



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 6XII / pdb_00006xii
EMDB ID : EMD-22192
Title : Escherichia coli transcription-translation complex B (TTC-B) containing an
24 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-06-20
Resolution : 7.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

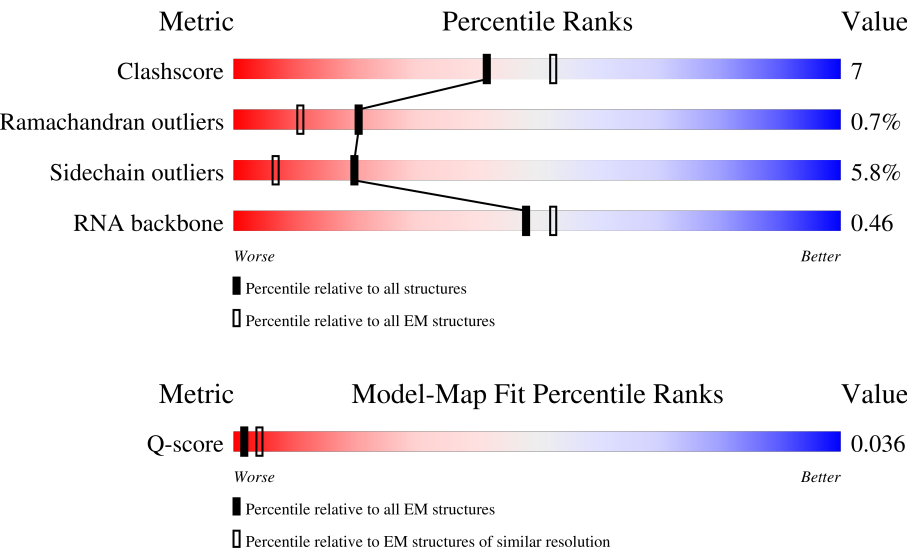
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	483 (6.50 - 7.50)

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	41	
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	C	75	
17	D	1542	
18	E	87	
19	F	71	
20	G	241	
21	H	557	
22	I	233	
23	J	206	
24	K	167	
25	L	135	
26	M	179	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	N	130	
28	O	130	
29	P	103	
30	Q	129	
31	R	124	
32	S	101	
33	T	89	
34	U	82	
35	V	84	
36	W	92	
37	X	118	
38	Y	142	
39	Z	121	
40	a	2904	
41	b	85	
42	c	78	
43	d	120	
44	e	63	
45	f	59	
46	g	70	
47	h	273	
48	i	57	
49	j	209	
50	k	55	
51	l	201	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	m	46	
53	n	179	
54	o	65	
55	p	177	
56	q	38	
57	r	149	
58	s	142	
59	t	123	
60	u	144	
61	v	136	
62	w	127	
63	x	117	
64	y	115	
65	z	118	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
67	ZN	AE	1502	-	-	X	-

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 276059 atoms, of which 99203 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 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			732	225	260	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	31	Total	C	N	O	P	0	0
			647	289	92	235	31		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	162	Total	C	N	O	S	0	0
			1282	816	222	237	7		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	66	Total	C	H	N	O	S	
			1103	344	559	102	97	1	0

- Molecule 17 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	1524	Total	C	H	N	O	P	
			49126	14585	16423	6003	10591	1524	0

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	86	Total	C	H	N	O	S	
			1388	414	719	138	114	3	0

- Molecule 19 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 21 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 22 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 23 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 24 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 25 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 26 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 27 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 29 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 30 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 31 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 32 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 33 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 34 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 36 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 37 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 38 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 40 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 43 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 47 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	k	52	Total	C	H	N	O	S	0	0
			890	275	464	78	73			

- Molecule 51 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 58 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 59 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 60 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 61 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 62 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 63 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 64 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 65 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	AE	1	Total	Mg	0
			1	1	

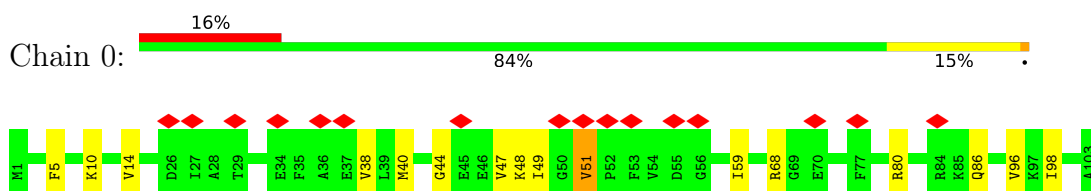
- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
67	AE	2	Total	Zn	0
			2	2	

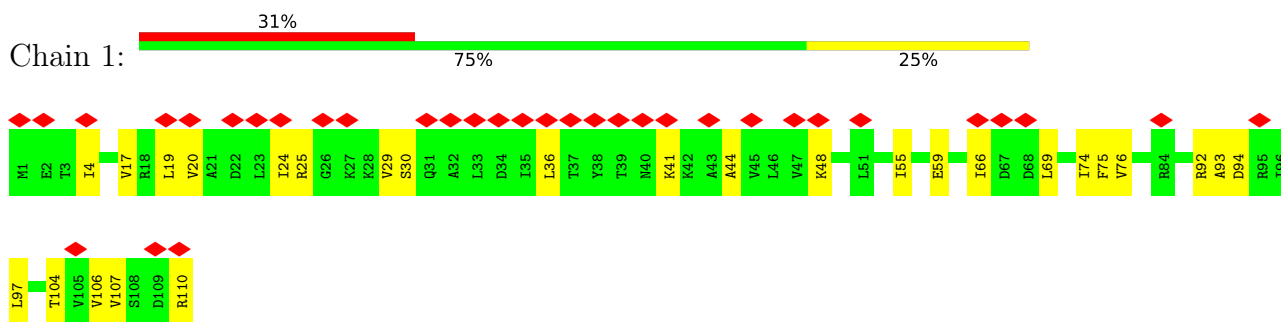
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

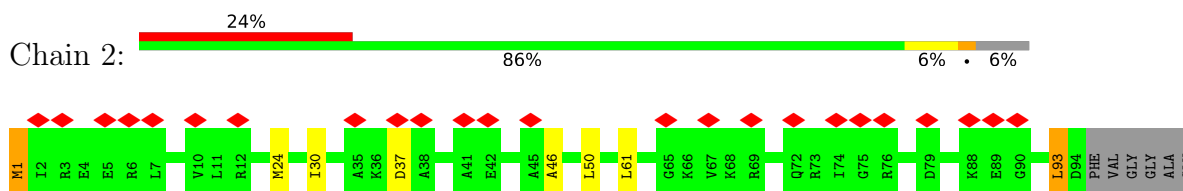
- Molecule 1: 50S ribosomal protein L21



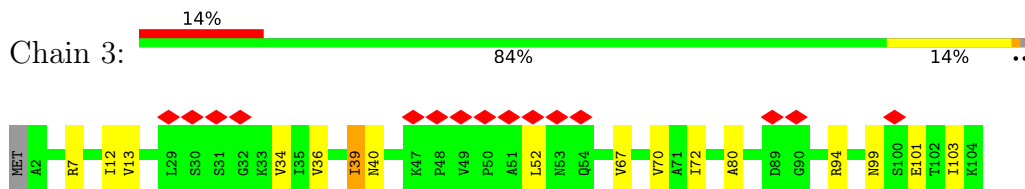
- Molecule 2: 50S ribosomal protein L22



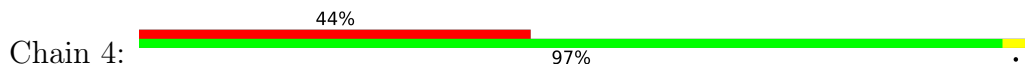
- Molecule 3: 50S ribosomal protein L23

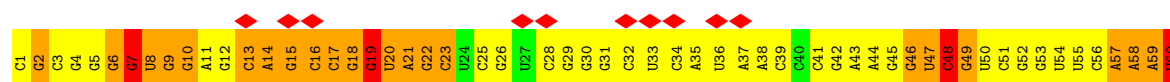


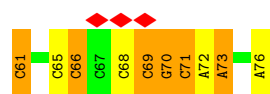
- Molecule 4: 50S ribosomal protein L24



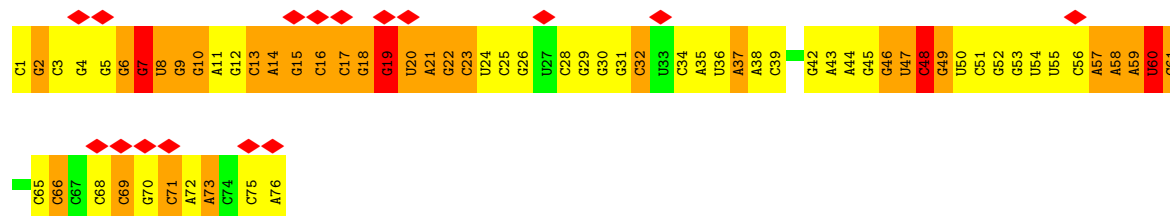
- Molecule 5: 50S ribosomal protein L25



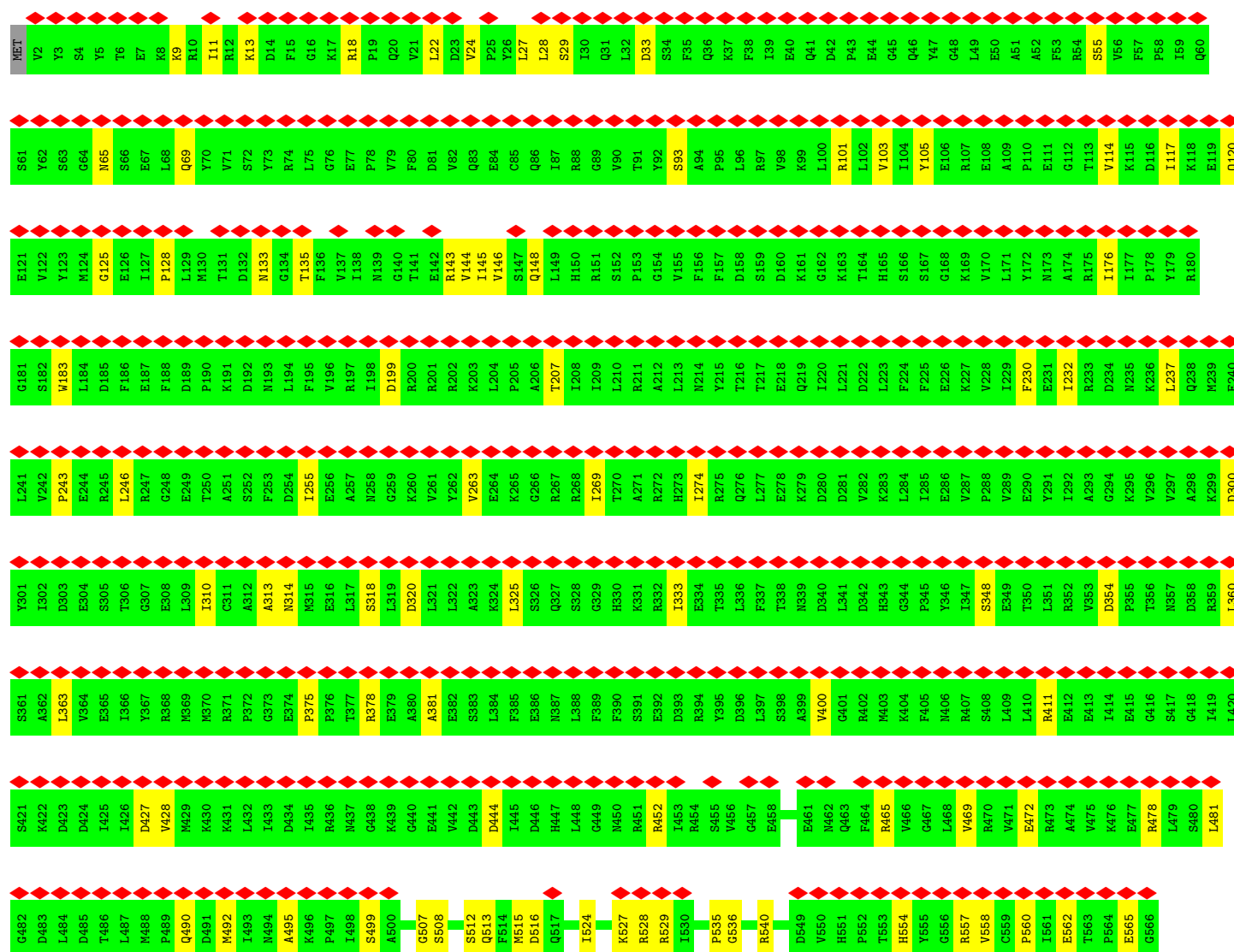
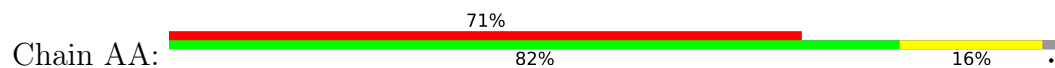


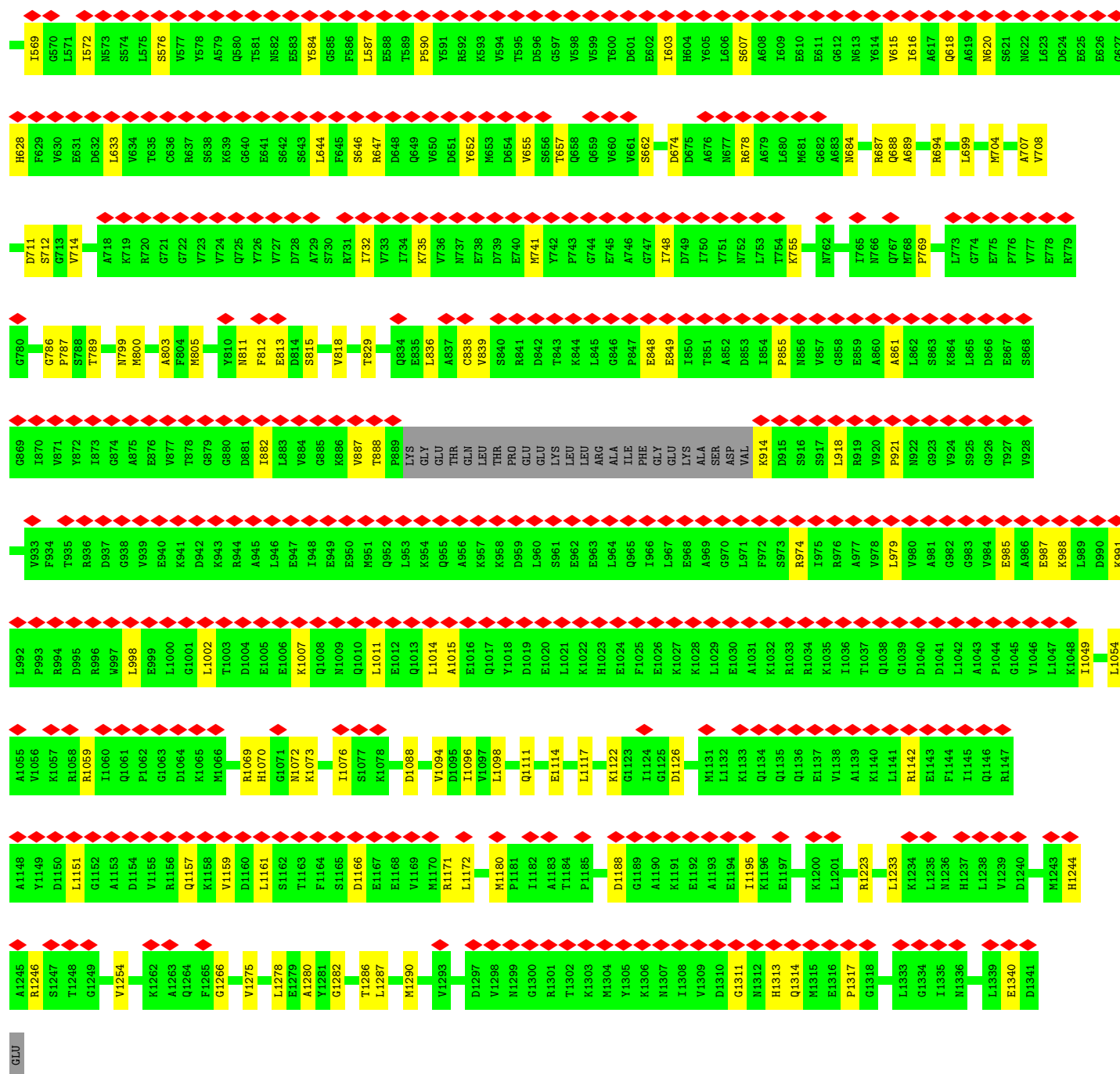


• Molecule 10: E-site and P-site tRNA (fMet)



• Molecule 11: DNA-directed RNA polymerase subunit beta





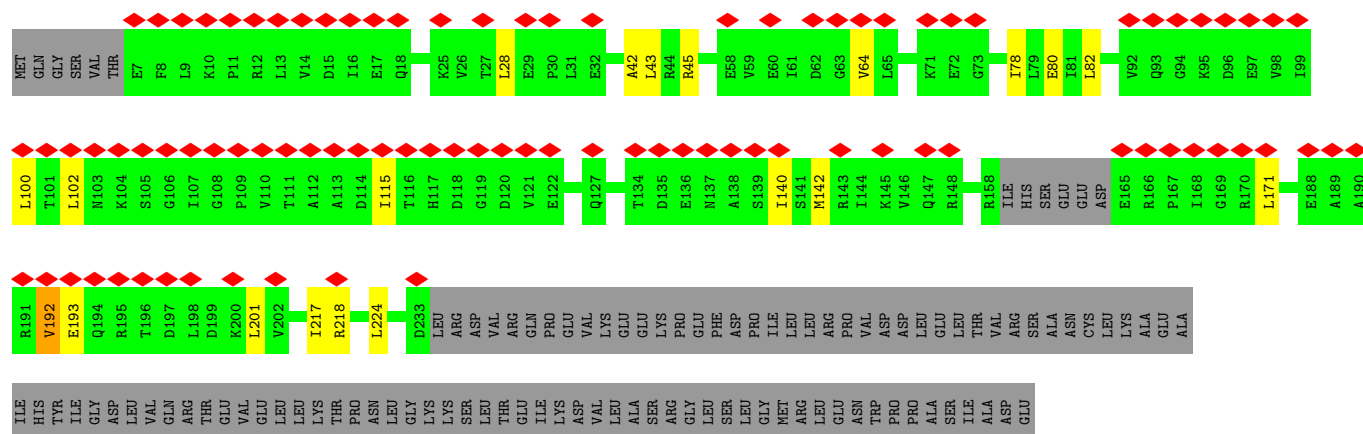
• Molecule 12: Transcription termination/antitermination protein NusG

Chain AB:

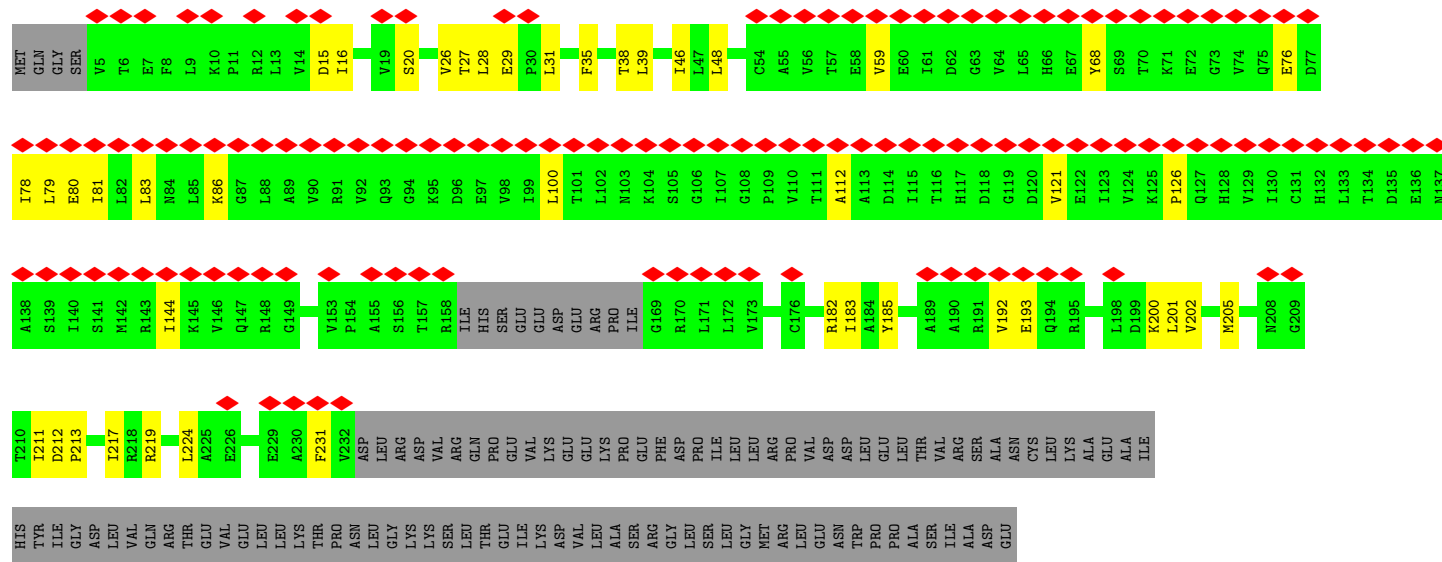
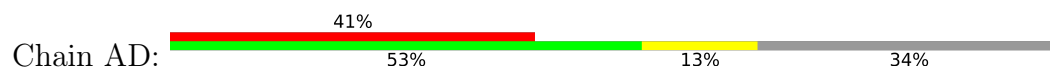




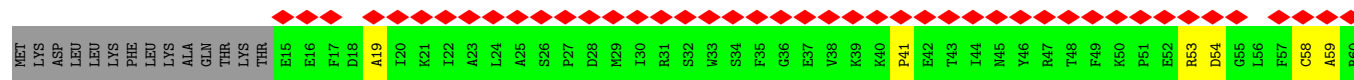
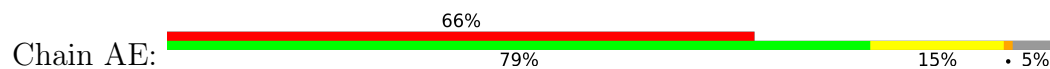
• Molecule 13: DNA-directed RNA polymerase subunit alpha



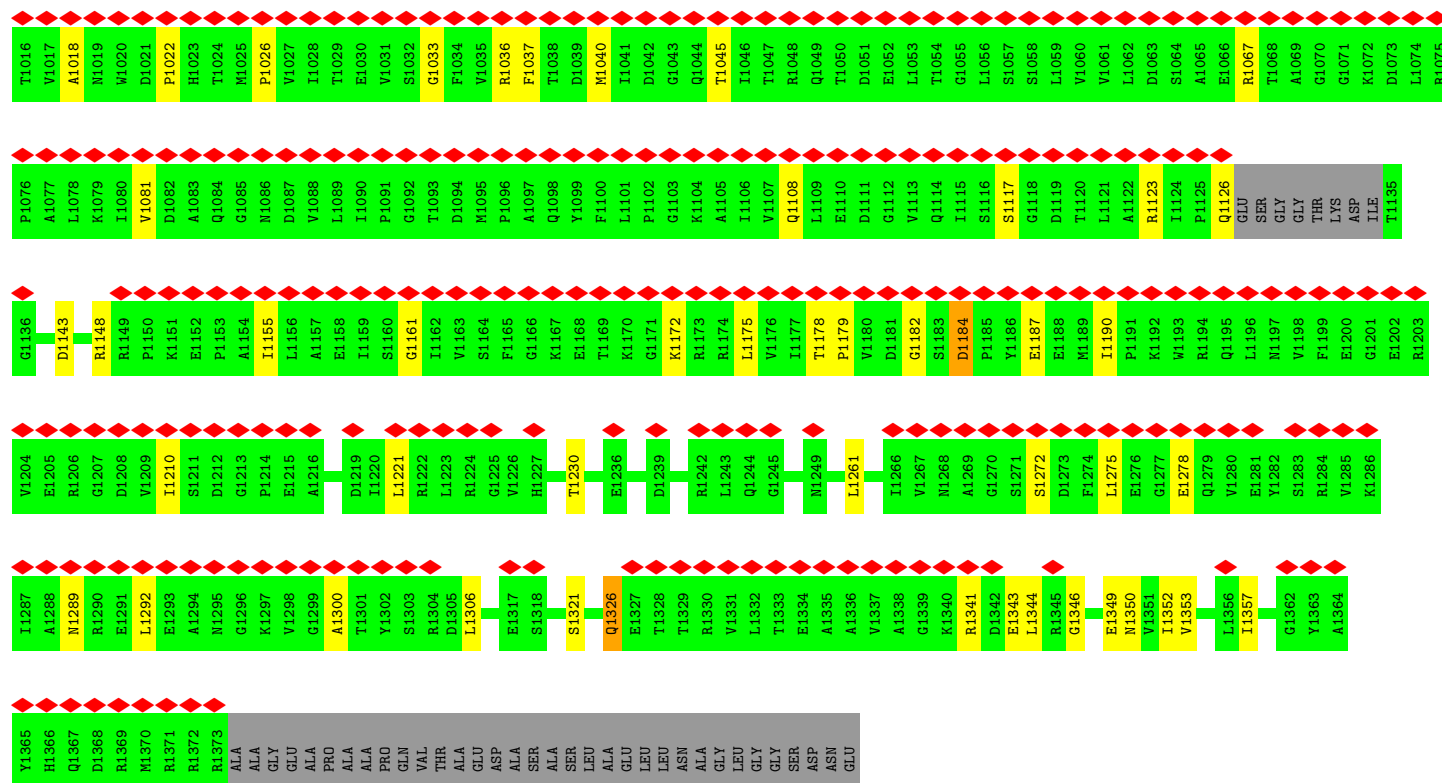
• Molecule 13: DNA-directed RNA polymerase subunit alpha



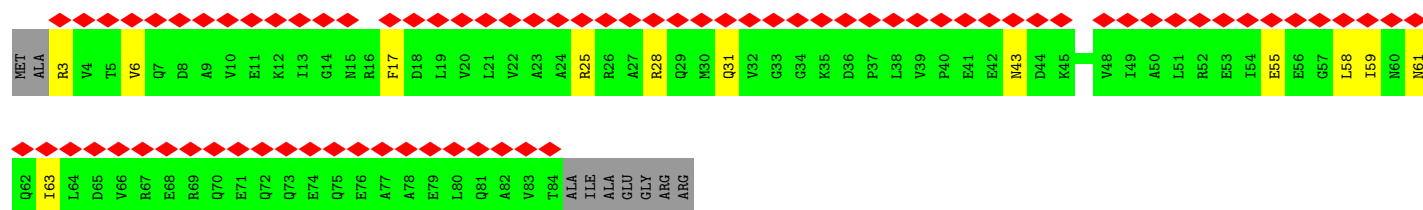
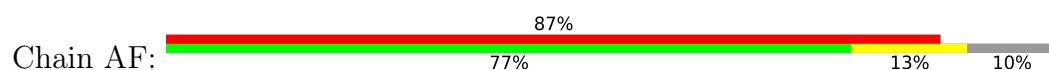
• Molecule 14: DNA-directed RNA polymerase subunit beta'



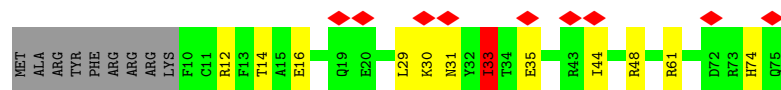
G956	S957	I958	K959	L960	S961	N962	V963	K964	S965	V966	V967	N968	S969	S970	G971	K972	L973	V974	T975	T976	S977	R978	N979	T980	V981	L982	K983	L984	I985	D986	E987	F988	G989	THR	PHE	HIS	ILE	GLY	ALA	ALA	ALA	ALA	GLU	S948	S949	V1002	L1003	A1004	K1005	G1006	D1007	G1008	E1009	Q1010	V1011	A1012	G1013	G1014	E1015
S876	V877	D878	A879	V880	K881	V882	R883	V886	S887	C888	D889	T890	D891	A896	H897	R901	D902	L903	A904	R905	G906	H907	I908	K911	T918	A919	A920	G924	E925	R933	THR	PHE	HIS	ILE	GLY	ALA	ALA	ALA	ALA	GLU	S948	S949	V1002	L1003	A1004	K1005	G1006	D1007	G1008	E1009	Q1010	V1011	A1012	G1013	G1014	E1015			
D812	D813	C814	G815	T816	H817	E818	P824	V825	I826	E827	G828	G829	D830	V831	K832	E833	P834	L835	R836	D837	R838	V839	L840	G841	R842	V843	T844	A845	E846	D847	V848	L849	K850	P851	G852	T853	A854	D855	L856	L857	V858	P859	R860	H861	T862	L863	L864	H865	E866	Q867	R868	C869	D870	L871	L872	E873	E874	H875	
R738	A741	G742	M743	R744	G745	L746	M747	A748	K749	P750	D751	G752	S753	T754	I755	E756	T757	P758	L759	T760	A761	N762	G766	L767	N768	V769	L770	Q771	Y772	F773	L774	S775	T776	H777	G778	A779	R780	K781	G782	L783	A784	D785	K789	Y795	L796	T797	L800	A804	Q805	D806	T810	E811							
E652	T653	I654	S655	E656	A657	E658	A659	E660	V661	A662	E663	I664	Q665	E666	Q667	F668	S670	L671	G672	V673	T674	A675	G676	E677	R678	Y679	M680	K681	V682	T683	D684	T685	M686	A687	A688	M689	D691	V693	S694	K695	D699	V706	T707	M708	R709	D710	G711	Q712	E713	E714	K715	S721							
D460	F461	D462	G463	D464	Q465	M466	A467	V468	L472	T473	L474	E475	A476	Q477	L478	R481	A482	M485	S486	L490	L491	S492	N495	G496	E497	S503	Q504	D505	V506	L510	M513	T514	R515	D516	C517	V518	M519	A520	V526	E532	A533	E534	A546	K549	V550	R551	L552												
A397	K398	K399	M400	V401	E402	R403	E404	A406	V407	V408	V409	D410	L411	L412	D413	E414	V415	L416	R417	E418	H419	P420	V421	L422	L423	N424	R425	A426	L429	H430	R431	L432	Q435	A436	F437	E438	P439	V440	L441	L442	E443	G444	K445	A446	L447	Q448	L449	H450	P451	L452	V453	C454	A455	M458	A459				
A315	I316	T317	S318	N320	K321	R322	P323	L324	K325	S326	K332	L342	Y349	V354	I355	T356	V357	G358	L361	R362	L363	H364	Q365	C366	G367	L368	P369	K370	K371	M372	A373	L374	E375	L376	P379	F380	I381	Y382	G383	K384	L385	E386	L387	R388	G389	L390	A391	T392	T393	I394	K395	A396							
V241	L242	P243	V253	D256	G257	G258	R259	F260	D267	L268	Y269	R270	R271	V272	I273	N274	R275	N276	N277	R278	L279	K280	R281	L282	L283	D284	L285	A286	A287	P288	D289	I290	I291	V292	R293	N294	E295	K296	R297	M298	L299	Q300	E301	A302	V303	D304	A305	L306	L307	D308	N309	G310	R311	G312	G313	R314			
G181	A182	E183	A184	I185	Q186	A187	L188	L189	K190	S191	M192	D193	L194	E195	Q196	C198	E199	Q200	L201	R202	E203	E204	L205	N206	E207	T208	N209	S210	E211	T212	K213	K215	K216	L217	T218	K219	R220	I221	K222	L223	L224	E225	A226	F227	V228	Q229	D230	S230	G231	N232	K233	P234	D174	E175	F176	D177	K179	M180	
P121	S122	R123	I124	G125	L126	L127	L128	D129	M130	P131	L132	R133	D134	I135	E136	R137	V138	L139	Y140	F141	E142	S143	Y144	V145	V146	I147	E148	G149	S150	E151	T152	K153	N154	E155	R156	Q157	Q158	I159	L160	T161	G162	E163	Q164	Y165	L166	D167	A168	L169	E170	T171	F172	G173	D174	E175	F176	D177	K179	M180	
I61	F62	G63	P64	V65	K66	D67	Y68	E69	C70	L71	C72	G73	K74	Y75	K76	R77	L78	K79	H80	R81	G82	V83	I84	C85	E86	K87	C88	G89	V90	E91	V92	T93	Q94	T95	K96	V97	R98	R99	E100	R101	M102	G103	H104	I105	E106	L107	A108	S109	P110	T111	A112	H113	W115	F116	L117	K118	S119	L120	



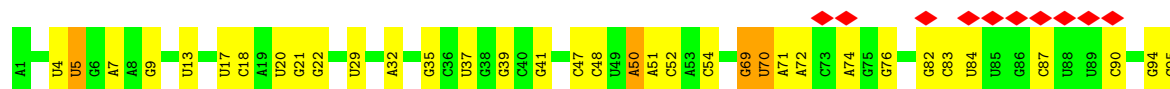
• Molecule 15: DNA-directed RNA polymerase subunit omega

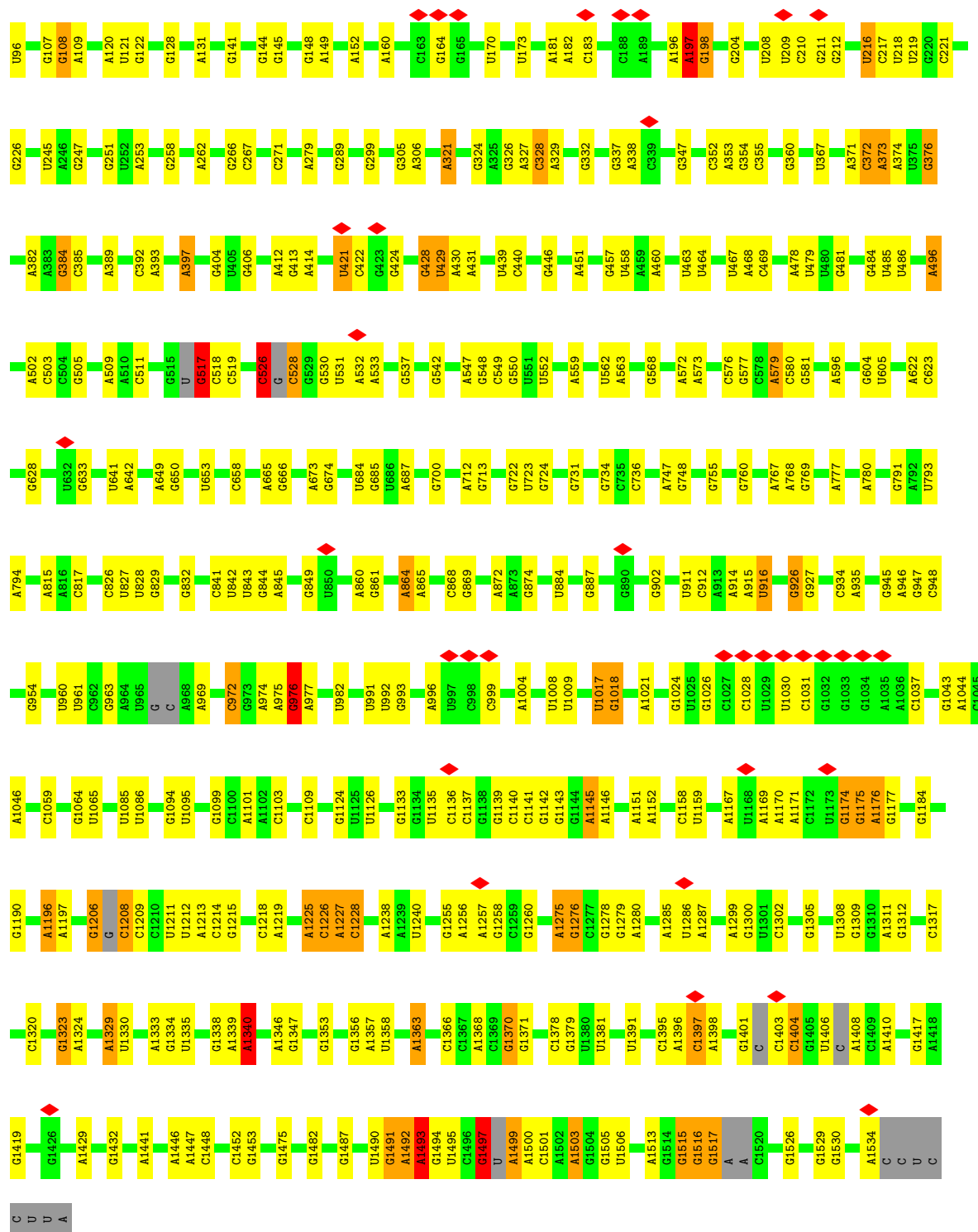


• Molecule 16: 30S ribosomal protein S18



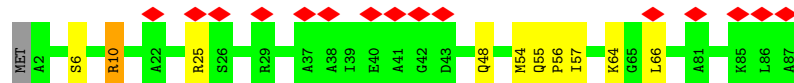
• Molecule 17: 16S rRNA



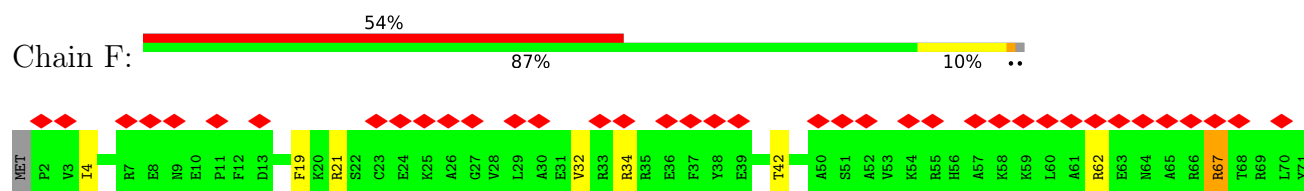


• Molecule 18: 30S ribosomal protein S20

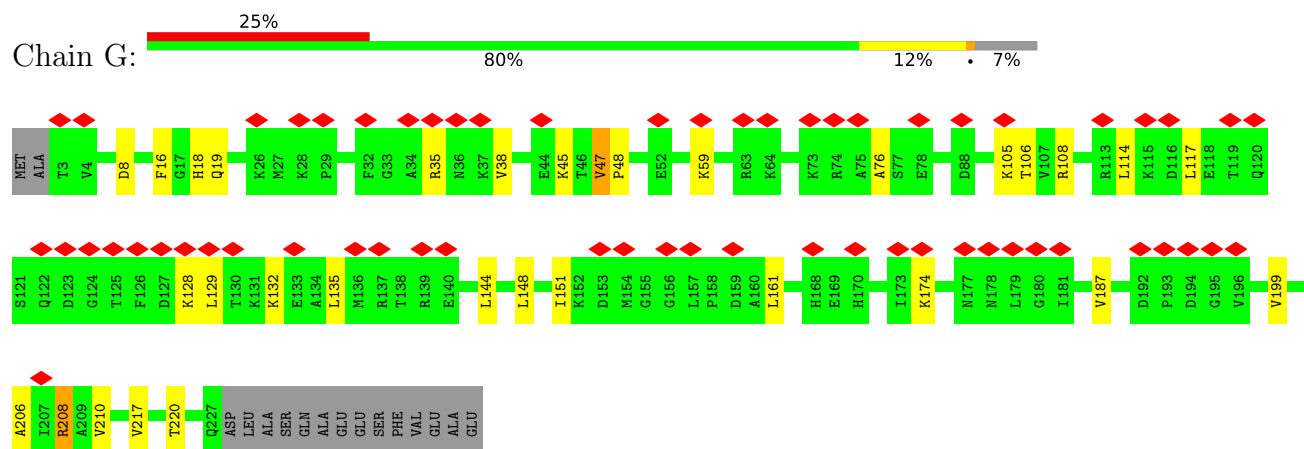
Chain E: 17% 87% 10% ..



