



Full wwPDB EM Validation Report ⓘ

May 23, 2026 – 02:37 PM EDT

PDB ID : 9PJ7 / pdb_00009pj7
EMDB ID : EMD-71682
Title : C. acnes 70S ribosome bound to Doxycycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-12
Resolution : 2.40 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:

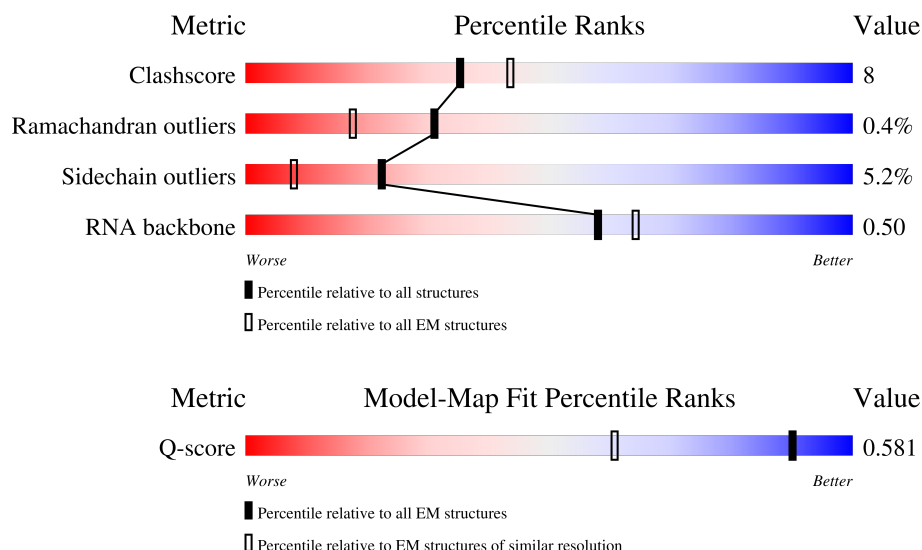
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.40 Å.

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



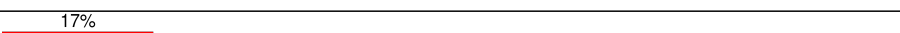
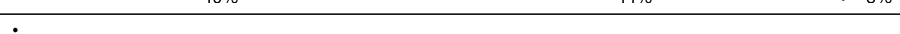
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	44	
3	2	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	37	
5	4	69	
6	A	1537	
7	B	283	
8	C	76	
9	D	201	
10	E	215	
11	F	96	
12	G	269	
13	H	135	
14	I	156	
15	J	173	
16	K	135	
17	L	123	
18	M	103	
19	N	123	
20	O	87	
21	P	147	
22	Q	90	
23	R	79	
24	S	61	
25	T	88	
26	U	93	
27	V	24	
28	X	33	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Y	22	
30	a	3086	
31	b	120	
32	c	278	
33	d	223	
34	e	301	
35	f	210	
36	g	180	
37	i	147	
38	j	122	
39	k	146	
40	l	139	
41	m	187	
42	n	127	
43	o	117	
44	p	123	
45	q	102	
46	r	153	
47	s	102	
48	t	122	
49	u	205	
50	v	89	
51	w	61	
52	x	77	
53	y	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	z	63	84% 11%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1512	Total	C	N	O	P	0	0
			32480	14471	5911	10586	1512		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 8 is a RNA chain called initiator tRNA Met (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	75	Total	C	N	O	P S	0	0
			1605	716	291	522	75 1		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	122	Total	C	N	O	S	0	0
			976	598	205	173			

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	67	Total	C	N	O		0	0
			527	334	103	90			

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O		0	0
			673	408	144	121			

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 27 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	23	Total	C	N	O		0	0
			183	106	50	27			

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 29 is a RNA chain called mRNA 32MF.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2903	Total	C	N	O	P	0	0
			62408	27795	11386	20324	2903		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	x	69	Total	C	N	O	0	0
			564	348	108	108		

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

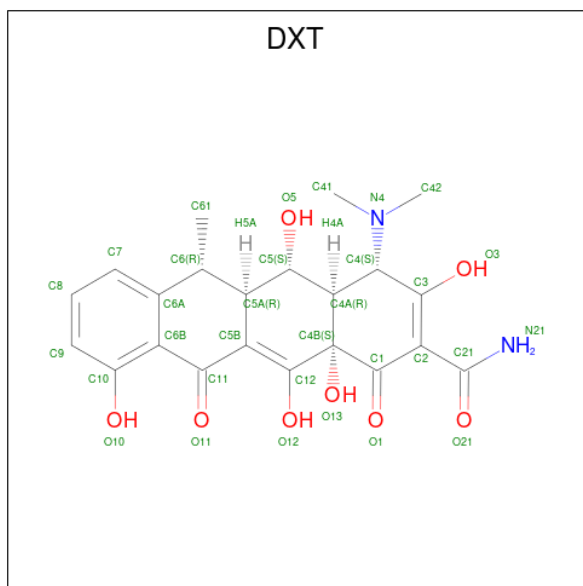
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	S	1	Total	Zn	0
			1	1	
55	w	1	Total	Zn	0
			1	1	
55	z	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	51	Total	Mg	0
			51	51	
56	a	230	Total	Mg	0
			230	230	
56	b	2	Total	Mg	0
			2	2	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	
56	o	1	Total	Mg	0
			1	1	

- Molecule 57 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: $C_{22}H_{24}N_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	a	1	Total	C	N	O	0
			32	22	2	8	
57	r	1	Total	C	N	O	0
			32	22	2	8	
57	s	1	Total	C	N	O	0
			32	22	2	8	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	12	Total	O	0
			12	12	
58	C	1	Total	O	0
			1	1	

Continued on next page...

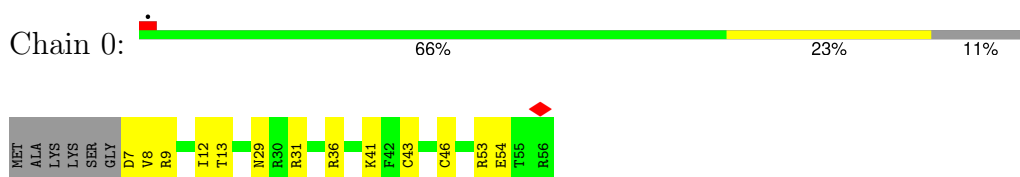
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	S	1	Total 1	O 1	0
58	a	115	Total 115	O 115	0
58	b	1	Total 1	O 1	0
58	c	1	Total 1	O 1	0
58	d	1	Total 1	O 1	0
58	s	1	Total 1	O 1	0

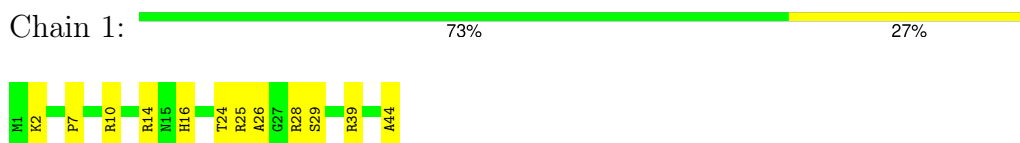
3 Residue-property plots [i](#)

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

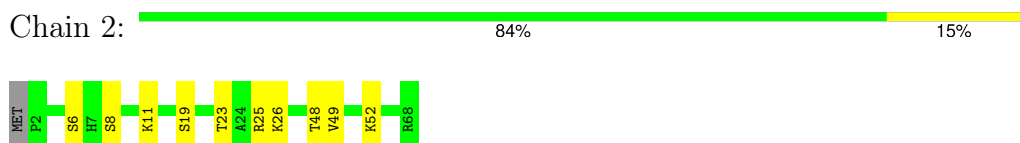
- Molecule 1: 50S ribosomal protein L33



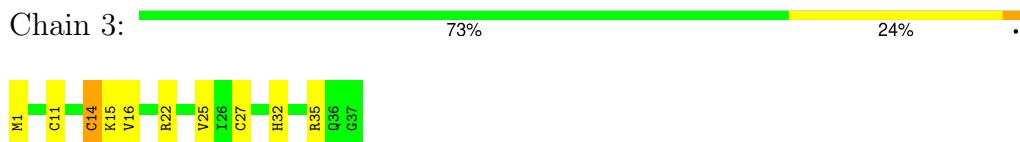
- Molecule 2: 50S ribosomal protein L34



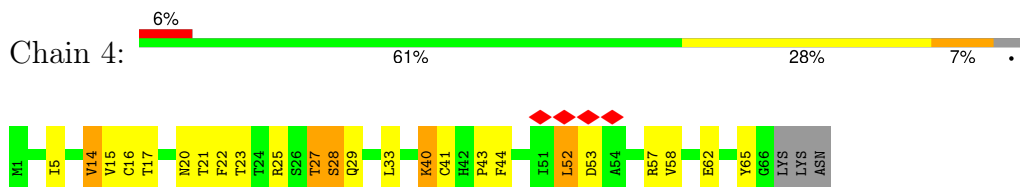
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: 50S ribosomal protein L36



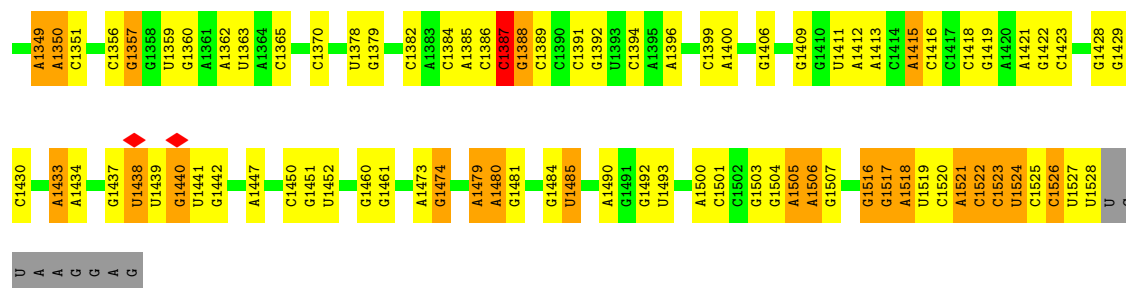
- Molecule 5: 50S ribosomal protein L31



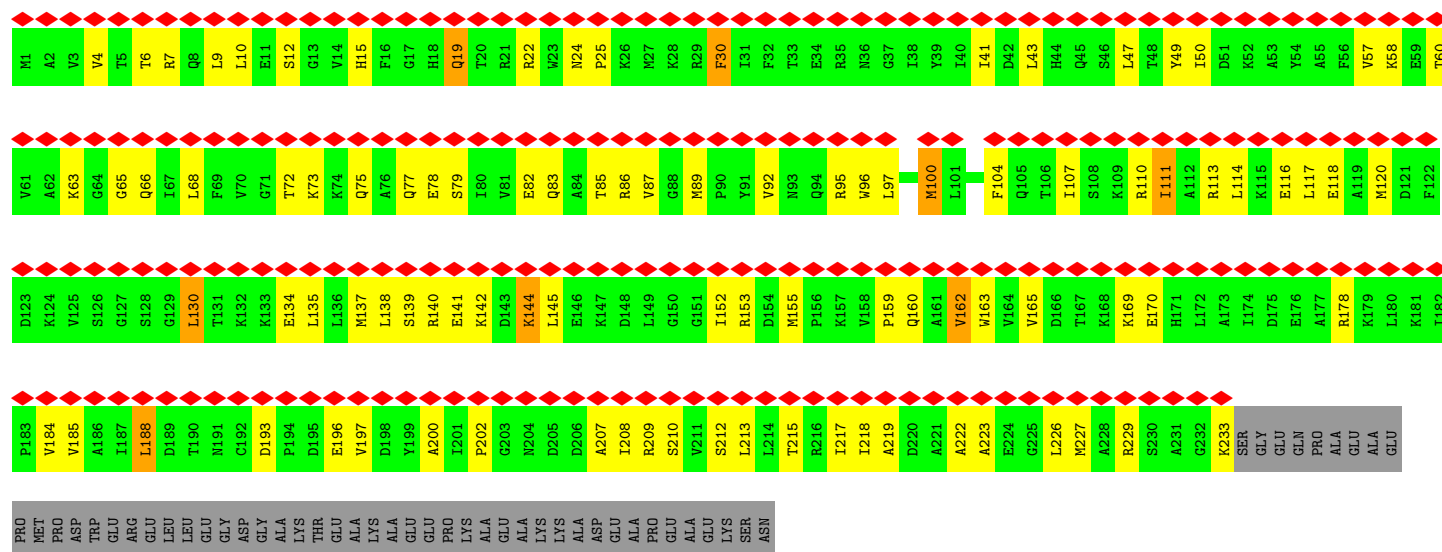
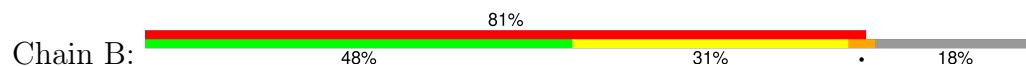
- Molecule 6: 16S rRNA

Response	Percentage
Yes	55%
No	35%
Don't know	8%





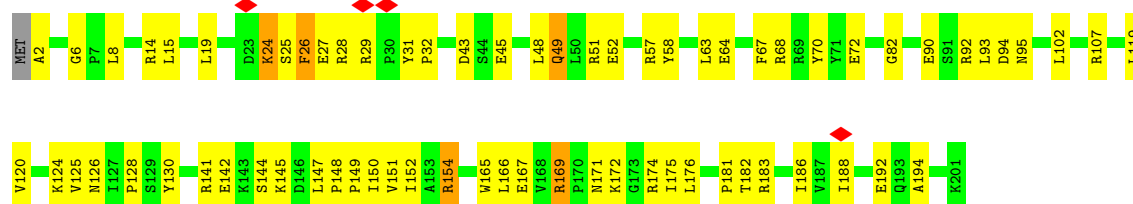
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: initiator tRNA Met (76-MER)

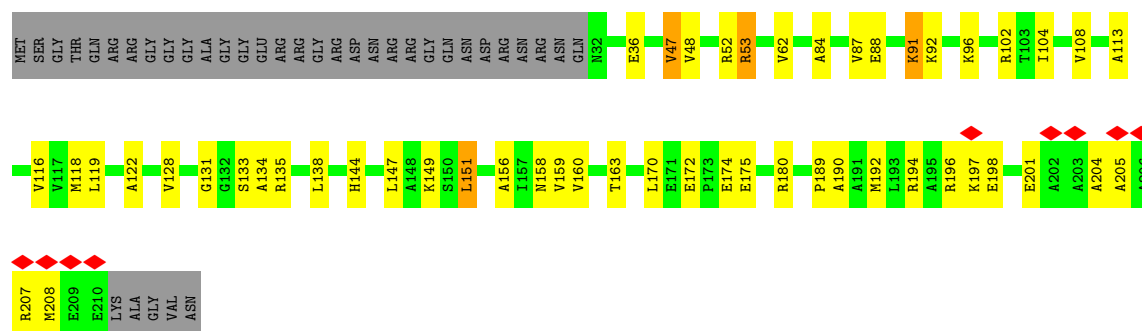


• Molecule 9: 30S ribosomal protein S4



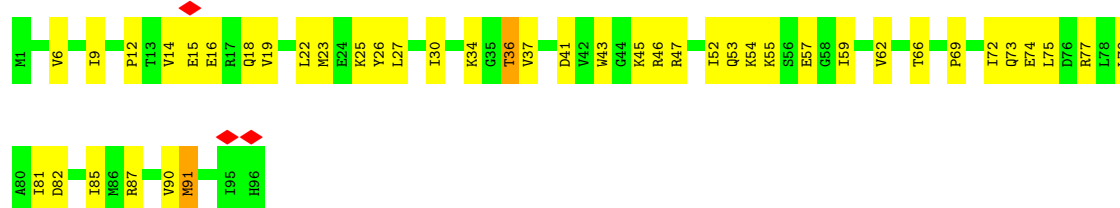
• Molecule 10: Small ribosomal subunit protein uS5

Chain E: 



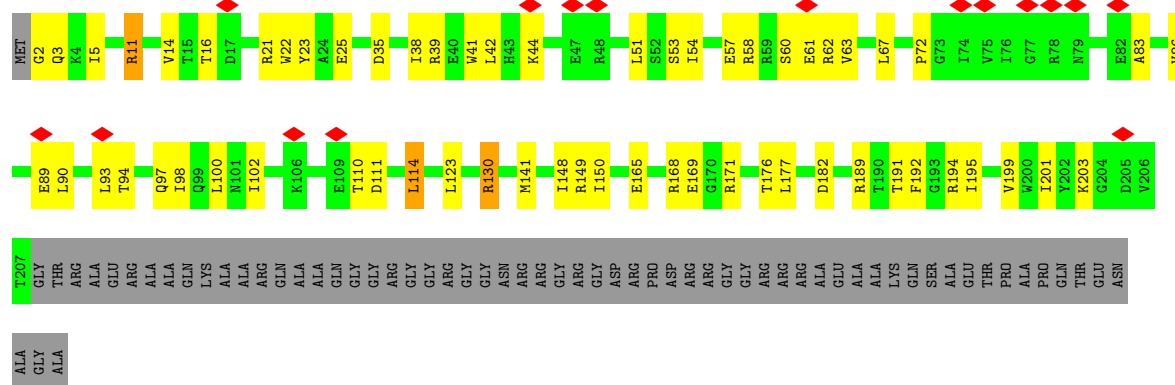
- Molecule 11: 30S ribosomal protein S6

Chain F: 



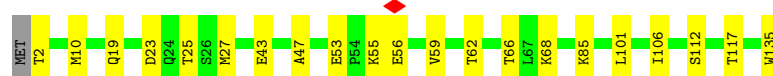
- Molecule 12: 30S ribosomal protein S3

Chain G: 

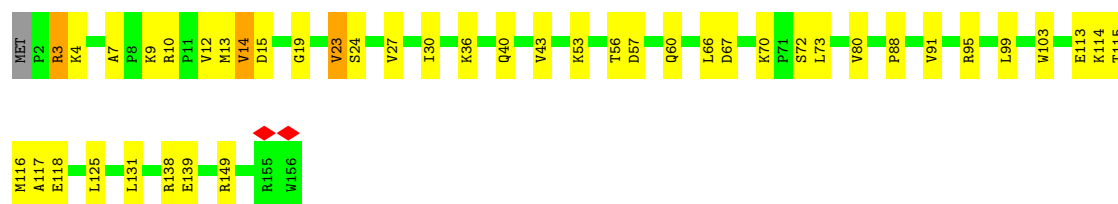


- Molecule 13: 30S ribosomal protein S8

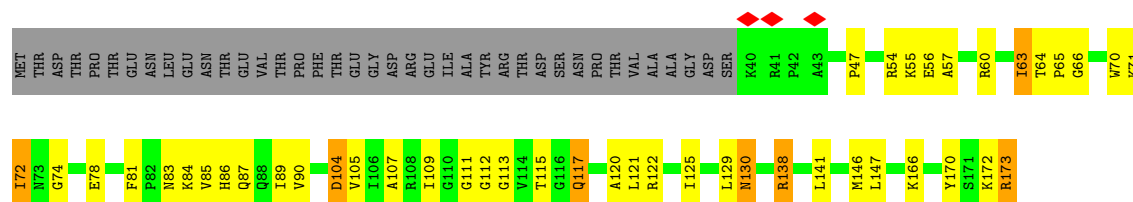
Chain H: 



- Molecule 14: 30S ribosomal protein S7



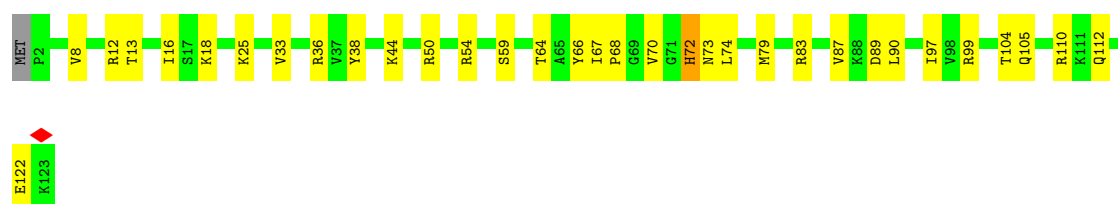
- Molecule 15: 30S ribosomal protein S9



- Molecule 16: 30S ribosomal protein S11

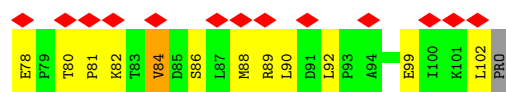


- Molecule 17: 30S ribosomal protein S12



- Molecule 18: Small ribosomal subunit protein uS10

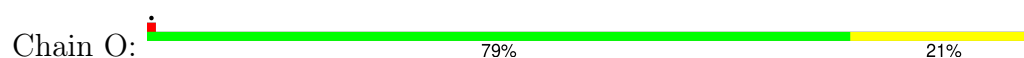




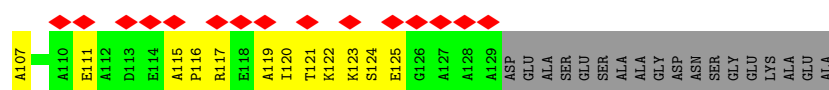
- Molecule 19: 30S ribosomal protein S13



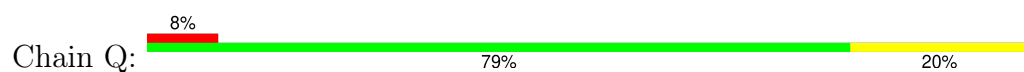
- Molecule 20: 30S ribosomal protein S15



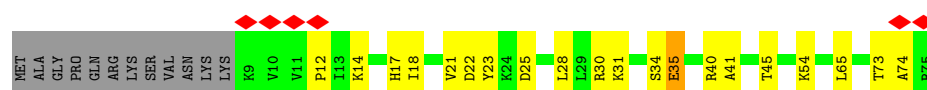
- Molecule 21: 30S ribosomal protein S16



- Molecule 22: 30S ribosomal protein S17



- Molecule 23: 30S ribosomal protein S18



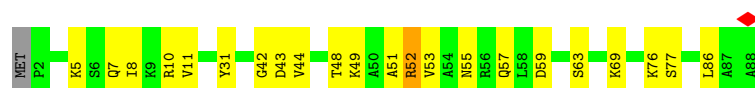
- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  59% 34% 5% .



