



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:10 AM UTC

PDB ID : 6YAL / pdb_00006yal
EMDB ID : EMD-10760
Title : Mammalian 48S late-stage initiation complex with beta-globin mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.00 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:

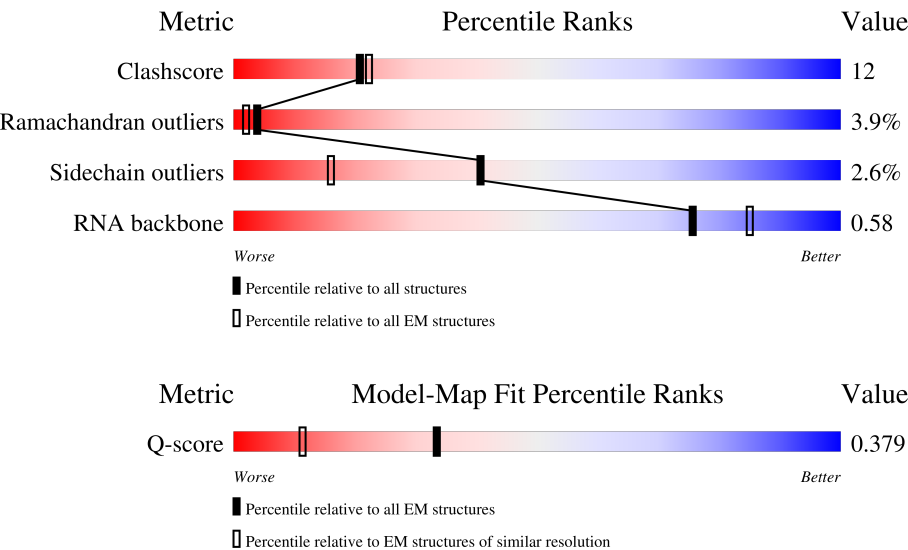
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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	14081 (2.50 - 3.50)

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	1	75	79% 61% 28% 7% .
2	1	25	28% 100%
3	C	209	12% 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	264	
5	E	226	
6	F	243	
7	G	263	
8	H	191	
9	I	237	
10	J	192	
11	K	206	
12	L	182	
13	M	98	
14	N	158	
15	O	132	
16	P	150	
17	Q	151	
18	S	141	
19	T	135	
20	V	141	
21	W	119	
22	X	82	
23	Y	130	
24	Z	143	
25	a	133	
26	b	115	
27	c	84	
28	d	69	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	e	56	
30	f	71	
31	g	313	
32	n	124	
33	i	133	
34	2	1863	
35	A	284	
36	B	422	
37	j	111	
38	k	595	
39	U	152	
40	R	145	
41	3	42	

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
34	C4J	2	1244	X	-	-	-
42	SF4	k	701	-	-	X	-
42	SF4	k	702	-	-	X	-
44	GNP	k	704	-	-	X	-
44	GNP	k	705	-	-	X	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 90085 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

- Molecule 2 is a protein called 60s ribosomal protein ul41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 3 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 4 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 5 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 6 is a protein called 40S Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 7 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 8 is a protein called 40S Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 9 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 10 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 11 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 12 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 13 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 14 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 15 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 16 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 17 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 18 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 19 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 20 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 21 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 22 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 23 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

- Molecule 25 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 26 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 27 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 28 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 29 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 30 is a protein called 40S ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 31 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 32 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	1744	Total	C	N	O	P	0	0
			37204	16614	6663	12187	1740		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2146	1354	376	405	11		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	109	Total	C	N	O	S	0	0
			883	549	168	162	4		

- Molecule 38 is a protein called ATP-binding cassette sub-family E member 1 (ABCE1).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

- Molecule 39 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

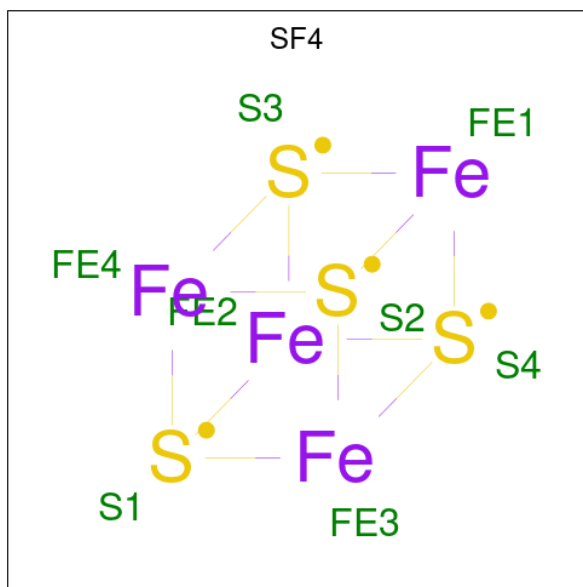
- Molecule 40 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 41 is a RNA chain called beta-globin mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	42	Total	C	N	O	P	0	0
			892	401	166	284	41		

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

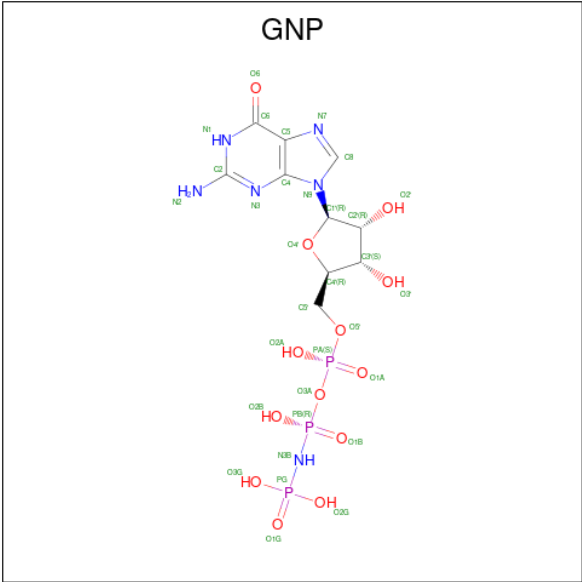


Mol	Chain	Residues	Atoms			AltConf
42	k	1	Total	Fe	S	0
			8	4	4	
42	k	1	Total	Fe	S	0
			8	4	4	

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	k	1	Total	Mg	0
			1	1	

- Molecule 44 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

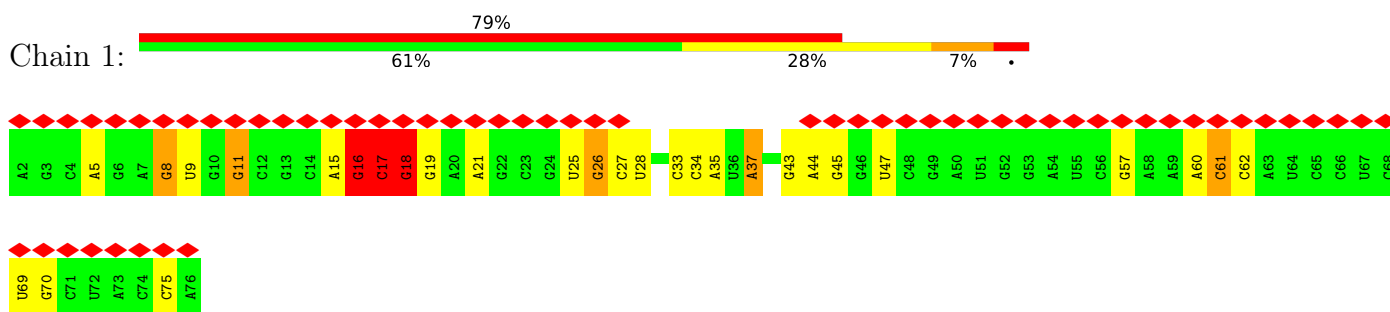


Mol	Chain	Residues	Atoms					AltConf
44	k	1	Total	C	N	O	P	0
			32	10	6	13	3	
44	k	1	Total	C	N	O	P	0
			32	10	6	13	3	

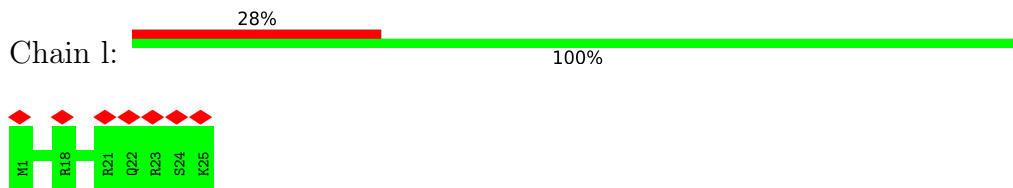
3 Residue-property plots [i](#)

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.

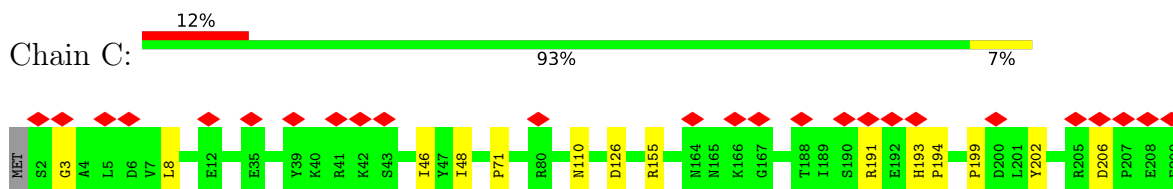
- Molecule 1: initiator methionylated tRNA



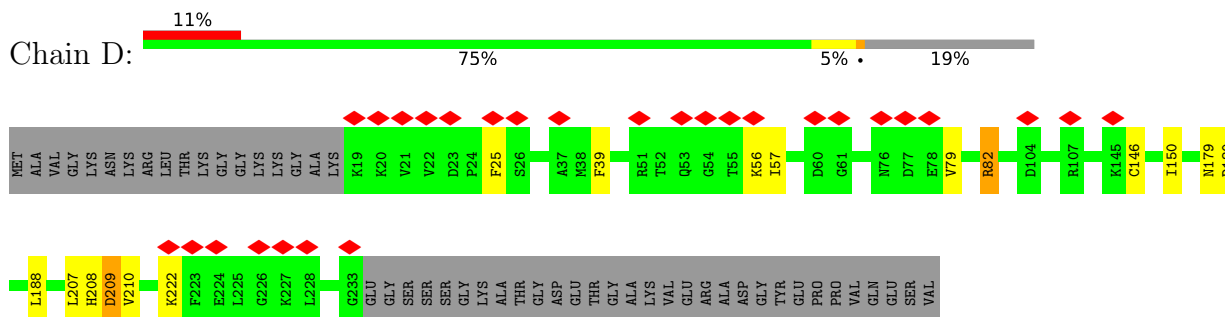
- Molecule 2: 60s ribosomal protein ul41



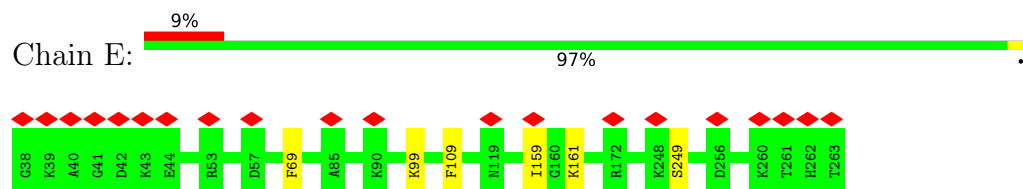
- Molecule 3: 40S ribosomal protein uS2



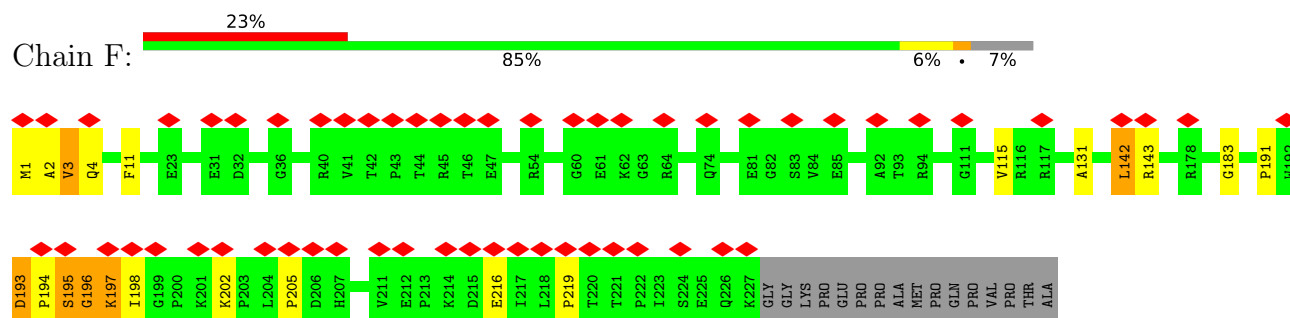
- Molecule 4: 40S ribosomal protein eS1



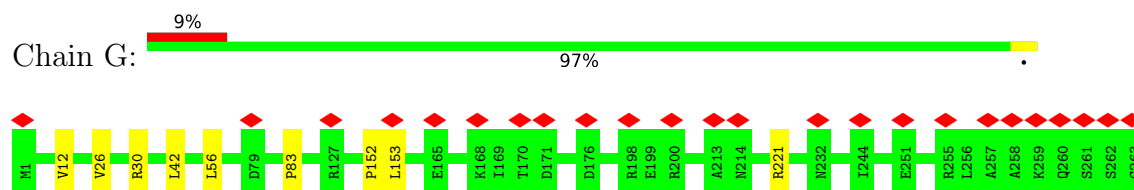
- Molecule 5: 40S ribosomal protein uS5



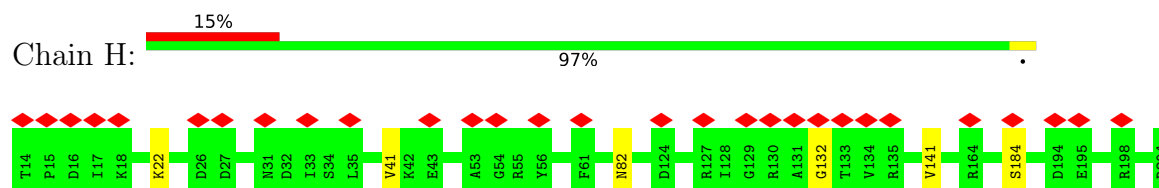
- Molecule 6: 40S Ribosomal protein uS3



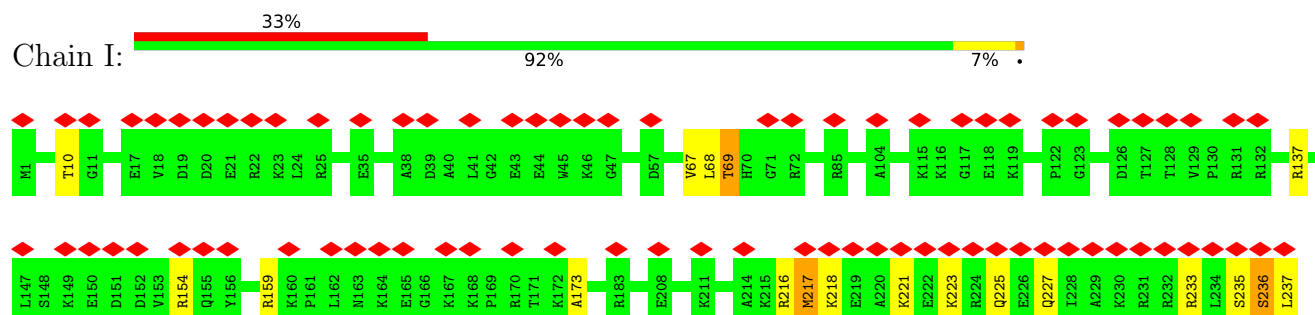
- Molecule 7: 40S ribosomal protein eS4



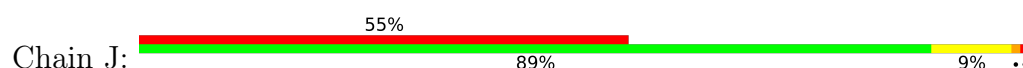
- Molecule 8: 40S Ribosomal protein uS7

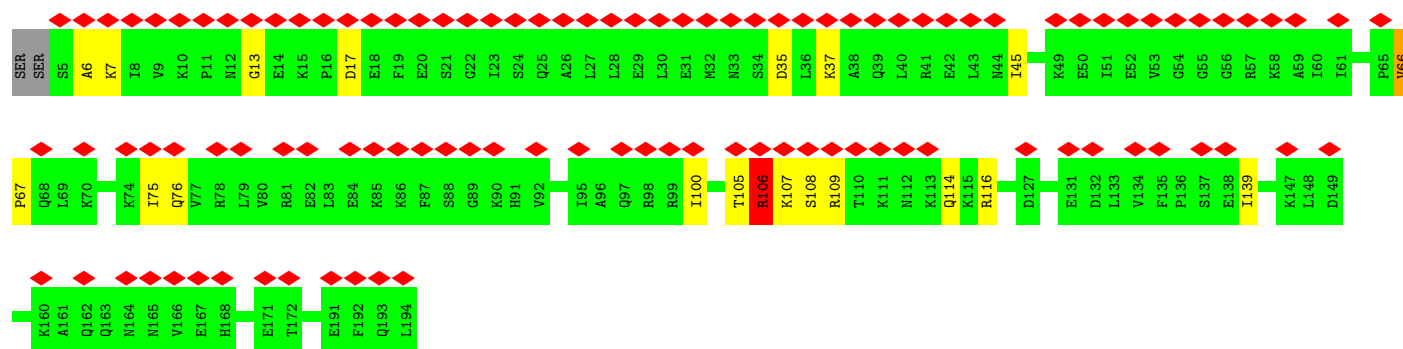


- Molecule 9: 40S ribosomal protein eS6

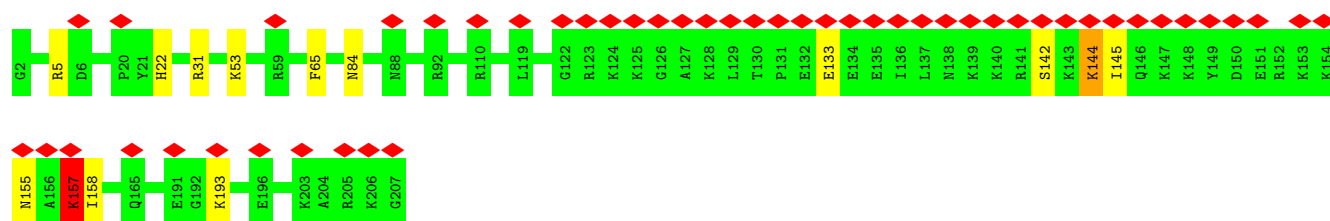


- Molecule 10: 40S ribosomal protein eS7

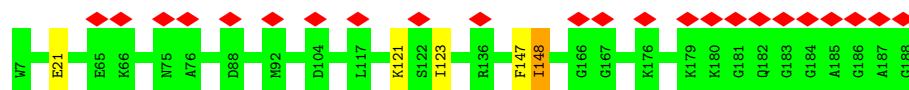




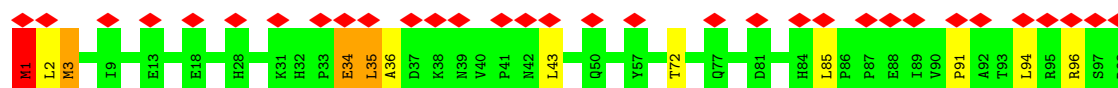
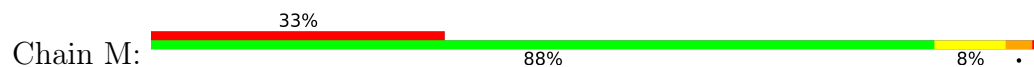
• Molecule 11: 40S ribosomal protein eS8



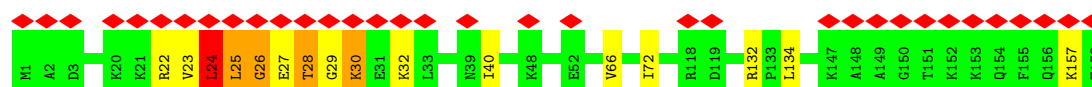
• Molecule 12: 40S ribosomal protein uS4



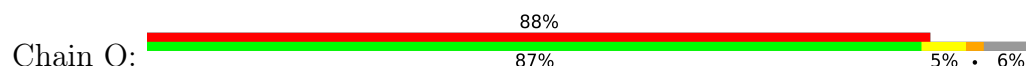
• Molecule 13: 40S ribosomal protein eS10

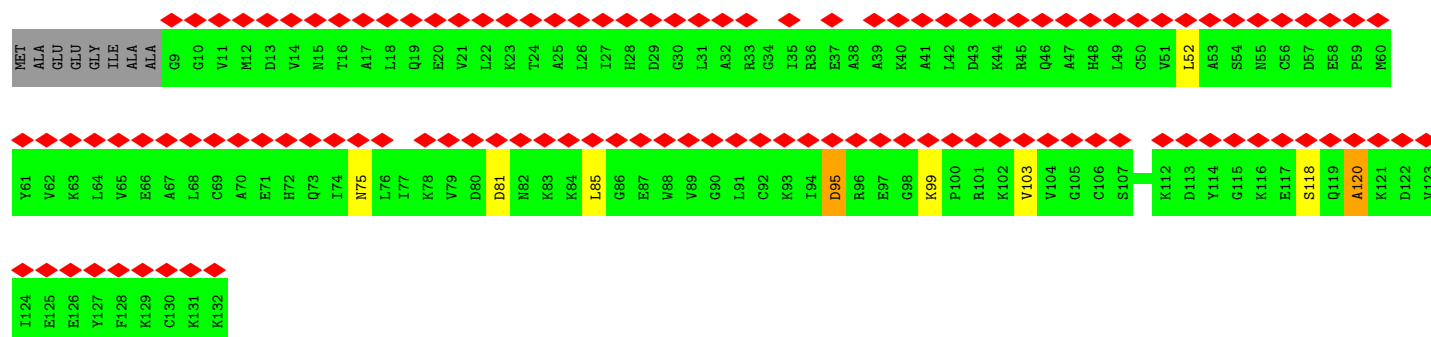


• Molecule 14: 40S ribosomal protein uS17

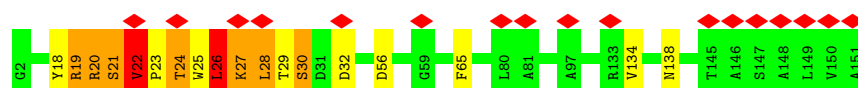
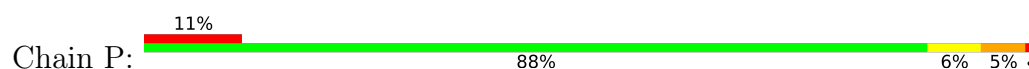


• Molecule 15: 40S ribosomal protein eS12

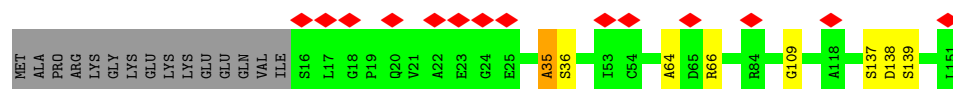
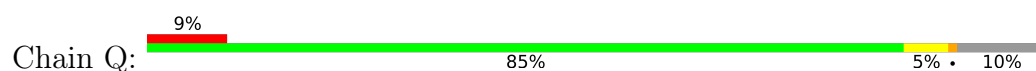




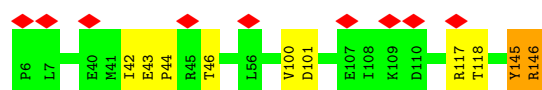
- Molecule 16: 40S ribosomal protein uS15



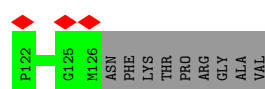
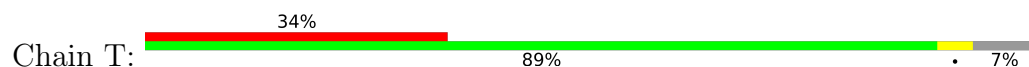
- Molecule 17: 40S ribosomal protein uS11



- Molecule 18: 40S ribosomal protein uS9

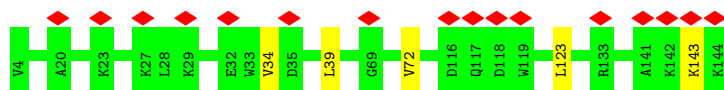


- Molecule 19: 40S ribosomal protein eS17

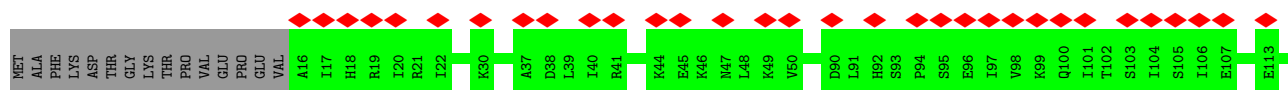
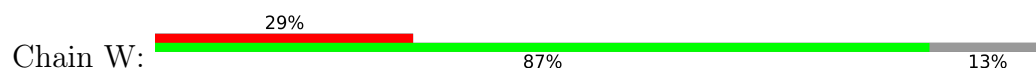


- Molecule 20: 40S ribosomal protein eS19

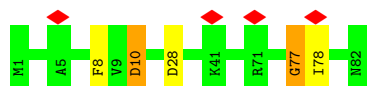




- Molecule 21: 40S ribosomal protein uS10



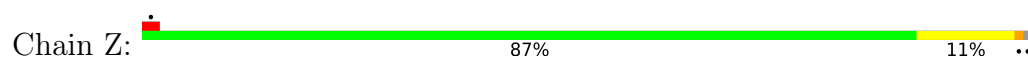
- Molecule 22: 40S ribosomal protein eS21



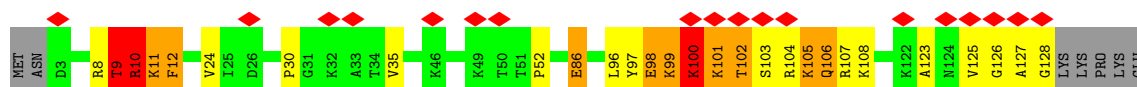
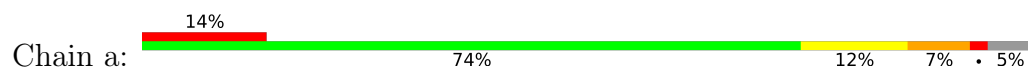
- Molecule 23: 40S ribosomal protein uS8



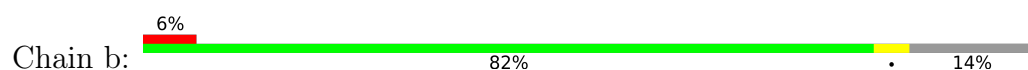
- Molecule 24: 40S ribosomal protein uS12

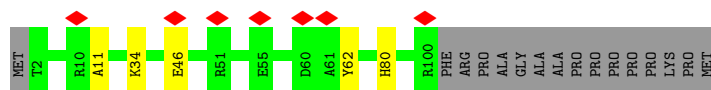


- Molecule 25: 40S ribosomal protein eS24

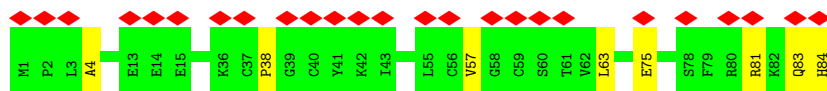


- Molecule 26: 40S ribosomal protein eS26

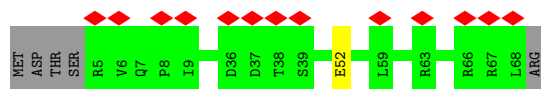




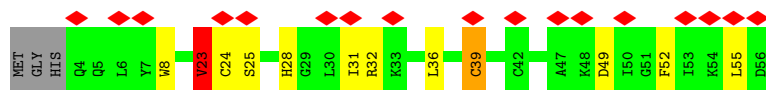
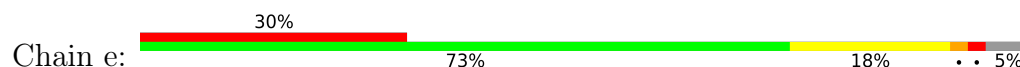
- Molecule 27: 40S ribosomal protein eS27



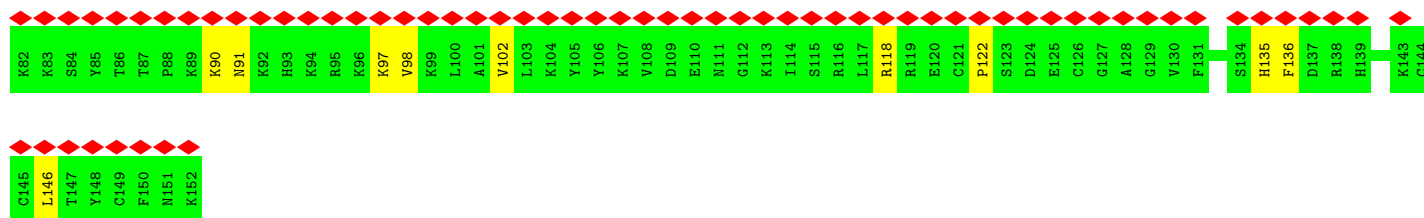
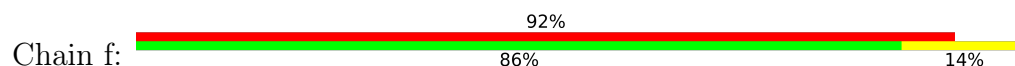
- Molecule 28: 40S ribosomal protein eS28



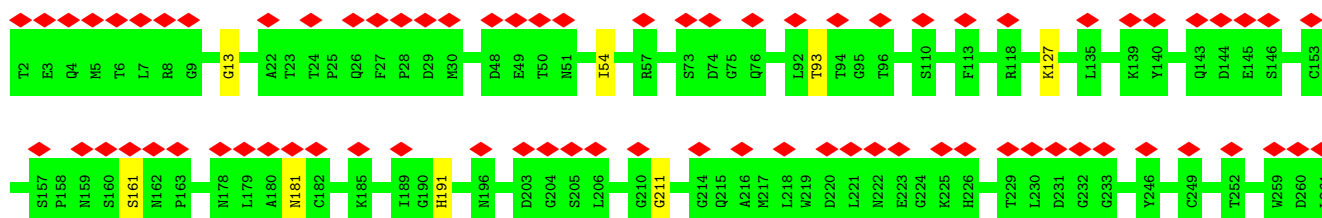
- Molecule 29: 40S ribosomal protein uS14

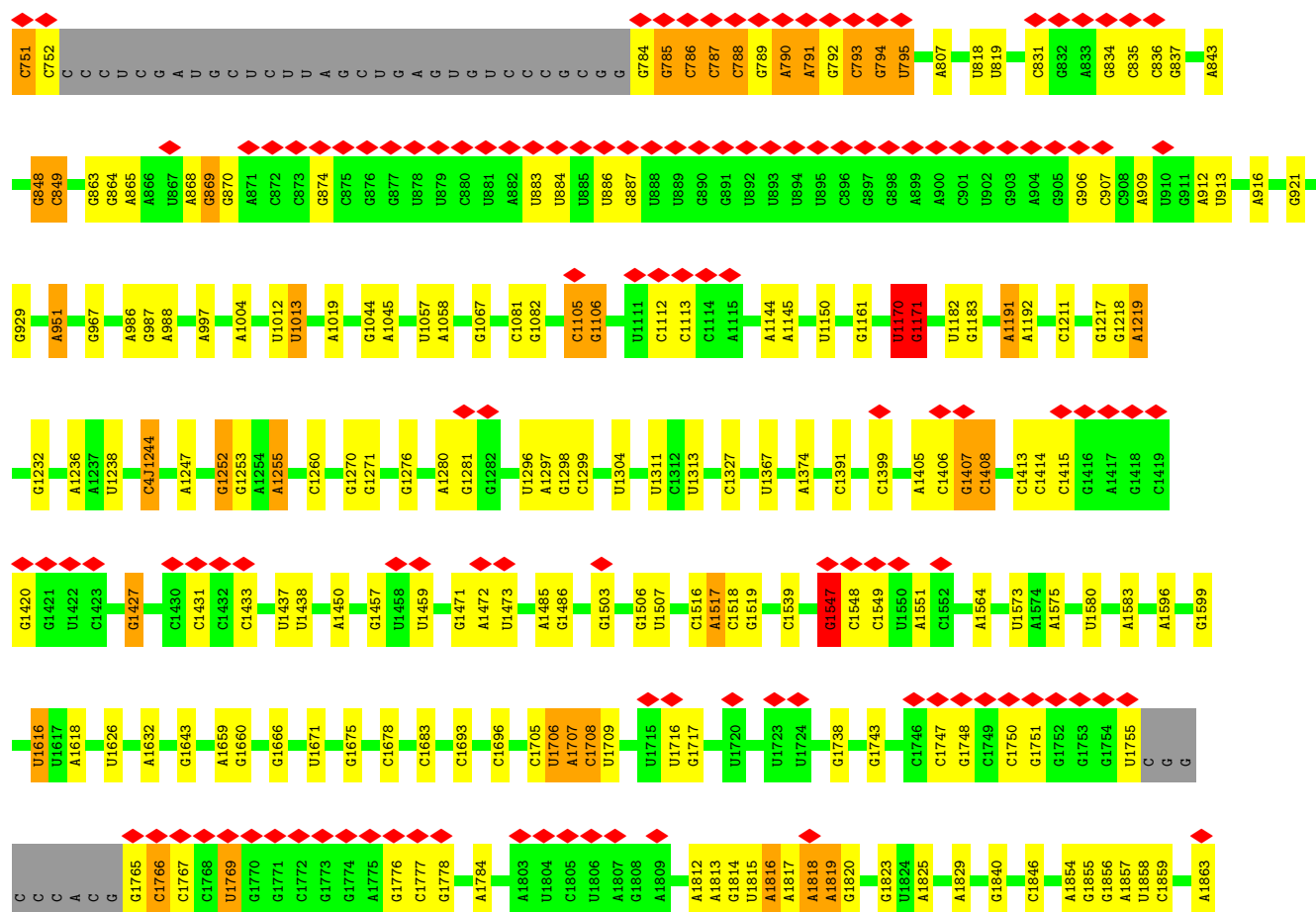


- Molecule 30: 40S ribosomal protein eS31



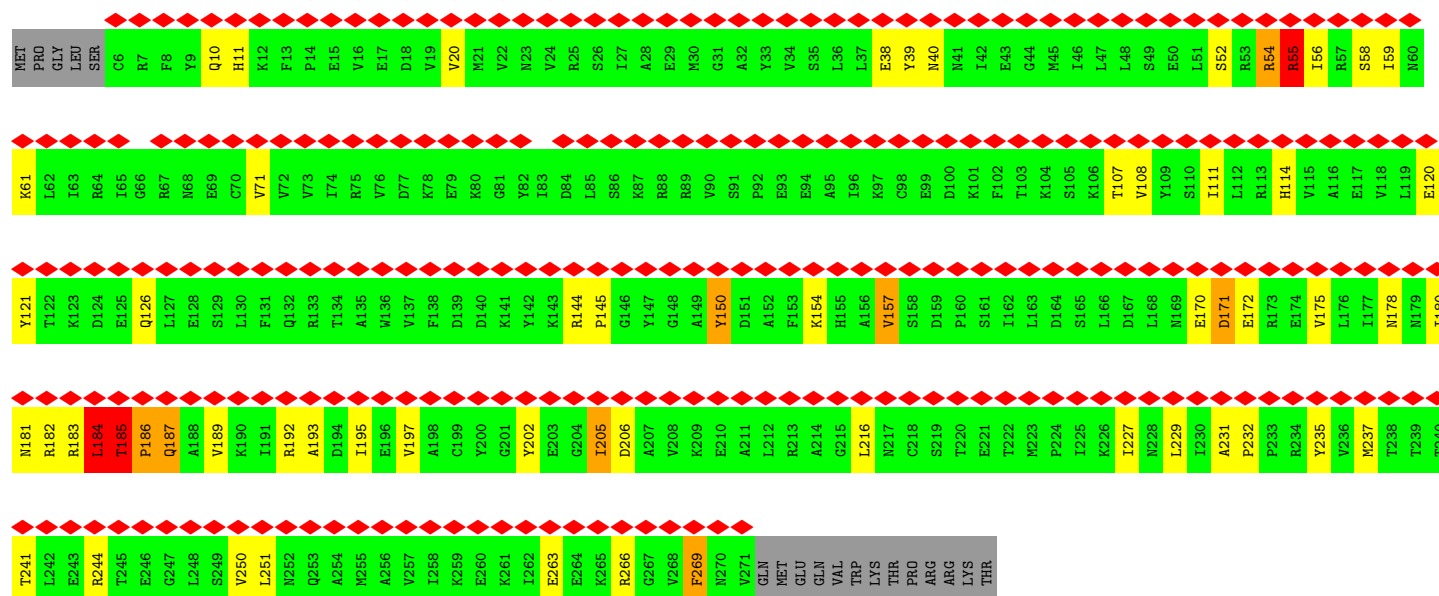
- Molecule 31: ribosomal protein RACK1



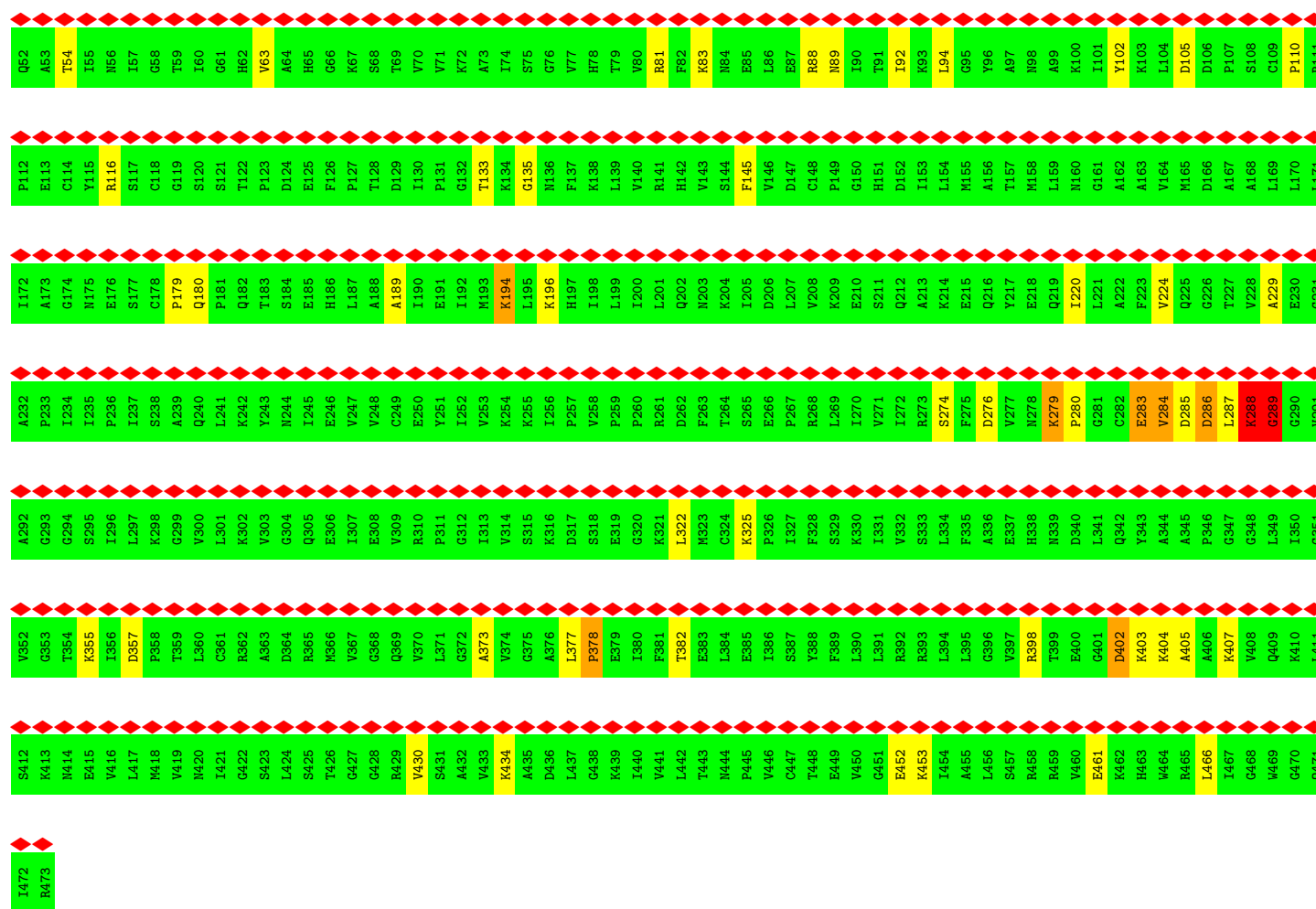
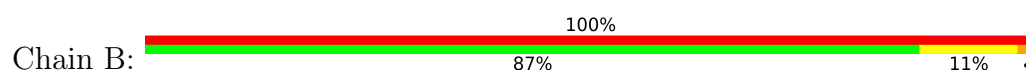