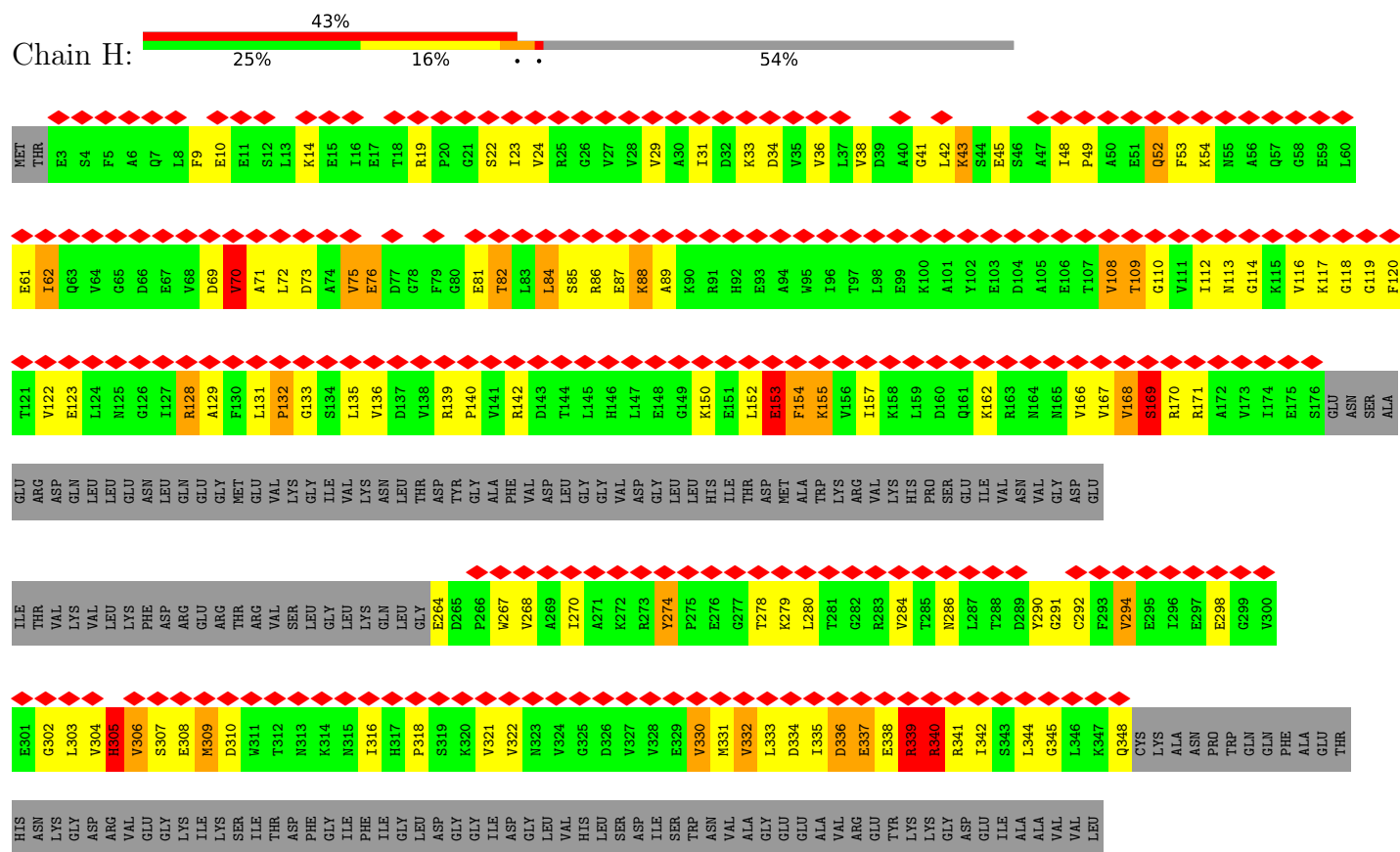
• Molecule 19: 30S ribosomal protein S21

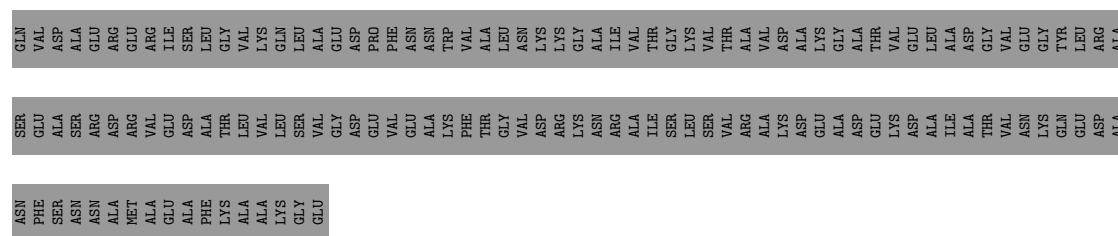


• Molecule 20: 30S ribosomal protein S2

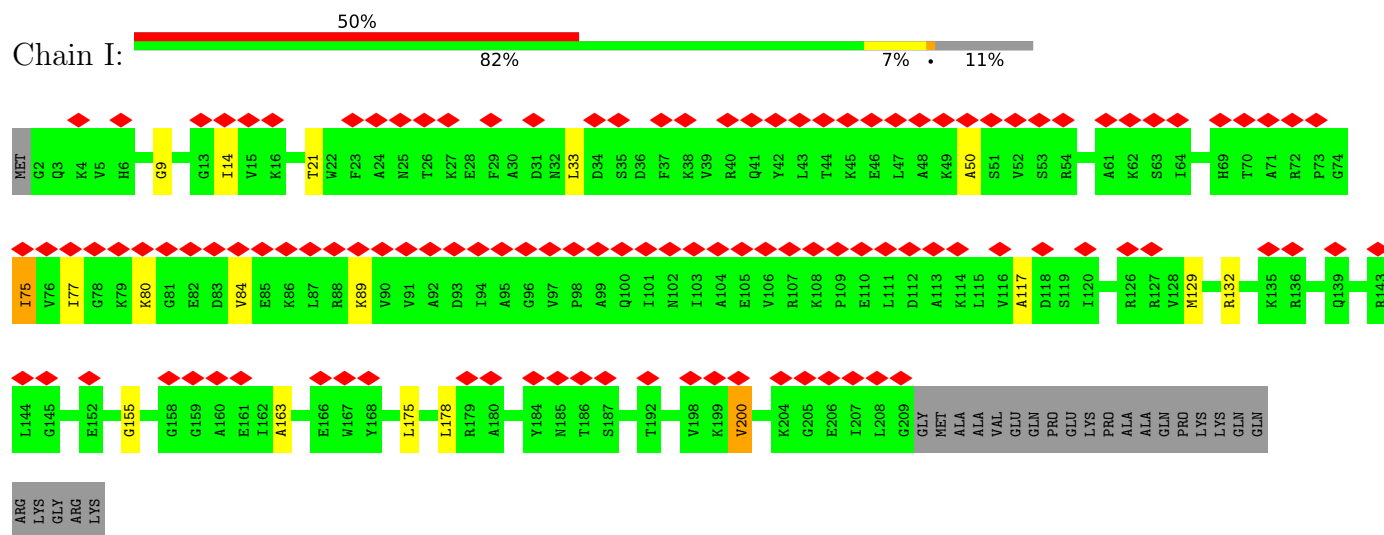


• Molecule 21: 30S ribosomal protein S1

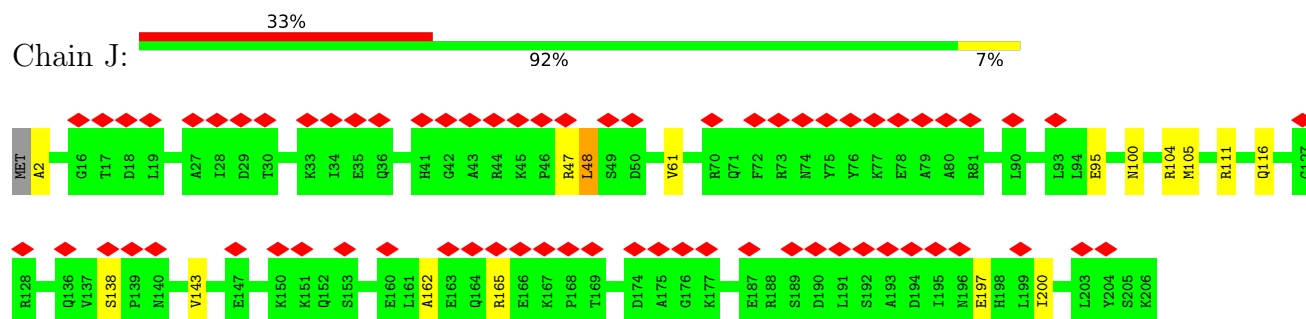




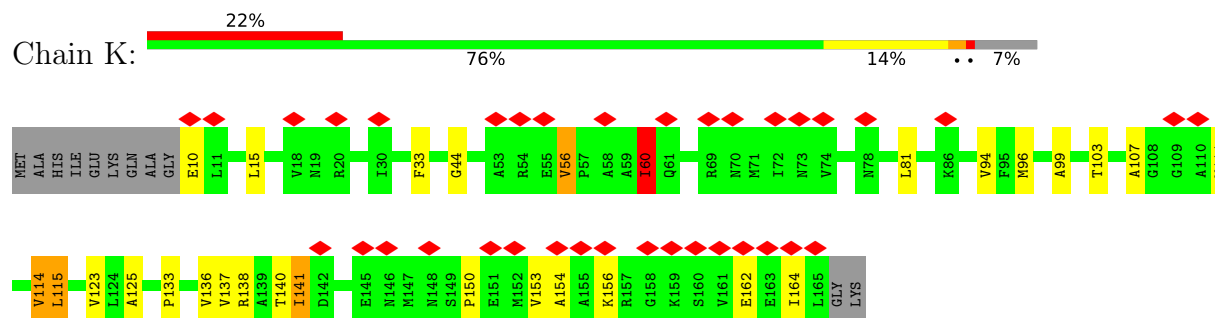
- Molecule 22: 30S ribosomal protein S3



- Molecule 23: 30S ribosomal protein S4

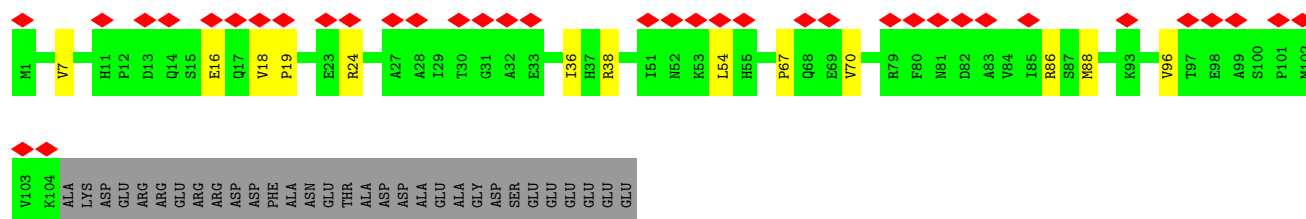


- Molecule 24: 30S ribosomal protein S5

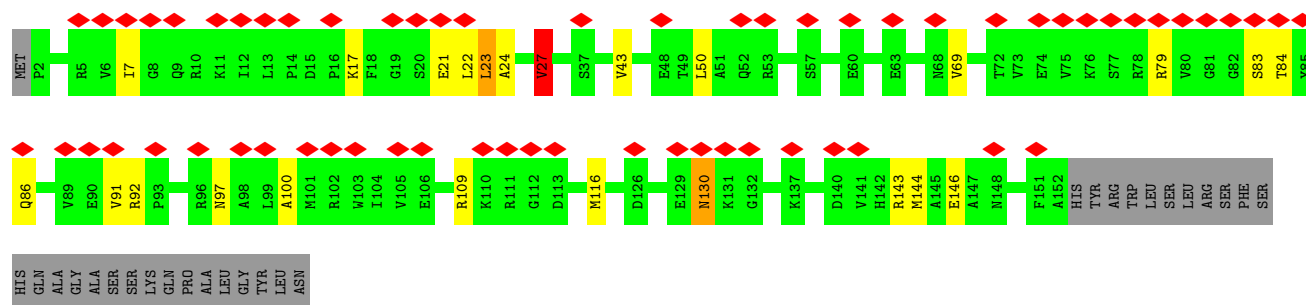


- Molecule 25: 30S ribosomal protein S6

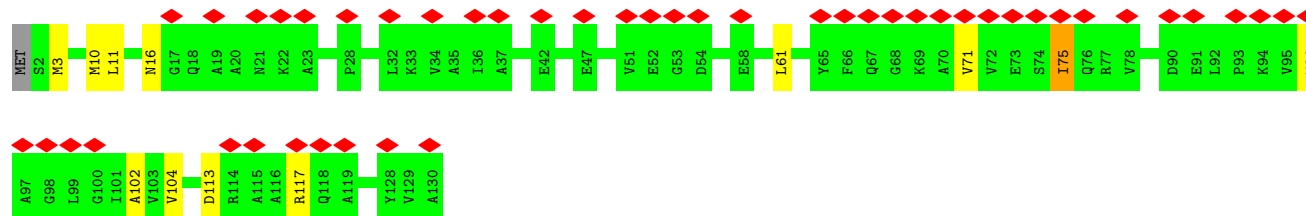
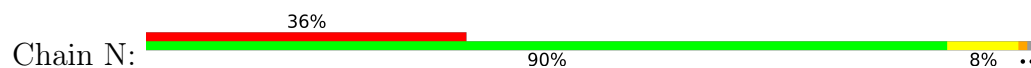




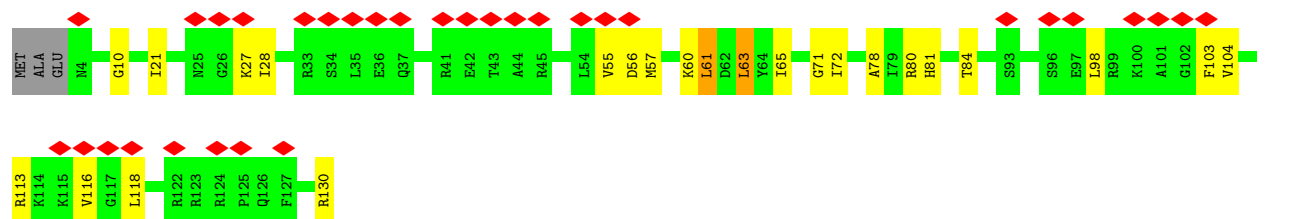
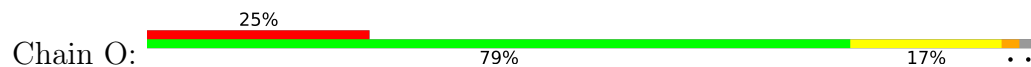
• Molecule 26: 30S ribosomal protein S7



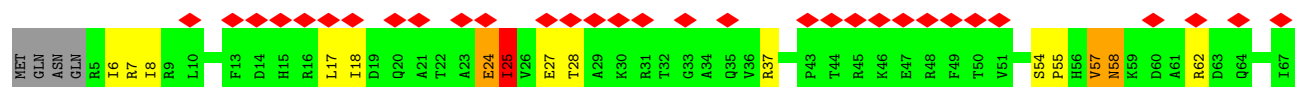
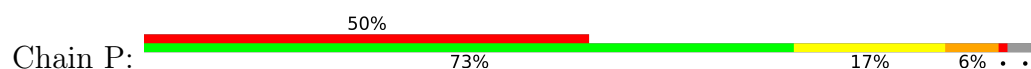
• Molecule 27: 30S ribosomal protein S8

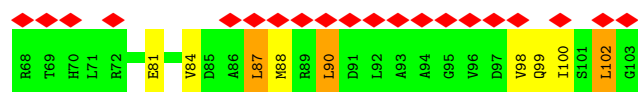


• Molecule 28: 30S ribosomal protein S9

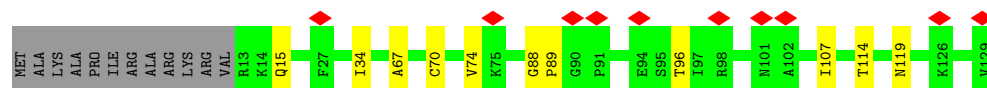
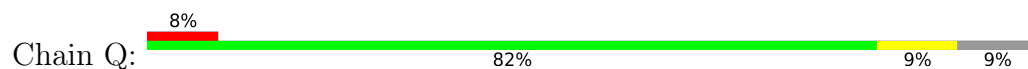


• Molecule 29: 30S ribosomal protein S10

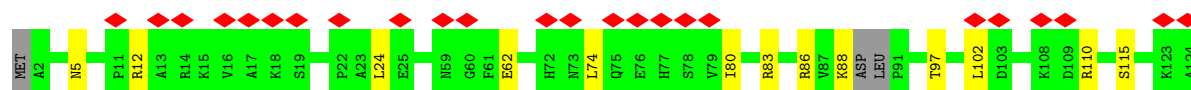
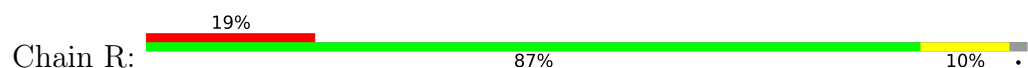




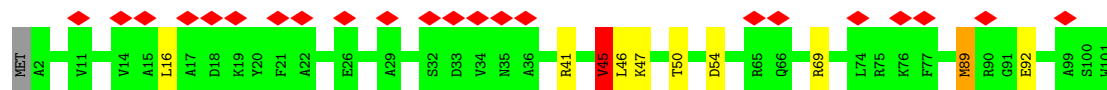
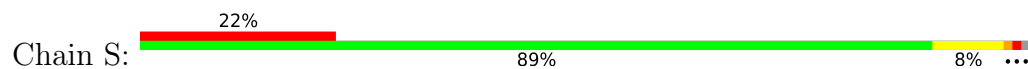
- Molecule 30: 30S ribosomal protein S11



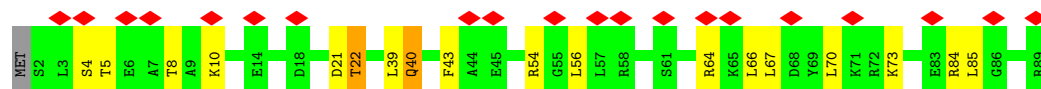
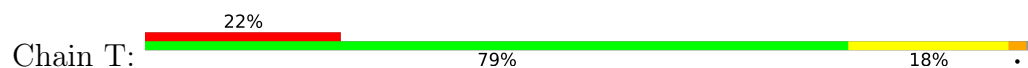
- Molecule 31: 30S ribosomal protein S12



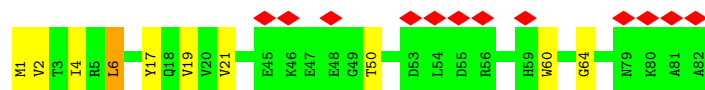
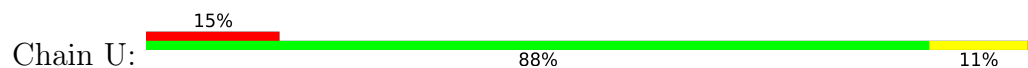
- Molecule 32: 30S ribosomal protein S14



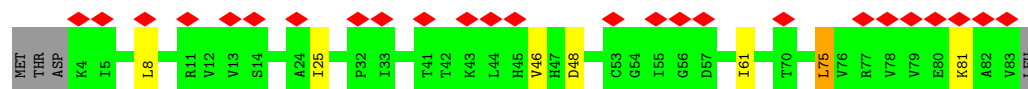
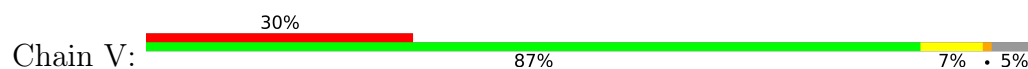
- Molecule 33: 30S ribosomal protein S15



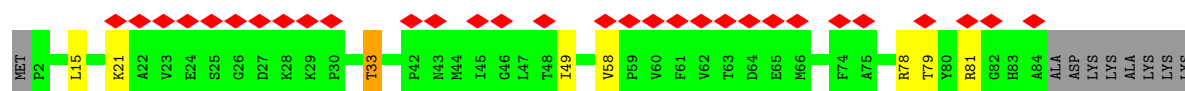
- Molecule 34: 30S ribosomal protein S16



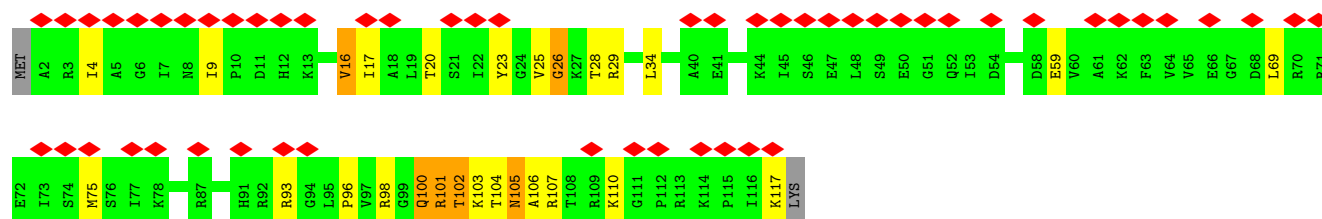
- Molecule 35: 30S ribosomal protein S17



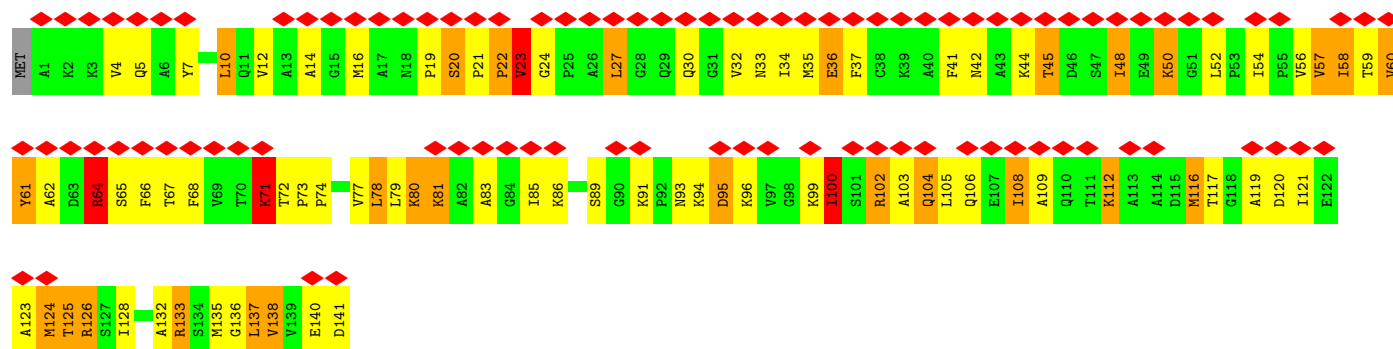
- Molecule 36: 30S ribosomal protein S19



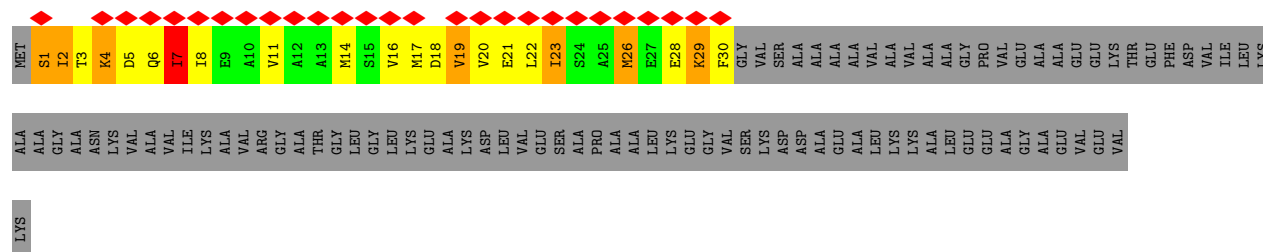
Chain X: 46% 75% 18% 5%



Chain Y: 66% 38% 39% 19%

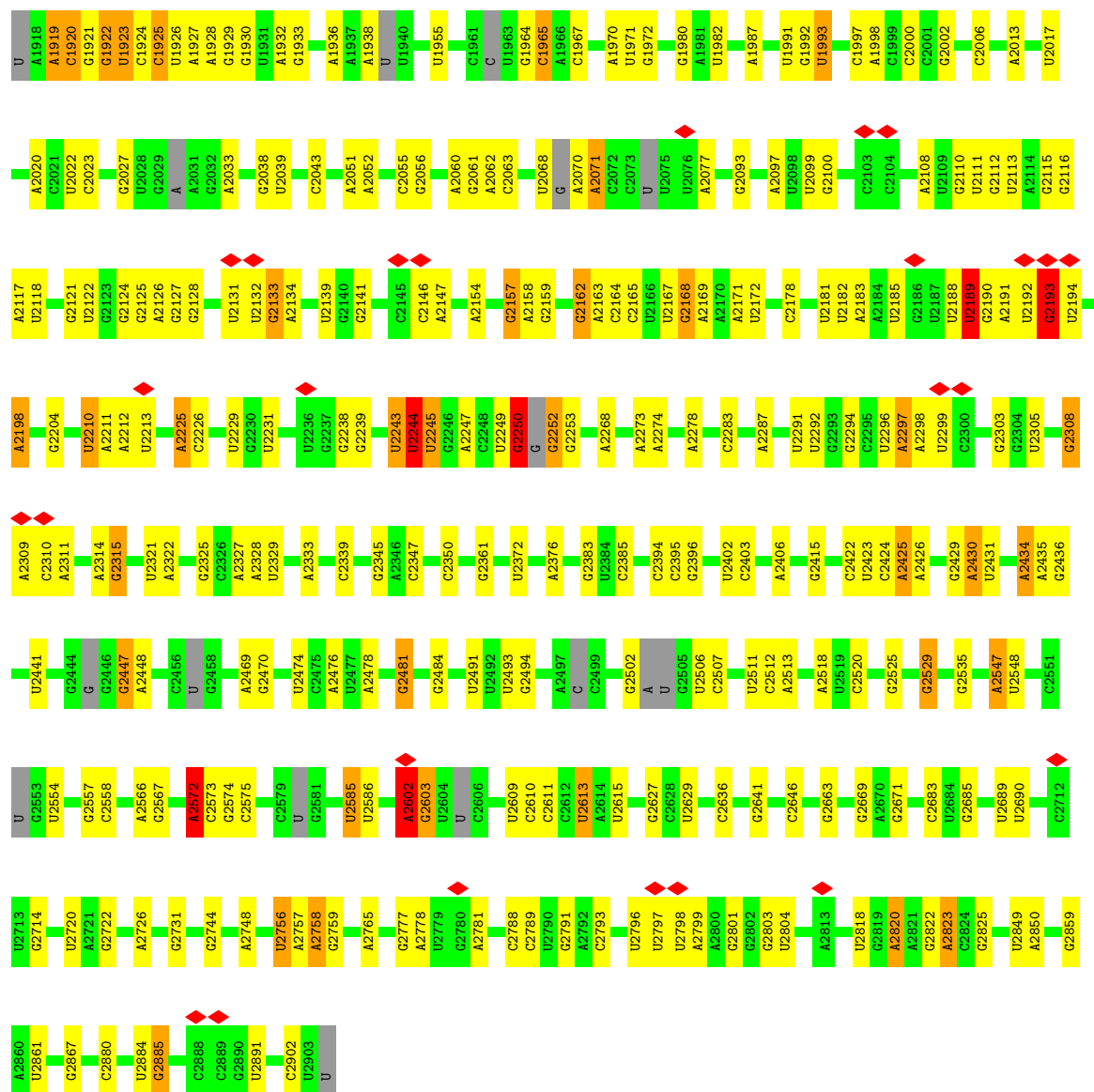


Chain Z: 7% 12% 6% . 75%

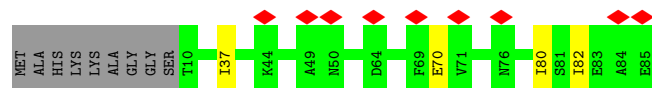
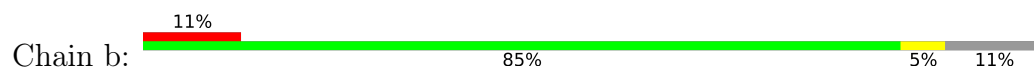


Chain a: 73% 23%

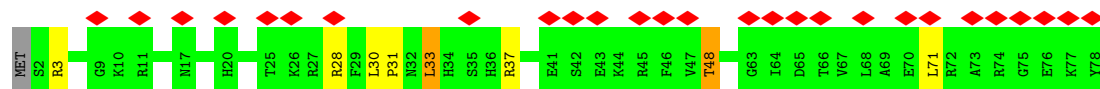
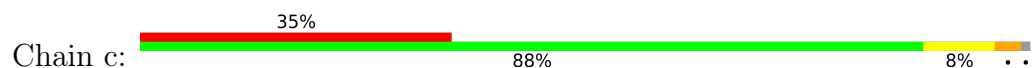




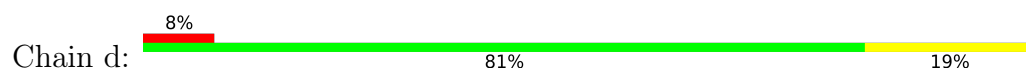
- Molecule 41: 50S ribosomal protein L27



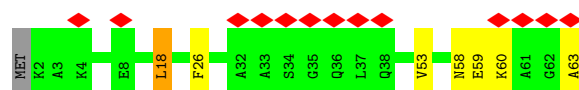
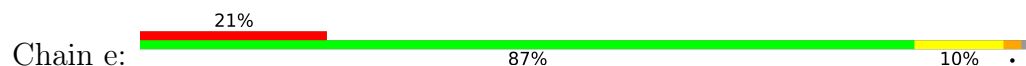
- Molecule 42: 50S ribosomal protein L28



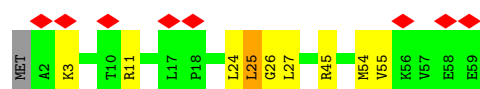
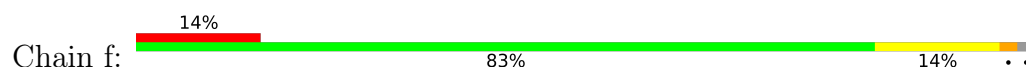
- Molecule 43: 5S rRNA



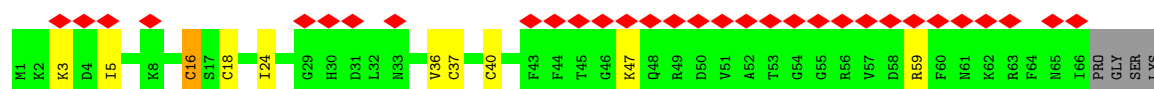
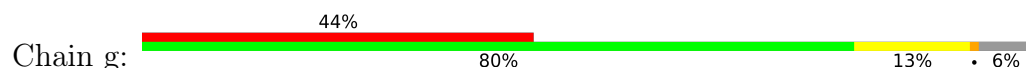
- Molecule 44: 50S ribosomal protein L29



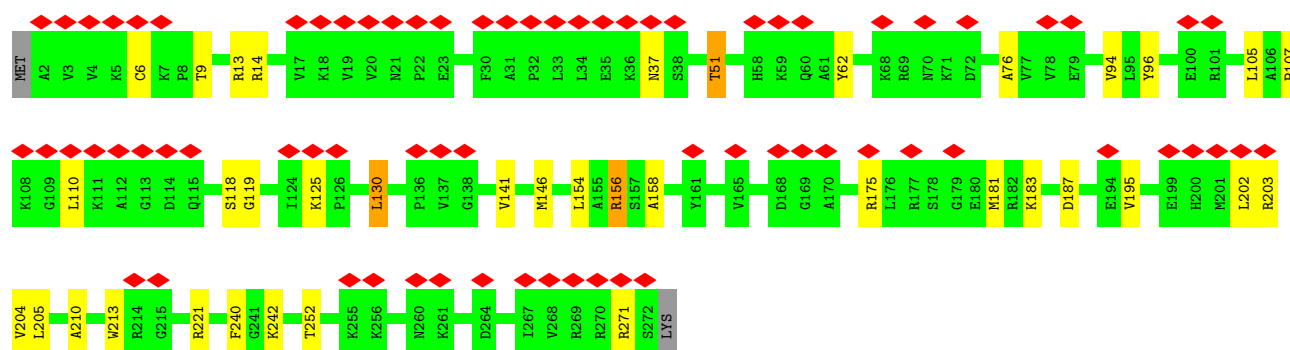
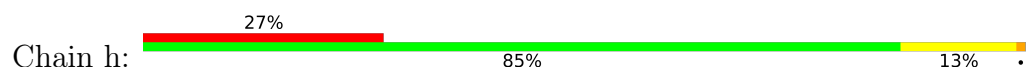
- Molecule 45: 50S ribosomal protein L30



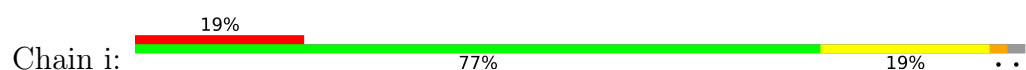
- Molecule 46: 50S ribosomal protein L31



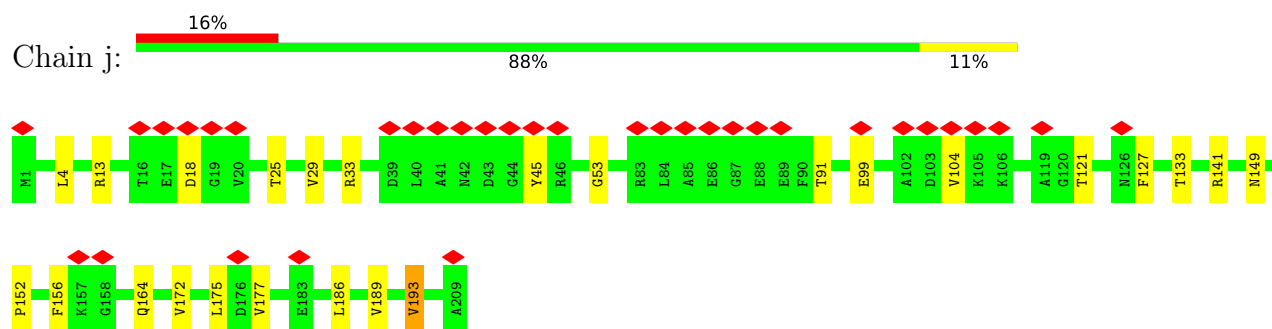
- Molecule 47: 50S ribosomal protein L2



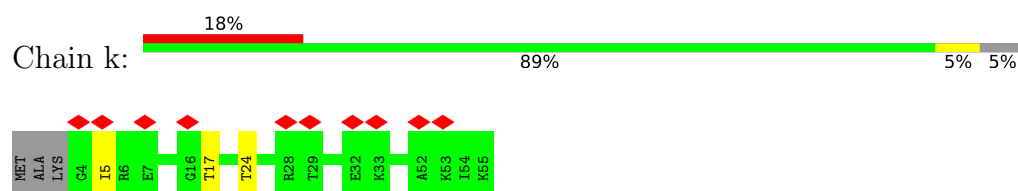
- Molecule 48: 50S ribosomal protein L32



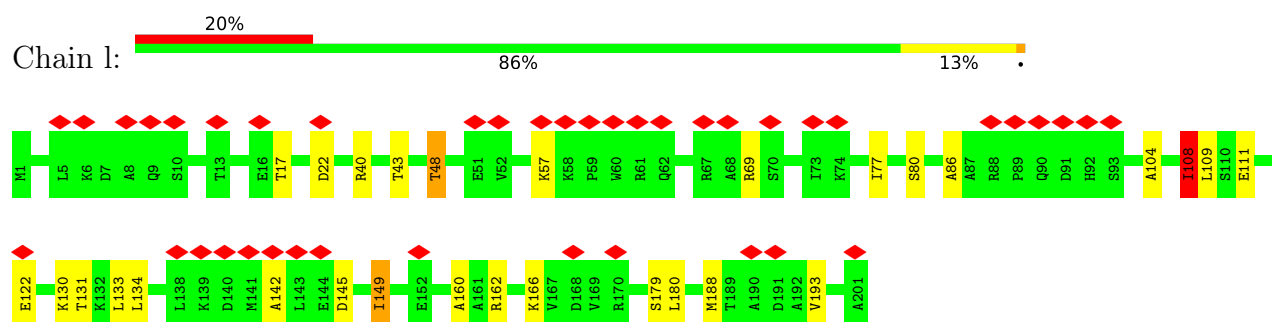
- Molecule 49: 50S ribosomal protein L3



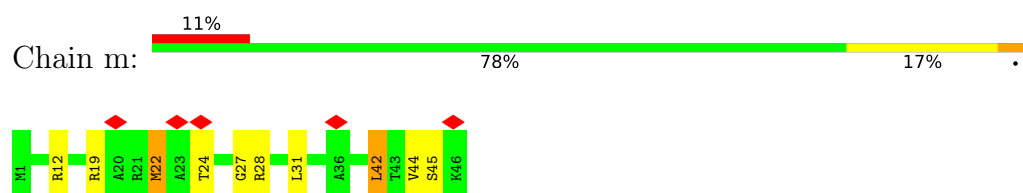
- Molecule 50: 50S ribosomal protein L33



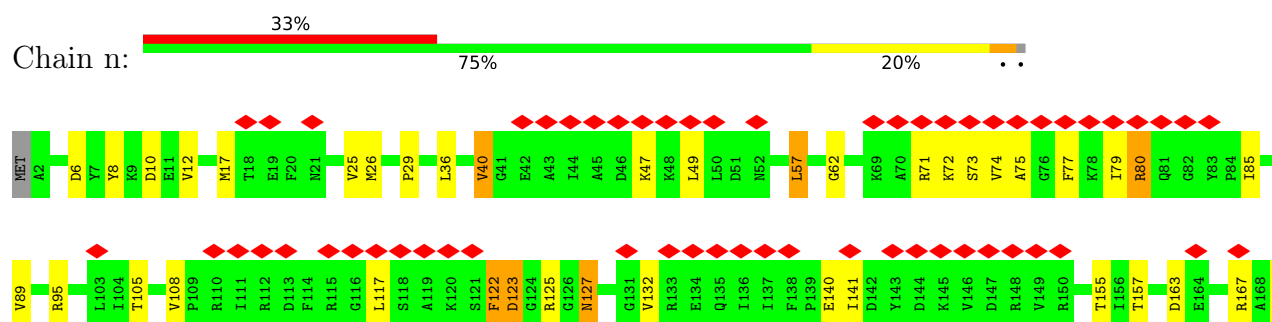
- Molecule 51: 50S ribosomal protein L4

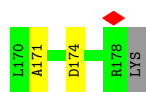


- Molecule 52: 50S ribosomal protein L34

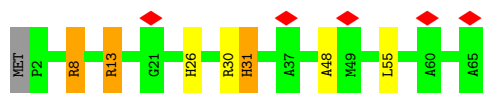
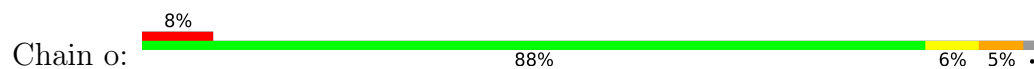


- Molecule 53: 50S ribosomal protein L5

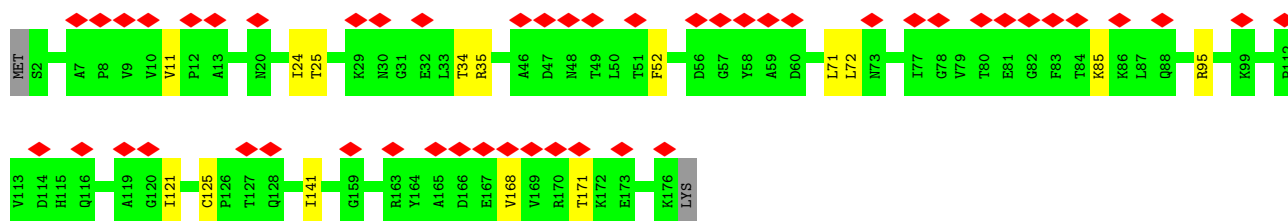
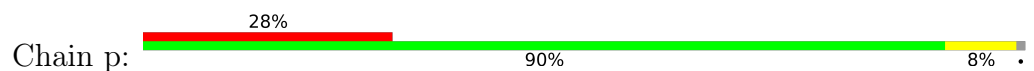




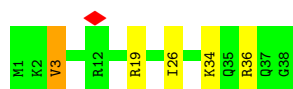
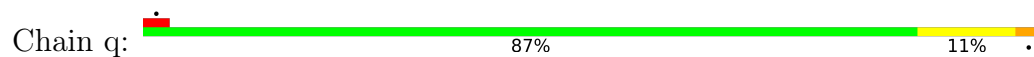
- Molecule 54: 50S ribosomal protein L35



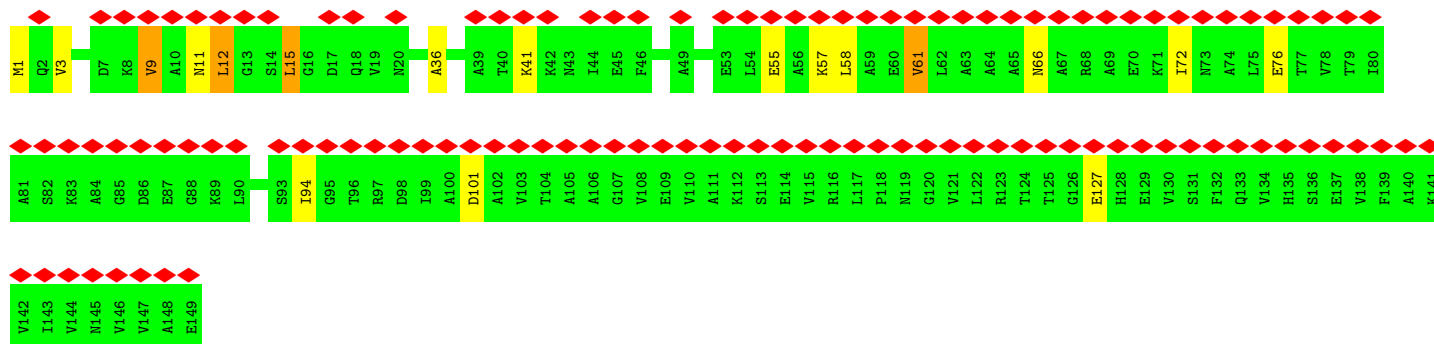
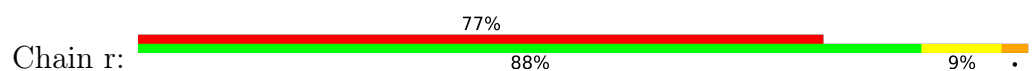
- Molecule 55: 50S ribosomal protein L6



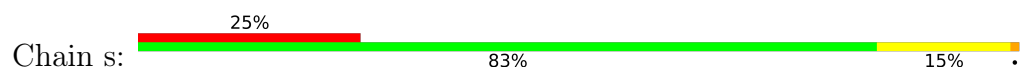
- Molecule 56: 50S ribosomal protein L36

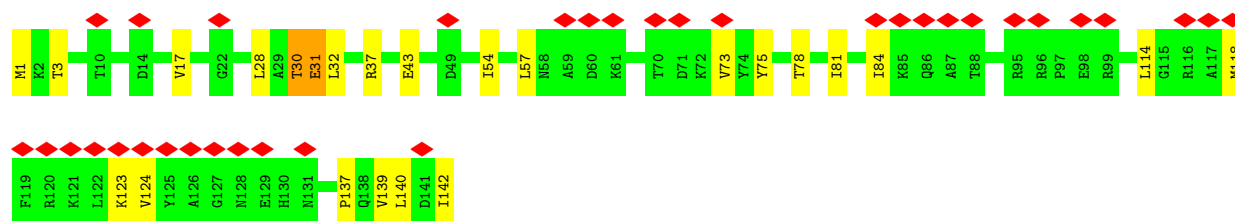


- Molecule 57: 50S ribosomal protein L9

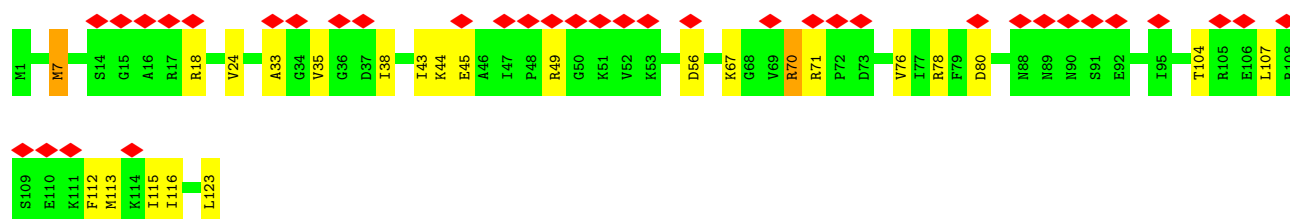
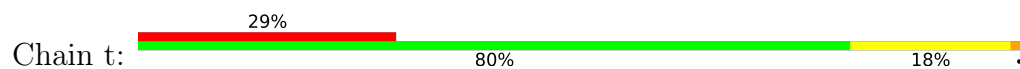


- Molecule 58: 50S ribosomal protein L13

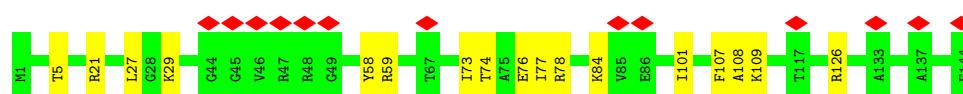
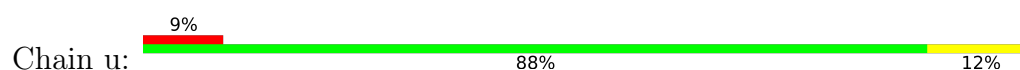




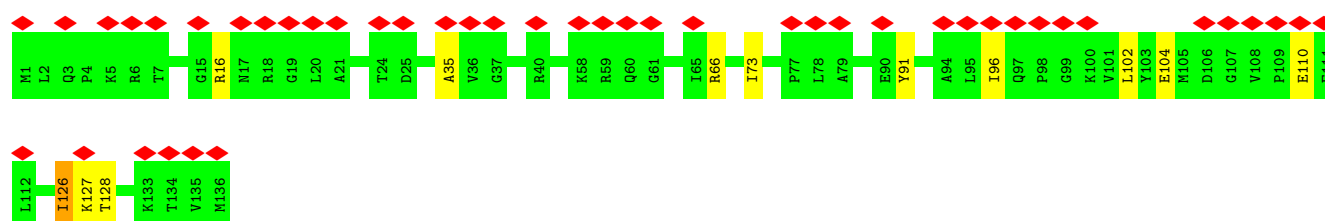
• Molecule 59: 50S ribosomal protein L14



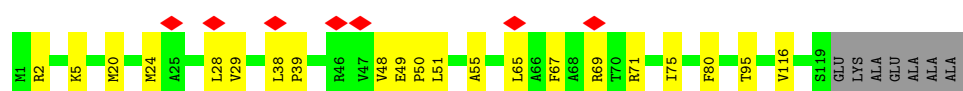
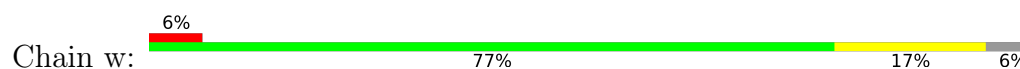
• Molecule 60: 50S ribosomal protein L15