- Molecule 25: 30S ribosomal protein S20

Chain T:  74% 24% ..



- Molecule 26: 30S ribosomal protein S19

Chain U:  58% 30% . 10%



- Molecule 27: 50S ribosomal protein bL37

Chain V:  83% 12% .



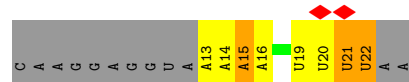
- Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X:  76% 18% . .



- Molecule 29: mRNA 32MF

Chain Y:  9% 9% 23% 14% 55%



- Molecule 30: 23S rRNA

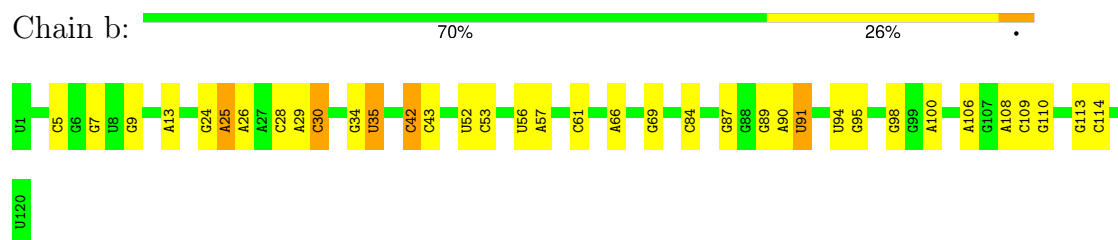
Chain a:  59% 29% 6% 6%



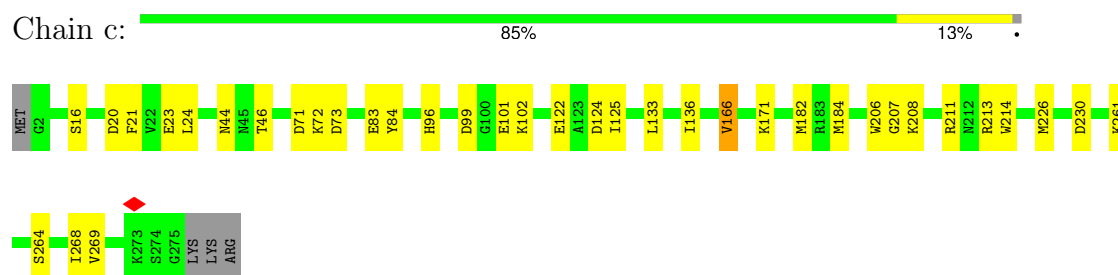


A3053	A2923	G2774	C2665	C2564	A2455	G	U2290	G2193	U2065	G1933	A1787	C1686
C3054	C2924	A2784	U2673	G2566	A2456	A	U2291	A2197	A2066	G1939	U1791	U1687
C2925	G2926	G2785	C2680	A2567	G2461	A	U	A2198	A2067	G1939	U1791	U1688
A3063	G2929	U2786	C2681	G2571	C2465	U	U	U2199	C2069	G1947	A1792	A1690
U3065	A2930	U2787	C2681	U2572	C2466	C	U	U2200	A2072	G1956	G1797	A1691
G3066	G2933	G2791	G2684	C2573	C2467	C	G	C2201	A2072	A1956	U1818	G1692
A3071	C2934	C2792	U2685	U2573	A2468	A	A	C2202	A2073	C1965	U1818	G1693
G3072	C2935	C2794	C2687	C2580	A2469	C	G	A2203	A2073	C1965	U1818	A1594
G3073	U2936	U2795	U2688	C2580	C2580	C	U	U2204	A2084	C1973	U1830	G1596
A3074	C2937	G2807	U2695	U2583	U2473	U	A	U2205	C2085	A1974	U1831	G1501
C3075	A2947	C2808	G2696	G2584	U2474	G	G	A2206	G2089	G1978	U1831	A1607
U3076	G2948	U2695	U2588	G2584	C2475	U	U	C2207	G2089	C1978	C1832	C1608
U3077	A2811	U2588	U2589	U2589	U2484	G	G	A2208	U2094	C1978	U1836	G1609
U3078	G2812	A2700	C2589	U2589	U2487	A	U	G2210	A2095	C1978	U1837	G1612
C3079	A2816	G2706	G2592	G2592	U2487	G	A	G2211	C2096	C1983	A1838	U1613
U	U2816	U2710	C2598	C2598	G2490	G	U	U2220	A2101	A1992	G1851	U1618
A	U2819	G2711	C2606	C2606	G2500	G	U	C2221	G2112	A1993	G1858	A1619
A	G2820	A2712	C2607	C2607	U2501	U	U	G2222	G2113	A1993	C1859	G1620
C	G2827	G2714	U2610	G2610	U2502	U	A	C2226	U2114	G1984	A1860	C1623
A	C2828	U2715	A2612	G2611	G2503	U	A	U2230	A2115	A1985	A1861	U1524
U	U2829	C2716	U2612	U2608	U2504	U	U	C2231	G2116	C1996	A1862	U1625
A	G2830	G2717	U2613	A2509	A2504	G	U	C2232	A2116	U1999	A1863	C1626
C	U2831	U2718	U2613	A2509	A2504	U	U	C2233	A2119	A2008	C1866	C1627
A	G2832	U2719	U2617	A2510	A2504	U	U	C2234	A2120	C2009	C1867	C1628
A	U2833	C2720	A2617	A2511	G2511	G	G	C2238	A2121	C2009	C1868	C1629
A	U2834	C2721	C2623	U2512	U2512	C	C	G2239	G2128	A2012	G1887	G1630
U	G2843	C2722	C2627	A2517	A2517	A	A	A2243	U2129	G2018	U1726	U1632
A	A2844	G2726	A2630	A2518	A2518	C	C	G2244	G2138	G2018	G1897	U1633
A	G2845	U2734	U2631	G2527	G2527	U	U	A2245	U2139	G2025	C1898	G1725
U	U2859	C2739	U2639	A2528	C2529	A	U	U2256	C2140	A2031	U1901	G1726
U	G2860	C2740	G2640	A2532	C2532	G	G	U2257	C2141	A2031	C1902	U1727
U	A2861	C2748	U2642	U2533	U2532	U	U	A2264	C2145	A2036	G1903	U1638
U	U2864	G2749	C2643	G2533	G2533	U	U	G2265	A2149	A2037	U1904	U1639
U	U2871	C2750	U2644	A2536	A2536	G	G	U2268	C2150	G2040	C1905	G1640
U	U2871	C2750	U2644	A2536	A2536	U	U	G2269	C2150	G2040	C1906	U1641
U	U2880	A2754	U2651	A2540	A2540	G	G	U2272	A2153	G2040	A1907	C1642
U	U2881	C2755	C2652	A2542	A2542	U	U	A2272	U2154	G2042	U1911	G1647
U	G2896	C2757	C2652	G2543	G2543	G	G	G2280	G2155	A2043	G1913	A1743
U	U2906	C2761	C2655	C2546	C2546	A	A	U2281	U2174	G2047	C1914	A1749
U	A2907	U2762	U2656	C2547	C2547	U	U	G2282	G2175	G2048	G1915	A1550
U	C2908	G2763	A2658	A2548	A2548	C	C	G2283	C2177	U2047	G1916	A1551
U	U2915	G2764	U2659	A2551	A2551	U	U	G2284	U2178	G2048	U1917	G1751
U	U2916	G2765	A2660	A2551	A2551	U	U	A2285	C2179	G2048	U1918	G1752
U	G2917	U2766	C2661	G2561	G2561	U	U	G2286	C2179	U2055	U1919	G1751
U	G2917	U2767	C2662	U2562	U2562	G	G	G2287	U2185	G2056	G1920	G1752
U	A2922	C2773	A2664	C2563	C2563	U	U	U2288	G2186	A2060	U1921	G1753
U	A2922	C2773	A2664	C2563	C2563	U	U	U2289	G2186	A2060	U1922	G1754
U	A2922	C2773	A2664	C2563	C2563	U	U	U2290	G2186	A2060	U1923	G1755

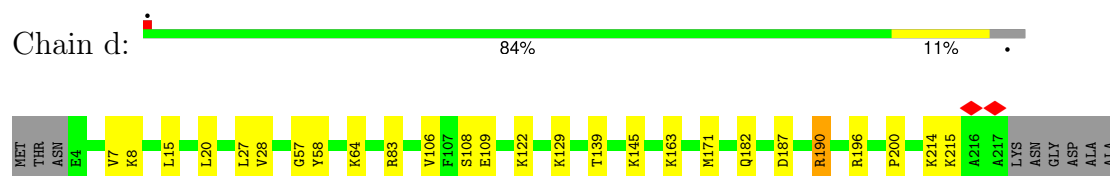
- Molecule 31: 5S rRNA



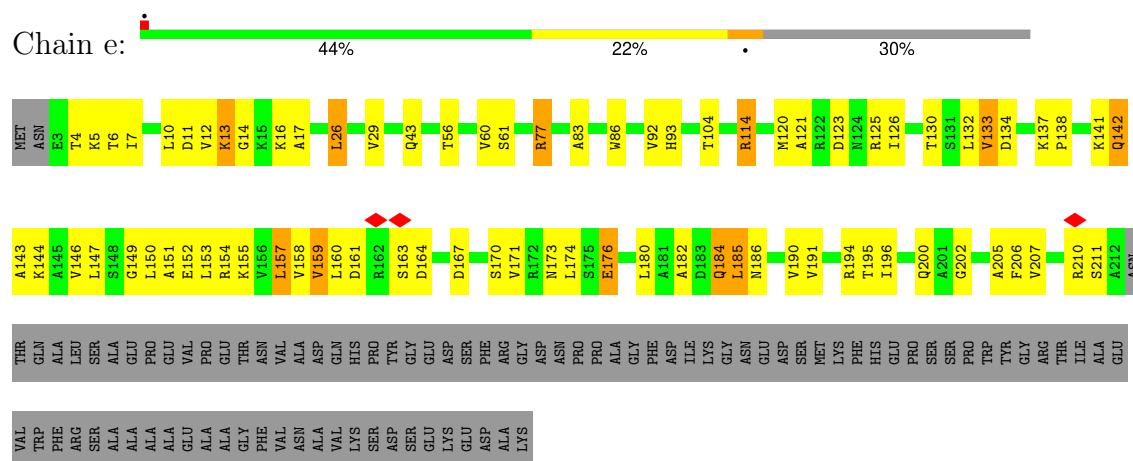
- Molecule 32: 50S ribosomal protein L2



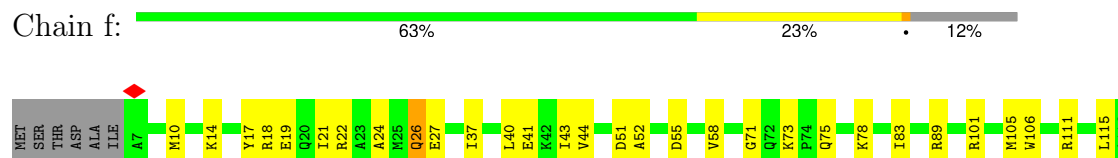
- Molecule 33: 50S ribosomal protein L3

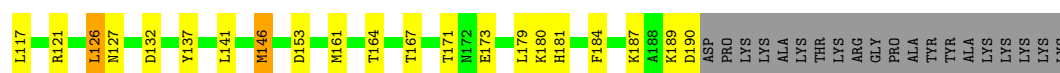


- Molecule 34: 50S ribosomal protein L4

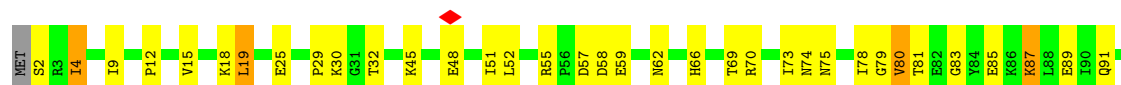


- Molecule 35: 50S ribosomal protein L5

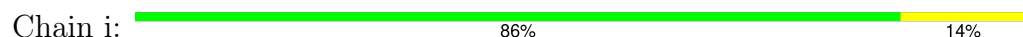




- Molecule 36: 50S ribosomal protein L6



- Molecule 37: 50S ribosomal protein L13



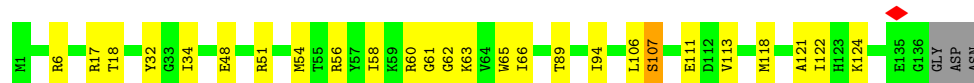
- Molecule 38: 50S ribosomal protein L14



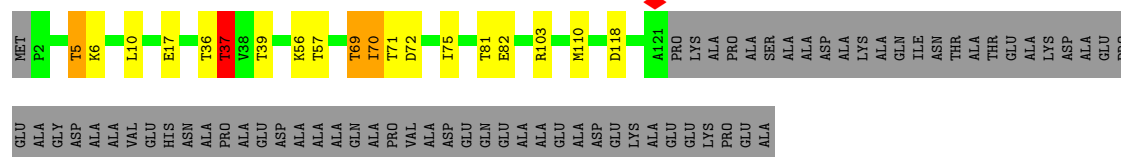
- Molecule 39: 50S ribosomal protein L15



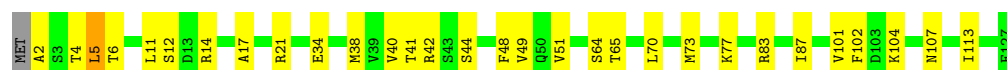
- Molecule 40: 50S ribosomal protein L16



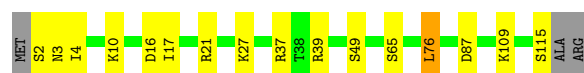
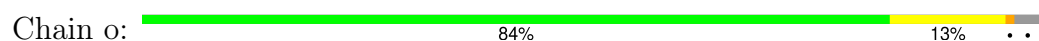
- Molecule 41: Large ribosomal subunit protein bL17



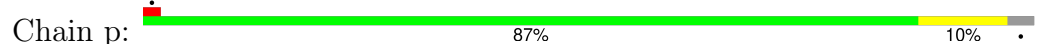
- Molecule 42: 50S ribosomal protein L18



- Molecule 43: 50S ribosomal protein L19



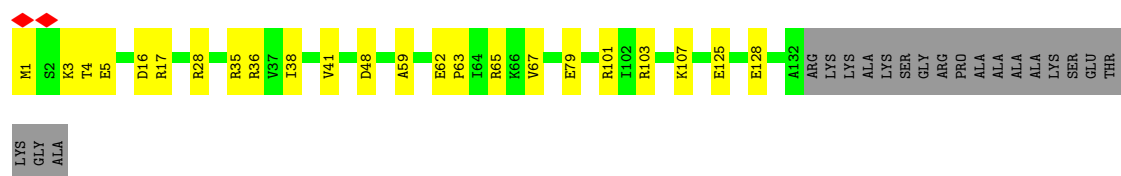
- Molecule 44: 50S ribosomal protein L20



- Molecule 45: Large ribosomal subunit protein bL21



- Molecule 46: 50S ribosomal protein L22



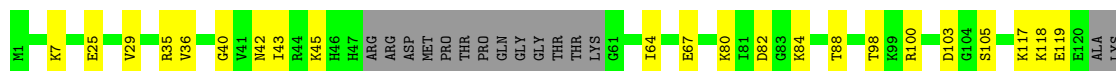
- Molecule 47: 50S ribosomal protein L23

Chain s:  77% 14% 7%



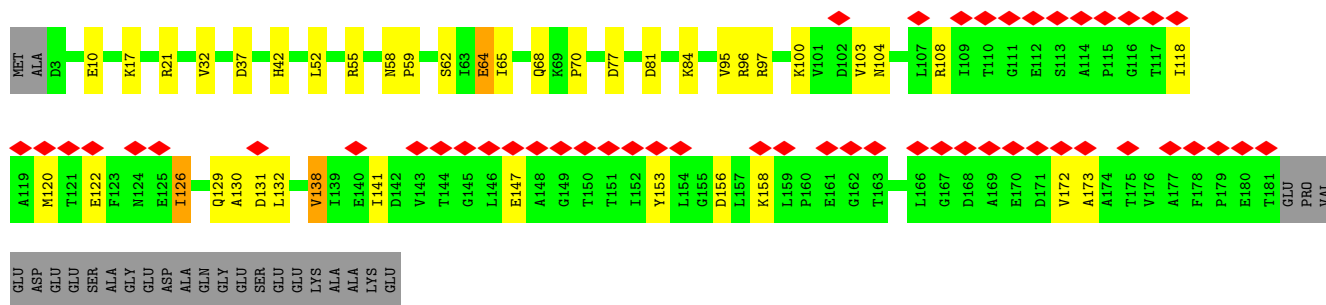
- Molecule 48: Large ribosomal subunit protein uL24

Chain t:  70% 18% 12%



- Molecule 49: 50S ribosomal protein L25

Chain u:  25% 67% 19% 13%



- Molecule 50: 50S ribosomal protein L27

Chain v:  82% 6% 12%



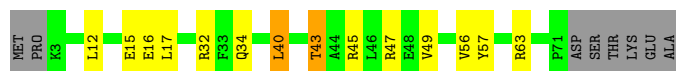
- Molecule 51: 50S ribosomal protein L28

Chain w:  80% 16% 2%

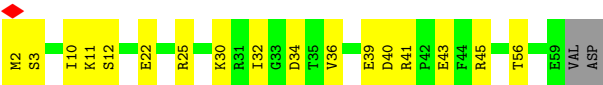


- Molecule 52: 50S ribosomal protein L29

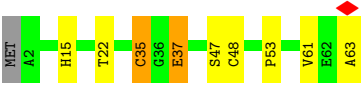
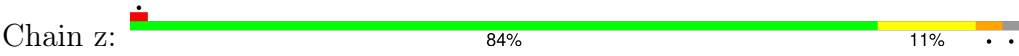
Chain x:  71% 16% 10%