• Molecule 35: Eukaryotic translation initiation factor 2 subunit alpha

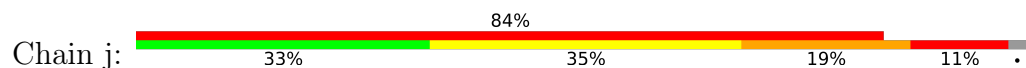
Chain A: 93% 72% 18% 6%



• Molecule 36: Eukaryotic translation initiation factor 2 subunit gamma

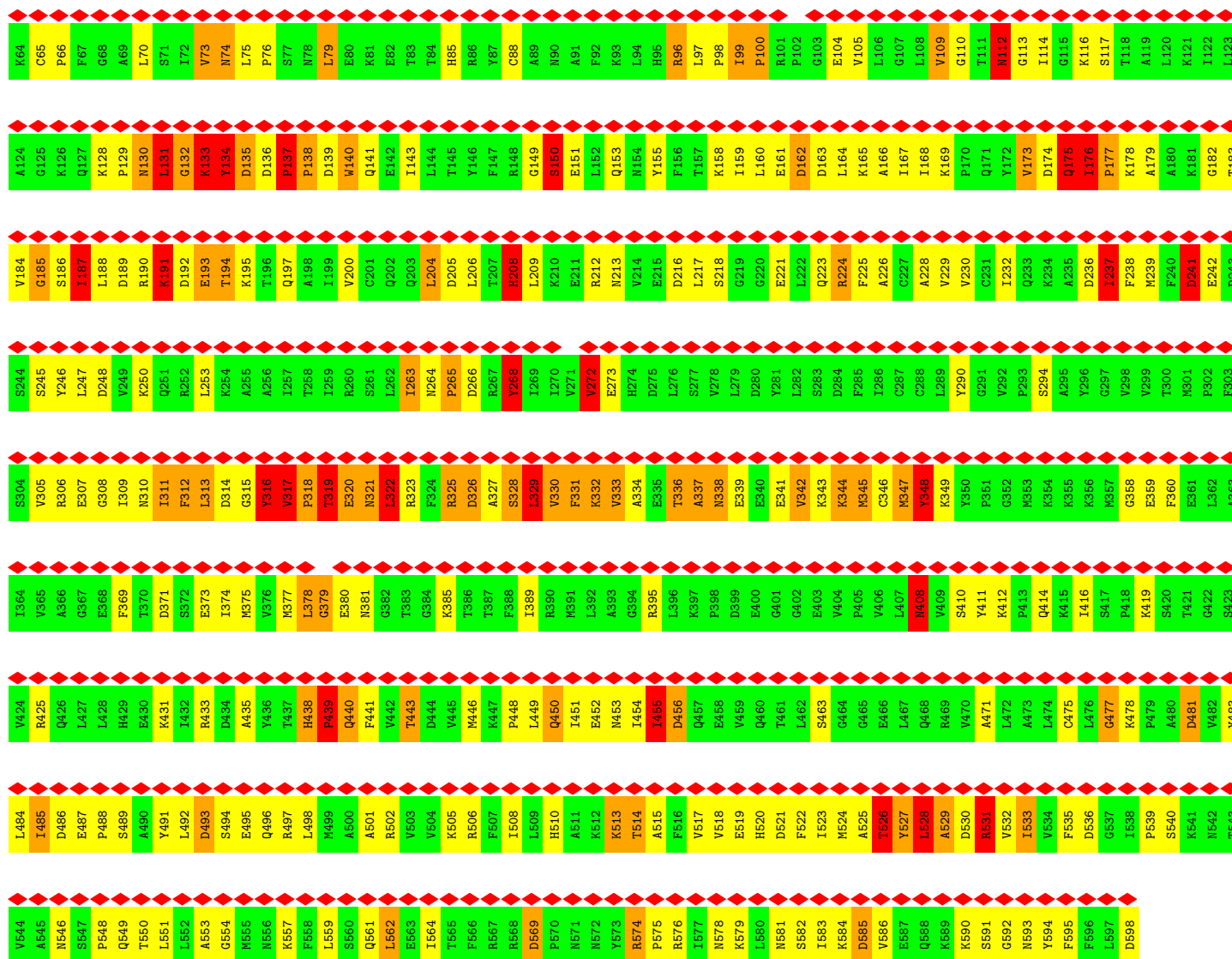


• Molecule 37: eukaryotic translation initiation factor 1A

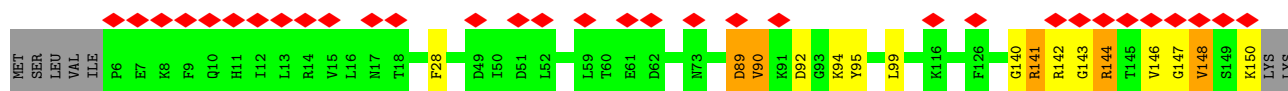
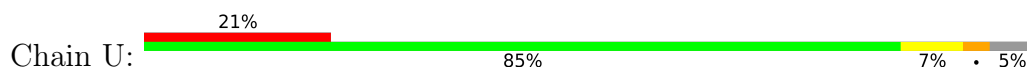


• Molecule 38: ATP-binding cassette sub-family E member 1 (ABCE1)

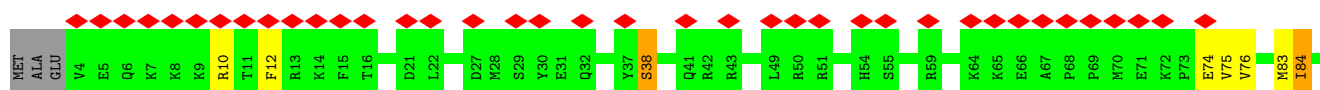
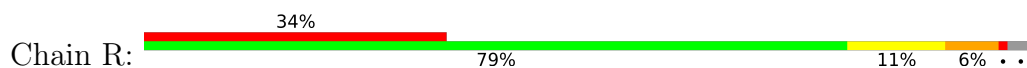


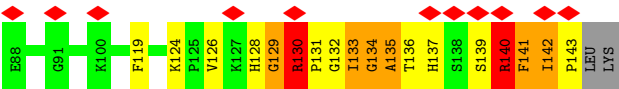


• Molecule 39: 40S ribosomal protein uS13

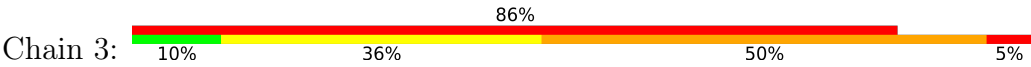


• Molecule 40: 40S ribosomal protein uS19





• Molecule 41: beta-globin mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	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	0.147	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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, C4J, SF4, GNP, T6A

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	1	1.44	8/1770 (0.5%)	1.29	11/2759 (0.4%)
2	l	1.60	0/241	1.35	0/305
3	C	1.24	0/1680	1.43	4/2283 (0.2%)
4	D	1.19	0/1769	1.44	16/2367 (0.7%)
5	E	1.18	0/1779	1.34	4/2399 (0.2%)
6	F	1.24	1/1792 (0.1%)	1.36	5/2412 (0.2%)
7	G	1.26	0/2125	1.36	7/2856 (0.2%)
8	H	1.26	0/1531	1.40	1/2059 (0.0%)
9	I	1.28	1/1947 (0.1%)	1.33	3/2590 (0.1%)
10	J	1.22	0/1553	1.43	6/2079 (0.3%)
11	K	1.29	0/1709	1.42	6/2278 (0.3%)
12	L	1.33	1/1523 (0.1%)	1.40	0/2031
13	M	1.25	0/852	1.49	7/1147 (0.6%)
14	N	1.22	0/1319	1.30	5/1761 (0.3%)
15	O	1.20	0/968	1.50	5/1296 (0.4%)
16	P	1.19	0/1232	1.43	3/1656 (0.2%)
17	Q	1.31	0/1029	1.45	4/1380 (0.3%)
18	S	1.31	0/1142	1.45	6/1528 (0.4%)
19	T	1.25	0/1031	1.39	2/1383 (0.1%)
20	V	1.25	0/1133	1.45	4/1517 (0.3%)
21	W	1.29	0/832	1.37	0/1117
22	X	1.42	1/627 (0.2%)	1.44	4/839 (0.5%)
23	Y	1.28	0/1051	1.39	2/1406 (0.1%)
24	Z	1.27	0/1124	1.35	0/1500
25	a	1.37	1/1038 (0.1%)	1.47	7/1380 (0.5%)
26	b	1.32	0/802	1.37	1/1076 (0.1%)
27	c	1.24	0/673	1.38	2/902 (0.2%)
28	d	1.39	0/508	1.17	0/680
29	e	1.35	0/455	1.46	2/603 (0.3%)
30	f	1.24	0/594	1.47	3/786 (0.4%)
31	g	1.23	0/2494	1.33	6/3394 (0.2%)
32	n	1.25	0/604	1.34	2/810 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	1.35	0/478	1.40	2/628 (0.3%)
34	2	0.89	8/41567 (0.0%)	0.99	23/64783 (0.0%)
35	A	0.97	3/2177 (0.1%)	1.50	11/2935 (0.4%)
36	B	1.19	2/3267 (0.1%)	1.46	24/4415 (0.5%)
37	j	0.96	2/893 (0.2%)	1.54	10/1186 (0.8%)
38	k	2.27	16/4772 (0.3%)	2.46	72/6428 (1.1%)
39	U	1.31	0/1211	1.45	3/1618 (0.2%)
40	R	1.24	0/1177	1.40	8/1571 (0.5%)
41	3	0.67	1/998 (0.1%)	0.80	3/1553 (0.2%)
All	All	1.18	45/95467 (0.0%)	1.30	284/137696 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	3	2
3	C	0	1
4	D	0	1
9	I	0	3
10	J	0	2
11	K	0	2
12	L	0	2
13	M	0	5
17	Q	0	2
18	S	0	2
22	X	0	1
25	a	0	1
26	b	0	1
27	c	0	1
29	e	0	4
30	f	0	1
33	i	0	3
34	2	1	47
35	A	0	7
36	B	0	8
37	j	0	12
38	k	0	33
39	U	0	3
All	All	4	144

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	455	ILE	C-N	-63.41	0.45	1.33
38	k	562	LEU	C-N	-59.66	0.52	1.33
38	k	408	ASN	C-N	-48.21	0.68	1.33
38	k	481	ASP	C-N	-43.98	0.79	1.33
38	k	378	LEU	C-N	42.00	1.94	1.33
38	k	104	GLU	C-N	-39.92	0.75	1.33
38	k	440	GLN	C-N	37.11	1.85	1.33
38	k	531	ARG	C-N	-30.24	0.82	1.33
38	k	109	VAL	C-N	29.11	1.79	1.34
1	1	17	C	O3'-P	25.70	1.99	1.61
38	k	241	ASP	C-N	-23.70	0.84	1.33
38	k	268	TYR	C-N	-22.63	1.02	1.33
1	1	17	C	C2'-O2'	-22.53	1.07	1.41
38	k	513	LYS	C-N	22.14	1.64	1.33
38	k	150	SER	C-N	-22.03	1.02	1.33
38	k	160	LEU	C-N	-20.73	1.05	1.33
25	a	9	THR	C-N	19.38	1.60	1.33
1	1	37	T6A	O3'-P	18.93	1.75	1.56
38	k	493	ASP	C-N	-18.75	1.09	1.33
34	2	80	G	O3'-P	-17.57	1.34	1.61
1	1	18	G	O3'-P	17.35	1.87	1.61
34	2	239	U	O3'-P	-16.47	1.36	1.61
1	1	18	G	C3'-O3'	-15.57	1.18	1.42
22	X	77	GLY	C-N	15.23	1.54	1.33
34	2	350	A	O3'-P	15.19	1.83	1.61
36	B	289	GLY	N-CA	-14.40	1.24	1.45
41	3	39	U	O3'-P	-14.22	1.39	1.61
37	j	95	TYR	C-N	-11.95	1.16	1.33
35	A	184	LEU	C-N	11.46	1.57	1.33
34	2	351	U	O3'-P	-10.84	1.44	1.61
1	1	16	G	O3'-P	-10.11	1.46	1.61
38	k	179	ALA	C-N	10.09	1.48	1.33
34	2	1170	U	O3'-P	-8.25	1.48	1.61
1	1	18	G	C1'-N9	-8.12	1.35	1.48
37	j	19	ASN	C-N	-7.63	1.23	1.33
34	2	1171	G	O3'-P	-7.34	1.50	1.61
9	I	217	MET	C-N	-7.07	1.25	1.33
36	B	288	LYS	C-N	-6.51	1.24	1.33
34	2	1170	U	C1'-N1	6.27	1.57	1.48
34	2	67	C	O3'-P	6.21	1.70	1.61
1	1	17	C	C3'-O3'	-5.93	1.34	1.43
35	A	10	GLN	C-O	-5.76	1.17	1.24
35	A	10	GLN	C-N	5.29	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	121	LYS	CA-C	-5.18	1.50	1.53
6	F	183	GLY	CA-C	-5.01	1.48	1.52

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	531	ARG	CA-C-N	-67.13	35.77	122.37
38	k	531	ARG	C-N-CA	-67.13	35.77	122.37
38	k	160	LEU	O-C-N	53.40	178.73	122.12
38	k	160	LEU	CA-C-N	-38.23	59.19	122.65
38	k	160	LEU	C-N-CA	-38.23	59.19	122.65
38	k	408	ASN	O-C-N	-30.93	81.45	122.59
38	k	481	ASP	O-C-N	-27.20	88.48	122.21
38	k	348	TYR	O-C-N	-25.85	88.21	122.59
1	1	17	C	C4'-C3'-O3'	24.17	145.65	109.40
38	k	531	ARG	O-C-N	24.04	154.79	122.57
38	k	378	LEU	CA-C-N	-22.59	77.13	121.41
38	k	378	LEU	C-N-CA	-22.59	77.13	121.41
38	k	481	ASP	CA-C-N	22.59	157.26	122.70
38	k	481	ASP	C-N-CA	22.59	157.26	122.70
38	k	104	GLU	O-C-N	-22.53	97.87	123.33
38	k	513	LYS	O-C-N	-20.72	95.03	122.59
38	k	455	ILE	O-C-N	-19.86	97.74	122.57
38	k	104	GLU	CA-C-N	19.84	149.03	121.66
38	k	104	GLU	C-N-CA	19.84	149.03	121.66
38	k	493	ASP	O-C-N	18.08	148.80	122.76
38	k	493	ASP	CA-C-N	-17.93	96.25	120.28
38	k	493	ASP	C-N-CA	-17.93	96.25	120.28
1	1	17	C	O3'-P-O5'	17.59	130.38	104.00
1	1	18	G	O3'-P-O5'	16.98	129.46	104.00
34	2	271	G	P-O3'-C3'	16.75	145.33	120.20
1	1	16	G	O3'-P-O5'	16.72	129.08	104.00
38	k	109	VAL	O-C-N	-16.61	98.12	122.20
25	a	12	PHE	CB-CA-C	16.46	139.75	109.46
38	k	455	ILE	CA-C-N	-15.46	92.02	121.54
38	k	455	ILE	C-N-CA	-15.46	92.02	121.54
34	2	351	U	P-O3'-C3'	14.62	142.12	120.20
37	j	29	LYS	CA-C-N	-14.16	94.49	121.54
37	j	29	LYS	C-N-CA	-14.16	94.49	121.54
37	j	29	LYS	O-C-N	-13.70	104.37	122.59
38	k	510	HIS	O-C-N	-13.50	107.50	122.09
34	2	1171	G	O3'-P-O5'	13.17	123.75	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1854	A	P-O3'-C3'	12.32	138.68	120.20
38	k	268	TYR	O-C-N	-12.28	107.61	123.21
38	k	272	VAL	O-C-N	11.76	135.55	122.97
34	2	350	A	O3'-P-O5'	-11.48	86.77	104.00
38	k	241	ASP	O-C-N	11.36	136.19	123.13
38	k	513	LYS	CA-C-N	11.27	143.06	121.54
38	k	513	LYS	C-N-CA	11.27	143.06	121.54
38	k	317	VAL	C-N-CD	-11.22	79.00	125.00
41	3	39	U	P-O3'-C3'	10.46	135.89	120.20
34	2	351	U	O3'-P-O5'	10.29	119.43	104.00
22	X	78	ILE	N-CA-CB	-10.02	94.47	111.50
36	B	288	LYS	CA-C-N	9.89	140.80	121.41
36	B	288	LYS	C-N-CA	9.89	140.80	121.41
38	k	263	ILE	N-CA-C	9.69	119.64	110.53
11	K	142	SER	CA-C-N	9.17	138.20	121.70
11	K	142	SER	C-N-CA	9.17	138.20	121.70
35	A	184	LEU	CA-C-N	9.12	144.05	121.80
35	A	184	LEU	C-N-CA	9.12	144.05	121.80
30	f	135	HIS	CA-CB-CG	8.95	122.75	113.80
38	k	408	ASN	CA-C-N	8.92	138.03	121.97
38	k	408	ASN	C-N-CA	8.92	138.03	121.97
38	k	109	VAL	CA-C-N	8.88	130.89	121.48
38	k	109	VAL	C-N-CA	8.88	130.89	121.48
38	k	150	SER	CA-C-N	-8.79	106.03	120.71
38	k	150	SER	C-N-CA	-8.79	106.03	120.71
34	2	1766	C	O3'-P-O5'	8.78	117.17	104.00
38	k	272	VAL	CA-C-N	-8.73	102.11	122.19
38	k	272	VAL	C-N-CA	-8.73	102.11	122.19
35	A	184	LEU	O-C-N	8.70	136.01	122.61
1	1	8	G	P-O3'-C3'	8.52	132.99	120.20
38	k	112	ASN	CA-CB-CG	-8.48	104.12	112.60
31	g	181	ASN	N-CA-C	-8.27	105.19	114.62
38	k	510	HIS	CA-C-N	8.23	138.77	122.31
38	k	510	HIS	C-N-CA	8.23	138.77	122.31
35	A	269	PHE	CA-CB-CG	-8.09	105.71	113.80
34	2	1170	U	P-O3'-C3'	8.03	132.24	120.20
34	2	67	C	O3'-P-O5'	-8.01	91.98	104.00
37	j	19	ASN	CA-C-N	7.94	136.71	121.54
37	j	19	ASN	C-N-CA	7.94	136.71	121.54
22	X	78	ILE	N-CA-C	7.81	132.88	111.00
34	2	351	U	OP1-P-O3'	-7.78	84.66	108.00
38	k	241	ASP	CA-C-N	-7.76	102.86	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	241	ASP	C-N-CA	-7.76	102.86	121.80
25	a	125	VAL	CA-C-N	-7.75	106.22	121.41
25	a	125	VAL	C-N-CA	-7.75	106.22	121.41
31	g	54	ILE	N-CA-C	-7.73	102.85	109.19
38	k	150	SER	O-C-N	7.56	134.47	122.61
34	2	1218	G	O3'-P-O5'	-7.51	92.73	104.00
16	P	22	VAL	C-N-CD	7.46	137.00	120.60
38	k	208	HIS	CA-CB-CG	7.42	121.22	113.80
1	1	16	G	OP2-P-O3'	-7.41	85.77	108.00
41	3	40	C	O3'-P-O5'	7.36	115.04	104.00
1	1	18	G	C4'-C3'-O3'	7.35	124.02	113.00
37	j	95	TYR	CA-C-N	7.26	134.49	122.07
37	j	95	TYR	C-N-CA	7.26	134.49	122.07
38	k	440	GLN	O-C-N	-7.26	112.93	122.59
25	a	86	GLU	N-CA-CB	7.05	122.91	110.37
34	2	834	G	O4'-C1'-N9	7.02	119.03	108.50
34	2	1671	U	P-O3'-C3'	7.02	130.72	120.20
36	B	94	LEU	CA-C-N	7.01	127.00	120.34
36	B	94	LEU	C-N-CA	7.01	127.00	120.34
38	k	136	ASP	CA-C-N	-6.91	113.26	120.38
38	k	136	ASP	C-N-CA	-6.91	113.26	120.38
35	A	206	ASP	CA-CB-CG	-6.88	105.72	112.60
36	B	289	GLY	N-CA-C	6.87	129.45	113.18
38	k	529	ALA	N-CA-C	6.85	121.03	110.42
5	E	69	PHE	CA-CB-CG	-6.82	106.98	113.80
36	B	286	ASP	CA-C-N	-6.80	111.40	122.82
36	B	286	ASP	C-N-CA	-6.80	111.40	122.82
23	Y	46	TYR	N-CA-C	-6.76	106.24	114.75
39	U	28	PHE	CA-CB-CG	-6.75	107.06	113.80
18	S	46	THR	N-CA-C	-6.69	106.33	114.75
34	2	80	G	O3'-P-O5'	6.62	113.92	104.00
38	k	35	GLY	N-CA-C	6.57	121.48	113.79
6	F	197	LYS	CA-C-N	6.57	133.53	121.70
6	F	197	LYS	C-N-CA	6.57	133.53	121.70
13	M	1	MET	CA-C-N	6.56	133.51	121.70
13	M	1	MET	C-N-CA	6.56	133.51	121.70
4	D	25	PHE	CA-CB-CG	-6.54	107.26	113.80
1	1	17	C	P-O3'-C3'	6.50	129.95	120.20
36	B	220	ILE	N-CA-CB	6.50	118.15	110.55
18	S	145	TYR	CA-C-N	-6.49	110.02	121.70
18	S	145	TYR	C-N-CA	-6.49	110.02	121.70
38	k	116	LYS	CA-C-N	6.46	128.94	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	116	LYS	C-N-CA	6.46	128.94	120.28
15	O	120	ALA	CA-C-N	6.45	129.25	120.54
15	O	120	ALA	C-N-CA	6.45	129.25	120.54
37	j	98	ASP	CA-CB-CG	-6.37	106.23	112.60
6	F	115	VAL	N-CA-C	-6.31	106.38	111.81
14	N	72	ILE	N-CA-C	-6.21	100.16	108.35
18	S	117	ARG	N-CA-C	-6.19	104.54	113.21
38	k	162	ASP	CA-CB-CG	6.17	118.77	112.60
34	2	1671	U	O3'-P-O5'	6.08	113.13	104.00
34	2	848	G	P-O3'-C3'	6.07	129.31	120.20
27	c	63	LEU	N-CA-C	-6.05	107.72	114.62
39	U	92	ASP	N-CA-C	-6.04	107.73	114.62
29	e	23	VAL	N-CA-CB	6.04	117.62	110.55
10	J	107	LYS	N-CA-C	-6.04	107.14	114.75
9	I	10	THR	N-CA-C	-6.00	106.94	114.56
1	1	18	G	OP1-P-O3'	-5.98	90.06	108.00
31	g	211	GLY	CA-C-N	5.97	128.28	120.28
31	g	211	GLY	C-N-CA	5.97	128.28	120.28
4	D	150	ILE	N-CA-C	-5.96	106.44	113.42
29	e	55	LEU	N-CA-C	-5.94	107.27	114.75
36	B	54	THR	N-CA-C	-5.92	107.87	114.62
41	3	40	C	OP2-P-O3'	-5.90	90.30	108.00
19	T	102	THR	N-CA-C	-5.89	105.76	113.12
38	k	463	SER	CA-C-N	5.87	126.62	119.99
38	k	463	SER	C-N-CA	5.87	126.62	119.99
34	2	1407	G	P-O3'-C3'	5.84	128.96	120.20
37	j	21	SER	N-CA-CB	5.80	120.30	110.49
38	k	237	ILE	O-C-N	-5.80	115.32	122.57
7	G	56	LEU	N-CA-C	-5.77	107.48	114.75
22	X	8	PHE	CA-CB-CG	-5.75	108.05	113.80
36	B	357	ASP	CA-C-N	5.74	127.02	119.84
36	B	357	ASP	C-N-CA	5.74	127.02	119.84
34	2	536	G	O3'-P-O5'	5.74	112.60	104.00
38	k	378	LEU	O-C-N	5.72	130.20	122.59
3	C	202	TYR	N-CA-C	-5.72	106.34	113.38
16	P	56	ASP	N-CA-C	5.69	117.57	111.36
40	R	119	PHE	CA-CB-CG	-5.69	108.11	113.80
11	K	65	PHE	CA-CB-CG	-5.68	108.12	113.80
22	X	10	ASP	N-CA-CB	5.67	120.08	110.49
36	B	377	LEU	CA-C-N	5.67	126.93	119.84
36	B	377	LEU	C-N-CA	5.67	126.93	119.84
36	B	180	GLN	CA-C-N	5.67	126.93	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	180	GLN	C-N-CA	5.67	126.93	119.84
13	M	91	PRO	N-CA-C	-5.66	106.72	114.98
36	B	145	PHE	CA-CB-CG	-5.64	108.16	113.80
38	k	439	PRO	N-CA-C	5.63	124.07	112.47
35	A	185	THR	N-CA-C	5.63	122.26	109.81
5	E	109	PHE	CA-CB-CG	-5.63	108.17	113.80
4	D	57	ILE	CA-C-N	5.60	128.09	120.54
4	D	57	ILE	C-N-CA	5.60	128.09	120.54
13	M	85	LEU	CA-C-N	5.59	126.14	120.38
13	M	85	LEU	C-N-CA	5.59	126.14	120.38
1	1	17	C	OP2-P-O3'	-5.58	91.25	108.00
34	2	73	C	P-O3'-C3'	5.57	128.56	120.20
34	2	1219	A	P-O3'-C3'	-5.57	111.85	120.20
38	k	438	HIS	CA-C-N	5.56	126.79	119.84
38	k	438	HIS	C-N-CA	5.56	126.79	119.84
32	n	103	HIS	CA-C-N	5.56	127.73	120.28
32	n	103	HIS	C-N-CA	5.56	127.73	120.28
35	A	232	PRO	N-CA-C	5.55	117.47	110.70
40	R	130	ARG	CA-C-N	-5.53	114.26	119.90
40	R	130	ARG	C-N-CA	-5.53	114.26	119.90
3	C	8	LEU	N-CA-C	-5.52	107.80	114.75
7	G	26	VAL	N-CA-C	5.51	116.24	110.62
36	B	194	LYS	N-CA-CB	5.51	119.81	110.49
4	D	188	LEU	CA-C-N	5.49	124.72	120.33
4	D	188	LEU	C-N-CA	5.49	124.72	120.33
7	G	12	VAL	N-CA-C	-5.47	105.34	113.39
39	U	90	VAL	N-CA-C	-5.45	98.00	109.34
36	B	325	LYS	CA-C-N	5.44	125.44	119.89
36	B	325	LYS	C-N-CA	5.44	125.44	119.89
27	c	57	VAL	N-CA-C	-5.44	107.50	113.43
25	a	35	VAL	CA-C-N	5.43	125.43	119.89
25	a	35	VAL	C-N-CA	5.43	125.43	119.89
23	Y	62	VAL	N-CA-C	-5.41	100.05	108.81
16	P	134	VAL	N-CA-C	-5.40	107.54	113.43
38	k	162	ASP	N-CA-C	5.40	119.02	111.90
15	O	95	ASP	N-CA-CB	5.38	119.59	110.49
35	A	10	GLN	N-CA-CB	5.38	118.04	110.12
19	T	89	SER	N-CA-C	-5.37	106.60	114.39
20	V	72	VAL	CA-C-N	5.37	125.80	119.94
20	V	72	VAL	C-N-CA	5.37	125.80	119.94
34	2	1067	G	O3'-P-O5'	5.36	112.04	104.00
4	D	39	PHE	CA-CB-CG	-5.35	108.45	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	i	118	ASN	CA-C-N	5.33	131.30	121.70
33	i	118	ASN	C-N-CA	5.33	131.30	121.70
36	B	189	ALA	CA-C-N	5.32	127.37	120.56
36	B	189	ALA	C-N-CA	5.32	127.37	120.56
11	K	157	LYS	CA-C-N	5.32	131.55	121.97
11	K	157	LYS	C-N-CA	5.32	131.55	121.97
36	B	382	THR	N-CA-C	-5.30	107.46	114.04
4	D	209	ASP	N-CA-CB	5.29	119.43	110.49
14	N	40	ILE	N-CA-C	-5.29	107.67	112.96
14	N	134	LEU	N-CA-C	-5.29	107.38	113.88
40	R	38	SER	CA-C-N	5.28	128.74	120.82
40	R	38	SER	C-N-CA	5.28	128.74	120.82
7	G	42	LEU	CA-C-N	5.27	125.27	119.89
7	G	42	LEU	C-N-CA	5.27	125.27	119.89
13	M	72	THR	CA-C-N	5.26	127.34	120.28
13	M	72	THR	C-N-CA	5.26	127.34	120.28
31	g	93	THR	N-CA-C	-5.26	108.62	114.62
38	k	137	PRO	CA-C-N	-5.26	113.26	119.84
38	k	137	PRO	C-N-CA	-5.26	113.26	119.84
38	k	128	LYS	CA-C-N	-5.26	113.26	119.84
38	k	128	LYS	C-N-CA	-5.26	113.26	119.84
38	k	176	ILE	CA-C-N	-5.24	113.28	119.84
38	k	176	ILE	C-N-CA	-5.24	113.28	119.84
11	K	155	ASN	N-CA-C	-5.23	104.70	111.71
40	R	124	LYS	CA-C-N	5.23	125.28	119.32
40	R	124	LYS	C-N-CA	5.23	125.28	119.32
3	C	48	ILE	CA-C-N	5.22	127.50	120.50
3	C	48	ILE	C-N-CA	5.22	127.50	120.50
10	J	7	LYS	N-CA-C	-5.21	108.68	114.62
1	1	18	G	P-O3'-C3'	5.19	127.99	120.20
17	Q	139	SER	CA-C-N	5.19	128.45	120.82
17	Q	139	SER	C-N-CA	5.19	128.45	120.82
5	E	249	SER	CA-C-N	5.18	124.50	118.85
5	E	249	SER	C-N-CA	5.18	124.50	118.85
36	B	92	ILE	N-CA-C	-5.18	108.08	113.10
4	D	210	VAL	N-CA-C	-5.18	101.18	108.27
10	J	35	ASP	CA-CB-CG	5.17	117.77	112.60
35	A	171	ASP	CA-C-N	5.16	127.19	120.28
35	A	171	ASP	C-N-CA	5.16	127.19	120.28
6	F	11	PHE	CA-CB-CG	-5.14	108.66	113.80
15	O	81	ASP	CA-C-N	5.14	127.88	120.38
15	O	81	ASP	C-N-CA	5.14	127.88	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	11	HIS	ND1-CG-CD2	5.13	111.23	106.10
40	R	76	VAL	N-CA-C	-5.13	101.09	108.53
4	D	222	LYS	CA-C-N	5.12	127.91	120.79
4	D	222	LYS	C-N-CA	5.12	127.91	120.79
36	B	434	LYS	N-CA-C	-5.12	102.20	110.14
7	G	221	ARG	CA-C-N	5.10	127.12	120.28
7	G	221	ARG	C-N-CA	5.10	127.12	120.28
20	V	123	LEU	CA-C-N	5.10	128.41	120.60
20	V	123	LEU	C-N-CA	5.10	128.41	120.60
25	a	9	THR	O-C-N	5.10	129.38	122.59
8	H	82	ASN	CA-CB-CG	-5.10	107.50	112.60
34	2	317	G	P-O3'-C3'	5.08	127.82	120.20
6	F	142	LEU	N-CA-CB	5.08	119.07	110.49
4	D	146	CYS	CA-C-N	5.08	127.39	120.54
4	D	146	CYS	C-N-CA	5.08	127.39	120.54
37	j	112	HIS	CB-CG-CD2	-5.08	124.60	131.20
17	Q	137	SER	CA-C-N	5.07	131.23	121.54
17	Q	137	SER	C-N-CA	5.07	131.23	121.54
10	J	114	GLN	CA-C-N	5.07	127.08	120.28
10	J	114	GLN	C-N-CA	5.07	127.08	120.28
38	k	161	GLU	CA-C-N	5.06	129.52	122.08
38	k	161	GLU	C-N-CA	5.06	129.52	122.08
9	I	137	ARG	CA-C-N	5.06	127.33	120.65
9	I	137	ARG	C-N-CA	5.06	127.33	120.65
30	f	97	LYS	CA-C-N	5.06	131.08	121.97
30	f	97	LYS	C-N-CA	5.06	131.08	121.97
18	S	117	ARG	CA-C-N	5.06	131.20	121.54
18	S	117	ARG	C-N-CA	5.06	131.20	121.54
4	D	180	ASP	CA-C-N	5.04	128.39	120.82
4	D	180	ASP	C-N-CA	5.04	128.39	120.82
26	b	34	LYS	N-CA-C	-5.04	108.16	114.56
38	k	11	VAL	N-CA-C	5.04	119.83	109.34
31	g	277	THR	N-CA-C	-5.04	101.42	109.07
4	D	82	ARG	N-CA-CB	5.03	119.00	110.49
10	J	106	ARG	N-CA-CB	5.03	118.99	110.49
14	N	132	ARG	CA-C-N	5.01	125.01	119.90
14	N	132	ARG	C-N-CA	5.01	125.01	119.90
34	2	79	A	C4'-C3'-C2'	-5.00	97.60	102.60

All (4) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
1	1	17	C	C3',C2'
1	1	18	G	C3'
34	2	1244	C4J	C4'