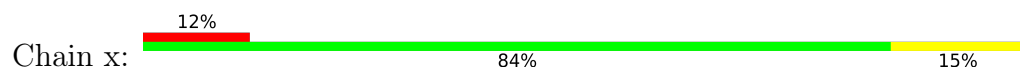
• Molecule 61: 50S ribosomal protein L16

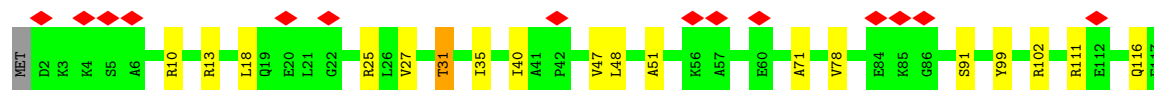


• Molecule 62: 50S ribosomal protein L17

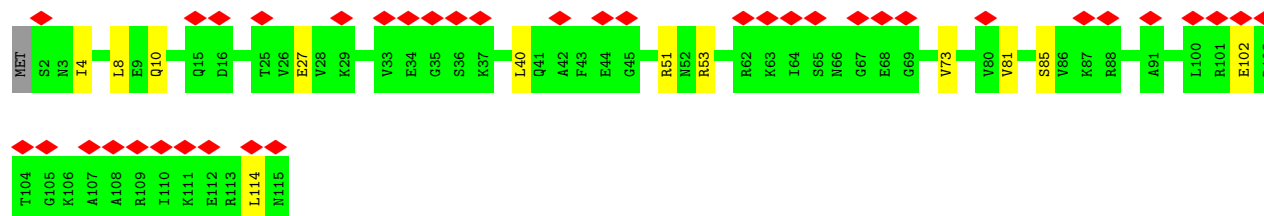
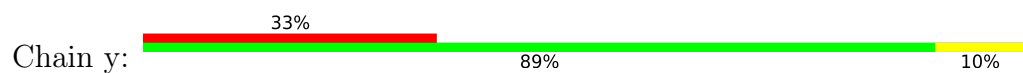


• Molecule 63: 50S ribosomal protein L18

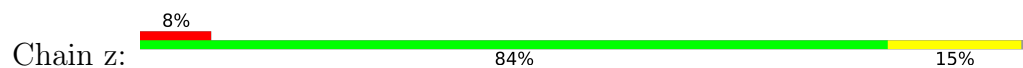




- Molecule 64: 50S ribosomal protein L19



- Molecule 65: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00722	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.50	0/829	0.74	0/1107
2	1	0.67	0/864	1.08	0/1156
3	2	0.54	0/752	0.89	0/1005
4	3	0.47	0/796	0.78	0/1062
5	4	0.52	0/766	0.88	0/1025
6	5	0.64	1/528 (0.2%)	0.55	0/810
7	6	0.55	1/603 (0.2%)	0.56	0/926
8	7	0.59	2/717 (0.3%)	0.90	4/1110 (0.4%)
9	9	1.15	3/1131 (0.3%)	1.30	4/1524 (0.3%)
10	A	0.36	0/1810	0.72	2/2821 (0.1%)
10	B	0.43	0/1810	0.87	9/2821 (0.3%)
11	AA	0.37	0/10547	0.62	0/14232
12	AB	0.86	0/1310	0.94	1/1766 (0.1%)
13	AC	0.37	0/1718	0.61	0/2328
13	AD	0.32	0/1696	0.60	0/2298
14	AE	0.38	0/10561	0.63	5/14258 (0.0%)
15	AF	0.29	0/652	0.61	0/879
16	C	0.66	0/553	1.14	2/743 (0.3%)
17	D	0.40	9/36610 (0.0%)	0.75	39/57091 (0.1%)
18	E	0.75	0/675	1.32	0/895
19	F	0.71	0/597	1.20	0/792
20	G	0.65	0/1791	1.08	1/2413 (0.0%)
21	H	0.76	4/1746 (0.2%)	1.58	34/2382 (1.4%)
22	I	0.58	0/1663	0.97	0/2241
23	J	0.63	0/1665	1.08	0/2227
24	K	0.63	1/1165 (0.1%)	1.06	2/1568 (0.1%)
25	L	0.58	0/867	0.94	0/1171
26	M	0.68	0/1195	1.19	3/1602 (0.2%)
27	N	0.55	0/989	0.91	0/1326
28	O	0.58	0/1034	1.02	1/1375 (0.1%)
29	P	0.60	0/800	1.10	4/1082 (0.4%)
30	Q	0.55	0/893	0.91	0/1205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	R	0.49	0/952	0.81	0/1274
32	S	0.64	0/817	1.11	1/1088 (0.1%)
33	T	0.69	0/722	1.21	0/964
34	U	0.58	0/659	0.99	0/884
35	V	0.45	0/657	0.73	0/881
36	W	0.51	0/680	0.83	0/915
37	X	0.67	0/909	1.21	3/1215 (0.2%)
38	Y	1.04	0/1046	1.09	1/1410 (0.1%)
39	Z	1.02	0/227	1.12	0/304
40	a	0.40	3/69247 (0.0%)	0.75	56/107985 (0.1%)
41	b	0.51	0/589	0.76	0/779
42	c	0.63	0/635	0.97	0/848
43	d	0.37	0/2872	0.69	0/4478
44	e	0.69	0/502	1.19	0/667
45	f	0.62	0/452	1.02	0/605
46	g	0.55	0/531	0.99	1/709 (0.1%)
47	h	0.54	0/2121	0.85	0/2852
48	i	0.52	0/450	0.94	0/599
49	j	0.60	0/1586	0.87	0/2134
50	k	0.46	0/433	0.80	0/576
51	l	0.61	0/1571	1.03	1/2113 (0.0%)
52	m	0.68	0/380	1.22	0/498
53	n	0.62	0/1434	1.18	10/1926 (0.5%)
54	o	0.63	0/513	1.10	1/676 (0.1%)
55	p	0.58	0/1333	0.89	0/1805
56	q	0.50	0/303	0.88	0/397
57	r	0.63	0/1122	0.97	1/1515 (0.1%)
58	s	0.68	0/1152	1.02	2/1551 (0.1%)
59	t	0.57	0/955	0.88	0/1279
60	u	0.55	0/1062	0.96	1/1413 (0.1%)
61	v	0.60	0/1093	0.97	0/1460
62	w	0.67	0/964	1.13	0/1289
63	x	0.61	0/902	1.09	0/1209
64	y	0.52	0/929	0.79	0/1242
65	z	0.80	0/960	1.25	0/1278
All	All	0.48	24/190093 (0.0%)	0.82	189/280059 (0.1%)

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
10	A	0	2
10	B	0	2
12	AB	0	3
13	AC	0	1
13	AD	0	1
14	AE	0	4
21	H	0	3
37	X	0	1
All	All	0	17

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	18.16	1.70	1.47
21	H	169	SER	N-CA	11.77	1.61	1.46
17	D	1516	G	O3'-P	-10.74	1.45	1.61
17	D	1339	A	O3'-P	8.45	1.73	1.61
8	7	19	G	C1'-N9	-7.46	1.36	1.48
6	5	109	DT	O3'-P	7.02	1.71	1.61
8	7	-19	U	C1'-N1	7.01	1.58	1.48
21	H	88	LYS	N-CA	7.01	1.55	1.46
17	D	145	G	O3'-P	6.75	1.71	1.61
17	D	196	A	O3'-P	6.66	1.71	1.61
21	H	168	VAL	C-N	6.46	1.42	1.33
17	D	1275	A	O3'-P	6.22	1.70	1.61
40	a	2434	A	O3'-P	6.02	1.70	1.61
17	D	1515	G	O3'-P	-5.80	1.52	1.61
17	D	1395	C	O3'-P	5.79	1.69	1.61
21	H	88	LYS	CA-C	5.75	1.60	1.52
17	D	1490	U	O3'-P	5.49	1.69	1.61
7	6	10	DG	C1'-N9	-5.37	1.35	1.46
17	D	1492	A	O3'-P	5.31	1.69	1.61
40	a	1905	C	O3'-P	5.29	1.69	1.61
40	a	2167	U	O3'-P	5.21	1.69	1.61
9	9	129	LEU	C-N	5.14	1.45	1.33
9	9	116	GLU	N-CA	5.07	1.49	1.46
24	K	56	VAL	CA-CB	5.05	1.57	1.54

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1516	G	O3'-P-O5'	17.48	130.22	104.00
21	H	88	LYS	CA-C-N	16.96	143.61	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	88	LYS	C-N-CA	16.96	143.61	120.38
10	B	29	G	C3'-C2'-O2'	15.98	134.68	110.70
9	9	129	LEU	CA-C-N	15.84	139.64	119.84
9	9	129	LEU	C-N-CA	15.84	139.64	119.84
17	D	1516	G	P-O3'-C3'	-15.54	96.89	120.20
21	H	332	VAL	N-CA-C	13.67	124.56	110.62
21	H	169	SER	N-CA-C	12.74	137.94	110.80
21	H	330	VAL	N-CA-C	12.21	126.97	109.51
21	H	305	HIS	N-CA-C	11.97	131.12	111.37
40	a	2244	U	C1'-C2'-O2'	-9.76	93.77	108.40
53	n	73	SER	N-CA-CB	-9.59	94.56	110.47
17	D	1206	G	C4'-C3'-O3'	9.55	127.33	113.00
29	P	54	SER	CA-C-N	9.35	129.04	118.85
29	P	54	SER	C-N-CA	9.35	129.04	118.85
40	a	2250	G	C4'-C3'-O3'	-9.23	95.56	109.40
17	D	1401	G	C4'-C3'-O3'	8.83	126.25	113.00
17	D	428	G	C4'-C3'-O3'	8.72	122.48	109.40
8	7	-20	A	O3'-P-O5'	-8.60	91.09	104.00
9	9	130	PRO	CA-N-CD	-8.59	99.98	112.00
21	H	339	ARG	CA-C-N	8.55	137.87	121.54
21	H	339	ARG	C-N-CA	8.55	137.87	121.54
32	S	45	VAL	N-CA-CB	8.49	120.49	110.55
17	D	1515	G	O3'-P-O5'	-8.46	91.31	104.00
40	a	2296	U	C4'-C3'-O3'	8.44	122.06	109.40
40	a	404	A	C2'-C3'-O3'	8.35	122.03	109.50
29	P	57	VAL	N-CA-C	8.27	120.01	107.77
8	7	-17	U	C2'-C3'-O3'	8.26	121.89	109.50
17	D	197	A	C2'-C3'-O3'	8.21	121.81	109.50
40	a	2252	G	N9-C1'-C2'	-8.16	99.76	112.00
17	D	1401	G	N9-C1'-C2'	-7.92	100.12	112.00
40	a	2425	A	C2'-C3'-O3'	7.82	121.23	109.50
21	H	155	LYS	CA-C-N	-7.76	110.95	121.66
21	H	155	LYS	C-N-CA	-7.76	110.95	121.66
40	a	2071	A	C4'-C3'-O3'	-7.72	101.41	113.00
21	H	168	VAL	CA-C-N	7.64	136.14	121.54
21	H	168	VAL	C-N-CA	7.64	136.14	121.54
53	n	75	ALA	CA-C-N	7.62	129.67	120.14
53	n	75	ALA	C-N-CA	7.62	129.67	120.14
17	D	1493	A	C2'-C3'-O3'	7.62	125.13	113.70
21	H	84	LEU	N-CA-C	7.61	120.97	110.24
21	H	52	GLN	N-CA-C	-7.60	104.15	113.50
37	X	102	THR	CB-CA-C	7.58	123.42	110.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1499	A	N9-C1'-C2'	-7.58	100.64	112.00
17	D	1339	A	P-O3'-C3'	7.57	131.56	120.20
24	K	60	ILE	N-CA-CB	7.52	119.35	110.55
17	D	528	C	N1-C1'-C2'	-7.52	100.72	112.00
21	H	336	ASP	CB-CA-C	-7.44	98.66	110.79
53	n	73	SER	CB-CA-C	7.43	122.90	110.79
24	K	56	VAL	O-C-N	7.38	125.15	120.42
53	n	108	VAL	O-C-N	7.37	125.30	120.07
10	B	28	C	P-O3'-C3'	7.34	131.21	120.20
40	a	2602	A	C4'-C3'-O3'	7.32	120.38	109.40
20	G	47	VAL	O-C-N	7.30	125.09	120.42
40	a	783	A	C4'-C3'-O3'	7.27	123.90	113.00
10	B	29	G	N9-C1'-C2'	-7.15	101.27	112.00
17	D	1497	G	C1'-C2'-O2'	-7.14	97.69	108.40
17	D	196	A	P-O3'-C3'	7.13	130.90	120.20
40	a	2162	G	C4'-C3'-O3'	7.11	120.06	109.40
40	a	896	A	C4'-C3'-O3'	7.06	119.98	109.40
40	a	2225	A	C4'-C3'-O3'	6.98	119.86	109.40
26	M	27	VAL	N-CA-CB	6.96	118.70	110.55
40	a	1379	U	C2'-C3'-O3'	6.96	124.13	113.70
21	H	140	PRO	N-CA-CB	6.90	110.50	103.25
40	a	2244	U	C4'-C3'-O3'	6.88	123.32	113.00
21	H	340	ARG	CA-C-N	-6.80	112.56	123.23
21	H	340	ARG	C-N-CA	-6.80	112.56	123.23
40	a	2252	G	C4'-C3'-O3'	6.78	123.17	113.00
53	n	71	ARG	CA-C-N	6.73	133.95	122.37
53	n	71	ARG	C-N-CA	6.73	133.95	122.37
40	a	2243	U	C4'-C3'-O3'	6.68	123.03	113.00
21	H	170	ARG	N-CA-C	6.65	119.62	110.24
17	D	517	G	C5'-C4'-C3'	6.63	125.15	115.20
21	H	87	GLU	N-CA-C	-6.60	104.08	111.28
21	H	303	LEU	N-CA-C	6.59	121.16	112.13
40	a	2189	U	C1'-C2'-O2'	-6.59	101.92	111.80
40	a	2167	U	P-O3'-C3'	6.56	130.03	120.20
21	H	132	PRO	N-CA-CB	6.54	110.25	103.38
17	D	526	C	C4'-C3'-O3'	6.54	122.80	113.00
21	H	155	LYS	N-CA-C	-6.53	98.25	108.90
40	a	894	U	C2'-C3'-O3'	6.53	119.30	109.50
57	r	61	VAL	N-CA-CB	6.53	118.19	110.55
53	n	127	ASN	CB-CA-C	6.51	121.64	110.77
21	H	112	ILE	N-CA-C	6.51	117.07	106.72
17	D	526	C	N1-C1'-C2'	-6.49	102.26	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	o	13	ARG	N-CA-C	6.49	121.03	113.18
28	O	72	ILE	N-CA-C	-6.49	105.38	111.48
53	n	127	ASN	CA-CB-CG	-6.46	106.14	112.60
17	D	1340	A	C1'-C2'-O2'	6.46	118.09	108.40
12	AB	122	PRO	N-CA-CB	6.40	109.97	103.25
40	a	754	U	N1-C1'-C2'	6.40	121.60	112.00
17	D	69	G	C4'-C3'-O3'	-6.37	103.44	113.00
17	D	1208	C	N1-C1'-C2'	-6.29	102.56	112.00
16	C	33	ILE	CA-C-O	-6.28	114.90	121.93
40	a	2434	A	P-O3'-C3'	6.26	129.59	120.20
21	H	153	GLU	N-CA-C	-6.24	97.50	110.80
10	B	28	C	O3'-P-O5'	-6.21	94.69	104.00
40	a	2425	A	C4'-C3'-O3'	6.21	118.71	109.40
21	H	113	ASN	N-CA-C	6.16	118.07	111.36
17	D	1206	G	N9-C1'-C2'	-6.15	102.78	112.00
8	7	9	U	C2'-C3'-O3'	6.08	122.82	113.70
40	a	271	G	C4'-C3'-O3'	6.07	118.50	109.40
17	D	1516	G	OP1-P-O3'	-6.05	89.85	108.00
40	a	2820	A	C4'-C3'-O3'	-6.00	103.99	113.00
17	D	1408	A	C4'-C3'-O3'	6.00	122.00	113.00
17	D	550	G	C3'-C2'-O2'	5.99	119.69	110.70
40	a	2210	U	C4'-C3'-O3'	5.99	118.38	109.40
40	a	1913	A	C2'-C3'-O3'	5.98	118.47	109.50
26	M	92	ARG	CA-C-N	5.92	125.40	119.24
26	M	92	ARG	C-N-CA	5.92	125.40	119.24
21	H	109	THR	N-CA-C	-5.88	99.07	109.06
40	a	2308	G	C2'-C3'-O3'	-5.86	104.92	113.70
21	H	150	LYS	N-CA-C	5.84	118.23	110.53
40	a	2756	U	C4'-C3'-O3'	5.83	118.15	109.40
51	l	108	ILE	N-CA-CB	5.83	118.47	110.54
53	n	72	LYS	N-CA-C	-5.82	99.16	109.06
21	H	75	VAL	N-CA-C	5.80	116.47	108.12
37	X	26	GLY	N-CA-C	-5.78	104.38	112.13
10	B	29	G	O5'-C5'-C4'	-5.78	102.83	111.50
40	a	1905	C	P-O3'-C3'	5.77	128.86	120.20
40	a	70	G	C4'-C3'-O3'	5.76	118.04	109.40
17	D	1275	A	P-O3'-C3'	5.75	128.83	120.20
14	AE	853	THR	CA-C-N	5.75	131.02	122.74
14	AE	853	THR	C-N-CA	5.75	131.02	122.74
10	B	48	C	N1-C1'-C2'	5.72	120.58	112.00
17	D	1406	U	N1-C1'-C2'	-5.71	103.43	112.00
40	a	2168	G	C4'-C3'-O3'	-5.71	104.43	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	1492	A	P-O3'-C3'	5.71	128.76	120.20
10	A	48	C	N1-C1'-C2'	5.70	120.55	112.00
17	D	976	G	C4'-C3'-O3'	-5.70	104.45	113.00
17	D	1340	A	C5'-C4'-C3'	5.69	124.54	116.00
40	a	1757	A	C4'-C3'-O3'	-5.69	104.47	113.00
17	D	1490	U	P-O3'-C3'	5.68	128.72	120.20
40	a	2017	U	C2'-C3'-O3'	-5.64	105.25	113.70
21	H	114	GLY	N-CA-C	5.61	121.23	111.14
17	D	780	A	C4'-C3'-O3'	-5.55	104.67	113.00
40	a	2447	G	C2'-C3'-O3'	-5.53	101.20	109.50
40	a	1568	G	C4'-C3'-O3'	-5.51	104.74	113.00
40	a	2731	G	C4'-C3'-O3'	-5.50	104.75	113.00
14	AE	1184	ASP	N-CA-C	5.44	121.83	109.81
40	a	2481	G	C4'-C3'-O3'	-5.40	104.90	113.00
40	a	2572	A	C4'-C3'-O3'	-5.40	101.30	109.40
40	a	2068	U	C4'-C3'-O3'	-5.39	104.92	113.00
10	B	35	A	P-O3'-C3'	5.38	128.27	120.20
40	a	944	C	C4'-C3'-O3'	-5.38	104.93	113.00
17	D	864	A	N9-C1'-C2'	5.38	120.06	112.00
17	D	1145	A	C4'-C3'-O3'	-5.36	104.96	113.00
17	D	517	G	C4'-C3'-O3'	-5.35	101.37	109.40
17	D	1499	A	C4'-C3'-O3'	5.35	121.02	113.00
40	a	2231	U	C1'-C2'-O2'	5.34	116.41	108.40
46	g	5	ILE	N-CA-C	5.33	117.72	111.05
40	a	375	G	C2'-C3'-O3'	5.33	121.69	113.70
17	D	145	G	P-O3'-C3'	5.32	128.17	120.20
40	a	2020	A	C4'-C3'-O3'	-5.31	105.04	113.00
40	a	1270	C	C2'-C3'-O3'	-5.30	105.75	113.70
37	X	102	THR	CA-C-O	-5.29	114.83	121.02
17	D	1395	C	P-O3'-C3'	5.26	128.09	120.20
8	7	-11	U	C2'-C3'-O3'	5.25	117.37	109.50
40	a	2529	G	C4'-C3'-O3'	-5.24	105.14	113.00
40	a	423	A	C2'-C3'-O3'	-5.19	105.92	113.70
40	a	2245	U	N1-C1'-C2'	-5.19	104.22	112.00
10	B	60	U	C2'-C3'-O3'	5.18	117.28	109.50
21	H	128	ARG	CA-C-N	-5.17	114.13	122.81
21	H	128	ARG	C-N-CA	-5.17	114.13	122.81
60	u	101	ILE	N-CA-C	5.16	116.46	112.12
40	a	528	A	C4'-C3'-O3'	-5.15	105.28	113.00
10	A	60	U	C2'-C3'-O3'	5.14	117.21	109.50
40	a	1834	U	C4'-C3'-O3'	-5.13	105.31	113.00
17	D	1335	U	C4'-C3'-O3'	-5.12	105.32	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Y	5	GLN	O-C-N	5.12	124.62	120.83
29	P	25	ILE	N-CA-CB	5.11	117.49	110.54
40	a	328	U	C4'-C3'-O3'	-5.10	105.36	113.00
21	H	154	PHE	N-CA-C	-5.09	100.40	109.06
14	AE	709	ARG	CA-C-N	5.09	135.46	126.45
14	AE	709	ARG	C-N-CA	5.09	135.46	126.45
40	a	126	A	C4'-C3'-O3'	-5.09	105.37	113.00
40	a	479	A	C4'-C3'-O3'	5.07	117.01	109.40
16	C	35	GLU	N-CA-C	-5.06	105.95	111.82
58	s	28	LEU	CA-C-N	5.05	127.01	120.44
58	s	28	LEU	C-N-CA	5.05	127.01	120.44
40	a	1864	U	C4'-C3'-O3'	-5.05	105.42	113.00
40	a	2193	G	C2'-C3'-O3'	5.05	121.27	113.70
9	9	115	GLY	CA-C-O	-5.03	118.22	122.29
17	D	70	U	C2'-C3'-O3'	5.03	117.04	109.50
21	H	108	VAL	N-CA-C	-5.03	98.89	109.34
40	a	1025	G	C4'-C3'-O3'	5.03	116.94	109.40
10	B	19	G	N9-C1'-C2'	5.02	119.54	112.00
40	a	614	A	C2'-C3'-O3'	5.02	117.03	109.50