- Molecule 53: 50S ribosomal protein L30



• Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.757	Depositor
Minimum map value	-0.231	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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, 5MU, UR3, G7M, ZN, PSU, OMU, H2U, DXT, 2MA, MA6, 5MC, 4SU, OMG, OMC, 4OC, 2MG, 3TD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.27	0/429	0.40	0/569
2	1	0.28	0/365	0.36	0/478
3	2	0.29	0/519	0.38	0/682
4	3	0.29	0/305	0.39	0/401
5	4	0.69	0/521	0.93	0/700
6	A	0.37	0/36052	0.47	0/56250
7	B	0.17	0/1864	0.48	0/2509
8	C	0.34	0/1703	0.42	0/2655
9	D	0.26	0/1662	0.47	0/2239
10	E	0.22	0/1325	0.46	0/1789
11	F	0.24	0/794	0.50	0/1069
12	G	0.19	0/1638	0.45	0/2201
13	H	0.21	0/1036	0.38	0/1395
14	I	0.23	0/1246	0.45	0/1679
15	J	0.36	0/1027	0.58	0/1376
16	K	0.34	0/874	0.56	0/1177
17	L	0.23	0/960	0.39	0/1283
18	M	0.19	0/800	0.43	0/1080
19	N	0.21	0/985	0.43	0/1317
20	O	0.23	0/718	0.43	0/959
21	P	0.36	0/1013	0.53	0/1370
22	Q	0.27	0/734	0.47	0/978
23	R	0.20	0/532	0.42	0/713
24	S	0.34	0/484	0.46	0/644
25	T	0.23	0/676	0.30	0/897
26	U	0.19	0/675	0.50	0/908
27	V	0.30	0/184	0.46	0/236
28	X	0.22	0/277	0.39	0/355
29	Y	0.22	0/235	0.29	0/363
30	a	0.39	1/69445 (0.0%)	0.48	2/108364 (0.0%)
31	b	0.32	0/2871	0.37	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.30	0/2132	0.44	0/2871
33	d	0.29	0/1611	0.42	0/2172
34	e	0.36	0/1600	0.60	0/2165
35	f	0.25	0/1493	0.41	0/2001
36	g	0.21	0/1398	0.41	0/1884
37	i	0.28	0/1164	0.40	0/1574
38	j	0.29	0/957	0.46	0/1282
39	k	0.28	0/1090	0.57	0/1465
40	l	0.29	0/1108	0.42	0/1488
41	m	0.29	0/949	0.43	0/1277
42	n	0.39	0/959	0.57	0/1281
43	o	0.26	0/909	0.37	0/1216
44	p	0.42	0/969	0.63	0/1292
45	q	0.37	0/785	0.50	0/1050
46	r	0.35	0/1028	0.49	0/1379
47	s	0.29	0/759	0.47	0/1022
48	t	0.21	0/840	0.37	0/1123
49	u	0.19	0/1396	0.41	0/1896
50	v	0.28	0/598	0.39	0/800
51	w	0.89	0/483	1.22	0/648
52	x	0.22	0/567	0.38	0/759
53	y	0.37	0/471	0.52	0/627
54	z	0.31	0/487	0.40	0/654
All	All	0.36	1/155702 (0.0%)	0.47	2/233037 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	D	0	1
14	I	0	1
22	Q	0	1
44	p	0	2
51	w	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2734	OMU	O3'-P	5.28	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	272	A	C1'-O4'-C4'	-5.36	104.54	109.90
30	a	271	G	C4'-C3'-C2'	-5.09	97.50	102.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	D	154	ARG	Sidechain
14	I	3	ARG	Sidechain
22	Q	8	ARG	Sidechain
44	p	14	ARG	Sidechain
44	p	92	ARG	Sidechain
51	w	11	ARG	Sidechain
51	w	28	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	0	423	0	429	8	0
2	1	362	0	388	7	0
3	2	513	0	565	7	0
4	3	302	0	330	7	0
5	4	512	0	498	17	0
6	A	32480	0	16339	377	0
7	B	1836	0	1902	69	0
8	C	1605	0	818	10	0
9	D	1632	0	1663	60	0
10	E	1309	0	1349	36	0
11	F	785	0	818	36	0
12	G	1613	0	1626	43	0
13	H	1021	0	1059	11	0
14	I	1225	0	1275	32	0
15	J	1012	0	1069	45	0
16	K	858	0	884	17	0
17	L	948	0	1031	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	786	0	823	36	0
19	N	976	0	1031	23	0
20	O	708	0	737	10	0
21	P	994	0	1008	36	0
22	Q	728	0	772	15	0
23	R	527	0	580	17	0
24	S	474	0	499	21	0
25	T	673	0	726	13	0
26	U	658	0	671	23	0
27	V	183	0	202	2	0
28	X	277	0	338	5	0
29	Y	211	0	106	7	0
30	a	62408	0	31296	593	0
31	b	2567	0	1297	21	0
32	c	2091	0	2150	22	0
33	d	1586	0	1634	16	0
34	e	1577	0	1619	68	0
35	f	1468	0	1487	36	0
36	g	1376	0	1421	41	0
37	i	1139	0	1163	14	0
38	j	946	0	1011	26	0
39	k	1072	0	1106	25	0
40	l	1082	0	1117	18	0
41	m	936	0	997	13	0
42	n	952	0	995	17	0
43	o	896	0	928	8	0
44	p	958	0	986	7	0
45	q	778	0	824	15	0
46	r	1017	0	1070	13	0
47	s	751	0	803	10	0
48	t	833	0	883	13	0
49	u	1376	0	1397	29	0
50	v	591	0	581	3	0
51	w	474	0	488	4	0
52	x	564	0	582	9	0
53	y	467	0	504	11	0
54	z	477	0	479	7	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	z	1	0	0	0	0
56	A	51	0	0	0	0
56	a	230	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
56	o	1	0	0	0	0
57	A	32	0	22	1	0
57	a	128	0	88	4	0
57	r	32	0	22	1	0
57	s	32	0	22	0	0
58	A	12	0	0	0	0
58	C	1	0	0	0	0
58	S	1	0	0	0	0
58	a	115	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	s	1	0	0	0	0
All	All	144663	0	96508	1858	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 8.