All (144) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	18	G	Sidechain
1	1	26	G	Sidechain
34	2	1044	G	Sidechain
34	2	1105	C	Sidechain
34	2	1161	G	Sidechain
34	2	1170	U	Sidechain
34	2	1171	G	Sidechain
34	2	1182	U	Sidechain
34	2	1183	G	Sidechain
34	2	1191	A	Sidechain
34	2	1192	A	Sidechain
34	2	1236	A	Sidechain
34	2	1252	G	Sidechain
34	2	1255	A	Sidechain
34	2	126	G	Sidechain
34	2	1304	U	Sidechain
34	2	1405	A	Sidechain
34	2	1427	G	Sidechain
34	2	1437	U	Sidechain
34	2	1438	U	Sidechain
34	2	146	G	Sidechain
34	2	148	U	Sidechain
34	2	1547	G	Sidechain
34	2	1564	A	Sidechain
34	2	1599	G	Sidechain
34	2	1616	U	Sidechain
34	2	1626	U	Sidechain
34	2	1738	G	Sidechain
34	2	1750	C	Sidechain
34	2	1769	U	Sidechain
34	2	1776	G	Sidechain
34	2	1784	A	Sidechain
34	2	1840	G	Sidechain
34	2	195	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
34	2	240	C	Sidechain
34	2	318	U	Sidechain
34	2	39	A	Sidechain
34	2	435	A	Sidechain
34	2	526	A	Sidechain
34	2	554	A	Sidechain
34	2	574	A	Sidechain
34	2	576	G	Sidechain
34	2	660	A	Sidechain
34	2	71	G	Sidechain
34	2	76	U	Sidechain
34	2	82	G	Sidechain
34	2	869	G	Sidechain
34	2	951	A	Sidechain
34	2	997	A	Sidechain
35	A	150	TYR	Sidechain
35	A	184	LEU	Peptide
35	A	185	THR	Peptide
35	A	186	PRO	Peptide
35	A	187	GLN	Peptide
35	A	192	ARG	Sidechain
35	A	39	TYR	Sidechain
36	B	110	PRO	Peptide
36	B	133	THR	Peptide
36	B	287	LEU	Peptide
36	B	288	LYS	Mainchain,Peptide
36	B	289	GLY	Peptide
36	B	322	LEU	Peptide
36	B	373	ALA	Peptide
3	C	193	HIS	Peptide
4	D	208	HIS	Peptide
9	I	217	MET	Mainchain
9	I	68	LEU	Peptide
9	I	69	THR	Peptide
10	J	105	THR	Peptide
10	J	66	VAL	Peptide
11	K	144	LYS	Peptide
11	K	157	LYS	Peptide
12	L	147	PHE	Peptide
12	L	148	ILE	Peptide
13	M	1	MET	Peptide
13	M	34	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	M	35	LEU	Peptide
13	M	43	LEU	Peptide
13	M	96	ARG	Sidechain
17	Q	35	ALA	Peptide
17	Q	36	SER	Peptide
18	S	42	ILE	Peptide
18	S	43	GLU	Peptide
39	U	89	ASP	Peptide
39	U	94	LYS	Peptide
39	U	99	LEU	Peptide
22	X	77	GLY	Mainchain
25	a	126	GLY	Peptide
26	b	46	GLU	Peptide
27	c	81	ARG	Peptide
29	e	28	HIS	Peptide
29	e	32	ARG	Peptide
29	e	49	ASP	Peptide
29	e	52	PHE	Peptide
30	f	90	LYS	Peptide
33	i	126	LYS	Peptide
33	i	78	GLY	Peptide
33	i	82	ARG	Sidechain
37	j	15	GLY	Peptide
37	j	16	LYS	Peptide
37	j	18	GLU	Peptide
37	j	19	ASN	Peptide
37	j	22	GLU	Peptide
37	j	23	LYS	Peptide
37	j	24	ARG	Peptide
37	j	25	GLU	Peptide
37	j	28	PHE	Peptide
37	j	29	LYS	Mainchain,Peptide
37	j	92	ILE	Peptide
38	k	129	PRO	Peptide
38	k	130	ASN	Peptide
38	k	131	LEU	Peptide
38	k	132	GLY	Peptide
38	k	133	LYS	Peptide
38	k	134	TYR	Peptide
38	k	137	PRO	Peptide
38	k	138	PRO	Peptide
38	k	150	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
38	k	173	VAL	Peptide
38	k	175	GLN	Peptide
38	k	176	ILE	Peptide
38	k	192	ASP	Peptide
38	k	193	GLU	Peptide
38	k	208	HIS	Sidechain
38	k	237	ILE	Mainchain
38	k	241	ASP	Mainchain
38	k	268	TYR	Mainchain
38	k	272	VAL	Mainchain
38	k	290	TYR	Sidechain
38	k	348	TYR	Mainchain,Peptide
38	k	408	ASN	Mainchain
38	k	438	HIS	Peptide
38	k	455	ILE	Mainchain,Peptide
38	k	481	ASP	Mainchain
38	k	513	LYS	Mainchain
38	k	531	ARG	Mainchain
38	k	535	PHE	Sidechain
38	k	569	ASP	Peptide
38	k	574	ARG	Sidechain
38	k	96	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1614	0	822	49	0
2	l	240	0	289	0	0
3	C	1643	0	1646	0	0
4	D	1741	0	1815	0	0
5	E	1743	0	1836	1	0
6	F	1764	0	1863	23	0
7	G	2083	0	2189	0	0
8	H	1509	0	1563	1	0
9	I	1924	0	2089	16	0
10	J	1530	0	1627	22	0
11	K	1680	0	1762	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1499	0	1608	0	0
13	M	828	0	854	1	0
14	N	1296	0	1374	29	0
15	O	958	0	993	1	0
16	P	1208	0	1294	62	0
17	Q	1016	0	1039	1	0
18	S	1124	0	1193	7	0
19	T	1019	0	1075	0	0
20	V	1113	0	1149	0	0
21	W	822	0	887	0	0
22	X	620	0	622	0	0
23	Y	1034	0	1080	1	0
24	Z	1106	0	1179	48	0
25	a	1021	0	1085	77	0
26	b	789	0	839	1	0
27	c	659	0	683	2	0
28	d	506	0	536	0	0
29	e	445	0	442	1	0
30	f	582	0	599	1	0
31	g	2437	0	2393	0	0
32	n	598	0	656	0	0
33	i	473	0	524	34	0
34	2	37204	0	18784	424	0
35	A	2146	0	2191	130	0
36	B	3214	0	3353	49	0
37	j	883	0	903	254	0
38	k	4693	0	4798	728	0
39	U	1194	0	1252	60	0
40	R	1154	0	1213	93	0
41	3	892	0	458	129	0
42	k	16	0	0	14	0
43	k	1	0	0	0	0
44	k	64	0	26	30	0
All	All	90085	0	72583	1862	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 12.