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
12	AB	135	ARG	Sidechain
12	AB	157	ARG	Sidechain
12	AB	167	ARG	Sidechain
13	AC	192	VAL	Peptide
13	AD	20	SER	Peptide
14	AE	1326	GLN	Peptide
14	AE	1344	LEU	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
10	B	19	G	Sidechain
10	B	7	G	Sidechain
21	H	274	TYR	Peptide
21	H	81	GLU	Peptide
21	H	82	THR	Peptide
37	X	100	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	8	0
2	1	857	922	922	14	0
3	2	746	811	811	6	0
4	3	788	844	844	10	0
5	4	753	780	780	0	0
6	5	472	260	260	16	0
7	6	542	305	306	28	0
8	7	647	0	321	101	0
9	9	1117	0	1153	165	0
10	A	1620	826	826	173	0
10	B	1620	813	827	141	0
11	AA	10381	0	10391	139	0
12	AB	1282	0	1252	110	0
13	AC	1698	0	1718	11	0
13	AD	1677	0	1713	28	0
14	AE	10404	0	10622	189	0
15	AF	650	0	658	10	0
16	C	544	559	560	23	0
17	D	32703	16423	16459	214	0
18	E	669	719	719	4	0
19	F	589	629	629	8	0
20	G	1760	1785	1785	45	0
21	H	1730	1454	1454	209	0
22	I	1636	1710	1710	9	0
23	J	1643	1707	1707	16	0
24	K	1152	1196	1196	22	0
25	L	848	846	846	3	0
26	M	1181	1235	1235	33	0
27	N	979	1031	1031	6	0
28	O	1022	1070	1070	13	0
29	P	790	831	831	61	0
30	Q	877	887	887	4	0
31	R	939	1001	1001	7	0
32	S	805	844	844	5	0
33	T	714	734	734	8	0
34	U	649	666	666	3	0
35	V	648	691	691	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	W	663	688	688	2	0
37	X	900	964	964	57	0
38	Y	1032	0	1088	82	0
39	Z	227	0	237	18	0
40	a	61841	31077	31123	301	0
41	b	582	599	599	2	0
42	c	625	652	652	4	0
43	d	2569	1301	1301	3	0
44	e	501	531	531	4	0
45	f	448	488	488	6	0
46	g	522	520	520	10	0
47	h	2082	2154	2154	18	0
48	i	444	459	458	6	0
49	j	1565	1617	1616	14	0
50	k	426	464	464	0	0
51	l	1552	1619	1619	12	0
52	m	377	418	418	10	0
53	n	1410	1443	1444	28	0
54	o	504	572	572	4	0
55	p	1313	1358	1358	7	0
56	q	302	343	343	2	0
57	r	1111	1148	1148	6	0
58	s	1129	1162	1162	13	0
59	t	946	1023	1023	12	0
60	u	1053	1129	1129	8	0
61	v	1074	1157	1157	5	0
62	w	951	994	994	8	0
63	x	892	923	923	8	0
64	y	917	962	962	4	0
65	z	947	1020	1019	12	0
66	AE	1	0	0	0	0
67	AE	2	0	0	3	0
All	All	176856	99203	128452	2060	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2060) 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)
21:H:131:LEU:CB	21:H:167:VAL:CA	1.78	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:12:ARG:HG3	21:H:264:GLU:CB	1.30	1.57
14:AE:79:LYS:HA	14:AE:81:ARG:CZ	1.26	1.52
12:AB:165:PHE:CE2	29:P:100:ILE:CD1	1.95	1.48
21:H:131:LEU:CB	21:H:167:VAL:HA	1.03	1.47
14:AE:79:LYS:HA	14:AE:81:ARG:NH1	1.20	1.43
12:AB:167:ARG:NH2	29:P:99:GLN:HB2	1.25	1.43
14:AE:72:CYS:SG	67:AE:1502:ZN:ZN	1.03	1.43
12:AB:165:PHE:CD2	29:P:100:ILE:HD12	1.52	1.41
9:9:31:ARG:NE	40:a:1054:A:H5'	1.31	1.40
21:H:71:ALA:C	21:H:72:LEU:HD12	1.49	1.37
9:9:130:PRO:N	9:9:130:PRO:CA	1.70	1.36
21:H:118:GLY:O	21:H:133:GLY:CA	1.74	1.35
17:D:1358:U:O4	17:D:1363:A:N1	1.60	1.34
40:a:1839:G:H1'	40:a:1927:A:C8	1.62	1.33
9:9:57:ASN:OD1	9:9:62:ARG:CG	1.75	1.33
14:AE:79:LYS:CA	14:AE:81:ARG:NH1	1.90	1.33
12:AB:165:PHE:CZ	29:P:87:LEU:HB3	1.65	1.32
14:AE:79:LYS:CA	14:AE:81:ARG:CZ	2.06	1.31
40:a:1021:A:N1	40:a:1141:U:O4	1.63	1.31
9:9:31:ARG:CZ	40:a:1054:A:H5'	1.63	1.27
17:D:1227:A:OP2	37:X:110:LYS:HE3	1.35	1.27
17:D:1308:U:H2'	37:X:98:ARG:NH2	1.48	1.26
16:C:12:ARG:CG	21:H:264:GLU:CB	2.15	1.24
7:6:5:DT:OP1	14:AE:1172:LYS:NZ	1.68	1.24
17:D:948:C:OP2	37:X:105:ASN:OD1	1.53	1.23
10:A:18:G:N7	10:A:57:A:N6	1.87	1.23
10:A:32:C:O4'	26:M:144:MET:HE1	1.09	1.23
21:H:267:TRP:CZ2	21:H:340:ARG:HG2	1.75	1.22
9:9:88:HIS:HB3	9:9:89:PRO:CD	1.70	1.22
10:B:18:G:N7	10:B:57:A:N6	1.87	1.21
17:D:1308:U:H3'	37:X:98:ARG:CZ	1.43	1.20
12:AB:165:PHE:HE2	29:P:100:ILE:CD1	1.39	1.20
17:D:1308:U:C2'	37:X:98:ARG:NH2	2.03	1.20
17:D:563:A:N1	17:D:884:U:O4	1.73	1.19
9:9:142:THR:HG21	39:Z:7:ILE:HG12	1.21	1.19
12:AB:165:PHE:CD2	29:P:100:ILE:CD1	2.17	1.19
21:H:118:GLY:O	21:H:133:GLY:HA3	1.27	1.18
12:AB:47:GLU:HG3	12:AB:64:PHE:CE1	1.80	1.17
9:9:31:ARG:NE	40:a:1054:A:C5'	2.07	1.16
12:AB:47:GLU:HG3	12:AB:64:PHE:HE1	1.02	1.15
16:C:44:ILE:HD13	21:H:339:ARG:HG2	1.18	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:70:G:H2'	10:A:71:C:H5''	1.22	1.14
6:5:100:DA:H5'	14:AE:278:ARG:NH1	1.61	1.13
10:B:70:G:H2'	10:B:71:C:H5''	1.23	1.13
17:D:1329:A:OP1	37:X:28:THR:HB	1.47	1.13
20:G:19:GLN:CD	21:H:76:GLU:HB3	1.67	1.13
21:H:119:GLY:HA2	21:H:133:GLY:HA2	1.14	1.12
16:C:44:ILE:HD13	21:H:339:ARG:CG	1.78	1.12
21:H:135:LEU:CB	21:H:167:VAL:CB	2.27	1.12
10:A:32:C:O4'	26:M:144:MET:CE	1.97	1.11
21:H:267:TRP:CH2	21:H:340:ARG:HG2	1.87	1.10
17:D:1308:U:C2'	37:X:98:ARG:HH21	1.63	1.10
21:H:267:TRP:CE2	21:H:340:ARG:HG2	1.84	1.10
9:9:129:LEU:N	9:9:130:PRO:HD3	1.66	1.10
40:a:1839:G:C8	40:a:1927:A:H1'	1.87	1.10
14:AE:79:LYS:HA	14:AE:81:ARG:NH2	1.66	1.09
9:9:88:HIS:CB	9:9:89:PRO:HD3	1.82	1.09
9:9:50:VAL:HG22	38:Y:119:ALA:CB	1.82	1.08
23:J:162:ALA:HA	23:J:165:ARG:CZ	1.83	1.08
17:D:1308:U:C3'	37:X:98:ARG:NH2	2.16	1.08
9:9:57:ASN:OD1	9:9:62:ARG:HG3	1.44	1.08
20:G:19:GLN:CD	21:H:76:GLU:CB	2.19	1.07
21:H:71:ALA:O	21:H:72:LEU:HD12	1.54	1.07
12:AB:165:PHE:CE2	29:P:100:ILE:HD11	1.84	1.07
17:D:1308:U:C3'	37:X:98:ARG:CZ	2.31	1.07
12:AB:165:PHE:HE2	29:P:100:ILE:HD13	1.13	1.06
20:G:19:GLN:CG	21:H:75:VAL:HG22	1.84	1.06
8:7:-18:G:H5''	17:D:1500:A:N6	1.69	1.05
10:A:18:G:N2	10:A:55:U:O2	1.90	1.05
12:AB:140:PRO:CB	29:P:84:VAL:HB	1.85	1.05
8:7:14:U:H4'	14:AE:322:ARG:CD	1.88	1.04
12:AB:167:ARG:NH2	29:P:99:GLN:CB	2.19	1.04
10:B:56:C:O4'	53:n:80:ARG:NH2	1.91	1.04
21:H:19:ARG:O	21:H:72:LEU:HB2	1.58	1.04
10:B:18:G:N2	10:B:55:U:O2	1.90	1.03
8:7:-10:U:O2'	24:K:33:PHE:CE1	2.11	1.03
17:D:1329:A:OP1	37:X:28:THR:CB	2.07	1.03
21:H:162:LYS:CB	21:H:298:GLU:CD	2.30	1.03
17:D:1227:A:OP2	37:X:110:LYS:CE	2.06	1.02
10:A:56:C:H2'	10:A:57:A:H5''	1.39	1.02
20:G:19:GLN:HG3	21:H:75:VAL:HG22	1.38	1.02
9:9:93:ALA:O	9:9:129:LEU:HD12	1.60	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:70:G:C2'	10:A:71:C:H5''	1.89	1.02
10:B:56:C:H5'	53:n:80:ARG:CZ	1.90	1.02
10:B:56:C:H2'	10:B:57:A:H5''	1.39	1.01
9:9:129:LEU:H	9:9:130:PRO:HD3	0.90	1.01
10:B:70:G:C2'	10:B:71:C:H5''	1.89	1.01
21:H:290:TYR:O	21:H:305:HIS:O	1.77	1.01
12:AB:165:PHE:HZ	29:P:87:LEU:CB	1.73	1.00
14:AE:85:CYS:HG	67:AE:1502:ZN:ZN	0.70	1.00
17:D:13:U:N3	17:D:915:A:C6	2.29	1.00
20:G:38:VAL:CG2	21:H:75:VAL:HG21	1.90	1.00
40:a:2297:A:N1	40:a:2321:U:C4	2.29	1.00
12:AB:167:ARG:CZ	29:P:99:GLN:HB2	1.92	1.00
10:A:32:C:C4'	26:M:144:MET:HE1	1.93	0.99
17:D:13:U:O4	17:D:20:U:O4	1.79	0.99
12:AB:165:PHE:CE2	29:P:100:ILE:HD12	1.78	0.98
8:7:12:G:H1'	14:AE:253:VAL:HG11	1.43	0.98
40:a:1839:G:O4'	40:a:1927:A:O4'	1.82	0.98
9:9:57:ASN:OD1	9:9:62:ARG:HG2	1.65	0.97
21:H:131:LEU:CB	21:H:167:VAL:CB	2.40	0.97
12:AB:47:GLU:CG	12:AB:64:PHE:HE1	1.76	0.97
9:9:129:LEU:H	9:9:130:PRO:CD	1.77	0.97
12:AB:140:PRO:HB2	29:P:84:VAL:HB	1.45	0.97
9:9:31:ARG:CD	40:a:1054:A:H5'	1.94	0.97
17:D:1308:U:H3'	37:X:98:ARG:NH2	1.76	0.97
12:AB:167:ARG:NH1	29:P:98:VAL:O	1.97	0.97
40:a:1839:G:C1'	40:a:1927:A:C8	2.46	0.97
8:7:-19:U:P	17:D:1505:G:H8	1.87	0.96
21:H:119:GLY:CA	21:H:133:GLY:HA2	1.95	0.96
9:9:142:THR:HG21	39:Z:7:ILE:CG1	1.95	0.96
10:A:32:C:O2'	26:M:86:GLN:CG	2.12	0.96
17:D:1308:U:H2'	37:X:98:ARG:HH21	1.06	0.96
21:H:118:GLY:O	21:H:133:GLY:HA2	1.63	0.96
10:A:72:A:H2'	10:A:73:A:H5''	1.48	0.95
20:G:38:VAL:HG22	21:H:75:VAL:HG21	1.43	0.95
10:B:72:A:H2'	10:B:73:A:H5''	1.49	0.94
40:a:67:U:N3	40:a:74:A:C6	2.35	0.94
8:7:12:G:C1'	14:AE:253:VAL:HG11	1.97	0.94
17:D:13:U:C4	17:D:915:A:N6	2.36	0.94
7:6:15:DC:N4	7:6:16:DC:N4	2.14	0.94
21:H:135:LEU:HA	21:H:157:ILE:CB	1.98	0.94
9:9:88:HIS:CB	9:9:89:PRO:CD	2.41	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:a:1839:G:O4'	40:a:1927:A:C1'	2.15	0.94
17:D:13:U:N3	17:D:915:A:N6	2.16	0.93
12:AB:165:PHE:HZ	29:P:87:LEU:HB3	1.11	0.93
21:H:119:GLY:HA3	21:H:131:LEU:O	1.68	0.92
10:B:68:C:H2'	10:B:69:C:H5''	1.50	0.92
14:AE:59:ALA:CB	14:AE:71:LEU:HD21	1.99	0.92
10:A:32:C:O2'	26:M:86:GLN:HG3	1.68	0.92
10:B:75:C:OP1	40:a:2602:A:C8	2.23	0.92
8:7:14:U:H4'	14:AE:322:ARG:HD3	1.49	0.92
9:9:88:HIS:HB3	9:9:89:PRO:HD3	0.92	0.92
7:6:5:DT:P	14:AE:1172:LYS:HZ1	1.92	0.92
7:6:5:DT:P	14:AE:1172:LYS:NZ	2.43	0.91
10:A:68:C:H2'	10:A:69:C:H5''	1.51	0.91
8:7:-19:U:P	17:D:1505:G:C8	2.64	0.91
12:AB:165:PHE:HD2	29:P:100:ILE:HD12	1.14	0.91
10:A:56:C:H1'	40:a:2112:G:C6	2.06	0.91
17:D:13:U:C4	17:D:20:U:O4	2.23	0.91
9:9:50:VAL:HG22	38:Y:119:ALA:HB1	1.51	0.90
38:Y:104:GLN:HG2	38:Y:108:ILE:HD11	1.53	0.90
12:AB:167:ARG:HH22	29:P:99:GLN:HB2	1.12	0.90
40:a:2013:A:N6	40:a:2613:U:H3	1.68	0.90
8:7:-18:G:C5'	17:D:1500:A:H62	1.85	0.90
8:7:-17:U:O2'	17:D:1403:C:O2	1.87	0.90
9:9:93:ALA:O	9:9:129:LEU:CD1	2.19	0.90
40:a:1406:U:O2'	40:a:1407:G:C5'	2.19	0.90
21:H:71:ALA:C	21:H:72:LEU:CD1	2.42	0.89
10:B:18:G:N2	10:B:58:A:N7	2.19	0.89
9:9:129:LEU:N	9:9:130:PRO:CD	2.34	0.89
21:H:279:LYS:HA	21:H:331:MET:HB3	1.54	0.89
38:Y:21:PRO:HB2	38:Y:22:PRO:HD3	1.54	0.89
21:H:119:GLY:HA2	21:H:133:GLY:CA	2.01	0.89
14:AE:59:ALA:CB	14:AE:71:LEU:CD2	2.51	0.88
14:AE:79:LYS:HA	14:AE:81:ARG:HH12	1.32	0.88
10:A:18:G:N2	10:A:58:A:N7	2.19	0.88
21:H:162:LYS:N	21:H:298:GLU:OE2	2.06	0.88
21:H:131:LEU:CB	21:H:167:VAL:N	2.37	0.88
14:AE:79:LYS:N	14:AE:81:ARG:NH1	2.22	0.88
9:9:50:VAL:CG2	38:Y:119:ALA:HB3	2.04	0.88
7:6:21:DA:N1	8:7:15:G:N2	2.22	0.87
14:AE:78:LEU:C	14:AE:81:ARG:HH11	1.79	0.87
16:C:31:ASN:OD1	21:H:268:VAL:HG22	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:g:16:CYS:CB	46:g:37:CYS:HB3	2.05	0.87
40:a:2314:A:H1'	53:n:155:THR:HG21	1.54	0.87
21:H:348:GLN:N	21:H:348:GLN:OE1	2.07	0.87
10:A:33:U:H5''	26:M:84:THR:HG21	1.55	0.86
38:Y:81:LYS:O	38:Y:81:LYS:HE3	1.75	0.86
9:9:52:MET:C	9:9:52:MET:HE3	2.00	0.86
9:9:142:THR:CG2	39:Z:7:ILE:HG12	2.03	0.86
4:3:34:VAL:HG13	4:3:67:VAL:HG22	1.58	0.86
9:9:31:ARG:CD	40:a:1054:A:H4'	2.06	0.86
12:AB:123:ARG:H	12:AB:124:PRO:HD3	1.39	0.86
40:a:783:A:N3	40:a:783:A:H2'	1.89	0.86
10:B:18:G:N7	10:B:57:A:C6	2.44	0.85
20:G:18:HIS:HA	21:H:43:LYS:HD2	1.55	0.85
17:D:197:A:C6	17:D:221:C:H4'	2.11	0.85
21:H:332:VAL:HG11	21:H:335:ILE:HG13	1.57	0.85
9:9:31:ARG:HH11	9:9:31:ARG:HG3	1.41	0.85
9:9:31:ARG:CZ	40:a:1054:A:C5'	2.49	0.85
23:J:162:ALA:HB2	23:J:165:ARG:NH2	1.90	0.85
10:A:18:G:N7	10:A:57:A:C6	2.44	0.85
21:H:267:TRP:CD2	21:H:340:ARG:HG2	2.11	0.85
12:AB:151:VAL:HG13	12:AB:158:LEU:CD2	2.07	0.84
21:H:135:LEU:CB	21:H:167:VAL:C	2.50	0.84
9:9:125:ARG:NH1	9:9:125:ARG:HA	1.92	0.84
23:J:61:VAL:HG21	23:J:200:ILE:HD11	1.57	0.84
16:C:12:ARG:HH22	21:H:268:VAL:CG2	1.90	0.84
21:H:267:TRP:CZ3	21:H:340:ARG:HG2	2.11	0.84
40:a:67:U:N3	40:a:74:A:N6	2.25	0.84
40:a:2303:G:C2	40:a:2314:A:C2	2.66	0.84
10:A:16:C:O2	40:a:2181:U:H5'	1.76	0.84
24:K:111:MET:HE2	24:K:125:ALA:HB1	1.59	0.84
10:A:68:C:C2'	10:A:69:C:H5''	2.08	0.83
7:6:21:DA:N1	8:7:15:G:C2	2.45	0.83
21:H:131:LEU:CB	21:H:166:VAL:O	2.26	0.83
21:H:267:TRP:CH2	21:H:340:ARG:CG	2.61	0.83
10:B:68:C:C2'	10:B:69:C:H5''	2.08	0.83
10:B:72:A:C2'	10:B:73:A:H5''	2.09	0.83
9:9:50:VAL:HG22	38:Y:119:ALA:HB3	1.60	0.83
8:7:-19:U:OP2	17:D:1505:G:C8	2.32	0.83
14:AE:78:LEU:C	14:AE:81:ARG:NH1	2.24	0.83
9:9:3:LEU:HD13	9:9:5:LEU:HG	1.62	0.82
12:AB:148:VAL:CA	12:AB:160:VAL:HG22	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:16:PHE:HB3	21:H:43:LYS:HA	1.60	0.82
9:9:28:ALA:H	9:9:110:ALA:HA	1.44	0.82
10:A:54:U:H3	10:A:58:A:N6	1.78	0.82
10:A:72:A:C2'	10:A:73:A:H5''	2.08	0.82
10:B:56:C:H5'	53:n:80:ARG:NE	1.93	0.82
21:H:267:TRP:CZ3	21:H:340:ARG:CG	2.63	0.82
38:Y:20:SER:HB3	38:Y:21:PRO:HD3	1.59	0.82
8:7:-19:U:OP1	17:D:1505:G:H8	1.62	0.82
8:7:-18:G:C5'	17:D:1500:A:N6	2.42	0.82
9:9:57:ASN:OD1	9:9:62:ARG:CD	2.27	0.82
9:9:31:ARG:CD	40:a:1054:A:C4'	2.56	0.82
12:AB:141:PHE:CZ	29:P:102:LEU:HD23	2.14	0.82
17:D:37:U:N3	17:D:397:A:N6	2.28	0.82
38:Y:60:VAL:HG13	38:Y:66:PHE:HB3	1.58	0.82
40:a:1019:U:H3	40:a:1142:A:N6	1.77	0.82
17:D:1227:A:H5'	37:X:110:LYS:NZ	1.94	0.82
40:a:1839:G:C1'	40:a:1927:A:N9	2.43	0.82
40:a:1021:A:N6	40:a:1141:U:H3	1.77	0.81
9:9:31:ARG:HD2	40:a:1054:A:H4'	1.62	0.81
40:a:1019:U:H3	40:a:1142:A:H61	1.28	0.81
9:9:50:VAL:CG2	38:Y:119:ALA:CB	2.59	0.81
10:A:56:C:C2'	10:A:57:A:H5''	2.11	0.81
8:7:-19:U:OP1	17:D:1505:G:C8	2.32	0.81
16:C:12:ARG:CB	21:H:264:GLU:CB	2.59	0.81
21:H:155:LYS:CB	21:H:169:SER:CB	2.58	0.81
38:Y:102:ARG:HB3	38:Y:141:ASP:HA	1.61	0.81
40:a:1406:U:O2'	40:a:1407:G:H5''	1.79	0.81
10:B:22:G:H2'	10:B:23:C:C6	2.16	0.81
17:D:972:C:O2'	29:P:57:VAL:CG2	2.29	0.81
10:B:76:A:H1'	40:a:2494:G:P	2.20	0.81
10:B:7:G:H4'	10:B:8:U:OP1	1.81	0.81
21:H:122:VAL:O	21:H:129:ALA:N	2.13	0.81
12:AB:148:VAL:HA	12:AB:160:VAL:HG22	1.63	0.81
10:B:54:U:H3	10:B:58:A:N6	1.78	0.81
40:a:585:G:N7	65:z:6:ARG:NH1	2.29	0.81
10:A:22:G:H2'	10:A:23:C:C6	2.16	0.81
23:J:162:ALA:CB	23:J:165:ARG:NH2	2.44	0.81
40:a:1021:A:H61	40:a:1141:U:H3	1.29	0.81
9:9:62:ARG:HG2	9:9:62:ARG:HH21	1.43	0.80
12:AB:165:PHE:CZ	29:P:87:LEU:CB	2.51	0.80
14:AE:81:ARG:H	14:AE:81:ARG:HD2	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:27:LEU:HD12	38:Y:27:LEU:O	1.81	0.80
46:g:18:CYS:HB3	46:g:40:CYS:CB	2.12	0.80
53:n:125:ARG:O	53:n:127:ASN:ND2	2.14	0.80
10:B:58:A:O2'	10:B:59:A:H3'	1.81	0.80
23:J:162:ALA:CA	23:J:165:ARG:NH2	2.44	0.80
21:H:123:GLU:HA	21:H:128:ARG:HA	1.63	0.80
46:g:16:CYS:HB2	46:g:37:CYS:HB3	1.63	0.80
17:D:1397:C:OP1	17:D:1397:C:H2'	1.81	0.80
21:H:305:HIS:CD2	21:H:306:VAL:H	1.98	0.80
9:9:3:LEU:H	9:9:3:LEU:HD12	1.47	0.80
10:A:7:G:H4'	10:A:8:U:OP1	1.81	0.80
10:A:58:A:O2'	10:A:59:A:H3'	1.82	0.80
10:B:18:G:N2	10:B:58:A:C5	2.50	0.80
10:B:56:C:C2'	10:B:57:A:H5''	2.11	0.80
38:Y:72:THR:OG1	38:Y:73:PRO:HD2	1.81	0.80
40:a:2189:U:OP1	40:a:2189:U:O4'	2.00	0.80
9:9:78:GLY:N	9:9:79:PRO:HD2	1.97	0.80
23:J:162:ALA:HA	23:J:165:ARG:NH2	1.95	0.80
10:A:18:G:N2	10:A:58:A:C5	2.50	0.79
9:9:39:THR:HA	9:9:42:ARG:HD2	1.64	0.79
40:a:2297:A:N1	40:a:2321:U:O4	2.14	0.79
40:a:2298:A:C4	40:a:2321:U:C5	2.70	0.79
9:9:43:LYS:HD2	9:9:43:LYS:C	2.05	0.79
21:H:270:ILE:CG2	21:H:337:GLU:HB3	2.12	0.79
21:H:162:LYS:CA	21:H:298:GLU:OE2	2.17	0.79
49:j:4:LEU:HD23	49:j:29:VAL:HG11	1.65	0.79
23:J:162:ALA:HB2	23:J:165:ARG:HH22	1.47	0.78
17:D:1329:A:P	37:X:28:THR:HB	2.22	0.78
38:Y:32:VAL:HG13	38:Y:60:VAL:HG21	1.65	0.78
9:9:31:ARG:CD	40:a:1054:A:C5'	2.58	0.78
21:H:19:ARG:HD3	21:H:73:ASP:CG	2.09	0.78
20:G:16:PHE:CZ	21:H:41:GLY:O	2.36	0.78
10:A:15:G:N1	10:A:20:U:O2	2.17	0.78
20:G:35:ARG:HD2	21:H:14:LYS:HD3	1.66	0.78
40:a:1406:U:O2'	40:a:1407:G:P	2.41	0.78
9:9:11:ILE:HD11	9:9:62:ARG:HA	1.66	0.78
40:a:1406:U:O2'	40:a:1407:G:O5'	2.01	0.77
40:a:2756:U:N3	40:a:2758:A:C6	2.53	0.77
10:B:5:G:H2'	10:B:6:G:H5'	1.66	0.77
10:A:18:G:C5	10:A:57:A:C6	2.72	0.77
10:A:33:U:O3'	26:M:84:THR:OG1	2.02	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:76:A:H2'	40:a:2394:C:H42	1.48	0.77
12:AB:169:THR:O	12:AB:169:THR:HG22	1.83	0.77
10:B:15:G:N1	10:B:20:U:O2	2.17	0.77
40:a:2756:U:N3	40:a:2758:A:N6	2.32	0.77
9:9:27:VAL:HG23	9:9:83:ALA:HB3	1.67	0.77
14:AE:59:ALA:HB1	14:AE:71:LEU:CD2	2.15	0.77
10:B:18:G:C5	10:B:57:A:C6	2.72	0.77
10:B:68:C:C3'	10:B:69:C:H5''	2.15	0.76
7:6:15:DC:C4	7:6:16:DC:N4	2.53	0.76
21:H:305:HIS:CD2	21:H:306:VAL:N	2.53	0.76
10:A:70:G:H2'	10:A:71:C:C5'	2.11	0.76
10:A:5:G:H2'	10:A:6:G:H5'	1.66	0.76
7:6:18:DC:H42	8:7:17:G:H1	1.34	0.76
9:9:31:ARG:NE	40:a:1054:A:C4'	2.48	0.76
20:G:35:ARG:HG3	21:H:10:GLU:OE2	1.86	0.76
38:Y:74:PRO:HG2	38:Y:77:VAL:HB	1.67	0.75
40:a:2298:A:C4	40:a:2321:U:H5	2.04	0.75
4:3:36:VAL:HG11	4:3:39:ILE:HD12	1.68	0.75
21:H:109:THR:HA	21:H:153:GLU:HA	1.69	0.75
10:A:68:C:C3'	10:A:69:C:H5''	2.15	0.75
20:G:19:GLN:CD	21:H:76:GLU:HB2	2.08	0.75
63:x:31:THR:O	63:x:102:ARG:NH1	2.19	0.75
9:9:97:LYS:HD3	9:9:127:ALA:HA	1.68	0.75
16:C:44:ILE:CD1	21:H:339:ARG:CG	2.62	0.75
10:A:32:C:C1'	26:M:144:MET:HE1	2.16	0.75
38:Y:85:ILE:H	38:Y:85:ILE:HD12	1.52	0.75
46:g:18:CYS:CB	46:g:40:CYS:HB3	2.16	0.75
10:B:70:G:H2'	10:B:71:C:C5'	2.11	0.75
24:K:137:VAL:O	24:K:140:THR:OG1	2.04	0.75
17:D:197:A:N6	17:D:221:C:H4'	2.01	0.75
17:D:1227:A:H5'	37:X:110:LYS:HZ2	1.52	0.75
21:H:131:LEU:CB	21:H:166:VAL:C	2.60	0.74
29:P:24:GLU:OE2	29:P:90:LEU:HD11	1.87	0.74
9:9:60:LEU:HD23	9:9:64:VAL:HG21	1.67	0.74
9:9:52:MET:HG3	9:9:95:LEU:HD11	1.68	0.74
10:A:41:C:O4'	26:M:143:ARG:NH1	2.20	0.74
10:B:18:G:H1'	10:B:58:A:C2	2.23	0.74
21:H:110:GLY:CA	21:H:153:GLU:O	2.36	0.74
21:H:304:VAL:HG12	21:H:309:MET:SD	2.28	0.74
9:9:78:GLY:N	9:9:79:PRO:CD	2.51	0.74
17:D:1228:C:OP1	37:X:107:ARG:NH1	2.21	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:41:C:H1'	26:M:143:ARG:HH12	1.52	0.73
10:A:70:G:C3'	10:A:71:C:H5''	2.18	0.73
10:A:6:G:O2'	10:A:7:G:O5'	2.05	0.73
17:D:517:G:O2'	17:D:530:G:H4'	1.88	0.73
20:G:19:GLN:CG	21:H:76:GLU:HB2	2.18	0.73
10:A:18:G:H1'	10:A:58:A:C2	2.23	0.73
10:B:70:G:C3'	10:B:71:C:H5''	2.17	0.73
10:B:76:A:H2'	10:B:76:A:N3	2.02	0.73
21:H:19:ARG:HB2	21:H:73:ASP:OD2	1.88	0.73
10:A:18:G:O2'	10:A:60:U:C2	2.41	0.73
10:A:33:U:H5''	26:M:84:THR:CG2	2.19	0.73
12:AB:123:ARG:N	12:AB:124:PRO:HD3	2.03	0.73
10:B:6:G:O2'	10:B:7:G:O5'	2.05	0.73
16:C:44:ILE:HD13	21:H:339:ARG:HG3	1.70	0.73
21:H:109:THR:CA	21:H:153:GLU:HA	2.18	0.73
7:6:21:DA:C6	8:7:15:G:N2	2.56	0.73
7:6:21:DA:C2	8:7:15:G:N2	2.56	0.73
14:AE:81:ARG:HD2	14:AE:81:ARG:N	2.03	0.73
40:a:1021:A:N1	40:a:1141:U:C4	2.55	0.73
21:H:267:TRP:CE3	21:H:340:ARG:CG	2.72	0.73
28:O:84:THR:HG21	28:O:103:PHE:HB3	1.71	0.73
14:AE:59:ALA:HB1	14:AE:71:LEU:HD22	1.71	0.72
17:D:1358:U:C4	17:D:1363:A:N1	2.53	0.72
12:AB:148:VAL:HG13	12:AB:148:VAL:O	1.89	0.72
20:G:19:GLN:OE1	21:H:75:VAL:O	1.85	0.72
40:a:1839:G:H1'	40:a:1927:A:N9	2.03	0.72
10:B:6:G:HO2'	10:B:7:G:H8	1.37	0.72
10:B:18:G:O2'	10:B:60:U:C2	2.41	0.72
10:B:76:A:H1'	40:a:2494:G:OP1	1.88	0.72
8:7:-3:U:H5''	8:7:-3:U:C6	2.24	0.72
21:H:267:TRP:CE3	21:H:340:ARG:HG2	2.25	0.72
9:9:18:VAL:HA	9:9:86:MET:HE2	1.71	0.72
40:a:1839:G:C1'	40:a:1927:A:C1'	2.67	0.72
14:AE:79:LYS:CA	14:AE:81:ARG:NH2	2.40	0.72
21:H:70:VAL:HA	21:H:85:SER:CB	2.20	0.72
38:Y:36:GLU:OE1	38:Y:36:GLU:HA	1.88	0.72
8:7:14:U:H4'	14:AE:322:ARG:CZ	2.20	0.72
40:a:1913:A:OP2	40:a:1913:A:H3'	1.89	0.72
8:7:-12:U:N3	17:D:1196:A:C8	2.57	0.72
9:9:77:VAL:HG12	9:9:82:ILE:HG21	1.71	0.72
20:G:16:PHE:CB	21:H:43:LYS:HA	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:46:G:H1'	10:B:47:U:C5	2.25	0.71
17:D:1308:U:O5'	37:X:98:ARG:HG3	1.90	0.71
10:A:72:A:C3'	10:A:73:A:H5''	2.20	0.71
40:a:67:U:C4	40:a:74:A:N6	2.57	0.71
14:AE:64:PRO:HG3	14:AE:90:VAL:CG1	2.20	0.71
10:B:72:A:C3'	10:B:73:A:H5''	2.20	0.71
16:C:12:ARG:HB2	21:H:264:GLU:CB	2.19	0.71
14:AE:68:TYR:HA	14:AE:92:VAL:HG23	1.72	0.71
14:AE:77:ARG:NE	14:AE:77:ARG:HA	2.04	0.71
17:D:827:U:H3	17:D:872:A:N6	1.87	0.71
8:7:-12:U:O4	17:D:1196:A:N9	2.24	0.71
9:9:3:LEU:HD12	9:9:3:LEU:N	2.05	0.71
17:D:1309:G:H8	37:X:98:ARG:NH2	1.89	0.71
37:X:96:PRO:HG2	37:X:102:THR:CG2	2.21	0.71
40:a:2314:A:C1'	53:n:155:THR:HG21	2.21	0.71
10:A:46:G:H1'	10:A:47:U:C5	2.25	0.71
11:AA:65:ASN:HB3	11:AA:105:TYR:HB2	1.73	0.70
10:B:18:G:C5	10:B:57:A:N6	2.59	0.70
10:B:76:A:H2'	40:a:2493:U:H5''	1.72	0.70
21:H:86:ARG:O	21:H:89:ALA:HB3	1.91	0.70
12:AB:123:ARG:N	12:AB:124:PRO:CD	2.54	0.70
21:H:70:VAL:HA	21:H:85:SER:CA	2.22	0.70
10:A:18:G:C5	10:A:57:A:N6	2.59	0.70
31:R:86:ARG:HG3	31:R:86:ARG:O	1.89	0.70
10:A:15:G:H2'	10:A:15:G:N3	2.06	0.70
46:g:18:CYS:CB	46:g:40:CYS:CB	2.69	0.70
21:H:19:ARG:HD3	21:H:73:ASP:OD1	1.92	0.70
10:A:16:C:O2	40:a:2181:U:C5'	2.40	0.70
10:A:41:C:C1'	26:M:143:ARG:NH1	2.55	0.70
9:9:58:THR:HG21	9:9:81:LEU:HG	1.74	0.70
14:AE:59:ALA:HB2	14:AE:71:LEU:HD21	1.74	0.70
8:7:14:U:H4'	14:AE:322:ARG:NE	2.07	0.69
47:h:146:MET:HE3	47:h:154:LEU:HD21	1.74	0.69
9:9:31:ARG:HD2	40:a:1054:A:C5'	2.22	0.69
10:A:11:A:H2'	10:A:12:G:O4'	1.92	0.69
10:B:15:G:H2'	10:B:15:G:N3	2.06	0.69
40:a:742:A:H2'	40:a:743:A:C8	2.26	0.69
9:9:73:LYS:HB2	9:9:117:LEU:HD21	1.75	0.69
40:a:1021:A:H3'	40:a:1021:A:N3	2.07	0.69
40:a:2310:C:O2'	53:n:74:VAL:CG1	2.40	0.69
10:B:11:A:H2'	10:B:12:G:O4'	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:37:U:H3	17:D:397:A:N6	1.90	0.69
17:D:1308:U:C3'	37:X:98:ARG:HH21	1.92	0.69
17:D:563:A:N1	17:D:884:U:C4	2.60	0.69
17:D:915:A:N6	17:D:916:U:C4	2.60	0.69
1:0:80:ARG:NH2	40:a:572:A:OP2	2.25	0.69
10:A:32:C:C4'	26:M:144:MET:CE	2.66	0.69
12:AB:165:PHE:CE2	29:P:100:ILE:HD13	1.97	0.69
10:A:32:C:C1'	26:M:144:MET:CE	2.69	0.69
21:H:110:GLY:HA3	21:H:153:GLU:O	1.93	0.69
40:a:927:A:H2'	40:a:928:A:C8	2.28	0.68
7:6:18:DC:N3	8:7:17:G:N2	2.38	0.68
14:AE:1033:GLY:HA3	14:AE:1081:VAL:O	1.93	0.68
21:H:117:LYS:CB	21:H:279:LYS:O	2.41	0.68
9:9:50:VAL:HG13	38:Y:119:ALA:CB	2.22	0.68
21:H:19:ARG:HD3	21:H:73:ASP:OD2	1.92	0.68
37:X:96:PRO:CG	37:X:102:THR:CG2	2.71	0.68
13:AD:48:LEU:HB2	13:AD:183:ILE:HD11	1.76	0.68
40:a:1839:G:C4	40:a:1927:A:C4	2.81	0.68
9:9:118:ILE:HB	9:9:119:PRO:HD3	1.76	0.68
10:A:19:G:N2	40:a:2112:G:C8	2.62	0.68
40:a:1596:A:H2'	40:a:1597:A:C8	2.28	0.68
7:6:8:DC:C6	7:6:9:DT:H72	2.29	0.68
17:D:13:U:O4	17:D:21:G:C2	2.46	0.68
40:a:2756:U:C4	40:a:2758:A:N6	2.61	0.68
8:7:14:U:H4'	14:AE:322:ARG:NH1	2.07	0.68
9:9:43:LYS:HD2	9:9:43:LYS:O	1.94	0.68
40:a:2310:C:O2'	53:n:74:VAL:HG12	1.94	0.68
6:5:100:DA:H5'	14:AE:278:ARG:HH11	1.56	0.68
38:Y:58:ILE:HD13	38:Y:58:ILE:N	2.09	0.68
40:a:1920:C:O5'	40:a:1920:C:H6	1.77	0.68
17:D:972:C:O2'	29:P:57:VAL:HG23	1.92	0.67
21:H:267:TRP:CD2	21:H:340:ARG:CG	2.76	0.67
37:X:96:PRO:CG	37:X:102:THR:HG22	2.25	0.67
38:Y:21:PRO:CB	38:Y:22:PRO:HD3	2.22	0.67
40:a:1839:G:H8	40:a:1927:A:H1'	1.54	0.67
10:A:5:G:H2'	10:A:6:G:C5'	2.24	0.67
6:5:100:DA:H5'	14:AE:278:ARG:HH12	1.54	0.67
9:9:11:ILE:CD1	9:9:62:ARG:HD3	2.24	0.67
12:AB:167:ARG:HH22	29:P:99:GLN:CB	1.99	0.67
21:H:70:VAL:HA	21:H:85:SER:HA	1.77	0.67
8:7:-10:U:O2'	24:K:33:PHE:HE1	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:142:ALA:O	12:AB:143:ASP:HB2	1.94	0.67
10:B:5:G:H2'	10:B:6:G:C5'	2.24	0.67
22:I:75:ILE:O	22:I:75:ILE:HD13	1.95	0.67
21:H:118:GLY:C	21:H:133:GLY:CA	2.67	0.67
8:7:14:U:C4'	14:AE:322:ARG:NH1	2.58	0.67
38:Y:14:ALA:HB2	38:Y:54:ILE:HD12	1.76	0.67
38:Y:116:MET:HB3	38:Y:124:MET:HG2	1.76	0.67
14:AE:85:CYS:SG	67:AE:1502:ZN:ZN	1.79	0.67
9:9:60:LEU:HA	9:9:64:VAL:HB	1.77	0.66
21:H:270:ILE:HG23	21:H:337:GLU:HB3	1.77	0.66
20:G:16:PHE:HZ	21:H:41:GLY:O	1.77	0.66
21:H:110:GLY:N	21:H:153:GLU:C	2.53	0.66
40:a:1153:C:OP1	65:z:92:ARG:NH1	2.27	0.66
21:H:110:GLY:H	21:H:153:GLU:CA	2.08	0.66
9:9:67:THR:N	9:9:68:PRO:CD	2.58	0.66
21:H:267:TRP:CE2	21:H:340:ARG:CG	2.73	0.66
37:X:96:PRO:HG3	37:X:102:THR:HG22	1.78	0.66
21:H:162:LYS:CB	21:H:298:GLU:OE1	2.44	0.66
8:7:-12:U:N3	17:D:1196:A:N7	2.44	0.66
8:7:-12:U:O4	17:D:1196:A:O4'	2.13	0.66
14:AE:58:CYS:SG	14:AE:59:ALA:N	2.69	0.66
9:9:61:ARG:NH1	40:a:1047:G:N7	2.44	0.66
9:9:142:THR:HG21	39:Z:7:ILE:CD1	2.26	0.65
10:A:56:C:C5	40:a:2168:G:C6	2.83	0.65
55:p:24:ILE:HD13	55:p:72:LEU:HD21	1.77	0.65
9:9:50:VAL:CG1	38:Y:119:ALA:HB3	2.26	0.65
10:B:66:C:H5'	10:B:66:C:H6	1.60	0.65
21:H:72:LEU:HD12	21:H:72:LEU:N	2.11	0.65
35:V:25:ILE:HD11	35:V:61:ILE:HD11	1.77	0.65
40:a:1779:U:H5	40:a:1784:A:N7	1.93	0.65
12:AB:165:PHE:HE1	29:P:88:MET:HA	1.61	0.65
10:B:56:C:H5'	53:n:80:ARG:NH2	2.10	0.65
21:H:52:GLN:O	21:H:53:PHE:CD1	2.50	0.65
17:D:1329:A:P	37:X:28:THR:CB	2.83	0.65
21:H:135:LEU:CA	21:H:157:ILE:CB	2.74	0.65
21:H:332:VAL:HG12	21:H:334:ASP:H	1.62	0.65
12:AB:151:VAL:HG13	12:AB:158:LEU:HD23	1.78	0.65
10:B:76:A:H1'	40:a:2493:U:O3'	1.97	0.65
38:Y:116:MET:HE2	38:Y:116:MET:HA	1.79	0.65
9:9:11:ILE:HG13	9:9:65:GLU:HB3	1.79	0.65
20:G:38:VAL:HG22	21:H:75:VAL:CG2	2.24	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:21:A:H4'	10:A:21:A:OP1	1.95	0.65
10:B:75:C:OP1	40:a:2602:A:N9	2.30	0.65
21:H:85:SER:O	21:H:88:LYS:CB	2.45	0.65
10:A:66:C:H6	10:A:66:C:H5'	1.60	0.65
10:B:21:A:H4'	10:B:21:A:OP1	1.95	0.65
54:o:26:HIS:CE1	54:o:48:ALA:HB2	2.32	0.65
9:9:78:GLY:H	9:9:79:PRO:CD	2.10	0.65
10:A:18:G:C8	10:A:57:A:C6	2.85	0.65
17:D:1227:A:OP2	37:X:110:LYS:NZ	2.29	0.65
40:a:1839:G:C8	40:a:1927:A:C1'	2.74	0.65
10:B:18:G:C8	10:B:57:A:C6	2.85	0.65
17:D:1308:U:H5''	37:X:98:ARG:HG2	1.78	0.65
17:D:827:U:N3	17:D:872:A:N6	2.45	0.64
21:H:267:TRP:CZ2	21:H:340:ARG:CG	2.68	0.64
23:J:162:ALA:CB	23:J:165:ARG:HH22	2.08	0.64
40:a:1082:U:N3	40:a:1086:A:N6	2.45	0.64
8:7:12:G:H1'	14:AE:253:VAL:CG1	2.22	0.64
10:B:3:C:H2'	10:B:4:G:H8	1.62	0.64
20:G:18:HIS:HA	21:H:43:LYS:CD	2.28	0.64
20:G:35:ARG:HH21	21:H:10:GLU:HG2	1.62	0.64
14:AE:84:ILE:HG22	14:AE:91:GLU:HG3	1.79	0.64
10:B:37:A:H3'	10:B:37:A:OP2	1.96	0.64
17:D:1308:U:O5'	37:X:98:ARG:CG	2.45	0.64
7:6:15:DC:N4	7:6:16:DC:H41	1.96	0.64
8:7:-13:U:OP2	17:D:1397:C:N3	2.30	0.64
17:D:1358:U:N3	17:D:1363:A:N6	2.46	0.64
20:G:19:GLN:CG	21:H:76:GLU:CB	2.76	0.64
40:a:1923:U:H2'	40:a:1923:U:OP2	1.96	0.64
10:A:41:C:C4'	26:M:143:ARG:NH1	2.60	0.64
10:A:50:U:H2'	10:A:51:C:C6	2.33	0.64
11:AA:528:ARG:NH2	11:AA:576:SER:O	2.30	0.64
17:D:1358:U:H3	17:D:1363:A:N6	1.96	0.64
9:9:57:ASN:OD1	9:9:62:ARG:HD2	1.98	0.64
9:9:57:ASN:CG	9:9:62:ARG:CG	2.68	0.64
10:A:31:G:O2'	26:M:144:MET:SD	2.56	0.64
14:AE:79:LYS:C	14:AE:81:ARG:NH2	2.56	0.64
10:B:50:U:H2'	10:B:51:C:C6	2.33	0.64
58:s:114:LEU:HG	58:s:118:MET:HE3	1.78	0.64
40:a:2885:G:N7	48:i:40:ARG:NH2	2.46	0.64
40:a:1909:C:O5'	40:a:1909:C:H6	1.81	0.63
2:1:36:LEU:HD13	2:1:48:LYS:HA	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:1358:U:O4	17:D:1363:A:C2	2.47	0.63
40:a:2303:G:N3	40:a:2314:A:C2	2.66	0.63
10:A:3:C:H2'	10:A:4:G:H8	1.62	0.63
10:A:56:C:O2	40:a:2112:G:C4	2.52	0.63
10:B:22:G:H2'	10:B:23:C:H6	1.62	0.63
40:a:1839:G:O4'	40:a:1927:A:H1'	1.97	0.63
55:p:121:ILE:HD12	55:p:141:ILE:HG22	1.79	0.63
9:9:11:ILE:HD12	9:9:62:ARG:HD3	1.80	0.63
11:AA:120:GLN:NE2	11:AA:490:GLN:OE1	2.32	0.63
14:AE:79:LYS:C	14:AE:81:ARG:CZ	2.71	0.63
21:H:162:LYS:CB	21:H:298:GLU:OE2	2.45	0.63
40:a:2297:A:C2	40:a:2321:U:C4	2.86	0.63
11:AA:314:ASN:HD21	11:AA:348:SER:HA	1.62	0.63
21:H:267:TRP:CE3	21:H:340:ARG:HG3	2.32	0.63
11:AA:1282:GLY:HA3	15:AF:17:PHE:HE1	1.63	0.63
17:D:13:U:O4	17:D:20:U:C4	2.52	0.63
17:D:197:A:C6	17:D:221:C:C4'	2.80	0.63
20:G:19:GLN:CG	21:H:75:VAL:CG2	2.70	0.63
40:a:1789:A:OP2	47:h:221:ARG:NH1	2.32	0.63
17:D:37:U:O2	17:D:548:G:C2	2.52	0.63
1:0:40:MET:HE1	65:z:105:ALA:HB1	1.80	0.62
9:9:23:LEU:HB3	9:9:92:ALA:HA	1.81	0.62
9:9:29:ASP:HB2	9:9:56:ARG:HD3	1.79	0.62
12:AB:151:VAL:HG13	12:AB:158:LEU:HD22	1.81	0.62
6:5:98:DA:C2'	6:5:99:DT:H72	2.28	0.62
10:A:37:A:O2'	10:A:38:A:H5'	1.99	0.62
17:D:1059:C:O2	29:P:55:PRO:HG3	1.99	0.62
40:a:2013:A:N6	40:a:2613:U:N3	2.33	0.62
10:A:69:C:H2'	10:A:70:G:O4'	1.99	0.62
10:B:69:C:H2'	10:B:70:G:O4'	1.99	0.62
40:a:1998:A:OP2	49:j:141:ARG:NH2	2.32	0.62
9:9:57:ASN:CG	9:9:62:ARG:HG2	2.25	0.62
9:9:92:ALA:HB3	9:9:129:LEU:HB2	1.82	0.62
13:AD:211:ILE:HG12	13:AD:219:ARG:HH12	1.65	0.62
17:D:13:U:C5	17:D:20:U:O4	2.53	0.62
17:D:1309:G:C8	37:X:98:ARG:NH2	2.66	0.62
8:7:-14:U:H5''	8:7:-14:U:H6	1.64	0.62
21:H:49:PRO:CD	21:H:84:LEU:HD11	2.29	0.62
21:H:270:ILE:HG21	21:H:337:GLU:HB3	1.80	0.62
10:B:42:G:H2'	10:B:43:A:H8	1.65	0.62
38:Y:32:VAL:HA	38:Y:60:VAL:HG11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:a:754:U:H2'	40:a:755:U:C6	2.35	0.62
10:A:22:G:H2'	10:A:23:C:H6	1.62	0.62
10:A:65:C:H2'	10:A:66:C:H5'	1.82	0.62
12:AB:165:PHE:HD2	29:P:100:ILE:CD1	1.85	0.62
21:H:110:GLY:N	21:H:153:GLU:O	2.32	0.62
26:M:23:LEU:O	26:M:27:VAL:HG13	1.99	0.62
9:9:18:VAL:HG13	9:9:71:CYS:HB2	1.81	0.62
11:AA:55:SER:OG	11:AA:465:ARG:NH1	2.33	0.62
10:B:65:C:H2'	10:B:66:C:H5'	1.82	0.62
21:H:270:ILE:CG2	21:H:337:GLU:CB	2.77	0.62
40:a:2189:U:O4'	40:a:2189:U:P	2.57	0.62
16:C:29:LEU:O	16:C:33:ILE:HG23	2.00	0.62
40:a:1839:G:N9	40:a:1927:A:N9	2.48	0.62
10:B:54:U:N3	10:B:58:A:N6	2.47	0.61
9:9:62:ARG:CG	9:9:62:ARG:HH21	2.14	0.61
21:H:304:VAL:HG12	21:H:304:VAL:O	1.99	0.61
24:K:107:ALA:HB2	24:K:125:ALA:HB3	1.82	0.61
40:a:1021:A:C2	40:a:1141:U:O4	2.51	0.61
40:a:2683:C:OP1	64:y:51:ARG:NH2	2.32	0.61
10:A:33:U:H4'	26:M:84:THR:HB	1.82	0.61
10:A:41:C:C1'	26:M:143:ARG:HH12	2.12	0.61
12:AB:123:ARG:H	12:AB:124:PRO:CD	2.09	0.61
12:AB:165:PHE:CD2	29:P:100:ILE:HD11	2.11	0.61
3:2:50:LEU:HD23	44:e:26:PHE:CE1	2.35	0.61
14:AE:86:GLU:OE1	14:AE:86:GLU:N	2.34	0.61
9:9:136:ILE:HD12	9:9:139:LEU:HD12	1.83	0.61
10:B:56:C:C4'	53:n:80:ARG:NH2	2.63	0.61
20:G:19:GLN:HG3	21:H:76:GLU:HB2	1.82	0.61
9:9:77:VAL:HG12	9:9:77:VAL:O	2.01	0.61
13:AC:45:ARG:HD3	13:AD:38:THR:HB	1.82	0.61
14:AE:506:VAL:HG23	14:AE:628:GLY:HA3	1.83	0.61
20:G:19:GLN:CD	21:H:75:VAL:HG22	2.25	0.61
21:H:84:LEU:HD22	21:H:84:LEU:N	2.16	0.61
40:a:84:A:N1	40:a:98:G:O2'	2.33	0.61
6:5:110:DA:N7	11:AA:183:TRP:CH2	2.69	0.61
7:6:15:DC:C4	7:6:16:DC:C4	2.89	0.61
13:AD:112:ALA:HB3	13:AD:126:PRO:HA	1.83	0.61
14:AE:785:ASP:O	14:AE:789:LYS:HB2	2.01	0.61
16:C:44:ILE:CD1	21:H:339:ARG:HG2	2.12	0.61
38:Y:54:ILE:O	38:Y:54:ILE:HG22	2.00	0.61
10:A:3:C:H2'	10:A:4:G:C8	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:140:PRO:CG	29:P:84:VAL:HB	2.31	0.61
14:AE:741:ALA:O	14:AE:762:ASN:ND2	2.32	0.61
14:AE:1161:GLY:HA3	14:AE:1179:PRO:HA	1.83	0.61
10:B:3:C:H2'	10:B:4:G:C8	2.36	0.61
29:P:57:VAL:O	29:P:58:ASN:CG	2.43	0.61
38:Y:112:LYS:HZ2	38:Y:112:LYS:HB3	1.65	0.61
9:9:6:GLN:OE1	9:9:6:GLN:HA	2.00	0.60
10:A:41:C:H4'	26:M:143:ARG:CZ	2.31	0.60
32:S:47:LYS:O	32:S:50:THR:OG1	2.12	0.60
17:D:1308:U:C5'	37:X:98:ARG:HG2	2.32	0.60
38:Y:21:PRO:HB2	38:Y:22:PRO:CD	2.30	0.60
40:a:2297:A:C2	40:a:2321:U:C5	2.89	0.60
40:a:2720:U:OP1	64:y:53:ARG:NH2	2.34	0.60
9:9:47:GLU:HG3	9:9:95:LEU:HD21	1.83	0.60
10:A:6:G:HO2'	10:A:7:G:H8	1.50	0.60
37:X:101:ARG:O	37:X:101:ARG:HD3	2.00	0.60
10:A:42:G:H2'	10:A:43:A:H8	1.65	0.60
14:AE:1275:LEU:HB3	14:AE:1278:GLU:HB2	1.83	0.60
21:H:305:HIS:O	21:H:306:VAL:HB	2.00	0.60
34:U:21:VAL:HG21	34:U:60:TRP:CD1	2.36	0.60
40:a:1406:U:HO2'	40:a:1407:G:C5'	2.08	0.60
12:AB:47:GLU:CG	12:AB:64:PHE:CE1	2.64	0.60
21:H:119:GLY:CA	21:H:131:LEU:O	2.46	0.60
8:7:14:U:C4'	14:AE:322:ARG:CZ	2.79	0.60
21:H:117:LYS:CB	21:H:278:THR:HG23	2.32	0.60
21:H:305:HIS:CD2	21:H:307:SER:H	2.20	0.60
11:AA:1072:ASN:ND2	11:AA:1111:GLN:OE1	2.34	0.60
21:H:331:MET:N	21:H:331:MET:SD	2.75	0.60
34:U:4:ILE:HG12	34:U:21:VAL:HG22	1.84	0.60
14:AE:92:VAL:HG22	14:AE:92:VAL:O	2.01	0.60
17:D:1218:C:H2'	17:D:1219:A:C8	2.36	0.60
20:G:217:VAL:O	20:G:220:THR:HG22	2.02	0.60
11:AA:69:GLN:HE21	11:AA:101:ARG:HD2	1.67	0.60
14:AE:64:PRO:HG3	14:AE:90:VAL:HG12	1.83	0.60
17:D:321:A:N7	17:D:328:C:O2'	2.34	0.60
39:Z:7:ILE:HG23	39:Z:7:ILE:O	2.01	0.60
40:a:1921:G:O5'	40:a:1921:G:H8	1.84	0.60
10:A:47:U:O2'	10:A:50:U:P	2.60	0.59
12:AB:141:PHE:HZ	29:P:102:LEU:HD23	1.64	0.59
17:D:404:G:N7	23:J:2:ALA:HB3	2.17	0.59
17:D:1227:A:H5'	37:X:110:LYS:HZ1	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:20:G:OP1	11:AA:1073:LYS:NZ	2.24	0.59
14:AE:814:CYS:SG	14:AE:883:ARG:NH2	2.74	0.59
17:D:13:U:C2	17:D:915:A:N6	2.70	0.59
40:a:70:G:H4'	40:a:71:A:OP1	2.02	0.59
7:6:21:DA:N6	8:7:15:G:H1	2.00	0.59
21:H:36:VAL:HB	21:H:48:ILE:HB	1.84	0.59
21:H:280:LEU:N	21:H:330:VAL:O	2.32	0.59
4:3:36:VAL:CG1	4:3:39:ILE:HD12	2.32	0.59
6:5:100:DA:C5'	14:AE:278:ARG:NH1	2.53	0.59
20:G:35:ARG:HD2	21:H:14:LYS:CD	2.32	0.59
39:Z:20:VAL:O	39:Z:20:VAL:HG12	2.02	0.59
45:f:24:LEU:HD11	45:f:54:MET:HE2	1.84	0.59
17:D:1225:A:H4'	36:W:78:ARG:NH1	2.18	0.59
21:H:118:GLY:C	21:H:133:GLY:HA2	2.27	0.59
21:H:19:ARG:O	21:H:72:LEU:CB	2.41	0.59
9:9:52:MET:HE3	9:9:52:MET:O	2.02	0.59
14:AE:888:CYS:SG	14:AE:889:ASP:N	2.74	0.59
17:D:658:C:H1'	33:T:22:THR:HG21	1.83	0.59
9:9:19:ALA:HA	9:9:70:GLU:HG2	1.84	0.59
18:E:25:ARG:HA	18:E:66:LEU:HD21	1.85	0.59
21:H:284:VAL:HG12	21:H:294:VAL:HB	1.84	0.59
11:AA:1142:ARG:NH1	11:AA:1161:LEU:O	2.36	0.59
17:D:439:U:O2	17:D:440:C:C6	2.56	0.59
8:7:-3:U:C6	8:7:-3:U:C5'	2.85	0.59
10:A:76:A:H2'	40:a:2394:C:N4	2.11	0.59
11:AA:838:CYS:HB2	11:AA:918:LEU:HD22	1.85	0.59
10:B:47:U:O2'	10:B:50:U:P	2.60	0.59
16:C:44:ILE:CD1	21:H:339:ARG:HG3	2.28	0.59
21:H:270:ILE:HG21	21:H:337:GLU:CB	2.32	0.59
40:a:2572:A:C8	49:j:149:ASN:OD1	2.56	0.59
9:9:31:ARG:HG3	9:9:31:ARG:NH1	2.17	0.58
10:A:35:A:H2'	10:A:36:U:C6	2.38	0.58
26:M:69:VAL:HG23	26:M:100:ALA:HB1	1.83	0.58
10:A:34:C:P	26:M:84:THR:OG1	2.60	0.58
33:T:5:THR:O	33:T:8:THR:OG1	2.18	0.58
38:Y:78:LEU:HD13	38:Y:108:ILE:HG22	1.85	0.58
49:j:33:ARG:NH1	49:j:53:GLY:O	2.36	0.58
52:m:31:LEU:HD22	52:m:42:LEU:HD13	1.84	0.58
8:7:-11:U:H5''	8:7:-11:U:O2	2.03	0.58
8:7:-10:U:O2'	24:K:33:PHE:CZ	2.52	0.58
19:F:4:ILE:CD1	19:F:19:PHE:HA	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:54:U:N3	10:A:58:A:N6	2.48	0.58
10:A:58:A:H1'	10:A:60:U:C5	2.38	0.58
40:a:2314:A:O2'	53:n:155:THR:CG2	2.52	0.58
17:D:563:A:N6	17:D:884:U:N3	2.51	0.58
21:H:119:GLY:HA3	21:H:132:PRO:C	2.28	0.58
8:7:-12:U:O4	17:D:1196:A:C1'	2.52	0.58
21:H:267:TRP:CH2	21:H:340:ARG:CB	2.86	0.58
11:AA:1254:VAL:O	14:AE:99:ARG:NH2	2.37	0.58
14:AE:1221:LEU:HD22	14:AE:1306:LEU:HB2	1.85	0.58
10:B:56:C:C5'	53:n:80:ARG:CZ	2.76	0.58
40:a:1590:A:H2'	40:a:1591:A:C8	2.38	0.58
6:5:99:DT:H2''	6:5:100:DA:H5''	1.86	0.58
20:G:19:GLN:HG3	21:H:75:VAL:CG2	2.23	0.58
21:H:291:GLY:HA2	21:H:305:HIS:HA	1.86	0.58
38:Y:137:LEU:N	38:Y:137:LEU:HD23	2.19	0.58
8:7:-14:U:H5''	8:7:-14:U:C6	2.39	0.58
14:AE:144:TYR:OH	14:AE:293:ARG:NH2	2.37	0.58
21:H:110:GLY:N	21:H:153:GLU:CA	2.67	0.58
38:Y:7:TYR:HB2	38:Y:57:VAL:HG22	1.86	0.58
10:B:58:A:H1'	10:B:60:U:C5	2.38	0.57
20:G:19:GLN:NE2	21:H:75:VAL:HG22	2.19	0.57
21:H:330:VAL:HB	21:H:344:LEU:HD23	1.86	0.57
8:7:-9:U:H5''	24:K:56:VAL:HG21	1.86	0.57
10:A:34:C:P	26:M:84:THR:HG1	2.26	0.57
14:AE:1143:ASP:OD1	14:AE:1148:ARG:NH1	2.37	0.57
10:B:56:C:C5'	53:n:80:ARG:NH2	2.67	0.57
10:B:60:U:P	10:B:61:C:H41	2.27	0.57
8:7:-12:U:O4	17:D:1196:A:C8	2.57	0.57
10:A:11:A:H2'	10:A:12:G:C8	2.40	0.57
10:B:50:U:H2'	10:B:51:C:H6	1.69	0.57
46:g:16:CYS:HB3	46:g:37:CYS:HB3	1.86	0.57
9:9:61:ARG:CZ	40:a:1047:G:N7	2.67	0.57
11:AA:1223:ARG:NH2	14:AE:721:SER:OG	2.38	0.57
17:D:1526:G:OP2	19:F:42:THR:HG23	2.04	0.57
24:K:56:VAL:O	24:K:60:ILE:HG23	2.04	0.57
29:P:6:ILE:HG23	29:P:100:ILE:HG23	1.87	0.57
10:A:60:U:P	10:A:61:C:H41	2.27	0.57
11:AA:707:ALA:O	11:AA:711:ASP:HB2	2.03	0.57
17:D:1329:A:P	37:X:28:THR:OG1	2.62	0.57
60:u:77:ILE:HD11	60:u:108:ALA:HB1	1.87	0.57
27:N:10:MET:HE3	27:N:61:LEU:HD11	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AC:82:LEU:HD11	13:AC:171:LEU:HD23	1.86	0.57
17:D:496:A:N3	17:D:496:A:H2'	2.18	0.57
37:X:104:THR:O	37:X:104:THR:HG22	2.03	0.57
9:9:31:ARG:HD2	40:a:1054:A:C4'	2.29	0.57
10:A:76:A:C2'	40:a:2394:C:H42	2.16	0.57
8:7:12:G:O4'	14:AE:253:VAL:HG11	2.04	0.57
11:AA:818:VAL:HG22	11:AA:1096:ILE:HG12	1.87	0.57
20:G:148:LEU:HD22	20:G:151:ILE:HD11	1.86	0.57
21:H:110:GLY:H	21:H:153:GLU:C	2.12	0.57
9:9:54:VAL:O	9:9:54:VAL:HG22	2.03	0.57
40:a:1839:G:N9	40:a:1927:A:C4	2.72	0.57
40:a:2245:U:O2'	40:a:2436:G:OP2	2.22	0.57
42:c:31:PRO:HG2	42:c:33:LEU:HD13	1.87	0.57
8:7:-9:U:H3'	8:7:-9:U:H6	1.69	0.56
30:Q:67:ALA:HB2	30:Q:96:THR:HG23	1.86	0.56
10:B:11:A:H2'	10:B:12:G:C8	2.40	0.56
2:1:20:VAL:HG11	2:1:44:ALA:HA	1.86	0.56
8:7:-12:U:C4	17:D:1196:A:C8	2.93	0.56
9:9:31:ARG:HH11	9:9:31:ARG:CG	2.14	0.56
11:AA:13:LYS:HB2	11:AA:1180:MET:HE2	1.86	0.56
11:AA:1142:ARG:NH2	11:AA:1166:ASP:OD1	2.38	0.56
12:AB:129:GLU:OE1	12:AB:129:GLU:HA	2.05	0.56
46:g:16:CYS:CB	46:g:37:CYS:CB	2.82	0.56
51:l:104:ALA:O	51:l:108:ILE:HG23	2.05	0.56
9:9:31:ARG:HD2	40:a:1054:A:H5'	1.80	0.56
10:A:50:U:H2'	10:A:51:C:H6	1.69	0.56
10:A:60:U:O2'	10:A:61:C:OP1	2.23	0.56
2:1:93:ALA:HB2	40:a:1614:A:C2	2.40	0.56
9:9:34:THR:HG22	9:9:38:MET:HE3	1.85	0.56
9:9:35:VAL:HA	9:9:38:MET:HB2	1.88	0.56
10:A:56:C:C6	40:a:2168:G:C6	2.94	0.56
11:AA:1122:LYS:NZ	11:AA:1126:ASP:OD1	2.38	0.56
38:Y:96:LYS:HE3	38:Y:136:GLY:HA3	1.87	0.56
8:7:14:U:C1'	14:AE:322:ARG:NH1	2.69	0.56
38:Y:77:VAL:O	38:Y:77:VAL:HG12	2.05	0.56
40:a:404:A:O2'	40:a:405:U:OP2	2.22	0.56
21:H:305:HIS:HD2	21:H:306:VAL:H	1.49	0.56
38:Y:59:THR:HG22	38:Y:61:TYR:HE1	1.69	0.56
40:a:1818:U:OP2	47:h:156:ARG:NH1	2.38	0.56
8:7:-20:A:H2'	8:7:-19:U:H6	1.70	0.56
8:7:12:G:H1'	14:AE:253:VAL:HG21	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:17:GLU:HB3	9:9:86:MET:HB2	1.87	0.56
10:A:11:A:O5'	10:A:11:A:H8	1.89	0.56
21:H:49:PRO:HD3	21:H:84:LEU:HD11	1.87	0.56
21:H:267:TRP:CH2	21:H:340:ARG:HB3	2.41	0.56
10:A:18:G:C8	10:A:57:A:N6	2.69	0.56
40:a:580:U:O3'	65:z:31:VAL:HG13	2.05	0.56
11:AA:839:VAL:HG12	11:AA:1049:ILE:HG12	1.87	0.55
61:v:66:ARG:NH1	61:v:104:GLU:OE1	2.39	0.55
8:7:-10:U:O2	8:7:-10:U:H2'	2.06	0.55
8:7:-3:U:O2	8:7:-3:U:H2'	2.06	0.55
12:AB:141:PHE:CZ	29:P:102:LEU:CD2	2.87	0.55
17:D:769:G:H4'	17:D:1513:A:H4'	1.88	0.55
8:7:-18:G:H5''	17:D:1501:C:N4	2.21	0.55
10:B:32:C:OP2	28:O:130:ARG:NH2	2.38	0.55
17:D:1227:A:P	37:X:110:LYS:HZ2	2.29	0.55
10:B:11:A:H8	10:B:11:A:O5'	1.89	0.55
1:0:51:VAL:HG23	65:z:86:ALA:O	2.05	0.55
11:AA:516:ASP:OD1	11:AA:516:ASP:O	2.23	0.55
17:D:927:G:O2'	17:D:1503:A:N7	2.36	0.55
51:l:130:LYS:HB2	51:l:133:LEU:HD12	1.89	0.55
38:Y:116:MET:HG3	38:Y:124:MET:HB3	1.89	0.55
51:l:108:ILE:HD11	51:l:180:LEU:HD13	1.89	0.55
11:AA:360:LEU:HD13	11:AA:378:ARG:HH11	1.72	0.55
21:H:154:PHE:CB	21:H:168:VAL:CB	2.85	0.55
21:H:332:VAL:CG1	21:H:335:ILE:HG13	2.33	0.55
11:AA:103:VAL:HB	11:AA:114:VAL:HG11	1.89	0.55
11:AA:985:GLU:HB3	11:AA:988:LYS:HB2	1.89	0.55
21:H:45:GLU:OE1	21:H:45:GLU:N	2.40	0.55
21:H:71:ALA:O	21:H:72:LEU:CD1	2.42	0.55
8:7:11:U:H3'	8:7:11:U:H6	1.71	0.55
12:AB:134:VAL:CG2	12:AB:160:VAL:HG11	2.37	0.55
36:W:15:LEU:HD13	36:W:33:THR:HG21	1.88	0.55
17:D:528:C:H6	17:D:528:C:H5''	1.71	0.54
40:a:2314:A:O2'	53:n:155:THR:HG21	2.06	0.54
9:9:50:VAL:HG13	38:Y:119:ALA:HB3	1.88	0.54
13:AC:28:LEU:HD22	13:AC:201:LEU:HD23	1.88	0.54
14:AE:886:VAL:HG11	14:AE:1230:THR:HG21	1.89	0.54
10:B:18:G:C8	10:B:57:A:N6	2.70	0.54
17:D:439:U:O2	17:D:440:C:C5	2.61	0.54
40:a:2249:U:H3'	40:a:2250:G:C5'	2.36	0.54
40:a:2303:G:C4	40:a:2314:A:C2	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:51:TYR:CD1	9:9:51:TYR:C	2.85	0.54
10:A:38:A:H2'	10:A:39:C:H5'	1.88	0.54
11:AA:1117:LEU:HD12	11:AA:1195:ILE:HG12	1.90	0.54
10:B:17:C:O2	10:B:17:C:H2'	2.08	0.54
21:H:22:SER:N	21:H:69:ASP:OD2	2.40	0.54
21:H:119:GLY:CA	21:H:133:GLY:CA	2.74	0.54
24:K:99:ALA:HB1	24:K:103:THR:HG21	1.89	0.54
40:a:811:U:H2'	60:u:21:ARG:HA	1.89	0.54
40:a:1056:G:O2'	40:a:1103:A:N6	2.41	0.54
46:g:18:CYS:HB3	46:g:40:CYS:HB2	1.88	0.54
7:6:2:DC:H2''	7:6:3:DC:C5	2.43	0.54
7:6:22:DC:H4'	11:AA:508:SER:OG	2.07	0.54
8:7:-13:U:H5'	17:D:1397:C:N3	2.22	0.54
10:A:56:C:H2'	10:A:57:A:C5'	2.27	0.54
31:R:80:ILE:HD12	31:R:97:THR:HG22	1.89	0.54
8:7:-18:G:C3'	17:D:1500:A:N6	2.71	0.54
11:AA:143:ARG:NH2	11:AA:512:SER:O	2.40	0.54
21:H:84:LEU:HD22	21:H:84:LEU:H	1.72	0.54
63:x:27:VAL:HG21	63:x:40:ILE:HD12	1.89	0.54
8:7:-20:A:C4	8:7:-19:U:C5	2.95	0.54
11:AA:811:ASN:HA	11:AA:815:SER:HB2	1.90	0.54
10:B:12:G:H2'	10:B:13:C:OP1	2.08	0.54
51:l:131:THR:HG22	51:l:160:ALA:O	2.08	0.54
12:AB:148:VAL:HA	12:AB:160:VAL:CG2	2.37	0.54
17:D:13:U:C2	17:D:915:A:C6	2.95	0.54
38:Y:12:VAL:HG12	38:Y:23:VAL:HG21	1.90	0.54
3:2:50:LEU:HD23	44:e:26:PHE:CZ	2.42	0.54
8:7:-18:G:C4'	17:D:1500:A:H62	2.21	0.54
9:9:139:LEU:HD11	39:Z:11:VAL:HG13	1.90	0.54
11:AA:29:SER:O	11:AA:33:ASP:HB2	2.07	0.54
17:D:945:G:C2	17:D:946:A:C8	2.96	0.54
6:5:110:DA:N7	11:AA:183:TRP:HH2	2.06	0.54
7:6:26:DT:H2''	7:6:27:DG:H5'	1.88	0.54
9:9:62:ARG:HG2	9:9:62:ARG:NH2	2.20	0.54
10:A:56:C:C2	40:a:2112:G:C8	2.96	0.54
17:D:961:U:O4	17:D:974:A:N1	2.40	0.54
17:D:1515:G:H2'	17:D:1516:G:H8	1.72	0.54
21:H:84:LEU:H	21:H:84:LEU:CD2	2.21	0.54
29:P:8:ILE:HD12	29:P:25:ILE:HD11	1.89	0.54
38:Y:109:ALA:HB2	38:Y:128:ILE:HG13	1.89	0.54
39:Z:2:ILE:HB	39:Z:5:ASP:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:66:LYS:HB2	14:AE:69:GLU:CB	2.38	0.54
14:AE:1000:GLY:HA3	14:AE:1026:PRO:HG2	1.90	0.54
29:P:24:GLU:OE2	29:P:90:LEU:CD1	2.56	0.54
57:r:58:LEU:O	57:r:61:VAL:HG22	2.08	0.54
8:7:-8:U:H5''	8:7:-8:U:H6	1.73	0.53
10:B:18:G:C2	10:B:58:A:C5	2.97	0.53
21:H:290:TYR:C	21:H:305:HIS:O	2.47	0.53
38:Y:19:PRO:HG2	38:Y:24:GLY:H	1.73	0.53
40:a:2192:U:H2'	40:a:2193:G:C8	2.43	0.53
9:9:123:ILE:O	9:9:123:ILE:HG12	2.08	0.53
10:A:18:G:C2	10:A:58:A:C5	2.96	0.53
14:AE:901:ARG:HH21	14:AE:906:GLY:HA2	1.73	0.53
21:H:332:VAL:O	21:H:334:ASP:N	2.40	0.53
40:a:523:C:O2	40:a:554:U:O2'	2.25	0.53
11:AA:633:LEU:HD13	11:AA:644:LEU:HD23	1.89	0.53
11:AA:684:ASN:OD1	11:AA:687:ARG:NH2	2.41	0.53
21:H:52:GLN:OE1	21:H:86:ARG:CB	2.55	0.53
63:x:35:ILE:HG21	63:x:71:ALA:HA	1.89	0.53
9:9:78:GLY:H	9:9:79:PRO:HD2	1.68	0.53
10:A:12:G:H2'	10:A:13:C:OP1	2.08	0.53
12:AB:167:ARG:CZ	29:P:99:GLN:CB	2.76	0.53
13:AC:43:LEU:HD13	13:AC:217:ILE:HD11	1.90	0.53
10:B:76:A:N3	40:a:2493:U:H4'	2.23	0.53
40:a:1906:G:H5''	40:a:1906:G:H8	1.73	0.53
41:b:37:ILE:HD11	41:b:82:ILE:HD11	1.90	0.53
4:3:13:VAL:CG2	4:3:39:ILE:HD13	2.39	0.53
9:9:125:ARG:HA	9:9:125:ARG:CZ	2.38	0.53
14:AE:77:ARG:HD3	14:AE:78:LEU:H	1.73	0.53
14:AE:1045:THR:O	14:AE:1067:ARG:NH2	2.41	0.53
14:AE:1175:LEU:O	14:AE:1187:GLU:HA	2.08	0.53
14:AE:1346:GLY:O	14:AE:1350:ASN:ND2	2.41	0.53
38:Y:138:VAL:HG12	38:Y:138:VAL:O	2.08	0.53
8:7:-18:G:H3'	17:D:1500:A:N6	2.23	0.53
8:7:15:G:H2'	8:7:16:A:C8	2.43	0.53
12:AB:141:PHE:HZ	29:P:102:LEU:CD2	2.20	0.53
13:AC:100:LEU:HD23	13:AC:115:ILE:HG21	1.89	0.53
13:AD:100:LEU:HD21	13:AD:121:VAL:HG11	1.90	0.53
14:AE:514:THR:HG21	14:AE:596:LEU:HD12	1.90	0.53
17:D:767:A:H2'	17:D:768:A:O4'	2.09	0.53
21:H:116:VAL:C	21:H:279:LYS:HB2	2.33	0.53
59:t:7:MET:HE1	59:t:44:LYS:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:43:LYS:HG2	9:9:98:GLU:HG2	1.90	0.53
10:A:72:A:H2'	10:A:73:A:C5'	2.32	0.53
13:AD:16:ILE:HG23	13:AD:26:VAL:HG22	1.91	0.53
14:AE:526:VAL:HG12	14:AE:549:LYS:HB2	1.91	0.53
14:AE:795:TYR:OH	14:AE:1326:GLN:NE2	2.42	0.53
38:Y:57:VAL:O	38:Y:57:VAL:HG12	2.07	0.53
40:a:2298:A:C5	40:a:2321:U:O4	2.62	0.53
40:a:2636:C:HO2'	49:j:45:TYR:HH	1.56	0.53
8:7:17:G:H2'	8:7:18:A:C8	2.44	0.53
9:9:58:THR:HG21	9:9:81:LEU:HA	1.90	0.53
10:A:38:A:C2'	10:A:39:C:H5'	2.39	0.53
11:AA:243:PRO:HB2	11:AA:274:ILE:HG23	1.90	0.53
10:B:6:G:O2'	10:B:7:G:H8	1.92	0.53
17:D:1228:C:OP2	37:X:110:LYS:NZ	2.41	0.53
2:1:59:GLU:CG	2:1:66:ILE:HD11	2.38	0.53
8:7:10:U:O2	8:7:10:U:H2'	2.09	0.53
14:AE:968:ASN:HA	14:AE:1117:SER:HB2	1.90	0.53
38:Y:33:ASN:H	38:Y:66:PHE:HE1	1.56	0.53
40:a:2315:G:O2'	53:n:125:ARG:HD3	2.09	0.53
13:AD:182:ARG:NH1	14:AE:534:GLU:OE1	2.42	0.52
21:H:24:VAL:HG12	21:H:69:ASP:H	1.74	0.52
38:Y:116:MET:HE2	38:Y:117:THR:H	1.74	0.52
40:a:1980:G:O2'	40:a:1982:U:OP2	2.28	0.52
53:n:8:TYR:HA	53:n:12:VAL:HB	1.91	0.52
12:AB:140:PRO:HD3	29:P:81:GLU:HA	1.92	0.52
12:AB:161:SER:HB3	12:AB:170:PRO:N	2.24	0.52
13:AD:205:MET:HE3	13:AD:213:PRO:HB3	1.91	0.52
14:AE:122:SER:HB2	14:AE:132:LEU:HD12	1.91	0.52
16:C:61:ARG:NH2	17:D:736:C:OP1	2.43	0.52
17:D:563:A:N6	17:D:884:U:H3	2.05	0.52
21:H:321:VAL:HG13	21:H:322:VAL:HG23	1.90	0.52
28:O:98:LEU:HB3	28:O:104:VAL:HG13	1.92	0.52
40:a:995:C:O2	58:s:3:THR:OG1	2.24	0.52
11:AA:628:HIS:HB3	11:AA:647:ARG:HH21	1.73	0.52
13:AC:140:ILE:HD12	13:AC:142:MET:HE3	1.91	0.52
10:B:22:G:O2'	10:B:23:C:P	2.67	0.52
17:D:13:U:C4	17:D:21:G:C2	2.96	0.52
20:G:38:VAL:CG2	21:H:75:VAL:CG2	2.77	0.52
2:1:93:ALA:HB2	40:a:1614:A:N1	2.25	0.52
10:A:17:C:O2	10:A:17:C:H2'	2.08	0.52
11:AA:1287:LEU:HD13	14:AE:1357:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:30:LYS:HA	16:C:33:ILE:HD13	1.91	0.52
17:D:673:A:H2'	17:D:674:G:C8	2.44	0.52
40:a:1406:U:HO2'	40:a:1407:G:P	2.30	0.52
11:AA:246:LEU:HB3	11:AA:269:ILE:HD13	1.91	0.52
11:AA:714:VAL:HB	11:AA:787:PRO:HD2	1.92	0.52
14:AE:342:LEU:HD23	14:AE:1352:ILE:HG23	1.90	0.52
20:G:35:ARG:NH2	21:H:10:GLU:HG2	2.25	0.52
40:a:523:C:H4'	40:a:540:C:O2	2.10	0.52
40:a:2328:A:H2'	40:a:2329:U:C6	2.45	0.52
62:w:38:LEU:N	62:w:39:PRO:CD	2.73	0.52
9:9:93:ALA:O	9:9:129:LEU:HD13	2.06	0.52
12:AB:140:PRO:HB2	29:P:84:VAL:CB	2.28	0.52
40:a:1266:G:OP2	48:i:17:ARG:NE	2.43	0.52
10:A:22:G:O2'	10:A:23:C:P	2.68	0.52
14:AE:959:LYS:HB3	14:AE:983:LYS:HB2	1.92	0.52
10:B:16:C:O2	10:B:16:C:H2'	2.08	0.52
21:H:19:ARG:O	21:H:72:LEU:HD22	2.09	0.52
2:1:59:GLU:HG3	2:1:66:ILE:HD11	1.92	0.52
8:7:-8:U:H5''	8:7:-8:U:C6	2.45	0.52
8:7:17:G:OP2	11:AA:540:ARG:NH1	2.42	0.52
9:9:125:ARG:HG3	9:9:125:ARG:O	2.10	0.52
10:B:15:G:N3	10:B:15:G:C2'	2.73	0.52
10:B:56:C:H2'	10:B:57:A:C5'	2.27	0.52
21:H:135:LEU:CB	21:H:157:ILE:CB	2.87	0.52
33:T:40:GLN:CA	33:T:40:GLN:HE21	2.23	0.52
38:Y:59:THR:HG22	38:Y:61:TYR:CE1	2.45	0.52
40:a:929:U:H1'	45:f:26:GLY:O	2.10	0.52
40:a:1693:U:O2'	47:h:14:ARG:NH2	2.43	0.52
52:m:31:LEU:HD22	52:m:42:LEU:CD1	2.40	0.52
7:6:23:DC:N4	8:7:12:G:O6	2.34	0.52
10:A:12:G:C2'	10:A:13:C:OP1	2.57	0.52
11:AA:1070:HIS:NE2	11:AA:1114:GLU:OE1	2.36	0.52
12:AB:133:MET:HG2	12:AB:147:VAL:HG22	1.91	0.52
24:K:94:VAL:HG13	24:K:111:MET:HE1	1.91	0.52
40:a:1814:G:H4'	47:h:51:THR:HG21	1.92	0.52
65:z:58:ARG:HA	65:z:61:TRP:CE3	2.45	0.52
4:3:94:ARG:HB3	4:3:103:ILE:HD12	1.91	0.52
11:AA:974:ARG:HD2	11:AA:1014:LEU:HD21	1.92	0.52
12:AB:169:THR:O	12:AB:169:THR:CG2	2.56	0.52
13:AD:28:LEU:HD12	13:AD:201:LEU:HD23	1.91	0.52
10:B:12:G:C2'	10:B:13:C:OP1	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:1228:C:OP1	37:X:107:ARG:CZ	2.58	0.52
17:D:1499:A:O2'	17:D:1500:A:H5'	2.10	0.52
21:H:49:PRO:HD2	21:H:84:LEU:CD1	2.39	0.52
22:I:77:ILE:HA	22:I:84:VAL:HG23	1.91	0.52
24:K:81:LEU:HD13	24:K:123:VAL:HG12	1.92	0.52
40:a:587:C:OP2	60:u:21:ARG:NH1	2.43	0.52
8:7:-19:U:H2'	8:7:-18:G:C8	2.45	0.51
10:A:18:G:C2	10:A:58:A:C6	2.99	0.51
14:AE:79:LYS:CA	14:AE:81:ARG:HH12	1.96	0.51
17:D:864:A:C2	17:D:865:A:C2	2.98	0.51
17:D:1329:A:OP1	37:X:28:THR:N	2.42	0.51
38:Y:27:LEU:HD12	38:Y:27:LEU:C	2.35	0.51
55:p:121:ILE:HD12	55:p:141:ILE:CG2	2.41	0.51
7:6:21:DA:N6	8:7:15:G:N1	2.59	0.51
9:9:23:LEU:HA	9:9:118:ILE:HG13	1.92	0.51
10:A:6:G:O2'	10:A:7:G:H8	1.92	0.51
17:D:1308:U:P	37:X:98:ARG:HG3	2.50	0.51
38:Y:112:LYS:NZ	38:Y:112:LYS:CB	2.73	0.51
8:7:15:G:H2'	8:7:16:A:H8	1.75	0.51
10:A:15:G:N3	10:A:15:G:C2'	2.73	0.51
11:AA:93:SER:HA	11:AA:128:PRO:HA	1.92	0.51
10:B:60:U:O2'	10:B:61:C:OP1	2.23	0.51
8:7:-18:G:C4'	17:D:1500:A:N6	2.73	0.51
11:AA:125:GLY:HA2	11:AA:499:SER:HB2	1.92	0.51
11:AA:255:ILE:HB	11:AA:263:VAL:HB	1.92	0.51
11:AA:481:LEU:HD21	12:AB:25:SER:OG	2.10	0.51
11:AA:524:ILE:HG21	11:AA:708:VAL:HG13	1.92	0.51
21:H:135:LEU:CB	21:H:167:VAL:CA	2.86	0.51
8:7:16:A:H2'	8:7:17:G:C8	2.45	0.51
10:A:16:C:O2	10:A:16:C:H2'	2.09	0.51
11:AA:855:PRO:HD2	11:AA:887:VAL:HG11	1.91	0.51
38:Y:37:PHE:CZ	38:Y:56:VAL:HG11	2.44	0.51
10:A:76:A:O2'	40:a:2395:C:C2	2.64	0.51
14:AE:1179:PRO:HB2	14:AE:1182:GLY:H	1.75	0.51
17:D:1404:C:H2'	17:D:1404:C:O2	2.10	0.51
9:9:11:ILE:CD1	9:9:11:ILE:N	2.73	0.51
12:AB:136:VAL:HG11	12:AB:141:PHE:HB2	1.92	0.51
10:B:5:G:C2'	10:B:6:G:H5'	2.40	0.51
17:D:1276:G:O5'	17:D:1276:G:H8	1.93	0.51
9:9:3:LEU:HD13	9:9:5:LEU:H	1.75	0.51
9:9:71:CYS:HA	9:9:117:LEU:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:56:C:H1'	40:a:2112:G:C5	2.46	0.51
14:AE:67:ASP:C	14:AE:69:GLU:H	2.18	0.51
14:AE:71:LEU:HD22	14:AE:90:VAL:HG21	1.93	0.51
10:B:34:C:O2	10:B:34:C:H2'	2.11	0.51
21:H:332:VAL:C	21:H:334:ASP:H	2.18	0.51
38:Y:100:ILE:HB	38:Y:105:LEU:HD11	1.92	0.51
43:d:106:G:H2'	43:d:107:G:O4'	2.10	0.51
9:9:41:LEU:HD12	38:Y:117:THR:HG22	1.92	0.51
14:AE:510:LEU:HD22	14:AE:601:ILE:HD12	1.91	0.51
21:H:308:GLU:O	21:H:310:ASP:N	2.43	0.51
40:a:2627:G:O2'	40:a:2781:A:N1	2.37	0.51
59:t:71:ARG:NH2	59:t:123:LEU:O	2.42	0.51
8:7:-6:U:OP1	22:l:132:ARG:NH2	2.43	0.51
10:A:56:C:C3'	10:A:57:A:H5''	2.40	0.51
10:B:24:U:O2'	40:a:1922:G:O3'	2.29	0.51
17:D:13:U:C4	17:D:915:A:C6	2.92	0.51
17:D:1410:A:C2	17:D:1491:G:C2	2.99	0.51
40:a:118:A:C8	40:a:119:A:C8	2.99	0.51
40:a:1824:G:O2'	47:h:252:THR:HG21	2.11	0.51
40:a:1839:G:N9	40:a:1927:A:H1'	2.23	0.51
40:a:2000:C:OP1	62:w:5:LYS:NZ	2.36	0.51
43:d:5:U:OP1	43:d:61:G:O2'	2.26	0.51
59:t:43:ILE:HD12	59:t:56:ASP:HB2	1.93	0.51
11:AA:232:ILE:HG12	11:AA:237:LEU:HG	1.93	0.50
40:a:783:A:N3	40:a:783:A:C2'	2.70	0.50
7:6:5:DT:P	14:AE:1172:LYS:HZ3	2.23	0.50
11:AA:812:PHE:O	14:AE:504:GLN:NE2	2.40	0.50
17:D:1366:C:O2'	29:P:62:ARG:NH2	2.44	0.50
4:3:12:ILE:HG21	4:3:80:ALA:HB2	1.92	0.50
9:9:51:TYR:CG	9:9:89:PRO:HD2	2.47	0.50
10:A:28:C:H2'	10:A:29:G:H8	1.76	0.50
11:AA:786:GLY:N	11:AA:789:THR:OG1	2.41	0.50
10:B:48:C:O2	10:B:48:C:H2'	2.11	0.50
10:B:56:C:C3'	10:B:57:A:H5''	2.40	0.50
29:P:57:VAL:O	29:P:57:VAL:HG13	2.11	0.50
40:a:639:U:H2'	40:a:640:C:C6	2.45	0.50
40:a:1869:G:N2	40:a:1871:A:O2'	2.44	0.50
2:1:55:ILE:HG23	2:1:66:ILE:HD12	1.93	0.50
9:9:52:MET:HE3	9:9:52:MET:CA	2.42	0.50
11:AA:400:VAL:HG21	11:AA:452:ARG:HE	1.77	0.50
10:B:18:G:C2	10:B:58:A:C6	2.99	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:49:PRO:HD2	21:H:84:LEU:HD11	1.92	0.50
40:a:2298:A:N3	40:a:2321:U:C5	2.80	0.50
14:AE:430:HIS:HB3	14:AE:925:GLU:HG3	1.93	0.50
23:J:61:VAL:HG21	23:J:200:ILE:CD1	2.35	0.50
40:a:2557:G:H2'	40:a:2558:C:C6	2.46	0.50
6:5:96:DT:H2''	6:5:97:DC:C5	2.46	0.50
12:AB:71:VAL:HG12	12:AB:73:MET:HB2	1.93	0.50
10:B:47:U:H2'	10:B:48:C:H4'	1.94	0.50
10:B:72:A:H2'	10:B:73:A:C5'	2.32	0.50
21:H:117:LYS:CB	21:H:278:THR:CG2	2.90	0.50
58:s:30:THR:HG22	58:s:31:GLU:N	2.27	0.50
2:1:24:ILE:HD13	2:1:36:LEU:HD11	1.93	0.50
6:5:98:DA:N9	6:5:99:DT:H72	2.26	0.50
8:7:9:U:H3'	8:7:9:U:O2	2.11	0.50
10:A:48:C:H2'	10:A:48:C:O2	2.11	0.50
14:AE:77:ARG:HB3	14:AE:80:HIS:HB2	1.93	0.50
14:AE:209:ASN:HB3	14:AE:214:ARG:HH21	1.76	0.50
14:AE:412:LEU:HD22	14:AE:441:LEU:HD21	1.94	0.50
14:AE:417:ARG:NH1	15:AF:43:ASN:O	2.45	0.50
15:AF:3:ARG:NH1	15:AF:55:GLU:OE2	2.40	0.50
17:D:108:G:H5''	17:D:108:G:N3	2.27	0.50
40:a:1141:U:O2	40:a:1142:A:N6	2.44	0.50
40:a:1910:G:O5'	40:a:1910:G:H8	1.93	0.50
12:AB:165:PHE:HE1	29:P:88:MET:CA	2.25	0.50
40:a:1964:G:H4'	40:a:1965:C:OP2	2.11	0.50
9:9:31:ARG:NH1	9:9:31:ARG:CG	2.73	0.50
9:9:44:ALA:HB1	9:9:52:MET:HB3	1.93	0.50
10:A:41:C:H4'	26:M:143:ARG:NH1	2.25	0.50
10:A:56:C:C5	40:a:2168:G:O6	2.64	0.50
14:AE:157:GLN:HE22	14:AE:188:LEU:HD22	1.76	0.50
10:B:59:A:H2'	10:B:60:U:H5'	1.94	0.50
40:a:2297:A:C6	40:a:2321:U:O4	2.65	0.50
52:m:22:MET:O	52:m:28:ARG:NH1	2.45	0.50
65:z:47:TYR:CD1	65:z:47:TYR:C	2.90	0.50
11:AA:146:VAL:HG21	11:AA:513:GLN:HE21	1.77	0.49
12:AB:156:SER:O	12:AB:156:SER:OG	2.27	0.49
17:D:1208:C:H2'	17:D:1209:C:C6	2.47	0.49
19:F:4:ILE:HD12	19:F:19:PHE:HA	1.93	0.49
24:K:114:VAL:HG21	24:K:141:ILE:HD12	1.94	0.49
33:T:21:ASP:O	33:T:22:THR:HG22	2.12	0.49
35:V:48:ASP:HB3	35:V:75:LEU:HD23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:h:107:PRO:HD2	47:h:110:LEU:HD22	1.94	0.49
55:p:35:ARG:HD3	55:p:71:LEU:HD13	1.93	0.49
58:s:32:LEU:CD2	58:s:54:ILE:HG21	2.42	0.49
59:t:113:MET:O	59:t:116:ILE:HG13	2.11	0.49
1:0:14:VAL:HG21	1:0:98:ILE:HG13	1.93	0.49
8:7:-19:U:OP2	17:D:926:G:N2	2.45	0.49
11:AA:529:ARG:HH11	11:AA:572:ILE:HG22	1.77	0.49
14:AE:679:TYR:OH	14:AE:754:ILE:O	2.23	0.49
21:H:120:PHE:CB	21:H:136:VAL:CB	2.91	0.49
21:H:132:PRO:N	21:H:167:VAL:CB	2.75	0.49
21:H:267:TRP:CZ3	21:H:340:ARG:HG3	2.43	0.49
27:N:3:MET:HA	27:N:3:MET:HE3	1.94	0.49
28:O:81:HIS:O	28:O:84:THR:OG1	2.23	0.49
49:j:25:THR:HG21	49:j:193:VAL:HG22	1.94	0.49
10:A:11:A:H2'	10:A:12:G:C1'	2.42	0.49
12:AB:158:LEU:HD21	12:AB:175:PHE:CE1	2.46	0.49
12:AB:173:LEU:HB3	12:AB:178:VAL:HG13	1.93	0.49
17:D:50:A:O2'	17:D:360:G:N2	2.45	0.49
17:D:1311:A:OP1	46:g:59:ARG:NH1	2.45	0.49
17:D:1356:G:H2'	17:D:1357:A:C8	2.47	0.49
33:T:4:SER:O	33:T:8:THR:HG23	2.12	0.49
40:a:742:A:C2	40:a:743:A:C6	3.00	0.49
63:x:51:ALA:HB3	63:x:78:VAL:HB	1.94	0.49
8:7:-13:U:OP2	17:D:1397:C:C2	2.65	0.49
14:AE:107:LEU:HD22	14:AE:299:LEU:HD21	1.94	0.49
14:AE:814:CYS:SG	14:AE:815:GLY:N	2.85	0.49
10:B:11:A:H2'	10:B:12:G:C1'	2.43	0.49
21:H:318:PRO:HA	21:H:321:VAL:HG12	1.95	0.49
38:Y:80:LYS:HG3	38:Y:86:LYS:HA	1.93	0.49
10:A:37:A:H2'	10:A:38:A:H8	1.77	0.49
10:A:47:U:H2'	10:A:48:C:H4'	1.94	0.49
10:B:25:C:H2'	10:B:26:G:H5'	1.94	0.49
17:D:1499:A:H3'	17:D:1499:A:OP2	2.12	0.49
40:a:2243:U:H2'	40:a:2244:U:C6	2.46	0.49
40:a:2303:G:C6	40:a:2314:A:N1	2.81	0.49
57:r:3:VAL:HG22	57:r:36:ALA:HB1	1.95	0.49
62:w:55:ALA:HA	62:w:80:PHE:CE1	2.47	0.49
10:A:18:G:C5	10:A:57:A:C5	3.01	0.49
10:A:59:A:H2'	10:A:60:U:H5'	1.94	0.49
14:AE:425:ARG:NH1	14:AE:458:ASN:O	2.45	0.49
25:L:18:VAL:N	25:L:19:PRO:CD	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:-15:U:C2	17:D:1493:A:C2	3.00	0.49
10:A:19:G:C5	40:a:2112:G:H4'	2.44	0.49
12:AB:148:VAL:HG21	12:AB:151:VAL:HG22	1.95	0.49
17:D:13:U:O4	17:D:21:G:N3	2.46	0.49
17:D:552:U:O2'	31:R:83:ARG:O	2.27	0.49
17:D:872:A:H2'	17:D:872:A:N3	2.27	0.49
38:Y:21:PRO:CB	38:Y:22:PRO:CD	2.90	0.49
49:j:156:PHE:CE1	58:s:81:ILE:HD13	2.48	0.49
53:n:127:ASN:ND2	53:n:127:ASN:N	2.60	0.49
13:AD:86:LYS:NZ	14:AE:532:GLU:OE2	2.41	0.49
41:b:37:ILE:HG21	41:b:80:ILE:HG21	1.95	0.49
52:m:24:THR:HG23	52:m:27:GLY:H	1.78	0.49
9:9:31:ARG:HE	40:a:1054:A:C4'	2.26	0.49
11:AA:1340:GLU:HB2	14:AE:19:ALA:HB3	1.94	0.49
17:D:1169:A:H2'	17:D:1170:A:C8	2.48	0.49
58:s:17:VAL:HG23	58:s:137:PRO:HB2	1.93	0.49
8:7:12:G:C4	14:AE:253:VAL:HG21	2.48	0.49
14:AE:678:ARG:NH1	14:AE:756:GLU:OE1	2.46	0.49
17:D:1308:U:H2'	37:X:98:ARG:HH22	1.61	0.49
40:a:1412:U:C4	40:a:1413:A:N7	2.81	0.49
47:h:210:ALA:HA	47:h:213:TRP:CE3	2.48	0.49
62:w:67:PHE:O	62:w:71:ARG:N	2.45	0.49
7:6:21:DA:C6	8:7:15:G:C2	3.01	0.48
12:AB:136:VAL:HG22	12:AB:173:LEU:CD1	2.42	0.48
14:AE:693:VAL:HG21	14:AE:743:MET:HE3	1.94	0.48
10:B:11:A:C2'	10:B:12:G:O4'	2.60	0.48
40:a:464:U:O3'	52:m:12:ARG:NH2	2.45	0.48
7:6:18:DC:N4	8:7:17:G:H1	2.06	0.48
11:AA:18:ARG:HE	11:AA:620:ASN:HA	1.77	0.48
10:B:18:G:C5	10:B:57:A:C5	3.01	0.48
35:V:75:LEU:C	35:V:75:LEU:HD12	2.38	0.48
44:e:18:LEU:HB2	44:e:53:VAL:HG11	1.94	0.48
2:1:29:VAL:HB	2:1:55:ILE:HD11	1.95	0.48
7:6:16:DC:H1'	14:AE:426:ALA:HB1	1.95	0.48
8:7:14:U:H5''	14:AE:322:ARG:HD2	1.95	0.48
9:9:31:ARG:NE	40:a:1054:A:O4'	2.46	0.48
9:9:125:ARG:NH1	9:9:125:ARG:CA	2.73	0.48
10:A:11:A:C2'	10:A:12:G:O4'	2.60	0.48
10:A:76:A:N6	40:a:2422:C:O4'	2.46	0.48
11:AA:554:HIS:HD2	11:AA:558:VAL:HB	1.77	0.48
11:AA:836:LEU:HD13	11:AA:1054:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:749:LYS:HD3	14:AE:753:SER:HB2	1.94	0.48
10:B:49:G:O5'	10:B:49:G:H8	1.96	0.48
17:D:974:A:OP1	32:S:69:ARG:NH1	2.46	0.48
17:D:1017:U:O2'	17:D:1018:G:O4'	2.31	0.48
17:D:1174:G:H2'	17:D:1175:G:H5'	1.95	0.48
40:a:2685:G:OP1	59:t:78:ARG:NH2	2.47	0.48
49:j:4:LEU:HD23	49:j:29:VAL:CG1	2.39	0.48
8:7:-15:U:C2	17:D:1493:A:H2	2.31	0.48
9:9:8:LYS:NZ	40:a:1046:A:H61	2.11	0.48
10:A:15:G:C2	10:A:20:U:O2	2.66	0.48
11:AA:143:ARG:NH1	11:AA:507:GLY:O	2.32	0.48
11:AA:1280:ALA:HB1	14:AE:918:ILE:HG22	1.96	0.48
12:AB:148:VAL:O	12:AB:148:VAL:CG1	2.61	0.48
12:AB:157:ARG:CZ	12:AB:174:ASP:OD1	2.61	0.48
10:B:39:C:O5'	10:B:39:C:H6	1.95	0.48
38:Y:77:VAL:HG13	38:Y:80:LYS:CE	2.44	0.48
40:a:565:C:H2'	40:a:566:U:O4'	2.13	0.48
40:a:2038:G:H2'	40:a:2039:U:O4'	2.13	0.48
9:9:23:LEU:HD22	9:9:92:ALA:HB1	1.95	0.48
10:A:37:A:H2'	10:A:38:A:C8	2.48	0.48
13:AD:182:ARG:O	13:AD:205:MET:HA	2.14	0.48
14:AE:210:SER:O	14:AE:214:ARG:N	2.43	0.48
14:AE:520:ALA:HB3	14:AE:546:ALA:HB2	1.95	0.48
14:AE:977:SER:OG	14:AE:980:THR:OG1	2.31	0.48
29:P:6:ILE:HG23	29:P:100:ILE:CG2	2.43	0.48
45:f:24:LEU:HD11	45:f:54:MET:CE	2.42	0.48
3:2:61:LEU:C	3:2:61:LEU:HD12	2.39	0.48
8:7:-13:U:H5'	17:D:1397:C:C2	2.48	0.48
9:9:51:TYR:CD1	9:9:88:HIS:HB2	2.49	0.48
10:A:76:A:C2'	40:a:2394:C:N4	2.75	0.48
11:AA:9:LYS:HG2	11:AA:1171:ARG:HH12	1.77	0.48
11:AA:411:ARG:NH2	11:AA:427:ASP:OD2	2.44	0.48
11:AA:618:GLN:HG3	14:AE:770:LEU:HD13	1.95	0.48
14:AE:67:ASP:C	14:AE:69:GLU:N	2.71	0.48
10:B:76:A:N3	10:B:76:A:C2'	2.74	0.48
40:a:2585:U:O2	40:a:2585:U:O4'	2.32	0.48
2:1:4:ILE:HG12	2:1:106:VAL:HG22	1.96	0.48
10:A:49:G:H8	10:A:49:G:O5'	1.96	0.48
14:AE:429:LEU:HB3	14:AE:925:GLU:HG2	1.95	0.48
17:D:5:U:O2	17:D:5:U:O4'	2.29	0.48
21:H:330:VAL:HG12	21:H:345:GLY:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:K:99:ALA:CB	24:K:103:THR:HG21	2.43	0.48
42:c:3:ARG:HD2	42:c:30:LEU:HD22	1.94	0.48
8:7:14:U:H4'	14:AE:322:ARG:HH11	1.79	0.48
10:A:15:G:H22	10:A:20:U:H3	1.59	0.48
10:A:33:U:H2'	10:A:35:A:OP2	2.14	0.48
12:AB:161:SER:HA	12:AB:170:PRO:HA	1.95	0.48
10:B:15:G:C2	10:B:20:U:O2	2.66	0.48
17:D:13:U:O2	17:D:915:A:N7	2.47	0.48
40:a:1433:A:H2'	40:a:1434:A:O4'	2.13	0.48
1:0:14:VAL:CG2	1:0:98:ILE:HG13	2.43	0.48
6:5:108:DT:H73	11:AA:199:ASP:HB3	1.95	0.48
8:7:-14:U:C6	8:7:-14:U:C3'	2.97	0.48
9:9:43:LYS:HZ1	9:9:95:LEU:HD13	1.79	0.48
10:A:5:G:C2'	10:A:6:G:H5'	2.40	0.48
17:D:911:U:H2'	17:D:912:C:C6	2.49	0.48
21:H:23:ILE:N	21:H:69:ASP:OD2	2.46	0.48
21:H:279:LYS:HA	21:H:331:MET:CB	2.33	0.48
40:a:1588:G:C6	40:a:1589:U:O4	2.67	0.48
40:a:2646:C:O5'	40:a:2646:C:H6	1.95	0.48
1:0:40:MET:HE3	1:0:49:ILE:CD1	2.44	0.48
4:3:7:ARG:HB2	40:a:85:G:OP2	2.13	0.48
8:7:-2:U:O2	8:7:-2:U:H2'	2.12	0.48
8:7:14:U:O4'	14:AE:322:ARG:NH1	2.47	0.48
10:A:42:G:H2'	10:A:43:A:C8	2.47	0.48
10:A:58:A:OP2	10:A:58:A:C8	2.67	0.48
10:A:60:U:OP2	10:A:61:C:N4	2.45	0.48
11:AA:400:VAL:HG11	11:AA:452:ARG:HD2	1.94	0.48
11:AA:732:ILE:HD11	11:AA:769:PRO:HB3	1.95	0.48
12:AB:174:ASP:O	12:AB:178:VAL:HG22	2.14	0.48
14:AE:616:PRO:HA	14:AE:619:ILE:HG22	1.96	0.48
17:D:371:A:H2'	17:D:372:C:O4'	2.14	0.48
29:P:6:ILE:CG2	29:P:100:ILE:HG23	2.43	0.48
40:a:686:U:O4	52:m:12:ARG:HB2	2.14	0.48
40:a:2168:G:H8	40:a:2168:G:OP1	1.97	0.48
40:a:2303:G:C2	40:a:2314:A:N3	2.82	0.48
9:9:17:GLU:HG2	9:9:88:HIS:NE2	2.29	0.47
10:A:9:G:H5''	10:A:10:G:OP2	2.14	0.47
11:AA:848:GLU:HG2	11:AA:888:THR:HG22	1.96	0.47
20:G:35:ARG:CD	21:H:14:LYS:HD3	2.40	0.47
10:A:25:C:H2'	10:A:26:G:H5'	1.94	0.47
11:AA:400:VAL:HG22	11:AA:584:TYR:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:560:PRO:O	14:AE:780:ARG:NH2	2.47	0.47
10:B:14:A:N3	10:B:14:A:H2'	2.29	0.47
40:a:742:A:C2	40:a:755:U:N3	2.80	0.47
2:1:25:ARG:NH1	2:1:74:ILE:O	2.47	0.47
11:AA:363:LEU:HB3	11:AA:381:ALA:HB1	1.96	0.47
11:AA:565:GLU:HA	11:AA:569:ILE:HG12	1.95	0.47
12:AB:134:VAL:HG21	12:AB:160:VAL:HG21	1.97	0.47
12:AB:164:ILE:HG12	12:AB:165:PHE:CD1	2.49	0.47
10:B:9:G:H5''	10:B:10:G:OP2	2.14	0.47
21:H:52:GLN:O	21:H:53:PHE:HD1	1.95	0.47
38:Y:133:ARG:O	38:Y:133:ARG:HG2	2.14	0.47
40:a:1814:G:C4'	47:h:51:THR:HG21	2.44	0.47
40:a:1993:U:H4'	49:j:133:THR:HG22	1.96	0.47
10:A:41:C:H5'	26:M:143:ARG:HD2	1.96	0.47
13:AD:100:LEU:HB2	13:AD:144:ILE:HG23	1.94	0.47
17:D:946:A:H2'	17:D:947:G:C8	2.50	0.47
49:j:121:THR:HB	49:j:127:PHE:CD2	2.49	0.47
12:AB:148:VAL:N	12:AB:160:VAL:HG22	2.30	0.47
14:AE:79:LYS:CB	14:AE:81:ARG:HH12	2.28	0.47
10:B:68:C:C4	10:B:69:C:C5	3.02	0.47
38:Y:77:VAL:HG13	38:Y:80:LYS:HE3	1.95	0.47
40:a:1020:A:C6	40:a:1141:U:O2	2.68	0.47
10:A:18:G:C6	10:A:57:A:N7	2.83	0.47
12:AB:135:ARG:HG2	12:AB:135:ARG:HH11	1.80	0.47
13:AD:15:ASP:OD1	13:AD:27:THR:OG1	2.30	0.47
10:B:18:G:N3	10:B:58:A:C6	2.82	0.47
17:D:526:C:P	31:R:88:LYS:HE3	2.54	0.47
25:L:67:PRO:O	25:L:70:VAL:HG22	2.15	0.47
39:Z:29:LYS:HE2	39:Z:29:LYS:HB2	1.45	0.47
8:7:11:U:C3'	8:7:11:U:C6	2.97	0.47
9:9:43:LYS:NZ	9:9:95:LEU:HD13	2.30	0.47
9:9:132:TYR:CE1	39:Z:19:VAL:HG22	2.50	0.47
10:A:60:U:H4'	10:A:61:C:OP2	2.14	0.47
10:A:68:C:C4	10:A:69:C:C5	3.02	0.47
11:AA:103:VAL:HG12	11:AA:117:ILE:HG22	1.97	0.47
11:AA:207:THR:OG1	11:AA:354:ASP:OD2	2.32	0.47
11:AA:1311:GLY:O	15:AF:31:GLN:NE2	2.47	0.47
12:AB:158:LEU:HD21	12:AB:175:PHE:CZ	2.50	0.47
12:AB:161:SER:CA	12:AB:170:PRO:HA	2.44	0.47
13:AD:35:PHE:HA	13:AD:38:THR:HG22	1.97	0.47
14:AE:79:LYS:CB	14:AE:81:ARG:NH1	2.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:516:ASP:OD1	14:AE:516:ASP:N	2.47	0.47
10:B:42:G:H2'	10:B:43:A:C8	2.48	0.47
10:B:60:U:H4'	10:B:61:C:OP2	2.14	0.47
17:D:604:G:H2'	17:D:605:U:O4'	2.14	0.47
21:H:72:LEU:CD1	21:H:72:LEU:N	2.73	0.47
23:J:61:VAL:CG2	23:J:200:ILE:HD11	2.39	0.47
37:X:16:VAL:HG23	37:X:17:ILE:HD12	1.97	0.47
49:j:152:PRO:HG3	49:j:156:PHE:CZ	2.50	0.47
54:o:13:ARG:HD3	60:u:58:TYR:O	2.14	0.47
9:9:67:THR:H	9:9:68:PRO:HD3	1.80	0.47
11:AA:1314:GLN:HB2	15:AF:28:ARG:HH12	1.79	0.47
13:AC:102:LEU:HD12	13:AC:115:ILE:HG12	1.96	0.47
14:AE:59:ALA:HB3	14:AE:71:LEU:CD2	2.42	0.47
14:AE:66:LYS:HB2	14:AE:69:GLU:HB3	1.96	0.47
14:AE:77:ARG:HA	14:AE:77:ARG:CZ	2.44	0.47
14:AE:86:GLU:N	14:AE:86:GLU:CD	2.73	0.47
16:C:33:ILE:O	16:C:33:ILE:HG12	2.15	0.47
17:D:1308:U:P	37:X:98:ARG:CG	3.03	0.47
17:D:1308:U:OP1	37:X:100:GLN:OE1	2.23	0.47
21:H:135:LEU:CB	21:H:167:VAL:O	2.63	0.47
39:Z:18:ASP:HB3	39:Z:22:LEU:CD1	2.45	0.47
3:2:30:ILE:HD13	3:2:93:LEU:HD12	1.97	0.47
9:9:27:VAL:HG22	9:9:99:PHE:HE2	1.80	0.47
10:A:14:A:H2'	10:A:14:A:N3	2.29	0.47
12:AB:140:PRO:HG3	29:P:84:VAL:CG2	2.45	0.47
13:AD:59:VAL:HG22	13:AD:144:ILE:HA	1.97	0.47
17:D:373:A:C2	17:D:374:A:C8	3.03	0.47
17:D:1064:G:O2'	17:D:1190:G:N2	2.47	0.47
21:H:69:ASP:O	21:H:85:SER:CB	2.63	0.47
1:0:51:VAL:HG22	1:0:51:VAL:O	2.15	0.47
10:A:18:G:N3	10:A:58:A:C6	2.82	0.47
11:AA:562:GLU:OE1	11:AA:662:SER:OG	2.28	0.47
12:AB:140:PRO:HB3	29:P:84:VAL:HB	1.89	0.47
14:AE:437:PHE:HZ	14:AE:453:VAL:HG11	1.79	0.47
10:B:15:G:H22	10:B:20:U:H3	1.59	0.47
10:B:18:G:C8	10:B:57:A:N1	2.83	0.47
17:D:1103:C:O2	20:G:106:THR:HG21	2.15	0.47
21:H:309:MET:HE2	21:H:318:PRO:HB3	1.97	0.47
23:J:162:ALA:O	23:J:165:ARG:O	2.32	0.47
27:N:102:ALA:HB3	27:N:113:ASP:HB3	1.96	0.47
58:s:84:ILE:HG23	58:s:84:ILE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:t:18:ARG:HB2	59:t:45:GLU:HB3	1.97	0.47
63:x:27:VAL:CG2	63:x:40:ILE:HD12	2.44	0.47
8:7:-20:A:H2'	8:7:-19:U:C6	2.50	0.46
11:AA:735:LYS:HA	11:AA:748:ILE:HG22	1.98	0.46
13:AC:64:VAL:HG11	13:AC:78:ILE:HG21	1.97	0.46
14:AE:218:THR:HA	14:AE:221:ILE:HG22	1.96	0.46
10:B:18:G:C6	10:B:57:A:N7	2.83	0.46
10:B:58:A:C8	10:B:58:A:OP2	2.67	0.46
39:Z:4:LYS:O	39:Z:4:LYS:HD2	2.15	0.46
40:a:2756:U:C4	40:a:2759:G:C6	3.03	0.46
53:n:36:LEU:HB3	53:n:57:LEU:HD21	1.97	0.46
8:7:16:A:H2'	8:7:17:G:H8	1.79	0.46
8:7:17:G:H2'	8:7:18:A:H8	1.80	0.46
9:9:1:MET:SD	9:9:2:ALA:N	2.88	0.46
11:AA:230:PHE:HB2	11:AA:333:ILE:HB	1.97	0.46
11:AA:318:SER:OG	11:AA:320:ASP:OD1	2.31	0.46
11:AA:1286:THR:O	11:AA:1290:MET:HB2	2.14	0.46
12:AB:135:ARG:O	12:AB:178:VAL:HA	2.16	0.46
17:D:1225:A:OP1	37:X:101:ARG:HB2	2.15	0.46
17:D:1329:A:OP1	37:X:28:THR:OG1	2.31	0.46
38:Y:79:LEU:HD13	38:Y:132:ALA:HA	1.97	0.46
40:a:517:C:OP2	48:i:10:ARG:NH2	2.48	0.46
40:a:1021:A:N3	40:a:1021:A:C3'	2.78	0.46
9:9:118:ILE:HB	9:9:119:PRO:CD	2.45	0.46
14:AE:438:GLU:OE2	14:AE:481:ARG:NH1	2.44	0.46
14:AE:1108:GLN:HE21	14:AE:1123:ARG:HH12	1.62	0.46
14:AE:1350:ASN:HA	14:AE:1353:VAL:HG12	1.97	0.46
17:D:35:G:N3	31:R:115:SER:OG	2.47	0.46
17:D:915:A:C8	17:D:915:A:H3'	2.50	0.46
20:G:18:HIS:CA	21:H:43:LYS:HD2	2.29	0.46
21:H:84:LEU:N	21:H:84:LEU:CD2	2.78	0.46
24:K:96:MET:CE	24:K:115:LEU:HD11	2.46	0.46
40:a:784:G:H5'	40:a:785:G:OP1	2.15	0.46
40:a:1839:G:N9	40:a:1927:A:C1'	2.77	0.46
10:A:18:G:C8	10:A:57:A:N1	2.83	0.46
17:D:1517:G:H1'	40:a:1919:A:O2'	2.16	0.46
35:V:8:LEU:HD23	35:V:25:ILE:HG21	1.97	0.46
40:a:2291:U:H2'	40:a:2292:U:C6	2.51	0.46
1:0:5:PHE:HB3	1:0:59:ILE:HD12	1.96	0.46
9:9:24:SER:HB2	9:9:116:GLU:HG2	1.97	0.46
9:9:139:LEU:HD21	39:Z:11:VAL:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:5:G:C2'	10:A:6:G:C5'	2.93	0.46
11:AA:1314:GLN:HA	15:AF:28:ARG:HH22	1.80	0.46
14:AE:482:ALA:HA	15:AF:6:VAL:HG21	1.98	0.46
14:AE:804:ALA:O	14:AE:806:ASP:N	2.47	0.46
10:B:6:G:O2'	10:B:7:G:C5'	2.64	0.46
17:D:1175:G:N3	17:D:1176:A:C8	2.83	0.46
21:H:332:VAL:HG13	21:H:342:ILE:HG23	1.98	0.46
22:I:75:ILE:HD13	22:I:75:ILE:C	2.40	0.46
40:a:2168:G:OP1	40:a:2168:G:C8	2.69	0.46
55:p:24:ILE:CD1	55:p:72:LEU:HD21	2.44	0.46
4:3:94:ARG:CB	4:3:103:ILE:HD12	2.45	0.46
11:AA:689:ALA:HB2	11:AA:1233:LEU:HD23	1.97	0.46
14:AE:420:PRO:HA	14:AE:437:PHE:O	2.16	0.46
16:C:61:ARG:HG2	25:L:88:MET:HE1	1.98	0.46
18:E:54:MET:O	18:E:57:ILE:HG22	2.15	0.46
21:H:316:ILE:HD11	21:H:321:VAL:HG11	1.97	0.46
40:a:2298:A:C6	40:a:2299:U:C2	3.04	0.46
51:l:149:ILE:CD1	51:l:188:MET:HE3	2.46	0.46
9:9:7:ASP:OD1	9:9:7:ASP:N	2.36	0.46
9:9:48:ALA:HB3	9:9:51:TYR:CD2	2.50	0.46
10:A:14:A:H1'	10:A:22:G:N2	2.31	0.46
10:A:29:G:H2'	10:A:30:G:O4'	2.15	0.46
13:AD:185:TYR:HA	13:AD:202:VAL:O	2.16	0.46
14:AE:1037:PHE:HB3	14:AE:1040:MET:HB2	1.97	0.46
17:D:1228:C:P	37:X:107:ARG:HH12	2.38	0.46
22:I:117:ALA:HB2	22:I:200:VAL:CG1	2.46	0.46
30:Q:34:ILE:HG12	30:Q:70:CYS:SG	2.56	0.46
10:A:68:C:H3'	10:A:69:C:H5''	1.96	0.46
14:AE:797:THR:HG22	14:AE:924:GLY:HA3	1.97	0.46
28:O:63:LEU:HD13	28:O:65:ILE:HD11	1.97	0.46
40:a:2093:G:O2'	40:a:2198:A:N1	2.41	0.46
8:7:-13:U:OP2	17:D:1397:C:O2	2.34	0.46
10:A:41:C:C5'	26:M:143:ARG:HD2	2.46	0.46
10:A:58:A:C1'	10:A:60:U:C5	2.99	0.46
11:AA:812:PHE:HZ	14:AE:503:SER:HB2	1.80	0.46
10:B:14:A:H1'	10:B:22:G:N2	2.31	0.46
20:G:114:LEU:HA	20:G:144:LEU:HD13	1.98	0.46
29:P:99:GLN:O	29:P:99:GLN:HG2	2.16	0.46
40:a:1668:A:O2'	40:a:1674:G:N7	2.44	0.46
49:j:186:LEU:HD21	64:y:4:ILE:HG21	1.98	0.46
6:5:108:DT:O4	11:AA:199:ASP:OD2	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:28:LEU:HD21	11:AA:524:ILE:HG13	1.98	0.46
12:AB:47:GLU:HG3	12:AB:64:PHE:CD1	2.44	0.46
12:AB:165:PHE:CD1	12:AB:165:PHE:N	2.82	0.46
12:AB:165:PHE:CE1	29:P:87:LEU:C	2.94	0.46
14:AE:79:LYS:HZ2	14:AE:79:LYS:HB3	1.81	0.46
10:B:48:C:N4	10:B:59:A:C5	2.84	0.46
20:G:16:PHE:CD2	21:H:42:LEU:O	2.69	0.46
38:Y:125:THR:HA	38:Y:128:ILE:HG12	1.98	0.46
40:a:1695:G:N7	47:h:14:ARG:NH2	2.64	0.46
9:9:39:THR:HA	9:9:42:ARG:HH11	1.81	0.45
12:AB:138:ASP:OD1	12:AB:139:GLY:N	2.49	0.45
14:AE:230:SER:OG	14:AE:231:GLY:N	2.49	0.45
14:AE:1022:PRO:O	14:AE:1126:GLN:NE2	2.45	0.45
14:AE:1321:SER:OG	14:AE:1349:GLU:OE2	2.32	0.45
17:D:429:U:N3	17:D:431:A:N6	2.64	0.45
19:F:67:ARG:HD3	19:F:67:ARG:N	2.31	0.45
40:a:1266:G:OP1	48:i:16:ARG:NE	2.45	0.45
40:a:2315:G:H5'	53:n:157:THR:HG23	1.97	0.45
11:AA:176:ILE:HD11	11:AA:428:VAL:HG21	1.98	0.45
17:D:1176:A:H2'	17:D:1177:G:O4'	2.16	0.45
17:D:1240:U:OP1	26:M:116:MET:HB2	2.16	0.45
26:M:24:ALA:O	26:M:27:VAL:HG22	2.16	0.45
26:M:27:VAL:HG12	26:M:43:VAL:HG11	1.98	0.45
40:a:1327:A:H2'	40:a:1328:A:O4'	2.17	0.45
40:a:1394:U:H4'	40:a:1603:A:H4'	1.97	0.45
47:h:76:ALA:HB2	47:h:96:TYR:CD1	2.51	0.45
61:v:96:ILE:HG21	61:v:126:ILE:HD12	1.98	0.45
2:1:17:VAL:HG12	2:1:76:VAL:HG21	1.98	0.45
9:9:50:VAL:CG2	38:Y:120:ASP:N	2.79	0.45
9:9:57:ASN:CG	9:9:62:ARG:HG3	2.30	0.45
9:9:111:ALA:HB3	9:9:114:GLU:HG3	1.98	0.45
14:AE:388:ARG:NH2	14:AE:414:GLU:OE1	2.49	0.45
14:AE:1289:ASN:ND2	14:AE:1300:ALA:O	2.46	0.45
21:H:291:GLY:HA2	21:H:305:HIS:O	2.15	0.45
29:P:28:THR:HG21	29:P:87:LEU:CD1	2.46	0.45
38:Y:23:VAL:HB	38:Y:24:GLY:H	1.65	0.45
40:a:1906:G:H4'	40:a:1906:G:OP1	2.17	0.45
9:9:60:LEU:HB2	9:9:61:ARG:NH2	2.31	0.45
9:9:62:ARG:CG	9:9:62:ARG:NH2	2.73	0.45
10:A:48:C:N4	10:A:59:A:C5	2.84	0.45
14:AE:781:LYS:HD2	14:AE:933:ARG:HH12	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Z:23:ILE:HD12	39:Z:23:ILE:HA	1.77	0.45
53:n:57:LEU:HD22	53:n:89:VAL:CG2	2.46	0.45
9:9:106:PHE:O	9:9:106:PHE:CG	2.69	0.45
12:AB:161:SER:OG	12:AB:170:PRO:HA	2.16	0.45
10:B:48:C:C5	10:B:59:A:C8	3.05	0.45
17:D:868:C:H2'	17:D:869:G:O4'	2.16	0.45
17:D:1255:G:O2'	17:D:1258:G:N3	2.47	0.45
17:D:1340:A:H8	17:D:1340:A:O5'	2.00	0.45
21:H:19:ARG:O	21:H:72:LEU:HD13	2.16	0.45
40:a:645:C:H2'	40:a:647:G:C8	2.52	0.45
40:a:954:G:OP2	61:v:16:ARG:NH2	2.50	0.45
12:AB:147:VAL:O	12:AB:160:VAL:HG13	2.15	0.45
14:AE:640:GLY:N	14:AE:643:ASP:OD2	2.42	0.45
16:C:12:ARG:CZ	21:H:264:GLU:HA	2.46	0.45
20:G:114:LEU:HD13	20:G:144:LEU:CB	2.46	0.45
29:P:28:THR:HG21	29:P:87:LEU:HD12	1.99	0.45
46:g:18:CYS:HB2	46:g:40:CYS:HB3	1.96	0.45
58:s:30:THR:CG2	58:s:31:GLU:N	2.79	0.45
62:w:28:LEU:HD23	62:w:48:VAL:HG21	1.98	0.45
6:5:110:DA:N1	11:AA:536:GLY:O	2.50	0.45
8:7:14:U:H2'	8:7:15:G:C8	2.51	0.45
10:A:48:C:C5	10:A:59:A:C8	3.05	0.45
11:AA:557:ARG:NH2	11:AA:607:SER:O	2.50	0.45
15:AF:25:ARG:NH1	15:AF:61:ASN:OD1	2.49	0.45
17:D:17:U:H2'	17:D:18:C:C6	2.52	0.45
17:D:915:A:H8	17:D:915:A:O5'	2.00	0.45
17:D:1308:U:O5'	37:X:98:ARG:HG2	2.16	0.45
37:X:106:ALA:HB3	37:X:110:LYS:CD	2.47	0.45
38:Y:42:ASN:HA	38:Y:45:THR:HB	1.98	0.45
40:a:998:C:OP2	65:z:58:ARG:NH2	2.49	0.45
40:a:1082:U:H3	40:a:1086:A:N6	2.15	0.45
40:a:2070:A:H2'	40:a:2071:A:O4'	2.16	0.45
57:r:55:GLU:HA	57:r:58:LEU:HD12	1.99	0.45
9:9:31:ARG:HE	40:a:1054:A:C5'	2.18	0.45
10:A:32:C:O2'	26:M:86:GLN:CD	2.31	0.45
11:AA:674:ASP:OD2	11:AA:1070:HIS:ND1	2.50	0.45
13:AC:218:ARG:NH1	13:AD:231:PHE:O	2.50	0.45
14:AE:41:PRO:HB2	14:AE:270:ARG:HG3	1.99	0.45
14:AE:1341:ARG:NH1	14:AE:1343:GLU:OE2	2.49	0.45
17:D:526:C:OP2	31:R:88:LYS:HE3	2.15	0.45
17:D:1493:A:C8	17:D:1493:A:OP1	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:55:GLN:N	18:E:56:PRO:HD2	2.32	0.45
29:P:8:ILE:HD12	29:P:25:ILE:CD1	2.46	0.45
45:f:25:LEU:C	45:f:25:LEU:HD13	2.41	0.45
47:h:6:CYS:SG	47:h:13:ARG:NH1	2.89	0.45
63:x:18:LEU:HD23	63:x:25:ARG:HD2	1.99	0.45
9:9:9:GLN:CD	9:9:9:GLN:C	2.85	0.45
9:9:50:VAL:HG22	38:Y:119:ALA:C	2.41	0.45
9:9:67:THR:H	9:9:68:PRO:CD	2.29	0.45
10:B:58:A:C1'	10:B:60:U:C5	2.99	0.45
21:H:33:LYS:HA	21:H:34:ASP:HA	1.61	0.45
21:H:38:VAL:HG22	21:H:48:ILE:HD11	1.99	0.45
38:Y:95:ASP:OD2	38:Y:95:ASP:N	2.50	0.45
40:a:560:C:O2	65:z:48:ARG:NH1	2.41	0.45
40:a:2547:A:H2'	40:a:2548:U:C6	2.52	0.45
53:n:77:PHE:N	53:n:77:PHE:CD1	2.82	0.45
9:9:31:ARG:HD3	40:a:1054:A:H4'	1.96	0.45
11:AA:694:ARG:HH22	13:AC:80:GLU:HG3	1.82	0.45
14:AE:907:HIS:ND1	14:AE:908:ILE:O	2.48	0.45
10:B:25:C:C2'	10:B:26:G:H5'	2.47	0.45
17:D:109:A:C6	17:D:326:G:C6	3.05	0.45
17:D:198:G:OP2	17:D:198:G:C8	2.70	0.45
23:J:165:ARG:NH1	23:J:165:ARG:HB2	2.32	0.45
37:X:75:MET:HA	37:X:75:MET:HE3	1.99	0.45
38:Y:7:TYR:CD2	38:Y:7:TYR:O	2.70	0.45
9:9:58:THR:HB	9:9:82:ILE:H	1.80	0.44
10:A:34:C:OP1	26:M:84:THR:OG1	2.35	0.44
12:AB:128:PHE:CD2	12:AB:128:PHE:O	2.70	0.44
10:B:9:G:O2'	10:B:45:G:H2'	2.18	0.44
20:G:76:ALA:CB	20:G:210:VAL:HG11	2.47	0.44
21:H:294:VAL:HG21	21:H:330:VAL:HG21	1.99	0.44
23:J:197:GLU:HA	23:J:200:ILE:HD12	1.99	0.44
38:Y:37:PHE:CD2	38:Y:37:PHE:O	2.70	0.44
38:Y:140:GLU:OE1	38:Y:140:GLU:N	2.50	0.44
57:r:15:LEU:HD13	57:r:15:LEU:C	2.42	0.44
7:6:15:DC:N3	7:6:16:DC:C4	2.84	0.44
8:7:-12:U:C6	8:7:-12:U:OP2	2.70	0.44
9:9:16:SER:HB2	9:9:20:LYS:NZ	2.33	0.44
10:A:18:G:O2'	10:A:60:U:N3	2.48	0.44
10:A:57:A:O5'	10:A:58:A:P	2.76	0.44
11:AA:24:VAL:HG11	11:AA:704:MET:HE1	1.99	0.44
12:AB:164:ILE:HG22	12:AB:169:THR:OG1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:167:ARG:NH2	29:P:99:GLN:OE1	2.49	0.44
12:AB:167:ARG:NH1	29:P:99:GLN:HA	2.32	0.44
37:X:106:ALA:HB3	37:X:110:LYS:HD2	1.98	0.44
38:Y:37:PHE:CE1	38:Y:56:VAL:HG11	2.51	0.44
40:a:930:G:H1'	45:f:25:LEU:HD11	1.98	0.44
40:a:1927:A:C8	40:a:1927:A:O5'	2.71	0.44
9:9:34:THR:HG22	9:9:38:MET:CE	2.46	0.44
9:9:139:LEU:CD2	39:Z:11:VAL:HG22	2.47	0.44
10:A:49:G:C2'	10:A:50:U:H5'	2.47	0.44
11:AA:560:PRO:HB2	14:AE:776:THR:HG21	2.00	0.44
11:AA:998:LEU:HG	11:AA:1011:LEU:HB3	1.99	0.44
11:AA:1002:LEU:HD21	11:AA:1007:LYS:HB2	1.98	0.44
12:AB:140:PRO:HB3	29:P:81:GLU:O	2.17	0.44
12:AB:173:LEU:HD13	12:AB:178:VAL:CG1	2.47	0.44
13:AD:29:GLU:HB3	13:AD:200:LYS:HG3	1.99	0.44
33:T:21:ASP:OD1	33:T:22:THR:N	2.49	0.44
37:X:96:PRO:HG2	37:X:102:THR:HG23	1.97	0.44
9:9:127:ALA:O	9:9:130:PRO:HG2	2.16	0.44
10:A:6:G:O2'	10:A:7:G:C5'	2.64	0.44
11:AA:813:GLU:HB2	14:AE:461:PHE:HD2	1.83	0.44
11:AA:829:THR:HG23	11:AA:1059:ARG:HG2	1.99	0.44
13:AD:83:LEU:HD11	14:AE:526:VAL:HB	1.99	0.44
14:AE:68:TYR:CA	14:AE:92:VAL:HG23	2.45	0.44
14:AE:774:ILE:HA	14:AE:777:HIS:HD2	1.82	0.44
10:B:34:C:O5'	10:B:34:C:C6	2.70	0.44
10:B:60:U:OP2	10:B:61:C:N4	2.45	0.44
17:D:337:G:H2'	17:D:338:A:C8	2.52	0.44
17:D:376:G:C2	17:D:389:A:C2	3.05	0.44
21:H:332:VAL:HG11	21:H:335:ILE:CG1	2.38	0.44
9:9:50:VAL:CG1	38:Y:119:ALA:CB	2.88	0.44
10:A:22:G:O2'	10:A:23:C:O5'	2.36	0.44
13:AD:68:TYR:HE1	13:AD:79:LEU:HD13	1.82	0.44
17:D:1397:C:O5'	17:D:1397:C:C6	2.70	0.44
38:Y:34:ILE:HG22	38:Y:34:ILE:O	2.18	0.44
40:a:1007:C:OP1	58:s:37:ARG:NH2	2.50	0.44
40:a:1720:U:H2'	40:a:1721:G:O4'	2.16	0.44
9:9:71:CYS:CA	9:9:117:LEU:HD13	2.48	0.44
11:AA:1246:ARG:HH11	11:AA:1266:GLY:HA2	1.82	0.44
14:AE:848:VAL:HB	14:AE:858:VAL:HG22	1.98	0.44
10:B:26:G:N2	10:B:45:G:N2	2.66	0.44
10:B:49:G:C2'	10:B:50:U:H5'	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:57:A:O5'	10:B:58:A:P	2.76	0.44
22:I:155:GLY:HA2	22:I:163:ALA:HB1	1.99	0.44
8:7:-9:U:C3'	8:7:-9:U:C6	3.00	0.44
9:9:106:PHE:O	9:9:106:PHE:CD2	2.70	0.44
10:A:9:G:O2'	10:A:45:G:H2'	2.18	0.44
12:AB:134:VAL:HG22	12:AB:160:VAL:HG11	2.00	0.44
12:AB:161:SER:CB	12:AB:170:PRO:HA	2.48	0.44
14:AE:288:PRO:HG2	14:AE:291:ILE:HD12	2.00	0.44
14:AE:319:SER:HA	14:AE:320:ASN:HA	1.74	0.44
14:AE:708:ASN:OD1	14:AE:708:ASN:N	2.50	0.44
10:B:1:C:C5	10:B:2:G:N7	2.86	0.44
10:B:34:C:C5	10:B:34:C:OP1	2.70	0.44
10:B:37:A:N3	10:B:37:A:H5''	2.32	0.44
10:B:49:G:O5'	10:B:49:G:C8	2.71	0.44
21:H:136:VAL:HA	21:H:168:VAL:O	2.18	0.44
21:H:290:TYR:O	21:H:305:HIS:C	2.56	0.44
38:Y:71:LYS:HB3	38:Y:72:THR:H	1.58	0.44
40:a:1589:U:C2	40:a:1590:A:C8	3.06	0.44
40:a:1925:C:C5	40:a:1925:C:OP2	2.70	0.44
40:a:2822:G:OP1	49:j:164:GLN:NE2	2.47	0.44
53:n:17:MET:HE2	53:n:25:VAL:HA	1.99	0.44
7:6:15:DC:C4	7:6:16:DC:C5	3.05	0.44
9:9:72:LEU:HD22	9:9:72:LEU:C	2.42	0.44
10:A:22:G:H2'	10:A:23:C:C5	2.52	0.44
10:A:58:A:HO2'	10:A:60:U:H5	1.62	0.44
10:A:76:A:C2	54:o:31:HIS:NE2	2.85	0.44
13:AD:182:ARG:HD2	14:AE:581:MET:HE1	1.98	0.44
14:AE:975:ILE:HG22	14:AE:977:SER:H	1.83	0.44
17:D:397:A:H3'	17:D:397:A:N3	2.33	0.44
20:G:35:ARG:CG	21:H:10:GLU:OE2	2.63	0.44
20:G:206:ALA:O	20:G:210:VAL:HG23	2.18	0.44
21:H:109:THR:C	21:H:153:GLU:HA	2.43	0.44
40:a:57:C:H2'	40:a:58:G:O4'	2.18	0.44
40:a:1386:C:H2'	40:a:1387:A:C8	2.53	0.44
40:a:2133:G:O2'	40:a:2157:G:N2	2.51	0.44
10:A:1:C:C5	10:A:2:G:N7	2.86	0.44
10:A:26:G:N2	10:A:45:G:N2	2.66	0.44
10:A:56:C:OP1	40:a:2168:G:C4	2.71	0.44
13:AD:192:VAL:HG12	13:AD:193:GLU:H	1.83	0.44
14:AE:79:LYS:HG3	14:AE:81:ARG:HH12	1.83	0.44
15:AF:58:LEU:HD12	15:AF:59:ILE:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:5:G:C2'	10:B:6:G:C5'	2.93	0.44
10:B:22:G:O2'	10:B:23:C:O5'	2.36	0.44
16:C:12:ARG:HD3	16:C:16:GLU:OE1	2.18	0.44
17:D:13:U:C2	17:D:915:A:C5	3.06	0.44
17:D:1417:G:C6	17:D:1482:G:C6	3.06	0.44
40:a:340:A:O2'	51:l:162:ARG:NH1	2.50	0.44
40:a:2252:G:O2'	40:a:2253:G:H5'	2.18	0.44
43:d:48:U:H2'	43:d:49:C:C6	2.52	0.44
20:G:208:ARG:HH12	21:H:29:VAL:HG11	1.82	0.43
22:I:50:ALA:HB2	22:I:75:ILE:HD12	2.00	0.43
24:K:111:MET:CE	24:K:125:ALA:HB1	2.39	0.43
37:X:23:TYR:CD2	37:X:69:LEU:HD23	2.53	0.43
38:Y:123:ALA:HA	38:Y:126:ARG:HG3	2.00	0.43
8:7:11:U:H3'	8:7:11:U:C6	2.53	0.43
9:9:106:PHE:CD2	9:9:106:PHE:C	2.95	0.43
11:AA:444:ASP:OD1	11:AA:444:ASP:N	2.51	0.43
17:D:324:G:N2	17:D:327:A:C8	2.86	0.43
19:F:21:ARG:HH22	21:H:341:ARG:HD2	1.82	0.43
21:H:123:GLU:CA	21:H:128:ARG:HA	2.43	0.43
28:O:80:ARG:O	28:O:84:THR:HG23	2.17	0.43
40:a:74:A:N7	40:a:88:G:C5	2.86	0.43
40:a:813:U:H2'	40:a:814:C:C6	2.53	0.43
61:v:35:ALA:HB2	61:v:102:LEU:HD11	2.00	0.43
8:7:18:A:O3'	11:AA:688:GLN:NE2	2.51	0.43
11:AA:375:PRO:HD3	12:AB:98:ASP:HA	1.99	0.43
11:AA:646:SER:OG	11:AA:647:ARG:N	2.52	0.43
13:AD:78:ILE:HA	13:AD:81:ILE:HG22	2.00	0.43
13:AD:212:ASP:OD1	13:AD:212:ASP:N	2.48	0.43
14:AE:362:ARG:H	14:AE:365:GLN:HE21	1.66	0.43
14:AE:859:PRO:HD2	14:AE:862:THR:HG21	2.01	0.43
17:D:1499:A:O2'	17:D:1500:A:C5'	2.67	0.43
28:O:84:THR:HG21	28:O:103:PHE:CB	2.45	0.43
8:7:-14:U:H6	8:7:-14:U:H3'	1.84	0.43
9:9:18:VAL:HA	9:9:86:MET:CE	2.44	0.43
14:AE:658:GLU:HA	14:AE:661:VAL:HG22	2.00	0.43
16:C:44:ILE:HG21	21:H:339:ARG:HA	2.01	0.43
53:n:29:PRO:HB2	53:n:169:LEU:HD22	1.99	0.43
58:s:73:VAL:HG11	58:s:75:TYR:CZ	2.53	0.43
10:A:36:U:H2'	10:A:37:A:O4'	2.19	0.43
11:AA:1313:HIS:CD2	15:AF:31:GLN:HE22	2.37	0.43
12:AB:122:PRO:CB	12:AB:124:PRO:HD3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:1036:ARG:HE	14:AE:1081:VAL:HG21	1.83	0.43
10:B:58:A:HO2'	10:B:60:U:H5	1.58	0.43
17:D:684:U:H2'	17:D:685:G:O4'	2.18	0.43
20:G:114:LEU:HD13	20:G:144:LEU:HB3	1.99	0.43
40:a:39:G:H1'	51:l:43:THR:HG21	1.99	0.43
10:A:18:G:N3	10:A:58:A:C5	2.87	0.43
12:AB:165:PHE:HZ	29:P:87:LEU:HB2	1.71	0.43
10:B:46:G:O2'	10:B:47:U:H5''	2.19	0.43
17:D:384:G:H2'	17:D:385:C:C6	2.54	0.43
17:D:1371:G:O3'	28:O:71:GLY:HA3	2.19	0.43
21:H:76:GLU:HA	21:H:76:GLU:OE2	2.19	0.43
38:Y:121:ILE:HA	38:Y:124:MET:SD	2.58	0.43
40:a:1020:A:C2	40:a:1141:U:C2	3.07	0.43
40:a:1142:A:H2'	40:a:1142:A:N3	2.34	0.43
40:a:1385:A:O2'	40:a:1396:U:O2	2.35	0.43
65:z:76:TYR:OH	65:z:92:ARG:NH1	2.51	0.43
4:3:12:ILE:CG2	4:3:80:ALA:HB2	2.49	0.43
10:B:58:A:OP2	10:B:58:A:H8	2.02	0.43
21:H:280:LEU:HB2	21:H:330:VAL:O	2.19	0.43
24:K:156:LYS:HG2	27:N:71:VAL:HG13	2.00	0.43
38:Y:64:ARG:HE	38:Y:64:ARG:HB2	1.51	0.43
40:a:2395:C:H2'	40:a:2396:G:O4'	2.18	0.43
52:m:12:ARG:HG3	52:m:44:VAL:HG11	2.00	0.43
10:A:25:C:C2'	10:A:26:G:H5'	2.47	0.43
11:AA:1244:HIS:NE2	11:AA:1266:GLY:O	2.44	0.43
14:AE:117:LEU:HG	14:AE:118:LYS:HG3	2.00	0.43
14:AE:450:HIS:HA	14:AE:451:PRO:HD3	1.92	0.43
14:AE:694:SER:OG	14:AE:738:ARG:NE	2.52	0.43
17:D:976:G:C8	17:D:1358:U:O2	2.71	0.43
21:H:61:GLU:HG2	21:H:62:ILE:HG23	2.00	0.43
30:Q:88:GLY:H	30:Q:114:THR:HG22	1.84	0.43
40:a:973:A:O4'	40:a:1188:U:C6	2.72	0.43
40:a:1047:G:N2	40:a:1110:G:O2'	2.50	0.43
40:a:1932:A:H2'	40:a:1933:G:O4'	2.19	0.43
42:c:37:ARG:HG2	42:c:48:THR:HG23	2.00	0.43
59:t:76:VAL:HG12	64:y:73:VAL:HB	2.00	0.43
62:w:49:GLU:HB2	62:w:50:PRO:HD3	2.00	0.43
9:9:72:LEU:HD22	9:9:72:LEU:O	2.19	0.43
10:A:46:G:O2'	10:A:47:U:H5''	2.19	0.43
12:AB:150:GLU:HB3	12:AB:159:LYS:HD3	2.00	0.43
10:B:18:G:N3	10:B:58:A:C5	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:53:G:C2	10:B:54:U:C5	3.07	0.43
16:C:12:ARG:O	16:C:16:GLU:HG3	2.19	0.43
17:D:1126:U:OP1	29:P:7:ARG:NH2	2.51	0.43
17:D:1333:A:H2'	17:D:1334:G:O4'	2.19	0.43
17:D:1515:G:H2'	17:D:1516:G:C8	2.52	0.43
23:J:48:LEU:HD13	23:J:48:LEU:N	2.33	0.43
40:a:68:G:N2	40:a:74:A:OP2	2.49	0.43
44:e:59:GLU:O	44:e:63:ALA:HB3	2.18	0.43
47:h:37:ASN:HB2	47:h:62:TYR:HB2	2.01	0.43
10:A:49:G:O5'	10:A:49:G:C8	2.71	0.43
11:AA:300:ASP:OD1	11:AA:313:ALA:N	2.51	0.43
11:AA:811:ASN:ND2	11:AA:1098:LEU:O	2.51	0.43
11:AA:1278:LEU:HD23	11:AA:1278:LEU:HA	1.86	0.43
12:AB:135:ARG:O	12:AB:178:VAL:CA	2.67	0.43
10:B:22:G:H2'	10:B:23:C:C5	2.52	0.43
20:G:16:PHE:CG	21:H:43:LYS:HA	2.53	0.43
20:G:47:VAL:N	20:G:48:PRO:HD2	2.34	0.43
21:H:152:LEU:CB	21:H:171:ARG:H	2.32	0.43
24:K:150:PRO:O	24:K:153:VAL:HG22	2.19	0.43
28:O:55:VAL:O	28:O:57:MET:N	2.52	0.43
40:a:879:G:H2'	40:a:880:G:O4'	2.19	0.43
40:a:1095:A:H2'	40:a:1096:A:C8	2.54	0.43
40:a:1363:C:O2'	40:a:1809:A:N3	2.46	0.43
40:a:2469:A:N6	40:a:2481:G:O2'	2.52	0.43
6:5:98:DA:H2'	6:5:99:DT:H72	2.01	0.42
7:6:12:DC:O5'	7:6:12:DC:H6	2.01	0.42
11:AA:557:ARG:HB3	11:AA:587:LEU:HD13	2.00	0.42
12:AB:132:GLU:OE2	12:AB:180:LYS:HG3	2.19	0.42
12:AB:158:LEU:HD11	12:AB:175:PHE:CD1	2.54	0.42
40:a:1394:U:C4	40:a:1395:A:C6	3.07	0.42
40:a:2683:C:O2	59:t:70:ARG:NH2	2.52	0.42
48:i:43:ILE:HG22	48:i:49:TYR:HB2	2.01	0.42
58:s:32:LEU:HD23	58:s:54:ILE:HD13	2.01	0.42
58:s:114:LEU:HD12	58:s:114:LEU:HA	1.87	0.42
9:9:52:MET:HE1	9:9:85:SER:HB2	2.00	0.42
13:AD:31:LEU:HD21	13:AD:39:LEU:HD12	2.00	0.42
38:Y:41:PHE:HA	38:Y:68:PHE:CE2	2.55	0.42
49:j:172:VAL:HG11	49:j:175:LEU:HD21	2.01	0.42
59:t:24:VAL:HG13	59:t:33:ALA:HB2	2.00	0.42
6:5:116:DG:C6	6:5:117:DA:C6	3.06	0.42
10:A:26:G:H1	10:A:44:A:N6	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:469:VAL:HA	11:AA:472:GLU:HG2	2.02	0.42
11:AA:1275:VAL:HG13	11:AA:1287:LEU:HD11	2.01	0.42
12:AB:136:VAL:HG22	12:AB:178:VAL:HG12	2.01	0.42
14:AE:134:ASP:HB3	14:AE:159:ILE:HG21	2.01	0.42
10:B:22:G:HO2'	10:B:23:C:P	2.42	0.42
17:D:842:U:H3'	17:D:843:U:C5'	2.48	0.42
21:H:274:TYR:HD1	21:H:335:ILE:HD12	1.85	0.42
21:H:335:ILE:HG12	21:H:342:ILE:HG23	2.00	0.42
40:a:67:U:C4	40:a:74:A:C6	3.04	0.42
40:a:214:G:N2	40:a:216:A:N3	2.66	0.42
40:a:2252:G:H2'	40:a:2253:G:H8	1.83	0.42
40:a:2511:U:O4	40:a:2575:C:N3	2.52	0.42
63:x:99:TYR:OH	63:x:111:ARG:NH1	2.53	0.42
4:3:39:ILE:HG22	4:3:40:ASN:N	2.34	0.42
11:AA:478:ARG:HD2	11:AA:492:MET:HA	2.02	0.42
12:AB:175:PHE:O	12:AB:178:VAL:O	2.38	0.42
14:AE:412:LEU:HA	14:AE:415:VAL:HG22	2.01	0.42
17:D:429:U:O2	17:D:430:A:C8	2.72	0.42
17:D:537:G:OP1	31:R:110:ARG:NH2	2.48	0.42
17:D:622:A:C8	17:D:623:C:C6	3.08	0.42
21:H:119:GLY:O	21:H:120:PHE:C	2.62	0.42
38:Y:19:PRO:HG2	38:Y:24:GLY:N	2.32	0.42
38:Y:58:ILE:N	38:Y:58:ILE:CD1	2.76	0.42
40:a:705:A:O4'	47:h:9:THR:HG21	2.18	0.42
40:a:819:A:C4	40:a:1189:A:C2	3.07	0.42
40:a:2803:G:H2'	40:a:2804:U:C5	2.55	0.42
65:z:65:ILE:CD1	65:z:92:ARG:HB2	2.49	0.42
8:7:13:G:H5''	8:7:13:G:H8	1.84	0.42
13:AD:46:ILE:HD11	13:AD:224:LEU:HD13	2.02	0.42
14:AE:708:ASN:HA	14:AE:713:GLU:HA	2.00	0.42
10:B:18:G:O2'	10:B:60:U:N3	2.48	0.42
17:D:197:A:C5	17:D:221:C:H4'	2.53	0.42
24:K:136:VAL:O	24:K:140:THR:HG23	2.20	0.42
34:U:6:LEU:HG	34:U:17:TYR:HB3	2.00	0.42
40:a:48:G:O2'	40:a:118:A:N1	2.51	0.42
40:a:244:A:OP2	54:o:8:ARG:NH2	2.50	0.42
40:a:299:A:N1	40:a:322:A:O2'	2.47	0.42
40:a:1925:C:OP2	40:a:1925:C:C6	2.73	0.42
40:a:2615:U:C2	48:i:4:GLN:HA	2.55	0.42
40:a:2756:U:C4	40:a:2759:G:O6	2.72	0.42
59:t:107:LEU:HD21	59:t:115:ILE:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:98:DA:C2'	6:5:99:DT:C7	2.96	0.42
10:A:58:A:OP2	10:A:58:A:H8	2.02	0.42
11:AA:125:GLY:H	11:AA:495:ALA:HB1	1.84	0.42
11:AA:741:MET:SD	11:AA:974:ARG:NH2	2.93	0.42
11:AA:861:ALA:HB1	11:AA:882:ILE:HD13	2.01	0.42
14:AE:289:ASP:HA	14:AE:292:VAL:HG22	2.01	0.42
29:P:57:VAL:O	29:P:58:ASN:ND2	2.53	0.42
40:a:320:A:H2'	51:l:131:THR:HG21	2.01	0.42
40:a:567:U:OP2	60:u:29:LYS:NZ	2.53	0.42
40:a:1921:G:C2'	40:a:1922:G:H5'	2.49	0.42
10:A:53:G:C2	10:A:54:U:C5	3.07	0.42
11:AA:11:ILE:HG22	11:AA:1172:LEU:HD11	1.99	0.42
11:AA:22:LEU:HB3	11:AA:655:VAL:HG11	2.01	0.42
12:AB:7:LYS:HG2	12:AB:74:VAL:HG13	2.00	0.42
14:AE:513:MET:HE1	14:AE:579:LEU:HD13	2.01	0.42
10:B:68:C:H3'	10:B:69:C:H5''	1.96	0.42
17:D:502:A:H2'	17:D:503:C:O4'	2.20	0.42
24:K:153:VAL:HG23	24:K:164:ILE:HD13	2.00	0.42
38:Y:72:THR:OG1	38:Y:73:PRO:CD	2.62	0.42
40:a:126:A:O5'	52:m:19:ARG:HG3	2.19	0.42
40:a:984:A:N3	40:a:984:A:H2'	2.35	0.42
40:a:2602:A:H5''	40:a:2603:G:C5'	2.49	0.42
3:2:1:MET:N	40:a:142:A:O2'	2.47	0.42
9:9:25:ALA:HA	9:9:96:PHE:HE1	1.85	0.42
11:AA:849:GLU:HB2	11:AA:887:VAL:HG23	2.02	0.42
14:AE:211:GLU:HA	14:AE:214:ARG:HD2	2.01	0.42
10:B:26:G:H1	10:B:44:A:N6	2.18	0.42
21:H:119:GLY:CA	21:H:132:PRO:C	2.92	0.42
32:S:41:ARG:O	32:S:45:VAL:HG12	2.20	0.42
39:Z:18:ASP:HB3	39:Z:22:LEU:HD12	2.00	0.42
40:a:126:A:OP1	52:m:45:SER:OG	2.38	0.42
51:l:48:THR:HG23	51:l:86:ALA:HB3	2.02	0.42
51:l:134:LEU:HB2	51:l:160:ALA:HB1	2.02	0.42
55:p:25:THR:HG22	55:p:34:THR:HG23	2.02	0.42
59:t:38:ILE:HD11	59:t:112:PHE:CZ	2.54	0.42
11:AA:800:MET:HE3	11:AA:800:MET:HB2	1.69	0.42
11:AA:1157:GLN:HG3	11:AA:1159:VAL:HG13	2.00	0.42
12:AB:148:VAL:CG2	12:AB:151:VAL:HG22	2.50	0.42
13:AD:76:GLU:HB3	13:AD:80:GLU:HB3	2.01	0.42
14:AE:224:LEU:HA	14:AE:224:LEU:HD23	1.83	0.42
20:G:208:ARG:NH1	21:H:29:VAL:HG11	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:302:GLY:HA3	21:H:344:LEU:HD13	2.00	0.42
28:O:28:ILE:HD12	28:O:28:ILE:N	2.35	0.42
9:9:8:LYS:HZ1	40:a:1046:A:H61	1.68	0.42
11:AA:27:LEU:O	11:AA:528:ARG:NH1	2.43	0.42
17:D:826:C:O2	27:N:16:ASN:ND2	2.52	0.42
17:D:1329:A:OP1	37:X:28:THR:CA	2.67	0.42
40:a:1028:A:N6	40:a:1125:G:H2'	2.34	0.42
40:a:1250:G:OP2	60:u:21:ARG:NH2	2.53	0.42
56:q:3:VAL:HA	56:q:36:ARG:O	2.19	0.42
8:7:-8:U:C6	8:7:-8:U:C3'	3.03	0.41
9:9:67:THR:N	9:9:68:PRO:HD3	2.34	0.41
11:AA:741:MET:HE3	11:AA:974:ARG:HH12	1.85	0.41
12:AB:136:VAL:HG11	12:AB:141:PHE:CB	2.48	0.41
14:AE:800:LEU:HB3	14:AE:920:ALA:HB1	2.02	0.41
17:D:216:U:H2'	17:D:217:C:C6	2.55	0.41
17:D:548:G:C6	17:D:549:C:C4	3.08	0.41
17:D:791:G:N2	17:D:1497:G:O3'	2.53	0.41
21:H:292:CYS:SG	21:H:304:VAL:HB	2.60	0.41
37:X:17:ILE:O	37:X:20:THR:OG1	2.22	0.41
40:a:631:A:N3	40:a:2415:G:O2'	2.48	0.41
40:a:948:C:H1'	40:a:984:A:C8	2.55	0.41
47:h:240:PHE:CD2	47:h:240:PHE:O	2.73	0.41
3:2:46:ALA:O	3:2:50:LEU:HB2	2.20	0.41
7:6:27:DG:H1'	7:6:28:DA:C5	2.55	0.41
11:AA:755:LYS:HA	11:AA:755:LYS:HD2	1.86	0.41
14:AE:438:GLU:HG3	14:AE:485:MET:HE1	2.03	0.41
17:D:37:U:O2	17:D:548:G:N2	2.53	0.41
17:D:421:U:O2	17:D:421:U:O4'	2.37	0.41
21:H:110:GLY:H	21:H:153:GLU:N	2.17	0.41
40:a:36:G:N3	40:a:450:G:O2'	2.53	0.41
40:a:1406:U:H3	40:a:1596:A:H2	1.59	0.41
40:a:2273:A:H2'	40:a:2274:A:C8	2.55	0.41
51:l:145:ASP:HA	51:l:166:LYS:HB3	2.02	0.41
59:t:113:MET:HE3	59:t:116:ILE:HD11	2.01	0.41
9:9:48:ALA:HB3	9:9:51:TYR:HD2	1.86	0.41
9:9:80:THR:O	40:a:1108:U:OP1	2.38	0.41
10:A:56:C:C2	40:a:2112:G:C5	3.07	0.41
11:AA:1088:ASP:OD1	11:AA:1088:ASP:N	2.51	0.41
17:D:1208:C:H2'	17:D:1209:C:H6	1.85	0.41
17:D:1323:G:H2'	17:D:1324:A:C8	2.55	0.41
19:F:67:ARG:HD3	19:F:67:ARG:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:9:GLY:HA3	32:S:89:MET:HE3	2.01	0.41
40:a:1067:A:O2'	40:a:1068:G:O4'	2.31	0.41
40:a:1570:A:H2'	40:a:1571:A:C8	2.55	0.41
40:a:2602:A:H5''	40:a:2603:G:H5''	2.03	0.41
47:h:119:GLY:O	47:h:130:LEU:HB3	2.20	0.41
53:n:123:ASP:OD1	53:n:123:ASP:C	2.62	0.41
9:9:61:ARG:C	9:9:65:GLU:HB2	2.45	0.41
10:A:56:C:OP1	40:a:2168:G:N3	2.53	0.41
11:AA:133:ASN:O	11:AA:527:LYS:NZ	2.42	0.41
11:AA:148:GLN:NE2	11:AA:535:PRO:O	2.40	0.41
12:AB:151:VAL:O	12:AB:152:ASP:OD1	2.39	0.41
14:AE:97:VAL:HG12	14:AE:101:ARG:HG3	2.02	0.41
16:C:12:ARG:NH2	21:H:268:VAL:CG2	2.71	0.41
21:H:155:LYS:O	21:H:169:SER:CB	2.69	0.41
40:a:197:A:N6	40:a:2430:A:H2'	2.36	0.41
40:a:851:C:H2'	40:a:852:U:C6	2.55	0.41
40:a:1082:U:N3	40:a:1086:A:C6	2.87	0.41
40:a:1169:A:H5''	40:a:1169:A:N3	2.36	0.41
40:a:1406:U:C2'	40:a:1407:G:OP2	2.69	0.41
52:m:12:ARG:CG	52:m:44:VAL:HG11	2.50	0.41
57:r:9:VAL:HG11	57:r:12:LEU:HD21	2.03	0.41
62:w:67:PHE:O	62:w:71:ARG:HG2	2.21	0.41
65:z:66:ASN:OD1	65:z:70:ARG:NE	2.54	0.41
9:9:8:LYS:NZ	40:a:1046:A:N6	2.69	0.41
11:AA:144:VAL:HG23	11:AA:515:MET:HB2	2.02	0.41
11:AA:616:ILE:HG13	11:AA:652:TYR:HB2	2.02	0.41
11:AA:699:LEU:HG	11:AA:799:ASN:HD22	1.85	0.41
12:AB:136:VAL:HB	12:AB:141:PHE:O	2.20	0.41
14:AE:138:VAL:HG21	14:AE:145:VAL:HB	2.03	0.41
14:AE:975:ILE:HD11	14:AE:1003:LEU:HG	2.02	0.41
10:B:8:U:O2'	10:B:47:U:C4	2.72	0.41
19:F:32:VAL:HG11	30:Q:89:PRO:HG3	2.01	0.41
27:N:11:LEU:HD22	27:N:75:ILE:HD11	2.03	0.41
38:Y:14:ALA:HB3	38:Y:50:LYS:HA	2.03	0.41
38:Y:102:ARG:HD2	38:Y:103:ALA:N	2.36	0.41
38:Y:116:MET:CB	38:Y:124:MET:HG2	2.46	0.41
40:a:476:G:H4'	40:a:502:A:N1	2.35	0.41
40:a:742:A:N1	40:a:755:U:O4	2.53	0.41
40:a:829:A:N7	40:a:2247:A:O2'	2.49	0.41
40:a:1421:G:C2	40:a:1422:G:C8	3.09	0.41
40:a:2298:A:C5	40:a:2321:U:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:p:52:PHE:CZ	55:p:72:LEU:HD22	2.56	0.41
10:A:15:G:H1	10:A:20:U:H3	1.68	0.41
10:A:26:G:C2	10:A:45:G:N2	2.89	0.41
11:AA:590:PRO:HB2	11:AA:655:VAL:HG21	2.01	0.41
12:AB:165:PHE:CE1	29:P:88:MET:HA	2.49	0.41
14:AE:836:ARG:HG3	14:AE:869:CYS:HB3	2.02	0.41
16:C:14:THR:CG2	16:C:48:ARG:HE	2.33	0.41
39:Z:26:MET:HE2	39:Z:26:MET:HB2	1.71	0.41
40:a:1365:A:O5'	42:c:28:ARG:NH2	2.52	0.41
40:a:2311:A:C2	53:n:85:ILE:HD11	2.55	0.41
62:w:29:VAL:HG11	62:w:75:ILE:HG23	2.03	0.41
2:1:75:PHE:CZ	2:1:104:THR:HG21	2.56	0.41
8:7:-7:U:OP1	22:l:129:MET:HE1	2.21	0.41
8:7:13:G:H8	8:7:13:G:C5'	2.33	0.41
11:AA:22:LEU:HD22	11:AA:603:ILE:HG21	2.02	0.41
11:AA:805:MET:HE3	11:AA:805:MET:HB2	1.86	0.41
13:AD:205:MET:HE1	13:AD:217:ILE:HG13	2.03	0.41
14:AE:367:GLY:HA3	14:AE:448:GLN:HB2	2.03	0.41
21:H:342:ILE:HG22	21:H:344:LEU:HD12	2.01	0.41
37:X:16:VAL:HG13	37:X:34:LEU:CD1	2.51	0.41
38:Y:78:LEU:HD22	38:Y:78:LEU:HA	1.92	0.41
39:Z:1:SER:HB3	39:Z:2:ILE:H	1.61	0.41
40:a:1839:G:C4	40:a:1927:A:C5	3.08	0.41
57:r:57:LYS:O	57:r:61:VAL:HG13	2.21	0.41
9:9:72:LEU:C	9:9:72:LEU:CD2	2.94	0.41
11:AA:979:LEU:HD11	11:AA:1011:LEU:HD11	2.03	0.41
11:AA:1069:ARG:NH2	11:AA:1114:GLU:OE2	2.44	0.41
13:AC:42:ALA:HB1	13:AC:224:LEU:HD11	2.03	0.41
14:AE:1272:SER:HB2	14:AE:1292:LEU:HD11	2.02	0.41
10:B:26:G:C2	10:B:45:G:N2	2.88	0.41
17:D:977:A:H1'	17:D:982:U:O4	2.20	0.41
17:D:1526:G:P	19:F:42:THR:HG23	2.61	0.41
37:X:4:ILE:CG1	37:X:9:ILE:HD12	2.50	0.41
40:a:17:G:H2'	40:a:18:U:C6	2.56	0.41
40:a:2006:C:O2'	40:a:2823:A:N3	2.47	0.41
40:a:2294:G:OP1	63:x:10:ARG:HD3	2.21	0.41
47:h:175:ARG:NH1	47:h:181:MET:HE2	2.36	0.41
60:u:109:LYS:HG2	60:u:126:ARG:HB2	2.02	0.41
2:1:92:ARG:NE	2:1:94:ASP:OD1	2.53	0.41
10:A:34:C:H41	26:M:83:SER:HA	1.86	0.41
11:AA:836:LEU:HD21	11:AA:921:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:53:ARG:HA	14:AE:54:ASP:HA	1.59	0.41
14:AE:609:TYR:HD2	14:AE:610:ARG:HD2	1.85	0.41
10:B:15:G:N2	10:B:20:U:C2	2.88	0.41
10:B:46:G:H2'	10:B:47:U:OP2	2.21	0.41
17:D:218:U:H2'	17:D:219:U:O4'	2.21	0.41
17:D:860:A:H2'	17:D:861:G:O4'	2.20	0.41
17:D:972:C:O2'	29:P:57:VAL:HG21	2.18	0.41
20:G:187:VAL:HG21	20:G:199:VAL:HG23	2.02	0.41
23:J:100:ASN:OD1	23:J:111:ARG:NH1	2.54	0.41
38:Y:10:LEU:HD13	38:Y:10:LEU:HA	1.79	0.41
38:Y:35:MET:O	38:Y:35:MET:SD	2.79	0.41
38:Y:133:ARG:HG3	38:Y:136:GLY:HA2	2.03	0.41
40:a:548:G:H3'	40:a:549:G:O4'	2.20	0.41
40:a:1095:A:O2'	40:a:1096:A:O4'	2.33	0.41
51:l:188:MET:HE2	51:l:193:VAL:HA	2.03	0.41
9:9:118:ILE:H	9:9:119:PRO:HD2	1.85	0.41
11:AA:803:ALA:HB2	11:AA:1094:VAL:HG21	2.03	0.41
11:AA:987:GLU:HG2	11:AA:991:LYS:HE3	2.03	0.41
11:AA:998:LEU:HD21	11:AA:1015:ALA:HB2	2.02	0.41
12:AB:148:VAL:HB	12:AB:160:VAL:CG2	2.51	0.41
17:D:429:U:O2	17:D:430:A:N7	2.53	0.41
17:D:580:C:H2'	17:D:581:G:O4'	2.21	0.41
17:D:1330:U:OP2	37:X:26:GLY:HA3	2.21	0.41
24:K:154:ALA:HA	24:K:164:ILE:HD11	2.03	0.41
26:M:22:LEU:HD13	26:M:97:ASN:ND2	2.35	0.41
33:T:43:PHE:CE2	33:T:56:LEU:HD22	2.56	0.41
40:a:637:A:N1	40:a:651:G:O2'	2.51	0.41
40:a:753:A:C5	40:a:754:U:C5	3.09	0.41
40:a:1548:A:H2'	40:a:1549:A:C8	2.55	0.41
40:a:2788:C:H2'	40:a:2789:C:C6	2.55	0.41
61:v:73:ILE:HG21	61:v:91:TYR:CZ	2.55	0.41
9:9:73:LYS:CB	9:9:117:LEU:HD11	2.51	0.40
11:AA:657:THR:HG21	11:AA:1188:ASP:HB2	2.03	0.40
12:AB:132:GLU:OE2	12:AB:180:LYS:HE3	2.20	0.40
14:AE:79:LYS:HA	14:AE:81:ARG:HH22	1.74	0.40
14:AE:1155:ILE:HG13	14:AE:1210:ILE:HB	2.02	0.40
10:B:8:U:OP2	10:B:8:U:H6	2.04	0.40
40:a:207:A:H2'	40:a:208:C:O4'	2.21	0.40
40:a:1082:U:C4	40:a:1086:A:N6	2.88	0.40
45:f:27:LEU:HD23	45:f:27:LEU:HA	1.94	0.40
47:h:76:ALA:HB2	47:h:96:TYR:CE1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:n:171:ALA:O	53:n:174:ASP:N	2.53	0.40
9:9:71:CYS:SG	9:9:117:LEU:HB2	2.60	0.40
9:9:118:ILE:CB	9:9:119:PRO:HD3	2.49	0.40
10:A:15:G:N2	10:A:20:U:H3	2.20	0.40
10:A:46:G:H2'	10:A:47:U:OP2	2.21	0.40
12:AB:171:VAL:HG22	12:AB:172:GLU:N	2.35	0.40
14:AE:74:LYS:HB2	14:AE:74:LYS:HE2	1.60	0.40
14:AE:591:ILE:HG23	14:AE:592:VAL:HG13	2.03	0.40
17:D:579:A:O2'	33:T:54:ARG:NH1	2.54	0.40
17:D:1225:A:H2'	17:D:1226:C:C5	2.56	0.40
29:P:90:LEU:HD22	29:P:90:LEU:HA	1.86	0.40
32:S:16:LEU:HD13	32:S:54:ASP:HB2	2.03	0.40
40:a:67:U:C2	40:a:74:A:N6	2.89	0.40
40:a:493:G:H2'	40:a:494:G:O4'	2.20	0.40
40:a:1182:G:H2'	40:a:1183:U:O4'	2.21	0.40
40:a:2641:G:OP1	58:s:78:THR:HG22	2.21	0.40
40:a:2756:U:OP2	56:q:19:ARG:NE	2.54	0.40
8:7:-11:U:O2	8:7:-11:U:C3'	2.69	0.40
11:AA:310:ILE:HG21	11:AA:325:LEU:HB3	2.03	0.40
12:AB:173:LEU:CD1	12:AB:178:VAL:CG1	3.00	0.40
14:AE:66:LYS:HB2	14:AE:69:GLU:HB2	2.02	0.40
14:AE:1175:LEU:HD22	14:AE:1190:ILE:HD11	2.04	0.40
10:B:15:G:N2	10:B:20:U:H3	2.20	0.40
10:B:25:C:H2'	10:B:26:G:C5'	2.51	0.40
17:D:107:G:N7	18:E:10:ARG:NH2	2.60	0.40
17:D:152:A:N6	17:D:170:U:C2	2.89	0.40
17:D:915:A:C6	17:D:916:U:C4	3.08	0.40
17:D:1368:A:OP1	28:O:113:ARG:NH2	2.54	0.40
21:H:286:ASN:OD1	21:H:286:ASN:N	2.55	0.40
24:K:133:PRO:HA	24:K:136:VAL:HG12	2.02	0.40
40:a:2315:G:C5'	53:n:157:THR:HG23	2.52	0.40
60:u:74:THR:HG22	60:u:107:PHE:HB2	2.04	0.40
10:A:8:U:H6	10:A:8:U:OP2	2.04	0.40
10:A:25:C:H2'	10:A:26:G:C5'	2.51	0.40
11:AA:135:THR:HG22	11:AA:144:VAL:HG22	2.03	0.40
11:AA:524:ILE:HD12	11:AA:712:SER:HB2	2.02	0.40
11:AA:678:ARG:HD3	11:AA:678:ARG:HA	1.84	0.40
12:AB:173:LEU:HD12	12:AB:178:VAL:HG11	2.04	0.40
14:AE:1003:LEU:HD23	14:AE:1018:ALA:HB2	2.02	0.40
14:AE:1178:THR:HG23	14:AE:1184:ASP:HB3	2.04	0.40
17:D:1370:G:C2	17:D:1371:G:C8	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:a:1406:U:O2'	40:a:1407:G:OP2	2.38	0.40
10:A:60:U:O3'	10:A:61:C:C6	2.75	0.40
10:B:15:G:H1	10:B:20:U:H3	1.68	0.40
17:D:712:A:H2'	17:D:713:G:O4'	2.21	0.40
17:D:915:A:C8	17:D:915:A:C3'	3.04	0.40
24:K:94:VAL:CG1	24:K:111:MET:HE1	2.52	0.40
28:O:10:GLY:HA3	28:O:78:ALA:O	2.21	0.40
28:O:21:ILE:HD12	28:O:61:LEU:HD13	2.04	0.40
53:n:122:PHE:CZ	53:n:167:ARG:HA	2.56	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	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	48
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	12	48
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	7
11	AA	1312/1342 (98%)	1199 (91%)	112 (8%)	1 (0%)	48	83
12	AB	158/181 (87%)	142 (90%)	12 (8%)	4 (2%)	4	26
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14	51
13	AD	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
14	AE	1331/1407 (95%)	1217 (91%)	111 (8%)	3 (0%)	43	78
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
19	F	68/71 (96%)	68 (100%)	0	0	100	100
20	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
21	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	16
22	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	24	63
23	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
24	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	59
25	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12	48
26	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	18	56
27	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	54
28	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	54
29	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	12	48
30	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	36
31	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
32	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
33	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
34	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	9	42
35	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
36	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
37	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	6	34
38	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	0	9
39	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	11
41	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
42	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
44	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
45	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
46	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
47	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	67
48	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
49	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
50	k	50/55 (91%)	50 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	63
52	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	11	46
54	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
56	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
58	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
59	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
60	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
61	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
62	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
63	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
64	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
65	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	51
All	All	9485/10577 (90%)	8776 (92%)	640 (7%)	69 (1%)	20	56