All (1858) 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)
30:a:1281:C:H5	30:a:1318:G:H1	1.07	0.98
30:a:2282:G:H1	30:a:2371:U:H3	1.09	0.97
34:e:133:VAL:HG21	34:e:138:PRO:HD2	1.47	0.96
34:e:160:LEU:HB3	34:e:164:ASP:HB2	1.47	0.96
30:a:2706:G:H1	30:a:2721:C:H5	1.07	0.95
7:B:66:GLN:HB2	7:B:160:GLN:HG2	1.47	0.95
34:e:125:ARG:HH22	34:e:150:LEU:HD13	1.32	0.93
35:f:21:ILE:HD12	35:f:181:HIS:HB3	1.48	0.93
10:E:205:ALA:HA	10:E:208:MET:HE1	1.52	0.92
9:D:147:LEU:HG	9:D:149:PRO:HD2	1.53	0.90
34:e:120:MET:HE2	34:e:196:ILE:HD12	1.53	0.90
10:E:116:VAL:HB	10:E:151:LEU:O	1.74	0.86
15:J:130:ASN:HD22	15:J:138:ARG:HD3	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:15:HIS:HA	7:B:41:ILE:HG22	1.59	0.83
31:b:87:G:H21	31:b:90:A:H2	1.27	0.83
36:g:57:ASP:OD1	36:g:58:ASP:N	2.10	0.83
36:g:120:PRO:HG2	36:g:123:ILE:HD13	1.60	0.83
30:a:360:A:H2	30:a:444:G:H22	1.27	0.82
6:A:1428:G:H8	6:A:1447:A:H62	1.27	0.82
30:a:288:G:N3	30:a:310:C:N4	2.28	0.81
30:a:337:G:H22	30:a:355:U:H2'	1.46	0.81
12:G:51:LEU:HD23	12:G:54:ILE:HD11	1.60	0.81
30:a:1130:G:N2	30:a:1194:A:H62	1.79	0.80
30:a:1130:G:H21	30:a:1194:A:N6	1.79	0.80
15:J:109:ILE:HG21	15:J:117:GLN:HG3	1.62	0.80
32:c:16:SER:HB3	32:c:207:GLY:HA3	1.62	0.80
6:A:1342:G:H2'	6:A:1343:A:C8	2.17	0.80
30:a:1143:U:H4'	30:a:1144:U:H5'	1.66	0.78
30:a:439:C:H2'	30:a:440:A:H8	1.48	0.78
6:A:977:G:H2'	6:A:979:C:H41	1.47	0.78
30:a:1492:C:H2'	30:a:1493:G:C8	2.19	0.78
9:D:172:LYS:HE3	21:P:115:ALA:HB1	1.66	0.77
30:a:669:A:H62	30:a:1328:A:H2	1.27	0.77
15:J:72:ILE:HG22	15:J:107:ALA:HB3	1.64	0.77
6:A:1409:G:H5'	38:j:48:PRO:HB3	1.67	0.76
47:s:62:MET:HE2	47:s:85:ILE:HD11	1.68	0.76
30:a:1698:G:H22	30:a:1915:G:N2	1.83	0.75
30:a:2712:G:H8	30:a:2713:A:H5''	1.50	0.75
32:c:21:PHE:HB3	32:c:24:LEU:HD22	1.69	0.75
37:i:92:MET:HE2	37:i:99:ARG:HG2	1.69	0.75
12:G:90:LEU:HB3	12:G:98:ILE:HD13	1.70	0.74
30:a:198:A:H2'	30:a:199:G:C8	2.22	0.74
40:l:60:ARG:HD3	40:l:60:ARG:H	1.52	0.74
6:A:1342:G:H2'	6:A:1343:A:H8	1.52	0.74
6:A:94:G:H1	6:A:97:C:H41	1.33	0.74
6:A:655:G:H2'	6:A:656:G:C8	2.23	0.74
14:I:40:GLN:HA	14:I:43:VAL:HG22	1.70	0.74
35:f:173:GLU:OE2	35:f:173:GLU:N	2.21	0.73
45:q:10:ARG:NH1	45:q:23:ASP:OD1	2.21	0.73
30:a:1623:C:H5	30:a:1731:G:H1	1.32	0.73
30:a:2040:G:N2	30:a:2067:A:O2'	2.21	0.73
9:D:145:LYS:HB2	21:P:122:LYS:HZ1	1.53	0.73
9:D:169:ARG:HB3	9:D:172:LYS:HZ1	1.52	0.73
12:G:14:VAL:HG11	12:G:177:LEU:HG	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:92:VAL:HG11	7:B:96:TRP:HD1	1.54	0.73
26:U:28:HIS:O	26:U:29:ASN:ND2	2.20	0.73
30:a:179:G:N2	30:a:180:U:O4	2.22	0.73
6:A:1298:G:H5'	26:U:5:LEU:HD11	1.71	0.73
30:a:142:G:H22	30:a:147:G:H22	1.37	0.73
6:A:646:G:H22	6:A:723:G:H1	1.36	0.72
10:E:96:LYS:HA	10:E:96:LYS:HE2	1.72	0.72
21:P:93:LYS:H	21:P:93:LYS:HD3	1.55	0.72
7:B:118:GLU:HA	7:B:142:LYS:HE2	1.70	0.72
18:M:9:ARG:HB2	18:M:99:GLU:HB3	1.70	0.72
30:a:1727:G:H2'	30:a:1728:A:C8	2.24	0.72
6:A:619:U:OP1	22:Q:11:ARG:NH2	2.21	0.72
16:K:94:GLY:H	16:K:120:THR:HG22	1.54	0.72
23:R:31:LYS:O	23:R:31:LYS:NZ	2.18	0.72
6:A:916:C:H5''	14:I:4:LYS:HE3	1.72	0.72
36:g:80:VAL:HA	36:g:138:ILE:HD11	1.71	0.72
30:a:332:U:H3	30:a:449:G:H1	1.35	0.72
45:q:24:LYS:HA	45:q:93:THR:HG23	1.71	0.71
24:S:40:CYS:H	24:S:43:CYS:HB2	1.55	0.71
18:M:45:GLU:HB2	18:M:69:THR:HB	1.72	0.71
34:e:13:LYS:HB2	34:e:130:THR:HG23	1.72	0.71
36:g:117:VAL:HG11	36:g:150:ILE:HD11	1.72	0.71
30:a:1708:G:H22	30:a:1729:G:H1	1.37	0.71
36:g:139:ASP:HB3	36:g:142:VAL:HG22	1.73	0.71
9:D:119:LEU:HD23	9:D:124:LYS:H	1.55	0.71
30:a:1985:A:H2'	30:a:1986:A:C8	2.26	0.71
22:Q:65:ARG:HG2	22:Q:86:ILE:HB	1.72	0.70
30:a:2755:C:OP1	30:a:2756:G:OP1	2.09	0.70
34:e:142:GLN:NE2	34:e:142:GLN:H	1.89	0.70
15:J:113:GLY:O	15:J:117:GLN:HB2	1.90	0.70
9:D:14:ARG:HA	9:D:32:PRO:HB3	1.74	0.70
18:M:42:LEU:HD12	18:M:71:LYS:HD3	1.73	0.70
12:G:23:TYR:OH	18:M:11:ARG:NH1	2.24	0.70
30:a:2536:A:H4'	50:v:35:GLU:HG2	1.72	0.70
30:a:347:C:H3'	30:a:348:G:H8	1.57	0.69
15:J:63:ILE:HG22	15:J:105:VAL:HG12	1.74	0.69
30:a:1632:U:O2'	30:a:1633:G:N2	2.24	0.69
6:A:659:U:H3	6:A:695:G:H22	1.40	0.69
30:a:1349:U:H2'	57:a:3123:DXT:O10	1.92	0.69
6:A:930:A:H2'	6:A:931:G:C8	2.27	0.69
9:D:169:ARG:HB2	9:D:174:ARG:HB3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:379:A:O2'	30:a:380:G:O4'	2.10	0.69
36:g:19:LEU:HD11	36:g:45:LYS:HD3	1.75	0.69
6:A:1127:U:H2'	6:A:1128:G:C8	2.28	0.69
3:2:8:SER:HA	3:2:11:LYS:HE2	1.74	0.69
34:e:155:LYS:HD2	34:e:180:LEU:HD12	1.75	0.69
49:u:65:ILE:HB	49:u:68:GLN:HB2	1.75	0.69
30:a:361:G:H22	30:a:443:G:H22	1.41	0.69
30:a:2052:G:H21	30:a:2055:U:H5	1.40	0.69
30:a:392:G:H21	30:a:415:A:H62	1.41	0.68
30:a:2706:G:N1	30:a:2721:C:H5	1.87	0.68
30:a:2906:U:OP1	33:d:129:LYS:NZ	2.26	0.68
30:a:1690:A:H1'	30:a:1691:A:H5'	1.75	0.68
30:a:1650:A:H2'	30:a:1651:A:C8	2.27	0.68
34:e:207:VAL:O	34:e:211:SER:HB3	1.93	0.68
30:a:130:G:N2	30:a:154:G:H22	1.91	0.68
18:M:24:LYS:HE2	18:M:90:LEU:HD21	1.75	0.67
30:a:130:G:H22	30:a:154:G:H22	1.42	0.67
30:a:94:G:H21	52:x:43:THR:HG21	1.59	0.67
30:a:1139:G:H22	30:a:1185:C:H3'	1.60	0.67
46:r:17:ARG:NH1	46:r:125:GLU:OE1	2.28	0.67
41:m:103:ARG:HG3	41:m:110:MET:HE3	1.75	0.67
6:A:1128:G:H3'	6:A:1129:G:H8	1.60	0.67
9:D:141:ARG:HH21	9:D:144:SER:HB3	1.59	0.67
30:a:941:G:H2'	30:a:942:A:C8	2.30	0.67
30:a:1253:U:N3	30:a:1254:G:O6	2.22	0.67
33:d:163:LYS:HB3	37:i:80:ARG:HB3	1.77	0.67
38:j:17:LYS:HD2	38:j:47:ILE:HD13	1.75	0.67
30:a:361:G:H1	30:a:443:G:H22	1.43	0.67
6:A:983:G:H1	6:A:1027:U:H3	1.43	0.67
30:a:153:U:H2'	30:a:154:G:C8	2.30	0.67
4:3:15:LYS:NZ	30:a:2935:A:O2'	2.28	0.67
7:B:12:SER:HB2	7:B:209:ARG:HE	1.60	0.67
7:B:79:SER:O	7:B:83:GLN:HG2	1.95	0.67
1:0:41:LYS:NZ	30:a:2529:C:OP1	2.26	0.66
30:a:106:G:H4'	30:a:379:A:H5''	1.76	0.66
9:D:148:PRO:O	9:D:152:ILE:HG12	1.95	0.66
30:a:83:A:H62	30:a:101:G:H8	1.44	0.66
30:a:263:A:H2'	30:a:264:A:C8	2.31	0.66
30:a:2510:A:H2'	30:a:2511:G:C8	2.31	0.66
30:a:1722:U:H2'	30:a:1723:G:H8	1.61	0.66
35:f:43:ILE:HD12	35:f:105:MET:HG3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:58:ILE:HD13	40:l:106:LEU:HD11	1.78	0.66
14:I:118:GLU:OE2	14:I:118:GLU:N	2.23	0.66
6:A:656:G:H2'	6:A:657:A:H8	1.61	0.66
17:L:67:ILE:HG12	17:L:97:ILE:HD12	1.78	0.66
6:A:1422:G:H2'	6:A:1423:C:C6	2.32	0.65
7:B:60:THR:HA	7:B:63:LYS:HE2	1.77	0.65
30:a:130:G:H22	30:a:154:G:H1	1.43	0.65
19:N:79:ARG:O	19:N:83:GLU:HG2	1.96	0.65
30:a:2843:G:O6	36:g:177:LYS:NZ	2.28	0.65
38:j:108:GLU:O	38:j:109:LYS:HG3	1.95	0.65
16:K:74:GLU:HG3	16:K:78:ARG:HH21	1.61	0.65
30:a:1698:G:H22	30:a:1915:G:H22	1.44	0.65
37:i:11:VAL:HG11	37:i:50:THR:HG23	1.77	0.65
7:B:47:LEU:HD23	7:B:50:ILE:HD11	1.78	0.65
15:J:71:LYS:HE3	15:J:74:GLY:HA2	1.78	0.65
34:e:123:ASP:OD2	39:k:2:ALA:N	2.28	0.65
36:g:59:GLU:OE1	36:g:62:ASN:ND2	2.30	0.65
14:I:15:ASP:OD1	14:I:19:GLY:N	2.30	0.65
49:u:122:GLU:HB2	49:u:173:ALA:HA	1.79	0.65
2:l:25:ARG:NH2	30:a:218:G:OP1	2.28	0.65
6:A:429:U:OP2	9:D:28:ARG:NH2	2.27	0.65
30:a:1638:U:O2'	30:a:1640:G:N2	2.30	0.65
2:l:2:LYS:HE2	30:a:772:C:H5''	1.79	0.64
49:u:141:ILE:HA	49:u:158:LYS:HZ3	1.61	0.64
6:A:987:G:H2'	6:A:988:G:C8	2.32	0.64
6:A:1346:A:OP2	24:S:35:ARG:NH2	2.31	0.64
30:a:361:G:H22	30:a:443:G:N2	1.96	0.64
30:a:1169:A:H1'	30:a:1186:A:H61	1.61	0.64
34:e:157:LEU:HD21	34:e:185:LEU:HG	1.78	0.64
5:4:16:CYS:SG	5:4:17:THR:N	2.71	0.64
5:4:15:VAL:HG12	5:4:21:THR:HG22	1.80	0.64
21:P:45:ASP:HB2	21:P:46:PRO:HD3	1.79	0.64
19:N:69:ASP:OD1	19:N:69:ASP:N	2.24	0.64
30:a:6:G:H1	30:a:3076:U:H3	1.45	0.64
30:a:50:G:O2'	30:a:118:A:N6	2.31	0.64
30:a:1327:G:N7	39:k:20:ARG:NH2	2.45	0.64
34:e:132:LEU:O	34:e:133:VAL:HG12	1.98	0.64
41:m:37:THR:HG22	41:m:110:MET:HE1	1.80	0.64
30:a:1488:U:H3	30:a:1774:C:H42	1.46	0.63
38:j:93:PRO:HG3	38:j:114:ILE:HG13	1.80	0.63
6:A:277:G:H5'	22:Q:23:LYS:HG3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:85:GLU:HG2	36:g:87:LYS:HE2	1.79	0.63
37:i:30:THR:HA	37:i:108:MET:HE1	1.79	0.63
6:A:1237:G:H4'	15:J:56:GLU:OE2	1.98	0.63
10:E:180:ARG:NH2	13:H:43:GLU:OE1	2.30	0.63
6:A:348:G:OP1	43:o:39:ARG:NH2	2.30	0.63
30:a:2533:G:O2'	30:a:2548:A:N6	2.32	0.63
31:b:9:G:N7	42:n:2:ALA:N	2.46	0.63
36:g:9:ILE:HG12	36:g:70:ARG:HH11	1.64	0.63
36:g:96:ARG:HG2	36:g:108:ASN:HD21	1.63	0.63
30:a:1402:U:HO2'	30:a:2193:G:HO2'	1.44	0.63
30:a:2282:G:N2	30:a:2371:U:O2	2.24	0.63
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.81	0.63
12:G:62:ARG:NE	12:G:97:GLN:OE1	2.31	0.63
30:a:1664:U:H3	30:a:1685:G:H1	1.47	0.63
30:a:2971:C:H1'	30:a:3071:A:H2	1.63	0.63
6:A:989:G:H3'	6:A:990:A:H8	1.64	0.62
48:t:88:THR:HG22	48:t:118:LYS:HD2	1.79	0.62
6:A:183:G:H2'	6:A:184:G:H2'	1.81	0.62
6:A:347:C:OP2	43:o:37:ARG:NH2	2.32	0.62
6:A:491:A:OP2	6:A:492:A:OP2	2.18	0.62
30:a:151:G:H4'	47:s:3:GLU:HG2	1.81	0.62
30:a:949:G:H21	30:a:951:A:H62	1.48	0.62
54:z:61:VAL:HG12	54:z:63:ALA:H	1.63	0.62
6:A:415:G:O2'	6:A:430:G:N2	2.33	0.62
7:B:188:LEU:HD21	7:B:200:ALA:HB1	1.80	0.62
45:q:33:ILE:HD11	45:q:95:VAL:HG21	1.81	0.62
30:a:73:A:OP1	52:x:47:ARG:NH2	2.31	0.62
30:a:2072:A:H2'	30:a:2073:A:C8	2.35	0.62
36:g:18:LYS:HB2	36:g:25:GLU:HG2	1.80	0.62
1:0:43:CYS:HB3	1:0:46:CYS:HB2	1.81	0.62
6:A:1033:G:H5''	24:S:3:LYS:HG2	1.81	0.62
7:B:19:GLN:OE1	7:B:22:ARG:NH1	2.31	0.62
22:Q:21:SER:HA	22:Q:62:MET:HE1	1.82	0.62
6:A:406:G:O6	9:D:2:ALA:N	2.32	0.62
11:F:12:PRO:HD2	11:F:55:LYS:HD2	1.80	0.62
14:I:113:GLU:OE1	14:I:114:LYS:N	2.32	0.62
30:a:2290:U:O2'	30:a:2363:G:N2	2.32	0.62
40:l:60:ARG:HH11	40:l:61:GLY:H	1.47	0.62
6:A:1237:G:H21	6:A:1356:C:H1'	1.63	0.62
23:R:21:VAL:HG11	23:R:54:LYS:HB3	1.81	0.62
43:o:2:SER:OG	43:o:3:ASN:N	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:14:CYS:SG	4:3:27:CYS:HB2	2.39	0.62
6:A:1015:U:H2'	6:A:1020:G:H8	1.64	0.62
30:a:2289:U:H3	30:a:2364:A:H2	1.48	0.62
5:4:65:TYR:CD2	26:U:9:PRO:HG3	2.34	0.61
30:a:439:C:H2'	30:a:440:A:C8	2.32	0.61
30:a:1698:G:H1	30:a:1915:G:H1	1.47	0.61
32:c:182:MET:HB2	32:c:269:VAL:HG22	1.82	0.61
10:E:174:GLU:OE2	10:E:196:ARG:NH1	2.34	0.61
30:a:82:G:N2	30:a:102:A:OP2	2.33	0.61
36:g:74:ASN:O	36:g:78:ILE:HG22	2.00	0.61
9:D:24:LYS:HG3	9:D:26:PHE:HB2	1.80	0.61
30:a:970:U:H3	30:a:975:G:H22	1.46	0.61
6:A:1386:C:H4'	6:A:1387:5MC:H3'	1.83	0.61
30:a:2761:C:H5'	33:d:145:LYS:HG3	1.83	0.61
23:R:18:ILE:HB	23:R:28:LEU:HD21	1.81	0.61
30:a:1862:A:H2'	30:a:1863:A:C8	2.36	0.61
49:u:10:GLU:N	49:u:10:GLU:OE2	2.33	0.61
19:N:69:ASP:O	19:N:73:GLU:HG3	2.00	0.61
6:A:183:G:H21	6:A:226:G:H4'	1.65	0.61
20:O:74:GLU:N	20:O:74:GLU:OE2	2.33	0.61
6:A:1127:U:H2'	6:A:1128:G:H8	1.63	0.61
6:A:1135:C:H2'	6:A:1136:A:C8	2.36	0.61
6:A:1500:A:H2'	6:A:1501:C:C6	2.36	0.61
12:G:89:GLU:O	12:G:93:LEU:HD23	2.01	0.61
18:M:6:ILE:HB	18:M:76:ILE:HB	1.82	0.60
30:a:653:G:H2'	30:a:2213:A:N7	2.16	0.60
34:e:159:VAL:HG21	34:e:205:ALA:HB3	1.83	0.60
11:F:74:GLU:O	11:F:77:ARG:HG3	2.00	0.60
26:U:36:ARG:NH2	26:U:75:ALA:O	2.34	0.60
7:B:92:VAL:HG11	7:B:96:TRP:CD1	2.35	0.60
25:T:43:ASP:OD1	25:T:44:VAL:N	2.35	0.60
9:D:142:GLU:HA	9:D:145:LYS:HD2	1.83	0.60
24:S:42:ILE:O	24:S:46:GLU:HG2	2.02	0.60
30:a:361:G:H1	30:a:443:G:H1	1.49	0.60
30:a:2971:C:H2'	30:a:2972:A:C8	2.36	0.60
34:e:142:GLN:H	34:e:142:GLN:CD	2.07	0.60
6:A:805:G:HO2'	13:H:2:THR:N	1.99	0.60
30:a:291:U:H5''	30:a:308:U:H5	1.66	0.60
30:a:2982:U:H3'	30:a:2983:C:H6	1.66	0.60
6:A:696:G:H2'	6:A:697:A:C8	2.36	0.60
6:A:1507:G:N7	28:X:15:LYS:NZ	2.48	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:44:THR:HG22	18:M:70:HIS:HA	1.84	0.60
37:i:42:PRO:O	44:p:64:ARG:HG2	2.02	0.60
30:a:1281:C:H5	30:a:1318:G:N1	1.90	0.60
30:a:2973:C:OP2	30:a:3073:G:N2	2.34	0.60
57:A:1615:DXT:N21	57:A:1615:DXT:O3	2.29	0.60
13:H:55:LYS:HD2	13:H:56:GLU:HG2	1.83	0.60
30:a:430:U:H5''	30:a:431:A:H5'	1.84	0.60
30:a:1138:G:H21	30:a:1168:A:H1'	1.67	0.60
30:a:2473:U:H2'	30:a:2474:U:C6	2.37	0.60
21:P:19:ARG:HD3	21:P:36:GLU:OE2	2.02	0.60
24:S:23:ARG:NH1	24:S:28:GLY:O	2.35	0.60
6:A:317:A:N7	6:A:330:U:H5	2.00	0.60
15:J:47:PRO:HG3	15:J:65:PRO:HD3	1.83	0.60
30:a:225:G:H22	30:a:242:U:H4'	1.67	0.60
30:a:1260:U:H5''	53:y:30:LYS:HE3	1.84	0.60
6:A:1523:C:H4'	6:A:1524:U:OP1	2.00	0.59
12:G:111:ASP:OD1	12:G:114:LEU:HB2	2.02	0.59
30:a:631:G:H4'	30:a:632:U:H3'	1.83	0.59
6:A:438:C:H4'	9:D:148:PRO:HG2	1.84	0.59
6:A:656:G:H2'	6:A:657:A:C8	2.37	0.59
29:Y:21:U:H2'	29:Y:22:U:H4'	1.84	0.59
30:a:641:G:OP1	37:i:112:ASN:HB3	2.02	0.59
30:a:2066:G:H2'	30:a:2067:A:C8	2.38	0.59
15:J:111:GLY:O	15:J:117:GLN:NE2	2.35	0.59
30:a:701:U:H1'	34:e:43:GLN:HG3	1.82	0.59
30:a:1486:U:H2'	30:a:1487:G:C8	2.37	0.59
39:k:79:LEU:HD22	39:k:117:LEU:HD22	1.84	0.59
7:B:170:GLU:N	7:B:170:GLU:OE2	2.35	0.59
11:F:52:ILE:HG22	11:F:53:GLN:HG3	1.85	0.59
21:P:74:LEU:HD22	21:P:79:ASP:HB2	1.85	0.59
6:A:822:C:H2'	6:A:823:A:C8	2.37	0.59
6:A:1105:C:H2'	6:A:1106:A:C8	2.36	0.59
6:A:1516:G:N7	28:X:7:LYS:NZ	2.49	0.59