All (1862) 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)
10:J:109:ARG:CB	34:2:740:G:H1'	1.18	1.62
35:A:235:TYR:CD1	36:B:285:ASP:CG	1.76	1.60
35:A:229:LEU:HD22	36:B:284:VAL:CG2	1.14	1.60
38:k:332:LYS:HG2	38:k:527:TYR:CD2	1.25	1.60
38:k:73:VAL:HB	38:k:322:LEU:CD2	1.30	1.59
37:j:92:ILE:HG22	37:j:93:LEU:CG	1.27	1.55
37:j:92:ILE:CG2	37:j:93:LEU:HG	1.31	1.54
39:U:146:VAL:CG1	40:R:131:PRO:CG	1.83	1.53
38:k:73:VAL:CB	38:k:322:LEU:HD22	1.38	1.52
34:2:1693:C:C6	41:3:58:C:N4	1.79	1.51
35:A:229:LEU:CD2	36:B:284:VAL:HG21	1.43	1.49
34:2:1518:C:C4'	39:U:144:ARG:HA	1.41	1.48
16:P:20:ARG:HD2	16:P:65:PHE:CE1	1.48	1.47
38:k:241:ASP:C	38:k:242:GLU:CA	1.84	1.47
38:k:414:GLN:CD	38:k:486:ASP:HB3	1.05	1.46
39:U:146:VAL:CG1	40:R:131:PRO:HG3	1.01	1.46
38:k:414:GLN:CD	38:k:486:ASP:CB	1.86	1.45
38:k:414:GLN:NE2	38:k:486:ASP:CB	1.78	1.45
34:2:1705:C:H1'	37:j:42:LEU:CD2	1.49	1.43
39:U:146:VAL:HG13	40:R:131:PRO:CG	1.43	1.43
10:J:109:ARG:CB	34:2:740:G:C1'	1.98	1.42
37:j:8:GLY:HA2	40:R:140:ARG:NH2	1.29	1.41
38:k:521:ASP:HB3	38:k:524:MET:CB	1.46	1.41
16:P:20:ARG:CD	16:P:65:PHE:CE1	2.05	1.39
38:k:241:ASP:CA	38:k:242:GLU:N	1.84	1.39
38:k:332:LYS:HG2	38:k:527:TYR:CE2	1.58	1.38
38:k:109:VAL:C	38:k:110:GLY:N	1.79	1.38
38:k:332:LYS:HE3	38:k:334:ALA:CB	1.52	1.36
37:j:70:TRP:CD1	40:R:143:PRO:HA	1.60	1.35
38:k:204:LEU:HG	38:k:224:ARG:NH1	1.34	1.35
10:J:109:ARG:HB2	34:2:740:G:C1'	1.56	1.33
38:k:440:GLN:C	38:k:441:PHE:N	1.85	1.32
38:k:522:PHE:O	38:k:526:THR:HG22	1.29	1.32
9:I:237:LEU:HD12	34:2:784:G:O3'	1.30	1.31
35:A:235:TYR:CG	36:B:285:ASP:OD2	1.82	1.31
37:j:8:GLY:CA	40:R:140:ARG:HH22	1.44	1.30
35:A:229:LEU:CD2	36:B:284:VAL:CG2	2.02	1.30
34:2:1327:C:H41	37:j:15:GLY:C	1.37	1.30
39:U:143:GLY:O	39:U:144:ARG:CG	1.78	1.30
38:k:414:GLN:HG3	38:k:486:ASP:C	1.54	1.29
40:R:143:PRO:HG2	41:3:55:G:N3	1.45	1.29
25:a:104:ARG:NH2	25:a:108:LYS:NZ	1.79	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1705:C:C1'	37:j:42:LEU:HD21	1.61	1.29
38:k:332:LYS:O	38:k:334:ALA:N	1.65	1.29
38:k:183:THR:O	38:k:187:ILE:HG22	1.23	1.28
38:k:332:LYS:CE	38:k:334:ALA:HB2	1.63	1.27
24:Z:68:LYS:HG3	37:j:84:TYR:OH	1.21	1.27
38:k:183:THR:O	38:k:187:ILE:CG2	1.82	1.26
38:k:318:PRO:CG	38:k:322:LEU:HA	1.63	1.26
24:Z:58:GLU:OE1	37:j:60:HIS:CE1	1.88	1.26
38:k:209:LEU:CD1	38:k:221:GLU:HG3	1.64	1.26
38:k:414:GLN:NE2	38:k:486:ASP:HB3	0.93	1.26
37:j:70:TRP:HZ2	41:3:55:G:C2'	1.47	1.25
37:j:93:LEU:O	37:j:94:LYS:O	1.54	1.25
38:k:374:ILE:HD11	38:k:529:ALA:C	1.63	1.24
11:K:193:LYS:NZ	14:N:32:LYS:HZ1	1.35	1.24
34:2:740:G:H21	34:2:794:G:C1'	1.50	1.24
6:F:3:VAL:HG11	34:2:1573:U:O4	1.35	1.23
37:j:8:GLY:C	40:R:140:ARG:HH22	1.47	1.23
35:A:229:LEU:CG	36:B:284:VAL:HG21	1.68	1.22
34:2:1812:A:C2	34:2:1813:A:C8	2.28	1.22
35:A:58:SER:OG	35:A:61:LYS:HG2	1.37	1.21
38:k:332:LYS:CG	38:k:527:TYR:CD2	2.21	1.21
38:k:329:LEU:O	38:k:498:LEU:HD12	1.37	1.21
38:k:374:ILE:CD1	38:k:528:LEU:O	1.88	1.21
1:1:17:C:O3'	1:1:18:G:P	1.99	1.20
34:2:1519:G:P	39:U:144:ARG:HB3	1.80	1.20
39:U:143:GLY:O	39:U:144:ARG:HG3	1.07	1.20
34:2:478:U:OP1	38:k:150:SER:HB2	1.38	1.20
34:2:1518:C:H4'	39:U:144:ARG:CA	1.71	1.20
34:2:1693:C:N1	41:3:58:C:N4	1.76	1.19
38:k:411:TYR:C	38:k:412:LYS:N	2.01	1.19
25:a:104:ARG:HH22	25:a:108:LYS:NZ	1.37	1.19
38:k:315:GLY:HA2	38:k:326:ASP:C	1.66	1.19
11:K:193:LYS:HZ3	14:N:32:LYS:NZ	1.40	1.19
34:2:1707:A:C2	34:2:1708:C:C2	2.30	1.19
10:J:109:ARG:HB3	34:2:740:G:C1'	1.66	1.19
1:1:18:G:H4'	1:1:61:C:OP1	1.43	1.18
34:2:1706:U:H2'	34:2:1707:A:H8	1.03	1.18
25:a:12:PHE:CE1	34:2:836:C:O2'	1.94	1.18
38:k:591:SER:C	38:k:592:GLY:N	2.02	1.17
33:i:78:GLY:N	37:j:33:GLN:OE1	1.76	1.17
11:K:193:LYS:NZ	14:N:32:LYS:NZ	1.93	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:97:ASN:OD1	38:k:34:MET:HE1	1.41	1.16
38:k:378:LEU:O	38:k:385:LYS:HD3	1.43	1.16
38:k:204:LEU:CG	38:k:224:ARG:NH1	2.08	1.16
38:k:315:GLY:CA	38:k:326:ASP:O	1.93	1.16
35:A:157:VAL:CG1	35:A:180:ILE:HG21	1.76	1.16
37:j:8:GLY:CA	40:R:140:ARG:NH2	2.04	1.16
41:3:76:A:H2'	41:3:77:A:H5'	1.26	1.16
24:Z:78:GLY:HA2	38:k:60:ILE:HD11	1.19	1.16
33:i:80:LEU:CD2	37:j:62:ARG:HH21	1.57	1.16
34:2:158:A:OP1	38:k:583:ILE:CG2	1.92	1.16
40:R:143:PRO:CG	41:3:55:G:N3	2.10	1.15
35:A:235:TYR:CD1	36:B:285:ASP:OD2	1.92	1.15
38:k:332:LYS:CE	38:k:502:ARG:HD3	1.75	1.15
38:k:375:MET:HE1	38:k:531:ARG:CD	1.76	1.15
1:1:34:C:N4	41:3:54:G:O6	1.80	1.15
24:Z:97:ASN:OD1	38:k:34:MET:CE	1.95	1.14
37:j:70:TRP:CZ2	41:3:55:G:H2'	1.80	1.14
38:k:375:MET:SD	38:k:533:ILE:HG23	1.88	1.14
33:i:82:ARG:HH22	33:i:84:GLY:C	1.54	1.14
38:k:209:LEU:HD11	38:k:221:GLU:CG	1.76	1.14
24:Z:58:GLU:OE1	37:j:60:HIS:HE1	1.23	1.14
38:k:315:GLY:O	38:k:325:ARG:O	1.63	1.14
38:k:378:LEU:C	38:k:379:GLY:CA	2.16	1.14
37:j:70:TRP:CZ2	41:3:55:G:C2'	2.29	1.14
35:A:227:ILE:CD1	35:A:237:MET:HE2	1.76	1.13
24:Z:78:GLY:CA	38:k:60:ILE:HD11	1.78	1.13
38:k:315:GLY:HA2	38:k:326:ASP:O	1.46	1.12
38:k:412:LYS:HB3	38:k:485:ILE:HA	1.19	1.12
38:k:332:LYS:HE2	38:k:502:ARG:CD	1.79	1.12
34:2:740:G:N2	34:2:794:G:H1'	1.62	1.12
35:A:229:LEU:HD22	36:B:284:VAL:HG23	1.24	1.12
34:2:1327:C:H41	37:j:16:LYS:N	1.48	1.12
38:k:412:LYS:HD3	38:k:485:ILE:HG13	1.31	1.12
34:2:472:G:OP1	38:k:63:LYS:HE3	1.50	1.12
35:A:157:VAL:HG21	35:A:180:ILE:CG2	1.80	1.11
38:k:374:ILE:HD12	38:k:528:LEU:O	0.94	1.11
38:k:374:ILE:HD12	38:k:528:LEU:C	1.76	1.11
35:A:58:SER:CB	35:A:61:LYS:HG2	1.81	1.11
35:A:185:THR:HB	35:A:187:GLN:HB2	1.28	1.11
35:A:227:ILE:HD11	35:A:237:MET:HE2	1.25	1.11
1:1:17:C:N4	1:1:60:A:N3	1.99	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:318:PRO:CB	38:k:322:LEU:HA	1.80	1.11
38:k:17:LYS:HG2	38:k:20:LYS:CE	1.80	1.10
38:k:73:VAL:CB	38:k:322:LEU:CD2	2.09	1.10
38:k:486:ASP:C	38:k:487:GLU:N	2.09	1.10
34:2:1707:A:C2	34:2:1708:C:N1	2.20	1.10
41:3:38:C:O2	41:3:39:U:O4	1.66	1.10
38:k:332:LYS:CG	38:k:527:TYR:CE2	2.32	1.10
38:k:375:MET:HE1	38:k:531:ARG:HD2	1.12	1.10
1:1:18:G:H1'	1:1:61:C:H5'	1.24	1.09
1:1:35:A:C4'	37:j:8:GLY:O	2.00	1.09
24:Z:60:LYS:NZ	34:2:1817:A:OP1	1.84	1.09
35:A:235:TYR:CE1	36:B:285:ASP:CG	2.29	1.09
38:k:217:LEU:HG	38:k:221:GLU:HG2	1.27	1.09
24:Z:97:ASN:CG	38:k:34:MET:HE1	1.77	1.09
38:k:212:ARG:HD2	38:k:359:GLU:OE2	1.51	1.09
35:A:157:VAL:HG11	35:A:180:ILE:HG21	1.26	1.08
37:j:78:LEU:HD23	37:j:93:LEU:HB2	1.25	1.08
37:j:78:LEU:CD2	37:j:93:LEU:HD12	1.82	1.08
40:R:133:ILE:HG23	40:R:134:GLY:H	0.96	1.08
41:3:58:C:O2	41:3:59:A:C5	2.05	1.08
38:k:412:LYS:N	38:k:484:LEU:O	1.86	1.08
39:U:146:VAL:HG11	40:R:131:PRO:HB3	1.35	1.08
39:U:146:VAL:HG12	40:R:131:PRO:HG3	1.23	1.07
6:F:3:VAL:HG22	6:F:4:GLN:H	1.15	1.07
25:a:104:ARG:HH21	25:a:108:LYS:CE	1.66	1.07
37:j:67:LYS:HE3	41:3:56:U:C4'	1.83	1.07
38:k:330:VAL:HG22	38:k:575:PRO:HD2	1.33	1.07
38:k:332:LYS:HE3	38:k:334:ALA:HB2	1.09	1.07
38:k:501:ALA:HB1	38:k:528:LEU:HD11	1.35	1.07
37:j:67:LYS:HE3	41:3:56:U:H4'	1.10	1.07
38:k:65:CYS:SG	42:k:702:SF4:FE3	1.44	1.07
38:k:498:LEU:HD11	38:k:523:ILE:HD12	1.29	1.07
39:U:143:GLY:C	39:U:144:ARG:HD2	1.79	1.07
38:k:4:LYS:HA	38:k:79:LEU:CG	1.84	1.06
35:A:157:VAL:HG11	35:A:180:ILE:CG2	1.83	1.06
35:A:229:LEU:CB	36:B:284:VAL:HG21	1.85	1.06
38:k:347:MET:O	38:k:348:TYR:O	1.73	1.06
37:j:10:LYS:CG	37:j:11:ASN:H	1.67	1.06
38:k:330:VAL:HG21	38:k:574:ARG:HD3	1.35	1.06
38:k:451:ILE:HG13	38:k:452:GLU:N	1.69	1.06
37:j:10:LYS:HG2	37:j:11:ASN:N	1.58	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:104:ARG:HH21	25:a:108:LYS:HE3	1.19	1.05
34:2:1706:U:H2'	34:2:1707:A:C8	1.89	1.05
38:k:330:VAL:HG21	38:k:574:ARG:CD	1.83	1.05
34:2:158:A:OP1	38:k:583:ILE:HG21	1.54	1.05
33:i:82:ARG:NH2	33:i:84:GLY:C	2.15	1.05
35:A:235:TYR:CD1	36:B:285:ASP:CB	2.38	1.05
39:U:146:VAL:HG11	40:R:131:PRO:CB	1.84	1.05
25:a:104:ARG:O	25:a:105:LYS:HB2	1.49	1.04
38:k:375:MET:CE	38:k:531:ARG:HD2	1.87	1.04
34:2:1518:C:H5'	39:U:144:ARG:HG3	1.36	1.04
38:k:311:ILE:HA	38:k:317:VAL:HG21	1.34	1.04
41:3:58:C:O2	41:3:59:A:C4	2.10	1.04
34:2:1518:C:OP1	39:U:143:GLY:CA	2.04	1.04
35:A:170:GLU:O	35:A:172:GLU:N	1.90	1.04
38:k:209:LEU:CD1	38:k:221:GLU:CG	2.31	1.04
39:U:146:VAL:CG1	40:R:131:PRO:CB	2.36	1.04
41:3:38:C:C2	41:3:39:U:O4	2.10	1.04
16:P:22:VAL:HG12	16:P:26:LEU:HG	1.32	1.03
38:k:70:LEU:CD1	42:k:702:SF4:S2	2.46	1.03
38:k:204:LEU:CB	38:k:224:ARG:CZ	2.28	1.03
38:k:518:VAL:C	38:k:519:GLU:N	2.16	1.03
37:j:70:TRP:NE1	40:R:143:PRO:HB3	1.72	1.03
1:1:35:A:O2'	37:j:8:GLY:HA3	1.57	1.03
16:P:22:VAL:H	16:P:23:PRO:HA	1.23	1.03
18:S:145:TYR:O	18:S:146:ARG:HG2	1.56	1.03
38:k:187:ILE:HG23	38:k:188:LEU:H	1.23	1.03
38:k:451:ILE:O	38:k:454:ILE:N	1.67	1.03
37:j:63:GLY:O	37:j:64:LYS:HG3	1.59	1.02
38:k:294:SER:OG	44:k:704:GNP:O3'	1.74	1.02
38:k:164:LEU:HD21	38:k:237:ILE:HB	1.41	1.02
35:A:157:VAL:HG21	35:A:180:ILE:HG22	1.39	1.02
37:j:41:MET:HA	37:j:47:LEU:HD13	1.39	1.02
38:k:218:SER:HB3	44:k:705:GNP:O2'	1.60	1.02
38:k:521:ASP:HB3	38:k:524:MET:HB2	1.35	1.02
38:k:253:LEU:HD11	38:k:564:ILE:CD1	1.90	1.02
40:R:141:PHE:C	40:R:142:ILE:HD12	1.85	1.02
40:R:143:PRO:CB	41:3:55:G:H1'	1.90	1.01
16:P:27:LYS:HZ2	16:P:28:LEU:HD23	1.26	1.01
38:k:241:ASP:O	38:k:242:GLU:N	1.93	1.01
38:k:374:ILE:HD11	38:k:529:ALA:CA	1.91	1.01
38:k:411:TYR:C	38:k:412:LYS:CA	2.34	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:521:ASP:CB	38:k:524:MET:CB	2.37	1.01
24:Z:78:GLY:HA2	38:k:60:ILE:CD1	1.91	1.01
34:2:742:C:C2'	34:2:743:U:H5'	1.91	1.01
24:Z:68:LYS:CG	37:j:84:TYR:OH	2.07	1.01
34:2:737:C:H3'	34:2:738:U:H5''	1.42	1.01
37:j:67:LYS:CE	41:3:56:U:H4'	1.90	1.01
37:j:94:LYS:HG2	37:j:95:TYR:N	1.74	1.00
38:k:4:LYS:CA	38:k:79:LEU:HG	1.91	1.00
38:k:329:LEU:O	38:k:498:LEU:CD1	2.08	1.00
38:k:578:ASN:HD21	38:k:585:ASP:HB2	1.24	1.00
6:F:2:ALA:HB1	6:F:3:VAL:HA	1.42	1.00
38:k:425:ARG:CZ	38:k:455:ILE:HD12	1.89	1.00
38:k:521:ASP:HB3	38:k:524:MET:HB3	1.05	1.00
34:2:1705:C:C1'	37:j:42:LEU:CD2	2.27	1.00
35:A:157:VAL:CG1	35:A:180:ILE:HD13	1.92	1.00
38:k:4:LYS:N	38:k:79:LEU:HG	1.76	1.00
6:F:196:GLY:HA2	6:F:197:LYS:C	1.85	1.00
10:J:106:ARG:HD3	34:2:794:G:O6	1.60	1.00
34:2:478:U:O4	38:k:99:ILE:HD11	1.62	1.00
34:2:683:G:N2	34:2:731:C:N3	2.10	1.00
34:2:1518:C:C5'	39:U:144:ARG:HA	1.91	1.00
34:2:1518:C:H5'	39:U:143:GLY:O	1.62	0.99
38:k:492:LEU:O	38:k:497:ARG:NE	1.95	0.99
34:2:1518:C:O3'	39:U:144:ARG:HB3	1.62	0.99
35:A:235:TYR:CE1	36:B:285:ASP:OD1	2.15	0.99
38:k:212:ARG:CD	38:k:359:GLU:OE2	2.10	0.99
1:1:35:A:O4'	37:j:8:GLY:O	1.81	0.99
37:j:70:TRP:HZ2	41:3:55:G:H2'	1.17	0.99
38:k:521:ASP:CB	38:k:524:MET:HB3	1.91	0.99
38:k:319:THR:CB	38:k:320:GLU:HB2	1.93	0.99
34:2:1327:C:N4	37:j:15:GLY:C	2.21	0.99
34:2:1696:C:O2	37:j:10:LYS:HG3	1.63	0.98
38:k:65:CYS:SG	42:k:702:SF4:S4	2.60	0.98
35:A:58:SER:CB	35:A:61:LYS:CG	2.41	0.98
37:j:78:LEU:HD23	37:j:93:LEU:HD12	1.45	0.98
37:j:47:LEU:HD12	37:j:48:GLU:H	1.25	0.98
34:2:1707:A:C6	34:2:1708:C:C4	2.50	0.98
25:a:12:PHE:HE1	34:2:836:C:C2'	1.76	0.98
37:j:70:TRP:NE1	40:R:143:PRO:CB	2.26	0.98
38:k:332:LYS:HE3	38:k:334:ALA:HB3	1.41	0.98
6:F:3:VAL:HG22	6:F:4:GLN:N	1.76	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:205:ILE:HD12	36:B:288:LYS:HB2	1.44	0.98
38:k:318:PRO:HG2	38:k:322:LEU:HA	1.42	0.98
34:2:472:G:OP1	38:k:63:LYS:CE	2.10	0.98
34:2:749:C:H3'	34:2:750:G:H5''	1.43	0.98
40:R:133:ILE:HG23	40:R:134:GLY:N	1.78	0.98
34:2:158:A:OP1	38:k:583:ILE:HG22	1.63	0.98
38:k:311:ILE:CA	38:k:317:VAL:HG21	1.92	0.98
6:F:193:ASP:H	6:F:194:PRO:HD2	1.25	0.97
35:A:58:SER:HB3	35:A:61:LYS:CG	1.92	0.97
38:k:85:HIS:HB2	38:k:130:ASN:ND2	1.77	0.97
34:2:1819:A:N6	37:j:66:ARG:O	1.94	0.97
35:A:229:LEU:HB2	36:B:284:VAL:HG11	1.43	0.97
35:A:235:TYR:CB	36:B:285:ASP:OD2	2.12	0.97
24:Z:50:ILE:CD1	38:k:58:CYS:HB3	1.94	0.97
34:2:684:A:C2	34:2:731:C:N3	2.32	0.97
34:2:740:G:H21	34:2:794:G:H1'	0.81	0.97
35:A:55:ARG:HG2	35:A:55:ARG:HH11	1.29	0.97
38:k:414:GLN:CD	38:k:486:ASP:CG	2.32	0.97
41:3:76:A:C2'	41:3:77:A:H5'	1.94	0.97
38:k:17:LYS:HG2	38:k:20:LYS:HG2	1.46	0.97
34:2:740:G:N2	34:2:794:G:C1'	2.22	0.96
37:j:70:TRP:NE1	40:R:143:PRO:HA	1.79	0.96
35:A:229:LEU:HD22	36:B:284:VAL:HG22	1.45	0.96
25:a:123:ALA:O	25:a:127:ALA:N	1.98	0.96
25:a:123:ALA:O	25:a:127:ALA:HB3	1.66	0.96
35:A:157:VAL:HG13	35:A:180:ILE:HD13	1.47	0.96
37:j:70:TRP:HZ2	41:3:55:G:O2'	1.48	0.96
34:2:1693:C:C5	41:3:58:C:N4	2.33	0.96
37:j:70:TRP:CD1	40:R:143:PRO:CA	2.48	0.96
38:k:17:LYS:NZ	38:k:20:LYS:CE	2.29	0.96
38:k:61:CYS:HG	42:k:701:SF4:FE3	0.66	0.96
38:k:378:LEU:C	38:k:379:GLY:O	2.09	0.96
35:A:235:TYR:OH	36:B:286:ASP:OD2	1.83	0.96
38:k:217:LEU:HD23	38:k:221:GLU:HB3	1.47	0.96
14:N:30:LYS:HE2	14:N:30:LYS:N	1.81	0.95
25:a:12:PHE:CE1	34:2:836:C:H1'	2.00	0.95
34:2:1707:A:C2	34:2:1708:C:C6	2.53	0.95
38:k:375:MET:SD	38:k:533:ILE:CG2	2.54	0.95
34:2:478:U:C5	38:k:99:ILE:HD13	2.01	0.95
16:P:20:ARG:CG	16:P:65:PHE:CE1	2.48	0.95
38:k:414:GLN:HG3	38:k:486:ASP:O	1.67	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:71:ILE:HD13	37:j:77:ILE:CD1	1.97	0.95
37:j:70:TRP:HZ2	41:3:55:G:HO2'	1.13	0.95
37:j:92:ILE:HG21	37:j:93:LEU:CD1	1.97	0.95
38:k:431:LYS:HE3	38:k:477:GLY:C	1.91	0.95
38:k:4:LYS:HA	38:k:79:LEU:HG	1.43	0.95
38:k:332:LYS:HE2	38:k:502:ARG:HD3	0.95	0.95
1:1:34:C:N3	41:3:54:G:N1	2.15	0.95
34:2:1707:A:N3	34:2:1708:C:C6	2.35	0.95
24:Z:61:GLN:HG2	34:2:1818:A:OP1	1.67	0.95
25:a:101:LYS:HG3	25:a:107:ARG:NH2	1.82	0.95
37:j:74:SER:O	37:j:75:ASP:HB2	1.65	0.94
39:U:143:GLY:O	39:U:144:ARG:CD	2.14	0.94
40:R:141:PHE:O	40:R:142:ILE:HD12	1.64	0.94
1:1:16:G:C6	1:1:17:C:H5	1.85	0.94
1:1:37:T6A:ODB	41:3:51:C:O2'	1.84	0.94
25:a:101:LYS:NZ	25:a:107:ARG:CZ	2.30	0.94
37:j:8:GLY:HA2	40:R:140:ARG:HH21	1.17	0.94
14:N:22:ARG:HH21	14:N:24:LEU:HB2	1.33	0.94
37:j:92:ILE:CG2	37:j:93:LEU:CD1	2.44	0.94
37:j:92:ILE:CG2	37:j:93:LEU:CG	2.11	0.94
41:3:75:G:H2'	41:3:76:A:H5'	1.49	0.94
34:2:1244:C4J:O36	34:2:1244:C4J:C3	2.14	0.94
34:2:745:U:H2'	34:2:746:C:C6	2.01	0.94
1:1:18:G:H1'	1:1:61:C:C5'	1.98	0.94
10:J:109:ARG:HB2	34:2:740:G:O4'	1.67	0.93
11:K:193:LYS:CE	14:N:32:LYS:HZ1	1.82	0.93
25:a:128:GLY:O	38:k:264:ASN:HB3	1.67	0.93
38:k:241:ASP:C	38:k:242:GLU:N	0.84	0.93
34:2:680:G:H1	34:2:734:C:H42	1.00	0.93
38:k:73:VAL:CG2	38:k:322:LEU:CD2	2.45	0.93
40:R:133:ILE:CG2	40:R:134:GLY:H	1.81	0.93
34:2:1817:A:O2'	37:j:46:ARG:NH2	2.02	0.93
38:k:17:LYS:HZ3	38:k:20:LYS:HE2	1.32	0.93
38:k:578:ASN:ND2	38:k:585:ASP:HB2	1.83	0.93
11:K:193:LYS:CE	14:N:32:LYS:NZ	2.31	0.93
35:A:235:TYR:CG	36:B:285:ASP:CG	2.39	0.93
37:j:48:GLU:OE2	37:j:49:ALA:N	2.02	0.93
38:k:583:ILE:HG23	38:k:584:LYS:H	1.33	0.93
25:a:106:GLN:OE1	38:k:266:ASP:OD2	1.86	0.92
34:2:478:U:O4	38:k:99:ILE:CD1	2.16	0.92
34:2:738:U:O2'	34:2:740:G:OP2	1.86	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:374:ILE:CD1	38:k:528:LEU:C	2.40	0.92
1:1:18:G:O4'	1:1:61:C:H5''	1.68	0.92
34:2:1518:C:H4'	39:U:144:ARG:HA	0.95	0.92
38:k:150:SER:HG	38:k:151:GLU:N	1.65	0.92
38:k:411:TYR:CA	38:k:412:LYS:N	2.32	0.92
39:U:146:VAL:HG11	40:R:131:PRO:CG	1.97	0.92
34:2:1519:G:OP1	39:U:144:ARG:HB3	1.70	0.92
34:2:742:C:H2'	34:2:743:U:H5'	1.49	0.92
34:2:742:C:O2'	34:2:743:U:H5'	1.68	0.92
34:2:605:C:OP1	37:j:63:GLY:HA3	1.69	0.92
1:1:18:G:N2	1:1:57:G:O6	2.02	0.92
37:j:70:TRP:NE1	40:R:143:PRO:CA	2.33	0.92
40:R:141:PHE:O	40:R:142:ILE:CD1	2.17	0.92
16:P:27:LYS:NZ	16:P:28:LEU:HD23	1.85	0.92
38:k:414:GLN:CG	38:k:486:ASP:C	2.43	0.92
38:k:61:CYS:SG	42:k:701:SF4:FE3	1.61	0.92
38:k:188:LEU:O	38:k:191:LYS:HB2	1.70	0.91
37:j:43:GLY:O	37:j:45:GLY:N	2.01	0.91
37:j:78:LEU:HD23	37:j:93:LEU:CB	2.00	0.91
37:j:78:LEU:CD2	37:j:93:LEU:HB2	1.99	0.91
38:k:17:LYS:HG2	38:k:20:LYS:HE2	1.51	0.91
38:k:55:CYS:SG	42:k:701:SF4:S3	2.67	0.91
40:R:143:PRO:CG	41:3:55:G:H1'	2.00	0.91
1:1:35:A:H4'	37:j:8:GLY:O	1.65	0.91
24:Z:68:LYS:HG3	37:j:84:TYR:HH	1.31	0.91
36:B:284:VAL:HG13	36:B:285:ASP:HB3	1.51	0.91
37:j:40:LYS:HB2	37:j:40:LYS:NZ	1.84	0.91
38:k:412:LYS:HD3	38:k:485:ILE:CG1	2.00	0.91
25:a:12:PHE:CZ	34:2:836:C:O2'	2.15	0.91
34:2:478:U:OP1	38:k:150:SER:CB	2.17	0.91
41:3:58:C:O2	41:3:59:A:C8	2.23	0.91
25:a:128:GLY:HA3	38:k:264:ASN:C	1.95	0.91
34:2:683:G:H1	34:2:731:C:H42	1.18	0.91
6:F:193:ASP:H	6:F:194:PRO:CD	1.81	0.91
38:k:17:LYS:CG	38:k:20:LYS:HG2	1.99	0.91
41:3:49:A:H5'	41:3:49:A:N3	1.85	0.91
25:a:104:ARG:NH2	25:a:108:LYS:HZ1	1.49	0.91
38:k:241:ASP:O	38:k:242:GLU:CA	2.18	0.91
38:k:521:ASP:O	38:k:525:ALA:N	2.02	0.91
34:2:680:G:H1	34:2:734:C:N4	1.68	0.91
34:2:1518:C:C4'	39:U:144:ARG:CA	2.37	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1518:C:OP1	39:U:143:GLY:HA3	1.71	0.91
34:2:1815:U:H2'	34:2:1816:A:H5''	1.53	0.91
25:a:123:ALA:O	25:a:127:ALA:CB	2.19	0.90
34:2:733:G:N7	34:2:738:U:O4	2.04	0.90
35:A:157:VAL:CG1	35:A:180:ILE:CD1	2.49	0.90
16:P:20:ARG:HD2	16:P:65:PHE:HE1	0.86	0.90
38:k:17:LYS:HZ2	38:k:20:LYS:CE	1.83	0.90
38:k:378:LEU:C	38:k:379:GLY:C	2.39	0.90
38:k:411:TYR:C	38:k:412:LYS:HA	1.95	0.90
38:k:377:MET:HB3	38:k:385:LYS:HD2	1.52	0.90
33:i:80:LEU:HD23	37:j:62:ARG:HH21	1.34	0.90
38:k:412:LYS:CD	38:k:485:ILE:HG13	2.01	0.90
34:2:734:C:H2'	34:2:735:C:H5''	1.53	0.90
34:2:1707:A:C2'	34:2:1708:C:H5'	2.00	0.90
38:k:164:LEU:CD2	38:k:237:ILE:HB	2.02	0.90
38:k:200:VAL:HG11	38:k:228:ALA:HA	1.54	0.90
38:k:411:TYR:HA	38:k:412:LYS:N	1.87	0.90
38:k:492:LEU:O	38:k:497:ARG:CZ	2.20	0.90
33:i:80:LEU:CD2	37:j:62:ARG:NH2	2.35	0.90
34:2:739:U:O2'	34:2:740:G:OP1	1.88	0.90
34:2:787:C:H2'	34:2:788:C:C6	2.06	0.90
38:k:315:GLY:HA3	38:k:326:ASP:O	1.72	0.90
25:a:104:ARG:NH2	25:a:108:LYS:CE	2.31	0.89
38:k:331:PHE:O	38:k:498:LEU:HD13	1.71	0.89
35:A:58:SER:CB	35:A:61:LYS:CD	2.49	0.89
38:k:112:ASN:HA	44:k:704:GNP:O3G	1.72	0.89
38:k:332:LYS:NZ	38:k:334:ALA:HB2	1.86	0.89
38:k:381:ASN:HB3	44:k:705:GNP:O1G	1.71	0.89
39:U:143:GLY:C	39:U:144:ARG:CD	2.45	0.89
1:1:16:G:C5	1:1:17:C:H5	1.89	0.89
16:P:26:LEU:HD22	16:P:27:LYS:N	1.88	0.89
25:a:12:PHE:HE1	34:2:836:C:C1'	1.85	0.89
25:a:104:ARG:HH22	25:a:108:LYS:HZ1	0.99	0.89
35:A:157:VAL:HG11	35:A:180:ILE:CB	2.03	0.89
1:1:18:G:C1'	1:1:61:C:H5'	2.03	0.89
37:j:78:LEU:HD21	37:j:93:LEU:HD12	1.53	0.89
38:k:17:LYS:NZ	38:k:20:LYS:HE2	1.85	0.89
38:k:521:ASP:CB	38:k:524:MET:HB2	2.01	0.89
40:R:133:ILE:O	40:R:139:SER:OG	1.89	0.89
24:Z:50:ILE:HD11	38:k:58:CYS:HB3	1.52	0.88
35:A:157:VAL:CG2	35:A:180:ILE:HG21	2.03	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:185:THR:HB	35:A:187:GLN:CB	2.02	0.88
38:k:55:CYS:SG	42:k:701:SF4:FE2	1.65	0.88
38:k:425:ARG:NH2	38:k:455:ILE:HD12	1.86	0.88
34:2:1707:A:N1	34:2:1708:C:N3	2.20	0.88
38:k:450:GLN:HG3	38:k:453:ASN:OD1	1.72	0.88
38:k:492:LEU:CB	38:k:497:ARG:HG3	2.03	0.88
24:Z:97:ASN:CG	38:k:34:MET:CE	2.43	0.88
34:2:1818:A:O2'	34:2:1819:A:OP2	1.90	0.88
34:2:605:C:OP1	37:j:63:GLY:CA	2.21	0.88
34:2:1707:A:N1	34:2:1708:C:C4	2.41	0.88
37:j:70:TRP:CE2	40:R:143:PRO:HB3	2.08	0.88
38:k:164:LEU:HD21	38:k:237:ILE:HD13	1.53	0.88
34:2:751:C:O2'	34:2:752:C:H5'	1.74	0.88
41:3:60:C:C3'	41:3:61:C:H4'	2.03	0.87
38:k:492:LEU:HB3	38:k:497:ARG:HG3	1.55	0.87
25:a:101:LYS:HZ3	25:a:107:ARG:CZ	1.87	0.87
37:j:78:LEU:HD23	37:j:93:LEU:CD1	2.03	0.87
37:j:78:LEU:CD2	37:j:93:LEU:CD1	2.53	0.87
25:a:128:GLY:C	38:k:264:ASN:HB3	1.99	0.87
34:2:742:C:O2'	34:2:743:U:C5'	2.23	0.87
34:2:746:C:H2'	34:2:747:G:C8	2.10	0.87
38:k:21:CYS:SG	42:k:702:SF4:FE2	1.66	0.87
34:2:1327:C:N4	37:j:16:LYS:N	2.21	0.86
39:U:143:GLY:C	39:U:144:ARG:CG	2.46	0.86
34:2:685:G:N2	34:2:730:C:N3	2.22	0.86
25:a:104:ARG:NH2	25:a:108:LYS:HZ2	1.67	0.86
33:i:82:ARG:NH2	33:i:85:LYS:N	2.23	0.86
24:Z:58:GLU:CD	37:j:60:HIS:CE1	2.53	0.86
38:k:315:GLY:HA2	38:k:326:ASP:HB3	1.58	0.86
38:k:345:MET:HG3	38:k:346:CYS:H	1.39	0.86
35:A:235:TYR:HB3	36:B:285:ASP:OD2	1.73	0.86
38:k:311:ILE:CB	38:k:317:VAL:HG21	2.04	0.86
16:P:20:ARG:CG	16:P:65:PHE:CD1	2.58	0.86
37:j:63:GLY:C	37:j:64:LYS:HG3	1.99	0.86
38:k:4:LYS:HG3	38:k:79:LEU:HD12	1.58	0.86
38:k:204:LEU:HB3	38:k:224:ARG:NE	1.90	0.86
38:k:345:MET:CG	38:k:346:CYS:H	1.89	0.86
25:a:101:LYS:HG3	25:a:107:ARG:HH21	1.40	0.86
37:j:8:GLY:C	40:R:140:ARG:NH2	2.32	0.86
34:2:740:G:N1	34:2:793:C:C2	2.44	0.86
35:A:229:LEU:HB2	36:B:284:VAL:HG21	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:229:LEU:HB2	36:B:284:VAL:CG1	2.04	0.85
38:k:204:LEU:HG	38:k:224:ARG:HH11	1.05	0.85
16:P:22:VAL:CG1	16:P:26:LEU:HG	2.04	0.85
38:k:182:GLY:HA2	38:k:187:ILE:HD13	1.57	0.85
38:k:209:LEU:HD11	38:k:221:GLU:HG3	0.87	0.85
38:k:318:PRO:CB	38:k:322:LEU:CA	2.52	0.85
34:2:684:A:H2'	34:2:685:G:C8	2.12	0.85
37:j:25:GLU:HG2	37:j:26:LEU:HG	1.58	0.85
38:k:332:LYS:C	38:k:334:ALA:H	1.84	0.85
16:P:22:VAL:HB	16:P:24:THR:N	1.90	0.85
25:a:101:LYS:O	25:a:102:THR:OG1	1.92	0.85
41:3:67:C:C2'	41:3:68:C:H5'	2.06	0.85
33:i:76:VAL:HG11	33:i:80:LEU:HD23	1.55	0.85
38:k:216:ASP:O	44:k:705:GNP:C4	2.25	0.85
38:k:217:LEU:HB3	38:k:221:GLU:HB2	1.59	0.85
38:k:522:PHE:O	38:k:526:THR:CG2	2.21	0.85
41:3:74:A:O2'	41:3:75:G:H5'	1.76	0.85
25:a:101:LYS:CG	25:a:107:ARG:NH2	2.40	0.85
37:j:72:ASN:HD22	37:j:72:ASN:H	1.24	0.85
34:2:740:G:N1	34:2:793:C:O2	2.09	0.84
35:A:55:ARG:HH11	35:A:55:ARG:CG	1.89	0.84
34:2:1518:C:OP1	39:U:143:GLY:C	2.20	0.84
35:A:108:VAL:CG2	35:A:150:TYR:HD1	1.90	0.84
38:k:550:THR:C	38:k:551:LEU:N	2.35	0.84
39:U:146:VAL:HG13	40:R:131:PRO:CD	2.07	0.84
6:F:3:VAL:CG2	6:F:4:GLN:H	1.90	0.84
34:2:732:C:H2'	34:2:733:G:O4'	1.76	0.84
35:A:178:ASN:O	35:A:182:ARG:HG2	1.78	0.84
25:a:12:PHE:HE1	34:2:836:C:O2'	1.42	0.84
37:j:71:ILE:HD13	37:j:77:ILE:HD11	1.58	0.84
1:1:11:G:H1	1:1:25:U:H3	1.21	0.84
41:3:73:G:OP2	41:3:74:A:N6	2.11	0.84
37:j:10:LYS:HG2	37:j:11:ASN:H	0.76	0.84
38:k:204:LEU:HB3	38:k:224:ARG:CZ	2.06	0.84
34:2:731:C:H2'	34:2:732:C:H5''	1.58	0.84
34:2:1705:C:C2'	37:j:42:LEU:HD21	2.07	0.84
41:3:74:A:H2'	41:3:75:G:C8	2.12	0.83
38:k:317:VAL:N	38:k:318:PRO:HD3	1.87	0.83
10:J:108:SER:OG	34:2:737:C:O2'	1.86	0.83
38:k:311:ILE:HA	38:k:317:VAL:CG2	2.08	0.83
34:2:1518:C:C3'	39:U:144:ARG:HA	2.07	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:188:LEU:HD12	38:k:225:PHE:HE1	1.43	0.83
38:k:318:PRO:HB3	38:k:322:LEU:N	1.94	0.83
39:U:143:GLY:C	39:U:144:ARG:HG3	2.01	0.83
38:k:489:SER:N	38:k:524:MET:HE1	1.94	0.83
10:J:109:ARG:HB3	34:2:740:G:H1'	0.83	0.82
35:A:229:LEU:HB2	36:B:284:VAL:CB	2.08	0.82
38:k:318:PRO:HB3	38:k:321:ASN:C	2.04	0.82
34:2:478:U:C4	38:k:99:ILE:HD13	2.15	0.82
34:2:1705:C:H1'	37:j:42:LEU:HD23	1.59	0.82
36:B:284:VAL:HG13	36:B:285:ASP:CB	2.08	0.82
38:k:414:GLN:HE21	38:k:486:ASP:HB3	1.43	0.82
35:A:108:VAL:HG23	35:A:150:TYR:HD1	1.43	0.82
38:k:17:LYS:HG2	38:k:20:LYS:CG	2.09	0.82
1:1:18:G:C1'	1:1:61:C:C5'	2.57	0.82
16:P:20:ARG:CD	16:P:65:PHE:HE1	1.64	0.82
24:Z:97:ASN:ND2	38:k:34:MET:SD	2.53	0.82
38:k:70:LEU:HD11	42:k:702:SF4:S2	2.16	0.82
38:k:204:LEU:HG	38:k:224:ARG:CZ	2.08	0.82
38:k:318:PRO:HB3	38:k:322:LEU:CA	2.10	0.82
40:R:130:ARG:HH11	40:R:130:ARG:HB2	1.41	0.82
40:R:143:PRO:HG2	41:3:55:G:H1'	1.59	0.82
41:3:75:G:C2'	41:3:76:A:H5'	2.10	0.82
38:k:253:LEU:HD11	38:k:564:ILE:HD11	1.61	0.82
34:2:1327:C:H5	37:j:16:LYS:H	1.25	0.82
38:k:70:LEU:HD13	42:k:702:SF4:S2	2.20	0.82
38:k:319:THR:H	38:k:320:GLU:C	1.88	0.82
16:P:20:ARG:HD3	16:P:65:PHE:CE1	2.15	0.81
24:Z:96:GLU:HG2	38:k:34:MET:CE	2.10	0.81
24:Z:96:GLU:HG2	38:k:34:MET:HE1	1.62	0.81
38:k:209:LEU:HD13	38:k:221:GLU:CG	2.10	0.81
35:A:157:VAL:CG2	35:A:180:ILE:CG2	2.55	0.81
38:k:176:ILE:HA	38:k:178:LYS:H	1.45	0.81
24:Z:52:LEU:O	38:k:34:MET:SD	2.39	0.81
34:2:1517:A:H5''	39:U:142:ARG:NH2	1.95	0.81
37:j:16:LYS:HE2	41:3:57:G:O2'	1.80	0.81
38:k:591:SER:C	38:k:593:ASN:H	1.88	0.81
39:U:140:GLY:O	39:U:141:ARG:HB2	1.77	0.81
16:P:22:VAL:N	16:P:23:PRO:HA	1.93	0.81
40:R:128:HIS:HB3	40:R:129:GLY:HA3	1.62	0.81
34:2:1693:C:C2	41:3:58:C:N4	2.37	0.81
34:2:1705:C:H1'	37:j:42:LEU:HD22	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1814:G:O2'	34:2:1815:U:H5'	1.79	0.81
38:k:73:VAL:CB	38:k:322:LEU:HD21	2.09	0.81
38:k:315:GLY:O	38:k:316:TYR:CB	2.29	0.81
38:k:315:GLY:C	38:k:316:TYR:CD1	2.59	0.81
11:K:193:LYS:HE2	14:N:32:LYS:NZ	1.96	0.81
39:U:148:VAL:HG21	40:R:131:PRO:O	1.80	0.81
38:k:166:ALA:HA	38:k:237:ILE:CG2	2.11	0.81
34:2:1518:C:O3'	39:U:144:ARG:CB	2.29	0.80
34:2:1816:A:O2'	34:2:1817:A:C8	2.35	0.80
37:j:30:GLU:H	37:j:33:GLN:HB3	1.46	0.80
38:k:55:CYS:SG	42:k:701:SF4:S1	2.78	0.80
38:k:307:GLU:O	38:k:311:ILE:HG23	1.81	0.80
1:1:17:C:H2'	1:1:18:G:H5'	1.63	0.80
24:Z:68:LYS:HG3	37:j:84:TYR:CZ	2.16	0.80
25:a:12:PHE:HE1	34:2:836:C:H1'	1.41	0.80
38:k:315:GLY:O	38:k:316:TYR:CG	2.34	0.80
41:3:58:C:H2'	41:3:59:A:C8	2.16	0.80
34:2:605:C:OP1	37:j:63:GLY:N	2.14	0.80
34:2:1707:A:N1	34:2:1708:C:C2	2.50	0.80
41:3:39:U:H4'	41:3:40:C:OP1	1.82	0.80
38:k:315:GLY:CA	38:k:326:ASP:HB3	2.11	0.80
16:P:24:THR:O	16:P:26:LEU:HD12	1.81	0.80
34:2:1518:C:P	39:U:143:GLY:HA3	2.22	0.80
35:A:58:SER:HB3	35:A:61:LYS:CD	2.12	0.80
9:I:237:LEU:HB2	34:2:785:G:OP1	1.81	0.80
37:j:70:TRP:HE1	40:R:143:PRO:HB3	1.46	0.80
38:k:241:ASP:HA	38:k:242:GLU:N	1.93	0.80
33:i:82:ARG:HH21	33:i:85:LYS:N	1.80	0.79
34:2:743:U:H1'	34:2:744:C:C1'	2.12	0.79
34:2:1518:C:OP1	39:U:143:GLY:O	2.00	0.79
40:R:143:PRO:HG2	41:3:55:G:C4	2.15	0.79
1:1:34:C:O2	37:j:10:LYS:HA	1.81	0.79
6:F:3:VAL:HG11	34:2:1573:U:C4	2.16	0.79
37:j:40:LYS:HD3	37:j:41:MET:H	1.48	0.79
38:k:166:ALA:HA	38:k:237:ILE:HG22	1.65	0.79
41:3:55:G:H5'	41:3:56:U:OP2	1.81	0.79
41:3:58:C:C2	41:3:59:A:C5	2.71	0.79
6:F:3:VAL:CG1	34:2:1573:U:O4	2.26	0.79
38:k:319:THR:OG1	38:k:320:GLU:HB2	1.81	0.79
34:2:748:G:O2'	34:2:749:C:O5'	2.01	0.79
14:N:25:LEU:HD22	14:N:28:THR:O	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:41:MET:HA	37:j:47:LEU:CD1	2.13	0.79
38:k:584:LYS:C	38:k:586:VAL:H	1.91	0.79
16:P:20:ARG:HG2	16:P:65:PHE:CD1	2.17	0.79
34:2:1707:A:O2'	34:2:1708:C:H5'	1.82	0.79
34:2:743:U:O2'	34:2:744:C:O4'	2.00	0.79
38:k:188:LEU:HD13	38:k:225:PHE:CD1	2.18	0.78
18:S:145:TYR:O	18:S:146:ARG:CG	2.30	0.78
38:k:414:GLN:CG	38:k:486:ASP:HB3	2.13	0.78
34:2:1812:A:N1	34:2:1813:A:N7	2.32	0.78
38:k:492:LEU:HB2	38:k:497:ARG:CG	2.13	0.78
41:3:43:A:H2'	41:3:44:C:C6	2.19	0.78
35:A:205:ILE:HD12	36:B:288:LYS:CB	2.13	0.78
38:k:150:SER:OG	38:k:151:GLU:N	2.01	0.78
38:k:311:ILE:HB	38:k:317:VAL:HG21	1.65	0.78
38:k:412:LYS:HB3	38:k:485:ILE:CA	2.08	0.78
34:2:604:G:OP2	37:j:64:LYS:NZ	2.17	0.78
34:2:734:C:C2'	34:2:735:C:H5''	2.13	0.78
1:1:16:G:H2'	1:1:17:C:H5''	1.66	0.78
35:A:235:TYR:HD1	36:B:285:ASP:CB	1.90	0.78
38:k:330:VAL:CG2	38:k:575:PRO:HD2	2.13	0.78
38:k:374:ILE:CD1	38:k:529:ALA:CA	2.61	0.78
38:k:414:GLN:CG	38:k:486:ASP:CB	2.60	0.78
38:k:431:LYS:HE3	38:k:478:LYS:N	1.99	0.78
41:3:67:C:H2'	41:3:68:C:H5'	1.63	0.78
38:k:237:ILE:C	38:k:238:PHE:CD2	2.62	0.78
38:k:319:THR:HG23	38:k:320:GLU:CB	2.13	0.78
38:k:337:ALA:O	38:k:338:ASN:HB2	1.83	0.78
40:R:133:ILE:HG12	40:R:139:SER:HB3	1.64	0.78
34:2:1705:C:O2'	37:j:42:LEU:HD21	1.84	0.78
37:j:27:VAL:HG12	37:j:28:PHE:H	1.48	0.78
37:j:29:LYS:HA	37:j:33:GLN:O	1.84	0.78
38:k:272:VAL:HG12	38:k:273:GLU:N	1.98	0.77
38:k:378:LEU:O	38:k:385:LYS:CD	2.30	0.77
38:k:241:ASP:C	38:k:242:GLU:C	2.51	0.77
38:k:487:GLU:N	38:k:518:VAL:O	2.16	0.77
16:P:27:LYS:NZ	16:P:27:LYS:HB2	1.99	0.77
34:2:1244:C4J:C31	34:2:1244:C4J:O2	2.31	0.77
35:A:111:ILE:HD11	35:A:183:ARG:HH12	1.48	0.77
38:k:519:GLU:CD	38:k:524:MET:HG2	2.10	0.77
10:J:106:ARG:CD	34:2:794:G:O6	2.32	0.77
38:k:76:PRO:HG3	38:k:323:ARG:CG	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:97:ASN:OD1	38:k:34:MET:HE2	1.81	0.77
34:2:452:C:O2'	38:k:306:ARG:HD3	1.83	0.77
34:2:743:U:O4	34:2:791:A:N1	2.18	0.77
35:A:229:LEU:HB2	36:B:284:VAL:CG2	2.14	0.77
38:k:450:GLN:HG3	38:k:453:ASN:CG	2.09	0.77
14:N:22:ARG:NH2	14:N:24:LEU:HB2	1.99	0.77
16:P:19:ARG:HH22	16:P:23:PRO:HB2	1.49	0.77
38:k:488:PRO:HG2	38:k:524:MET:HE2	1.66	0.77
24:Z:97:ASN:ND2	38:k:34:MET:CE	2.48	0.76
25:a:100:LYS:HA	25:a:101:LYS:C	2.09	0.76
38:k:183:THR:O	38:k:187:ILE:CB	2.33	0.76
38:k:414:GLN:HG2	38:k:486:ASP:OD1	1.83	0.76
38:k:17:LYS:HG2	38:k:20:LYS:CD	2.16	0.76
38:k:378:LEU:C	38:k:379:GLY:HA3	2.10	0.76
35:A:157:VAL:HG11	35:A:180:ILE:CD1	2.16	0.76
10:J:109:ARG:CG	34:2:740:G:H1'	2.15	0.76
35:A:54:ARG:HH21	35:A:54:ARG:CB	1.99	0.76
38:k:4:LYS:HA	38:k:79:LEU:CB	2.16	0.76
38:k:489:SER:CA	38:k:524:MET:HE1	2.16	0.76
38:k:188:LEU:CD1	38:k:225:PHE:CE1	2.69	0.76
38:k:226:ALA:O	38:k:229:VAL:HG12	1.84	0.76
38:k:546:ASN:OD1	38:k:557:LYS:NZ	2.17	0.76
41:3:73:G:N7	41:3:74:A:C5	2.54	0.76
37:j:70:TRP:CH2	41:3:55:G:H2'	2.20	0.76
38:k:4:LYS:HA	38:k:79:LEU:CD1	2.15	0.76
38:k:498:LEU:CD1	38:k:523:ILE:HD12	2.14	0.76
34:2:749:C:H2'	34:2:750:G:O4'	1.86	0.75
38:k:73:VAL:CG2	38:k:322:LEU:HD21	2.15	0.75
38:k:305:VAL:O	38:k:309:ILE:HG13	1.86	0.75
9:I:237:LEU:CB	34:2:785:G:OP1	2.34	0.75
38:k:253:LEU:CD1	38:k:564:ILE:CD1	2.64	0.75
38:k:319:THR:CG2	38:k:320:GLU:HB2	2.15	0.75
38:k:345:MET:CG	38:k:346:CYS:N	2.48	0.75
1:1:16:G:C5	1:1:17:C:C5	2.74	0.75
34:2:1812:A:C2	34:2:1813:A:N7	2.53	0.75
38:k:378:LEU:C	38:k:385:LYS:NZ	2.44	0.75
41:3:49:A:N3	41:3:49:A:C5'	2.49	0.75
35:A:227:ILE:CD1	35:A:237:MET:CE	2.62	0.75
38:k:217:LEU:HG	38:k:221:GLU:CG	2.14	0.75
38:k:412:LYS:CB	38:k:484:LEU:O	2.35	0.75
38:k:526:THR:HG23	38:k:527:TYR:H	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:58:SER:CB	35:A:61:LYS:HD2	2.16	0.75
38:k:591:SER:C	38:k:593:ASN:N	2.45	0.75
14:N:22:ARG:NH2	14:N:24:LEU:HD13	2.02	0.75
38:k:412:LYS:HB3	38:k:484:LEU:O	1.87	0.75
39:U:146:VAL:HG12	40:R:131:PRO:CG	1.91	0.75
41:3:73:G:C8	41:3:74:A:N7	2.55	0.74
38:k:165:LYS:H	38:k:236:ASP:HB3	1.49	0.74
1:1:35:A:HO2'	37:j:8:GLY:HA3	1.51	0.74
16:P:19:ARG:HH22	16:P:23:PRO:CB	2.00	0.74
40:R:141:PHE:O	40:R:142:ILE:CG1	2.34	0.74
9:I:237:LEU:CD1	34:2:784:G:O3'	2.25	0.74
41:3:58:C:O2	41:3:59:A:N7	2.19	0.74
34:2:597:U:O2	41:3:61:C:N4	2.21	0.74
34:2:1518:C:C5'	39:U:144:ARG:CA	2.64	0.74
35:A:114:HIS:CE1	35:A:175:VAL:HG21	2.23	0.74
38:k:311:ILE:HB	38:k:317:VAL:CG2	2.18	0.74
38:k:345:MET:HG3	38:k:371:ASP:HB3	1.69	0.74
34:2:1327:C:C5	37:j:16:LYS:N	2.56	0.74
25:a:12:PHE:CE1	34:2:836:C:C1'	2.65	0.74
25:a:103:SER:OG	25:a:104:ARG:N	2.21	0.74
35:A:202:TYR:HB2	36:B:355:LYS:HB3	1.69	0.74
37:j:92:ILE:HG21	37:j:93:LEU:HD12	1.68	0.74
6:F:193:ASP:N	6:F:194:PRO:HD2	2.02	0.74
38:k:348:TYR:HD2	38:k:369:PHE:O	1.71	0.74
16:P:27:LYS:C	16:P:28:LEU:HG	2.12	0.73
34:2:1709:U:O4	34:2:1813:A:N6	2.18	0.73
38:k:519:GLU:OE1	38:k:524:MET:HG2	1.87	0.73
38:k:188:LEU:HD12	38:k:225:PHE:CE1	2.23	0.73
34:2:454:A:C2	38:k:578:ASN:OD1	2.42	0.73
35:A:58:SER:HB3	35:A:61:LYS:HD2	1.70	0.73
35:A:202:TYR:HB2	36:B:355:LYS:CB	2.17	0.73
38:k:519:GLU:OE1	38:k:524:MET:HE2	1.89	0.73
34:2:748:G:C2	34:2:749:C:C2	2.77	0.73
35:A:58:SER:HB2	35:A:61:LYS:HE3	1.70	0.73
11:K:193:LYS:HZ3	14:N:32:LYS:HZ1	0.76	0.73
16:P:19:ARG:NH1	27:c:84:HIS:CE1	2.57	0.73
37:j:70:TRP:CE2	40:R:143:PRO:CB	2.72	0.73
38:k:425:ARG:CZ	38:k:455:ILE:CD1	2.66	0.73
38:k:253:LEU:CD1	38:k:564:ILE:HD12	2.18	0.73
38:k:583:ILE:HG23	38:k:584:LYS:N	2.03	0.73
25:a:104:ARG:HH22	25:a:108:LYS:HZ2	1.27	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:73:THR:O	37:j:74:SER:OG	2.05	0.73
38:k:591:SER:N	38:k:592:GLY:N	2.37	0.73
41:3:58:C:O2	41:3:59:A:N9	2.22	0.73
16:P:26:LEU:C	16:P:26:LEU:HD13	2.14	0.73
37:j:63:GLY:C	37:j:64:LYS:CG	2.61	0.73
38:k:187:ILE:HG23	38:k:188:LEU:N	2.02	0.73
25:a:104:ARG:O	25:a:105:LYS:CB	2.34	0.72
34:2:749:C:C3'	34:2:750:G:H5''	2.18	0.72
38:k:414:GLN:NE2	38:k:486:ASP:CA	2.52	0.72
40:R:134:GLY:HA2	40:R:139:SER:HB2	1.71	0.72
37:j:40:LYS:HD3	37:j:42:LEU:N	2.04	0.72
38:k:159:ILE:O	38:k:162:ASP:N	2.22	0.72
38:k:332:LYS:HG2	38:k:527:TYR:CG	2.14	0.72
38:k:164:LEU:HD21	38:k:237:ILE:CB	2.19	0.72
34:2:684:A:C2	34:2:731:C:C4	2.78	0.72
37:j:40:LYS:O	37:j:47:LEU:HD11	1.89	0.72
38:k:272:VAL:CG1	38:k:273:GLU:N	2.50	0.72
38:k:319:THR:CA	38:k:320:GLU:HB2	2.20	0.72
40:R:130:ARG:HA	40:R:130:ARG:NH1	2.04	0.72
35:A:55:ARG:C	35:A:56:ILE:HD12	2.14	0.72
33:i:82:ARG:HH22	33:i:84:GLY:CA	2.02	0.72
38:k:76:PRO:HG3	38:k:323:ARG:HG3	1.72	0.72
34:2:683:G:H1	34:2:731:C:N4	1.87	0.72
38:k:164:LEU:HD21	38:k:237:ILE:CD1	2.20	0.72
1:1:18:G:O4'	1:1:61:C:C5'	2.38	0.72
34:2:683:G:H2'	34:2:684:A:C8	2.24	0.72
34:2:1518:C:C5'	39:U:143:GLY:O	2.38	0.72
38:k:328:SER:O	38:k:329:LEU:HD22	1.90	0.72
6:F:3:VAL:CG2	6:F:4:GLN:N	2.49	0.72
34:2:748:G:N2	34:2:749:C:O2	2.23	0.72
38:k:310:ASN:O	38:k:314:ASP:N	2.22	0.72
38:k:378:LEU:C	38:k:385:LYS:HZ1	1.96	0.72
1:1:18:G:H4'	1:1:61:C:P	2.29	0.71
1:1:33:C:OP2	18:S:146:ARG:NH1	2.22	0.71
38:k:174:ASP:O	38:k:177:PRO:HD2	1.89	0.71
41:3:70:G:H3'	41:3:70:G:N3	2.04	0.71
37:j:21:SER:O	37:j:23:LYS:HG3	1.91	0.71
38:k:204:LEU:CD1	38:k:224:ARG:NH1	2.53	0.71
38:k:318:PRO:HB3	38:k:322:LEU:HA	1.65	0.71
24:Z:78:GLY:HA3	38:k:60:ILE:HD11	1.69	0.71
35:A:54:ARG:HH21	35:A:54:ARG:HB2	1.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:733:G:C5	34:2:738:U:O4	2.44	0.71
38:k:315:GLY:O	38:k:316:TYR:HB3	1.89	0.71
41:3:60:C:H3'	41:3:61:C:H4'	1.72	0.71
38:k:21:CYS:HG	42:k:702:SF4:FE2	0.49	0.71
38:k:450:GLN:HE21	38:k:452:GLU:HB3	1.55	0.71
34:2:1707:A:H2	34:2:1708:C:C2	2.02	0.71
38:k:218:SER:HB3	44:k:705:GNP:C2'	2.19	0.71
38:k:412:LYS:CB	38:k:485:ILE:HA	2.10	0.71
38:k:237:ILE:O	38:k:238:PHE:CD2	2.42	0.71
38:k:319:THR:HG23	38:k:320:GLU:HB2	1.70	0.71
34:2:745:U:H2'	34:2:746:C:C5	2.25	0.71
37:j:70:TRP:CE2	40:R:143:PRO:HG3	2.26	0.71
38:k:521:ASP:CG	38:k:524:MET:HB2	2.15	0.71
33:i:82:ARG:HH21	33:i:85:LYS:CA	2.03	0.70
34:2:80:G:H2'	34:2:81:U:C6	2.26	0.70
34:2:1518:C:O3'	39:U:144:ARG:CA	2.38	0.70
35:A:205:ILE:HD13	36:B:288:LYS:HG3	1.70	0.70
40:R:143:PRO:HG3	41:3:55:G:N3	2.05	0.70
34:2:80:G:H2'	34:2:81:U:H6	1.56	0.70
34:2:1707:A:C4	34:2:1708:C:C5	2.79	0.70
37:j:40:LYS:HD3	37:j:41:MET:N	2.04	0.70
38:k:188:LEU:CD1	38:k:225:PHE:HE1	2.04	0.70
40:R:133:ILE:C	40:R:139:SER:HG	1.98	0.70
34:2:1707:A:C4	34:2:1708:C:C6	2.80	0.70
34:2:740:G:N2	34:2:794:G:O4'	2.23	0.70
24:Z:96:GLU:OE2	38:k:34:MET:HE3	1.91	0.70
37:j:47:LEU:CD1	37:j:48:GLU:H	2.03	0.70
25:a:128:GLY:CA	38:k:264:ASN:HB3	2.22	0.70
38:k:204:LEU:CG	38:k:224:ARG:CZ	2.61	0.70
38:k:374:ILE:CD1	38:k:529:ALA:HA	2.21	0.70
38:k:591:SER:C	38:k:592:GLY:CA	2.64	0.70
33:i:80:LEU:HD23	37:j:62:ARG:NH2	2.04	0.70
38:k:246:TYR:HH	38:k:491:TYR:HH	0.78	0.70
38:k:311:ILE:O	38:k:317:VAL:HG23	1.92	0.70
41:3:58:C:N3	41:3:59:A:C6	2.60	0.70
16:P:19:ARG:NH1	27:c:84:HIS:NE2	2.40	0.70
41:3:71:A:H5''	41:3:73:G:H1'	1.74	0.70
34:2:1327:C:N4	37:j:15:GLY:O	2.25	0.69
35:A:185:THR:OG1	35:A:186:PRO:HA	1.92	0.69
40:R:130:ARG:HH11	40:R:130:ARG:CB	2.05	0.69
1:1:35:A:OP2	18:S:146:ARG:NH2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:96:GLU:CD	38:k:34:MET:HE3	2.16	0.69
37:j:47:LEU:HD12	37:j:48:GLU:N	2.04	0.69
38:k:85:HIS:HB2	38:k:130:ASN:HD21	1.57	0.69
38:k:223:GLN:HG2	38:k:247:LEU:HD11	1.73	0.69
38:k:316:TYR:C	38:k:318:PRO:HD3	2.18	0.69
38:k:375:MET:SD	38:k:531:ARG:HB2	2.32	0.69
34:2:1518:C:H5'	39:U:143:GLY:C	2.17	0.69
34:2:1818:A:O4'	37:j:44:ASN:O	2.11	0.69
6:F:196:GLY:CA	6:F:197:LYS:C	2.66	0.69
10:J:109:ARG:CG	34:2:794:G:H1'	2.22	0.69
34:2:1518:C:H5'	39:U:144:ARG:CG	2.18	0.69
38:k:492:LEU:CB	38:k:497:ARG:CG	2.69	0.69
41:3:63:G:H3'	41:3:63:G:N3	2.08	0.69
25:a:127:ALA:C	38:k:265:PRO:HB3	2.18	0.69
38:k:85:HIS:HA	38:k:131:LEU:H	1.56	0.69
38:k:331:PHE:CG	38:k:332:LYS:N	2.58	0.69
6:F:2:ALA:HA	6:F:3:VAL:O	1.93	0.69
1:1:16:G:C6	1:1:17:C:C5	2.75	0.68
38:k:73:VAL:CA	38:k:322:LEU:HD22	2.21	0.68
34:2:737:C:C3'	34:2:738:U:H5''	2.22	0.68
34:2:793:C:O2'	34:2:794:G:H4'	1.93	0.68
38:k:164:LEU:HD11	38:k:237:ILE:HD13	1.73	0.68
38:k:311:ILE:HB	38:k:317:VAL:CB	2.24	0.68
38:k:5:LEU:C	38:k:5:LEU:HD12	2.18	0.68
38:k:17:LYS:HZ2	38:k:20:LYS:HE3	1.57	0.68
38:k:315:GLY:HA2	38:k:326:ASP:CB	2.22	0.68
16:P:27:LYS:HG3	16:P:28:LEU:CD2	2.24	0.68
33:i:75:LYS:NZ	37:j:27:VAL:CG2	2.56	0.68
34:2:795:U:OP2	34:2:795:U:H4'	1.93	0.68
38:k:332:LYS:O	38:k:332:LYS:NZ	2.26	0.68
18:S:145:TYR:C	18:S:146:ARG:CG	2.66	0.68
24:Z:97:ASN:O	38:k:56:ILE:HD12	1.94	0.68
34:2:685:G:N2	34:2:730:C:C2	2.62	0.68
35:A:58:SER:HB2	35:A:61:LYS:CD	2.23	0.68
38:k:241:ASP:O	38:k:242:GLU:C	2.37	0.68
38:k:412:LYS:CD	38:k:485:ILE:CG1	2.67	0.68
41:3:74:A:H2'	41:3:75:G:H8	1.59	0.68
38:k:412:LYS:CA	38:k:484:LEU:O	2.40	0.68
35:A:111:ILE:HD11	35:A:183:ARG:NH1	2.09	0.68
11:K:193:LYS:CE	14:N:32:LYS:HZ3	2.07	0.67
33:i:75:LYS:HZ3	37:j:27:VAL:CG2	2.07	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1705:C:O2'	37:j:42:LEU:CD2	2.42	0.67
38:k:218:SER:CB	44:k:705:GNP:O2'	2.38	0.67
40:R:141:PHE:O	40:R:142:ILE:HG13	1.92	0.67
34:2:1518:C:C5'	39:U:143:GLY:C	2.67	0.67
37:j:9:GLY:N	40:R:140:ARG:HH22	1.90	0.67
6:F:196:GLY:HA2	6:F:198:ILE:N	2.08	0.67
25:a:100:LYS:HG2	25:a:101:LYS:O	1.95	0.67
25:a:123:ALA:O	25:a:127:ALA:CA	2.42	0.67
35:A:185:THR:CB	35:A:187:GLN:HB2	2.15	0.67
38:k:229:VAL:O	38:k:232:ILE:HG22	1.93	0.67
38:k:412:LYS:HB2	38:k:483:TYR:CE1	2.30	0.67
38:k:321:ASN:O	38:k:322:LEU:HB2	1.94	0.67
34:2:472:G:OP1	38:k:63:LYS:NZ	2.28	0.67
38:k:488:PRO:HG2	38:k:524:MET:CE	2.23	0.67
38:k:532:VAL:HG21	38:k:551:LEU:HA	1.76	0.67
38:k:212:ARG:NE	38:k:359:GLU:OE2	2.27	0.67
16:P:20:ARG:HD2	16:P:65:PHE:CD1	2.21	0.67
34:2:740:G:O6	34:2:793:C:N3	2.27	0.67
37:j:40:LYS:HB2	37:j:40:LYS:HZ3	1.58	0.67
38:k:329:LEU:HG	38:k:495:GLU:HA	1.76	0.67
38:k:451:ILE:CG1	38:k:452:GLU:N	2.53	0.67
38:k:578:ASN:ND2	38:k:585:ASP:CB	2.58	0.67
38:k:4:LYS:HA	38:k:79:LEU:HD12	1.77	0.67
38:k:85:HIS:HB2	38:k:130:ASN:CG	2.18	0.67
16:P:27:LYS:HZ2	16:P:27:LYS:HB2	1.60	0.66
33:i:81:ALA:CB	37:j:82:ARG:HD3	2.25	0.66
34:2:1518:C:H5'	39:U:144:ARG:CA	2.25	0.66
38:k:431:LYS:CE	38:k:477:GLY:C	2.68	0.66
38:k:431:LYS:HB3	38:k:477:GLY:O	1.94	0.66
33:i:80:LEU:HD21	37:j:62:ARG:HH21	1.56	0.66
35:A:235:TYR:CD1	36:B:285:ASP:HB2	2.28	0.66
38:k:241:ASP:C	38:k:242:GLU:CB	2.68	0.66
38:k:165:LYS:O	38:k:237:ILE:HG22	1.95	0.66
38:k:139:ASP:O	38:k:140:TRP:C	2.37	0.66
34:2:471:C:P	38:k:7:ARG:HH22	2.19	0.66
38:k:200:VAL:CG1	38:k:228:ALA:HA	2.25	0.66
38:k:332:LYS:O	38:k:333:VAL:C	2.38	0.66
16:P:19:ARG:O	16:P:20:ARG:HB2	1.96	0.66
25:a:101:LYS:C	25:a:102:THR:HG1	2.01	0.66
34:2:1705:C:O4'	37:j:42:LEU:HD21	1.96	0.66
39:U:148:VAL:CG2	40:R:131:PRO:O	2.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:9:THR:C	25:a:10:ARG:CG	2.68	0.66
34:2:1707:A:C5	34:2:1708:C:C5	2.84	0.66
34:2:80:G:C5	34:2:81:U:C4	2.84	0.66
38:k:489:SER:O	38:k:497:ARG:NH2	2.29	0.66
34:2:1518:C:O5'	39:U:143:GLY:C	2.39	0.65
38:k:348:TYR:CD2	38:k:369:PHE:O	2.48	0.65
38:k:412:LYS:HD3	38:k:485:ILE:CB	2.25	0.65
35:A:58:SER:HB2	35:A:61:LYS:CE	2.25	0.65
37:j:7:LYS:HG3	37:j:8:GLY:H	1.60	0.65
38:k:311:ILE:CA	38:k:317:VAL:CG2	2.68	0.65
38:k:582:SER:H	38:k:585:ASP:HB3	1.60	0.65
24:Z:52:LEU:HD22	38:k:33:ARG:CD	2.27	0.65
38:k:591:SER:CA	38:k:592:GLY:N	2.60	0.65
37:j:70:TRP:CZ2	41:3:55:G:C1'	2.79	0.65
38:k:337:ALA:O	38:k:338:ASN:CB	2.45	0.65
34:2:1518:C:P	39:U:143:GLY:C	2.80	0.65
41:3:38:C:C2	41:3:39:U:C4	2.85	0.65
11:K:157:LYS:HD3	14:N:23:VAL:HG11	1.77	0.65
38:k:73:VAL:HG21	38:k:322:LEU:HD21	1.78	0.65
38:k:237:ILE:O	38:k:238:PHE:CG	2.50	0.65
38:k:489:SER:O	38:k:497:ARG:CZ	2.45	0.65
25:a:101:LYS:HZ2	25:a:107:ARG:CZ	2.08	0.65
16:P:25:TRP:O	16:P:26:LEU:HB3	1.95	0.64
38:k:131:LEU:HD12	38:k:143:ILE:HG22	1.78	0.64
38:k:330:VAL:CG2	38:k:574:ARG:CD	2.69	0.64
25:a:128:GLY:HA3	38:k:264:ASN:HB3	1.80	0.64
34:2:743:U:H1'	34:2:744:C:H1'	1.78	0.64
38:k:135:ASP:O	38:k:138:PRO:HD3	1.96	0.64
41:3:69:U:H5	41:3:70:G:C8	2.15	0.64
41:3:76:A:H2'	41:3:77:A:C5'	2.17	0.64
25:a:10:ARG:HB2	25:a:24:VAL:HB	1.79	0.64
37:j:94:LYS:CE	37:j:95:TYR:O	2.45	0.64
38:k:188:LEU:HD13	38:k:225:PHE:CE1	2.31	0.64
24:Z:97:ASN:HD21	38:k:34:MET:CE	2.10	0.64
25:a:104:ARG:NH2	25:a:108:LYS:HE3	2.00	0.64
34:2:785:G:N2	34:2:786:C:O2	2.29	0.64
37:j:30:GLU:N	37:j:33:GLN:O	2.30	0.64
39:U:146:VAL:HG13	40:R:131:PRO:HG3	0.64	0.64
33:i:82:ARG:HH21	33:i:85:LYS:HA	1.63	0.64
35:A:185:THR:OG1	35:A:186:PRO:N	2.30	0.64
34:2:739:U:H4'	34:2:740:G:OP2	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1819:A:N1	37:j:70:TRP:HA	2.13	0.64
35:A:229:LEU:CB	36:B:284:VAL:HG11	2.23	0.64
34:2:683:G:C6	34:2:684:A:C6	2.86	0.64
37:j:70:TRP:CZ2	41:3:55:G:O2'	2.34	0.64
38:k:191:LYS:HG3	38:k:229:VAL:HG23	1.79	0.64
37:j:74:SER:O	37:j:75:ASP:CB	2.40	0.64
34:2:784:G:H2'	34:2:785:G:H5'	1.79	0.63
35:A:205:ILE:CD1	36:B:288:LYS:HG3	2.28	0.63
37:j:13:ARG:C	37:j:13:ARG:HD3	2.23	0.63
34:2:1707:A:H2'	34:2:1708:C:H5'	1.77	0.63
38:k:22:ARG:O	38:k:23:GLN:HG2	1.97	0.63
34:2:743:U:H1'	34:2:744:C:O4'	1.99	0.63
34:2:1327:C:H5	37:j:16:LYS:N	1.94	0.63
35:A:54:ARG:HB2	35:A:54:ARG:NH2	2.13	0.63
37:j:72:ASN:HD22	37:j:72:ASN:N	1.91	0.63
38:k:217:LEU:CG	38:k:221:GLU:HG2	2.17	0.63
38:k:218:SER:N	44:k:705:GNP:O2'	2.31	0.63
38:k:159:ILE:HD13	38:k:164:LEU:HB3	1.81	0.63
34:2:790:A:O5'	34:2:790:A:H8	1.81	0.63
37:j:94:LYS:HE2	37:j:95:TYR:O	1.99	0.63
38:k:441:PHE:CZ	38:k:454:ILE:HG21	2.33	0.63
40:R:141:PHE:C	40:R:142:ILE:CD1	2.67	0.63
35:A:235:TYR:CZ	36:B:285:ASP:OD1	2.52	0.63
38:k:17:LYS:HG2	38:k:20:LYS:HE3	1.78	0.63
38:k:7:ARG:C	38:k:8:ILE:HG12	2.22	0.63
25:a:9:THR:C	25:a:10:ARG:HG2	2.23	0.63
37:j:63:GLY:O	37:j:64:LYS:CG	2.43	0.63
37:j:92:ILE:HG22	37:j:93:LEU:CB	2.22	0.63
16:P:29:THR:N	16:P:32:ASP:OD2	2.32	0.62
35:A:108:VAL:HG23	35:A:150:TYR:CD1	2.32	0.62
35:A:235:TYR:CE1	36:B:285:ASP:CB	2.78	0.62
38:k:486:ASP:CA	38:k:487:GLU:N	2.62	0.62
14:N:22:ARG:HH21	14:N:24:LEU:CB	2.10	0.62
34:2:740:G:C2	34:2:793:C:O2	2.52	0.62
34:2:740:G:C6	34:2:793:C:N3	2.68	0.62
35:A:157:VAL:HG11	35:A:180:ILE:HB	1.80	0.62
35:A:181:ASN:O	35:A:185:THR:HG23	2.00	0.62
35:A:157:VAL:CB	35:A:180:ILE:HG21	2.27	0.62
38:k:32:VAL:O	38:k:32:VAL:HG12	1.99	0.62
34:2:746:C:H2'	34:2:747:G:N7	2.14	0.62
41:3:42:A:O5'	41:3:42:A:H8	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:185:THR:OG1	35:A:186:PRO:CA	2.46	0.62
34:2:688:U:O5'	34:2:688:U:H6	1.83	0.62
35:A:235:TYR:HD1	36:B:285:ASP:CG	1.85	0.62
38:k:272:VAL:CG1	38:k:273:GLU:H	2.13	0.62
38:k:450:GLN:O	38:k:453:ASN:HB2	1.94	0.62
34:2:685:G:H1	34:2:730:C:H42	1.47	0.62
34:2:1232:G:O2'	40:R:135:ALA:HB2	2.00	0.62
38:k:414:GLN:CG	38:k:486:ASP:CG	2.73	0.62
37:j:39:ILE:HB	37:j:48:GLU:HG3	1.81	0.62
38:k:112:ASN:CA	44:k:704:GNP:O3G	2.45	0.62
38:k:168:ILE:HG22	38:k:239:MET:HB2	1.81	0.62
38:k:176:ILE:CA	38:k:178:LYS:H	2.13	0.62
34:2:471:C:OP2	38:k:7:ARG:NH2	2.33	0.62
34:2:1707:A:C2	34:2:1708:C:C5	2.88	0.62
35:A:235:TYR:CE1	36:B:285:ASP:HB2	2.35	0.62
35:A:229:LEU:CB	36:B:284:VAL:CG2	2.68	0.61
38:k:346:CYS:C	38:k:347:MET:HG3	2.25	0.61
40:R:134:GLY:C	40:R:136:THR:H	2.08	0.61
38:k:517:VAL:HG12	38:k:519:GLU:HG2	1.82	0.61
33:i:81:ALA:HB1	37:j:82:ARG:CD	2.30	0.61
37:j:70:TRP:CE2	40:R:143:PRO:CG	2.83	0.61
38:k:39:ILE:HD11	42:k:701:SF4:S4	2.41	0.61
25:a:98:GLU:N	25:a:98:GLU:OE2	2.31	0.61
1:1:16:G:C4	1:1:17:C:C5	2.89	0.61
9:I:235:SER:O	9:I:236:SER:C	2.43	0.61
38:k:441:PHE:HZ	38:k:454:ILE:HG21	1.66	0.61
34:2:682:G:C2	34:2:683:G:N7	2.69	0.61
35:A:229:LEU:CD1	36:B:284:VAL:HG21	2.29	0.61
38:k:188:LEU:HD13	38:k:225:PHE:HD1	1.63	0.61
34:2:733:G:N7	34:2:738:U:C4	2.69	0.61
34:2:745:U:O2'	34:2:746:C:O4'	2.18	0.61
34:2:1816:A:C2	34:2:1817:A:N6	2.68	0.61
34:2:1518:C:P	39:U:143:GLY:CA	2.87	0.61
38:k:250:LYS:HE2	38:k:562:LEU:HD22	1.82	0.61
41:3:43:A:O2'	41:3:44:C:H5'	1.99	0.61
41:3:67:C:O2'	41:3:68:C:H5'	2.00	0.61
16:P:20:ARG:HG3	16:P:65:PHE:CE1	2.36	0.61
34:2:1766:C:O2'	34:2:1767:C:H5'	2.01	0.61
37:j:78:LEU:HD23	37:j:93:LEU:CG	2.30	0.61
38:k:345:MET:HG3	38:k:346:CYS:N	2.13	0.61
40:R:143:PRO:HB3	41:3:55:G:H1'	1.79	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:751:C:H2'	34:2:752:C:C6	2.35	0.60
34:2:790:A:C6	34:2:791:A:N6	2.69	0.60
38:k:158:LYS:O	38:k:163:ASP:HB2	2.01	0.60
38:k:309:ILE:O	38:k:313:LEU:HD23	2.01	0.60
34:2:478:U:H5	38:k:99:ILE:HD13	1.60	0.60
34:2:734:C:C3'	34:2:735:C:H5''	2.30	0.60
38:k:527:TYR:O	38:k:528:LEU:HD12	2.00	0.60
37:j:24:ARG:HA	37:j:25:GLU:HB2	1.83	0.60
33:i:81:ALA:HB1	37:j:82:ARG:HD3	1.82	0.60
34:2:472:G:P	38:k:63:LYS:NZ	2.74	0.60
38:k:410:SER:OG	38:k:475:CYS:O	2.18	0.60
33:i:76:VAL:HG11	37:j:62:ARG:NH2	2.16	0.60
34:2:470:G:OP1	38:k:74:ASN:ND2	2.34	0.60
34:2:744:C:C4	34:2:745:U:O4	2.55	0.60
37:j:13:ARG:HD3	37:j:13:ARG:O	2.01	0.60
38:k:311:ILE:HB	38:k:317:VAL:HB	1.82	0.60
35:A:235:TYR:CD1	36:B:285:ASP:OD1	2.33	0.60
37:j:61:ILE:HG22	37:j:62:ARG:N	2.17	0.60
38:k:188:LEU:CD1	38:k:225:PHE:CD1	2.85	0.60
34:2:793:C:C2'	34:2:794:G:H4'	2.31	0.60
35:A:178:ASN:O	35:A:182:ARG:CG	2.50	0.60
37:j:70:TRP:HD1	40:R:143:PRO:HA	1.51	0.60
41:3:49:A:OP2	41:3:49:A:H2	1.84	0.60
14:N:23:VAL:O	14:N:23:VAL:HG13	2.02	0.60
37:j:15:GLY:O	37:j:16:LYS:CG	2.50	0.60
10:J:109:ARG:HD2	34:2:794:G:H1'	1.83	0.60
25:a:101:LYS:HZ3	25:a:107:ARG:NE	1.99	0.60
34:2:686:G:H8	34:2:686:G:O5'	1.84	0.60
24:Z:52:LEU:HD22	38:k:33:ARG:HD3	1.84	0.59
34:2:1812:A:C2	34:2:1813:A:N9	2.69	0.59
34:2:1818:A:C4'	37:j:44:ASN:O	2.49	0.59
38:k:17:LYS:CG	38:k:20:LYS:CE	2.69	0.59
38:k:330:VAL:HG22	38:k:330:VAL:O	2.02	0.59
38:k:533:ILE:HG22	38:k:548:PRO:HB3	1.83	0.59
41:3:53:U:O5'	41:3:53:U:H6	1.85	0.59
1:1:18:G:C1'	1:1:61:C:H5''	2.29	0.59
38:k:414:GLN:OE1	38:k:486:ASP:CG	2.45	0.59
38:k:492:LEU:HB2	38:k:497:ARG:HG2	1.82	0.59
41:3:69:U:H3'	41:3:69:U:OP2	2.02	0.59
34:2:479:A:H4'	38:k:150:SER:C	2.28	0.59
34:2:1693:C:C1'	41:3:58:C:N4	2.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:425:ARG:NH1	38:k:455:ILE:CD1	2.65	0.59
37:j:10:LYS:HB2	41:3:54:G:H21	1.68	0.59
38:k:204:LEU:HD12	38:k:224:ARG:HH12	1.68	0.59
38:k:486:ASP:HA	38:k:487:GLU:N	2.17	0.59
37:j:76:ILE:HD13	37:j:76:ILE:N	2.16	0.59
38:k:112:ASN:HB3	44:k:704:GNP:O3G	2.01	0.59
41:3:59:A:H8	41:3:59:A:O5'	1.86	0.59
38:k:109:VAL:O	38:k:110:GLY:N	2.31	0.59
37:j:62:ARG:NH1	37:j:64:LYS:HD2	2.18	0.59
38:k:184:VAL:O	38:k:186:SER:N	2.36	0.59
38:k:498:LEU:HD11	38:k:523:ILE:CD1	2.19	0.59
34:2:790:A:H2'	34:2:791:A:C8	2.37	0.59
34:2:682:G:C2	34:2:683:G:C5	2.91	0.59
38:k:329:LEU:CD2	38:k:495:GLU:OE1	2.51	0.59
38:k:332:LYS:CD	38:k:527:TYR:CE2	2.85	0.59
38:k:450:GLN:O	38:k:453:ASN:CB	2.47	0.59
41:3:43:A:C2'	41:3:44:C:C6	2.86	0.59
24:Z:74:LEU:O	38:k:60:ILE:HD12	2.02	0.59
37:j:40:LYS:CD	37:j:41:MET:H	2.14	0.59
37:j:41:MET:HE2	37:j:47:LEU:HD22	1.85	0.59
38:k:348:TYR:O	38:k:349:LYS:HB3	2.01	0.59
38:k:590:LYS:C	38:k:592:GLY:N	2.61	0.59
41:3:72:G:H8	41:3:72:G:O5'	1.86	0.59
1:1:35:A:H4'	37:j:8:GLY:C	2.28	0.58
16:P:22:VAL:HB	16:P:24:THR:H	1.68	0.58
34:2:743:U:C6	34:2:744:C:C2	2.91	0.58
38:k:325:ARG:O	38:k:326:ASP:HB2	2.03	0.58
25:a:101:LYS:HG2	25:a:107:ARG:NH2	2.17	0.58
34:2:682:G:H2'	34:2:683:G:H8	1.68	0.58
34:2:683:G:N1	34:2:684:A:C6	2.71	0.58
38:k:550:THR:OG1	38:k:553:ALA:CB	2.51	0.58
34:2:743:U:HO2'	34:2:744:C:C1'	2.16	0.58
37:j:19:ASN:CG	37:j:20:GLU:HA	2.28	0.58
38:k:375:MET:HE1	38:k:531:ARG:HD3	1.80	0.58
41:3:73:G:N7	41:3:74:A:N7	2.51	0.58
16:P:19:ARG:NH2	16:P:21:SER:OG	2.37	0.58
25:a:12:PHE:HZ	34:2:836:C:O2'	1.85	0.58
34:2:1407:G:H3'	34:2:1408:C:H5''	1.85	0.58
35:A:205:ILE:CD1	36:B:288:LYS:CG	2.81	0.58
37:j:40:LYS:HB2	37:j:40:LYS:HZ2	1.68	0.58
38:k:414:GLN:HE21	38:k:486:ASP:CB	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:705:GNP:H3'	44:k:705:GNP:O1A	2.04	0.58
40:R:133:ILE:C	40:R:135:ALA:H	2.10	0.58
41:3:38:C:O2	41:3:39:U:C4	2.55	0.58
1:1:27:C:C4	1:1:28:U:C5	2.92	0.58
34:2:793:C:H4'	34:2:793:C:OP1	2.03	0.58
37:j:19:ASN:CB	37:j:20:GLU:HA	2.34	0.58
38:k:229:VAL:HA	38:k:232:ILE:HG22	1.86	0.58
38:k:521:ASP:OD2	38:k:524:MET:HB2	2.04	0.58
10:J:106:ARG:HD3	34:2:794:G:C6	2.38	0.58
34:2:471:C:P	38:k:7:ARG:NH2	2.76	0.58
34:2:526:A:H62	34:2:537:G:H21	1.51	0.58
34:2:743:U:H3	34:2:791:A:H2	1.51	0.58
34:2:784:G:C5	34:2:785:G:N7	2.71	0.58
34:2:1707:A:C6	34:2:1708:C:C5	2.92	0.58
37:j:70:TRP:CZ2	40:R:143:PRO:HB3	2.39	0.58
38:k:319:THR:HG23	38:k:320:GLU:HB3	1.85	0.58
16:P:23:PRO:O	16:P:25:TRP:N	2.37	0.58
16:P:27:LYS:HG3	16:P:28:LEU:HD21	1.84	0.58
25:a:123:ALA:C	25:a:127:ALA:HB3	2.27	0.58
33:i:80:LEU:HD11	37:j:92:ILE:HD13	1.85	0.58
35:A:157:VAL:CG1	35:A:180:ILE:HD12	2.33	0.58
34:2:784:G:C2'	34:2:785:G:H5'	2.33	0.58
38:k:4:LYS:CG	38:k:79:LEU:HD12	2.32	0.58
38:k:508:ILE:HD12	38:k:515:ALA:HB2	1.86	0.58
16:P:27:LYS:HE3	16:P:28:LEU:CD2	2.34	0.57
35:A:58:SER:OG	35:A:61:LYS:CG	2.30	0.57
34:2:683:G:N2	34:2:731:C:C2	2.66	0.57
37:j:94:LYS:HG2	37:j:95:TYR:H	1.65	0.57
38:k:583:ILE:CG2	38:k:584:LYS:H	2.13	0.57
1:1:18:G:O6	35:A:107:THR:HG21	2.04	0.57
33:i:77:HIS:HA	37:j:33:GLN:HE22	1.68	0.57
34:2:683:G:O2'	34:2:684:A:H5'	2.04	0.57
34:2:1518:C:O3'	39:U:144:ARG:HA	2.01	0.57
38:k:217:LEU:HB3	38:k:221:GLU:CB	2.32	0.57
38:k:331:PHE:HA	38:k:523:ILE:CG2	2.34	0.57
34:2:1170:U:H2'	34:2:1171:G:C8	2.39	0.57
38:k:105:VAL:HG23	38:k:263:ILE:HG12	1.86	0.57
34:2:1707:A:C2	34:2:1708:C:C4	2.92	0.57
37:j:16:LYS:HE2	41:3:57:G:HO2'	1.68	0.57
38:k:348:TYR:O	38:k:349:LYS:CB	2.52	0.57
38:k:373:GLU:O	38:k:514:THR:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:746:C:C2'	34:2:747:G:C8	2.86	0.57
34:2:750:G:C6	34:2:751:C:N4	2.73	0.57
34:2:787:C:H2'	34:2:788:C:C5	2.38	0.57
35:A:197:VAL:HG21	35:A:235:TYR:HE2	1.68	0.57
38:k:331:PHE:O	38:k:498:LEU:HD22	2.05	0.57
37:j:28:PHE:O	37:j:78:LEU:HD11	2.05	0.57
36:B:284:VAL:CG1	36:B:285:ASP:HB3	2.31	0.57
38:k:229:VAL:HG13	38:k:230:VAL:N	2.19	0.57
38:k:322:LEU:HG	38:k:323:ARG:N	2.18	0.57
34:2:454:A:N1	38:k:578:ASN:OD1	2.37	0.57
38:k:489:SER:N	38:k:524:MET:CE	2.67	0.57
34:2:1696:C:C2	37:j:11:ASN:OD1	2.58	0.57
37:j:9:GLY:CA	40:R:140:ARG:HH12	2.18	0.57
14:N:25:LEU:CD2	14:N:29:GLY:HA3	2.35	0.56
34:2:683:G:C6	34:2:684:A:N6	2.73	0.56
34:2:1518:C:OP1	39:U:143:GLY:N	2.37	0.56
37:j:19:ASN:HB3	37:j:20:GLU:HA	1.86	0.56
38:k:139:ASP:O	38:k:141:GLN:N	2.38	0.56
38:k:237:ILE:HG13	38:k:238:PHE:H	1.70	0.56
38:k:414:GLN:HE21	38:k:486:ASP:CA	2.17	0.56
41:3:49:A:H2'	41:3:50:C:O4'	2.05	0.56
34:2:740:G:H2'	34:2:741:C:H5''	1.87	0.56
38:k:21:CYS:O	38:k:24:GLU:OE2	2.22	0.56
16:P:29:THR:O	16:P:30:SER:C	2.48	0.56
34:2:1707:A:C6	34:2:1708:C:N4	2.73	0.56
38:k:315:GLY:HA2	38:k:326:ASP:CA	2.35	0.56
25:a:104:ARG:HD2	34:2:482:C:OP2	2.05	0.56
38:k:19:LYS:O	38:k:19:LYS:HG3	2.06	0.56
41:3:65:C:H1'	41:3:66:U:C6	2.40	0.56
34:2:745:U:C2	34:2:746:C:C4	2.94	0.56
14:N:22:ARG:NH2	14:N:23:VAL:O	2.38	0.56
34:2:80:G:C4	34:2:81:U:C5	2.93	0.56
34:2:848:G:H3'	34:2:849:C:H5''	1.87	0.56
34:2:1518:C:H4'	39:U:144:ARG:C	2.31	0.56
25:a:104:ARG:HB2	34:2:481:C:P	2.46	0.56
38:k:183:THR:O	38:k:187:ILE:HB	2.05	0.56
38:k:204:LEU:HD12	38:k:224:ARG:NH1	2.21	0.56
6:F:1:MET:O	6:F:2:ALA:HB2	2.06	0.55
38:k:76:PRO:CG	38:k:323:ARG:HG3	2.36	0.55
38:k:309:ILE:HG22	38:k:313:LEU:HD21	1.87	0.55
25:a:128:GLY:HA3	38:k:264:ASN:CB	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:315:GLY:O	38:k:316:TYR:CD1	2.58	0.55
38:k:318:PRO:O	38:k:319:THR:HG22	2.06	0.55
1:1:17:C:N4	1:1:60:A:C2	2.66	0.55
34:2:472:G:P	38:k:63:LYS:HZ1	2.30	0.55
35:A:263:GLU:HG2	35:A:269:PHE:CD1	2.41	0.55
38:k:489:SER:CA	38:k:524:MET:CE	2.84	0.55
38:k:559:LEU:HB2	38:k:594:TYR:CD2	2.41	0.55
16:P:22:VAL:HB	16:P:23:PRO:C	2.31	0.55
34:2:734:C:C5	34:2:737:C:N4	2.73	0.55
38:k:212:ARG:NH2	44:k:705:GNP:N3	2.53	0.55
38:k:330:VAL:HG22	38:k:575:PRO:CD	2.23	0.55
38:k:441:PHE:HZ	38:k:454:ILE:CG2	2.14	0.55
16:P:27:LYS:O	16:P:28:LEU:HG	2.06	0.55
38:k:381:ASN:CB	44:k:705:GNP:O1G	2.49	0.55
38:k:582:SER:H	38:k:585:ASP:CB	2.19	0.55
10:J:75:ILE:HG23	10:J:76:GLN:H	1.70	0.55
38:k:318:PRO:C	38:k:319:THR:HG22	2.32	0.55
38:k:374:ILE:HD11	38:k:529:ALA:HA	1.77	0.55
41:3:73:G:C5	41:3:74:A:C5	2.94	0.55
16:P:22:VAL:CG2	16:P:24:THR:H	2.20	0.55
16:P:27:LYS:CE	16:P:28:LEU:HD23	2.36	0.55
24:Z:58:GLU:OE1	37:j:60:HIS:ND1	2.34	0.55
37:j:40:LYS:HD3	37:j:41:MET:C	2.31	0.55
38:k:165:LYS:N	38:k:236:ASP:HB3	2.22	0.55
38:k:489:SER:HA	38:k:524:MET:HE1	1.85	0.55
38:k:492:LEU:C	38:k:497:ARG:NE	2.63	0.55
38:k:530:ASP:O	38:k:532:VAL:HG23	2.06	0.55
38:k:315:GLY:C	38:k:326:ASP:HB3	2.31	0.55
38:k:336:THR:O	38:k:337:ALA:HB2	2.05	0.55
34:2:687:G:H2'	34:2:688:U:H5'	1.89	0.55
38:k:316:TYR:N	38:k:316:TYR:HD1	2.05	0.55
38:k:318:PRO:HG2	38:k:322:LEU:CA	2.26	0.55
40:R:129:GLY:O	40:R:130:ARG:HB3	2.06	0.55
34:2:681:U:O2	34:2:681:U:H2'	2.07	0.55
34:2:1327:C:C4	37:j:16:LYS:N	2.75	0.55
38:k:385:LYS:HE2	38:k:518:VAL:HG13	1.89	0.55
10:J:109:ARG:CD	34:2:794:G:H1'	2.37	0.54
11:K:5:ARG:HH22	34:2:372:C:H41	1.55	0.54
14:N:30:LYS:HE2	14:N:30:LYS:CA	2.38	0.54
37:j:29:LYS:CA	37:j:33:GLN:O	2.55	0.54
38:k:113:GLY:HA2	44:k:704:GNP:O3A	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:451:ILE:HG22	38:k:454:ILE:HG23	1.89	0.54
40:R:143:PRO:HG2	41:3:55:G:C1'	2.34	0.54
25:a:128:GLY:O	38:k:264:ASN:CB	2.49	0.54
35:A:197:VAL:CG2	35:A:235:TYR:HE2	2.20	0.54
38:k:187:ILE:CG2	38:k:188:LEU:H	2.06	0.54
38:k:520:HIS:HE1	44:k:705:GNP:O1G	1.91	0.54
34:2:80:G:C5	34:2:81:U:C5	2.95	0.54
38:k:374:ILE:HD11	38:k:529:ALA:O	2.03	0.54
41:3:71:A:N6	41:3:72:G:O6	2.41	0.54
37:j:49:ALA:HB3	37:j:59:CYS:SG	2.47	0.54
38:k:204:LEU:HA	38:k:224:ARG:NH1	2.13	0.54
38:k:312:PHE:O	38:k:326:ASP:OD2	2.25	0.54
38:k:319:THR:CA	38:k:320:GLU:CB	2.85	0.54
38:k:475:CYS:HB3	38:k:483:TYR:CE1	2.43	0.54
34:2:478:U:C4	38:k:99:ILE:CD1	2.78	0.54
34:2:684:A:H8	34:2:684:A:O5'	1.91	0.54
37:j:70:TRP:HE1	40:R:143:PRO:CB	2.09	0.54
38:k:241:ASP:O	38:k:242:GLU:CB	2.56	0.54
38:k:312:PHE:CD1	38:k:312:PHE:C	2.86	0.54
41:3:43:A:H2'	41:3:44:C:H6	1.71	0.54
14:N:30:LYS:HE2	14:N:30:LYS:H	1.66	0.54
16:P:27:LYS:CE	16:P:28:LEU:CD2	2.86	0.54
34:2:786:C:H6	34:2:786:C:O5'	1.91	0.54
35:A:58:SER:CB	35:A:61:LYS:HE3	2.37	0.54
37:j:93:LEU:C	37:j:94:LYS:O	2.36	0.54
38:k:374:ILE:CD1	38:k:529:ALA:N	2.71	0.54
34:2:739:U:O2	34:2:739:U:H2'	2.07	0.54
34:2:787:C:N3	34:2:788:C:N4	2.55	0.54
37:j:93:LEU:O	37:j:94:LYS:C	2.39	0.54
16:P:26:LEU:HD13	16:P:26:LEU:O	2.07	0.54
35:A:58:SER:HB2	35:A:61:LYS:HD2	1.85	0.54
35:A:108:VAL:CG2	35:A:150:TYR:CD1	2.82	0.54
38:k:332:LYS:CE	38:k:334:ALA:CB	2.37	0.54
38:k:414:GLN:CG	38:k:486:ASP:OD1	2.55	0.54
38:k:209:LEU:HD13	38:k:221:GLU:CB	2.38	0.54
41:3:38:C:N3	41:3:39:U:O4	2.41	0.54
1:1:16:G:C2'	1:1:17:C:H5''	2.37	0.54
14:N:22:ARG:HG3	14:N:23:VAL:N	2.23	0.54
40:R:140:ARG:NH2	40:R:140:ARG:HG2	2.22	0.54
41:3:60:C:C2'	41:3:61:C:H4'	2.38	0.54
38:k:165:LYS:H	38:k:236:ASP:CB	2.20	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:315:GLY:C	38:k:316:TYR:CG	2.84	0.53
38:k:378:LEU:C	38:k:385:LYS:CE	2.81	0.53
41:3:57:G:H3'	41:3:57:G:OP2	2.09	0.53
41:3:58:C:N3	41:3:59:A:C5	2.76	0.53
16:P:22:VAL:HG11	16:P:26:LEU:CD1	2.37	0.53
9:I:237:LEU:HD12	34:2:784:G:C3'	2.33	0.53
38:k:321:ASN:O	38:k:322:LEU:CB	2.56	0.53
38:k:492:LEU:O	38:k:497:ARG:NH2	2.41	0.53
41:3:71:A:H8	41:3:71:A:O5'	1.92	0.53
9:I:237:LEU:HB3	34:2:785:G:OP1	2.07	0.53
34:2:1815:U:H2'	34:2:1816:A:C5'	2.31	0.53
37:j:70:TRP:CD2	40:R:143:PRO:HG3	2.43	0.53
38:k:174:ASP:O	38:k:176:ILE:N	2.38	0.53
38:k:584:LYS:C	38:k:586:VAL:N	2.57	0.53
25:a:101:LYS:NZ	25:a:107:ARG:NH2	2.56	0.53
34:2:685:G:H1	34:2:730:C:N4	2.06	0.53
34:2:744:C:C5	34:2:745:U:O4	2.62	0.53
34:2:1519:G:OP1	39:U:144:ARG:CB	2.51	0.53
38:k:164:LEU:CD2	38:k:237:ILE:HD13	2.31	0.53
38:k:176:ILE:HG23	38:k:176:ILE:O	2.07	0.53
41:3:58:C:O2	41:3:58:C:H2'	2.08	0.53
41:3:60:C:H3'	41:3:61:C:C4'	2.38	0.53
34:2:1696:C:N3	37:j:11:ASN:OD1	2.42	0.53
34:2:1818:A:HO2'	34:2:1819:A:P	2.27	0.53
35:A:154:LYS:HD2	35:A:184:LEU:CD2	2.39	0.53
37:j:27:VAL:HG12	37:j:28:PHE:N	2.22	0.53
38:k:217:LEU:CD2	38:k:221:GLU:HB3	2.28	0.53
38:k:451:ILE:HB	38:k:454:ILE:HG23	1.91	0.53
25:a:10:ARG:C	25:a:11:LYS:HG3	2.33	0.53
10:J:109:ARG:HB3	34:2:740:G:C2'	2.35	0.53
11:K:193:LYS:HE2	14:N:32:LYS:HZ1	1.62	0.53
34:2:794:G:O2'	34:2:795:U:OP1	2.20	0.53
34:2:1815:U:O2'	34:2:1816:A:O5'	2.25	0.53
38:k:73:VAL:HB	38:k:322:LEU:CG	2.28	0.53
38:k:208:HIS:CE1	38:k:540:SER:N	2.77	0.53
38:k:237:ILE:C	38:k:238:PHE:CG	2.86	0.53
38:k:316:TYR:CD1	38:k:316:TYR:N	2.73	0.53
10:J:109:ARG:CB	34:2:740:G:O4'	2.40	0.53
34:2:682:G:N3	34:2:683:G:C8	2.76	0.53
34:2:687:G:C5	34:2:729:C:N4	2.77	0.53
1:1:16:G:C2	1:1:17:C:C5	2.97	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:682:G:H8	34:2:682:G:O5'	1.92	0.52
34:2:683:G:C2	34:2:684:A:C4	2.97	0.52
9:I:223:LYS:HE2	9:I:227:GLN:NE2	2.24	0.52
34:2:469:C:O2'	38:k:319:THR:O	2.27	0.52
9:I:221:LYS:HE2	9:I:225:GLN:NE2	2.24	0.52
25:a:10:ARG:HH21	25:a:11:LYS:CE	2.22	0.52
37:j:24:ARG:HG3	37:j:25:GLU:N	2.24	0.52
38:k:319:THR:N	38:k:320:GLU:CB	2.72	0.52
38:k:345:MET:HG2	38:k:346:CYS:N	2.25	0.52
38:k:451:ILE:CG2	38:k:454:ILE:HG23	2.39	0.52
24:Z:68:LYS:CD	37:j:84:TYR:OH	2.57	0.52
37:j:78:LEU:HD21	37:j:93:LEU:CD1	2.31	0.52
38:k:455:ILE:HG13	38:k:456:ASP:N	2.23	0.52
39:U:143:GLY:CA	39:U:144:ARG:HD2	2.38	0.52
9:I:235:SER:O	9:I:237:LEU:N	2.43	0.52
34:2:747:G:O5'	34:2:747:G:H8	1.91	0.52
34:2:1705:C:O2'	37:j:42:LEU:HD11	2.10	0.52
38:k:177:PRO:O	38:k:178:LYS:HG3	2.09	0.52
38:k:455:ILE:CB	38:k:456:ASP:N	2.37	0.52
41:3:70:G:N3	41:3:70:G:C3'	2.73	0.52
34:2:225:C:H3'	34:2:226:A:C5'	2.40	0.52
37:j:28:PHE:HB3	37:j:35:TYR:OH	2.10	0.52
37:j:61:ILE:CG2	37:j:62:ARG:N	2.73	0.52
38:k:217:LEU:HD23	38:k:221:GLU:CB	2.32	0.52
40:R:133:ILE:C	40:R:139:SER:OG	2.48	0.52
14:N:22:ARG:HH21	14:N:24:LEU:HD13	1.73	0.52
14:N:30:LYS:C	14:N:32:LYS:H	2.18	0.52
33:i:82:ARG:NH2	33:i:83:VAL:O	2.43	0.52
37:j:68:LYS:HG2	41:3:57:G:O6	2.10	0.52
38:k:385:LYS:HE2	38:k:518:VAL:CG1	2.40	0.52
34:2:745:U:H3'	34:2:745:U:H6	1.75	0.52
34:2:749:C:H3'	34:2:750:G:C5'	2.29	0.52
37:j:30:GLU:N	37:j:33:GLN:HB3	2.21	0.52
38:k:360:PHE:HE2	44:k:705:GNP:N3	2.07	0.52
14:N:26:GLY:O	14:N:27:GLU:HB2	2.09	0.52
34:2:1105:C:H3'	34:2:1106:G:H5''	1.92	0.52
38:k:450:GLN:CG	38:k:453:ASN:CG	2.83	0.52
38:k:532:VAL:CG2	38:k:551:LEU:HA	2.39	0.52
25:a:105:LYS:C	25:a:107:ARG:H	2.18	0.51
34:2:734:C:C3'	34:2:735:C:C5'	2.88	0.51
34:2:790:A:C5	34:2:791:A:N6	2.78	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:92:ILE:CG2	37:j:93:LEU:HD12	2.34	0.51
38:k:112:ASN:HB3	44:k:704:GNP:O1G	2.10	0.51
38:k:381:ASN:HB3	44:k:705:GNP:PG	2.50	0.51
1:1:16:G:N1	1:1:17:C:C5	2.78	0.51
35:A:229:LEU:CD2	36:B:284:VAL:HG23	2.06	0.51
38:k:113:GLY:N	44:k:704:GNP:N3B	2.53	0.51
38:k:217:LEU:C	44:k:705:GNP:O2'	2.53	0.51
40:R:130:ARG:NH1	40:R:130:ARG:CB	2.73	0.51
1:1:16:G:N1	1:1:17:C:H5	2.08	0.51
38:k:22:ARG:O	38:k:23:GLN:CG	2.58	0.51
38:k:134:TYR:H	38:k:135:ASP:HA	1.73	0.51
38:k:451:ILE:CB	38:k:454:ILE:HG23	2.41	0.51
38:k:508:ILE:HD12	38:k:515:ALA:CB	2.39	0.51
40:R:140:ARG:HH21	40:R:140:ARG:HG2	1.76	0.51
41:3:77:A:O5'	41:3:77:A:H8	1.94	0.51
6:F:195:SER:HA	6:F:202:LYS:HD2	1.92	0.51
34:2:795:U:O2	34:2:863:G:H1'	2.11	0.51
38:k:32:VAL:HG13	38:k:37:LEU:HD23	1.93	0.51
38:k:164:LEU:HD21	38:k:237:ILE:CG1	2.41	0.51
39:U:143:GLY:N	39:U:144:ARG:HD2	2.25	0.51
34:2:80:G:C4	34:2:81:U:C6	2.99	0.51
34:2:682:G:C4	34:2:683:G:N7	2.79	0.51
34:2:687:G:C6	34:2:729:C:N4	2.78	0.51
37:j:71:ILE:CD1	37:j:77:ILE:HD11	2.34	0.51
38:k:212:ARG:CZ	44:k:705:GNP:HN22	2.24	0.51
25:a:105:LYS:C	25:a:107:ARG:N	2.67	0.51
34:2:787:C:H6	34:2:787:C:O5'	1.94	0.51
34:2:1709:U:C2	34:2:1814:G:C2	2.99	0.51
34:2:1819:A:C6	37:j:66:ARG:O	2.64	0.51
38:k:329:LEU:HD23	38:k:495:GLU:OE1	2.11	0.51
39:U:148:VAL:HG21	40:R:132:GLY:O	2.11	0.51
33:i:82:ARG:HA	37:j:83:ASP:OD2	2.11	0.51
38:k:378:LEU:CA	38:k:385:LYS:HE3	2.40	0.51
38:k:485:ILE:HD11	38:k:488:PRO:HG3	1.92	0.51
38:k:522:PHE:HZ	38:k:595:PHE:CD1	2.29	0.51
16:P:20:ARG:CD	16:P:65:PHE:CZ	2.85	0.51
34:2:1693:C:C4	41:3:58:C:N4	2.78	0.51
37:j:62:ARG:HH11	37:j:64:LYS:CD	2.24	0.51
38:k:450:GLN:NE2	38:k:452:GLU:HB3	2.25	0.51
38:k:489:SER:O	38:k:497:ARG:NE	2.44	0.51
24:Z:96:GLU:CG	38:k:34:MET:CE	2.86	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:105:LYS:O	25:a:107:ARG:N	2.44	0.50
33:i:75:LYS:NZ	37:j:27:VAL:HG22	2.26	0.50
41:3:63:G:N3	41:3:63:G:C2'	2.73	0.50
34:2:687:G:C2'	34:2:688:U:H5'	2.41	0.50
38:k:174:ASP:C	38:k:176:ILE:H	2.19	0.50
41:3:63:G:N3	41:3:63:G:C3'	2.73	0.50
38:k:113:GLY:H	44:k:704:GNP:PB	2.34	0.50
38:k:221:GLU:CD	38:k:221:GLU:H	2.19	0.50
38:k:226:ALA:O	38:k:230:VAL:HG23	2.10	0.50
16:P:20:ARG:HD3	16:P:65:PHE:CZ	2.46	0.50
38:k:73:VAL:HB	38:k:322:LEU:HD22	0.55	0.50
38:k:209:LEU:CD1	38:k:221:GLU:HG2	2.35	0.50
38:k:318:PRO:HG3	38:k:322:LEU:HA	1.79	0.50
38:k:523:ILE:HA	38:k:526:THR:CG2	2.42	0.50
38:k:17:LYS:NZ	38:k:20:LYS:NZ	2.60	0.50
38:k:21:CYS:C	38:k:23:GLN:H	2.18	0.50
38:k:139:ASP:O	38:k:141:GLN:OE1	2.30	0.50
38:k:315:GLY:C	38:k:316:TYR:HD1	2.16	0.50
6:F:3:VAL:HG13	6:F:4:GLN:N	2.27	0.50
33:i:75:LYS:NZ	37:j:27:VAL:HG21	2.26	0.50
38:k:248:ASP:HB2	38:k:381:ASN:OD1	2.12	0.50
38:k:294:SER:CB	44:k:704:GNP:O3'	2.58	0.50
40:R:133:ILE:O	40:R:135:ALA:N	2.44	0.50
37:j:7:LYS:O	40:R:140:ARG:HG2	2.12	0.50
38:k:17:LYS:CG	38:k:20:LYS:HE2	2.33	0.50
38:k:131:LEU:CD1	38:k:143:ILE:HG22	2.41	0.50
38:k:492:LEU:HB2	38:k:497:ARG:HE	1.77	0.50
41:3:49:A:O2'	41:3:50:C:H5'	2.11	0.50
6:F:2:ALA:CB	6:F:3:VAL:HA	2.22	0.50
25:a:12:PHE:CD1	34:2:836:C:H1'	2.46	0.50
37:j:15:GLY:O	37:j:16:LYS:CB	2.60	0.50
38:k:331:PHE:H	38:k:498:LEU:CD1	2.25	0.50
38:k:412:LYS:HB2	38:k:483:TYR:HE1	1.76	0.50
38:k:449:LEU:HG	38:k:496:GLN:OE1	2.11	0.50
15:O:85:LEU:HD23	15:O:85:LEU:H	1.77	0.50
38:k:319:THR:H	38:k:320:GLU:CA	2.24	0.50
40:R:133:ILE:CG1	40:R:139:SER:HB3	2.37	0.50
24:Z:52:LEU:O	24:Z:53:GLU:HB3	2.12	0.49
35:A:229:LEU:HD13	36:B:285:ASP:CB	2.42	0.49
37:j:11:ASN:O	37:j:12:ARG:HG2	2.12	0.49
38:k:173:VAL:O	38:k:177:PRO:HD3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:204:LEU:HG	38:k:224:ARG:HD2	1.92	0.49
38:k:455:ILE:CG1	38:k:456:ASP:N	2.73	0.49
34:2:679:U:H2'	34:2:680:G:C8	2.47	0.49
38:k:315:GLY:C	38:k:326:ASP:CB	2.85	0.49
38:k:320:GLU:O	38:k:321:ASN:HB2	2.12	0.49
34:2:683:G:C2	34:2:684:A:C5	3.00	0.49
34:2:1755:U:H3	34:2:1765:G:H1	1.60	0.49
37:j:94:LYS:HG2	37:j:95:TYR:O	2.12	0.49
38:k:112:ASN:CB	44:k:704:GNP:O3G	2.59	0.49
38:k:559:LEU:HB2	38:k:594:TYR:CE2	2.48	0.49
34:2:745:U:N3	34:2:746:C:N4	2.60	0.49
35:A:216:LEU:HD13	35:A:250:VAL:HG22	1.94	0.49
35:A:227:ILE:HD11	35:A:237:MET:CE	2.18	0.49
38:k:416:ILE:HD13	38:k:471:ALA:CB	2.42	0.49
40:R:134:GLY:O	40:R:136:THR:N	2.41	0.49
1:1:69:U:H2'	1:1:69:U:O2	2.12	0.49
16:P:27:LYS:HB2	16:P:27:LYS:HZ3	1.76	0.49
38:k:550:THR:OG1	38:k:553:ALA:HB3	2.12	0.49
33:i:82:ARG:NH2	33:i:85:LYS:HA	2.27	0.49
37:j:10:LYS:CG	37:j:11:ASN:N	2.39	0.49
34:2:740:G:C3'	34:2:741:C:H5''	2.43	0.49
34:2:795:U:C2	34:2:863:G:N3	2.80	0.49
38:k:209:LEU:HD13	38:k:221:GLU:HB3	1.95	0.49
34:2:16:G:H21	34:2:1191:A:H62	1.60	0.49
34:2:479:A:O4'	38:k:149:GLY:O	2.30	0.49
34:2:741:C:N3	34:2:792:G:O6	2.46	0.49
38:k:17:LYS:HZ2	38:k:20:LYS:NZ	2.10	0.49
38:k:318:PRO:C	38:k:319:THR:CG2	2.86	0.49
40:R:136:THR:OG1	40:R:137:HIS:N	2.44	0.49
34:2:1812:A:H2	34:2:1813:A:N9	2.10	0.49
37:j:27:VAL:CG1	37:j:28:PHE:H	2.23	0.49
37:j:40:LYS:CD	37:j:42:LEU:N	2.73	0.49
37:j:64:LYS:C	37:j:66:ARG:H	2.21	0.49
38:k:209:LEU:CD1	38:k:221:GLU:CB	2.91	0.49
38:k:5:LEU:C	38:k:5:LEU:CD1	2.86	0.48
38:k:332:LYS:O	38:k:334:ALA:CA	2.57	0.48
34:2:1817:A:HO2'	37:j:46:ARG:HH22	1.54	0.48
37:j:25:GLU:HG2	37:j:26:LEU:CG	2.35	0.48
38:k:342:VAL:HG13	38:k:342:VAL:O	2.13	0.48
38:k:414:GLN:HG2	38:k:486:ASP:CG	2.37	0.48
40:R:134:GLY:HA2	40:R:139:SER:CB	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:R:139:SER:O	40:R:140:ARG:HD2	2.13	0.48
1:1:34:C:N4	41:3:54:G:C6	2.66	0.48
25:a:128:GLY:HA3	38:k:264:ASN:O	2.11	0.48
33:i:79:SER:OG	37:j:80:GLY:CA	2.62	0.48
34:2:740:G:H3'	34:2:741:C:H5''	1.95	0.48
34:2:1407:G:H3'	34:2:1408:C:C5'	2.43	0.48
38:k:167:ILE:HG23	38:k:238:PHE:HA	1.94	0.48
38:k:216:ASP:O	44:k:705:GNP:N9	2.46	0.48
25:a:127:ALA:O	38:k:264:ASN:HB2	2.12	0.48
34:2:784:G:C6	34:2:785:G:C5	3.01	0.48
37:j:40:LYS:CG	37:j:41:MET:N	2.73	0.48
38:k:169:LYS:HE2	38:k:242:GLU:O	2.13	0.48
38:k:373:GLU:C	38:k:374:ILE:N	2.70	0.48
5:E:99:LYS:HA	34:2:10:G:H21	1.77	0.48
10:J:109:ARG:HG3	34:2:794:G:C4	2.48	0.48
25:a:101:LYS:HZ3	25:a:107:ARG:NH2	2.11	0.48
38:k:331:PHE:O	38:k:498:LEU:CD1	2.52	0.48
38:k:584:LYS:O	38:k:586:VAL:N	2.47	0.48
16:P:22:VAL:CB	16:P:24:THR:H	2.27	0.48
24:Z:50:ILE:CD1	38:k:58:CYS:CB	2.82	0.48
25:a:10:ARG:HH21	25:a:11:LYS:HE3	1.79	0.48
34:2:743:U:O4	34:2:791:A:C2	2.64	0.48
34:2:1707:A:N6	34:2:1708:C:N4	2.61	0.48
38:k:131:LEU:C	38:k:131:LEU:CD2	2.86	0.48
38:k:375:MET:SD	38:k:533:ILE:HG21	2.50	0.48
38:k:523:ILE:HG23	38:k:575:PRO:HG3	1.94	0.48
6:F:143:ARG:HD3	41:3:62:U:H5'	1.94	0.48
9:I:237:LEU:HB2	34:2:785:G:P	2.53	0.48
34:2:1812:A:C2	34:2:1813:A:C5	3.01	0.48
38:k:32:VAL:HG13	38:k:37:LEU:CD2	2.44	0.48
38:k:164:LEU:HD11	38:k:237:ILE:CD1	2.40	0.48
38:k:414:GLN:OE1	38:k:486:ASP:CB	2.52	0.48
40:R:128:HIS:CB	40:R:129:GLY:HA3	2.36	0.48
35:A:55:ARG:CG	35:A:55:ARG:NH1	2.57	0.48
38:k:112:ASN:HB3	44:k:704:GNP:PG	2.54	0.48
38:k:212:ARG:NH1	38:k:540:SER:HB3	2.28	0.48
40:R:130:ARG:NH1	40:R:130:ARG:CA	2.75	0.48
16:P:29:THR:O	16:P:32:ASP:N	2.45	0.48
34:2:745:U:C2	34:2:746:C:N4	2.81	0.48
38:k:518:VAL:CA	38:k:519:GLU:N	2.75	0.48
10:J:106:ARG:CG	34:2:794:G:O6	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3:58:C:C2	41:3:59:A:N7	2.82	0.48
41:3:65:C:O2	41:3:65:C:O2'	2.26	0.48
16:P:26:LEU:HD22	16:P:27:LYS:CA	2.44	0.47
34:2:80:G:C6	34:2:81:U:C4	3.02	0.47
35:A:244:ARG:HH22	35:A:251:LEU:HD22	1.78	0.47
38:k:22:ARG:HB3	38:k:27:LYS:NZ	2.29	0.47
38:k:229:VAL:CG1	38:k:230:VAL:N	2.76	0.47
38:k:550:THR:OG1	38:k:553:ALA:HB2	2.13	0.47
34:2:921:G:H1	34:2:1013:U:H3	1.62	0.47
34:2:1705:C:O2'	37:j:42:LEU:CD1	2.62	0.47
38:k:208:HIS:CE1	38:k:539:PRO:C	2.92	0.47
38:k:412:LYS:CD	38:k:485:ILE:CB	2.92	0.47
41:3:73:G:N7	41:3:74:A:C6	2.82	0.47
10:J:109:ARG:HG3	34:2:794:G:H1'	1.94	0.47
34:2:886:U:H5'	34:2:887:G:H5''	1.96	0.47
34:2:1519:G:P	39:U:144:ARG:CB	2.75	0.47
37:j:72:ASN:N	37:j:72:ASN:ND2	2.60	0.47
38:k:581:ASN:HA	38:k:585:ASP:OD1	2.15	0.47
24:Z:50:ILE:HD12	38:k:58:CYS:HB3	1.90	0.47
34:2:742:C:O2'	34:2:743:U:H5''	2.09	0.47
34:2:1815:U:HO2'	34:2:1816:A:P	2.36	0.47
34:2:1815:U:C2'	34:2:1816:A:H5''	2.35	0.47
35:A:189:VAL:HG21	35:A:241:THR:HA	1.96	0.47
38:k:22:ARG:HB3	38:k:27:LYS:HZ1	1.79	0.47
34:2:731:C:C2'	34:2:732:C:H5''	2.37	0.47
34:2:1276:G:H1	34:2:1313:U:H3	1.62	0.47
38:k:212:ARG:HH12	38:k:540:SER:HB3	1.79	0.47
41:3:60:C:O3'	41:3:61:C:H4'	2.12	0.47
24:Z:125:VAL:HG11	24:Z:140:ARG:HH12	1.80	0.47
34:2:597:U:C2	41:3:61:C:N4	2.81	0.47
37:j:62:ARG:HH11	37:j:64:LYS:HD2	1.78	0.47
38:k:536:ASP:CG	38:k:561:GLN:HE22	2.22	0.47
14:N:22:ARG:HH22	14:N:24:LEU:HD13	1.79	0.47
33:i:75:LYS:HZ2	37:j:27:VAL:CG2	2.27	0.47
33:i:81:ALA:HB1	37:j:82:ARG:HD2	1.96	0.47
34:2:741:C:H3'	34:2:741:C:H6	1.80	0.47
34:2:743:U:O2'	34:2:744:C:O5'	2.32	0.47
34:2:749:C:C3'	34:2:750:G:C5'	2.89	0.47
34:2:784:G:P	34:2:784:G:H8	2.38	0.47
34:2:784:G:C4	34:2:785:G:C8	3.02	0.47
34:2:1819:A:N7	37:j:66:ARG:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:55:ARG:O	35:A:56:ILE:HG13	2.13	0.47
38:k:166:ALA:HA	38:k:237:ILE:HG21	1.91	0.47
38:k:381:ASN:CB	44:k:705:GNP:PG	3.02	0.47
38:k:518:VAL:C	38:k:519:GLU:CA	2.88	0.47
9:I:159:ARG:HH11	9:I:173:ALA:HB2	1.79	0.47
9:I:237:LEU:HD12	34:2:785:G:P	2.49	0.47
35:A:205:ILE:HD12	36:B:288:LYS:CG	2.44	0.47
37:j:70:TRP:HE1	40:R:143:PRO:CA	2.19	0.47
38:k:6:THR:HB	38:k:75:LEU:O	2.14	0.47
38:k:7:ARG:O	38:k:8:ILE:HD13	2.15	0.47
35:A:263:GLU:HG2	35:A:269:PHE:HD1	1.78	0.47
38:k:334:ALA:O	38:k:336:THR:OG1	2.33	0.47
34:2:682:G:C2	34:2:683:G:C8	3.03	0.47
34:2:685:G:H8	34:2:685:G:O5'	1.98	0.47
34:2:793:C:H2'	34:2:794:G:H4'	1.97	0.47
37:j:40:LYS:CD	37:j:41:MET:N	2.73	0.47
38:k:130:ASN:O	38:k:133:LYS:N	2.48	0.47
38:k:378:LEU:N	38:k:385:LYS:HE3	2.30	0.47
38:k:450:GLN:CG	38:k:453:ASN:OD1	2.54	0.47
38:k:450:GLN:HB3	38:k:453:ASN:HD21	0.75	0.47
38:k:486:ASP:C	38:k:487:GLU:CA	2.87	0.47
38:k:520:HIS:CE1	44:k:705:GNP:O1G	2.68	0.47
14:N:25:LEU:CD1	14:N:29:GLY:HA3	2.45	0.46
25:a:100:LYS:HA	25:a:101:LYS:O	2.14	0.46
34:2:742:C:H3'	34:2:742:C:H6	1.80	0.46
35:A:58:SER:CB	35:A:61:LYS:CE	2.88	0.46
35:A:170:GLU:C	35:A:172:GLU:N	2.66	0.46
37:j:47:LEU:CD1	37:j:48:GLU:N	2.73	0.46
38:k:425:ARG:NH1	38:k:455:ILE:HD13	2.29	0.46
38:k:526:THR:O	38:k:528:LEU:N	2.48	0.46
41:3:66:U:H3'	41:3:66:U:O2	2.15	0.46
38:k:174:ASP:C	38:k:176:ILE:N	2.73	0.46
38:k:582:SER:OG	38:k:583:ILE:N	2.48	0.46
40:R:134:GLY:C	40:R:136:THR:N	2.73	0.46
40:R:135:ALA:O	40:R:136:THR:HB	2.16	0.46
1:1:62:C:O2'	35:A:186:PRO:HD3	2.16	0.46
34:2:1518:C:P	39:U:143:GLY:O	2.73	0.46
38:k:167:ILE:HG21	38:k:238:PHE:CD1	2.50	0.46
40:R:133:ILE:C	40:R:135:ALA:N	2.73	0.46
41:3:43:A:C1'	41:3:44:C:C5	2.98	0.46
37:j:71:ILE:O	37:j:71:ILE:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:159:ILE:CD1	38:k:164:LEU:HD22	2.45	0.46
1:l:17:C:H2'	1:l:18:G:C5'	2.41	0.46
34:2:479:A:H5'	38:k:150:SER:HA	1.97	0.46
34:2:684:A:H2'	34:2:685:G:H8	1.73	0.46
37:j:15:GLY:O	37:j:16:LYS:CD	2.64	0.46
37:j:84:TYR:CD1	37:j:84:TYR:N	2.83	0.46
34:2:1706:U:O2'	34:2:1707:A:O5'	2.27	0.46
37:j:68:LYS:HA	37:j:68:LYS:HD2	1.55	0.46
41:3:40:C:H2'	41:3:41:A:H5'	1.97	0.46
23:Y:2:VAL:HG23	23:Y:3:ARG:H	1.79	0.46
35:A:121:TYR:HA	35:A:126:GLN:HG3	1.98	0.46
38:k:168:ILE:HG22	38:k:239:MET:CB	2.45	0.46
41:3:68:C:O5'	41:3:68:C:H6	1.98	0.46
9:I:237:LEU:CD1	34:2:784:G:O2'	2.63	0.46
29:e:23:VAL:HG22	29:e:39:CYS:SG	2.56	0.46
33:i:79:SER:OG	37:j:80:GLY:HA3	2.16	0.46
34:2:741:C:H2'	34:2:742:C:O4'	2.15	0.46
37:j:9:GLY:N	40:R:140:ARG:HH12	2.14	0.46
37:j:64:LYS:C	37:j:66:ARG:N	2.73	0.46
38:k:475:CYS:SG	38:k:483:TYR:CE1	3.09	0.46
38:k:517:VAL:CG1	38:k:519:GLU:HG2	2.45	0.46
16:P:22:VAL:CG1	16:P:26:LEU:CG	2.86	0.46
24:Z:97:ASN:O	38:k:56:ILE:CD1	2.61	0.46
25:a:99:LYS:O	25:a:100:LYS:HB2	2.16	0.46
34:2:748:G:N2	34:2:749:C:C2	2.84	0.46
38:k:218:SER:N	38:k:221:GLU:OE1	2.42	0.46
18:S:100:VAL:HG12	18:S:101:ASP:H	1.81	0.46
34:2:785:G:C2	34:2:786:C:C2	3.04	0.46
34:2:1518:C:C5'	39:U:144:ARG:N	2.79	0.46
35:A:54:ARG:CB	35:A:54:ARG:NH2	2.73	0.46
35:A:195:ILE:HG21	35:A:235:TYR:HD2	1.81	0.46
9:I:216:ARG:C	9:I:218:LYS:H	2.22	0.45
34:2:740:G:C2'	34:2:741:C:H5''	2.46	0.45
34:2:1327:C:C6	37:j:17:ASN:ND2	2.84	0.45
34:2:1547:G:C8	34:2:1547:G:OP2	2.69	0.45
34:2:1819:A:N6	37:j:69:VAL:O	2.43	0.45
35:A:185:THR:CB	35:A:186:PRO:HA	2.46	0.45
37:j:11:ASN:C	37:j:13:ARG:N	2.73	0.45
38:k:341:GLU:C	38:k:342:VAL:HG12	2.41	0.45
38:k:431:LYS:HE3	38:k:477:GLY:O	2.14	0.45
25:a:12:PHE:CE1	34:2:836:C:C2'	2.66	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:679:U:H3'	34:2:679:U:H6	1.81	0.45
34:2:1813:A:C6	34:2:1814:G:C5	3.04	0.45
37:j:9:GLY:N	40:R:140:ARG:NH2	2.60	0.45
37:j:46:ARG:H	37:j:46:ARG:HG2	1.56	0.45
11:K:157:LYS:HE2	14:N:23:VAL:HB	1.97	0.45
34:2:190:A:H3'	34:2:191:C:H5''	1.98	0.45
40:R:84:ILE:H	40:R:84:ILE:HD12	1.81	0.45
34:2:751:C:C2'	34:2:752:C:H5'	2.44	0.45
37:j:68:LYS:C	37:j:69:VAL:HG23	2.42	0.45
38:k:105:VAL:CG2	38:k:263:ILE:HG12	2.46	0.45
38:k:250:LYS:CE	38:k:562:LEU:HD22	2.45	0.45
41:3:60:C:O2'	41:3:61:C:H4'	2.16	0.45
6:F:196:GLY:C	6:F:198:ILE:HA	2.42	0.45
34:2:452:C:O2'	38:k:306:ARG:CD	2.59	0.45
34:2:684:A:H2	34:2:731:C:N3	2.09	0.45
35:A:205:ILE:CD1	36:B:288:LYS:CB	2.91	0.45
37:j:10:LYS:HB2	41:3:54:G:N2	2.31	0.45
37:j:41:MET:CE	37:j:47:LEU:HD22	2.47	0.45
37:j:47:LEU:CG	37:j:48:GLU:N	2.79	0.45
40:R:142:ILE:HB	40:R:143:PRO:HD3	1.98	0.45
25:a:101:LYS:CG	25:a:107:ARG:HH21	2.12	0.45
34:2:1818:A:H4'	37:j:44:ASN:O	2.16	0.45
37:j:71:ILE:HD13	37:j:77:ILE:HD12	1.94	0.45
38:k:74:ASN:OD1	38:k:74:ASN:N	2.49	0.45
38:k:378:LEU:HD12	38:k:379:GLY:HA3	1.01	0.45
39:U:147:GLY:C	39:U:148:VAL:HG23	2.42	0.45
38:k:330:VAL:O	38:k:523:ILE:HG21	2.17	0.45
38:k:332:LYS:HA	38:k:332:LYS:HD2	1.70	0.45
41:3:43:A:N9	41:3:44:C:C5	2.85	0.45
16:P:22:VAL:N	16:P:23:PRO:CA	2.73	0.45
34:2:745:U:C2'	34:2:746:C:C6	2.89	0.45
38:k:140:TRP:CE3	38:k:140:TRP:HA	2.52	0.45
38:k:385:LYS:CE	38:k:518:VAL:HG13	2.47	0.45
16:P:22:VAL:H	16:P:23:PRO:CA	2.11	0.45
35:A:111:ILE:CD1	35:A:183:ARG:HH12	2.24	0.45
37:j:19:ASN:CB	37:j:20:GLU:CA	2.95	0.45
38:k:414:GLN:CG	38:k:486:ASP:CA	2.95	0.45
16:P:25:TRP:O	16:P:25:TRP:CG	2.70	0.45
34:2:743:U:H2'	34:2:743:U:OP2	2.17	0.45
37:j:62:ARG:HD3	37:j:63:GLY:O	2.16	0.45
37:j:67:LYS:O	37:j:70:TRP:CZ3	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:185:GLY:O	38:k:189:ASP:HB2	2.16	0.45
16:P:22:VAL:HG11	16:P:26:LEU:HD11	1.98	0.44
16:P:25:TRP:O	16:P:25:TRP:CD2	2.71	0.44
34:2:1707:A:C8	34:2:1707:A:OP2	2.70	0.44
25:a:98:GLU:C	25:a:98:GLU:CD	2.86	0.44
30:f:118:ARG:H	30:f:118:ARG:HD3	1.81	0.44
34:2:684:A:C6	34:2:685:G:O6	2.71	0.44
34:2:1815:U:C2'	34:2:1816:A:C5'	2.94	0.44
38:k:250:LYS:HE2	38:k:562:LEU:CD2	2.47	0.44
16:P:27:LYS:HE3	16:P:28:LEU:HD21	1.99	0.44
34:2:743:U:C5	34:2:744:C:N3	2.85	0.44
34:2:784:G:C5	34:2:785:G:C5	3.05	0.44
34:2:792:G:P	34:2:792:G:H8	2.41	0.44
38:k:168:ILE:HG22	38:k:239:MET:CG	2.47	0.44
38:k:374:ILE:HD11	38:k:529:ALA:N	2.31	0.44
26:b:80:HIS:CE1	41:3:48:C:C4	3.05	0.44
38:k:229:VAL:C	38:k:232:ILE:HG22	2.42	0.44
38:k:412:LYS:CD	38:k:485:ILE:HB	2.47	0.44
38:k:492:LEU:C	38:k:497:ARG:HE	2.25	0.44
33:i:82:ARG:NH2	33:i:85:LYS:CA	2.73	0.44
34:2:682:G:H2'	34:2:683:G:C8	2.52	0.44
35:A:154:LYS:HD2	35:A:184:LEU:HD23	1.99	0.44
37:j:29:LYS:HE2	37:j:35:TYR:CE2	2.53	0.44
38:k:344:LYS:O	38:k:345:MET:HB2	2.17	0.44
16:P:23:PRO:O	16:P:25:TRP:CD1	2.71	0.44
25:a:97:TYR:CE2	25:a:98:GLU:O	2.71	0.44
34:2:472:G:P	38:k:63:LYS:CE	3.05	0.44
38:k:76:PRO:HD3	38:k:323:ARG:HG3	1.98	0.44
38:k:549:GLN:NE2	38:k:557:LYS:HZ1	2.15	0.44
41:3:53:U:C2'	41:3:54:G:O5'	2.66	0.44
6:F:193:ASP:N	6:F:194:PRO:CD	2.56	0.44
16:P:18:TYR:O	16:P:19:ARG:O	2.36	0.44
34:2:1709:U:C2	34:2:1814:G:N2	2.86	0.44
37:j:11:ASN:C	37:j:13:ARG:H	2.24	0.44
38:k:17:LYS:CG	38:k:20:LYS:HE3	2.42	0.44
41:3:69:U:H3'	41:3:69:U:H6	1.82	0.44
1:1:17:C:H2'	1:1:18:G:P	2.58	0.44
34:2:158:A:P	38:k:583:ILE:HG22	2.55	0.44
37:j:19:ASN:HB3	37:j:20:GLU:CA	2.47	0.44
38:k:113:GLY:HA2	44:k:704:GNP:H5'1	1.99	0.44
38:k:140:TRP:HA	38:k:140:TRP:HE3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:206:LEU:HD23	38:k:224:ARG:HG3	2.00	0.44
38:k:241:ASP:O	38:k:242:GLU:HB3	2.17	0.44
38:k:246:TYR:OH	38:k:491:TYR:OH	1.81	0.44
38:k:322:LEU:HG	38:k:323:ARG:H	1.83	0.44
34:2:735:C:H3'	34:2:736:C:H5''	2.00	0.44
34:2:787:C:O5'	34:2:787:C:C6	2.70	0.44
34:2:1812:A:H2	34:2:1813:A:C4	2.36	0.44
37:j:67:LYS:NZ	41:3:56:U:H4'	2.32	0.44
38:k:412:LYS:HD3	38:k:485:ILE:CA	2.48	0.44
17:Q:35:ALA:HB1	17:Q:109:GLY:H	1.83	0.43
33:i:80:LEU:HD22	37:j:62:ARG:NH2	2.27	0.43
34:2:682:G:N3	34:2:683:G:N7	2.66	0.43
35:A:229:LEU:HD11	35:A:231:ALA:O	2.18	0.43
38:k:17:LYS:C	38:k:19:LYS:H	2.26	0.43
38:k:21:CYS:O	38:k:22:ARG:HB2	2.17	0.43
38:k:182:GLY:CA	38:k:187:ILE:HD13	2.38	0.43
38:k:332:LYS:HD3	38:k:527:TYR:CE2	2.53	0.43
41:3:71:A:C6	41:3:72:G:O6	2.70	0.43
34:2:1816:A:C2	34:2:1817:A:C6	3.06	0.43
35:A:20:VAL:CG2	35:A:71:VAL:HG23	2.49	0.43
37:j:72:ASN:H	37:j:72:ASN:ND2	2.01	0.43
37:j:77:ILE:HG13	37:j:94:LYS:HA	2.00	0.43
38:k:4:LYS:CA	38:k:79:LEU:HD12	2.46	0.43
38:k:347:MET:C	38:k:348:TYR:O	2.52	0.43
38:k:441:PHE:CZ	38:k:454:ILE:CG2	2.96	0.43
38:k:488:PRO:C	38:k:524:MET:HE1	2.43	0.43
38:k:550:THR:O	38:k:554:GLY:N	2.43	0.43
34:2:745:U:C2	34:2:746:C:N3	2.86	0.43
38:k:100:PRO:HG3	38:k:155:TYR:CE1	2.54	0.43
38:k:164:LEU:HD23	38:k:237:ILE:HB	1.94	0.43
41:3:58:C:OP2	41:3:58:C:C6	2.70	0.43
34:2:684:A:H2'	34:2:685:G:N7	2.32	0.43
34:2:734:C:H5	34:2:737:C:N4	2.17	0.43
34:2:785:G:C2	34:2:786:C:O2	2.71	0.43
35:A:120:GLU:O	35:A:126:GLN:HG3	2.18	0.43
35:A:193:ALA:HB3	35:A:237:MET:H	1.83	0.43
35:A:229:LEU:HD13	36:B:285:ASP:HB3	2.00	0.43
38:k:250:LYS:NZ	38:k:562:LEU:CD2	2.82	0.43
38:k:345:MET:HG2	38:k:346:CYS:H	1.77	0.43
34:2:737:C:H3'	34:2:738:U:C5'	2.30	0.43
34:2:746:C:H5''	34:2:747:G:OP2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:1708:C:H2'	34:2:1709:U:C6	2.53	0.43
38:k:229:VAL:CA	38:k:232:ILE:HG22	2.48	0.43
40:R:143:PRO:HB2	41:3:55:G:H1'	1.87	0.43
24:Z:52:LEU:O	38:k:34:MET:CG	2.66	0.43
24:Z:58:GLU:CD	37:j:60:HIS:ND1	2.75	0.43
34:2:748:G:O2'	34:2:749:C:C6	2.71	0.43
37:j:7:LYS:HG3	37:j:8:GLY:N	2.30	0.43
37:j:40:LYS:CG	37:j:48:GLU:HB3	2.48	0.43
38:k:22:ARG:HA	38:k:22:ARG:HD3	1.71	0.43
38:k:331:PHE:C	38:k:498:LEU:HD13	2.41	0.43
34:2:790:A:H8	34:2:790:A:P	2.41	0.43
38:k:416:ILE:HD13	38:k:471:ALA:HB2	2.00	0.43
1:1:27:C:N3	1:1:28:U:C5	2.87	0.43
8:H:132:GLY:HA3	41:3:49:A:H61	1.84	0.43
41:3:71:A:C5	41:3:72:G:O6	2.72	0.43
14:N:30:LYS:CA	14:N:30:LYS:CE	2.97	0.43
25:a:10:ARG:HE	25:a:10:ARG:HB3	1.48	0.43
34:2:682:G:N1	34:2:683:G:C5	2.87	0.43
35:A:144:ARG:HB2	35:A:145:PRO:HD3	2.01	0.43
38:k:4:LYS:CA	38:k:79:LEU:CG	2.61	0.43
38:k:216:ASP:HB3	44:k:705:GNP:N1	2.34	0.43
34:2:683:G:H2'	34:2:684:A:H8	1.78	0.42
34:2:790:A:N6	34:2:791:A:N6	2.67	0.42
37:j:7:LYS:CG	37:j:8:GLY:N	2.82	0.42
38:k:412:LYS:HD2	38:k:483:TYR:OH	2.18	0.42
38:k:440:GLN:O	38:k:443:THR:OG1	2.35	0.42
24:Z:52:LEU:O	24:Z:53:GLU:CB	2.66	0.42
34:2:737:C:H5'	34:2:738:U:OP2	2.19	0.42
38:k:331:PHE:H	38:k:498:LEU:HD13	1.83	0.42
38:k:502:ARG:HH22	38:k:506:ARG:HH21	1.67	0.42
34:2:734:C:H3'	34:2:735:C:C5'	2.49	0.42
34:2:791:A:C8	34:2:791:A:O5'	2.72	0.42
38:k:8:ILE:HG22	38:k:9:ALA:N	2.34	0.42
38:k:31:VAL:C	38:k:33:ARG:H	2.27	0.42
40:R:143:PRO:HB3	41:3:55:G:O2'	2.19	0.42
25:a:11:LYS:N	34:2:837:G:O6	2.42	0.42
38:k:176:ILE:O	38:k:176:ILE:HG12	2.19	0.42
38:k:451:ILE:HA	38:k:453:ASN:HB2	0.91	0.42
1:1:33:C:P	18:S:146:ARG:NH1	2.93	0.42
10:J:100:ILE:HG13	34:2:736:C:O2	2.19	0.42
24:Z:52:LEU:HD13	38:k:33:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:15:GLY:O	37:j:16:LYS:HG3	2.19	0.42
25:a:101:LYS:HG2	25:a:107:ARG:HH22	1.85	0.42
38:k:7:ARG:O	38:k:8:ILE:HG12	2.20	0.42
38:k:475:CYS:SG	38:k:483:TYR:HE1	2.42	0.42
34:2:795:U:C4	34:2:863:G:C2	3.07	0.42
34:2:1457:G:H3'	34:2:1459:U:H3	1.84	0.42
38:k:21:CYS:HB2	38:k:66:PRO:HG2	2.02	0.42
38:k:159:ILE:O	38:k:162:ASP:HA	2.20	0.42
25:a:8:ARG:CZ	34:2:831:C:H5	2.32	0.42
34:2:158:A:P	38:k:583:ILE:CG2	3.02	0.42
34:2:791:A:O5'	34:2:791:A:H8	2.03	0.42
34:2:1751:G:H1	34:2:1769:U:H3	1.66	0.42
16:P:23:PRO:HG2	16:P:25:TRP:NE1	2.35	0.42
38:k:414:GLN:HE21	38:k:486:ASP:N	2.18	0.42
40:R:140:ARG:O	40:R:141:PHE:HB2	2.20	0.42
41:3:49:A:OP2	41:3:49:A:C2	2.69	0.42
25:a:99:LYS:O	25:a:100:LYS:CB	2.68	0.41
34:2:741:C:C3'	34:2:741:C:C6	3.03	0.41
34:2:745:U:C4	34:2:746:C:N4	2.88	0.41
34:2:1327:C:C2'	37:j:17:ASN:HD21	2.33	0.41
37:j:70:TRP:CZ2	41:3:55:G:H1'	2.53	0.41
37:j:71:ILE:O	37:j:72:ASN:O	2.38	0.41
38:k:193:GLU:O	38:k:197:GLN:HG2	2.19	0.41
34:2:1706:U:C2'	34:2:1707:A:H8	1.97	0.41
35:A:229:LEU:HD13	36:B:284:VAL:CG2	2.50	0.41
37:j:62:ARG:NH1	37:j:64:LYS:CD	2.83	0.41
38:k:133:LYS:C	38:k:134:TYR:CG	2.97	0.41
38:k:485:ILE:HD11	38:k:488:PRO:HB3	2.02	0.41
10:J:106:ARG:CD	34:2:794:G:C6	3.00	0.41
24:Z:58:GLU:CG	37:j:60:HIS:CE1	3.01	0.41
25:a:103:SER:HG	25:a:104:ARG:H	1.64	0.41
34:2:786:C:O5'	34:2:786:C:C6	2.71	0.41
38:k:374:ILE:HD13	38:k:505:LYS:NZ	2.36	0.41
38:k:591:SER:C	38:k:592:GLY:C	2.88	0.41
1:1:18:G:O6	35:A:107:THR:CG2	2.68	0.41
34:2:686:G:O5'	34:2:686:G:C8	2.70	0.41
38:k:167:ILE:CG2	38:k:238:PHE:HA	2.50	0.41
38:k:493:ASP:O	38:k:494:SER:C	2.60	0.41
34:2:68:A:C6	34:2:69:C:C4	3.09	0.41
34:2:1327:C:O2'	37:j:17:ASN:ND2	2.47	0.41
35:A:202:TYR:HB2	36:B:355:LYS:HB2	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:28:PHE:HD1	37:j:35:TYR:OH	2.03	0.41
38:k:229:VAL:HA	38:k:232:ILE:CG2	2.50	0.41
38:k:347:MET:HE3	38:k:347:MET:HB2	1.66	0.41
38:k:451:ILE:HG22	38:k:454:ILE:CG2	2.51	0.41
34:2:471:C:OP1	38:k:7:ARG:NH2	2.46	0.41
34:2:742:C:C3'	34:2:742:C:C6	3.04	0.41
34:2:745:U:C3'	34:2:745:U:C6	3.03	0.41
34:2:1819:A:OP1	37:j:66:ARG:HD3	2.20	0.41
38:k:318:PRO:HB2	38:k:322:LEU:HB2	2.02	0.41
38:k:451:ILE:C	38:k:452:GLU:N	2.79	0.41
38:k:521:ASP:CA	38:k:524:MET:HB3	2.48	0.41
41:3:63:G:N3	41:3:63:G:H2'	2.33	0.41
16:P:19:ARG:NH2	16:P:23:PRO:CB	2.78	0.41
38:k:498:LEU:HD21	38:k:523:ILE:HB	2.02	0.41
34:2:746:C:C3'	34:2:747:G:C8	3.03	0.41
34:2:1707:A:C2	34:2:1708:C:C1'	3.00	0.41
35:A:20:VAL:HG23	35:A:71:VAL:HG23	2.02	0.41
37:j:67:LYS:HE2	37:j:67:LYS:HB2	1.88	0.41
38:k:308:GLY:HA2	38:k:311:ILE:HG12	2.03	0.41
38:k:330:VAL:O	38:k:331:PHE:HB2	2.21	0.41
40:R:141:PHE:C	40:R:142:ILE:CG1	2.93	0.41
41:3:73:G:C5	41:3:74:A:N7	2.89	0.41
6:F:3:VAL:HG13	6:F:4:GLN:H	1.85	0.41
13:M:1:MET:HA	13:M:3:MET:H	1.85	0.41
33:i:80:LEU:HD11	37:j:92:ILE:CD1	2.49	0.41
34:2:734:C:H41	34:2:737:C:N4	2.19	0.41
35:A:52:SER:OG	35:A:54:ARG:HG2	2.21	0.41
37:j:7:LYS:CG	37:j:8:GLY:H	2.29	0.41
38:k:159:ILE:C	38:k:162:ASP:H	2.22	0.41
38:k:169:LYS:CE	38:k:241:ASP:O	2.69	0.41
38:k:332:LYS:HG3	38:k:527:TYR:CE2	2.47	0.41
38:k:378:LEU:HD13	38:k:379:GLY:HA2	0.95	0.41
41:3:65:C:H4'	41:3:66:U:OP1	2.20	0.41
24:Z:50:ILE:HD11	38:k:58:CYS:CB	2.36	0.41
38:k:194:THR:HB	38:k:195:LYS:H	1.69	0.41
38:k:377:MET:HE1	38:k:389:ILE:HD11	2.02	0.41
40:R:140:ARG:HH21	40:R:140:ARG:CG	2.32	0.41
9:I:233:ARG:O	9:I:236:SER:HB2	2.21	0.40
16:P:20:ARG:HG3	16:P:65:PHE:CD1	2.51	0.40
38:k:4:LYS:CB	38:k:79:LEU:HD12	2.51	0.40
38:k:133:LYS:O	38:k:134:TYR:CG	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:175:GLN:O	38:k:176:ILE:HB	2.20	0.40
1:1:26:G:H1	1:1:44:A:H61	1.68	0.40
24:Z:140:ARG:HE	24:Z:142:ARG:HE	1.69	0.40
34:2:790:A:H2'	34:2:791:A:H8	1.83	0.40
38:k:209:LEU:HD13	38:k:221:GLU:HG2	1.96	0.40
41:3:56:U:H6	41:3:56:U:H5''	1.85	0.40
38:k:175:GLN:H	38:k:175:GLN:HG3	1.71	0.40
1:1:5:A:C2	1:1:70:G:C4	3.10	0.40
24:Z:96:GLU:CG	38:k:34:MET:HE3	2.48	0.40
34:2:1705:C:C4'	37:j:42:LEU:HD21	2.51	0.40
38:k:6:THR:O	38:k:74:ASN:HA	2.22	0.40
38:k:213:ASN:O	38:k:217:LEU:HD13	2.21	0.40
38:k:431:LYS:CE	38:k:478:LYS:N	2.77	0.40
41:3:73:G:C4	41:3:74:A:C8	3.09	0.40
34:2:679:U:C6	34:2:679:U:C3'	3.05	0.40
38:k:61:CYS:SG	42:k:701:SF4:S2	3.19	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	
2	l	23/25 (92%)	23 (100%)	0	0	100	100
3	C	206/209 (99%)	177 (86%)	21 (10%)	8 (4%)	2	14
4	D	213/264 (81%)	191 (90%)	16 (8%)	6 (3%)	4	21
5	E	224/226 (99%)	208 (93%)	14 (6%)	2 (1%)	14	48
6	F	225/243 (93%)	202 (90%)	14 (6%)	9 (4%)	2	14
7	G	261/263 (99%)	233 (89%)	24 (9%)	4 (2%)	8	35
8	H	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	7	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	235/237 (99%)	209 (89%)	22 (9%)	4 (2%)	7	32
10	J	188/192 (98%)	161 (86%)	18 (10%)	9 (5%)	2	11
11	K	204/206 (99%)	178 (87%)	20 (10%)	6 (3%)	3	20
12	L	180/182 (99%)	167 (93%)	11 (6%)	2 (1%)	11	43
13	M	96/98 (98%)	74 (77%)	16 (17%)	6 (6%)	1	6
14	N	156/158 (99%)	130 (83%)	22 (14%)	4 (3%)	4	23
15	O	122/132 (92%)	105 (86%)	13 (11%)	4 (3%)	3	17
16	P	148/150 (99%)	130 (88%)	11 (7%)	7 (5%)	2	11
17	Q	134/151 (89%)	118 (88%)	13 (10%)	3 (2%)	5	26
18	S	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	36
19	T	124/135 (92%)	112 (90%)	8 (6%)	4 (3%)	3	18
20	V	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	5	26
21	W	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
22	X	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	23
23	Y	127/130 (98%)	117 (92%)	6 (5%)	4 (3%)	3	19
24	Z	140/143 (98%)	128 (91%)	8 (6%)	4 (3%)	3	20
25	a	124/133 (93%)	104 (84%)	10 (8%)	10 (8%)	1	3
26	b	97/115 (84%)	90 (93%)	5 (5%)	2 (2%)	5	27
27	c	82/84 (98%)	69 (84%)	9 (11%)	4 (5%)	1	10
28	d	62/69 (90%)	57 (92%)	4 (6%)	1 (2%)	7	34
29	e	51/56 (91%)	40 (78%)	7 (14%)	4 (8%)	1	4
30	f	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	0	3
31	g	311/313 (99%)	273 (88%)	33 (11%)	5 (2%)	7	34
32	n	73/124 (59%)	69 (94%)	3 (4%)	1 (1%)	9	36
33	i	57/133 (43%)	49 (86%)	7 (12%)	1 (2%)	6	31
35	A	264/284 (93%)	233 (88%)	25 (10%)	6 (2%)	5	25
36	B	420/422 (100%)	352 (84%)	48 (11%)	20 (5%)	2	11
37	j	107/111 (96%)	64 (60%)	27 (25%)	16 (15%)	0	0
38	k	577/595 (97%)	431 (75%)	95 (16%)	51 (9%)	0	3
39	U	141/152 (93%)	123 (87%)	12 (8%)	6 (4%)	2	12
40	R	138/145 (95%)	107 (78%)	18 (13%)	13 (9%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6228/6625 (94%)	5362 (86%)	624 (10%)	242 (4%)	4	14