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
12	AB	122	PRO
21	H	139	ARG
21	H	153	GLU
21	H	169	SER
21	H	306	VAL
21	H	340	ARG
28	O	56	ASP
37	X	103	LYS
38	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
12	AB	124	PRO
14	AE	92	VAL
14	AE	175	GLU
21	H	108	VAL
21	H	309	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	H	333	LEU
38	Y	93	ASN
47	h	158	ALA
51	l	142	ALA
65	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
21	H	76	GLU
21	H	142	ARG
26	M	130	ASN
29	P	58	ASN
30	Q	119	ASN
38	Y	20	SER
38	Y	64	ARG
38	Y	106	GLN
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
12	AB	123	ARG
12	AB	130	PRO
13	AC	193	GLU
21	H	82	THR
22	I	80	LYS
37	X	105	ASN
38	Y	83	ALA
39	Z	21	GLU
53	n	40	VAL
9	9	28	ALA
14	AE	74	LYS
21	H	70	VAL
38	Y	22	PRO
38	Y	71	LYS
38	Y	89	SER
39	Z	7	ILE
4	3	39	ILE
13	AC	192	VAL
38	Y	62	ALA
25	L	96	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	Y	23	VAL
38	Y	100	ILE
1	0	44	GLY
24	K	44	GLY
30	Q	74	VAL
34	U	64	GLY
9	9	54	VAL
11	AA	1317	PRO
53	n	62	GLY
27	N	75	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	76 (90%)	8 (10%)	8	25
2	1	93/93 (100%)	86 (92%)	7 (8%)	12	33
3	2	81/84 (96%)	77 (95%)	4 (5%)	22	43
4	3	84/85 (99%)	79 (94%)	5 (6%)	17	39
5	4	78/78 (100%)	75 (96%)	3 (4%)	29	50
9	9	112/123 (91%)	63 (56%)	49 (44%)	0	0
11	AA	1135/1157 (98%)	1130 (100%)	5 (0%)	84	84
12	AB	138/158 (87%)	136 (99%)	2 (1%)	59	72
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1107 (99%)	15 (1%)	61	74
15	AF	70/75 (93%)	69 (99%)	1 (1%)	59	72
16	C	57/65 (88%)	55 (96%)	2 (4%)	32	53
18	E	65/66 (98%)	61 (94%)	4 (6%)	16	38
19	F	60/61 (98%)	57 (95%)	3 (5%)	22	43
20	G	187/199 (94%)	174 (93%)	13 (7%)	14	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	H	137/461 (30%)	124 (90%)	13 (10%)	8	25
22	I	171/190 (90%)	163 (95%)	8 (5%)	23	45
23	J	172/173 (99%)	164 (95%)	8 (5%)	23	45
24	K	119/126 (94%)	111 (93%)	8 (7%)	15	36
25	L	91/116 (78%)	84 (92%)	7 (8%)	12	32
26	M	124/147 (84%)	113 (91%)	11 (9%)	9	28
27	N	104/105 (99%)	101 (97%)	3 (3%)	37	58
28	O	105/107 (98%)	99 (94%)	6 (6%)	18	40
29	P	86/90 (96%)	77 (90%)	9 (10%)	6	21
30	Q	90/99 (91%)	88 (98%)	2 (2%)	45	64
31	R	101/104 (97%)	95 (94%)	6 (6%)	18	39
32	S	83/84 (99%)	79 (95%)	4 (5%)	23	44
33	T	76/77 (99%)	65 (86%)	11 (14%)	3	13
34	U	65/65 (100%)	60 (92%)	5 (8%)	12	32
35	V	74/78 (95%)	71 (96%)	3 (4%)	27	48
36	W	72/79 (91%)	66 (92%)	6 (8%)	10	30
37	X	94/96 (98%)	87 (93%)	7 (7%)	13	33
38	Y	109/110 (99%)	69 (63%)	40 (37%)	0	1
39	Z	26/85 (31%)	10 (38%)	16 (62%)	0	0
41	b	58/63 (92%)	57 (98%)	1 (2%)	53	69
42	c	67/68 (98%)	64 (96%)	3 (4%)	24	46
44	e	54/55 (98%)	51 (94%)	3 (6%)	19	40
45	f	48/49 (98%)	43 (90%)	5 (10%)	7	22
46	g	59/62 (95%)	54 (92%)	5 (8%)	10	29
47	h	216/218 (99%)	199 (92%)	17 (8%)	11	32
48	i	47/48 (98%)	41 (87%)	6 (13%)	4	15
49	j	164/164 (100%)	156 (95%)	8 (5%)	22	43
50	k	47/49 (96%)	44 (94%)	3 (6%)	16	37
51	l	165/165 (100%)	151 (92%)	14 (8%)	10	29
52	m	38/38 (100%)	36 (95%)	2 (5%)	20	41
53	n	148/150 (99%)	130 (88%)	18 (12%)	5	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	o	51/52 (98%)	47 (92%)	4 (8%)	11	32
55	p	136/138 (99%)	130 (96%)	6 (4%)	25	47
56	q	34/34 (100%)	31 (91%)	3 (9%)	9	28
57	r	114/114 (100%)	102 (90%)	12 (10%)	6	21
58	s	116/116 (100%)	106 (91%)	10 (9%)	10	29
59	t	104/104 (100%)	97 (93%)	7 (7%)	15	36
60	u	103/103 (100%)	96 (93%)	7 (7%)	14	36
61	v	109/109 (100%)	105 (96%)	4 (4%)	30	51
62	w	99/103 (96%)	91 (92%)	8 (8%)	11	31
63	x	86/87 (99%)	80 (93%)	6 (7%)	14	35
64	y	99/100 (99%)	91 (92%)	8 (8%)	11	31
65	z	89/90 (99%)	85 (96%)	4 (4%)	24	46
All	All	7887/8739 (90%)	7429 (94%)	458 (6%)	20	40