30:a:374:C:H2'	30:a:375:G:C8	2.37	0.59
30:a:971:U:H2'	30:a:972:A:C8	2.38	0.59
30:a:2291:U:H1'	30:a:2361:C:H42	1.68	0.59
6:A:700:A:H5'	16:K:125:ASN:HD22	1.68	0.59
6:A:1119:C:H3'	6:A:1120:G:H8	1.68	0.59
17:L:110:ARG:HD2	17:L:112:GLN:O	2.03	0.59
30:a:480:A:H1'	30:a:500:G:O4'	2.03	0.59
38:j:107:ARG:O	38:j:107:ARG:HG2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:48:PHE:HD1	42:n:64:SER:HB3	1.68	0.59
6:A:1077:A:H2'	6:A:1078:A:C8	2.38	0.59
15:J:60:ARG:O	15:J:107:ALA:HA	2.02	0.59
34:e:120:MET:HE3	34:e:125:ARG:HB2	1.84	0.59
47:s:88:VAL:HG13	47:s:92:ASP:HB2	1.84	0.59
30:a:1074:U:OP2	30:a:1263:G:OP2	2.21	0.59
30:a:2720:C:H2'	30:a:2721:C:O2	2.03	0.59
6:A:1204:C:H2'	6:A:1205:A:C8	2.37	0.58
30:a:3:A:H61	30:a:3079:C:H42	1.49	0.58
30:a:1722:U:H2'	30:a:1723:G:C8	2.37	0.58
12:G:67:LEU:HD11	12:G:102:ILE:HG13	1.85	0.58
30:a:341:U:H2'	30:a:342:G:C8	2.38	0.58
12:G:21:ARG:HB3	12:G:57:GLU:HG2	1.84	0.58
12:G:25:GLU:OE1	12:G:25:GLU:N	2.35	0.58
46:r:63:PRO:O	46:r:67:VAL:HG23	2.02	0.58
6:A:483:C:H2'	6:A:484:A:C8	2.38	0.58
6:A:720:U:H5''	11:F:69:PRO:HB3	1.84	0.58
6:A:1309:G:H2'	6:A:1310:A:C8	2.38	0.58
35:f:26:GLN:O	35:f:26:GLN:NE2	2.31	0.58
49:u:95:VAL:HB	49:u:132:LEU:HD21	1.85	0.58
6:A:1105:C:H2'	6:A:1106:A:H8	1.69	0.58
14:I:7:ALA:O	14:I:9:LYS:HE3	2.02	0.58
39:k:96:ASP:O	39:k:100:VAL:HG23	2.03	0.58
1:0:12:ILE:HB	1:0:54:GLU:HG3	1.85	0.58
9:D:172:LYS:HZ2	21:P:119:ALA:HB2	1.67	0.58
20:O:87:ARG:NH2	30:a:798:G:OP2	2.36	0.58
30:a:1912:U:H3'	30:a:1913:G:H3'	1.85	0.58
6:A:500:C:O2'	6:A:512:G:N2	2.36	0.58
34:e:184:GLN:HE21	34:e:184:GLN:HA	1.67	0.58
40:l:54:MET:HG3	40:l:121:ALA:HB2	1.85	0.58
18:M:84:VAL:O	18:M:88:MET:HG2	2.04	0.58
5:4:14:VAL:HB	5:4:33:LEU:HB2	1.86	0.58
7:B:72:THR:HB	7:B:169:LYS:HD3	1.85	0.58
30:a:82:G:H22	30:a:101:G:H2'	1.69	0.58
30:a:1185:C:H2'	30:a:1186:A:H8	1.67	0.58
30:a:1493:G:H5'	30:a:1595:A:H5''	1.85	0.58
39:k:94:VAL:HG22	39:k:97:LEU:HG	1.86	0.58
4:3:14:CYS:SG	4:3:32:HIS:HB3	2.44	0.58
6:A:934:U:OP2	19:N:102:ARG:HD2	2.04	0.58
15:J:78:GLU:OE1	15:J:78:GLU:N	2.34	0.58
30:a:631:G:O2'	30:a:633:G:OP1	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:138:PRO:HG2	34:e:142:GLN:HE22	1.68	0.58
36:g:129:ASN:HB2	36:g:132:LYS:HB2	1.86	0.58
6:A:1154:C:H3'	6:A:1155:A:H8	1.68	0.57
6:A:1307:U:O2'	26:U:78:ARG:NH2	2.37	0.57
30:a:2712:G:OP1	30:a:2717:G:N2	2.36	0.57
38:j:18:GLU:HG2	38:j:44:LYS:HB2	1.86	0.57
11:F:30:ILE:HD11	11:F:75:LEU:HD22	1.85	0.57
35:f:44:VAL:HB	35:f:164:THR:HG22	1.86	0.57
49:u:58:ASN:HD21	49:u:103:VAL:HB	1.70	0.57
52:x:17:LEU:HD22	52:x:56:VAL:HG13	1.86	0.57
7:B:6:THR:HG22	7:B:9:LEU:HD12	1.86	0.57
20:O:5:GLU:O	20:O:9:ILE:HG13	2.03	0.57
30:a:2711:G:H2'	30:a:2712:G:C8	2.40	0.57
6:A:271:U:H2'	6:A:272:A:C8	2.39	0.57
6:A:483:C:H2'	6:A:484:A:H8	1.69	0.57
6:A:1485:UR3:H4'	6:A:1506:MA6:H2	1.87	0.57
30:a:2115:A:H2'	30:a:2116:G:O4'	2.05	0.57
38:j:10:VAL:HG12	38:j:12:ASP:H	1.70	0.57
6:A:912:G:O2'	6:A:1520:C:OP1	2.23	0.57
30:a:142:G:H21	30:a:147:G:H1	1.50	0.57
6:A:405:C:H5''	9:D:128:PRO:HD2	1.86	0.57
6:A:1272:G:H2'	6:A:1273:A:H4'	1.87	0.57
30:a:725:U:H2'	30:a:726:C:C6	2.40	0.57
49:u:122:GLU:HG3	49:u:172:VAL:HG12	1.86	0.57
6:A:1048:C:H2'	6:A:1049:G:C8	2.40	0.57
6:A:1241:G:O2'	6:A:1244:G:N3	2.34	0.57
9:D:8:LEU:HD22	9:D:19:LEU:HD12	1.87	0.57
30:a:994:A:H2'	30:a:995:A:C8	2.40	0.57
32:c:96:HIS:CE1	32:c:102:LYS:HE2	2.39	0.57
6:A:25:G:H2'	6:A:26:G:C8	2.40	0.56
6:A:1439:U:H4'	6:A:1440:G:H5''	1.87	0.56
10:E:159:VAL:O	10:E:163:THR:HG22	2.05	0.56
19:N:106:ASN:O	19:N:108:ARG:HD2	2.05	0.56
6:A:668:G:N2	6:A:668:G:OP2	2.37	0.56
17:L:50:ARG:NH1	17:L:89:ASP:OD2	2.38	0.56
19:N:86:THR:HG22	19:N:88:GLN:H	1.69	0.56
30:a:132:A:H2'	30:a:133:A:C8	2.40	0.56
7:B:10:LEU:HD22	7:B:43:LEU:HD13	1.88	0.56
14:I:36:LYS:O	14:I:40:GLN:HG2	2.06	0.56
30:a:1317:U:H2'	30:a:1318:G:H8	1.69	0.56
30:a:2660:A:H1'	30:a:2710:U:O2'	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:19:GLU:OE1	35:f:19:GLU:N	2.38	0.56
7:B:86:ARG:NE	7:B:86:ARG:O	2.35	0.56
30:a:130:G:H22	30:a:154:G:N2	2.02	0.56
30:a:3078:U:H2'	30:a:3079:C:C6	2.41	0.56
21:P:107:ALA:O	21:P:111:GLU:HB2	2.06	0.56
30:a:1491:C:H2'	30:a:1492:C:H6	1.71	0.56
30:a:3073:G:O5'	30:a:3074:A:H5''	2.05	0.56
6:A:91:G:O2'	6:A:92:G:H5'	2.05	0.56
26:U:28:HIS:C	26:U:29:ASN:HD22	2.10	0.56
30:a:2283:G:H2'	30:a:2284:G:C8	2.40	0.56
6:A:718:U:H2'	6:A:719:C:C6	2.40	0.56
30:a:238:U:H2'	30:a:239:G:O4'	2.06	0.56
30:a:2423:A:H2'	30:a:2424:G:C8	2.40	0.56
36:g:2:SER:OG	36:g:66:HIS:ND1	2.27	0.56
6:A:1300:C:H2'	6:A:1301:U:C6	2.41	0.56
44:p:89:GLU:HB2	45:q:38:LEU:HD22	1.88	0.55
48:t:42:ASN:O	48:t:67:GLU:HA	2.05	0.55
6:A:1460:G:H2'	6:A:1461:G:C8	2.42	0.55
9:D:68:ARG:O	9:D:72:GLU:HG2	2.04	0.55
18:M:14:ASP:OD1	18:M:17:VAL:HG23	2.06	0.55
43:o:17:ILE:HG21	43:o:76:LEU:HD11	1.89	0.55
53:y:41:ARG:NH1	53:y:43:GLU:OE2	2.38	0.55
6:A:930:A:H2'	6:A:931:G:H8	1.72	0.55
30:a:361:G:N2	30:a:443:G:H22	2.04	0.55
30:a:975:G:H2'	30:a:976:G:C8	2.42	0.55
32:c:72:LYS:NZ	32:c:101:GLU:OE1	2.33	0.55
33:d:108:SER:OG	33:d:109:GLU:N	2.38	0.55
9:D:6:GLY:O	9:D:107:ARG:NH2	2.36	0.55
30:a:1688:U:H2'	30:a:1689:G:O4'	2.07	0.55
30:a:2929:G:OP1	36:g:75:ASN:ND2	2.35	0.55
33:d:122:LYS:HB2	33:d:171:MET:HG2	1.88	0.55
6:A:301:G:H2'	6:A:302:A:C8	2.41	0.55
6:A:1302:G:N1	6:A:1305:A:OP2	2.38	0.55
7:B:73:LYS:HE2	7:B:75:GLN:HB2	1.89	0.55
8:C:21:A:H61	8:C:46:G:H2'	1.71	0.55
12:G:5:ILE:HD11	24:S:58:LYS:HE2	1.89	0.55
30:a:82:G:N2	30:a:101:G:H2'	2.21	0.55
30:a:101:G:H4'	30:a:101:G:OP1	2.05	0.55
40:l:62:GLY:H	49:u:118:ILE:HG13	1.71	0.55
40:l:107:SER:HB3	49:u:120:MET:HE1	1.88	0.55
6:A:126:G:OP1	6:A:587:U:O2'	2.23	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:436:C:H2'	6:A:437:G:H8	1.72	0.55
30:a:1256:G:H3'	30:a:1256:G:N3	2.22	0.55
53:y:3:SER:OG	53:y:40:ASP:OD2	2.25	0.55
6:A:23:C:OP1	10:E:158:ASN:ND2	2.40	0.55
23:R:73:THR:OG1	23:R:74:ALA:N	2.40	0.55
30:a:63:A:H2'	30:a:64:C:C6	2.42	0.55
45:q:1:MET:HE3	45:q:42:ASP:HB2	1.88	0.55
53:y:10:ILE:HD13	53:y:56:THR:HG23	1.88	0.55
6:A:1022:U:H2'	6:A:1023:C:C6	2.41	0.55
6:A:1091:G:H5''	12:G:171:ARG:HE	1.72	0.55
15:J:57:ALA:HB2	15:J:112:GLY:HA3	1.89	0.55
25:T:42:GLY:HA2	25:T:86:LEU:HD21	1.88	0.55
30:a:2065:U:H2'	30:a:2066:G:H4'	1.88	0.55
6:A:1282:C:H4'	6:A:1288:U:O4	2.07	0.55
17:L:25:LYS:HD2	17:L:59:SER:HB2	1.89	0.55
30:a:225:G:N2	30:a:242:U:H4'	2.21	0.55
32:c:23:GLU:H	32:c:23:GLU:CD	2.14	0.55
32:c:166:VAL:HG21	32:c:182:MET:HE1	1.88	0.55
6:A:463:G:O2'	6:A:465:C:N4	2.40	0.54
30:a:2571:G:H5''	30:a:2572:U:O4'	2.07	0.54
41:m:36:THR:O	41:m:36:THR:OG1	2.24	0.54
6:A:21:U:H2'	6:A:22:C:C6	2.42	0.54
34:e:158:VAL:O	34:e:160:LEU:N	2.35	0.54
36:g:29:PRO:HB2	36:g:30:LYS:HZ3	1.72	0.54
30:a:663:C:H2'	30:a:664:C:C6	2.42	0.54
46:r:36:ARG:HD2	54:z:22:THR:HG23	1.88	0.54
6:A:172:A:H2'	6:A:173:A:C8	2.42	0.54
6:A:1324:G:H2'	6:A:1325:A:C8	2.42	0.54
6:A:1378:U:H2'	6:A:1379:G:C8	2.42	0.54
9:D:25:SER:C	9:D:27:GLU:H	2.15	0.54
11:F:15:GLU:OE1	11:F:15:GLU:N	2.39	0.54
30:a:1710:A:H61	30:a:1726:U:H5'	1.72	0.54
34:e:159:VAL:HG21	34:e:205:ALA:CB	2.37	0.54
6:A:537:C:H2'	6:A:538:C:C6	2.42	0.54
6:A:700:A:H5'	16:K:125:ASN:ND2	2.22	0.54
30:a:289:U:H1'	30:a:306:G:O2'	2.07	0.54
30:a:337:G:O4'	30:a:356:G:N2	2.40	0.54
30:a:405:G:N2	34:e:173:ASN:O	2.40	0.54
30:a:692:A:H2'	30:a:693:A:C8	2.42	0.54
34:e:4:THR:HG22	34:e:4:THR:O	2.08	0.54
11:F:14:VAL:HG13	11:F:18:GLN:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:898:U:H2'	30:a:899:C:C6	2.43	0.54
30:a:1142:G:N2	30:a:1163:C:O2	2.40	0.54
4:3:11:CYS:HB3	4:3:32:HIS:HE1	1.73	0.54
12:G:148:ILE:HD13	12:G:201:ILE:HD12	1.89	0.54
30:a:836:A:H5'	46:r:107:LYS:HA	1.89	0.54
30:a:976:G:H2'	30:a:977:C:C6	2.43	0.54
34:e:182:ALA:HB1	34:e:206:PHE:HB2	1.89	0.54
6:A:820:U:H2'	6:A:821:C:C6	2.43	0.54
14:I:15:ASP:OD2	14:I:23:VAL:HB	2.08	0.54
30:a:2365:U:H2'	30:a:2366:U:C6	2.43	0.54
6:A:634:U:H4'	13:H:59:VAL:HG23	1.89	0.54
9:D:45:GLU:OE2	10:E:135:ARG:HD3	2.07	0.54
18:M:10:LEU:HB3	18:M:18:ILE:HD11	1.90	0.54
18:M:86:SER:HA	18:M:89:ARG:HG2	1.89	0.54
26:U:22:GLN:HG2	26:U:31:ILE:HD11	1.89	0.54
30:a:1111:A:H2'	30:a:1112:A:C8	2.43	0.54
34:e:159:VAL:O	34:e:161:ASP:N	2.41	0.54
42:n:83:ARG:O	42:n:87:ILE:HG13	2.07	0.54
7:B:79:SER:O	7:B:82:GLU:HG2	2.08	0.54
8:C:43:A:H2'	8:C:44:A:C8	2.42	0.54
9:D:25:SER:C	9:D:27:GLU:N	2.63	0.54
20:O:68:ILE:HG22	20:O:76:TYR:HB2	1.89	0.54
30:a:2425:U:H2'	30:a:2426:U:C6	2.43	0.54
30:a:2712:G:C8	30:a:2713:A:H5''	2.38	0.54
34:e:16:LYS:HA	34:e:16:LYS:HE3	1.89	0.54
6:A:1023:C:H2'	6:A:1024:G:C8	2.43	0.53
14:I:40:GLN:NE2	15:J:85:VAL:HG22	2.23	0.53
6:A:94:G:H1'	6:A:95:U:H5''	1.90	0.53
6:A:697:A:H2'	6:A:698:A:C8	2.43	0.53
10:E:36:GLU:HG2	10:E:62:VAL:HG12	1.90	0.53
15:J:138:ARG:NH1	15:J:138:ARG:HB3	2.22	0.53
30:a:3009:G:H5''	33:d:83:ARG:HH12	1.73	0.53
34:e:12:VAL:HG12	34:e:14:GLY:N	2.22	0.53
51:w:5:CYS:SG	51:w:7:ILE:O	2.65	0.53
6:A:192:G:H21	22:Q:1:MET:N	2.06	0.53
19:N:13:LYS:O	19:N:45:VAL:HG23	2.09	0.53
30:a:503:C:H2'	30:a:504:A:C8	2.43	0.53
30:a:532:A:H8	30:a:1277:G:H21	1.56	0.53
6:A:191:U:H2'	6:A:192:G:C8	2.43	0.53
6:A:337:C:H2'	6:A:338:A:H8	1.74	0.53
30:a:337:G:O5'	30:a:356:G:N2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:142:GLN:O	34:e:146:VAL:HG22	2.08	0.53
47:s:64:ARG:HB3	47:s:81:THR:HG23	1.90	0.53
6:A:382:G:N2	6:A:385:A:OP2	2.40	0.53
6:A:512:G:C6	29:Y:22:U:H5''	2.44	0.53
7:B:152:ILE:HA	7:B:155:MET:HE1	1.89	0.53
15:J:84:LYS:HA	15:J:87:GLN:HG3	1.90	0.53
7:B:135:LEU:HD12	7:B:138:LEU:HD23	1.90	0.53
18:M:56:HIS:ND1	18:M:57:LYS:HB3	2.24	0.53
21:P:103:ASP:OD1	21:P:104:LEU:N	2.41	0.53
30:a:622:U:H2'	30:a:623:C:C6	2.44	0.53
30:a:1139:G:N2	30:a:1186:A:OP2	2.41	0.53
30:a:1194:A:N3	30:a:1195:G:H1'	2.23	0.53
30:a:1768:A:H2'	30:a:1769:G:O4'	2.09	0.53
6:A:1108:U:H4'	18:M:38:GLY:HA3	1.89	0.53
11:F:26:TYR:OH	11:F:82:ASP:OD2	2.26	0.53
6:A:384:A:H2'	6:A:385:A:H8	1.73	0.53
6:A:849:A:H2'	6:A:850:C:C6	2.44	0.53
6:A:1237:G:H2'	6:A:1238:A:C8	2.44	0.53
7:B:30:PHE:CE2	7:B:41:ILE:HD11	2.44	0.53
7:B:207:ALA:HB3	7:B:210:SER:HB3	1.91	0.53
21:P:3:THR:HG23	21:P:64:ALA:HA	1.90	0.53
38:j:109:LYS:O	38:j:109:LYS:HD2	2.08	0.53
42:n:4:THR:O	42:n:6:THR:N	2.42	0.53
6:A:148:G:H2'	6:A:149:G:C8	2.44	0.53
30:a:1399:A:C2	30:a:1409:C:H1'	2.44	0.53
32:c:44:ASN:HB3	32:c:46:THR:H	1.74	0.53
34:e:159:VAL:HB	34:e:202:GLY:HA2	1.89	0.53
6:A:240:G:H2'	6:A:241:G:C8	2.44	0.53
22:Q:12:ARG:HB2	22:Q:70:GLU:HG2	1.91	0.53
30:a:359:C:H2'	30:a:360:A:H8	1.74	0.53
30:a:1317:U:H2'	30:a:1318:G:C8	2.44	0.53
34:e:160:LEU:HG	34:e:163:SER:H	1.74	0.53
36:g:25:GLU:OE1	36:g:25:GLU:N	2.42	0.53
11:F:47:ARG:NE	11:F:57:GLU:OE2	2.43	0.52
19:N:6:GLY:O	35:f:121:ARG:NH1	2.37	0.52
30:a:272:A:N6	30:a:516:U:O2'	2.34	0.52
41:m:10:LEU:H	41:m:17:GLU:HG3	1.74	0.52
9:D:94:ASP:N	9:D:94:ASP:OD1	2.42	0.52
26:U:27:THR:HG23	26:U:47:HIS:CD2	2.44	0.52
30:a:133:A:OP2	30:a:134:U:N3	2.42	0.52
30:a:2527:G:N3	30:a:2563:C:H2'	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2925:C:O2'	36:g:152:LYS:HE2	2.09	0.52
6:A:140:U:O2	6:A:226:G:O6	2.28	0.52
30:a:889:A:OP1	39:k:43:LYS:NZ	2.34	0.52
30:a:1042:A:H2'	30:a:1043:A:C8	2.44	0.52
30:a:2791:U:O2	30:a:2791:U:H2'	2.09	0.52
30:a:2982:U:H3'	30:a:2983:C:C6	2.44	0.52
34:e:149:GLY:O	34:e:150:LEU:HB2	2.08	0.52
2:l:7:PRO:HB2	30:a:1385:G:H4'	1.90	0.52
6:A:454:A:H61	21:P:93:LYS:HB3	1.74	0.52
6:A:1359:U:H5''	15:J:115:THR:HG23	1.92	0.52
19:N:77:ASP:OD1	19:N:80:ARG:NH2	2.38	0.52
27:V:21:ARG:NH2	30:a:1065:C:N3	2.57	0.52
30:a:631:G:O2'	30:a:633:G:O4'	2.24	0.52
30:a:3029:G:O6	43:o:21:ARG:NH1	2.37	0.52
36:g:9:ILE:HG12	36:g:70:ARG:NH1	2.24	0.52
36:g:45:LYS:HE3	36:g:48:GLU:HA	1.90	0.52
49:u:131:ASP:N	49:u:131:ASP:OD1	2.36	0.52
6:A:6:C:O2	10:E:190:ALA:N	2.38	0.52
6:A:129:U:H5'	22:Q:12:ARG:HH21	1.74	0.52
6:A:1056:C:H2'	6:A:1057:G:H8	1.73	0.52
6:A:1265:A:O2'	6:A:1268:C:N4	2.42	0.52
9:D:142:GLU:O	9:D:145:LYS:HG2	2.09	0.52
12:G:150:ILE:HG12	12:G:199:VAL:HG22	1.92	0.52
15:J:90:VAL:HG21	15:J:121:LEU:HD23	1.92	0.52
25:T:7:GLN:O	25:T:11:VAL:HG13	2.10	0.52
30:a:1083:A:H2'	30:a:1084:A:C8	2.45	0.52
30:a:1904:U:H5	30:a:1921:G:H21	1.56	0.52
4:3:1:MET:SD	4:3:35:ARG:HB2	2.50	0.52
5:4:14:VAL:HA	5:4:33:LEU:HB2	1.92	0.52
6:A:392:U:H2'	6:A:393:G:C8	2.43	0.52
6:A:966:U:H5''	24:S:6:LEU:HD21	1.92	0.52
7:B:97:LEU:HD11	7:B:100:MET:HG3	1.91	0.52
9:D:26:PHE:O	9:D:29:ARG:HB3	2.08	0.52
15:J:72:ILE:HD12	15:J:72:ILE:O	2.10	0.52
30:a:433:G:H2'	30:a:435:G:O4'	2.10	0.52
30:a:993:A:H2'	30:a:996:C:C5	2.44	0.52
1:0:36:ARG:CZ	1:0:53:ARG:HE	2.22	0.52
6:A:1503:2MG:HM21	6:A:1506:MA6:N7	2.24	0.52
7:B:73:LYS:O	7:B:77:GLN:HG2	2.09	0.52
9:D:145:LYS:HB2	21:P:122:LYS:NZ	2.23	0.52
30:a:341:U:H2'	30:a:342:G:H8	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:350:A:H2'	30:a:351:G:C8	2.45	0.52
30:a:943:G:N3	30:a:2450:A:H2'	2.25	0.52