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ARG
4	D	209	ASP
6	F	3	VAL
6	F	193	ASP
6	F	219	PRO
8	H	41	VAL
9	I	69	THR
10	J	106	ARG
11	K	158	ILE
12	L	148	ILE
13	M	35	LEU
14	N	66	VAL
14	N	157	LYS
15	O	95	ASP
16	P	19	ARG
16	P	20	ARG
20	V	34	VAL
23	Y	30	CYS
25	a	10	ARG
25	a	100	LYS
25	a	102	THR
25	a	105	LYS
29	e	25	SER
30	f	102	VAL
35	A	171	ASP
35	A	185	THR
35	A	266	ARG
36	B	194	LYS
36	B	279	LYS
36	B	280	PRO
36	B	283	GLU
36	B	289	GLY
36	B	402	ASP
36	B	405	ALA
37	j	16	LYS
37	j	20	GLU
37	j	21	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	j	24	ARG
37	j	44	ASN
37	j	66	ARG
37	j	72	ASN
37	j	75	ASP
37	j	94	LYS
38	k	20	LYS
38	k	58	CYS
38	k	134	TYR
38	k	140	TRP
38	k	176	ILE
38	k	316	TYR
38	k	318	PRO
38	k	331	PHE
38	k	333	VAL
38	k	348	TYR
38	k	435	ALA
38	k	439	PRO
38	k	456	ASP
38	k	526	THR
38	k	528	LEU
39	U	90	VAL
39	U	144	ARG
40	R	126	VAL
40	R	142	ILE
3	C	46	ILE
4	D	82	ARG
5	E	159	ILE
6	F	131	ALA
10	J	17	ASP
10	J	67	PRO
10	J	139	ILE
13	M	34	GLU
13	M	36	ALA
14	N	24	LEU
15	O	118	SER
16	P	24	THR
17	Q	66	ARG
17	Q	138	ASP
18	S	44	PRO
20	V	143	LYS
22	X	10	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Y	58	ALA
24	Z	87	ASN
25	a	86	GLU
30	f	98	VAL
36	B	63	VAL
36	B	224	VAL
36	B	229	ALA
36	B	398	ARG
36	B	403	LYS
36	B	452	GLU
37	j	29	LYS
37	j	42	LEU
37	j	46	ARG
38	k	132	GLY
38	k	185	GLY
38	k	187	ILE
38	k	322	LEU
38	k	329	LEU
38	k	338	ASN
38	k	342	VAL
38	k	345	MET
38	k	358	GLY
38	k	408	ASN
38	k	514	THR
38	k	527	TYR
40	R	12	PHE
40	R	133	ILE
40	R	134	GLY
40	R	135	ALA
4	D	207	LEU
6	F	205	PRO
8	H	22	LYS
9	I	236	SER
10	J	13	GLY
12	L	21	GLU
15	O	75	ASN
16	P	30	SER
18	S	118	THR
19	T	83	ASN
19	T	94	GLU
23	Y	71	LYS
24	Z	86	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Z	109	GLY
25	a	30	PRO
25	a	52	PRO
25	a	106	GLN
26	b	62	TYR
27	c	83	GLN
28	d	52	GLU
29	e	24	CYS
31	g	13	GLY
31	g	161	SER
32	n	112	ASN
33	i	79	SER
35	A	55	ARG
36	B	89	ASN
36	B	135	GLY
36	B	179	PRO
36	B	378	PRO
37	j	74	SER
38	k	88	CYS
38	k	98	PRO
38	k	175	GLN
38	k	327	ALA
38	k	380	GLU
38	k	395	ARG
38	k	448	PRO
38	k	477	GLY
38	k	585	ASP
40	R	10	ARG
40	R	83	MET
3	C	71	PRO
3	C	155	ARG
4	D	56	LYS
5	E	161	LYS
7	G	30	ARG
7	G	153	LEU
10	J	6	ALA
10	J	37	LYS
10	J	116	ARG
11	K	22	HIS
11	K	31	ARG
11	K	144	LYS
13	M	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	120	ALA
16	P	22	VAL
16	P	26	LEU
16	P	138	ASN
17	Q	64	ALA
19	T	84	TYR
22	X	28	ASP
24	Z	53	GLU
25	a	9	THR
26	b	11	ALA
29	e	8	TRP
30	f	91	ASN
30	f	122	PRO
31	g	127	LYS
35	A	40	ASN
38	k	133	LYS
38	k	265	PRO
38	k	321	ASN
38	k	337	ALA
38	k	446	MET
38	k	450	GLN
39	U	89	ASP
39	U	95	TYR
40	R	140	ARG
3	C	199	PRO
4	D	179	ASN
6	F	142	LEU
6	F	216	GLU
7	G	83	PRO
8	H	184	SER
11	K	53	LYS
11	K	133	GLU
19	T	120	THR
20	V	39	LEU
25	a	96	LEU
27	c	4	ALA
27	c	75	GLU
30	f	136	PHE
30	f	146	LEU
35	A	59	ILE
36	B	196	LYS
36	B	461	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	j	25	GLU
38	k	191	LYS
38	k	330	VAL
38	k	379	GLY
39	U	141	ARG
39	U	148	VAL
40	R	38	SER
40	R	74	GLU
40	R	130	ARG
3	C	126	ASP
3	C	206	ASP
6	F	191	PRO
9	I	154	ARG
13	M	2	LEU
29	e	36	LEU
31	g	191	HIS
36	B	105	ASP
37	j	23	LYS
37	j	27	VAL
38	k	319	THR
3	C	3	GLY
7	G	152	PRO
13	M	3	MET
14	N	26	GLY
27	c	38	PRO
38	k	99	ILE
38	k	100	PRO
38	k	137	PRO
4	D	79	VAL
6	F	196	GLY
10	J	45	ILE
23	Y	29	PRO
31	g	275	ILE
38	k	177	PRO
38	k	237	ILE
9	I	67	VAL
40	R	129	GLY