All (458) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	38	VAL
1	0	47	VAL
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
1	0	96	VAL
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	93	LEU
4	3	52	LEU
4	3	70	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3	72	ILE
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	31	ARG
9	9	33	VAL
9	9	34	THR
9	9	35	VAL
9	9	36	ASP
9	9	37	LYS
9	9	39	THR
9	9	42	ARG
9	9	43	LYS
9	9	52	MET
9	9	54	VAL
9	9	55	VAL
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	69	PHE
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU
9	9	73	LYS
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR
9	9	143	MET
11	AA	145	ILE
11	AA	615	VAL
11	AA	914	LYS
11	AA	1076	ILE
11	AA	1151	LEU
12	AB	128	PHE
12	AB	129	GLU
14	AE	69	GLU
14	AE	70	CYS
14	AE	71	LEU
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	79	LYS
14	AE	81	ARG
14	AE	84	ILE
14	AE	85	CYS
14	AE	92	VAL
14	AE	93	THR
14	AE	514	THR
14	AE	1261	LEU
15	AF	63	ILE
16	C	33	ILE
16	C	74	HIS
18	E	6	SER
18	E	10	ARG
18	E	48	GLN
18	E	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	F	34	ARG
19	F	62	ARG
19	F	67	ARG
20	G	8	ASP
20	G	45	LYS
20	G	59	LYS
20	G	105	LYS
20	G	108	ARG
20	G	117	LEU
20	G	128	LYS
20	G	129	LEU
20	G	132	LYS
20	G	135	LEU
20	G	161	LEU
20	G	174	LYS
20	G	208	ARG
21	H	9	PHE
21	H	31	ILE
21	H	43	LYS
21	H	54	LYS
21	H	62	ILE
21	H	70	VAL
21	H	294	VAL
21	H	305	HIS
21	H	336	ASP
21	H	337	GLU
21	H	338	GLU
21	H	339	ARG
21	H	340	ARG
22	I	14	ILE
22	I	21	THR
22	I	33	LEU
22	I	75	ILE
22	I	89	LYS
22	I	175	LEU
22	I	178	LEU
22	I	200	VAL
23	J	47	ARG
23	J	48	LEU
23	J	95	GLU
23	J	104	ARG
23	J	105	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	J	116	GLN
23	J	138	SER
23	J	143	VAL
24	K	10	GLU
24	K	15	LEU
24	K	60	ILE
24	K	114	VAL
24	K	115	LEU
24	K	138	ARG
24	K	141	ILE
24	K	162	GLU
25	L	7	VAL
25	L	16	GLU
25	L	24	ARG
25	L	36	ILE
25	L	38	ARG
25	L	54	LEU
25	L	86	ARG
26	M	7	ILE
26	M	17	LYS
26	M	21	GLU
26	M	23	LEU
26	M	27	VAL
26	M	50	LEU
26	M	79	ARG
26	M	91	VAL
26	M	109	ARG
26	M	130	ASN
26	M	146	GLU
27	N	96	MET
27	N	104	VAL
27	N	117	ARG
28	O	27	LYS
28	O	60	LYS
28	O	61	LEU
28	O	63	LEU
28	O	116	VAL
28	O	118	LEU
29	P	17	LEU
29	P	18	ILE
29	P	24	GLU
29	P	25	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	P	27	GLU
29	P	37	ARG
29	P	87	LEU
29	P	90	LEU
29	P	102	LEU
30	Q	15	GLN
30	Q	107	ILE
31	R	5	ASN
31	R	12	ARG
31	R	24	LEU
31	R	62	GLU
31	R	74	LEU
31	R	102	LEU
32	S	45	VAL
32	S	46	LEU
32	S	89	MET
32	S	92	GLU
33	T	10	LYS
33	T	22	THR
33	T	39	LEU
33	T	40	GLN
33	T	64	ARG
33	T	66	LEU
33	T	67	LEU
33	T	70	LEU
33	T	73	LYS
33	T	84	ARG
33	T	85	LEU
34	U	1	MET
34	U	2	VAL
34	U	6	LEU
34	U	19	VAL
34	U	50	THR
35	V	46	VAL
35	V	75	LEU
35	V	81	LYS
36	W	21	LYS
36	W	33	THR
36	W	49	ILE
36	W	58	VAL
36	W	79	THR
36	W	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	X	16	VAL
37	X	25	VAL
37	X	29	ARG
37	X	59	GLU
37	X	93	ARG
37	X	101	ARG
37	X	117	LYS
38	Y	4	VAL
38	Y	10	LEU
38	Y	16	MET
38	Y	23	VAL
38	Y	27	LEU
38	Y	30	GLN
38	Y	36	GLU
38	Y	44	LYS
38	Y	45	THR
38	Y	48	ILE
38	Y	50	LYS
38	Y	52	LEU
38	Y	57	VAL
38	Y	58	ILE
38	Y	60	VAL
38	Y	61	TYR
38	Y	64	ARG
38	Y	65	SER
38	Y	67	THR
38	Y	71	LYS
38	Y	78	LEU
38	Y	80	LYS
38	Y	81	LYS
38	Y	91	LYS
38	Y	94	LYS
38	Y	95	ASP
38	Y	99	LYS
38	Y	100	ILE
38	Y	102	ARG
38	Y	104	GLN
38	Y	108	ILE
38	Y	112	LYS
38	Y	116	MET
38	Y	124	MET
38	Y	125	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	Y	126	ARG
38	Y	133	ARG
38	Y	135	MET
38	Y	137	LEU
38	Y	138	VAL
39	Z	1	SER
39	Z	2	ILE
39	Z	3	THR
39	Z	4	LYS
39	Z	6	GLN
39	Z	7	ILE
39	Z	8	ILE
39	Z	14	MET
39	Z	16	VAL
39	Z	17	MET
39	Z	19	VAL
39	Z	23	ILE
39	Z	26	MET
39	Z	28	GLU
39	Z	29	LYS
39	Z	30	PHE
41	b	70	GLU
42	c	33	LEU
42	c	48	THR
42	c	71	LEU
44	e	18	LEU
44	e	58	ASN
44	e	60	LYS
45	f	3	LYS
45	f	11	ARG
45	f	25	LEU
45	f	45	ARG
45	f	55	VAL
46	g	3	LYS
46	g	16	CYS
46	g	24	ILE
46	g	36	VAL
46	g	47	LYS
47	h	51	THR
47	h	94	VAL
47	h	105	LEU
47	h	118	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	h	125	LYS
47	h	130	LEU
47	h	141	VAL
47	h	156	ARG
47	h	183	LYS
47	h	187	ASP
47	h	195	VAL
47	h	202	LEU
47	h	203	ARG
47	h	204	VAL
47	h	205	LEU
47	h	242	LYS
47	h	271	ARG
48	i	9	THR
48	i	12	LYS
48	i	26	THR
48	i	27	SER
48	i	29	SER
48	i	40	ARG
49	j	13	ARG
49	j	18	ASP
49	j	91	THR
49	j	99	GLU
49	j	104	VAL
49	j	177	VAL
49	j	189	VAL
49	j	193	VAL
50	k	5	ILE
50	k	17	THR
50	k	24	THR
51	l	17	THR
51	l	22	ASP
51	l	40	ARG
51	l	48	THR
51	l	57	LYS
51	l	69	ARG
51	l	77	ILE
51	l	80	SER
51	l	108	ILE
51	l	109	LEU
51	l	111	GLU
51	l	122	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	l	149	ILE
51	l	179	SER
52	m	22	MET
52	m	42	LEU
53	n	6	ASP
53	n	10	ASP
53	n	26	MET
53	n	40	VAL
53	n	47	LYS
53	n	49	LEU
53	n	57	LEU
53	n	79	ILE
53	n	80	ARG
53	n	95	ARG
53	n	105	THR
53	n	117	LEU
53	n	122	PHE
53	n	123	ASP
53	n	132	VAL
53	n	140	GLU
53	n	141	ILE
53	n	163	ASP
54	o	8	ARG
54	o	30	ARG
54	o	31	HIS
54	o	55	LEU
55	p	11	VAL
55	p	85	LYS
55	p	95	ARG
55	p	125	CYS
55	p	168	VAL
55	p	171	THR
56	q	3	VAL
56	q	26	ILE
56	q	34	LYS
57	r	1	MET
57	r	9	VAL
57	r	11	ASN
57	r	12	LEU
57	r	15	LEU
57	r	41	LYS
57	r	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	r	72	ILE
57	r	76	GLU
57	r	94	ILE
57	r	101	ASP
57	r	127	GLU
58	s	1	MET
58	s	30	THR
58	s	31	GLU
58	s	43	GLU
58	s	57	LEU
58	s	123	LYS
58	s	124	VAL
58	s	139	VAL
58	s	140	LEU
58	s	142	ILE
59	t	7	MET
59	t	35	VAL
59	t	49	ARG
59	t	67	LYS
59	t	70	ARG
59	t	80	ASP
59	t	104	THR
60	u	5	THR
60	u	27	LEU
60	u	59	ARG
60	u	73	ILE
60	u	76	GLU
60	u	78	ARG
60	u	84	LYS
61	v	110	GLU
61	v	126	ILE
61	v	127	LYS
61	v	128	THR
62	w	2	ARG
62	w	20	MET
62	w	24	MET
62	w	51	LEU
62	w	65	LEU
62	w	69	ARG
62	w	95	THR
62	w	116	VAL
63	x	13	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	x	31	THR
63	x	47	VAL
63	x	48	LEU
63	x	91	SER
63	x	116	GLN
64	y	8	LEU
64	y	10	GLN
64	y	27	GLU
64	y	40	LEU
64	y	81	VAL
64	y	85	SER
64	y	102	GLU
64	y	114	LEU
65	z	18	LEU
65	z	51	ARG
65	z	109	LEU
65	z	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	86	GLN
2	1	61	ASN
3	2	28	ASN
3	2	59	ASN
4	3	54	GLN
9	9	103	ASN
9	9	122	GLN
11	AA	69	GLN
11	AA	314	ASN
11	AA	330	HIS
11	AA	343	HIS
11	AA	513	GLN
11	AA	554	HIS
11	AA	688	GLN
11	AA	808	ASN
11	AA	1237	HIS
11	AA	1288	GLN
11	AA	1313	HIS
13	AD	66	HIS
13	AD	84	ASN
13	AD	117	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AD	128	HIS
13	AD	227	GLN
14	AE	80	HIS
14	AE	157	GLN
14	AE	164	GLN
14	AE	232	ASN
14	AE	365	GLN
14	AE	424	ASN
14	AE	450	HIS
14	AE	469	HIS
14	AE	777	HIS
14	AE	865	HIS
14	AE	910	ASN
14	AE	1108	GLN
14	AE	1197	ASN
14	AE	1235	ASN
14	AE	1238	GLN
14	AE	1326	GLN
15	AF	31	GLN
15	AF	62	GLN
18	E	3	ASN
18	E	55	GLN
18	E	61	GLN
20	G	18	HIS
20	G	58	ASN
20	G	94	HIS
22	I	6	HIS
22	I	123	GLN
23	J	36	GLN
23	J	40	GLN
23	J	41	HIS
24	K	97	GLN
25	L	11	HIS
25	L	46	GLN
25	L	63	ASN
25	L	94	HIS
26	M	97	ASN
26	M	148	ASN
28	O	81	HIS
29	P	58	ASN
30	Q	15	GLN
31	R	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	R	72	HIS
33	T	40	GLN
34	U	59	HIS
37	X	12	HIS
37	X	105	ASN
46	g	33	ASN
47	h	70	ASN
50	k	26	ASN
53	n	63	GLN
54	o	28	ASN
55	p	88	GLN
57	r	20	ASN
57	r	133	GLN
59	t	88	ASN
64	y	15	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
17	D	1515/1542 (98%)	290 (19%)	35 (2%)
40	a	2859/2904 (98%)	540 (18%)	0
43	d	119/120 (99%)	17 (14%)	0
8	7	30/41 (73%)	19 (63%)	5 (16%)
All	All	4673/4759 (98%)	930 (19%)	52 (1%)