30:a:2711:G:H3'	30:a:2712:G:H5''	1.91	0.52
34:e:157:LEU:HD23	34:e:182:ALA:HA	1.91	0.52
41:m:5:THR:O	41:m:6:LYS:HB3	2.09	0.52
13:H:10:MET:HG3	13:H:27:MET:HE2	1.92	0.52
18:M:51:VAL:O	18:M:62:ARG:HG3	2.10	0.52
27:V:12:ARG:NH2	31:b:89:G:OP1	2.40	0.52
30:a:50:G:HO2'	30:a:118:A:N6	2.06	0.52
30:a:1133:A:H3'	30:a:1134:A:H8	1.75	0.52
30:a:1687:G:N2	30:a:1688:U:O4	2.43	0.52
39:k:99:SER:OG	39:k:105:ASP:HB3	2.09	0.52
6:A:378:G:H5''	21:P:6:ARG:HB3	1.91	0.52
6:A:1428:G:H8	6:A:1447:A:N6	2.01	0.52
9:D:93:LEU:HB2	9:D:130:TYR:HB3	1.92	0.52
10:E:104:ILE:HD12	10:E:170:LEU:HD11	1.92	0.52
12:G:22:TRP:CD1	12:G:58:ARG:HG3	2.45	0.52
30:a:1965:C:H1'	30:a:2791:U:H5''	1.92	0.52
30:a:2256:U:H2'	30:a:2257:U:C6	2.45	0.52
6:A:7:A:H2'	6:A:8:U:O4'	2.10	0.52
6:A:191:U:H2'	6:A:192:G:H8	1.74	0.52
6:A:446:U:H3	6:A:472:G:H1	1.57	0.52
6:A:1236:A:H4'	15:J:111:GLY:HA2	1.91	0.52
11:F:19:VAL:HA	11:F:22:LEU:HD12	1.92	0.52
14:I:67:ASP:HA	14:I:70:LYS:HG3	1.90	0.52
30:a:2773:C:H2'	30:a:2774:G:C8	2.45	0.52
6:A:1175:U:H5''	12:G:5:ILE:HD12	1.91	0.51
21:P:66:PRO:HB2	21:P:71:VAL:HG23	1.92	0.51
30:a:373:G:H2'	30:a:373:G:N3	2.25	0.51
51:w:3:ALA:HB1	51:w:12:PRO:HG3	1.91	0.51
5:4:5:ILE:HD12	35:f:73:LYS:HD3	1.92	0.51
5:4:14:VAL:HG21	35:f:115:LEU:HD21	1.91	0.51
6:A:1341:A:H2'	6:A:1342:G:H8	1.73	0.51
7:B:162:VAL:HG22	7:B:184:VAL:HG12	1.92	0.51
9:D:154:ARG:HG2	9:D:171:ASN:HB3	1.92	0.51
14:I:13:MET:SD	14:I:14:VAL:N	2.83	0.51
18:M:59:LYS:HE2	18:M:62:ARG:HH12	1.74	0.51
30:a:1224:U:OP2	37:i:65:THR:OG1	2.26	0.51
34:e:5:LYS:HE2	34:e:5:LYS:HA	1.91	0.51
46:r:1:MET:HB3	46:r:3:LYS:NZ	2.26	0.51
6:A:234:A:H2'	6:A:235:C:C6	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:521:A:H2'	6:A:522:G:H8	1.76	0.51
6:A:1437:G:H21	6:A:1440:G:H21	1.58	0.51
7:B:114:LEU:HG	7:B:145:LEU:HD13	1.93	0.51
12:G:11:ARG:HB3	12:G:16:THR:HG23	1.93	0.51
15:J:141:LEU:HB3	15:J:147:LEU:HD23	1.91	0.51
49:u:37:ASP:OD2	49:u:96:ARG:NH1	2.43	0.51
6:A:386:G:H2'	6:A:387:C:H6	1.75	0.51
11:F:18:GLN:O	11:F:22:LEU:HD12	2.11	0.51
16:K:124:HIS:O	16:K:125:ASN:HB2	2.11	0.51
18:M:66:GLU:HB2	24:S:59:SER:HB3	1.93	0.51
24:S:35:ARG:HG2	24:S:35:ARG:HH11	1.76	0.51
30:a:1904:U:OP2	30:a:1921:G:N2	2.43	0.51
30:a:2268:U:H2'	30:a:2269:G:C8	2.46	0.51
40:l:65:TRP:HZ3	40:l:107:SER:HB2	1.75	0.51
49:u:64:GLU:HG3	49:u:70:PRO:HB3	1.92	0.51
6:A:1412:A:H2'	6:A:1413:A:O4'	2.10	0.51
12:G:11:ARG:HD3	12:G:177:LEU:HD12	1.92	0.51
16:K:91:PHE:HB3	16:K:119:VAL:HG21	1.92	0.51
24:S:16:PHE:HB2	24:S:19:ARG:HD2	1.92	0.51
30:a:1123:U:H2'	30:a:1124:U:O4'	2.10	0.51
6:A:907:A:O2'	6:A:1386:C:OP2	2.27	0.51
7:B:24:ASN:HD22	7:B:25:PRO:HD2	1.76	0.51
7:B:47:LEU:HA	7:B:50:ILE:HG12	1.92	0.51
7:B:130:LEU:HD23	7:B:135:LEU:HD13	1.92	0.51
30:a:142:G:N2	30:a:147:G:H22	2.05	0.51
52:x:45:ARG:O	52:x:49:VAL:HG23	2.10	0.51
6:A:992:U:H2'	6:A:993:G:H8	1.76	0.51
8:C:56:C:N3	35:f:89:ARG:NH1	2.58	0.51
12:G:60:SER:O	12:G:61:GLU:HG3	2.10	0.51
18:M:78:GLU:HG2	18:M:80:THR:HG23	1.93	0.51
30:a:433:G:OP2	30:a:433:G:N2	2.40	0.51
30:a:631:G:H5''	30:a:632:U:H5'	1.92	0.51
30:a:759:G:O2'	34:e:77:ARG:HD3	2.11	0.51
30:a:1429:A:H2'	30:a:1430:A:C8	2.46	0.51
30:a:1601:G:H1'	30:a:1763:G:O6	2.11	0.51
2:1:24:THR:HG22	2:1:26:ALA:H	1.76	0.51
6:A:69:A:C2	6:A:220:G:H8	2.28	0.51
6:A:506:G:H2'	6:A:507:C:C6	2.46	0.51
6:A:848:A:H2'	6:A:849:A:C8	2.46	0.51
6:A:1441:U:H2'	6:A:1442:G:C8	2.46	0.51
6:A:1479:A:H4'	6:A:1480:A:C5	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:87:VAL:HG21	7:B:219:ALA:HB1	1.93	0.51
11:F:36:THR:HG23	11:F:66:THR:HB	1.93	0.51
11:F:87:ARG:HH11	11:F:87:ARG:HG3	1.76	0.51
16:K:71:MET:HE2	16:K:71:MET:HA	1.93	0.51
18:M:51:VAL:HG13	24:S:41:ARG:HG2	1.92	0.51
22:Q:7:GLU:C	22:Q:9:THR:H	2.19	0.51
30:a:384:A:N3	30:a:404:C:O2'	2.43	0.51
38:j:105:GLU:N	38:j:105:GLU:OE1	2.43	0.51
48:t:67:GLU:OE2	48:t:67:GLU:N	2.36	0.51
6:A:527:C:H5'	9:D:64:GLU:HB2	1.93	0.51
21:P:115:ALA:HB3	21:P:116:PRO:HD3	1.92	0.51
30:a:503:C:H2'	30:a:504:A:H8	1.76	0.51
30:a:935:U:H2'	30:a:936:U:C6	2.46	0.51
30:a:1901:U:H2'	30:a:1902:C:C6	2.46	0.51
33:d:15:LEU:HD13	43:o:4:ILE:HG21	1.93	0.51
6:A:386:G:H2'	6:A:387:C:C6	2.45	0.51
6:A:475:U:H2'	6:A:476:A:C4	2.46	0.51
10:E:172:GLU:HB3	10:E:175:GLU:OE2	2.11	0.51
20:O:5:GLU:H	20:O:5:GLU:CD	2.19	0.51
30:a:975:G:H2'	30:a:976:G:H8	1.76	0.51
42:n:65:THR:HA	42:n:70:LEU:HD22	1.92	0.51
49:u:17:LYS:O	49:u:21:ARG:HG3	2.11	0.51
54:z:35:CYS:O	54:z:37:GLU:HG2	2.11	0.51
2:1:16:HIS:HB2	2:1:44:ALA:HB3	1.92	0.50
30:a:3:A:N6	30:a:3079:C:H42	2.10	0.50
30:a:712:U:H4'	30:a:739:G:N7	2.26	0.50
35:f:22:ARG:HD2	35:f:37:ILE:HG21	1.93	0.50
5:4:25:ARG:O	35:f:111:ARG:NH1	2.43	0.50
6:A:378:G:OP1	21:P:67:THR:HG21	2.11	0.50
6:A:436:C:H2'	6:A:437:G:C8	2.47	0.50
6:A:975:U:H1'	6:A:977:G:C8	2.46	0.50
9:D:48:LEU:HD23	9:D:51:ARG:NH2	2.26	0.50
10:E:134:ALA:O	10:E:138:LEU:HD23	2.11	0.50
30:a:838:U:H2'	30:a:839:G:H8	1.76	0.50
30:a:979:U:H2'	30:a:981:C:H41	1.76	0.50
30:a:1628:C:O2'	30:a:1727:G:N3	2.40	0.50
30:a:1906:C:H2'	30:a:1907:A:C8	2.45	0.50
30:a:2712:G:H1'	30:a:2716:C:N4	2.26	0.50
30:a:2915:U:H3	33:d:214:LYS:HD3	1.75	0.50
30:a:2922:A:H2'	30:a:2923:A:C8	2.46	0.50
6:A:1437:G:H21	6:A:1440:G:N2	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:58:A:O2'	8:C:60:U:OP2	2.23	0.50
28:X:3:SER:C	28:X:5:ILE:H	2.19	0.50
30:a:400:G:H2'	30:a:401:U:O4'	2.11	0.50
30:a:720:G:H2'	30:a:721:C:C6	2.46	0.50
36:g:103:LYS:HB3	36:g:119:ALA:HB3	1.93	0.50
37:i:30:THR:CA	37:i:108:MET:HE1	2.42	0.50
7:B:15:HIS:HB3	7:B:43:LEU:HD11	1.92	0.50
11:F:6:VAL:HG22	11:F:90:VAL:HG22	1.93	0.50
11:F:12:PRO:HB2	11:F:45:LYS:HE3	1.93	0.50
30:a:279:A:H5'	30:a:280:C:OP2	2.11	0.50
30:a:672:U:H2'	30:a:673:A:H8	1.77	0.50
47:s:72:ARG:O	47:s:73:THR:OG1	2.28	0.50
6:A:90:U:O2'	6:A:91:G:O5'	2.22	0.50
6:A:1252:G:N2	6:A:1255:A:OP2	2.32	0.50
6:A:1301:U:O2'	6:A:1346:A:N3	2.40	0.50
7:B:209:ARG:HA	7:B:212:SER:HB2	1.94	0.50
10:E:84:ALA:O	10:E:88:GLU:HG2	2.11	0.50
23:R:22:ASP:O	23:R:25:ASP:N	2.43	0.50
30:a:1866:C:H2'	30:a:1867:C:C6	2.47	0.50
30:a:2828:C:H2'	30:a:2829:U:O4'	2.11	0.50
34:e:152:GLU:HB3	34:e:176:GLU:HB2	1.94	0.50
6:A:1056:C:H2'	6:A:1057:G:C8	2.46	0.50
6:A:1485:UR3:C4'	6:A:1506:MA6:H2	2.41	0.50
37:i:143:THR:OG1	37:i:144:GLN:N	2.45	0.50
46:r:128:GLU:N	46:r:128:GLU:OE1	2.45	0.50
6:A:384:A:H2'	6:A:385:A:C8	2.47	0.50
9:D:90:GLU:OE1	9:D:95:ASN:ND2	2.39	0.50
9:D:126:ASN:O	9:D:126:ASN:ND2	2.41	0.50
23:R:30:ARG:HG2	23:R:30:ARG:HH11	1.77	0.50
26:U:20:THR:HA	26:U:23:ASN:ND2	2.27	0.50
30:a:332:U:H3	30:a:449:G:H22	1.60	0.50
30:a:610:G:H2'	30:a:611:C:C6	2.47	0.50
30:a:1172:G:H22	30:a:1185:C:H42	1.58	0.50
30:a:3037:G:N2	30:a:3040:A:OP2	2.34	0.50
38:j:9:LYS:HD2	38:j:81:GLU:HG3	1.94	0.50
52:x:15:GLU:HG2	52:x:16:GLU:N	2.26	0.50
6:A:607:C:H5''	21:P:10:LEU:HD12	1.94	0.50
6:A:1438:U:O2'	6:A:1439:U:H5'	2.11	0.50
30:a:1047:U:O2'	30:a:2455:A:N3	2.37	0.50
30:a:2503:G:O2'	30:a:2504:A:OP1	2.29	0.50
38:j:24:VAL:HG13	38:j:33:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:195:G:H2'	6:A:196:C:H2'	1.93	0.50
6:A:508:C:C4	6:A:509:G7M:H1'	2.47	0.50
7:B:113:ARG:O	7:B:116:GLU:HG3	2.12	0.50
7:B:140:ARG:NH1	7:B:141:GLU:OE2	2.45	0.50
7:B:193:ASP:N	7:B:193:ASP:OD1	2.40	0.50
12:G:44:LYS:HD3	12:G:44:LYS:C	2.36	0.50
15:J:86:HIS:O	15:J:89:ILE:HG22	2.11	0.50
19:N:5:ILE:H	19:N:5:ILE:HD12	1.77	0.50
30:a:671:U:H2'	30:a:672:U:C6	2.46	0.50
49:u:153:TYR:H	49:u:153:TYR:HD1	1.60	0.50
1:0:9:ARG:NH1	30:a:2467:C:OP2	2.40	0.49
7:B:223:ALA:HA	7:B:226:LEU:HD23	1.94	0.49
15:J:54:ARG:HH21	15:J:55:LYS:HE3	1.77	0.49
29:Y:21:U:C4	29:Y:22:U:H1'	2.47	0.49
42:n:73:MET:SD	42:n:83:ARG:HG3	2.52	0.49
6:A:521:A:H2'	6:A:522:G:C8	2.47	0.49
6:A:1246:G:H8	6:A:1261:A:H62	1.60	0.49
10:E:128:VAL:O	10:E:135:ARG:NH2	2.45	0.49
11:F:23:MET:O	11:F:27:LEU:HG	2.12	0.49
46:r:35:ARG:HA	46:r:38:ILE:HG22	1.94	0.49
6:A:1336:A:OP1	15:J:166:LYS:HD2	2.12	0.49
7:B:24:ASN:HD22	7:B:25:PRO:CD	2.25	0.49
9:D:145:LYS:HG3	21:P:122:LYS:HE3	1.94	0.49
17:L:33:VAL:HG22	17:L:79:MET:SD	2.52	0.49
19:N:90:ARG:NH1	26:U:76:PRO:HG3	2.28	0.49
30:a:291:U:H5''	30:a:308:U:C5	2.46	0.49
30:a:1977:U:H2'	30:a:1978:C:H6	1.78	0.49
6:A:660:U:H2'	6:A:661:C:C6	2.48	0.49
6:A:1277:C:H2'	6:A:1278:C:C6	2.47	0.49
6:A:1505:MA6:H2'	6:A:1506:MA6:H8	1.94	0.49
7:B:78:GLU:OE1	7:B:78:GLU:N	2.45	0.49
10:E:47:VAL:HA	10:E:52:ARG:HA	1.95	0.49
14:I:66:LEU:O	14:I:70:LYS:HG2	2.12	0.49
18:M:34:ALA:HA	18:M:78:GLU:HB3	1.93	0.49
22:Q:86:ILE:HG22	22:Q:87:GLU:HG2	1.95	0.49
25:T:31:TYR:CE2	25:T:57:GLN:HG2	2.47	0.49
30:a:14:G:O2'	54:z:15:HIS:ND1	2.43	0.49
30:a:418:G:O2'	30:a:419:U:OP1	2.28	0.49
30:a:1665:C:H2'	30:a:1666:U:C6	2.47	0.49
31:b:5:C:OP1	31:b:61:C:O2'	2.30	0.49
6:A:660:U:H2'	6:A:661:C:H6	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:14:ALA:HB1	20:O:19:ASP:HB3	1.95	0.49
30:a:306:G:H4'	30:a:307:U:O5'	2.11	0.49
30:a:742:U:H2'	30:a:743:C:C6	2.47	0.49
6:A:657:A:H1'	16:K:124:HIS:CD2	2.48	0.49
10:E:102:ARG:HD2	10:E:144:HIS:ND1	2.28	0.49
21:P:100:ASN:OD1	21:P:101:LYS:N	2.45	0.49
30:a:198:A:H2'	30:a:199:G:H8	1.76	0.49
30:a:554:G:H2'	30:a:555:A:C8	2.48	0.49
30:a:1595:A:H2'	30:a:1596:G:O4'	2.12	0.49
6:A:1418:C:H2'	6:A:1419:G:O4'	2.13	0.49
18:M:50:CYS:SG	18:M:62:ARG:HG2	2.52	0.49
18:M:67:MET:HE1	24:S:36:LYS:HE3	1.95	0.49
19:N:24:GLY:HA3	19:N:66:VAL:HG12	1.94	0.49
30:a:1182:G:H2'	30:a:1183:C:C6	2.47	0.49
30:a:1491:C:H2'	30:a:1492:C:C6	2.47	0.49
30:a:1698:G:N2	30:a:1915:G:H22	2.09	0.49
32:c:124:ASP:OD1	32:c:125:ILE:N	2.46	0.49
36:g:96:ARG:HG2	36:g:108:ASN:ND2	2.27	0.49
49:u:52:LEU:HD22	49:u:55:ARG:HH21	1.76	0.49
6:A:509:G7M:O2'	6:A:517:A:N1	2.35	0.49
6:A:534:U:H5'	17:L:83:ARG:HH11	1.77	0.49
17:L:87:VAL:HG23	17:L:90:LEU:HB2	1.95	0.49
30:a:374:C:H42	30:a:436:U:H3	1.60	0.49
30:a:1040:A:N1	30:a:2640:G:H4'	2.27	0.49
30:a:1462:C:H2'	30:a:1463:C:C6	2.48	0.49
48:t:29:VAL:HG22	48:t:36:VAL:HG12	1.94	0.49
49:u:58:ASN:ND2	49:u:104:ASN:O	2.46	0.49
52:x:12:LEU:O	52:x:63:ARG:NH2	2.41	0.49
6:A:904:U:H2'	6:A:905:U:C6	2.48	0.49
14:I:95:ARG:HD3	14:I:99:LEU:HD23	1.95	0.49
30:a:580:A:H2'	30:a:581:G:O4'	2.13	0.49
30:a:1486:U:H2'	30:a:1487:G:H8	1.75	0.49
35:f:17:TYR:HA	35:f:21:ILE:HG12	1.95	0.49
36:g:123:ILE:HD11	36:g:142:VAL:HG23	1.94	0.49
48:t:80:LYS:HA	48:t:84:LYS:O	2.11	0.49
6:A:449:G:O6	6:A:467:G:O2'	2.26	0.49
30:a:337:G:N2	30:a:355:U:H2'	2.22	0.49
30:a:788:U:H2'	30:a:789:G:O4'	2.13	0.49
30:a:799:U:O2'	30:a:801:A:N7	2.31	0.49
30:a:970:U:C5	30:a:971:U:H1'	2.48	0.49
30:a:1977:U:H2'	30:a:1978:C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:22:VAL:HG21	16:K:48:ILE:HD13	1.95	0.48
30:a:214:A:H2'	30:a:215:C:O4'	2.12	0.48
30:a:1781:G:OP2	47:s:45:LYS:NZ	2.44	0.48
30:a:2579:A:H2'	30:a:2580:C:C6	2.48	0.48
39:k:93:THR:HA	39:k:97:LEU:HD12	1.94	0.48
6:A:201:U:H2'	6:A:202:G:H8	1.78	0.48
6:A:1399:C:H2'	6:A:1400:A:C8	2.48	0.48
29:Y:13:A:C2	29:Y:14:A:H1'	2.48	0.48
30:a:2610:G:H5''	30:a:2611:G:H5'	1.94	0.48
30:a:2640:G:O2'	30:a:2642:U:O4	2.31	0.48
33:d:187:ASP:OD2	33:d:190:ARG:HD3	2.13	0.48
34:e:185:LEU:O	34:e:186:ASN:ND2	2.46	0.48
6:A:457:G:N2	6:A:460:A:OP2	2.44	0.48
6:A:1027:U:H2'	6:A:1028:C:C6	2.48	0.48
6:A:1208:G:OP2	6:A:1308:C:N4	2.34	0.48
6:A:1226:U:C5	14:I:116:MET:HG2	2.49	0.48
7:B:139:SER:O	7:B:142:LYS:HB2	2.13	0.48
7:B:163:TRP:HA	7:B:185:VAL:O	2.13	0.48
9:D:28:ARG:HG2	9:D:31:TYR:OH	2.14	0.48
15:J:138:ARG:HB3	15:J:138:ARG:HH11	1.77	0.48
30:a:993:A:H2'	30:a:996:C:H5	1.79	0.48
30:a:1912:U:H4'	30:a:1914:C:C2	2.49	0.48
30:a:2428:G:H2'	30:a:2429:A:C8	2.48	0.48
30:a:3065:A:H2'	30:a:3066:G:O4'	2.13	0.48
34:e:16:LYS:HD3	34:e:17:ALA:H	1.79	0.48
35:f:40:LEU:HD23	35:f:167:THR:HG22	1.94	0.48
6:A:512:G:N1	29:Y:22:U:H5''	2.27	0.48
9:D:148:PRO:O	9:D:151:VAL:HG22	2.13	0.48
18:M:7:ARG:HD2	18:M:73:LEU:HD11	1.95	0.48
20:O:2:ASP:N	20:O:5:GLU:OE1	2.46	0.48
30:a:453:U:H1'	30:a:454:G:OP2	2.13	0.48
30:a:491:A:H2'	30:a:492:U:O4'	2.14	0.48
30:a:2989:A:H2'	30:a:2990:A:C8	2.48	0.48
36:g:119:ALA:HB2	36:g:125:PHE:CE2	2.49	0.48
41:m:69:THR:O	41:m:71:THR:N	2.46	0.48
6:A:337:C:H2'	6:A:338:A:C8	2.47	0.48
6:A:503:G:H4'	17:L:70:VAL:HG22	1.94	0.48
6:A:975:U:H1'	6:A:977:G:H8	1.77	0.48
7:B:60:THR:HG22	7:B:65:GLY:HA2	1.95	0.48
9:D:49:GLN:HG3	9:D:194:ALA:O	2.14	0.48
30:a:672:U:H2'	30:a:673:A:C8	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2197:A:H2'	30:a:2198:A:C8	2.49	0.48
35:f:117:LEU:HD21	35:f:126:LEU:HD11	1.95	0.48
6:A:476:A:C2'	6:A:478:A:H8	2.26	0.48
6:A:1112:G:H22	6:A:1131:G:H1	1.61	0.48
10:E:207:ARG:NH1	10:E:208:MET:HA	2.29	0.48
30:a:3:A:H61	30:a:3079:C:N4	2.12	0.48
30:a:2996:C:O2	30:a:3063:A:O2'	2.28	0.48
34:e:29:VAL:HG21	34:e:114:ARG:HB3	1.94	0.48
36:g:2:SER:N	36:g:55:ARG:HH12	2.11	0.48
6:A:268:G:H3'	22:Q:76:ALA:HB2	1.96	0.48
6:A:487:G:H2'	6:A:488:G:H8	1.79	0.48
6:A:693:G:OP1	11:F:54:LYS:NZ	2.36	0.48
