22	2:C:592:PHE:HB2	2.01	0.43
4:E:86:G:C6	4:E:87:U:C4	3.06	0.43
5:L:1102:C:C2	5:L:1103:C:C5	3.06	0.43
10:O:437:GLU:OE1	10:O:438:PRO:HA	2.17	0.43
13:R:207:PRO:O	13:R:212:TRP:NE1	2.50	0.43
1:A:426:PRO:HG3	16:Z:201:ARG:NE	2.32	0.43
1:A:1865:THR:HG21	1:A:1869:ASN:HD22	1.84	0.43
1:A:1932:GLN:HG2	1:A:1955:ALA:HB3	1.99	0.43
1:A:831:ARG:HD2	1:A:831:ARG:HA	1.75	0.43
1:A:936:GLU:O	1:A:939:LEU:N	2.52	0.43
2:C:223:ASP:OD2	2:C:647:ASN:ND2	2.40	0.43
2:C:231:ALA:O	2:C:487:ARG:NH1	2.52	0.43
2:C:473:LEU:HD12	2:C:485:LEU:CD2	2.49	0.43
2:C:760:LEU:C	2:C:764:ASN:HD22	2.22	0.43
2:C:952:PRO:HG3	2:C:957:ALA:HA	2.00	0.43
5:L:1120:G:C8	5:L:1120:G:H5"	2.51	0.43
5:L:15:C:C1'	5:L:16:U:C6	2.92	0.43
13:R:105:ARG:HG2	13:R:109:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:HIS:O	2:C:294:ASN:HB2	2.19	0.43
2:C:353:TYR:CD1	2:C:371:PRO:HA	2.53	0.43
2:C:373:PHE:O	2:C:377:ILE:HB	2.18	0.43
2:C:133:ILE:HD12	2:C:560:GLN:HB3	2.00	0.43
2:C:864:VAL:HG12	2:C:866:ILE:HG13	2.00	0.43
4:E:75:A:C2'	4:E:76:A:H5'	2.49	0.43
21:H:20:ALA:HB1	21:H:26:TYR:HB3	2.01	0.43
22:I:173:LYS:O	22:I:177:GLU:HG2	2.19	0.43
11:P:178:TYR:HD1	22:I:200:ASN:OD1	2.02	0.43
11:P:115:VAL:HG21	12:Q:24:ARG:NH1	2.34	0.43
12:Q:203:LYS:HG3	12:Q:256:SER:OG	2.18	0.43
1:A:1285:VAL:HG22	1:A:1301:TYR:HD1	1.83	0.43
1:A:1468:ALA:HA	1:A:1473:ARG:CG	2.48	0.43
1:A:1812:LEU:HB3	1:A:1816:ARG:NH1	2.34	0.43
1:A:1934:ILE:HG12	1:A:1957:ARG:HB2	2.00	0.43
1:A:426:PRO:HG2	16:Z:201:ARG:HE	1.80	0.43
2:C:251:GLN:HE21	2:C:255:GLN:HE21	1.67	0.43
4:E:56:A:HO2'	4:E:57:U:P	2.42	0.43
22:I:190:TYR:CE2	22:I:195:PHE:HZ	2.35	0.43
12:Q:251:LEU:HD12	12:Q:252:ARG:N	2.33	0.43
12:Q:290:ILE:HG22	12:Q:292:PRO:HD2	2.00	0.43
13:R:55:PRO:HB3	13:R:93:ILE:HD11	2.00	0.43
16:Z:205:TYR:O	16:Z:207:SER:N	2.50	0.43
1:A:1094:ASP:OD2	11:P:172:TRP:NE1	2.49	0.43
1:A:1616:ARG:NH2	1:A:1744:ASP:OD1	2.44	0.43
4:E:89:U:H5	22:I:176:TYR:O	2.02	0.43
5:L:1100:A:H61	5:L:1116:A:N6	2.07	0.43
6:M:498:C:O2'	21:H:2:SER:CA	2.54	0.43
6:M:506:U:H2'	6:M:507:U:C6	2.54	0.43
10:O:181:HIS:CE1	10:O:207:LYS:HD2	2.53	0.43
10:O:418:GLU:OE1	10:O:424:LYS:NZ	2.30	0.43
13:R:92:HIS:HE1	13:R:98:ASP:OD2	2.01	0.43
16:Z:431:LEU:HB3	16:Z:435:GLU:HB3	2.01	0.43
1:A:1521:ARG:HD3	6:M:507:U:H5''	2.01	0.43
1:A:728:ASN:ND2	4:E:72:C:HO2'	2.11	0.43
2:C:176:ARG:NH1	2:C:179:ASP:OD2	2.52	0.43
2:C:387:TYR:HA	2:C:391:MET:HG2	2.00	0.43
8:N:114:U:C4'	13:R:231:ASP:HB3	2.48	0.43
1:A:856:TRP:NE1	14:S:174:VAL:HG11	2.34	0.43
16:Z:178:ARG:HB2	16:Z:198:PHE:CZ	2.43	0.43
1:A:676:GLN:HE21	1:A:714:PHE:HB2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:ASP:OD2	1:A:1511:ARG:NH1	2.51	0.42
2:C:348:LEU:O	2:C:372:THR:HB	2.19	0.42
2:C:77:LEU:O	2:C:77:LEU:HD12	2.19	0.42
20:G:7:ASN:O	20:G:13:ASN:ND2	2.52	0.42
22:I:110:ARG:O	22:I:114:THR:HG23	2.19	0.42
5:L:18:U:H5''	22:I:199:LYS:HG3	2.00	0.42
5:L:44:U:O5'	5:L:44:U:H6	2.02	0.42
10:O:263:VAL:O	10:O:293:TRP:HH2	2.03	0.42
10:O:132:SER:OG	10:O:425:ILE:O	2.25	0.42
12:Q:203:LYS:O	12:Q:251:LEU:O	2.37	0.42
13:R:94:PRO:HB2	13:R:191:ASN:ND2	2.34	0.42
13:R:245:GLU:HG3	13:R:249:MET:HE2	2.01	0.42
1:A:1438:PRO:HB2	1:A:1443:TYR:HE2	1.84	0.42
1:A:1602:PRO:HG2	1:A:1605:ARG:HB3	2.01	0.42
1:A:285:PRO:HD2	1:A:298:TYR:OH	2.19	0.42
2:C:81:LYS:O	2:C:82:ASN:ND2	2.52	0.42
5:L:19:U:C1'	11:P:178:TYR:CD2	3.03	0.42
12:Q:261:ARG:O	12:Q:264:SER:HB2	2.19	0.42
13:R:171:ASP:N	13:R:185:LYS:O	2.52	0.42