All (930) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-18	G
8	7	-17	U
8	7	-16	U
8	7	-14	U
8	7	-13	U
8	7	-12	U
8	7	-11	U
8	7	-10	U
8	7	-9	U
8	7	-8	U
8	7	-7	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	-6	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U
8	7	10	U
8	7	11	U
8	7	12	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
17	D	4	U
17	D	5	U
17	D	9	G
17	D	22	G
17	D	29	U
17	D	32	A
17	D	39	G
17	D	41	G
17	D	47	C
17	D	48	C
17	D	50	A
17	D	51	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	52	C
17	D	54	C
17	D	69	G
17	D	70	U
17	D	71	A
17	D	72	A
17	D	74	A
17	D	76	G
17	D	82	G
17	D	83	C
17	D	84	U
17	D	87	C
17	D	90	C
17	D	94	G
17	D	95	C
17	D	96	U
17	D	108	G
17	D	120	A
17	D	122	G
17	D	128	G
17	D	131	A
17	D	141	G
17	D	144	G
17	D	148	G
17	D	149	A
17	D	160	A
17	D	164	G
17	D	173	U
17	D	181	A
17	D	182	A
17	D	197	A
17	D	198	G
17	D	204	G
17	D	208	U
17	D	209	U
17	D	210	C
17	D	211	G
17	D	212	G
17	D	216	U
17	D	226	G
17	D	245	U
17	D	247	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	251	G
17	D	253	A
17	D	258	G
17	D	262	A
17	D	266	G
17	D	267	C
17	D	271	C
17	D	279	A
17	D	289	G
17	D	299	G
17	D	306	A
17	D	321	A
17	D	328	C
17	D	329	A
17	D	332	G
17	D	347	G
17	D	352	C
17	D	353	A
17	D	354	G
17	D	355	C
17	D	367	U
17	D	372	C
17	D	373	A
17	D	376	G
17	D	382	A
17	D	384	G
17	D	392	C
17	D	393	A
17	D	397	A
17	D	406	G
17	D	412	A
17	D	413	G
17	D	414	A
17	D	421	U
17	D	422	C
17	D	424	G
17	D	429	U
17	D	446	G
17	D	451	A
17	D	457	G
17	D	458	U
17	D	460	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	463	U
17	D	464	U
17	D	467	U
17	D	468	A
17	D	469	C
17	D	478	A
17	D	479	U
17	D	481	G
17	D	484	G
17	D	485	U
17	D	486	U
17	D	505	G
17	D	509	A
17	D	511	C
17	D	518	C
17	D	519	C
17	D	526	C
17	D	531	U
17	D	532	A
17	D	533	A
17	D	542	G
17	D	547	A
17	D	559	A
17	D	562	U
17	D	568	G
17	D	572	A
17	D	573	A
17	D	576	C
17	D	577	G
17	D	579	A
17	D	596	A
17	D	628	G
17	D	633	G
17	D	641	U
17	D	642	A
17	D	649	A
17	D	650	G
17	D	653	U
17	D	665	A
17	D	666	G
17	D	687	A
17	D	700	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	723	U
17	D	724	G
17	D	731	G
17	D	734	G
17	D	747	A
17	D	748	G
17	D	755	G
17	D	760	G
17	D	777	A
17	D	793	U
17	D	794	A
17	D	815	A
17	D	817	C
17	D	828	U
17	D	829	G
17	D	832	G
17	D	841	C
17	D	844	G
17	D	845	A
17	D	849	G
17	D	874	G
17	D	887	G
17	D	902	G
17	D	914	A
17	D	916	U
17	D	926	G
17	D	934	C
17	D	935	A
17	D	954	G
17	D	960	U
17	D	963	G
17	D	969	A
17	D	972	C
17	D	975	A
17	D	976	G
17	D	991	U
17	D	992	U
17	D	993	G
17	D	996	A
17	D	999	C
17	D	1004	A
17	D	1008	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	1009	U
17	D	1017	U
17	D	1018	G
17	D	1021	A
17	D	1024	G
17	D	1026	G
17	D	1028	C
17	D	1030	U
17	D	1031	C
17	D	1037	C
17	D	1043	G
17	D	1044	A
17	D	1046	A
17	D	1065	U
17	D	1085	U
17	D	1086	U
17	D	1094	G
17	D	1095	U
17	D	1099	G
17	D	1101	A
17	D	1124	G
17	D	1133	G
17	D	1135	U
17	D	1136	C
17	D	1137	C
17	D	1139	G
17	D	1140	C
17	D	1141	C
17	D	1142	G
17	D	1143	G
17	D	1145	A
17	D	1146	A
17	D	1151	A
17	D	1152	A
17	D	1158	C
17	D	1159	U
17	D	1167	A
17	D	1171	A
17	D	1174	G
17	D	1175	G
17	D	1176	A
17	D	1184	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	1196	A
17	D	1197	A
17	D	1206	G
17	D	1211	U
17	D	1212	U
17	D	1213	A
17	D	1214	C
17	D	1215	G
17	D	1226	C
17	D	1227	A
17	D	1228	C
17	D	1238	A
17	D	1256	A
17	D	1257	A
17	D	1260	G
17	D	1275	A
17	D	1276	G
17	D	1278	G
17	D	1279	G
17	D	1280	A
17	D	1285	A
17	D	1286	U
17	D	1287	A
17	D	1299	A
17	D	1300	G
17	D	1302	C
17	D	1305	G
17	D	1312	G
17	D	1317	C
17	D	1320	C
17	D	1323	G
17	D	1329	A
17	D	1338	G
17	D	1340	A
17	D	1346	A
17	D	1347	G
17	D	1353	G
17	D	1363	A
17	D	1370	G
17	D	1378	C
17	D	1379	G
17	D	1381	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	1391	U
17	D	1396	A
17	D	1397	C
17	D	1398	A
17	D	1404	C
17	D	1419	G
17	D	1429	A
17	D	1441	A
17	D	1446	A
17	D	1447	A
17	D	1448	C
17	D	1452	C
17	D	1453	G
17	D	1475	G
17	D	1487	G
17	D	1492	A
17	D	1493	A
17	D	1494	G
17	D	1495	U
17	D	1497	G
17	D	1503	A
17	D	1506	U
17	D	1517	G
17	D	1529	G
17	D	1530	G
17	D	1534	A
40	a	10	A
40	a	15	G
40	a	34	U
40	a	35	G
40	a	46	G
40	a	58	G
40	a	60	G
40	a	63	A
40	a	71	A
40	a	74	A
40	a	75	G
40	a	83	A
40	a	84	A
40	a	85	G
40	a	93	G
40	a	96	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	102	U
40	a	103	A
40	a	110	G
40	a	114	U
40	a	118	A
40	a	119	A
40	a	120	U
40	a	122	G
40	a	131	A
40	a	136	G
40	a	139	U
40	a	140	C
40	a	141	G
40	a	145	C
40	a	163	C
40	a	165	A
40	a	181	A
40	a	196	A
40	a	199	A
40	a	200	U
40	a	215	G
40	a	216	A
40	a	222	A
40	a	225	C
40	a	248	G
40	a	249	C
40	a	261	G
40	a	264	C
40	a	265	A
40	a	266	G
40	a	267	C
40	a	271	G
40	a	272	A
40	a	275	C
40	a	276	U
40	a	278	A
40	a	285	G
40	a	311	A
40	a	324	A
40	a	329	G
40	a	330	A
40	a	353	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	359	G
40	a	361	G
40	a	362	A
40	a	371	A
40	a	372	G
40	a	373	U
40	a	375	G
40	a	383	C
40	a	386	G
40	a	396	G
40	a	405	U
40	a	411	G
40	a	412	A
40	a	420	C
40	a	424	G
40	a	435	C
40	a	451	U
40	a	456	C
40	a	457	A
40	a	477	A
40	a	481	G
40	a	491	G
40	a	501	A
40	a	503	A
40	a	504	A
40	a	505	A
40	a	509	C
40	a	522	A
40	a	529	A
40	a	532	A
40	a	543	G
40	a	546	U
40	a	547	A
40	a	548	G
40	a	549	G
40	a	551	G
40	a	563	A
40	a	569	U
40	a	573	U
40	a	575	A
40	a	588	U
40	a	603	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	609	A
40	a	613	A
40	a	614	A
40	a	615	U
40	a	616	A
40	a	618	G
40	a	620	G
40	a	621	A
40	a	627	A
40	a	637	A
40	a	645	C
40	a	647	G
40	a	654	A
40	a	664	G
40	a	668	A
40	a	685	A
40	a	686	U
40	a	710	U
40	a	717	C
40	a	730	A
40	a	738	G
40	a	757	G
40	a	764	A
40	a	765	C
40	a	775	G
40	a	776	G
40	a	782	A
40	a	784	G
40	a	785	G
40	a	800	A
40	a	802	A
40	a	805	G
40	a	812	C
40	a	819	A
40	a	827	U
40	a	828	U
40	a	845	A
40	a	846	U
40	a	858	G
40	a	859	G
40	a	869	G
40	a	878	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	881	G
40	a	883	G
40	a	884	U
40	a	885	C
40	a	888	C
40	a	891	G
40	a	892	A
40	a	893	C
40	a	895	U
40	a	896	A
40	a	897	C
40	a	899	A
40	a	907	G
40	a	910	A
40	a	914	G
40	a	915	C
40	a	931	U
40	a	941	A
40	a	945	A
40	a	946	C
40	a	953	G
40	a	961	C
40	a	974	G
40	a	983	A
40	a	984	A
40	a	985	C
40	a	995	C
40	a	996	A
40	a	999	U
40	a	1005	C
40	a	1012	U
40	a	1013	C
40	a	1022	G
40	a	1023	U
40	a	1026	G
40	a	1033	U
40	a	1041	G
40	a	1042	G
40	a	1045	C
40	a	1046	A
40	a	1047	G
40	a	1060	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	1061	U
40	a	1062	G
40	a	1063	G
40	a	1064	C
40	a	1065	U
40	a	1066	U
40	a	1067	A
40	a	1068	G
40	a	1069	A
40	a	1070	A
40	a	1071	G
40	a	1073	A
40	a	1074	G
40	a	1076	C
40	a	1079	C
40	a	1080	A
40	a	1081	U
40	a	1082	U
40	a	1083	U
40	a	1084	A
40	a	1087	G
40	a	1088	A
40	a	1090	A
40	a	1095	A
40	a	1096	A
40	a	1107	G
40	a	1110	G
40	a	1111	A
40	a	1112	G
40	a	1119	U
40	a	1122	G
40	a	1132	U
40	a	1134	A
40	a	1135	C
40	a	1142	A
40	a	1143	A
40	a	1169	A
40	a	1170	C
40	a	1173	U
40	a	1174	U
40	a	1175	A
40	a	1176	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	1177	G
40	a	1178	C
40	a	1179	G
40	a	1180	U
40	a	1186	G
40	a	1238	G
40	a	1248	G
40	a	1253	A
40	a	1256	G
40	a	1266	G
40	a	1271	G
40	a	1272	A
40	a	1273	U
40	a	1301	A
40	a	1321	A
40	a	1345	C
40	a	1352	U
40	a	1365	A
40	a	1368	G
40	a	1378	A
40	a	1379	U
40	a	1380	G
40	a	1383	A
40	a	1387	A
40	a	1395	A
40	a	1406	U
40	a	1407	G
40	a	1408	G
40	a	1411	U
40	a	1414	C
40	a	1415	U
40	a	1416	G
40	a	1417	C
40	a	1419	A
40	a	1420	A
40	a	1428	C
40	a	1452	G
40	a	1453	A
40	a	1460	U
40	a	1478	G
40	a	1482	G
40	a	1490	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	1491	G
40	a	1497	U
40	a	1503	A
40	a	1508	A
40	a	1509	A
40	a	1510	G
40	a	1515	A
40	a	1529	G
40	a	1534	U
40	a	1535	A
40	a	1536	C
40	a	1537	G
40	a	1554	U
40	a	1559	U
40	a	1566	A
40	a	1569	A
40	a	1578	U
40	a	1580	A
40	a	1581	G
40	a	1582	C
40	a	1583	A
40	a	1584	U
40	a	1589	U
40	a	1590	A
40	a	1608	A
40	a	1609	A
40	a	1610	A
40	a	1647	U
40	a	1648	U
40	a	1649	G
40	a	1651	G
40	a	1674	G
40	a	1677	A
40	a	1703	G
40	a	1714	U
40	a	1715	G
40	a	1718	G
40	a	1729	U
40	a	1730	C
40	a	1732	C
40	a	1738	G
40	a	1750	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	1755	A
40	a	1758	U
40	a	1764	C
40	a	1773	A
40	a	1791	A
40	a	1800	C
40	a	1801	A
40	a	1808	A
40	a	1811	G
40	a	1816	C
40	a	1829	A
40	a	1833	C
40	a	1847	A
40	a	1848	A
40	a	1858	A
40	a	1859	U
40	a	1862	G
40	a	1864	U
40	a	1869	G
40	a	1870	C
40	a	1872	A
40	a	1873	G
40	a	1905	C
40	a	1906	G
40	a	1907	G
40	a	1913	A
40	a	1914	C
40	a	1919	A
40	a	1920	C
40	a	1922	G
40	a	1923	U
40	a	1924	C
40	a	1925	C
40	a	1926	U
40	a	1928	A
40	a	1929	G
40	a	1930	G
40	a	1936	A
40	a	1938	A
40	a	1955	U
40	a	1965	C
40	a	1967	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	1970	A
40	a	1971	U
40	a	1972	G
40	a	1987	A
40	a	1991	U
40	a	1992	G
40	a	1993	U
40	a	1997	C
40	a	2002	G
40	a	2022	U
40	a	2023	C
40	a	2027	G
40	a	2033	A
40	a	2043	C
40	a	2051	A
40	a	2052	A
40	a	2055	C
40	a	2056	G
40	a	2060	A
40	a	2061	G
40	a	2062	A
40	a	2063	C
40	a	2077	A
40	a	2097	A
40	a	2099	U
40	a	2100	G
40	a	2108	A
40	a	2110	G
40	a	2111	U
40	a	2113	U
40	a	2115	G
40	a	2116	G
40	a	2117	A
40	a	2118	U
40	a	2121	G
40	a	2122	U
40	a	2124	G
40	a	2125	G
40	a	2126	A
40	a	2127	G
40	a	2128	G
40	a	2131	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	2132	U
40	a	2133	G
40	a	2134	A
40	a	2139	U
40	a	2141	G
40	a	2146	C
40	a	2147	A
40	a	2154	A
40	a	2157	G
40	a	2158	A
40	a	2159	G
40	a	2162	G
40	a	2163	A
40	a	2164	C
40	a	2165	C
40	a	2169	A
40	a	2171	A
40	a	2172	U
40	a	2178	C
40	a	2182	U
40	a	2183	A
40	a	2185	U
40	a	2188	U
40	a	2189	U
40	a	2190	G
40	a	2191	A
40	a	2193	G
40	a	2194	U
40	a	2198	A
40	a	2204	G
40	a	2210	U
40	a	2211	A
40	a	2212	A
40	a	2213	U
40	a	2225	A
40	a	2226	C
40	a	2229	U
40	a	2238	G
40	a	2239	G
40	a	2244	U
40	a	2250	G
40	a	2268	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	2278	A
40	a	2283	C
40	a	2287	A
40	a	2297	A
40	a	2305	U
40	a	2308	G
40	a	2309	A
40	a	2315	G
40	a	2322	A
40	a	2325	G
40	a	2327	A
40	a	2333	A
40	a	2339	C
40	a	2345	G
40	a	2347	C
40	a	2350	C
40	a	2361	G
40	a	2372	U
40	a	2376	A
40	a	2383	G
40	a	2385	C
40	a	2402	U
40	a	2403	C
40	a	2406	A
40	a	2423	U
40	a	2424	C
40	a	2425	A
40	a	2426	A
40	a	2429	G
40	a	2430	A
40	a	2431	U
40	a	2434	A
40	a	2435	A
40	a	2441	U
40	a	2447	G
40	a	2448	A
40	a	2470	G
40	a	2474	U
40	a	2476	A
40	a	2478	A
40	a	2484	G
40	a	2491	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	2502	G
40	a	2506	U
40	a	2507	C
40	a	2512	C
40	a	2513	A
40	a	2518	A
40	a	2520	C
40	a	2525	G
40	a	2529	G
40	a	2535	G
40	a	2547	A
40	a	2554	U
40	a	2566	A
40	a	2567	G
40	a	2572	A
40	a	2573	C
40	a	2574	G
40	a	2585	U
40	a	2586	U
40	a	2602	A
40	a	2603	G
40	a	2609	U
40	a	2610	C
40	a	2611	C
40	a	2613	U
40	a	2629	U
40	a	2663	G
40	a	2669	G
40	a	2671	G
40	a	2689	U
40	a	2690	U
40	a	2714	G
40	a	2722	G
40	a	2726	A
40	a	2744	G
40	a	2748	A
40	a	2757	A
40	a	2758	A
40	a	2765	A
40	a	2777	G
40	a	2778	A
40	a	2791	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	a	2793	C
40	a	2796	U
40	a	2797	U
40	a	2798	U
40	a	2799	A
40	a	2801	G
40	a	2818	U
40	a	2820	A
40	a	2823	A
40	a	2825	G
40	a	2849	U
40	a	2850	A
40	a	2859	G
40	a	2861	U
40	a	2867	G
40	a	2880	C
40	a	2884	U
40	a	2885	G
40	a	2891	U
40	a	2902	C
43	d	2	G
43	d	9	G
43	d	13	G
43	d	16	G
43	d	17	C
43	d	35	C
43	d	36	C
43	d	45	A
43	d	51	G
43	d	56	G
43	d	64	G
43	d	66	A
43	d	88	C
43	d	89	U
43	d	90	C
43	d	99	A
43	d	109	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-17	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7	-14	U
8	7	-11	U
8	7	-3	U
8	7	9	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A
10	B	60	U
17	D	7	A
17	D	70	U
17	D	121	U
17	D	181	A
17	D	183	C
17	D	197	A
17	D	209	U
17	D	305	G
17	D	328	C
17	D	428	G
17	D	496	A
17	D	517	G
17	D	531	U
17	D	532	A
17	D	562	U
17	D	641	U
17	D	722	G
17	D	793	U
17	D	991	U
17	D	992	U
17	D	1109	C
17	D	1145	A
17	D	1196	A
17	D	1211	U
17	D	1212	U
17	D	1213	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	1214	C
17	D	1225	A
17	D	1299	A
17	D	1396	A
17	D	1432	G
17	D	1447	A
17	D	1491	G
17	D	1492	A
17	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