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	24/24 (100%)	24 (100%)	0	100	100
3	C	174/175 (99%)	172 (99%)	2 (1%)	65	83
4	D	196/231 (85%)	196 (100%)	0	100	100
5	E	187/187 (100%)	187 (100%)	0	100	100
6	F	190/202 (94%)	189 (100%)	1 (0%)	81	89
7	G	225/225 (100%)	225 (100%)	0	100	100
8	H	161/161 (100%)	160 (99%)	1 (1%)	78	88
9	I	207/207 (100%)	207 (100%)	0	100	100
10	J	170/172 (99%)	169 (99%)	1 (1%)	78	88
11	K	177/177 (100%)	175 (99%)	2 (1%)	65	83
12	L	157/157 (100%)	156 (99%)	1 (1%)	78	88
13	M	89/89 (100%)	89 (100%)	0	100	100
14	N	142/142 (100%)	138 (97%)	4 (3%)	38	70
15	O	104/108 (96%)	101 (97%)	3 (3%)	37	70
16	P	130/130 (100%)	125 (96%)	5 (4%)	29	63
17	Q	106/119 (89%)	106 (100%)	0	100	100
18	S	117/117 (100%)	116 (99%)	1 (1%)	70	85
19	T	114/121 (94%)	114 (100%)	0	100	100
20	V	113/113 (100%)	113 (100%)	0	100	100
21	W	94/107 (88%)	94 (100%)	0	100	100
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	112/113 (99%)	112 (100%)	0	100	100
24	Z	114/115 (99%)	114 (100%)	0	100	100
25	a	108/115 (94%)	102 (94%)	6 (6%)	19	52
26	b	87/99 (88%)	87 (100%)	0	100	100
27	c	76/76 (100%)	76 (100%)	0	100	100
28	d	57/62 (92%)	57 (100%)	0	100	100
29	e	47/49 (96%)	44 (94%)	3 (6%)	16	48
30	f	64/64 (100%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	g	272/272 (100%)	272 (100%)	0	100	100
32	n	66/102 (65%)	66 (100%)	0	100	100
33	i	49/106 (46%)	47 (96%)	2 (4%)	27	61
35	A	238/255 (93%)	232 (98%)	6 (2%)	42	72
36	B	354/354 (100%)	337 (95%)	17 (5%)	23	57
37	j	92/93 (99%)	67 (73%)	25 (27%)	0	2
38	k	523/523 (100%)	466 (89%)	57 (11%)	6	26
39	U	125/132 (95%)	124 (99%)	1 (1%)	73	86
40	R	126/130 (97%)	121 (96%)	5 (4%)	28	62
All	All	5454/5691 (96%)	5311 (97%)	143 (3%)	41	72