13:R:234:ALA:HA	13:R:237:ARG:HD3	2.01	0.42
1:A:1361:VAL:HG21	1:A:1407:ILE:HD11	2.01	0.42
1:A:404:ASN:OD1	1:A:405:ASN:N	2.51	0.42
2:C:463:THR:O	2:C:463:THR:OG1	2.32	0.42
2:C:602:VAL:HG13	2:C:860:PRO:HG2	2.01	0.42
2:C:829:VAL:HG12	2:C:830:ASN:N	2.31	0.42
4:E:34:A:N1	13:R:73:CYS:HA	2.34	0.42
6:M:483:U:O2	21:H:91:ARG:NH2	2.52	0.42
1:A:791:ARG:CZ	11:P:173:LYS:HE2	2.50	0.42
12:Q:213:SER:HA	13:R:237:ARG:CZ	2.49	0.42
13:R:72:PHE:HE1	13:R:90:LEU:HD12	1.84	0.42
11:P:86:ASN:ND2	14:S:24:GLY:O	2.52	0.42
15:T:156:THR:HG23	15:T:157:ASP:N	2.34	0.42
16:Z:184:GLN:NE2	16:Z:185:GLU:H	2.13	0.42
1:A:1158:ILE:HG12	1:A:1172:PHE:CE1	2.54	0.42
5:L:1097:G:H2'	5:L:1098:C:C6	2.54	0.42
1:A:134:MET:CE	15:T:107:ARG:HD2	2.49	0.42
1:A:1070:LEU:HA	1:A:1073:ILE:HG22	2.01	0.42
1:A:235:LYS:HB3	1:A:648:GLN:NE2	2.35	0.42
2:C:144:SER:HB2	2:C:238:VAL:HG12	2.02	0.42
19:F:58:ILE:HD12	19:F:64:PHE:HZ	1.84	0.42
5:L:36:A:N6	6:M:500:A:H61	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:110:A:H2	13:R:46:ARG:HD3	1.79	0.42
12:Q:259:GLY:O	12:Q:263:VAL:CG2	2.66	0.42
13:R:159:ARG:O	13:R:163:VAL:HG23	2.19	0.42
16:Z:67:LYS:HA	16:Z:67:LYS:HE2	2.02	0.42
1:A:2006:SER:O	1:A:2009:THR:OG1	2.27	0.42
1:A:607:THR:HG23	1:A:610:ARG:NH1	2.33	0.42
2:C:772:ASN:HD21	2:C:803:VAL:HG22	1.84	0.42
10:O:418:GLU:OE2	10:O:424:LYS:HD2	2.19	0.42
11:P:87:ASN:HB3	11:P:90:SER:H	1.84	0.42
4:E:42:A:C2	13:R:38:SER:O	2.72	0.42
16:Z:143:LEU:HD21	16:Z:177:LEU:HG	2.01	0.42
1:A:1219:ASP:OD2	1:A:1255:ASN:ND2	2.53	0.42
1:A:1663:PHE:CZ	1:A:1902:GLN:HG3	2.55	0.42
1:A:1756:PHE:CZ	1:A:1760:THR:HG21	2.55	0.42
1:A:2048:TRP:O	1:A:2052:GLU:HG3	2.20	0.42
1:A:2070:ASN:OD1	1:A:2071:ILE:N	2.52	0.42
4:E:58:C:H1'	20:G:2:GLY:O	2.20	0.42
5:L:1096:C:H2'	5:L:1097:G:H8	1.85	0.42
1:A:1870:VAL:CG2	5:L:46:C:H4'	2.49	0.42
8:N:113:U:O4'	13:R:183:PHE:HE2	2.02	0.42
1:A:1369:ASN:HB3	1:A:1378:LYS:NZ	2.35	0.42
1:A:1440:ILE:O	1:A:1443:TYR:N	2.44	0.42
1:A:1605:ARG:HD2	1:A:1823:LEU:O	2.20	0.42
1:A:1856:ASN:HD22	1:A:1969:MET:HG2	1.84	0.42
1:A:2013:ARG:NH1	1:A:2085:GLY:HA2	2.35	0.42
1:A:213:TYR:CZ	1:A:217:TRP:HD1	2.32	0.42
2:C:542:ILE:HA	2:C:563:LEU:O	2.20	0.42
7:B:90:A:N6	9:J:6:ILE:HD11	2.34	0.42
5:L:33:U:H2'	5:L:34:G:O4'	2.20	0.42
10:O:342:LEU:HB3	11:P:47:ARG:HD2	2.01	0.42
12:Q:291:ILE:HG23	12:Q:292:PRO:CA	2.50	0.42
13:R:150:HIS:CE1	13:R:205:LEU:HD11	2.55	0.42
1:A:1389:TYR:CZ	1:A:1401:SER:HB3	2.55	0.42
1:A:1708:GLU:HG3	1:A:1730:ASN:OD1	2.19	0.42
5:L:18:U:C6	22:I:202:GLN:CG	3.02	0.42
10:O:405:SER:HA	10:O:415:ILE:O	2.19	0.42
12:Q:125:ILE:CD1	12:Q:126:THR:N	2.82	0.42
12:Q:240:LEU:HD12	12:Q:241:ILE:H	1.85	0.42
15:T:147:HIS:HB2	15:T:148:CYS:SG	2.59	0.42
1:A:1028:TRP:HD1	1:A:1260:PHE:CZ	2.37	0.42
1:A:693:LYS:O	1:A:694:ASN:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:ILE:O	1:A:878:GLU:HB2	2.20	0.42
2:C:428:ILE:HG22	2:C:429:PHE:CD1	2.55	0.42
2:C:626:SER:HB2	2:C:634:ILE:HD13	2.01	0.42
2:C:757:TRP:HD1	2:C:762:SER:OG	2.03	0.42
4:E:66:C:H1'	12:Q:108:MET:SD	2.60	0.42
10:O:187:ASP:HB3	10:O:200:VAL:CG1	2.49	0.42
10:O:442:TRP:CG	10:O:442:TRP:O	2.70	0.42
12:Q:205:PHE:CE1	12:Q:293:TRP:HD1	2.37	0.42
16:Z:190:LEU:HD23	16:Z:191:ARG:CA	2.50	0.42
1:A:1419:ASP:OD1	1:A:1419:ASP:O	2.38	0.41
1:A:484:PHE:HE1	1:A:488:ARG:HD2	1.85	0.41
1:A:770:MET:CE	11:P:165:ILE:HD11	2.50	0.41
2:C:316:THR:O	2:C:319:GLY:N	2.48	0.41
1:A:458:PHE:HD1	2:C:335:SER:OG	2.02	0.41
2:C:338:SER:O	2:C:341:ILE:HG12	2.19	0.41