6:A:1517:G:H2'	6:A:1518:A:O4'	2.14	0.48
12:G:141:MET:HG3	12:G:169:GLU:OE2	2.13	0.48
25:T:69:LYS:H	25:T:69:LYS:HG2	1.42	0.48
30:a:350:A:H2'	30:a:351:G:H8	1.78	0.48
30:a:814:G:C5	32:c:208:LYS:HG3	2.49	0.48
30:a:949:G:H21	30:a:951:A:N6	2.12	0.48
30:a:1251:C:H2'	30:a:1252:C:C6	2.49	0.48
30:a:2220:U:H2'	30:a:2221:C:C6	2.49	0.48
30:a:2710:U:H3'	30:a:2711:G:O4'	2.14	0.48
40:l:34:ILE:HD12	40:l:122:ILE:HG13	1.95	0.48
5:4:27:THR:O	5:4:29:GLN:N	2.47	0.48
6:A:467:G:H1'	6:A:468:U:OP2	2.13	0.48
6:A:1362:A:H2'	6:A:1363:U:O4'	2.14	0.48
9:D:182:THR:O	9:D:186:ILE:HG13	2.13	0.48
11:F:41:ASP:HB3	11:F:62:VAL:HG22	1.95	0.48
26:U:13:GLU:HA	26:U:16:ALA:HB3	1.94	0.48
26:U:43:ASP:OD1	26:U:43:ASP:N	2.46	0.48
30:a:630:U:H2'	30:a:631:G:O4'	2.14	0.48
6:A:561:U:H2'	6:A:562:C:C6	2.49	0.48
9:D:148:PRO:HB2	9:D:149:PRO:HD3	1.96	0.48
10:E:108:VAL:HG23	10:E:119:LEU:HB2	1.94	0.48
11:F:91:MET:HE2	23:R:23:TYR:HE2	1.78	0.48
12:G:39:ARG:NH1	12:G:54:ILE:O	2.45	0.48
30:a:694:C:H2'	30:a:695:C:H6	1.79	0.48
30:a:1130:G:N2	30:a:1194:A:N6	2.45	0.48
6:A:373:A:H2'	6:A:374:C:O4'	2.14	0.48
6:A:992:U:H2'	6:A:993:G:C8	2.49	0.48
6:A:1271:G:H5'	6:A:1272:G:C4	2.49	0.48
12:G:35:ASP:OD1	12:G:58:ARG:NH2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1694:U:H2'	30:a:1695:U:O4'	2.14	0.48
32:c:184:MET:HG2	32:c:268:ILE:HD11	1.95	0.48
44:p:76:TYR:CZ	44:p:80:ILE:HG13	2.48	0.48
48:t:117:LYS:C	48:t:119:GLU:H	2.22	0.48
6:A:811:G:O2'	7:B:25:PRO:HG3	2.14	0.47
6:A:861:C:H5''	13:H:85:LYS:HD2	1.96	0.47
6:A:996:C:H2'	6:A:997:A:C8	2.48	0.47
8:C:17:U:H6	8:C:17:U:H5'	1.79	0.47
9:D:14:ARG:HG2	9:D:14:ARG:HH11	1.78	0.47
12:G:3:GLN:OE1	12:G:3:GLN:N	2.47	0.47
15:J:54:ARG:HE	15:J:55:LYS:HB2	1.79	0.47
16:K:41:THR:HG22	16:K:47:VAL:HA	1.96	0.47
30:a:693:A:H2'	30:a:694:C:O4'	2.14	0.47
30:a:2468:A:H4'	30:a:2469:A:O4'	2.14	0.47
31:b:29:A:H2'	31:b:30:C:C6	2.49	0.47
39:k:92:ILE:HD12	39:k:122:ASP:HB2	1.95	0.47
39:k:121:VAL:O	39:k:141:GLY:HA3	2.13	0.47
6:A:1024:G:H2'	6:A:1025:G:C8	2.49	0.47
8:C:74:C:H2'	8:C:75:C:C6	2.48	0.47
30:a:591:A:H4'	30:a:593:A:H5'	1.95	0.47
30:a:1156:A:O2'	30:a:2656:U:O3'	2.30	0.47
30:a:1159:C:H2'	30:a:1160:A:C8	2.49	0.47
6:A:615:G:H2'	6:A:616:C:H6	1.79	0.47
6:A:1134:U:O2'	15:J:60:ARG:NH1	2.47	0.47
6:A:1338:C:H2'	6:A:1339:G:C8	2.49	0.47
9:D:172:LYS:HG3	21:P:119:ALA:HB2	1.96	0.47
30:a:50:G:H1'	30:a:117:A:H61	1.79	0.47
30:a:50:G:H1'	30:a:117:A:N6	2.29	0.47
30:a:361:G:H21	30:a:368:A:N6	2.12	0.47
30:a:631:G:H5'	30:a:632:U:C6	2.49	0.47
30:a:1454:A:O2'	30:a:1456:G:N7	2.44	0.47
30:a:2644:U:H2'	30:a:2645:U:C6	2.48	0.47
35:f:40:LEU:HD23	35:f:40:LEU:HA	1.77	0.47
53:y:40:ASP:OD1	53:y:45:ARG:NH1	2.47	0.47
7:B:215:THR:HA	7:B:218:ILE:HG12	1.95	0.47
19:N:87:TYR:O	19:N:91:ARG:HG2	2.15	0.47
26:U:20:THR:HA	26:U:23:ASN:HD21	1.80	0.47
30:a:172:U:H2'	30:a:173:A:C8	2.49	0.47
30:a:349:C:O5'	30:a:349:C:H6	1.96	0.47
30:a:349:C:H2'	30:a:350:A:C8	2.50	0.47
30:a:565:G:N1	30:a:568:A:OP2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:851:U:H2'	30:a:852:U:C6	2.49	0.47
30:a:2193:G:H5''	46:r:59:ALA:HB2	1.96	0.47
30:a:2208:G:H2'	30:a:2209:A:C8	2.48	0.47
34:e:167:ASP:O	34:e:171:VAL:HG22	2.15	0.47
36:g:29:PRO:HB2	36:g:30:LYS:NZ	2.28	0.47
36:g:79:GLY:O	36:g:83:GLY:N	2.47	0.47
51:w:40:GLU:O	51:w:41:ASN:C	2.57	0.47
54:z:35:CYS:SG	54:z:47:SER:HB2	2.55	0.47
6:A:989:G:H3'	6:A:990:A:C8	2.46	0.47
30:a:974:C:H3'	30:a:975:G:C8	2.50	0.47
30:a:1010:A:H2'	30:a:1011:A:C8	2.50	0.47
49:u:81:ASP:HB3	49:u:84:LYS:O	2.14	0.47
6:A:139:U:H2'	6:A:140:U:C6	2.49	0.47
6:A:879:G:H2'	6:A:880:C:C6	2.49	0.47
6:A:1243:G:OP1	6:A:1243:G:N2	2.46	0.47
19:N:15:LEU:O	19:N:19:LEU:HG	2.14	0.47
30:a:373:G:N2	30:a:437:G:H1	2.13	0.47
30:a:430:U:H4'	30:a:431:A:H8	1.78	0.47
50:v:18:ALA:HB3	50:v:20:ARG:NH1	2.30	0.47
3:2:19:SER:OG	30:a:737:G:OP1	2.29	0.47
6:A:494:U:H2'	6:A:495:A:H8	1.80	0.47
6:A:718:U:H2'	6:A:719:C:H6	1.79	0.47
6:A:1415:A:H2'	6:A:1416:C:C6	2.50	0.47
7:B:111:ILE:HD12	7:B:153:ARG:HA	1.97	0.47
9:D:70:TYR:OH	9:D:92:ARG:NH1	2.48	0.47
13:H:47:ALA:HB2	13:H:68:LYS:HB3	1.97	0.47
17:L:8:VAL:HG11	22:Q:45:MET:HE1	1.96	0.47
18:M:81:PRO:HA	18:M:84:VAL:HG22	1.97	0.47
21:P:117:ARG:O	21:P:121:THR:HG23	2.14	0.47
24:S:7:LYS:HB2	24:S:7:LYS:HE3	1.73	0.47
30:a:257:G:H2'	30:a:258:A:C8	2.50	0.47
30:a:620:C:H2'	30:a:620:C:O2	2.14	0.47
30:a:1835:G:O5'	41:m:39:THR:HG21	2.14	0.47
34:e:26:LEU:HD23	34:e:114:ARG:HD2	1.97	0.47
35:f:52:ALA:HA	35:f:55:ASP:O	2.14	0.47
38:j:25:LEU:HD12	38:j:38:THR:HG22	1.96	0.47
40:l:65:TRP:CZ3	40:l:107:SER:HB2	2.49	0.47
46:r:62:GLU:HB3	46:r:63:PRO:HD3	1.96	0.47
6:A:364:G:N1	6:A:367:U:OP2	2.45	0.47
6:A:537:C:H2'	6:A:538:C:H6	1.79	0.47
10:E:92:LYS:HE3	10:E:92:LYS:HB3	1.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:189:ARG:HD3	12:G:189:ARG:N	2.30	0.47
17:L:44:LYS:HA	17:L:44:LYS:HD3	1.76	0.47
22:Q:12:ARG:HG3	22:Q:70:GLU:O	2.14	0.47
26:U:22:GLN:CD	26:U:29:ASN:HB2	2.39	0.47
30:a:106:G:C4'	30:a:379:A:H5''	2.43	0.47
30:a:343:C:H2'	30:a:344:U:O4'	2.14	0.47
30:a:517:A:H2'	30:a:518:A:C8	2.49	0.47
30:a:1139:G:N2	30:a:1185:C:H3'	2.29	0.47
30:a:1364:U:H5	30:a:1402:U:O2	1.97	0.47
30:a:1391:C:H2'	30:a:1392:A:C8	2.49	0.47
30:a:1647:G:H4'	30:a:1729:G:H21	1.80	0.47
30:a:2048:G:H1'	30:a:2060:A:N6	2.30	0.47
30:a:2971:C:H1'	30:a:3071:A:C2	2.48	0.47
34:e:153:LEU:HB3	34:e:194:ARG:HB2	1.97	0.47
37:i:4:TYR:CD2	44:p:100:VAL:HG11	2.50	0.47
6:A:1120:G:H2'	6:A:1120:G:N3	2.30	0.47
6:A:1285:A:O2'	6:A:1286:G:H4'	2.15	0.47
30:a:328:G:C4	30:a:329:G:C8	3.03	0.47
30:a:658:A:OP2	30:a:2681:C:O2'	2.32	0.47
30:a:968:G:H2'	30:a:969:C:H6	1.79	0.47
31:b:94:U:H2'	31:b:95:G:H8	1.79	0.47
38:j:111:PHE:O	38:j:115:VAL:HG13	2.15	0.47
42:n:40:VAL:HG22	42:n:49:VAL:HG23	1.97	0.47
1:O:31:ARG:HB2	1:O:31:ARG:CZ	2.45	0.47
6:A:220:G:H2'	6:A:221:C:O4'	2.15	0.47
6:A:1207:G:O3'	26:U:77:THR:HG21	2.14	0.47
7:B:178:ARG:NH1	7:B:196:GLU:O	2.47	0.47
18:M:84:VAL:HG23	18:M:88:MET:HE3	1.97	0.47
30:a:1149:U:H2'	30:a:1150:G:H5''	1.97	0.47
34:e:142:GLN:HG3	34:e:170:SER:HB3	1.95	0.47
39:k:80:ASP:OD1	39:k:81:LYS:N	2.48	0.47
9:D:63:LEU:HD23	9:D:63:LEU:HA	1.75	0.46
14:I:91:VAL:HG13	14:I:95:ARG:HD2	1.96	0.46
18:M:81:PRO:O	18:M:84:VAL:HG22	2.16	0.46
30:a:669:A:N1	30:a:894:G:O2'	2.42	0.46
30:a:1715:A:N6	30:a:1723:G:C6	2.81	0.46
30:a:2651:A:H4'	40:l:56:ARG:HD3	1.97	0.46
40:l:48:GLU:OE1	40:l:51:ARG:NH1	2.47	0.46
40:l:51:ARG:HG3	40:l:66:ILE:HD11	1.96	0.46
6:A:677:A:H2'	6:A:678:A:C8	2.49	0.46
6:A:1217:A:H2'	6:A:1218:U:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:21:VAL:HG21	21:P:23:MET:HE2	1.97	0.46
21:P:55:ARG:HA	21:P:55:ARG:HD2	1.64	0.46
30:a:629:C:H2'	30:a:630:U:O4'	2.15	0.46
30:a:664:C:H2'	30:a:665:U:C6	2.50	0.46
30:a:902:C:O2'	30:a:924:U:H5''	2.16	0.46
30:a:2712:G:O2'	30:a:2715:U:O4	2.32	0.46
31:b:87:G:N2	31:b:90:A:OP2	2.38	0.46
32:c:171:LYS:HB2	32:c:171:LYS:HE2	1.82	0.46
32:c:211:ARG:HG2	32:c:214:TRP:CZ2	2.50	0.46
34:e:16:LYS:HD3	34:e:17:ALA:O	2.15	0.46
37:i:105:VAL:O	37:i:109:MET:HG2	2.15	0.46
44:p:22:SER:O	44:p:22:SER:OG	2.30	0.46
6:A:201:U:H2'	6:A:202:G:C8	2.50	0.46
6:A:272:A:H2'	6:A:273:C:C6	2.50	0.46
6:A:535:G:H2'	6:A:536:U:C6	2.51	0.46
7:B:141:GLU:O	7:B:145:LEU:HG	2.16	0.46
11:F:15:GLU:HG2	11:F:15:GLU:O	2.16	0.46
20:O:75:HIS:HA	20:O:78:GLU:HG3	1.96	0.46
25:T:48:THR:HG23	25:T:52:ARG:NH1	2.30	0.46
30:a:709:U:H2'	30:a:710:C:C6	2.51	0.46
30:a:1192:C:H3'	30:a:1193:A:C8	2.50	0.46
30:a:1730:U:H2'	30:a:1731:G:C8	2.50	0.46
57:a:3138:DXT:H423	57:a:3138:DXT:H4A	1.75	0.46
40:l:48:GLU:HA	40:l:48:GLU:OE2	2.15	0.46
6:A:1481:G:H4'	30:a:2096:A:N7	2.29	0.46
21:P:49:ILE:HG12	21:P:73:LEU:HD22	1.98	0.46
23:R:14:LYS:HE3	23:R:14:LYS:HA	1.97	0.46
30:a:356:G:O2'	30:a:357:G:O5'	2.24	0.46
30:a:372:U:H3	30:a:439:C:H42	1.62	0.46
30:a:2532:U:H2'	30:a:2533:G:O4'	2.16	0.46
30:a:2546:C:H2'	30:a:2547:G:O4'	2.16	0.46
30:a:2710:U:C4	30:a:2711:G:N3	2.84	0.46
34:e:159:VAL:HA	34:e:182:ALA:H	1.80	0.46
35:f:141:LEU:HB3	35:f:146:MET:HE1	1.97	0.46
6:A:494:U:H2'	6:A:495:A:C8	2.51	0.46
6:A:963:C:O2	24:S:19:ARG:HG2	2.16	0.46
8:C:66:C:H2'	8:C:67:C:H6	1.81	0.46
15:J:54:ARG:HB3	15:J:120:ALA:N	2.31	0.46
20:O:39:GLU:O	20:O:43:VAL:HG23	2.14	0.46
24:S:35:ARG:HG2	24:S:35:ARG:NH1	2.31	0.46
30:a:545:G:C8	47:s:73:THR:HA	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:963:A:H2'	30:a:964:G:O4'	2.15	0.46
30:a:2929:G:O6	30:a:2937:C:H5''	2.15	0.46
34:e:92:VAL:HG12	34:e:93:HIS:CG	2.50	0.46
5:4:40:LYS:HE3	5:4:40:LYS:HB3	1.65	0.46
6:A:495:A:H2'	6:A:496:C:C6	2.51	0.46
6:A:576:C:H2'	6:A:577:G:O4'	2.16	0.46
6:A:674:U:O2'	6:A:676:G:N7	2.42	0.46
6:A:1038:G:N7	6:A:1186:C:H5'	2.30	0.46
6:A:1315:A:OP1	19:N:29:ARG:HB2	2.16	0.46
9:D:15:LEU:HD23	9:D:51:ARG:HG2	1.97	0.46
30:a:147:G:H1'	30:a:1780:C:O2'	2.15	0.46
30:a:2665:C:N3	40:l:124:LYS:NZ	2.60	0.46
30:a:2862:C:H5'	33:d:200:PRO:HA	1.97	0.46
34:e:133:VAL:HG23	34:e:141:LYS:HZ2	1.80	0.46
39:k:133:GLN:O	39:k:137:GLU:HG3	2.16	0.46
6:A:10:G:H4'	6:A:300:A:H4'	1.98	0.46
6:A:675:G:C8	29:Y:13:A:H1'	2.50	0.46
9:D:19:LEU:HD13	9:D:58:TYR:HB3	1.98	0.46
9:D:172:LYS:NZ	21:P:119:ALA:HB2	2.31	0.46
11:F:43:TRP:O	11:F:46:ARG:NH1	2.49	0.46
12:G:38:ILE:HD11	12:G:90:LEU:HD13	1.97	0.46
30:a:633:G:H3'	30:a:634:U:H5'	1.96	0.46
35:f:17:TYR:HA	35:f:21:ILE:CG1	2.45	0.46
36:g:4:ILE:O	36:g:70:ARG:HG2	2.15	0.46
39:k:123:LEU:HB2	39:k:143:VAL:HG12	1.97	0.46
48:t:100:ARG:HE	48:t:100:ARG:HB3	1.45	0.46
49:u:32:VAL:HG23	49:u:42:HIS:CD2	2.50	0.46
6:A:392:U:H2'	6:A:393:G:H8	1.80	0.46
7:B:95:ARG:NH1	7:B:97:LEU:HB3	2.30	0.46
26:U:17:LYS:HD3	26:U:17:LYS:HA	1.76	0.46
30:a:78:U:H2'	30:a:79:G:C8	2.50	0.46
30:a:361:G:H1	30:a:443:G:N2	2.09	0.46
30:a:702:G:H1'	34:e:184:GLN:NE2	2.31	0.46
30:a:1724:G:H3'	30:a:1725:G:C8	2.50	0.46
30:a:2047:U:OP1	30:a:2592:G:O2'	2.27	0.46
40:l:63:LYS:HG2	49:u:120:MET:HE3	1.97	0.46
47:s:66:GLY:N	47:s:80:ASP:OD1	2.37	0.46
6:A:96:G:H2'	6:A:97:C:O4'	2.16	0.46
6:A:574:A:H2'	6:A:575:U:C6	2.51	0.46
6:A:1055:U:H2'	6:A:1056:C:C6	2.51	0.46
6:A:1421:A:H2'	6:A:1422:G:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1473:A:H2'	6:A:1474:G:C8	2.51	0.46
15:J:89:ILE:HG13	15:J:122:ARG:HH11	1.81	0.46
25:T:59:ASP:OD1	25:T:76:LYS:HD3	2.16	0.46
30:a:2025:G:H2'	30:a:2026:C:C6	2.50	0.46
30:a:3065:A:H5'	54:z:53:PRO:HB3	1.97	0.46
32:c:206:TRP:O	32:c:211:ARG:HD3	2.15	0.46
34:e:10:LEU:HD22	34:e:16:LYS:HE2	1.98	0.46
42:n:38:MET:HE2	42:n:102:PHE:HE1	1.81	0.46
6:A:1225:A:H62	6:A:1285:A:N6	2.14	0.46
7:B:144:LYS:HG3	7:B:145:LEU:N	2.31	0.46
12:G:44:LYS:HD3	12:G:44:LYS:O	2.15	0.46
12:G:182:ASP:OD1	12:G:203:LYS:HG3	2.16	0.46
30:a:254:G:H4'	30:a:475:G:C6	2.51	0.46
30:a:347:C:H3'	30:a:348:G:C8	2.45	0.46
30:a:729:A:N1	30:a:2551:A:O2'	2.43	0.46
30:a:1084:A:H2'	30:a:1085:G:O4'	2.16	0.46
35:f:127:ASN:O	35:f:137:TYR:OH	2.24	0.46
6:A:428:U:H2'	6:A:429:U:C6	2.50	0.45
6:A:923:G:H2'	6:A:924:C:C6	2.51	0.45
15:J:170:TYR:OH	15:J:172:LYS:HB2	2.16	0.45
30:a:2366:U:C2	30:a:2367:G:C8	3.03	0.45
42:n:34:GLU:OE1	42:n:34:GLU:N	2.27	0.45
42:n:42:ARG:HB2	42:n:113:ILE:HD11	1.97	0.45
6:A:1020:G:H3'	6:A:1021:G:H8	1.80	0.45
6:A:1433:A:O2'	6:A:1434:A:H5'	2.16	0.45
6:A:1522:C:C6	6:A:1523:C:C5	3.04	0.45
12:G:83:ALA:O	12:G:86:VAL:HG12	2.16	0.45
17:L:72:HIS:CD2	17:L:74:LEU:HG	2.51	0.45
30:a:1350:G:O2'	30:a:1351:U:H3'	2.17	0.45
30:a:2453:G:OP1	50:v:18:ALA:HB1	2.16	0.45
6:A:695:G:H2'	6:A:696:G:C8	2.51	0.45
6:A:995:U:H2'	6:A:996:C:C6	2.51	0.45
9:D:120:VAL:HB	9:D:125:VAL:HG21	1.98	0.45
14:I:131:LEU:HD23	14:I:131:LEU:H	1.80	0.45
17:L:38:TYR:HE1	17:L:54:ARG:HG2	1.80	0.45
30:a:440:A:H2'	30:a:441:C:C6	2.52	0.45
30:a:750:U:H2'	30:a:751:C:C6	2.51	0.45
30:a:1014:G:H1'	53:y:25:ARG:HD2	1.98	0.45
30:a:1167:A:N6	30:a:1168:A:N1	2.63	0.45
30:a:1995:A:H2'	30:a:1996:C:C6	2.51	0.45
35:f:55:ASP:HB3	35:f:58:VAL:HG23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:187:LYS:HB2	35:f:187:LYS:HE2	1.73	0.45
36:g:69:THR:O	36:g:73:ILE:HG12	2.15	0.45
49:u:32:VAL:HG23	49:u:42:HIS:HD2	1.80	0.45
49:u:108:ARG:HG3	49:u:138:VAL:HG21	1.98	0.45
6:A:60:U:H2'	6:A:61:G:C8	2.51	0.45
6:A:90:U:H2'	6:A:91:G:C8	2.51	0.45
6:A:1396:A:H5''	30:a:2098:3TD:H10	1.97	0.45
9:D:167:GLU:HG3	9:D:176:LEU:HD12	1.99	0.45
12:G:130:ARG:H	12:G:130:ARG:HG3	1.58	0.45
14:I:91:VAL:CG1	14:I:95:ARG:HD2	2.47	0.45
17:L:16:ILE:HD12	17:L:16:ILE:N	2.32	0.45
21:P:10:LEU:HD21	21:P:19:ARG:HD2	1.97	0.45
30:a:203:A:C2	39:k:49:PHE:HZ	2.34	0.45
30:a:1407:U:H2'	30:a:1409:C:C5	2.51	0.45
30:a:1774:C:H2'	30:a:1775:G:N3	2.32	0.45
30:a:2042:A:N6	30:a:2066:G:O2'	2.50	0.45
31:b:94:U:H2'	31:b:95:G:C8	2.51	0.45
48:t:119:GLU:HG2	48:t:119:GLU:O	2.16	0.45
6:A:1020:G:H3'	6:A:1021:G:C8	2.52	0.45
6:A:1213:A:C8	19:N:117:VAL:HG11	2.52	0.45
6:A:1285:A:H2'	6:A:1285:A:N3	2.32	0.45
7:B:223:ALA:HA	7:B:226:LEU:CD2	2.46	0.45