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	110	ASN
3	C	194	PRO
6	F	195	SER
8	H	141	VAL
10	J	66	VAL
11	K	84	ASN
11	K	145	ILE
12	L	123	ILE
14	N	24	LEU
14	N	25	LEU
14	N	28	THR
14	N	30	LYS
15	O	52	LEU
15	O	99	LYS
15	O	103	VAL
16	P	21	SER
16	P	22	VAL
16	P	26	LEU
16	P	27	LYS
16	P	28	LEU
18	S	146	ARG
25	a	10	ARG
25	a	11	LYS
25	a	98	GLU
25	a	99	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	a	100	LYS
25	a	101	LYS
29	e	23	VAL
29	e	31	ILE
29	e	39	CYS
33	i	80	LEU
33	i	82	ARG
35	A	38	GLU
35	A	54	ARG
35	A	55	ARG
35	A	157	VAL
35	A	185	THR
35	A	205	ILE
36	B	81	ARG
36	B	83	LYS
36	B	88	ARG
36	B	102	TYR
36	B	116	ARG
36	B	274	SER
36	B	276	ASP
36	B	279	LYS
36	B	283	GLU
36	B	284	VAL
36	B	378	PRO
36	B	402	ASP
36	B	404	LYS
36	B	407	LYS
36	B	430	VAL
36	B	453	LYS
36	B	466	LEU
37	j	7	LYS
37	j	13	ARG
37	j	17	ASN
37	j	26	LEU
37	j	29	LYS
37	j	34	GLU
37	j	40	LYS
37	j	41	MET
37	j	42	LEU
37	j	44	ASN
37	j	46	ARG
37	j	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	j	64	LYS
37	j	65	LEU
37	j	66	ARG
37	j	67	LYS
37	j	68	LYS
37	j	72	ASN
37	j	76	ILE
37	j	82	ARG
37	j	91	VAL
37	j	101	ARG
37	j	103	LEU
37	j	111	GLU
37	j	115	ILE
38	k	20	LYS
38	k	33	ARG
38	k	40	GLU
38	k	45	SER
38	k	73	VAL
38	k	74	ASN
38	k	79	LEU
38	k	96	ARG
38	k	97	LEU
38	k	112	ASN
38	k	114	ILE
38	k	117	SER
38	k	131	LEU
38	k	133	LYS
38	k	135	ASP
38	k	150	SER
38	k	153	GLN
38	k	176	ILE
38	k	187	ILE
38	k	190	ARG
38	k	191	LYS
38	k	194	THR
38	k	204	LEU
38	k	205	ASP
38	k	224	ARG
38	k	245	SER
38	k	268	TYR
38	k	311	ILE
38	k	312	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	k	313	LEU
38	k	316	TYR
38	k	317	VAL
38	k	319	THR
38	k	320	GLU
38	k	322	LEU
38	k	325	ARG
38	k	326	ASP
38	k	328	SER
38	k	329	LEU
38	k	332	LYS
38	k	336	THR
38	k	339	GLU
38	k	343	LYS
38	k	344	LYS
38	k	347	MET
38	k	419	LYS
38	k	433	ARG
38	k	439	PRO
38	k	443	THR
38	k	485	ILE
38	k	526	THR
38	k	528	LEU
38	k	533	ILE
38	k	569	ASP
38	k	576	ARG
38	k	579	LYS
38	k	598	ASP
39	U	150	LYS
40	R	75	VAL
40	R	84	ILE
40	R	130	ARG
40	R	140	ARG
40	R	141	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	24	HIS
3	C	110	ASN
4	D	95	ASN
5	E	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	121	HIS
5	E	262	HIS
6	F	101	GLN
6	F	159	HIS
6	F	207	HIS
7	G	67	GLN
7	G	98	ASN
7	G	112	HIS
7	G	142	HIS
7	G	188	ASN
8	H	74	ASN
8	H	95	HIS
8	H	114	ASN
8	H	118	ASN
8	H	149	GLN
9	I	4	ASN
9	I	65	GLN
9	I	105	ASN
9	I	177	GLN
10	J	44	ASN
10	J	68	GLN
10	J	73	GLN
10	J	164	ASN
10	J	165	ASN
11	K	35	ASN
11	K	44	HIS
11	K	84	ASN
11	K	181	GLN
12	L	75	ASN
14	N	100	ASN
14	N	112	HIS
15	O	55	ASN
16	P	69	ASN
16	P	90	HIS
17	Q	79	GLN
18	S	11	GLN
18	S	24	HIS
18	S	29	ASN
18	S	48	GLN
18	S	97	GLN
19	T	121	GLN
20	V	42	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	V	85	ASN
21	W	85	HIS
21	W	92	HIS
23	Y	56	HIS
23	Y	92	ASN
24	Z	16	HIS
26	b	25	ASN
26	b	80	HIS
27	c	51	GLN
28	d	7	GLN
29	e	5	GLN
30	f	135	HIS
30	f	139	HIS
31	g	14	HIS
31	g	76	GLN
31	g	117	ASN
31	g	133	ASN
31	g	162	ASN
31	g	187	ASN
31	g	191	HIS
31	g	226	HIS
31	g	305	ASN
31	g	311	GLN
33	i	113	ASN
35	A	60	ASN
35	A	181	ASN
37	j	17	ASN
37	j	60	HIS
37	j	72	ASN
37	j	112	HIS
38	k	112	ASN
38	k	208	HIS
38	k	274	HIS
38	k	426	GLN
38	k	450	GLN
38	k	468	GLN
38	k	520	HIS
38	k	549	GLN
38	k	556	ASN
38	k	578	ASN
40	R	79	HIS
40	R	114	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	13 (17%)	3 (4%)
34	2	1737/1863 (93%)	242 (13%)	7 (0%)
41	3	41/42 (97%)	26 (63%)	1 (2%)
All	All	1852/1980 (93%)	281 (15%)	11 (0%)

All (281) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	9	U
1	1	11	G
1	1	15	A
1	1	16	G
1	1	17	C
1	1	18	G
1	1	19	G
1	1	21	A
1	1	43	G
1	1	45	G
1	1	47	U
1	1	61	C
1	1	75	C
34	2	4	C
34	2	33	G
34	2	41	G
34	2	42	A
34	2	44	U
34	2	46	A
34	2	56	G
34	2	67	C
34	2	68	A
34	2	72	C
34	2	73	C
34	2	74	G
34	2	76	U
34	2	77	A
34	2	79	A
34	2	80	G
34	2	113	G
34	2	143	U
34	2	147	A
34	2	148	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	181	A
34	2	182	C
34	2	191	C
34	2	197	U
34	2	202	U
34	2	223	A
34	2	226	A
34	2	274	G
34	2	277	U
34	2	278	U
34	2	296	U
34	2	297	C
34	2	299	G
34	2	300	G
34	2	309	A
34	2	310	G
34	2	311	C
34	2	315	C
34	2	316	C
34	2	317	G
34	2	322	G
34	2	337	G
34	2	347	C
34	2	352	C
34	2	354	A
34	2	358	U
34	2	373	G
34	2	375	G
34	2	376	C
34	2	399	C
34	2	418	U
34	2	438	A
34	2	439	A
34	2	440	C
34	2	457	G
34	2	462	C
34	2	463	A
34	2	464	G
34	2	472	G
34	2	477	U
34	2	483	A
34	2	492	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	515	A
34	2	522	C
34	2	542	G
34	2	543	U
34	2	546	U
34	2	547	U
34	2	554	A
34	2	558	C
34	2	577	A
34	2	579	G
34	2	580	A
34	2	583	C
34	2	584	A
34	2	596	G
34	2	597	U
34	2	598	C
34	2	618	A
34	2	633	A
34	2	658	A
34	2	659	A
34	2	661	A
34	2	662	A
34	2	678	U
34	2	679	U
34	2	680	G
34	2	681	U
34	2	682	G
34	2	729	C
34	2	732	C
34	2	733	G
34	2	734	C
34	2	735	C
34	2	736	C
34	2	737	C
34	2	738	U
34	2	739	U
34	2	740	G
34	2	741	C
34	2	742	C
34	2	743	U
34	2	744	C
34	2	746	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	747	G
34	2	748	G
34	2	749	C
34	2	750	G
34	2	751	C
34	2	785	G
34	2	786	C
34	2	787	C
34	2	788	C
34	2	789	G
34	2	790	A
34	2	791	A
34	2	793	C
34	2	794	G
34	2	795	U
34	2	807	A
34	2	818	U
34	2	819	U
34	2	835	C
34	2	843	A
34	2	849	C
34	2	864	G
34	2	865	A
34	2	868	A
34	2	869	G
34	2	870	G
34	2	874	G
34	2	883	U
34	2	884	U
34	2	906	G
34	2	907	C
34	2	909	A
34	2	913	U
34	2	916	A
34	2	929	G
34	2	951	A
34	2	967	G
34	2	986	A
34	2	987	G
34	2	988	A
34	2	1004	A
34	2	1013	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	1019	A
34	2	1045	A
34	2	1057	U
34	2	1058	A
34	2	1081	C
34	2	1082	G
34	2	1106	G
34	2	1112	C
34	2	1113	C
34	2	1144	A
34	2	1145	A
34	2	1150	U
34	2	1211	C
34	2	1217	G
34	2	1219	A
34	2	1238	U
34	2	1247	A
34	2	1252	G
34	2	1253	G
34	2	1255	A
34	2	1260	C
34	2	1270	G
34	2	1271	G
34	2	1280	A
34	2	1281	G
34	2	1296	U
34	2	1297	A
34	2	1298	G
34	2	1299	C
34	2	1311	U
34	2	1367	U
34	2	1374	A
34	2	1391	C
34	2	1399	C
34	2	1406	C
34	2	1408	C
34	2	1413	C
34	2	1414	C
34	2	1415	C
34	2	1420	G
34	2	1427	G
34	2	1431	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	1433	C
34	2	1450	A
34	2	1471	G
34	2	1472	A
34	2	1473	U
34	2	1485	A
34	2	1486	G
34	2	1503	G
34	2	1506	G
34	2	1507	U
34	2	1516	C
34	2	1517	A
34	2	1539	C
34	2	1547	G
34	2	1548	C
34	2	1549	C
34	2	1551	A
34	2	1575	A
34	2	1580	U
34	2	1583	A
34	2	1596	A
34	2	1616	U
34	2	1618	A
34	2	1632	A
34	2	1643	G
34	2	1659	A
34	2	1660	G
34	2	1666	G
34	2	1675	G
34	2	1678	C
34	2	1683	C
34	2	1706	U
34	2	1707	A
34	2	1708	C
34	2	1716	U
34	2	1717	G
34	2	1743	G
34	2	1747	C
34	2	1748	G
34	2	1777	C
34	2	1778	G
34	2	1816	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	1818	A
34	2	1819	A
34	2	1820	G
34	2	1823	G
34	2	1825	A
34	2	1829	A
34	2	1846	C
34	2	1855	G
34	2	1856	G
34	2	1858	U
34	2	1859	C
34	2	1863	A
41	3	37	C
41	3	39	U
41	3	40	C
41	3	41	A
41	3	42	A
41	3	43	A
41	3	45	A
41	3	47	A
41	3	48	C
41	3	49	A
41	3	55	G
41	3	56	U
41	3	57	G
41	3	58	C
41	3	59	A
41	3	61	C
41	3	62	U
41	3	65	C
41	3	66	U
41	3	67	C
41	3	69	U
41	3	70	G
41	3	71	A
41	3	72	G
41	3	73	G
41	3	74	A

All (11) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
-----	-------	-----	------

Mol	Chain	Res	Type
1	1	8	G
1	1	17	C
1	1	18	G
34	2	74	G
34	2	739	U
34	2	912	A
34	2	1012	U
34	2	1270	G
34	2	1716	U
34	2	1857	A
41	3	39	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	C4J	2	1244	34	25,29,30	1.04	2 (8%)	28,42,45	2.91	2 (7%)
1	T6A	1	37	1	31,34,35	1.42	4 (12%)	43,49,52	2.50	18 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	C4J	2	1244	34	1/1/7/7	8/16/34/35	0/2/2/2
1	T6A	1	37	1	-	6/23/41/42	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	C5-C4	4.76	1.47	1.39
34	2	1244	C4J	C4-C5	-3.49	1.39	1.47
1	1	37	T6A	C5-C6	2.80	1.48	1.41
1	1	37	T6A	C5-N7	-2.31	1.34	1.39
1	1	37	T6A	C8-N7	2.23	1.36	1.31
34	2	1244	C4J	C1'-C5	-2.16	1.45	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1244	C4J	C1'-C5-C4	14.42	139.49	117.61
1	1	37	T6A	C12-N11-C10	8.50	136.12	121.99
1	1	37	T6A	C5-C4-N3	-5.54	119.09	126.72
1	1	37	T6A	N3-C4-N9	4.45	134.73	127.17
1	1	37	T6A	C14-C12-C13	3.70	116.49	110.03
1	1	37	T6A	C2-N3-C4	3.69	120.85	111.83
1	1	37	T6A	N3-C2-N1	-3.67	123.03	128.58
34	2	1244	C4J	C4-N3-C2	-3.63	121.15	125.62
1	1	37	T6A	C2'-C1'-N9	-3.58	104.41	113.30
1	1	37	T6A	C4-C5-N7	-3.56	106.51	110.58
1	1	37	T6A	C6-C5-N7	3.51	136.26	132.43
1	1	37	T6A	C4-N9-C8	2.80	108.68	105.74
1	1	37	T6A	O10-C10-N6	-2.80	118.66	123.64
1	1	37	T6A	C5-N7-C8	2.69	107.68	103.45
1	1	37	T6A	C14-C12-N11	2.62	118.64	111.70
1	1	37	T6A	C2-N1-C6	2.24	122.66	115.24
1	1	37	T6A	N9-C8-N7	-2.11	110.95	113.94
1	1	37	T6A	O4'-C1'-N9	2.10	112.12	108.09
1	1	37	T6A	N6-C10-N11	2.10	116.65	113.77
1	1	37	T6A	N6-C6-N1	2.05	122.85	117.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	2	1244	C4J	C4'

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C14-C12-N11-C10
34	2	1244	C4J	C31-C3-N3-C2
34	2	1244	C4J	C31-C3-N3-C4
34	2	1244	C4J	C3-C31-C32-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	2	1244	C4J	C3-C31-C32-N33
1	1	37	T6A	N11-C12-C13-ODB
1	1	37	T6A	N11-C12-C13-ODA
34	2	1244	C4J	N3-C3-C31-C32
1	1	37	T6A	O4'-C4'-C5'-O5'
34	2	1244	C4J	N33-C32-C34-O35
34	2	1244	C4J	C31-C32-C34-O36
1	1	37	T6A	C13-C12-N11-C10
1	1	37	T6A	C13-C12-C14-C15
34	2	1244	C4J	C31-C32-C34-O35

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	2	1244	C4J	2	0
1	1	37	T6A	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	SF4	k	702	38	0,12,12	-	-	-		
44	GNP	k	704	43	34,34,34	1.34	3 (8%)	47,54,54	0.88	2 (4%)
44	GNP	k	705	-	34,34,34	1.38	3 (8%)	47,54,54	0.90	2 (4%)
42	SF4	k	701	38	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	SF4	k	702	38	-	-	0/6/5/5
42	SF4	k	701	38	-	-	0/6/5/5
44	GNP	k	704	43	-	3/18/38/38	0/3/3/3
44	GNP	k	705	-	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	705	GNP	PG-O2G	-4.62	1.44	1.56
44	k	704	GNP	PG-O2G	-4.61	1.44	1.56
44	k	705	GNP	PB-O2B	-4.09	1.45	1.56
44	k	704	GNP	PB-O2B	-3.81	1.46	1.56
44	k	705	GNP	PA-O3A	2.63	1.62	1.59
44	k	704	GNP	PA-O3A	2.32	1.62	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	704	GNP	O2G-PG-O3G	-2.52	100.82	107.59
44	k	705	GNP	O2G-PG-O3G	-2.47	100.96	107.59
44	k	704	GNP	O3G-PG-O1G	-2.16	108.02	113.45
44	k	705	GNP	O3G-PG-O1G	-2.12	108.14	113.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