2:C:492:LEU:HD22	2:C:557:HIS:ND1	2.35	0.41
4:E:15:C:C6	4:E:15:C:OP2	2.73	0.41
19:F:36:LYS:HE2	19:F:38:HIS:O	2.20	0.41
19:F:87:SER:HA	19:F:93:ASN:O	2.19	0.41
1:A:1424:HIS:CD2	9:J:6:ILE:HD13	2.55	0.41
5:L:34:G:H2'	5:L:35:U:O4'	2.20	0.41
12:Q:38:THR:O	12:Q:39:LEU:HD12	2.20	0.41
14:S:170:LEU:HA	14:S:170:LEU:HD23	1.81	0.41
1:A:134:MET:HE2	15:T:107:ARG:HD2	2.02	0.41
1:A:2054:GLN:O	1:A:2058:LEU:HG	2.21	0.41
1:A:266:LEU:CD2	1:A:268:LEU:H	2.33	0.41
1:A:386:ALA:O	1:A:401:PRO:HG3	2.21	0.41
1:A:563:ASP:OD2	1:A:640:ARG:NH2	2.54	0.41
1:A:780:ARG:NH2	5:L:20:G:C4	2.89	0.41
1:A:351:LYS:HE3	7:B:91:A:OP1	2.20	0.41
2:C:116:THR:OG1	2:C:120:ARG:HG3	2.20	0.41
3:D:64:C:H2'	3:D:65:U:C6	2.55	0.41
10:O:159:SER:OG	10:O:160:ASN:N	2.53	0.41
10:O:348:GLU:CD	10:O:349:LYS:N	2.73	0.41
1:A:891:GLU:OE2	11:P:219:ILE:HG12	2.21	0.41
12:Q:217:TRP:C	12:Q:217:TRP:CD1	2.93	0.41
13:R:210:LYS:HG3	13:R:211:GLU:N	2.36	0.41
15:T:123:ARG:O	15:T:154:ALA:HB2	2.20	0.41
1:A:1011:ASN:HD21	1:A:1142:ASN:C	2.23	0.41
1:A:1339:LEU:CD2	1:A:1440:ILE:HD12	2.50	0.41
1:A:834:ILE:O	1:A:837:GLY:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:TYR:CD1	2:C:199:LEU:HG	2.55	0.41
2:C:203:LEU:HD13	2:C:325:LYS:NZ	2.34	0.41
2:C:153:LEU:HD13	2:C:212:PHE:CZ	2.55	0.41
2:C:139:ILE:HG22	2:C:215:ALA:HB3	2.02	0.41
2:C:325:LYS:HE2	2:C:441:ARG:NH1	2.35	0.41
4:E:42:A:O2'	4:E:43:C:P	2.78	0.41
5:L:15:C:N4	22:I:209:ARG:HD3	2.34	0.41
10:O:250:LEU:HA	10:O:250:LEU:HD23	1.79	0.41
12:Q:263:VAL:O	12:Q:263:VAL:HG12	2.20	0.41
13:R:108:VAL:HG23	13:R:109:LEU:HG	2.03	0.41
1:A:364:TYR:HD1	1:A:1209:LYS:HE2	1.85	0.41
1:A:1667:GLN:O	1:A:1670:ASP:HB3	2.21	0.41
1:A:584:HIS:O	1:A:587:GLY:N	2.47	0.41
1:A:672:LYS:HB2	3:D:101:C:OP1	2.20	0.41
1:A:821:ASP:HA	14:S:160:MET:HG3	2.02	0.41
2:C:199:LEU:HD13	2:C:207:SER:HB2	2.01	0.41
2:C:237:ILE:HB	2:C:265:PHE:CD1	2.55	0.41
2:C:362:LYS:CG	2:C:363:PRO:HD2	2.51	0.41
2:C:452:LYS:O	2:C:455:HIS:N	2.54	0.41
2:C:772:ASN:OD1	2:C:772:ASN:N	2.54	0.41
13:R:154:ALA:O	13:R:158:SER:OG	2.26	0.41
13:R:159:ARG:NE	13:R:205:LEU:HA	2.35	0.41
16:Z:178:ARG:CD	16:Z:182:GLN:HE22	2.32	0.41
16:Z:195:GLU:O	16:Z:198:PHE:HB2	2.20	0.41
1:A:1069:LEU:HD23	1:A:1120:VAL:HG21	2.01	0.41
1:A:1624:LEU:HD23	1:A:1624:LEU:HA	1.90	0.41
1:A:1724:PHE:HD1	1:A:1791:PHE:HA	1.86	0.41
1:A:526:LEU:HA	1:A:526:LEU:HD23	1.90	0.41
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.83	0.41
1:A:859:ASN:ND2	14:S:170:LEU:HD12	2.34	0.41
1:A:899:PRO:HD2	1:A:1006:ARG:CZ	2.50	0.41
2:C:123:MET:HA	2:C:199:LEU:HD23	2.02	0.41
2:C:735:LEU:HB3	2:C:750:ILE:HG21	2.03	0.41
4:E:75:A:O2'	4:E:76:A:H5'	2.20	0.41
19:F:44:MET:HB2	20:G:7:ASN:HD21	1.86	0.41
19:F:76:LEU:HD13	20:G:30:LEU:HD12	2.02	0.41
21:H:3:ARG:HG2	21:H:3:ARG:H	1.50	0.41
10:O:389:THR:HG22	10:O:426:TRP:HZ2	1.86	0.41
1:A:770:MET:HE2	11:P:165:ILE:HD11	2.01	0.41
11:P:194:ASN:OD1	11:P:195:ASN:N	2.52	0.41
13:R:153:PRO:HB3	13:R:177:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:164:PHE:CE1	13:R:199:MET:HG3	2.56	0.41
4:E:28:U:C1'	15:T:121:ILE:HD13	2.51	0.41
16:Z:368:ASN:O	16:Z:373:ILE:HG12	2.21	0.41
1:A:1033:ASN:HD22	1:A:1288:LEU:CB	2.34	0.41
1:A:1054:LEU:HA	1:A:1054:LEU:HD23	1.80	0.41
1:A:151:SER:HB3	1:A:154:TYR:CD2	2.56	0.41
1:A:2058:LEU:O	1:A:2061:THR:OG1	2.33	0.41
1:A:376:ARG:HH11	2:C:910:GLU:CD	2.23	0.41
1:A:168:LEU:HB3	1:A:622:MET:CE	2.51	0.41
2:C:832:ASP:HA	2:C:835:LYS:HG2	2.02	0.41