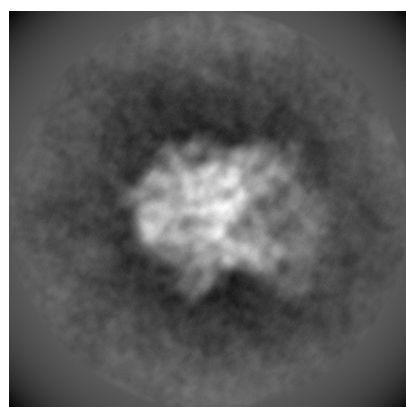
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22192. These allow visual inspection of the internal detail of the map and identification of artifacts.

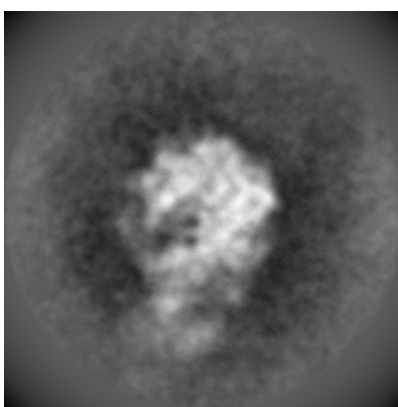
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

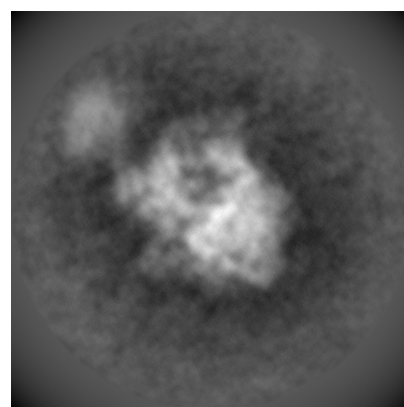
6.1.1 Primary map



X



Y

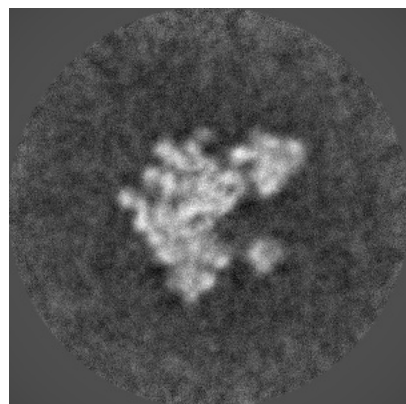


Z

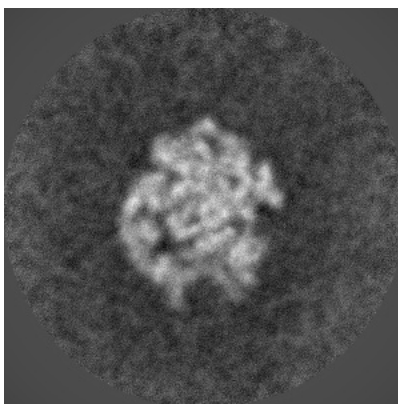
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

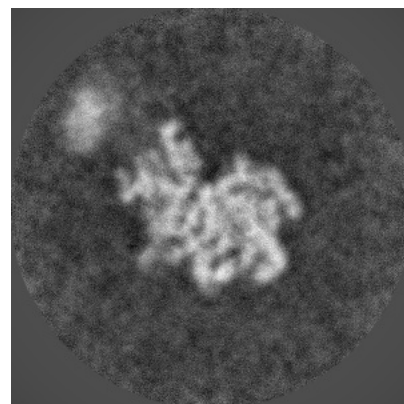
6.2.1 Primary map



X Index: 256



Y Index: 256

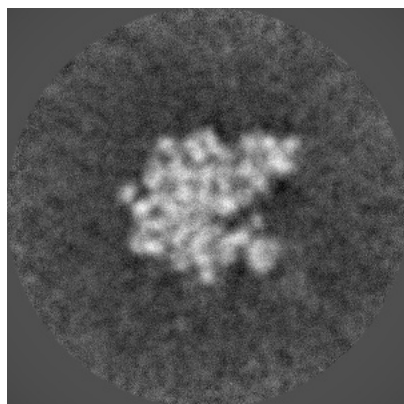


Z Index: 256

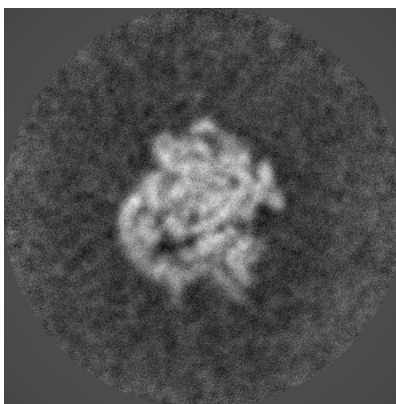
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

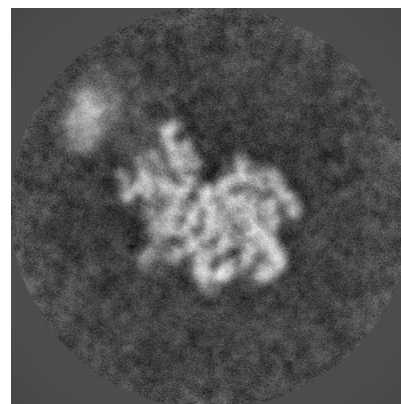
6.3.1 Primary map



X Index: 271



Y Index: 252

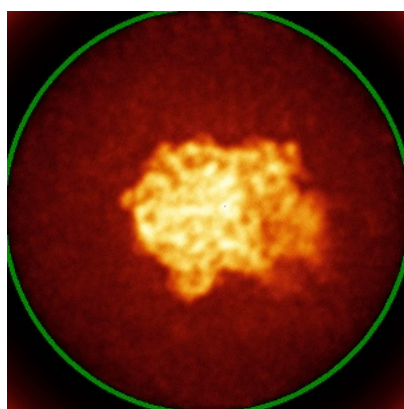


Z Index: 256

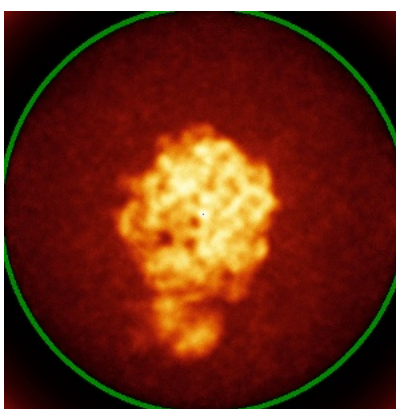
The images above show the largest variance slices of the map in three orthogonal directions.

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

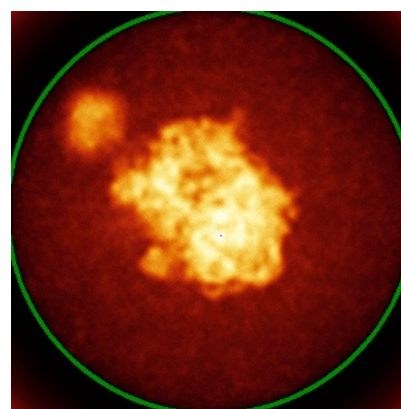
6.4.1 Primary map



X



Y

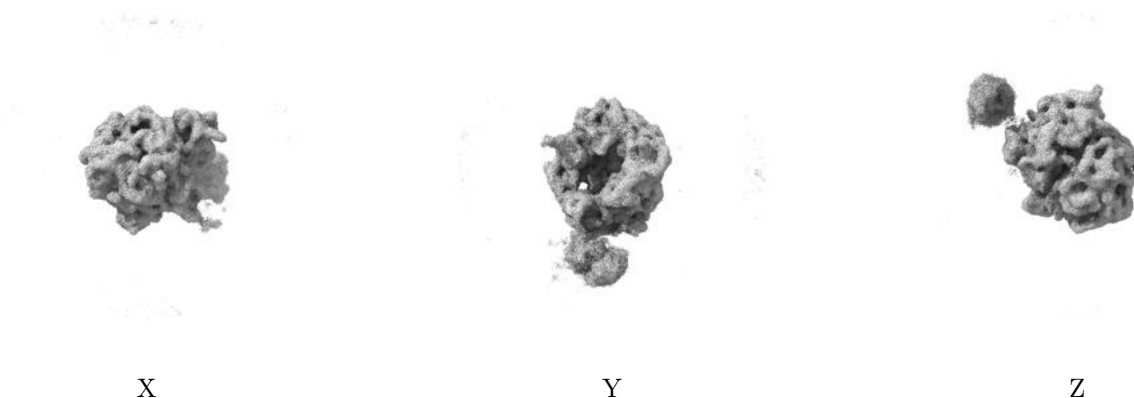


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00722. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

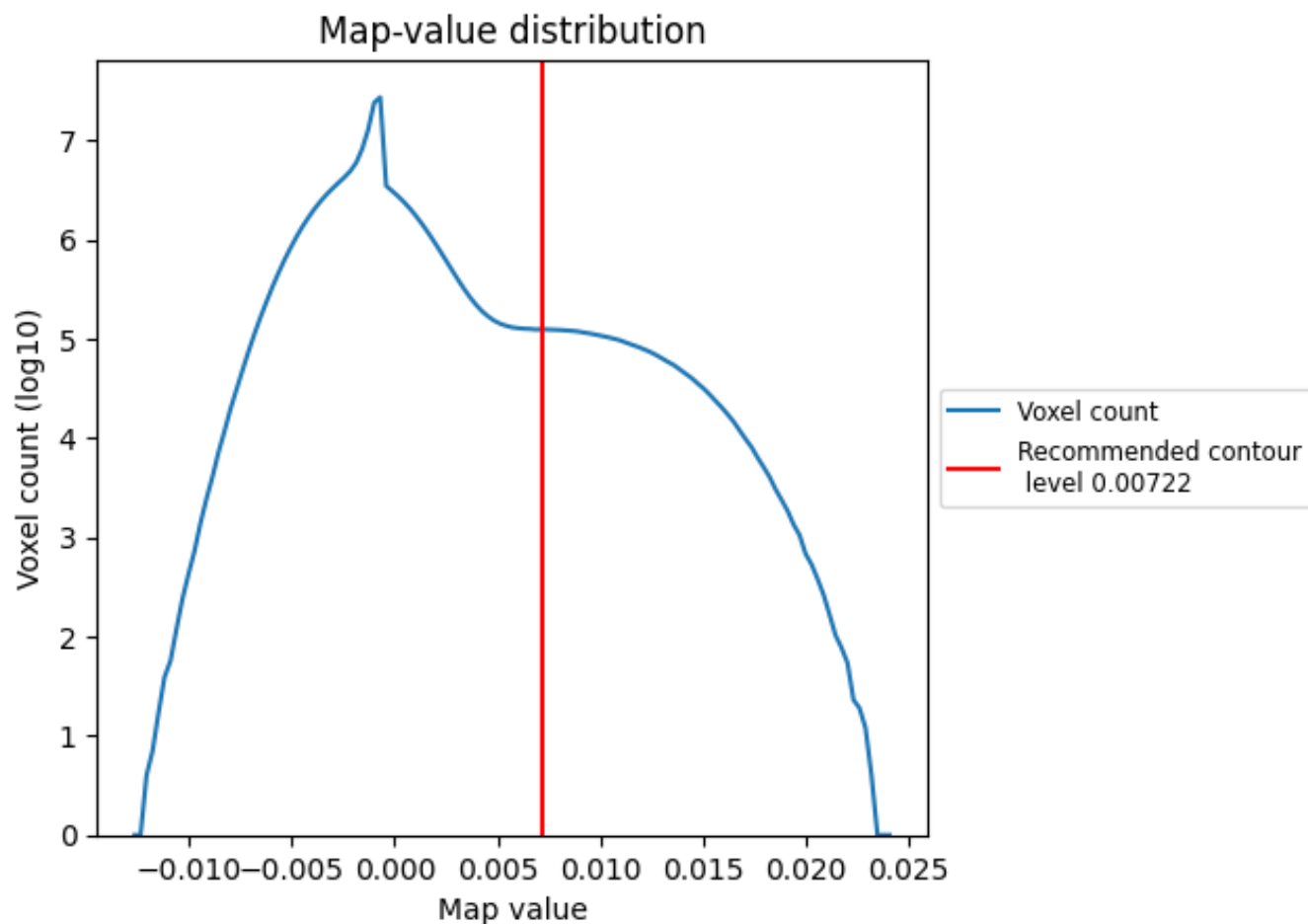
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

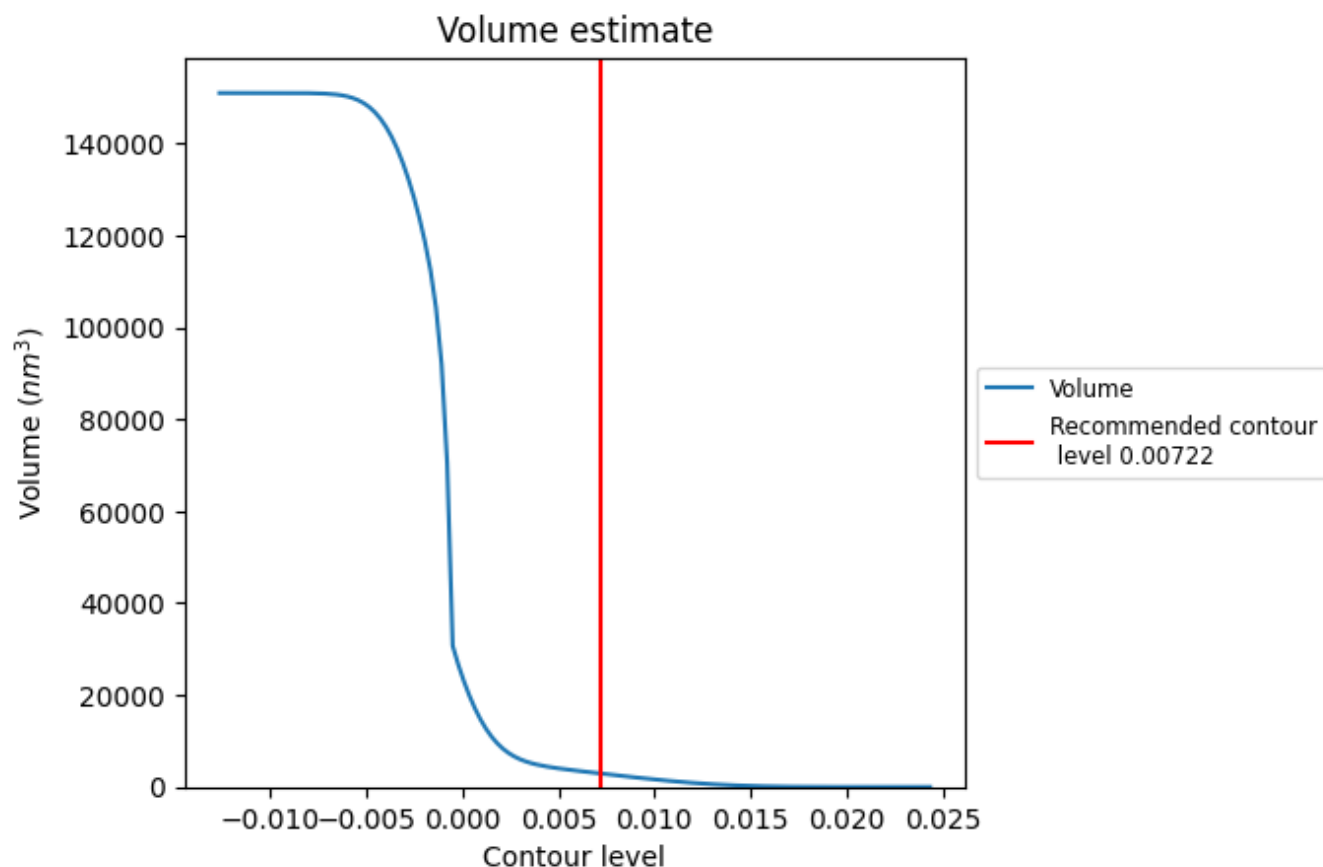
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

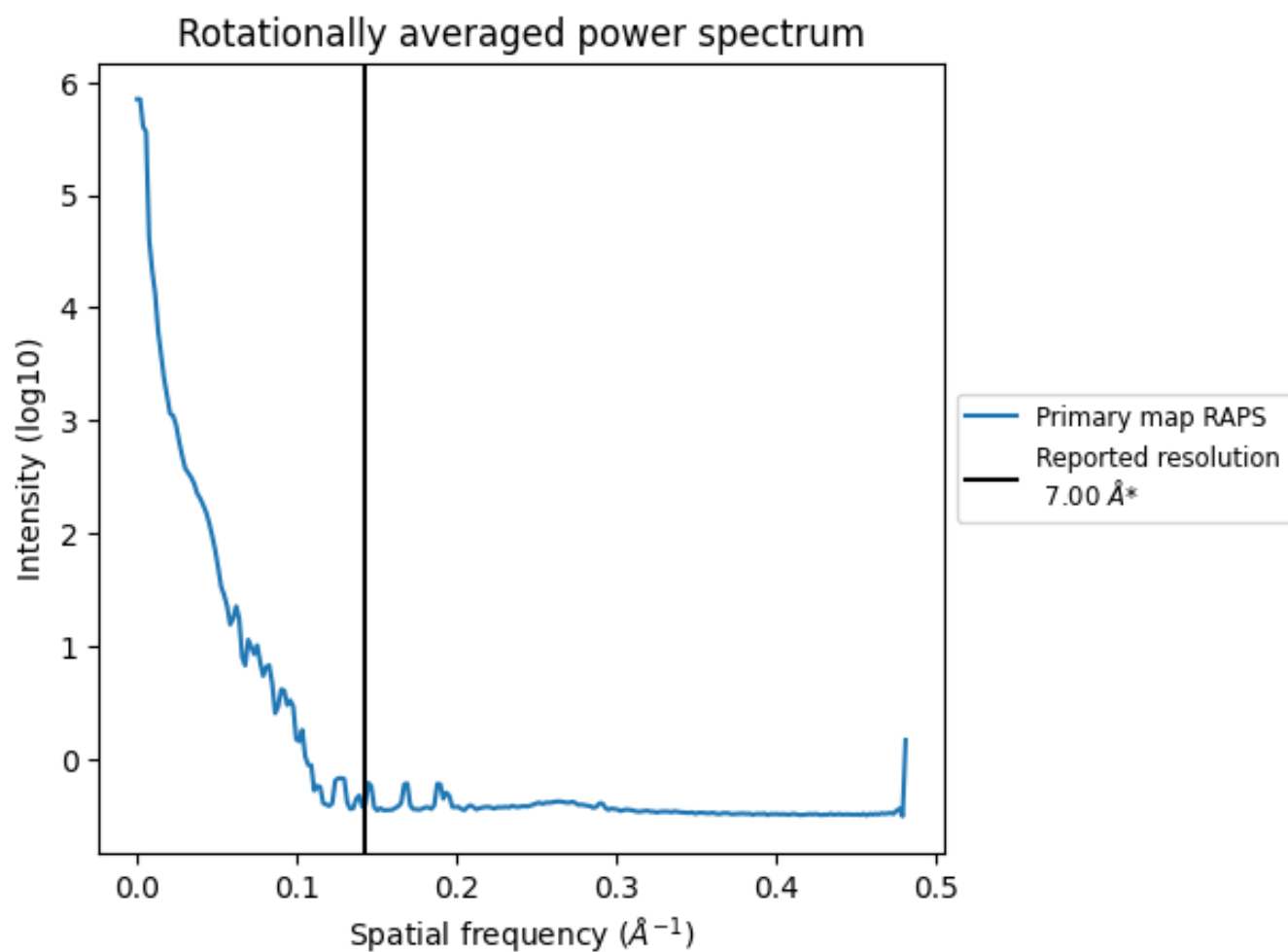
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2921 nm^3 ; this corresponds to an approximate mass of 2639 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

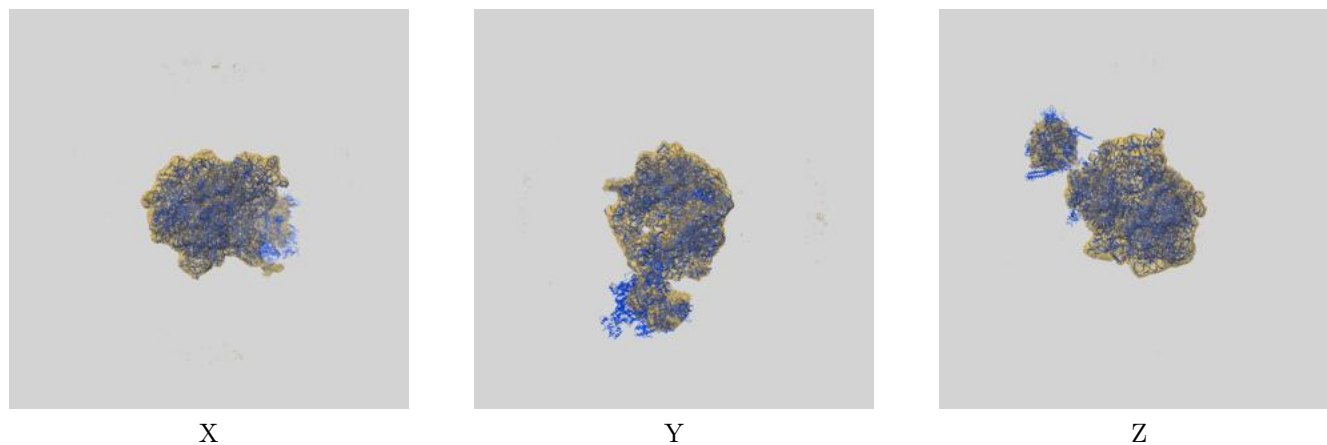
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

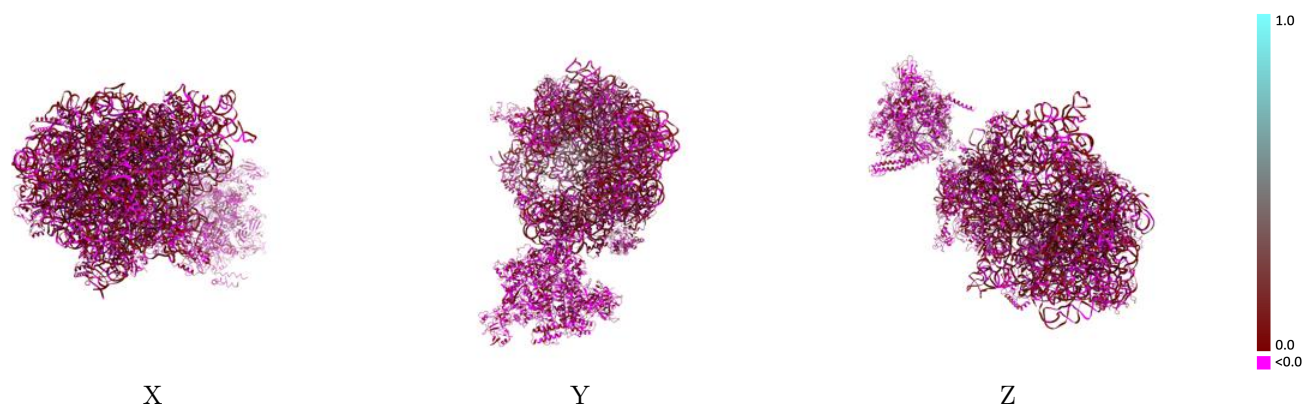
This section contains information regarding the fit between EMDB map EMD-22192 and PDB model 6XII. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



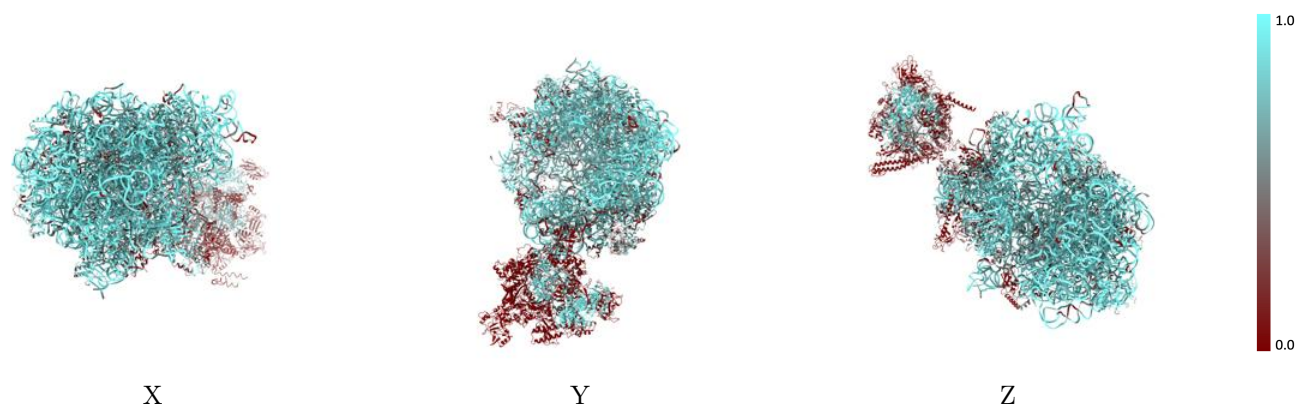
The images above show the 3D surface view of the map at the recommended contour level 0.00722 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



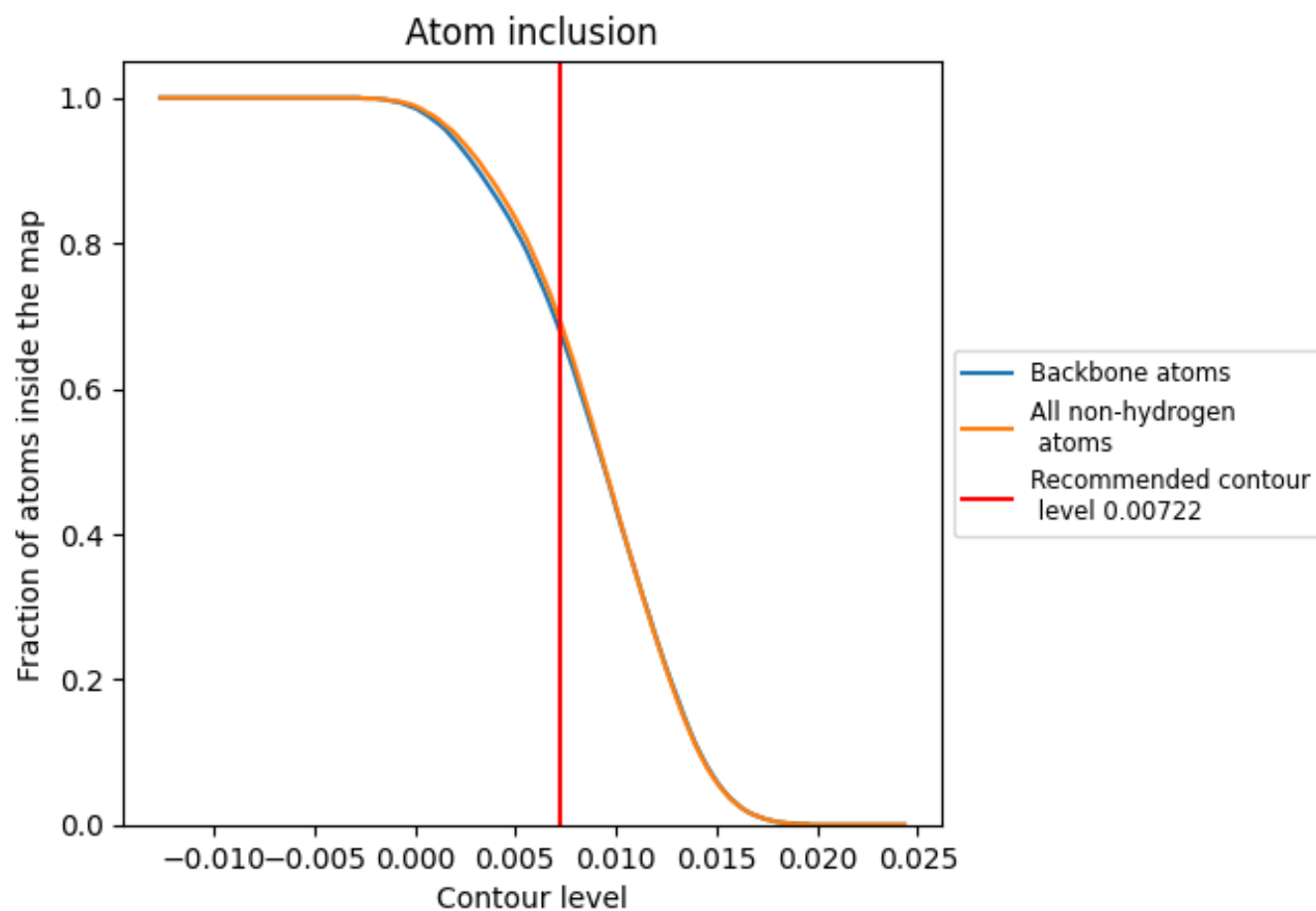
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00722).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00722) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.0360
0	 0.7780	 0.0240
1	 0.6460	 0.0250
2	 0.6700	 0.0120
3	 0.8220	 0.0080
4	 0.5150	 0.0320
5	 0.0980	 -0.0420
6	 0.3880	 -0.0060
7	 0.5550	 0.0240
9	 0.4560	 0.0150
A	 0.6890	 0.0340
AA	 0.2600	 -0.0040
AB	 0.1000	 0.0060
AC	 0.5430	 0.0130
AD	 0.3720	 0.0040
AE	 0.2890	 0.0030
AF	 0.0460	 -0.0100
B	 0.6970	 0.0220
C	 0.7760	 0.0220
D	 0.9040	 0.0550
E	 0.7660	 0.0090
F	 0.4440	 0.0480
G	 0.6440	 0.0490
H	 0.0840	 0.0280
I	 0.3880	 0.0420
J	 0.6160	 0.0240
K	 0.6890	 0.0440
L	 0.5820	 0.0360
M	 0.5040	 0.0340
N	 0.5810	 0.0450
O	 0.6590	 0.0100
P	 0.4350	 -0.0010
Q	 0.8460	 0.0310
R	 0.7170	 0.0280
S	 0.7000	 0.0420



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.7280	 0.0610
U	 0.8010	 0.0190
V	 0.6360	 -0.0130
W	 0.6140	 0.0220
X	 0.4480	 0.0240
Y	 0.2940	 0.0360
Z	 0.1230	 0.0250
a	 0.9080	 0.0500
b	 0.7630	 0.0440
c	 0.5870	 0.0040
d	 0.8640	 0.0470
e	 0.7950	 -0.0020
f	 0.7980	 0.0610
g	 0.4380	 0.0450
h	 0.6660	 0.0050
i	 0.7550	 0.0250
j	 0.7670	 0.0090
k	 0.7580	 0.0630
l	 0.7110	 0.0140
m	 0.8700	 -0.0210
n	 0.6290	 0.0490
o	 0.8410	 0.0120
p	 0.6500	 0.0340
q	 0.9180	 0.0210
r	 0.2320	 0.0310
s	 0.6610	 0.0180
t	 0.6640	 0.0480
u	 0.8370	 -0.0050
v	 0.6000	 0.0340
w	 0.8290	 0.0070
x	 0.8400	 0.0250
y	 0.6220	 0.0260
z	 0.8680	 0.0300