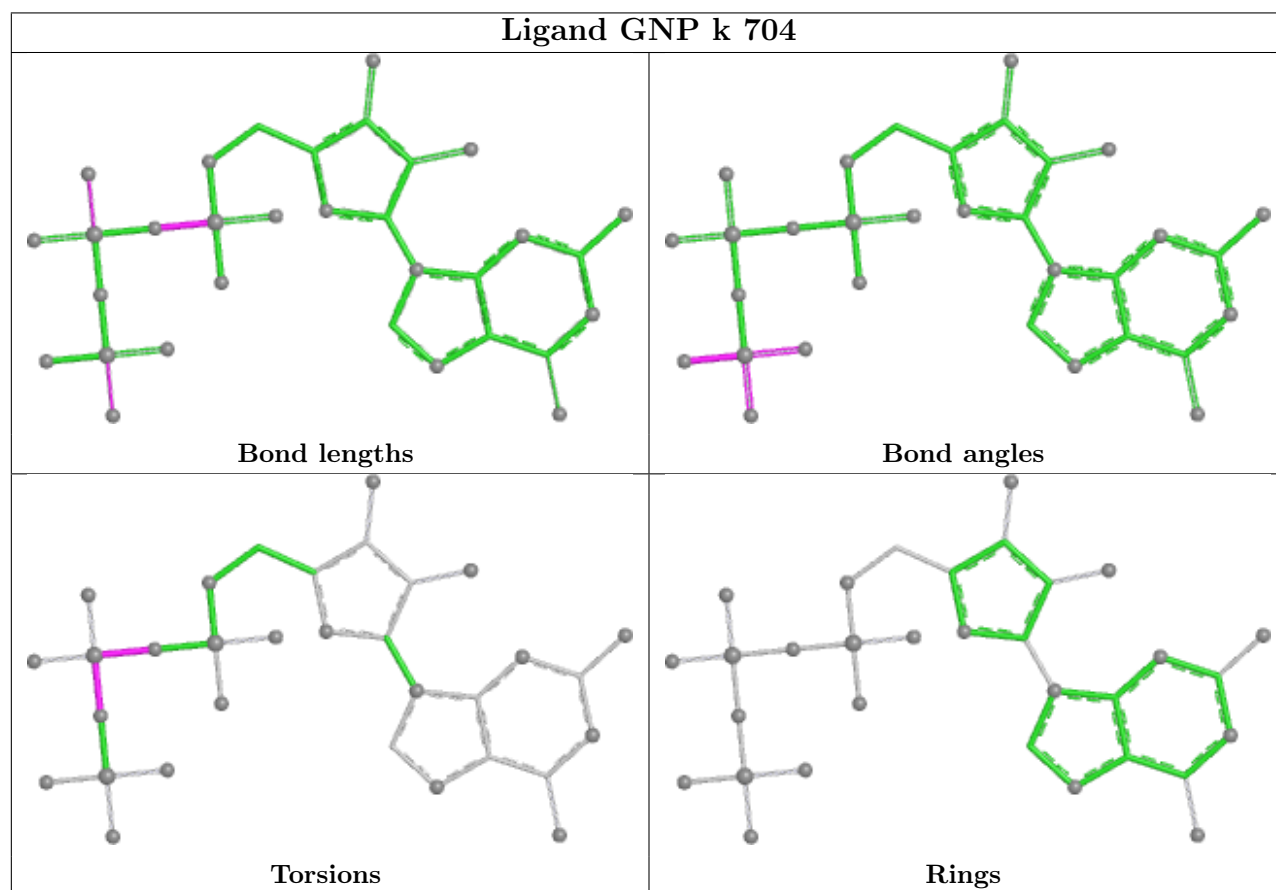
Mol	Chain	Res	Type	Atoms
44	k	704	GNP	PG-N3B-PB-O1B
44	k	704	GNP	PG-N3B-PB-O3A
44	k	704	GNP	PA-O3A-PB-O2B
44	k	705	GNP	PG-N3B-PB-O1B
44	k	705	GNP	C5'-O5'-PA-O3A
44	k	705	GNP	C5'-O5'-PA-O2A
44	k	705	GNP	C4'-C5'-O5'-PA

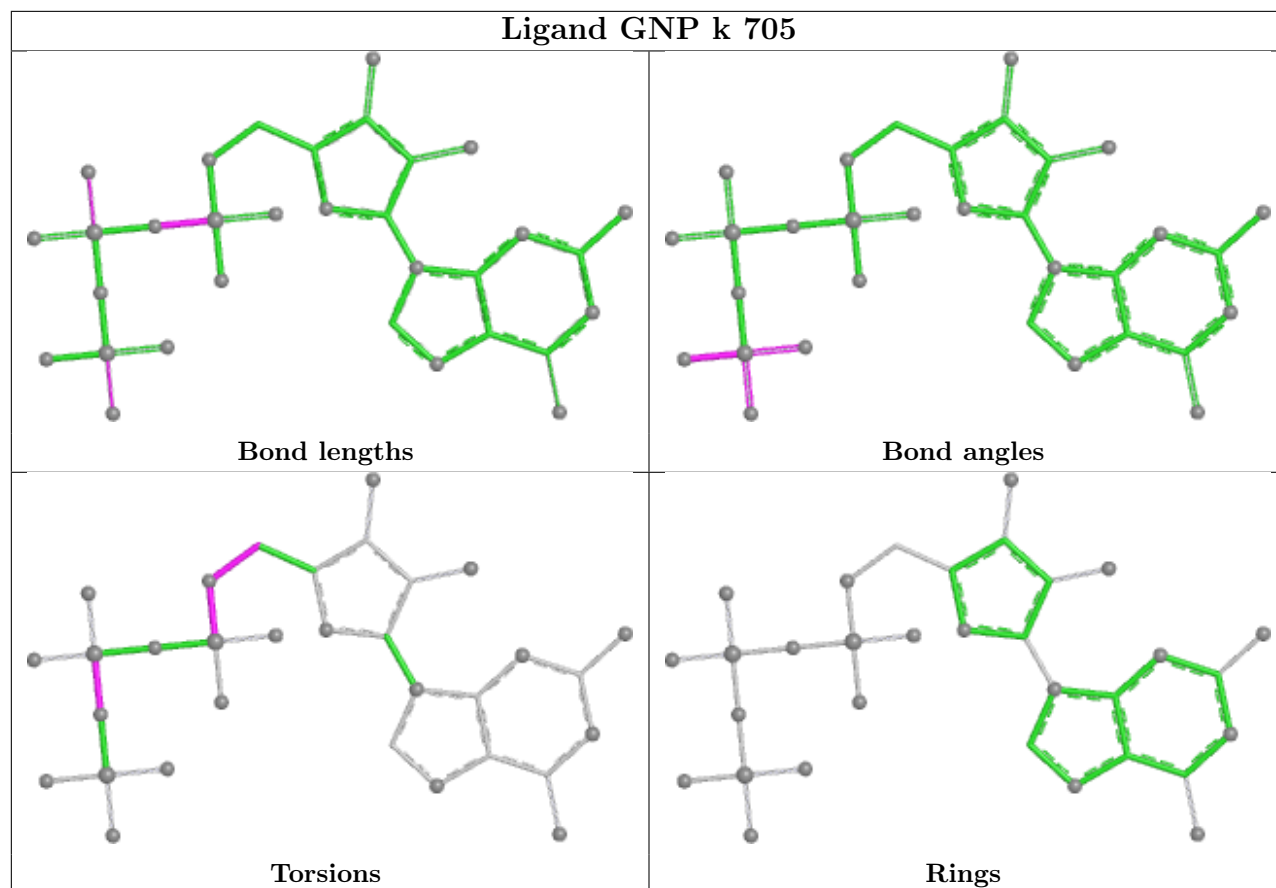
There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	k	702	SF4	7	0
44	k	704	GNP	12	0
44	k	705	GNP	18	0
42	k	701	SF4	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	k	23
34	2	4
1	1	2
39	U	1
25	a	1
41	3	1
37	j	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	k	521:ASP	C	522:PHE	N	2.98
1	U	142:ARG	C	143:GLY	N	2.92
1	k	451:ILE	C	452:GLU	N	2.79
1	k	373:GLU	C	374:ILE	N	2.70
1	k	550:THR	C	551:LEU	N	2.35
1	k	518:VAL	C	519:GLU	N	2.16
1	k	486:ASP	C	487:GLU	N	2.09
1	k	591:SER	C	592:GLY	N	2.02
1	k	411:TYR	C	412:LYS	N	2.01
1	1	17:C	O3'	18:G	P	1.99
1	k	378:LEU	C	379:GLY	N	1.94
1	1	18:G	O3'	19:G	P	1.87
1	k	440:GLN	C	441:PHE	N	1.85
1	2	350:A	O3'	351:U	P	1.83
1	k	109:VAL	C	110:GLY	N	1.79
1	k	513:LYS	C	514:THR	N	1.64
1	a	9:THR	C	10:ARG	N	1.60
1	3	39:U	O3'	40:C	P	1.39
1	2	239:U	O3'	240:C	P	1.36
1	2	80:G	O3'	81:U	P	1.34
1	j	95:TYR	C	96:ASN	N	1.16
1	k	493:ASP	C	494:SER	N	1.09
1	k	160:LEU	C	161:GLU	N	1.05
1	k	150:SER	C	151:GLU	N	1.02
1	k	268:TYR	C	269:ILE	N	1.02
1	k	241:ASP	C	242:GLU	N	0.84
1	k	531:ARG	C	532:VAL	N	0.82
1	k	481:ASP	C	482:VAL	N	0.79
1	k	104:GLU	C	105:VAL	N	0.75
1	k	408:ASN	C	409:VAL	N	0.68
1	k	562:LEU	C	563:GLU	N	0.52
1	k	455:ILE	C	456:ASP	N	0.44

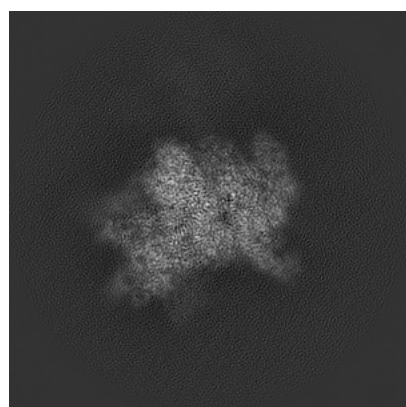
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10760. These allow visual inspection of the internal detail of the map and identification of artifacts.

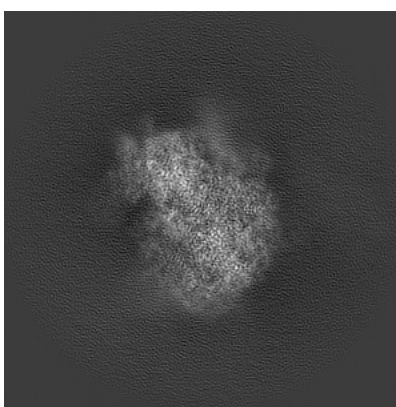
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

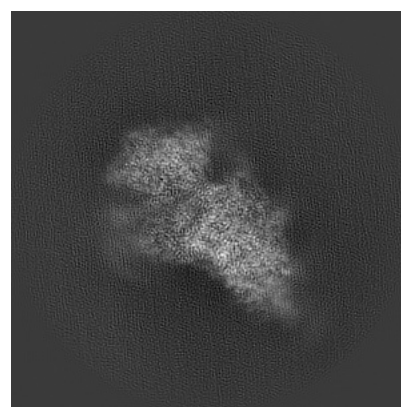
6.1.1 Primary map



X



Y

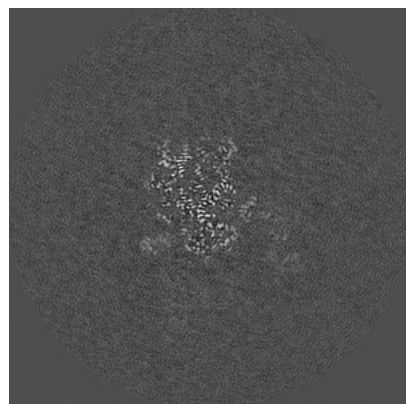


Z

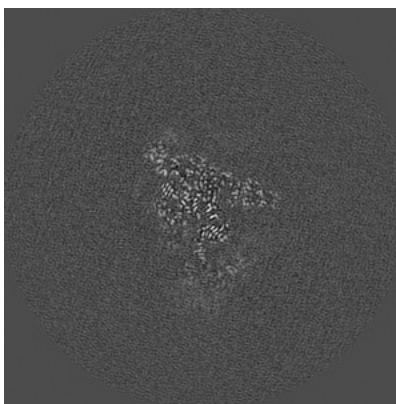
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

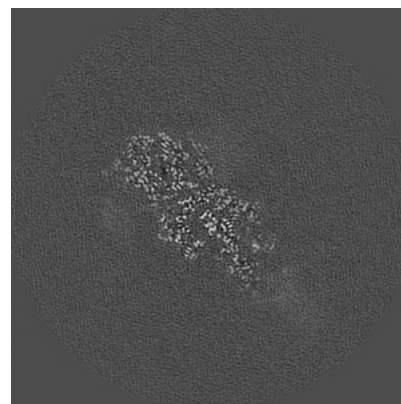
6.2.1 Primary map



X Index: 192



Y Index: 192

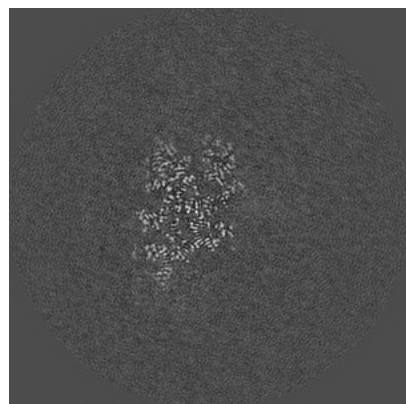


Z Index: 192

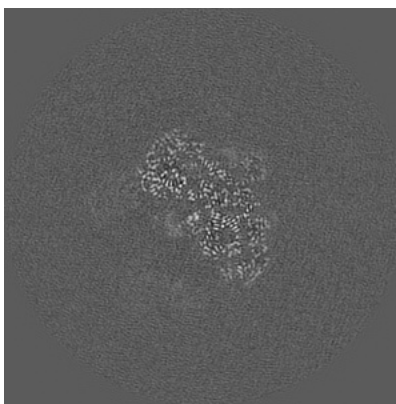
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

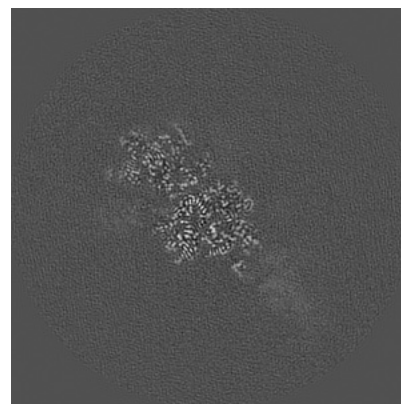
6.3.1 Primary map



X Index: 205



Y Index: 161

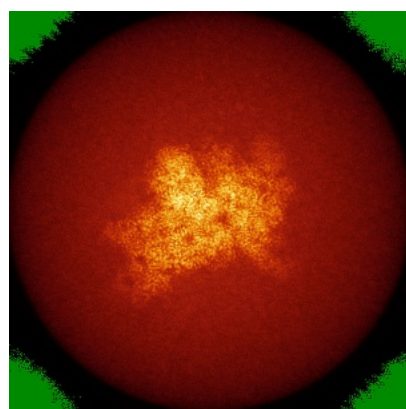


Z Index: 199

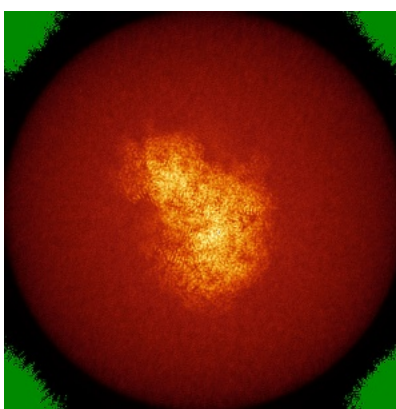
The images above show the largest variance slices of the map in three orthogonal directions.

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

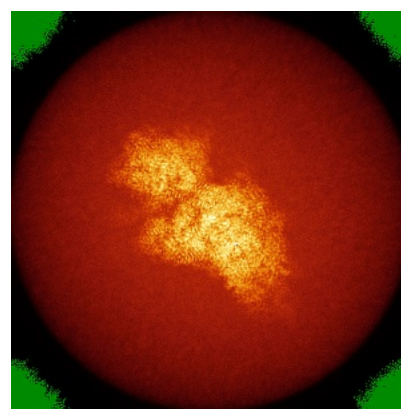
6.4.1 Primary map



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

This section was not generated.

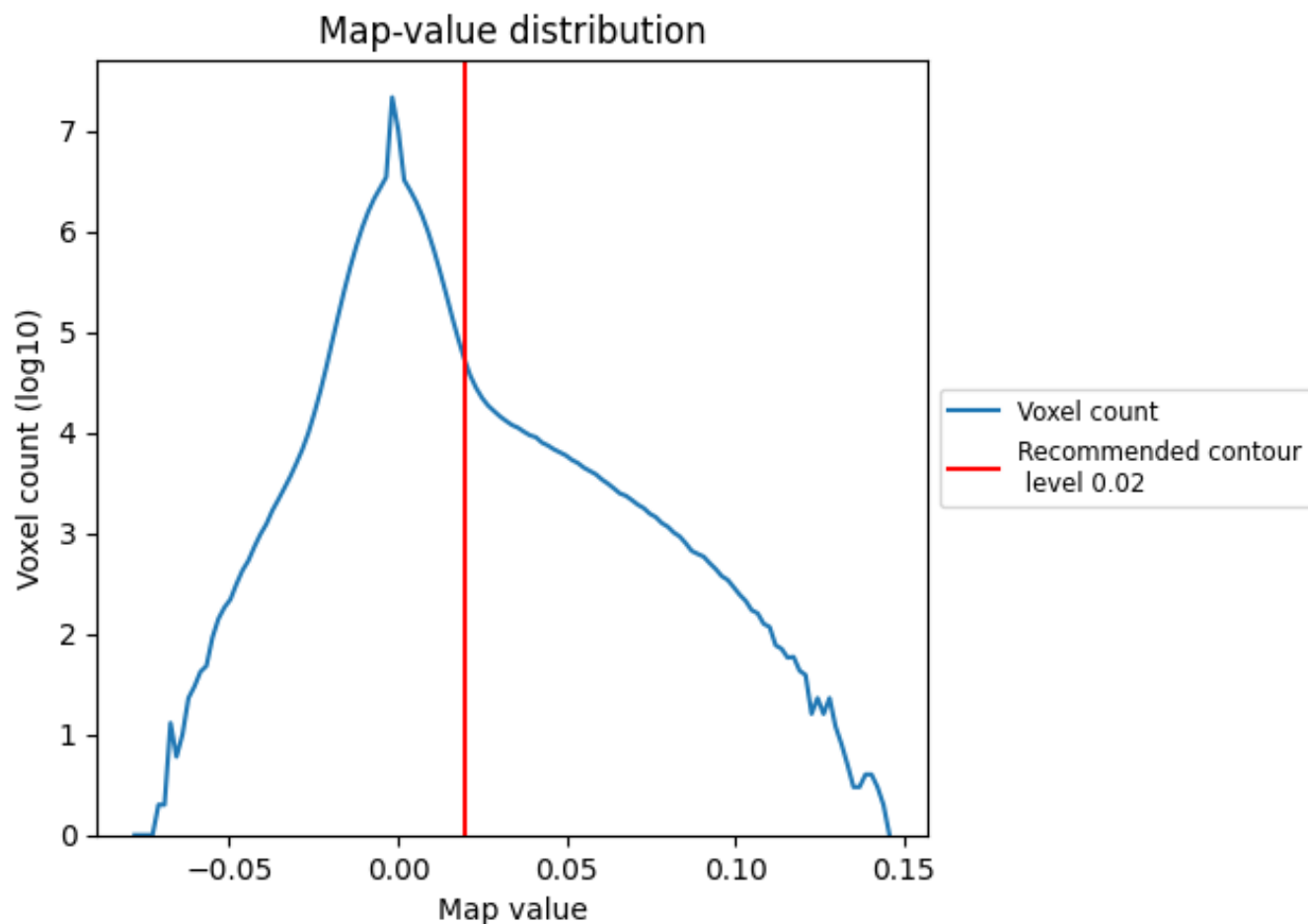
6.6 Mask visualisation

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

7 Map analysis [i](#)

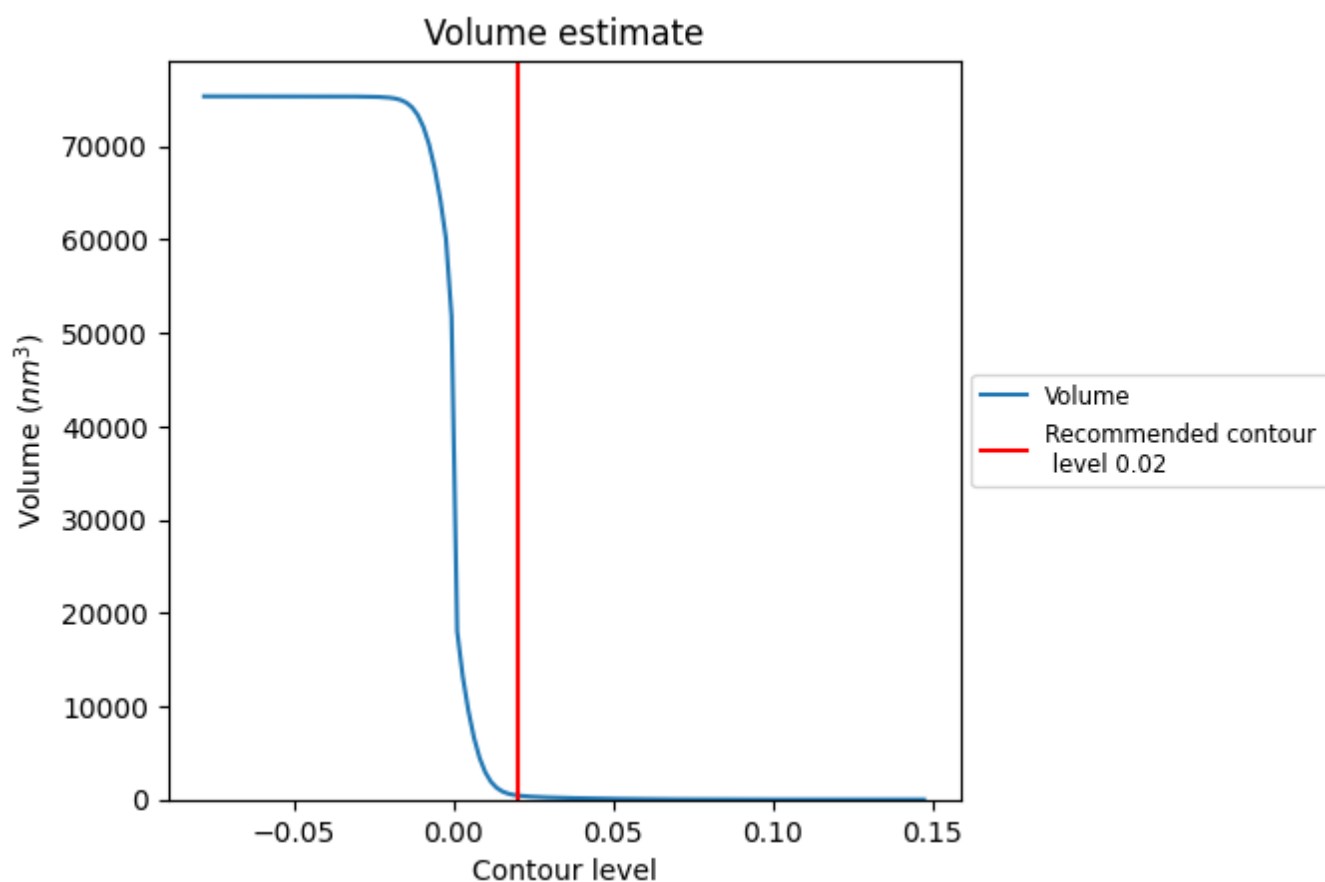
This section contains the results of statistical analysis of the map.

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.

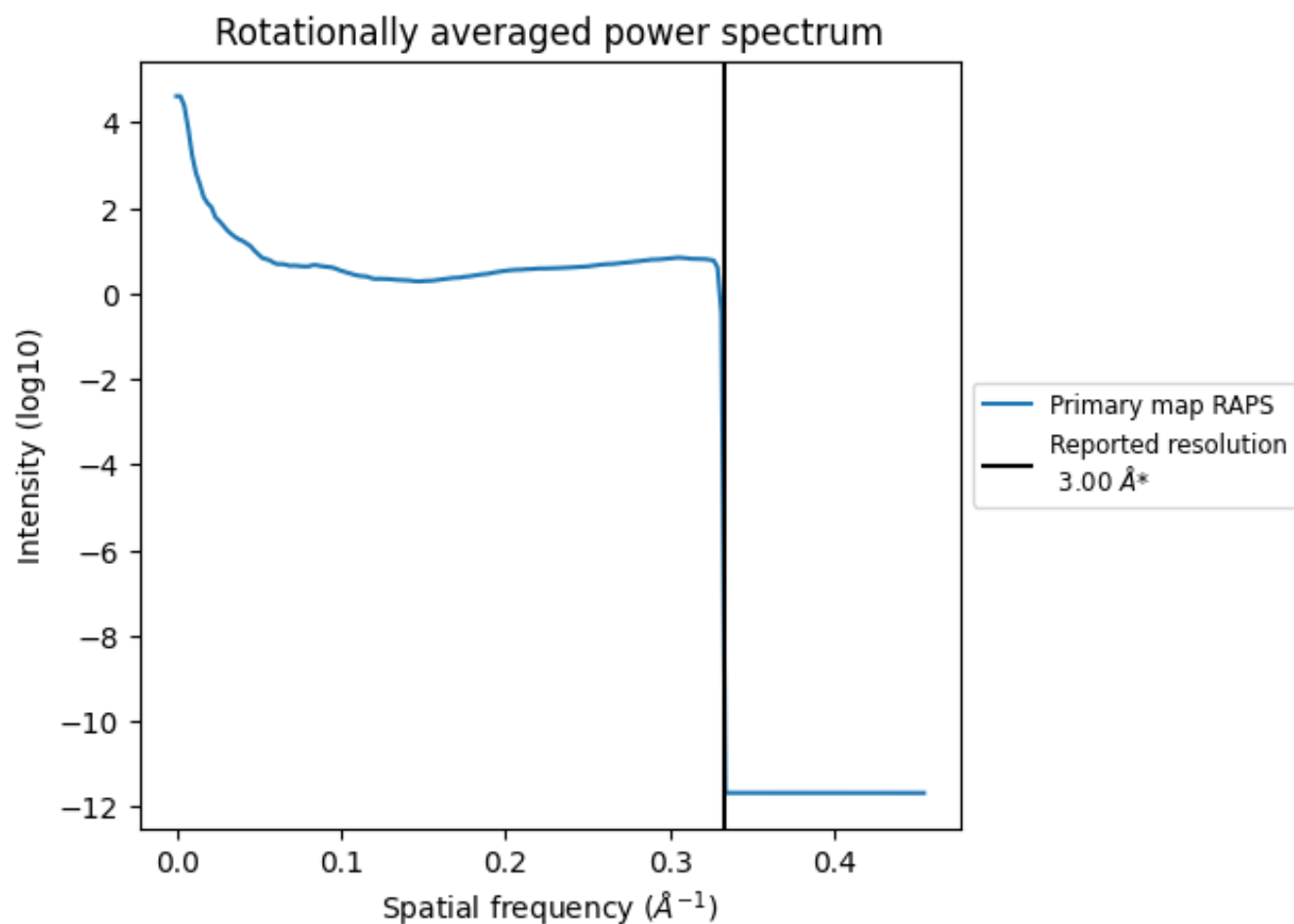
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 449 nm³; this corresponds to an approximate mass of 406 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 0.333 $\text{\AA}^{-1}$

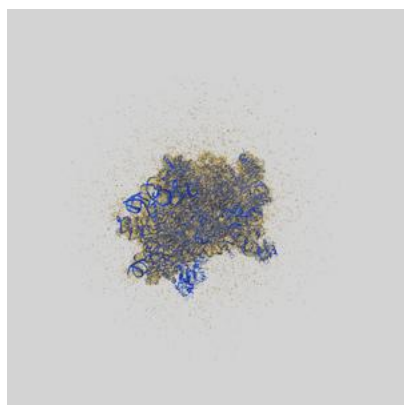
8 Fourier-Shell correlation ⓘ

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

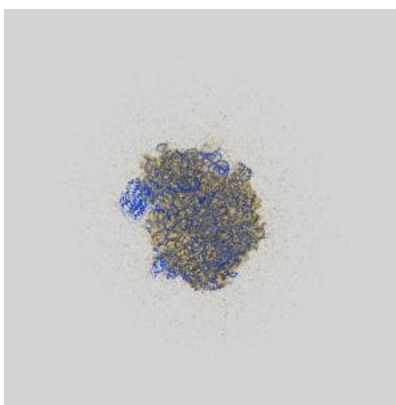
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10760 and PDB model 6YAL. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

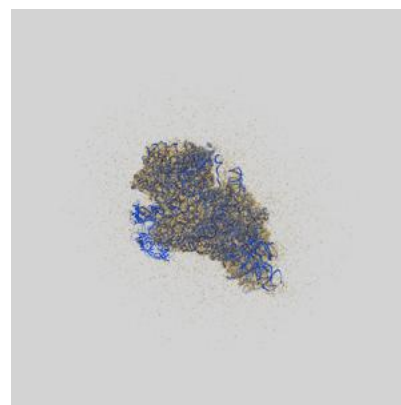
9.1 Map-model overlay [i](#)



X



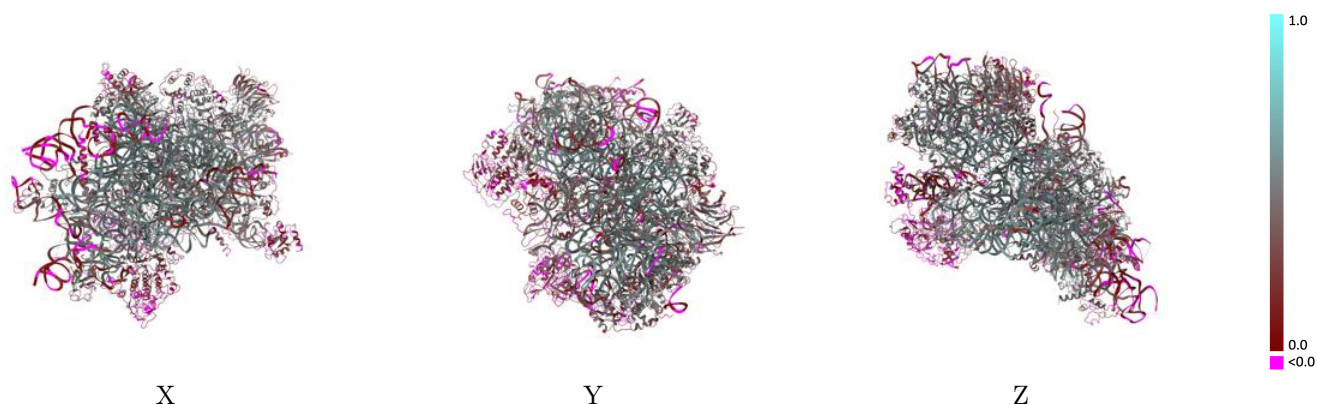
Y



Z

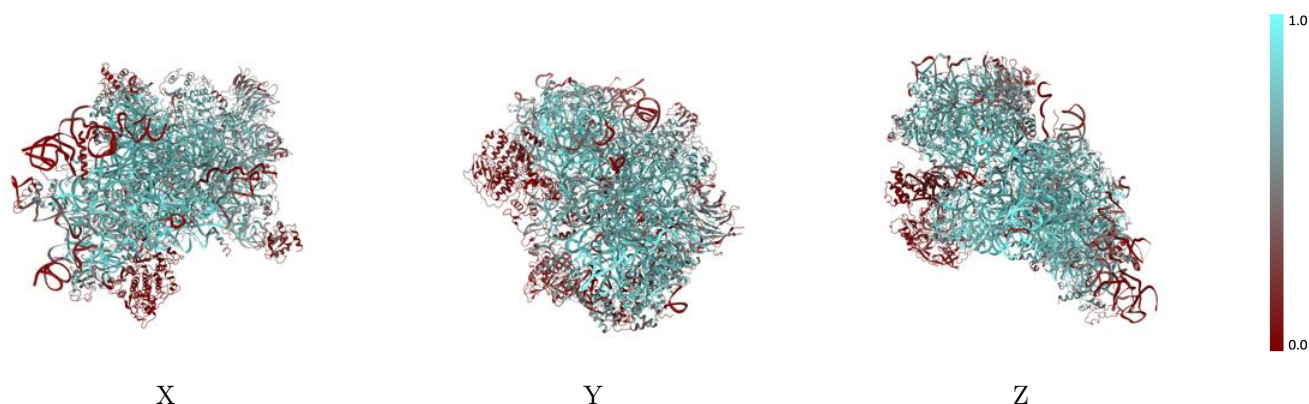
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



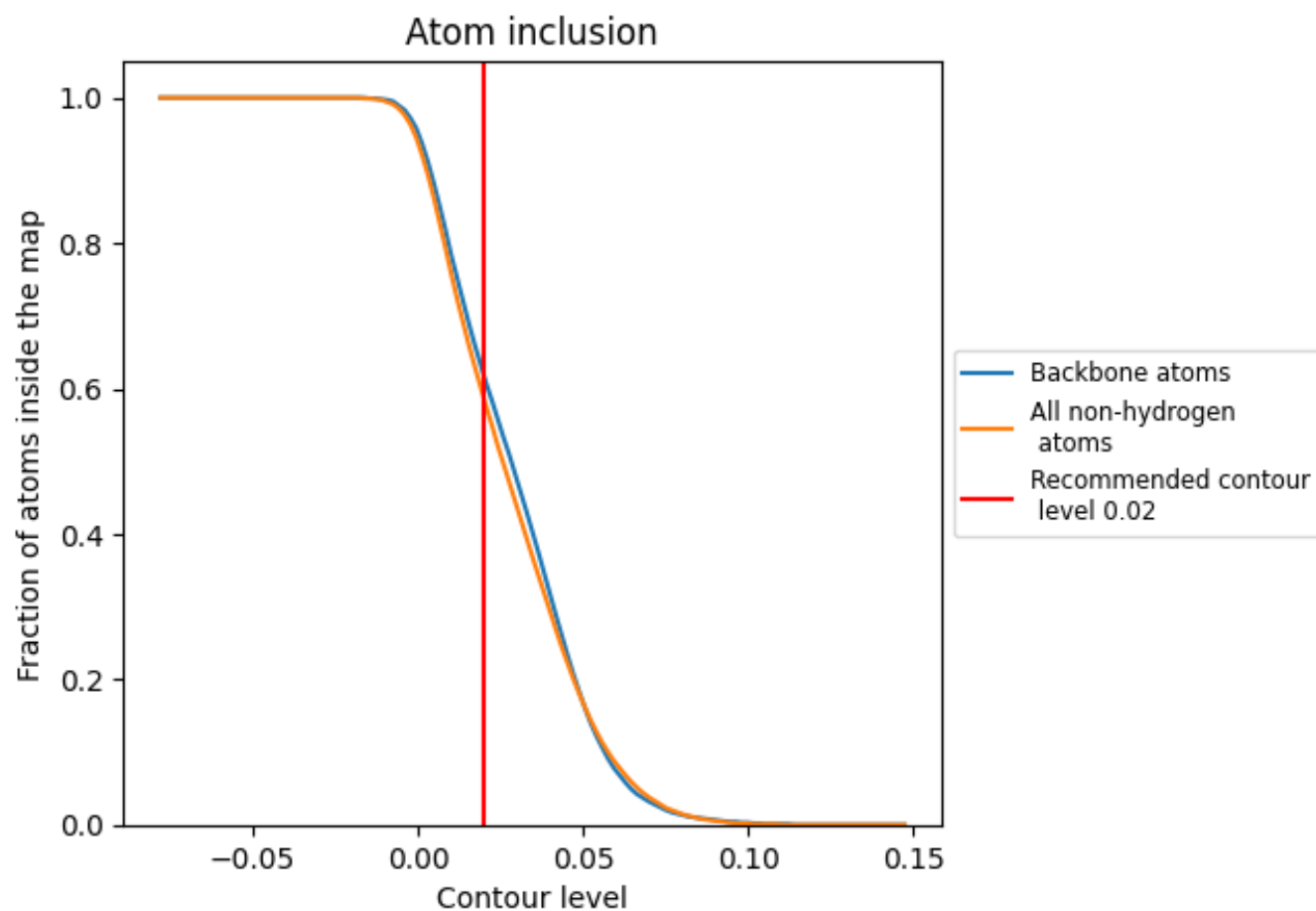
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 59% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.3790
1	 0.2280	 0.1570
2	 0.7700	 0.4650
3	 0.1330	 0.1270
A	 0.0440	 0.0980
B	 0.0020	 0.0100
C	 0.6800	 0.4320
D	 0.6480	 0.4170
E	 0.7120	 0.4660
F	 0.5430	 0.3560
G	 0.6900	 0.4550
H	 0.6310	 0.4090
I	 0.5000	 0.3310
J	 0.3730	 0.2690
K	 0.5910	 0.3850
L	 0.6780	 0.4330
M	 0.5200	 0.3330
N	 0.6270	 0.4100
O	 0.1320	 0.1360
P	 0.6790	 0.4410
Q	 0.6600	 0.4160
R	 0.4990	 0.3280
S	 0.6850	 0.4480
T	 0.5250	 0.3300
U	 0.5770	 0.3850
V	 0.6740	 0.4310
W	 0.5440	 0.3660
X	 0.6580	 0.4160
Y	 0.7660	 0.4940
Z	 0.7490	 0.4730
a	 0.6380	 0.4020
b	 0.7120	 0.4570
c	 0.5580	 0.3600
d	 0.5450	 0.3650
e	 0.5480	 0.2680



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.1480	 0.1270
g	 0.4910	 0.3590
i	 0.4630	 0.3140
j	 0.2020	 0.2240
k	 0.0400	 0.1780
l	 0.5750	 0.3940
n	 0.4600	 0.3510