19:F:14:ASP:CG	19:F:15:TYR:H	2.19	0.41
21:H:74:GLN:O	21:H:78:LEU:HG	2.20	0.41
5:L:1115:G:C6	5:L:1116:A:N6	2.89	0.41
12:Q:77:ASP:HB2	12:Q:87:ARG:HD2	2.02	0.41
15:T:4:ILE:HG22	15:T:5:LYS:N	2.36	0.41
1:A:1130:ARG:NH2	1:A:1158:ILE:O	2.54	0.41
1:A:1451:PHE:O	1:A:1454:SER:OG	2.23	0.41
1:A:1893:ILE:HG21	1:A:1981:ALA:HB3	2.03	0.41
1:A:1891:LEU:HD12	1:A:1989:PHE:CE2	2.56	0.41
1:A:806:ALA:N	1:A:807:PRO:HD2	2.35	0.41
3:D:89:U:H2'	3:D:90:C:O4'	2.21	0.41
4:E:51:A:H1'	4:E:52:G:P	2.60	0.41
4:E:56:A:C2'	4:E:57:U:O5'	2.69	0.41
10:O:406:THR:O	10:O:414:LEU:HD12	2.20	0.41
16:Z:205:TYR:C	16:Z:207:SER:H	2.23	0.41
1:A:1021:PRO:O	1:A:1024:LEU:HB3	2.20	0.41
1:A:1033:ASN:ND2	1:A:1297:THR:OG1	2.46	0.41
1:A:1405:ILE:HD12	16:Z:303:LEU:H	1.84	0.41
1:A:1686:VAL:HG12	1:A:1687:HIS:O	2.20	0.41
1:A:1690:LYS:HD2	1:A:1698:ALA:N	2.35	0.41
1:A:264:ILE:HG22	1:A:265:ASN:O	2.21	0.41
1:A:903:LEU:O	1:A:903:LEU:HD23	2.21	0.41
1:A:284:ARG:NE	3:D:33:U:O4	2.54	0.41
19:F:11:TYR:HE1	21:H:12:LEU:HD11	1.86	0.41
1:A:1050:LEU:CD2	1:A:1248:VAL:HG22	2.50	0.41
2:C:348:LEU:HD12	2:C:372:THR:HG22	2.02	0.41
2:C:801:TRP:NE1	2:C:843:LYS:HD2	2.35	0.41
2:C:927:MET:HG3	2:C:928:CYS:N	2.36	0.41
4:E:21:U:H2'	4:E:22:G:H8	1.85	0.41
21:H:41:VAL:HG21	21:H:92:TRP:CH2	2.56	0.41
10:O:340:SER:OG	10:O:341:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:157:THR:HG21	10:O:423:ILE:HD11	2.01	0.41
12:Q:222:THR:HA	12:Q:225:GLN:HE21	1.76	0.41
1:A:1442:ARG:NH2	16:Z:302:SER:O	2.54	0.41
1:A:1144:PHE:HD2	1:A:1145:MET:HG2	1.84	0.41
1:A:1328:PHE:CE1	1:A:1371:VAL:HG13	2.56	0.41
1:A:630:LYS:NZ	1:A:634:ASP:OD2	2.31	0.41
1:A:809:LYS:O	1:A:813:GLU:HG2	2.21	0.41
1:A:912:LEU:CD2	1:A:916:LEU:HD12	2.51	0.41
2:C:70:TYR:CE2	10:O:134:VAL:HG21	2.56	0.41
10:O:198:PHE:HE1	10:O:208:CYS:SG	2.44	0.41
10:O:257:ILE:O	10:O:259:VAL:N	2.54	0.41
12:Q:254:GLN:O	12:Q:255:SER:HB2	2.21	0.41
13:R:199:MET:HE3	13:R:202:GLN:HG3	2.03	0.41
14:S:5:HIS:C	14:S:6:ARG:CD	2.90	0.41
1:A:1699:ALA:HA	1:A:1735:ASP:OD1	2.21	0.41
1:A:1752:VAL:HG12	1:A:1787:TYR:HB3	2.03	0.41
1:A:1857:VAL:HG13	1:A:1894:ILE:HD12	2.03	0.41
1:A:1865:THR:OG1	1:A:1869:ASN:HB2	2.21	0.41
1:A:740:GLU:HG3	1:A:741:ILE:N	2.34	0.41
2:C:341:ILE:HG13	2:C:342:ASP:H	1.84	0.41
1:A:452:PHE:CZ	2:C:347:ARG:HG3	2.44	0.41
2:C:646:GLY:HA3	2:C:652:MET:CE	2.50	0.41
2:C:807:PRO:HB2	2:C:851:LEU:HD21	2.03	0.41
10:O:385:GLN:HE21	10:O:387:LEU:HD21	1.86	0.41
2:C:152:LEU:HD11	2:C:316:THR:HA	2.02	0.40
2:C:416:ASP:O	2:C:420:PHE:HB3	2.21	0.40
2:C:887:ARG:HD3	2:C:889:TYR:OH	2.22	0.40
4:E:74:U:O4	14:S:30:LEU:HG	2.22	0.40
19:F:56:GLU:HG3	19:F:90:ARG:HG3	2.03	0.40
22:I:182:GLN:O	22:I:186:ALA:CB	2.69	0.40
22:I:187:LYS:HA	22:I:201:LYS:HZ3	1.85	0.40
11:P:177:GLY:O	22:I:196:ILE:HD12	2.22	0.40
10:O:228:ARG:NH2	10:O:268:PRO:HB3	2.36	0.40
12:Q:208:TYR:HB2	12:Q:290:ILE:HB	2.02	0.40
12:Q:255:SER:CB	12:Q:257:GLU:HG2	2.50	0.40
13:R:246:SER:O	13:R:250:MET:HG3	2.22	0.40
16:Z:391:LEU:HD23	16:Z:391:LEU:HA	1.91	0.40
16:Z:462:ILE:HA	16:Z:474:THR:HG21	2.03	0.40
1:A:1192:ASP:OD2	1:A:1197:ASN:ND2	2.53	0.40
1:A:1372:LYS:HG2	1:A:1383:PHE:CE2	2.57	0.40
1:A:2050:THR:O	1:A:2053:SER:OG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PRO:O	1:A:392:ASN:HB3	2.21	0.40
1:A:426:PRO:HG2	16:Z:201:ARG:NH1	2.36	0.40
1:A:951:LEU:HD22	1:A:955:LYS:NZ	2.36	0.40
2:C:706:LEU:HA	2:C:824:SER:O	2.20	0.40
21:H:69:SER:O	21:H:70:LEU:HB2	2.21	0.40
7:B:90:A:C6	9:J:6:ILE:HD11	2.55	0.40
5:L:1102:C:H2'	5:L:1103:C:H5	1.70	0.40
5:L:81:G:C6	5:L:82:C:N4	2.90	0.40
10:O:370:ASN:OD1	10:O:370:ASN:N	2.46	0.40
5:L:19:U:C2	11:P:178:TYR:CD2	3.10	0.40
10:O:342:LEU:O	11:P:46:LYS:N	2.54	0.40
15:T:34:GLN:HE21	15:T:34:GLN:HB2	1.66	0.40
1:A:143:ILE:HD12	1:A:573:ARG:HH21	1.86	0.40
1:A:654:HIS:CE1	1:A:658:ASN:HD21	2.39	0.40
1:A:780:ARG:HH22	14:S:9:LEU:HD22	1.85	0.40
1:A:460:PRO:HG3	2:C:376:PHE:CE1	2.55	0.40
1:A:709:ARG:NH2	3:D:82:A:O3'	2.50	0.40
8:N:108:U:C1'	8:N:109:U:P	3.09	0.40
12:Q:214:ILE:HD11	12:Q:218:LYS:HB3	2.03	0.40
16:Z:180:ILE:HG22	16:Z:186:LEU:CD2	2.43	0.40
1:A:176:LEU:O	1:A:179:MET:HG3	2.22	0.40
1:A:1859:ARG:O	1:A:1874:ALA:HA	2.21	0.40
1:A:331:PHE:HD1	1:A:331:PHE:HA	1.73	0.40
2:C:544:LEU:HG	2:C:553:VAL:HG21	2.04	0.40
3:D:104:G:O2'	3:D:105:A:H5'	2.20	0.40
6:M:505:A:O3'	6:M:506:U:H4'	2.22	0.40
10:O:403:LEU:HD23	10:O:403:LEU:HA	1.86	0.40
12:Q:106:ASN:HB2	12:Q:109:MET:CG	2.51	0.40
12:Q:124:GLN:OE1	12:Q:124:GLN:HA	2.20	0.40
12:Q:65:ALA:O	12:Q:69:ASN:N	2.54	0.40
16:Z:424:PHE:O	16:Z:428:VAL:HG23	2.21	0.40
1:A:131:LYS:HD2	1:A:131:LYS:HA	1.95	0.40
1:A:1431:HIS:CG	1:A:1434:GLU:HA	2.56	0.40
1:A:1843:LEU:HD23	1:A:1849:LYS:NZ	2.36	0.40
1:A:603:LYS:HG2	1:A:604:THR:O	2.22	0.40
1:A:695:LEU:HD12	1:A:695:LEU:O	2.21	0.40
2:C:869:HIS:CD2	2:C:925:LEU:HD22	2.56	0.40
2:C:933:TRP:O	2:C:935:LYS:HG3	2.22	0.40
10:O:279:PRO:HG3	10:O:301:MET:SD	2.62	0.40
12:Q:215:PRO:HG3	12:Q:217:TRP:CZ2	2.56	0.40
13:R:9:ALA:HB2	13:R:60:GLY:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1902/2413 (79%)	1744 (92%)	149 (8%)	9 (0%)	34	75
2	C	872/1008 (86%)	796 (91%)	72 (8%)	4 (0%)	34	75
9	J	25/135 (18%)	20 (80%)	5 (20%)	0	100	100
10	O	335/451 (74%)	299 (89%)	31 (9%)	5 (2%)	13	54
11	P	193/379 (51%)	174 (90%)	17 (9%)	2 (1%)	19	63
12	Q	177/364 (49%)	154 (87%)	21 (12%)	2 (1%)	17	61
13	R	259/339 (76%)	241 (93%)	18 (7%)	0	100	100
14	S	63/175 (36%)	55 (87%)	5 (8%)	3 (5%)	3	25
15	T	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	15	57
16	Z	443/577 (77%)	390 (88%)	44 (10%)	9 (2%)	9	48
17	c	312/587 (53%)	291 (93%)	17 (5%)	4 (1%)	15	57
18	d	238/687 (35%)	221 (93%)	17 (7%)	0	100	100
19	F	113/278 (41%)	104 (92%)	8 (7%)	1 (1%)	21	65
20	G	39/179 (22%)	37 (95%)	1 (3%)	1 (3%)	7	42
21	H	93/235 (40%)	78 (84%)	14 (15%)	1 (1%)	17	61
22	I	98/215 (46%)	95 (97%)	3 (3%)	0	100	100
23	v	121/859 (14%)	110 (91%)	7 (6%)	4 (3%)	5	37
24	n	279/455 (61%)	242 (87%)	29 (10%)	8 (3%)	6	40
25	o	120/503 (24%)	115 (96%)	4 (3%)	1 (1%)	24	67
25	p	122/503 (24%)	116 (95%)	6 (5%)	0	100	100
25	q	355/503 (71%)	327 (92%)	16 (4%)	12 (3%)	5	36
25	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	7	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	t	150/175 (86%)	134 (89%)	13 (9%)	3 (2%)	9	48
27	k	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
27	s	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
28	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
28	u	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
29	h	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	13	54
29	w	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	13	54
30	j	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
30	x	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
31	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	15	57
31	y	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	15	57
32	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
32	z	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
33	e	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	12	53
33	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	17	61
34	a	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
35	b	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	12	53
All	All	7810/13649 (57%)	7124 (91%)	604 (8%)	82 (1%)	24	63

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	PRO
2	C	364	PHE
2	C	463	THR
16	Z	206	LYS
20	G	17	MET
23	v	616	PRO
24	n	246	LEU
24	n	428	PRO
25	q	53	ILE
25	q	77	ILE
25	q	172	PRO
25	q	174	TRP
25	q	239	PRO
25	q	246	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	q	362	PRO
25	q	442	SER
25	r	64	GLU
26	t	77	PRO
35	b	68	PRO
1	A	1405	ILE
12	Q	99	VAL
12	Q	255	SER
14	S	8	GLN
14	S	9	LEU
16	Z	67	LYS
16	Z	69	ASN
16	Z	234	GLU
16	Z	235	ALA
17	c	230	THR
21	H	27	LYS
23	v	601	VAL
23	v	618	GLU
24	n	61	LYS
24	n	291	HIS
24	n	406	ARG
25	q	196	PRO
26	t	110	GLU
1	A	484	PHE
2	C	829	VAL
16	Z	204	ASP
23	v	634	HIS
25	o	17	PRO
25	r	20	ARG
26	t	80	ASN
1	A	1628	ASP
10	O	444	PRO
11	P	86	ASN
11	P	112	ILE
14	S	10	GLU
17	c	231	SER
24	n	267	LEU
31	l	82	PRO
33	g	82	LYS
31	y	82	PRO
33	e	82	LYS
10	O	278	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	O	391	GLU
10	O	435	GLU
15	T	35	LYS
15	T	104	CYS
16	Z	146	ASN
16	Z	229	VAL
24	n	416	ARG
25	q	60	ALA
17	c	218	VAL
19	F	110	VAL
16	Z	214	ILE
25	q	36	GLY
29	h	15	PRO
29	w	15	PRO
35	b	52	LYS
1	A	407	VAL
1	A	562	ILE
10	O	277	VAL
25	q	175	PRO
1	A	264	ILE
1	A	377	VAL
1	A	741	ILE
17	c	16	VAL
24	n	387	ILE
2	C	363	PRO
25	r	36	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1736/2182 (80%)	1721 (99%)	15 (1%)	84	94
2	C	794/910 (87%)	789 (99%)	5 (1%)	90	96
9	J	21/121 (17%)	21 (100%)	0	100	100
10	O	295/397 (74%)	292 (99%)	3 (1%)	82	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	173/328 (53%)	172 (99%)	1 (1%)	90	96
12	Q	171/332 (52%)	154 (90%)	17 (10%)	10	39
13	R	224/296 (76%)	223 (100%)	1 (0%)	93	97
14	S	56/151 (37%)	53 (95%)	3 (5%)	27	67
15	T	141/141 (100%)	140 (99%)	1 (1%)	88	95
16	Z	417/538 (78%)	382 (92%)	35 (8%)	14	49
17	c	212/316 (67%)	206 (97%)	6 (3%)	51	83
18	d	219/249 (88%)	218 (100%)	1 (0%)	92	96
19	F	105/256 (41%)	103 (98%)	2 (2%)	65	87
20	G	39/163 (24%)	39 (100%)	0	100	100
21	H	88/216 (41%)	87 (99%)	1 (1%)	80	92
22	I	92/193 (48%)	92 (100%)	0	100	100
23	v	58/152 (38%)	48 (83%)	10 (17%)	2	13
24	n	124/413 (30%)	102 (82%)	22 (18%)	2	12
25	o	60/451 (13%)	53 (88%)	7 (12%)	7	30
25	p	62/451 (14%)	54 (87%)	8 (13%)	5	26
25	q	124/451 (28%)	107 (86%)	17 (14%)	4	23
25	r	60/451 (13%)	55 (92%)	5 (8%)	14	49
26	t	40/165 (24%)	29 (72%)	11 (28%)	0	3
27	k	70/176 (40%)	70 (100%)	0	100	100
27	s	67/176 (38%)	67 (100%)	0	100	100
28	i	65/83 (78%)	60 (92%)	5 (8%)	16	53
28	u	65/83 (78%)	60 (92%)	5 (8%)	16	53
29	h	61/77 (79%)	60 (98%)	1 (2%)	70	89
29	w	61/77 (79%)	60 (98%)	1 (2%)	70	89
30	j	58/66 (88%)	55 (95%)	3 (5%)	29	68
30	x	58/66 (88%)	55 (95%)	3 (5%)	29	68
31	l	69/89 (78%)	67 (97%)	2 (3%)	50	82
31	y	69/89 (78%)	67 (97%)	2 (3%)	50	82
32	m	77/129 (60%)	71 (92%)	6 (8%)	16	52
32	z	77/129 (60%)	71 (92%)	6 (8%)	16	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e	59/103 (57%)	55 (93%)	4 (7%)	20	60
33	g	79/103 (77%)	74 (94%)	5 (6%)	22	62
34	a	26/100 (26%)	25 (96%)	1 (4%)	40	76
35	b	47/219 (22%)	44 (94%)	3 (6%)	22	62
All	All	6319/11088 (57%)	6101 (97%)	218 (3%)	48	79

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	144	ASN
1	A	234	PHE
1	A	376	ARG
1	A	488	ARG
1	A	489	THR
1	A	495	ARG
1	A	588	LEU
1	A	612	LYS
1	A	640	ARG
1	A	737	ARG
1	A	900	PHE
1	A	903	LEU
1	A	908	ASP
1	A	928	ARG
2	C	176	ARG
2	C	177	TYR
2	C	458	ILE
2	C	461	LYS
2	C	465	GLU
10	O	443	ASN
10	O	445	ASN
10	O	446	LEU
11	P	185	ARG
12	Q	50	LYS
12	Q	51	ARG
12	Q	53	ASN
12	Q	55	ILE
12	Q	119	LYS
12	Q	120	LEU
12	Q	126	THR
12	Q	209	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Q	213	SER
12	Q	217	TRP
12	Q	220	THR
12	Q	222	THR
12	Q	226	LEU
12	Q	227	LEU
12	Q	245	LYS
12	Q	248	CYS
12	Q	252	ARG
13	R	10	LYS
14	S	4	SER
14	S	6	ARG
14	S	9	LEU
15	T	34	GLN
16	Z	12	LYS
16	Z	16	GLU
16	Z	34	MET
16	Z	67	LYS
16	Z	94	LEU
16	Z	132	GLU
16	Z	134	VAL
16	Z	138	ILE
16	Z	145	LYS
16	Z	149	ARG
16	Z	151	VAL
16	Z	162	LEU
16	Z	168	LYS
16	Z	174	TRP
16	Z	177	LEU
16	Z	179	TYR
16	Z	181	LEU
16	Z	183	THR
16	Z	184	GLN
16	Z	185	GLU
16	Z	186	LEU
16	Z	190	LEU
16	Z	192	GLU
16	Z	193	SER
16	Z	194	LEU
16	Z	195	GLU
16	Z	197	LEU
16	Z	198	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Z	199	GLU
16	Z	201	ARG
16	Z	203	LYS
16	Z	216	ASP
16	Z	229	VAL
16	Z	243	GLU
16	Z	245	CYS
17	c	504	PRO
17	c	505	PRO
17	c	517	VAL
17	c	523	LEU
17	c	532	PRO
17	c	550	PRO
18	d	155	LEU
19	F	42	ARG
19	F	62	ARG
21	H	3	ARG
23	v	616	PRO
23	v	617	PRO
23	v	641	PRO
23	v	706	LEU
23	v	712	CYS
23	v	722	PRO
23	v	723	SER
23	v	725	THR
23	v	726	ARG
23	v	733	ILE
24	n	51	PHE
24	n	55	GLU
24	n	57	LYS
24	n	58	ARG
24	n	59	ARG
24	n	61	LYS
24	n	62	THR
24	n	66	ASP
24	n	159	PRO
24	n	162	PRO
24	n	208	PRO
24	n	257	PRO
24	n	258	THR
24	n	260	PRO
24	n	295	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	n	306	SER
24	n	327	PRO
24	n	340	PRO
24	n	373	PRO
24	n	424	PRO
24	n	428	PRO
24	n	436	PRO
25	o	17	PRO
25	o	26	SER
25	o	44	PRO
25	o	63	THR
25	o	96	PHE
25	o	109	LEU
25	o	134	SER
25	p	17	PRO
25	p	44	PRO
25	p	63	THR
25	p	80	LEU
25	p	85	GLN
25	p	93	LEU
25	p	99	ARG
25	p	109	LEU
25	q	17	PRO
25	q	44	PRO
25	q	55	PRO
25	q	56	SER
25	q	61	SER
25	q	102	LEU
25	q	126	LEU
25	q	172	PRO
25	q	175	PRO
25	q	196	PRO
25	q	215	CYS
25	q	235	THR
25	q	239	PRO
25	q	262	PRO
25	q	271	SER
25	q	350	PRO
25	q	412	PRO
25	r	17	PRO
25	r	44	PRO
25	r	63	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	r	93	LEU
25	r	99	ARG
26	t	5	SER
26	t	7	VAL
26	t	13	PRO
26	t	77	PRO
26	t	96	PRO
26	t	100	THR
26	t	105	PRO
26	t	108	SER
26	t	133	PRO
26	t	136	VAL
26	t	150	THR
28	i	16	CYS
28	i	18	PHE
28	i	25	THR
28	i	79	LYS
28	i	81	LEU
29	h	79	LEU
30	j	18	ASN
30	j	41	ASP
30	j	71	LEU
31	l	10	LEU
31	l	76	ASP
32	m	20	LYS
32	m	26	TRP
32	m	30	GLN
32	m	77	ASP
32	m	99	ASP
32	m	104	ASP
33	g	24	PHE
33	g	49	ARG
33	g	77	THR
33	g	99	ASP
33	g	100	SER
28	u	16	CYS
28	u	18	PHE
28	u	25	THR
28	u	79	LYS
28	u	81	LEU
29	w	79	LEU
30	x	18	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	x	41	ASP
30	x	71	LEU
31	y	10	LEU
31	y	76	ASP
32	z	20	LYS
32	z	26	TRP
32	z	30	GLN
32	z	77	ASP
32	z	99	ASP
32	z	104	ASP
33	e	49	ARG
33	e	77	THR
33	e	99	ASP
33	e	100	SER
34	a	38	LYS
35	b	4	THR
35	b	44	PRO
35	b	71	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	265	ASN
1	A	405	ASN
1	A	429	ASN
1	A	658	ASN
1	A	659	HIS
1	A	705	GLN
1	A	848	ASN
1	A	868	GLN
1	A	1011	ASN
1	A	1156	HIS
1	A	1368	GLN
1	A	1376	ASN
1	A	1449	ASN
1	A	1529	ASN
1	A	1532	HIS
1	A	1652	HIS
1	A	1667	GLN
1	A	1737	GLN
1	A	1863	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1947	HIS
1	A	2018	ASN
2	C	82	ASN
2	C	101	GLN
2	C	158	HIS
2	C	183	GLN
2	C	251	GLN
2	C	289	ASN
2	C	683	ASN
2	C	764	ASN
2	C	817	GLN
2	C	830	ASN
2	C	869	HIS
10	O	126	HIS
10	O	215	GLN
10	O	344	ASN
10	O	382	HIS
10	O	428	GLN
11	P	37	ASN
11	P	174	ASN
12	Q	53	ASN
12	Q	209	ASN
12	Q	225	GLN
13	R	58	HIS
13	R	91	HIS
13	R	92	HIS
13	R	150	HIS
13	R	155	GLN
13	R	191	ASN
13	R	201	ASN
13	R	227	ASN
13	R	248	ASN
14	S	5	HIS
14	S	8	GLN
14	S	34	HIS
14	S	173	HIS
15	T	34	GLN
15	T	57	HIS
15	T	112	ASN
15	T	116	ASN
15	T	143	HIS
16	Z	170	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Z	184	GLN
16	Z	310	HIS
16	Z	354	HIS
16	Z	457	HIS
17	c	82	ASN
17	c	83	GLN
18	d	79	HIS
19	F	35	ASN
19	F	65	ASN
21	H	18	GLN
21	H	53	GLN
21	H	93	GLN
22	I	200	ASN
28	i	34	GLN
28	i	86	ASN
30	j	66	ASN
31	l	41	ASN
32	m	30	GLN
28	u	34	GLN
28	u	86	ASN
29	w	52	GLN
30	x	66	ASN
31	y	41	ASN
32	z	30	GLN
33	e	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	114/214 (53%)	30 (26%)	3 (2%)
4	E	102/112 (91%)	34 (33%)	7 (6%)
5	L	120/1175 (10%)	25 (20%)	5 (4%)
6	M	28/29 (96%)	7 (25%)	0
7	B	12/13 (92%)	5 (41%)	0
8	N	14/15 (93%)	7 (50%)	1 (7%)
All	All	390/1558 (25%)	108 (27%)	16 (4%)

All (108) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	29	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	31	G
3	D	32	G
3	D	33	U
3	D	42	A
3	D	44	A
3	D	74	U
3	D	75	A
3	D	76	U
3	D	77	A
3	D	79	C
3	D	80	G
3	D	81	A
3	D	82	A
3	D	84	A
3	D	90	C
3	D	92	U
3	D	94	C
3	D	101	C
3	D	104	G
3	D	127	U
3	D	164	C
3	D	165	A
3	D	166	U
3	D	170	U
3	D	171	U
3	D	172	U
3	D	173	U
3	D	174	G
3	D	175	G
4	E	12	A
4	E	13	A
4	E	14	C
4	E	15	C
4	E	16	C
4	E	30	G
4	E	33	C
4	E	36	U
4	E	37	U
4	E	39	G
4	E	43	C
4	E	50	G
4	E	51	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	52	G
4	E	54	U
4	E	57	U
4	E	60	G
4	E	62	A
4	E	65	U
4	E	66	C
4	E	67	C
4	E	68	C
4	E	73	A
4	E	74	U
4	E	75	A
4	E	80	U
4	E	81	G
4	E	85	C
4	E	86	G
4	E	87	U
4	E	88	U
4	E	90	U
4	E	91	A
4	E	92	C
5	L	16	U
5	L	17	U
5	L	18	U
5	L	19	U
5	L	20	G
5	L	25	A
5	L	26	G
5	L	30	A
5	L	31	A
5	L	32	G
5	L	85	A
5	L	111	C
5	L	115	U
5	L	116	U
5	L	117	U
5	L	118	U
5	L	119	G
5	L	120	G
5	L	1099	G
5	L	1107	C
5	L	1108	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	1111	U
5	L	1112	G
5	L	1114	G
5	L	1120	G
6	M	495	A
6	M	499	U
6	M	501	A
6	M	503	A
6	M	504	C
6	M	505	A
6	M	506	U
7	B	88	U
7	B	89	A
7	B	90	A
7	B	93	U
7	B	94	U
8	N	101	U
8	N	102	A
8	N	108	U
8	N	109	U
8	N	110	A
8	N	112	U
8	N	113	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	78	A
3	D	83	C
3	D	172	U
4	E	14	C
4	E	42	A
4	E	51	A
4	E	56	A
4	E	64	U
4	E	66	C
4	E	74	U
5	L	17	U
5	L	19	U
5	L	117	U
5	L	1107	C
5	L	1111	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	N	108	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	GTP	C	1500	37	26,34,34	1.04	1 (3%)	29,54,54	1.60	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GTP	C	1500	37	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C6-N1	2.41	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
36	C	1500	GTP	N3-C2-N1	-5.17	120.52	127.56
36	C	1500	GTP	C5-C6-N1	-2.87	119.77	123.52
36	C	1500	GTP	C2'-C1'-N9	-2.47	106.86	113.47
36	C	1500	GTP	C4'-O4'-C1'	2.07	111.83	109.64
36	C	1500	GTP	C6-N1-C2	3.03	119.44	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	1500	GTP	1	0

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.