23:R:41:ALA:O	23:R:45:THR:HG23	2.17	0.45
25:T:8:ILE:O	25:T:11:VAL:HG22	2.16	0.45
30:a:723:A:H4'	30:a:724:G:O5'	2.17	0.45
30:a:1657:U:H1'	30:a:1915:G:N2	2.32	0.45
30:a:2933:G:H4'	36:g:4:ILE:CD1	2.46	0.45
30:a:2982:U:OP2	30:a:2983:C:N4	2.50	0.45
45:q:14:VAL:HB	45:q:97:VAL:HG21	1.98	0.45
2:1:14:ARG:NH1	30:a:856:G:OP1	2.49	0.45
6:A:45:G:H2'	6:A:46:G:H8	1.81	0.45
6:A:113:G:H1'	6:A:356:G:H5'	1.98	0.45
6:A:917:G:N7	14:I:3:ARG:NH1	2.59	0.45
6:A:1271:G:H4'	6:A:1272:G:O5'	2.17	0.45
6:A:1521:A:N3	6:A:1521:A:H2'	2.31	0.45
10:E:156:ALA:O	10:E:160:VAL:HG23	2.17	0.45
15:J:83:ASN:C	15:J:85:VAL:H	2.24	0.45
30:a:367:A:H2'	30:a:368:A:C8	2.52	0.45
30:a:1687:G:H2'	30:a:1688:U:H5	1.81	0.45
30:a:1917:U:H2'	30:a:1918:G:C8	2.51	0.45
30:a:2264:A:H2'	30:a:2265:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2415:U:H2'	30:a:2416:G:C8	2.52	0.45
33:d:182:GLN:HB3	33:d:196:ARG:HD2	1.99	0.45
3:2:52:LYS:HB2	3:2:52:LYS:HE3	1.71	0.45
6:A:77:G:C2	6:A:78:G:H1'	2.52	0.45
6:A:938:G:H2'	6:A:939:A:C8	2.52	0.45
6:A:1274:A:H2'	6:A:1275:A:C8	2.51	0.45
9:D:166:LEU:HD21	9:D:175:ILE:HG23	1.98	0.45
17:L:122:GLU:OE1	17:L:122:GLU:HA	2.16	0.45
29:Y:14:A:H3'	29:Y:15:A:H8	1.82	0.45
30:a:968:G:H2'	30:a:969:C:C6	2.52	0.45
30:a:1002:A:H5''	31:b:98:G:O2'	2.16	0.45
30:a:1199:U:H2'	30:a:1200:U:C6	2.51	0.45
34:e:191:VAL:HG11	39:k:8:LEU:HD11	1.99	0.45
38:j:53:LYS:HA	38:j:53:LYS:HD3	1.64	0.45
6:A:562:C:H2'	6:A:563:G:O4'	2.17	0.45
6:A:745:G:H2'	6:A:746:C:C6	2.51	0.45
6:A:929:G:C2	6:A:930:A:C8	3.04	0.45
6:A:1301:U:H2'	6:A:1302:G:O4'	2.16	0.45
9:D:82:GLY:HA3	9:D:192:GLU:HG3	1.99	0.45
9:D:183:ARG:HD2	9:D:183:ARG:HA	1.70	0.45
21:P:44:ALA:HB3	21:P:47:SER:HA	1.99	0.45
26:U:13:GLU:O	26:U:13:GLU:HG2	2.17	0.45
30:a:406:G:OP2	34:e:138:PRO:HA	2.17	0.45
30:a:415:A:H2	30:a:1286:G:O2'	1.99	0.45
30:a:479:A:H4'	30:a:480:A:O5'	2.16	0.45
30:a:1137:A:N6	30:a:1189:G:O6	2.50	0.45
30:a:2977:A:H2	30:a:2982:U:H5	1.64	0.45
7:B:68:LEU:HD23	7:B:159:PRO:HB3	1.99	0.45
11:F:47:ARG:HA	11:F:57:GLU:OE1	2.16	0.45
11:F:69:PRO:O	11:F:72:ILE:HG22	2.16	0.45
15:J:66:GLY:HA3	15:J:104:ASP:HB2	1.99	0.45
25:T:48:THR:HG23	25:T:52:ARG:HH12	1.82	0.45
30:a:2651:A:H61	30:a:2663:G:H1'	1.81	0.45
30:a:2739:G:H2'	30:a:2740:C:C6	2.52	0.45
41:m:70:ILE:O	41:m:71:THR:OG1	2.30	0.45
52:x:34:GLN:HB3	52:x:40:LEU:HB2	1.99	0.45
6:A:162:A:H2'	6:A:163:A:C8	2.52	0.45
6:A:1248:G:H2'	6:A:1249:C:C6	2.51	0.45
12:G:102:ILE:N	12:G:102:ILE:HD12	2.32	0.45
14:I:115:THR:HG22	14:I:117:ALA:H	1.82	0.45
26:U:14:HIS:N	26:U:14:HIS:CD2	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:881:A:H2'	30:a:882:C:C6	2.52	0.45
30:a:1031:C:H1'	30:a:1067:G:C8	2.52	0.45
30:a:1470:U:H2'	30:a:1471:A:O4'	2.17	0.45
30:a:2627:2MG:OP1	34:e:77:ARG:NH2	2.41	0.45
30:a:2844:A:H2'	30:a:2845:G:O4'	2.17	0.45
34:e:125:ARG:HH21	34:e:195:THR:HG21	1.82	0.45
49:u:129:GLN:OE1	49:u:130:ALA:N	2.50	0.45
3:2:26:LYS:HD3	3:2:48:THR:HB	1.97	0.44
6:A:155:U:H2'	6:A:156:U:C6	2.52	0.44
6:A:451:C:H2'	6:A:452:G:O4'	2.17	0.44
6:A:454:A:H5''	6:A:455:G:H21	1.81	0.44
6:A:1130:G:N2	6:A:1132:A:H62	2.15	0.44
6:A:1211:U:H2'	6:A:1212:C:C5	2.53	0.44
23:R:34:SER:HA	23:R:40:ARG:HH11	1.82	0.44
24:S:32:SER:OG	24:S:41:ARG:HG3	2.17	0.44
28:X:30:ARG:HA	28:X:30:ARG:HD3	1.78	0.44
30:a:166:A:N3	30:a:2390:C:O2'	2.46	0.44
30:a:167:A:OP2	30:a:168:U:O2'	2.27	0.44
30:a:332:U:H2'	30:a:333:U:O4'	2.16	0.44
30:a:388:G:H2'	30:a:389:U:C6	2.52	0.44
30:a:432:A:H2'	30:a:433:G:O4'	2.18	0.44
30:a:2490:G:H2'	30:a:2490:G:N3	2.31	0.44
49:u:100:LYS:HB3	49:u:129:GLN:NE2	2.33	0.44
49:u:126:ILE:HD12	49:u:126:ILE:HA	1.77	0.44
53:y:12:SER:HB3	53:y:32:ILE:HD11	1.98	0.44
6:A:1038:G:H5''	6:A:1186:C:H5	1.83	0.44
6:A:1415:A:H2'	6:A:1416:C:H6	1.81	0.44
7:B:141:GLU:HA	7:B:144:LYS:HG2	2.00	0.44
30:a:406:G:N7	34:e:137:LYS:NZ	2.51	0.44
30:a:1154:G:O2'	30:a:1155:C:O4'	2.29	0.44
30:a:1837:G:C8	41:m:6:LYS:HG3	2.52	0.44
30:a:2041:G:C8	30:a:2067:A:N3	2.86	0.44
30:a:2511:G:H2'	30:a:2512:U:C6	2.52	0.44
3:2:6:SER:OG	30:a:250:U:OP1	2.35	0.44
6:A:161:A:H1'	6:A:346:A:N7	2.33	0.44
6:A:615:G:H2'	6:A:616:C:C6	2.52	0.44
6:A:828:A:H8	6:A:828:A:OP2	2.01	0.44
6:A:1186:C:H5''	6:A:1187:A:H3'	1.98	0.44
7:B:152:ILE:HD12	7:B:152:ILE:H	1.82	0.44
7:B:213:LEU:O	7:B:217:ILE:HG23	2.18	0.44
15:J:81:PHE:HD1	15:J:86:HIS:HE2	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:27:ASP:HB3	18:M:31:ARG:NH2	2.31	0.44
19:N:70:LEU:O	19:N:74:VAL:HG23	2.17	0.44
21:P:123:LYS:HG3	21:P:124:SER:N	2.31	0.44
23:R:34:SER:HA	23:R:40:ARG:NH1	2.31	0.44
30:a:426:A:H2'	30:a:427:C:O4'	2.17	0.44
30:a:1608:C:O2'	30:a:1752:A:OP2	2.22	0.44
30:a:2859:U:H2'	30:a:2860:G:C8	2.52	0.44
6:A:9:U:H1'	6:A:10:G:C2	2.53	0.44
6:A:161:A:H2'	6:A:162:A:O4'	2.17	0.44
6:A:810:A:N3	7:B:25:PRO:HG2	2.32	0.44
6:A:1154:C:H3'	6:A:1155:A:C8	2.49	0.44
12:G:11:ARG:NH1	12:G:176:THR:O	2.51	0.44
14:I:57:ASP:HB3	14:I:60:GLN:HG2	2.00	0.44
15:J:172:LYS:O	15:J:173:ARG:HB3	2.16	0.44
30:a:373:G:H22	30:a:437:G:H1	1.65	0.44
30:a:917:U:H2'	30:a:918:G:C8	2.53	0.44
30:a:974:C:H3'	30:a:975:G:H8	1.83	0.44
30:a:1199:U:H2'	30:a:1200:U:H6	1.82	0.44
30:a:1907:A:H2	30:a:1918:G:H22	1.65	0.44
30:a:2008:A:H2'	30:a:2009:C:C6	2.53	0.44
34:e:157:LEU:HD11	34:e:185:LEU:HD21	1.99	0.44
45:q:75:LYS:HD2	45:q:84:LYS:HD2	2.00	0.44
6:A:688:A:H2	16:K:47:VAL:HG21	1.83	0.44
11:F:22:LEU:O	11:F:25:LYS:HG2	2.18	0.44
12:G:189:ARG:HH11	12:G:194:ARG:NH2	2.15	0.44
30:a:311:A:O2'	30:a:312:U:OP1	2.34	0.44
30:a:1861:A:H2'	30:a:1862:A:C8	2.52	0.44
30:a:1973:C:H2'	30:a:1974:A:C5	2.53	0.44
30:a:2041:G:H2'	30:a:2042:A:O4'	2.17	0.44
30:a:2484:U:O2'	35:f:132:ASP:O	2.30	0.44
30:a:2663:G:H4'	30:a:2664:A:OP2	2.18	0.44
38:j:108:GLU:O	38:j:110:LYS:HG2	2.17	0.44
6:A:214:G:H2'	6:A:215:U:C6	2.53	0.44
10:E:91:LYS:HZ3	10:E:91:LYS:HG3	1.74	0.44
11:F:91:MET:HE2	23:R:23:TYR:CE2	2.51	0.44
13:H:101:LEU:HD22	13:H:135:TRP:HB2	1.99	0.44
18:M:15:HIS:O	18:M:18:ILE:HG22	2.17	0.44
19:N:102:ARG:HE	19:N:105:THR:HG22	1.83	0.44
26:U:46:GLY:HA2	26:U:61:PHE:CE1	2.52	0.44
28:X:33:LYS:HE3	28:X:33:LYS:HB2	1.82	0.44
30:a:51:A:H2'	30:a:52:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:201:G:H2'	30:a:202:A:O4'	2.18	0.44
30:a:2455:A:H2'	30:a:2456:A:C8	2.53	0.44
6:A:710:A:H2'	6:A:711:A:C8	2.53	0.44
6:A:1400:A:H2	6:A:1474:G:H22	1.66	0.44
6:A:1525:C:O2'	6:A:1526:C:H5''	2.18	0.44
7:B:229:ARG:HB3	7:B:233:LYS:NZ	2.33	0.44
9:D:165:TRP:CE2	9:D:181:PRO:HB3	2.52	0.44
10:E:204:ALA:O	10:E:208:MET:HE3	2.17	0.44
11:F:55:LYS:HB2	11:F:55:LYS:HE2	1.70	0.44
13:H:106:ILE:HB	13:H:117:THR:HG23	2.00	0.44
15:J:125:ILE:O	15:J:129:LEU:HG	2.18	0.44
25:T:51:ALA:O	25:T:55:ASN:ND2	2.47	0.44
30:a:344:U:O2'	30:a:347:C:N4	2.51	0.44
30:a:896:U:H2'	39:k:23:ARG:HA	2.00	0.44
30:a:976:G:H2'	30:a:977:C:H6	1.80	0.44
30:a:1917:U:H2'	30:a:1918:G:H8	1.83	0.44
30:a:2230:C:H2'	30:a:2231:A:C8	2.53	0.44
30:a:3055:U:H4'	43:o:2:SER:HA	2.00	0.44
6:A:751:G:H4'	6:A:1500:A:H4'	2.00	0.44
6:A:822:C:H2'	6:A:823:A:H8	1.80	0.44
6:A:1300:C:H2'	6:A:1301:U:H6	1.81	0.44
7:B:104:PHE:CD1	7:B:104:PHE:C	2.96	0.44
12:G:41:TRP:CZ3	12:G:42:LEU:HD23	2.53	0.44
21:P:66:PRO:HG2	21:P:80:TRP:HZ3	1.82	0.44
25:T:49:LYS:O	25:T:53:VAL:HG23	2.17	0.44
30:a:649:U:H2'	30:a:650:U:O4'	2.18	0.44
30:a:834:A:H4'	30:a:1348:G:N3	2.32	0.44
30:a:1690:A:H4'	30:a:1691:A:OP1	2.17	0.44
30:a:2149:A:N3	30:a:2774:G:O2'	2.49	0.44
32:c:23:GLU:OE2	32:c:23:GLU:N	2.40	0.44
45:q:14:VAL:HG12	45:q:20:VAL:HG21	1.99	0.44
6:A:32:G:O2'	6:A:298:U:OP1	2.33	0.44
6:A:487:G:H2'	6:A:488:G:C8	2.52	0.44
30:a:631:G:H2'	30:a:633:G:C8	2.53	0.44
30:a:806:U:H2'	30:a:807:C:C6	2.53	0.44
30:a:1629:C:H5'	30:a:1727:G:H1'	2.00	0.44
30:a:2036:A:H2'	30:a:2037:A:C8	2.53	0.44
30:a:2066:G:H2'	30:a:2067:A:C5	2.53	0.44
6:A:108:A:C2	25:T:10:ARG:HG3	2.53	0.43
6:A:271:U:H2'	6:A:272:A:H8	1.82	0.43
6:A:499:G:N1	6:A:515:A:OP2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:717:U:H2'	6:A:718:U:C6	2.53	0.43
6:A:733:U:H2'	6:A:734:G:O4'	2.18	0.43
18:M:82:LYS:HE2	18:M:82:LYS:HB2	1.87	0.43
20:O:45:LYS:HE2	20:O:45:LYS:HB3	1.75	0.43
30:a:1619:A:H2'	30:a:1620:G:O4'	2.18	0.43
30:a:2651:A:H2'	30:a:2652:G:O4'	2.17	0.43
30:a:2773:C:H2'	30:a:2774:G:H8	1.82	0.43
33:d:57:GLY:O	33:d:58:TYR:HB3	2.18	0.43
49:u:58:ASN:N	49:u:59:PRO:HD3	2.33	0.43
7:B:134:GLU:HG2	7:B:137:MET:HE2	2.00	0.43
7:B:222:ALA:O	7:B:226:LEU:HD23	2.18	0.43
10:E:122:ALA:HB2	10:E:147:LEU:HD13	1.99	0.43
30:a:1368:G:H2'	30:a:1369:U:C6	2.53	0.43
30:a:2880:U:H2'	30:a:2881:U:C6	2.53	0.43
57:a:3123:DXT:H413	57:a:3123:DXT:H4A	1.65	0.43
35:f:26:GLN:HE21	35:f:26:GLN:C	2.21	0.43
36:g:51:ILE:HD13	36:g:51:ILE:HA	1.88	0.43
38:j:9:LYS:O	38:j:83:ALA:HA	2.18	0.43
42:n:104:LYS:HE2	42:n:107:ASN:O	2.17	0.43
6:A:645:A:H2'	6:A:646:G:O4'	2.19	0.43
6:A:845:G:H5'	13:H:19:GLN:NE2	2.33	0.43
6:A:1134:U:H3'	6:A:1135:C:C6	2.53	0.43
6:A:1411:U:H2'	6:A:1412:A:C8	2.52	0.43
26:U:22:GLN:NE2	26:U:26:GLY:O	2.51	0.43
30:a:60:G:O4'	52:x:43:THR:HG23	2.18	0.43
30:a:171:A:H2'	30:a:172:U:C6	2.53	0.43
30:a:254:G:H4'	30:a:475:G:C5	2.53	0.43
30:a:1481:C:H2'	30:a:1482:G:C8	2.53	0.43
57:a:3146:DXT:H413	57:a:3146:DXT:H4A	1.59	0.43
34:e:133:VAL:HG23	34:e:141:LYS:HD3	1.99	0.43
45:q:91:LYS:H	45:q:91:LYS:HG2	1.54	0.43
49:u:97:ARG:HD3	49:u:97:ARG:HA	1.81	0.43
6:A:335:C:H2'	6:A:336:C:H6	1.83	0.43
6:A:1071:U:H3	6:A:1084:G:H22	1.67	0.43
12:G:114:LEU:HD13	12:G:114:LEU:HA	1.86	0.43
30:a:92:G:H2'	30:a:93:C:O4'	2.19	0.43
34:e:16:LYS:HD3	34:e:17:ALA:N	2.33	0.43
38:j:110:LYS:HD2	38:j:111:PHE:CE2	2.53	0.43
5:4:14:VAL:HG13	5:4:22:PHE:O	2.19	0.43
6:A:1137:G:H4'	18:M:70:HIS:HE1	1.81	0.43
7:B:4:VAL:HG13	7:B:7:ARG:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:110:ARG:HA	7:B:113:ARG:HD2	2.00	0.43
11:F:27:LEU:HD22	11:F:37:VAL:HG11	1.99	0.43
11:F:57:GLU:OE1	11:F:57:GLU:HA	2.18	0.43
30:a:718:A:H2'	30:a:719:A:C8	2.53	0.43
30:a:1264:G:H5'	45:q:82:TYR:CE1	2.54	0.43
30:a:2230:C:H2'	30:a:2231:A:H8	1.84	0.43
34:e:56:THR:O	34:e:60:VAL:HG23	2.19	0.43
6:A:895:U:H2'	6:A:896:C:C6	2.53	0.43
6:A:988:G:N2	6:A:1022:U:O2	2.52	0.43
8:C:9:G:O2'	8:C:10:G:N7	2.36	0.43
11:F:69:PRO:O	11:F:73:GLN:HG3	2.18	0.43
18:M:6:ILE:HD12	18:M:102:LEU:HD13	2.00	0.43
30:a:827:U:H2'	30:a:828:C:C6	2.53	0.43
30:a:2726:G:H1'	30:a:2828:C:H5'	2.01	0.43
35:f:24:ALA:O	35:f:27:GLU:HG3	2.18	0.43
36:g:135:VAL:HG23	36:g:143:VAL:HG13	2.00	0.43
6:A:94:G:N2	6:A:96:G:OP2	2.52	0.43
6:A:401:G:H2'	6:A:402:C:C6	2.54	0.43
6:A:987:G:H2'	6:A:988:G:N7	2.34	0.43
6:A:1505:MA6:H2'	6:A:1506:MA6:C8	2.49	0.43
9:D:48:LEU:HD23	9:D:51:ARG:HH21	1.84	0.43
10:E:104:ILE:HG23	10:E:170:LEU:HD11	2.00	0.43
12:G:100:LEU:HD23	12:G:100:LEU:H	1.83	0.43
30:a:305:U:O2'	30:a:307:U:H1'	2.19	0.43
30:a:924:U:H2'	30:a:925:U:C6	2.53	0.43
30:a:1275:U:H2'	30:a:1276:C:C6	2.53	0.43
30:a:2094:PSU:H2'	30:a:2101:A:N1	2.34	0.43
30:a:2509:A:H2'	30:a:2510:A:C8	2.54	0.43
37:i:125:TYR:OH	37:i:132:HIS:NE2	2.39	0.43
46:r:1:MET:HB3	46:r:3:LYS:HZ1	1.84	0.43
6:A:439:U:H2'	6:A:440:U:C6	2.54	0.43
6:A:795:U:H2'	6:A:796:A:H5''	2.01	0.43
6:A:1305:A:C8	6:A:1309:G:C6	3.07	0.43
8:C:66:C:H2'	8:C:67:C:C6	2.54	0.43
9:D:166:LEU:HD23	9:D:167:GLU:N	2.33	0.43
10:E:131:GLY:O	10:E:135:ARG:HB3	2.19	0.43
15:J:109:ILE:HD12	15:J:109:ILE:N	2.34	0.43
30:a:365:G:O3'	30:a:366:A:H4'	2.19	0.43
30:a:2540:A:H2'	30:a:2541:C:O4'	2.18	0.43
5:4:52:LEU:HB3	5:4:53:ASP:H	1.69	0.43
6:A:1248:G:H2'	6:A:1249:C:H6	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1396:A:H1'	6:A:1479:A:H61	1.84	0.43
7:B:73:LYS:HD3	7:B:165:VAL:HG12	2.01	0.43
9:D:25:SER:O	9:D:27:GLU:N	2.52	0.43
16:K:41:THR:HG22	16:K:47:VAL:HG22	2.01	0.43
21:P:13:ILE:O	21:P:14:ARG:HG2	2.19	0.43
22:Q:23:LYS:H	22:Q:23:LYS:HG2	1.61	0.43
30:a:172:U:H2'	30:a:173:A:H8	1.84	0.43
30:a:178:U:H2'	30:a:179:G:O4'	2.19	0.43
30:a:684:G:H2'	30:a:685:C:C6	2.54	0.43
30:a:1618:U:H2'	30:a:1619:A:H8	1.84	0.43
30:a:2819:U:H2'	30:a:2820:G:O4'	2.18	0.43
34:e:143:ALA:O	34:e:147:LEU:HG	2.19	0.43
38:j:14:THR:HB	38:j:52:VAL:HG21	2.00	0.43
39:k:138:LYS:C	39:k:138:LYS:HD3	2.44	0.43
6:A:325:U:H2'	6:A:326:G:O4'	2.19	0.43
6:A:1014:U:H4'	6:A:1015:U:O4'	2.19	0.43
7:B:107:ILE:HD12	7:B:107:ILE:HA	1.79	0.43
19:N:113:LYS:HA	19:N:113:LYS:HD2	1.73	0.43
30:a:1252:C:H2'	30:a:1253:U:C6	2.53	0.43
30:a:1392:A:H2'	30:a:1393:G:C8	2.53	0.43
30:a:2980:G:H2'	30:a:2981:U:C2	2.54	0.43
31:b:42:C:C6	35:f:75:GLN:HB2	2.54	0.43
34:e:121:ALA:HB2	34:e:126:ILE:HD12	2.01	0.43
40:l:63:LYS:HD3	40:l:65:TRP:CZ2	2.53	0.43
2:1:24:THR:O	2:1:28:ARG:HG3	2.19	0.42
6:A:55:A:N7	6:A:114:U:O2'	2.48	0.42
6:A:1227:G:H2'	6:A:1228:G:H8	1.83	0.42
10:E:87:VAL:O	10:E:91:LYS:HG2	2.18	0.42
30:a:1171:A:H4'	30:a:1172:G:H8	1.84	0.42
30:a:2178:U:H3'	30:a:2179:C:H2'	2.00	0.42
30:a:2272:A:O2'	51:w:51:THR:HG21	2.19	0.42
34:e:11:ASP:OD2	34:e:200:GLN:HG3	2.19	0.42
38:j:107:ARG:HG3	38:j:107:ARG:NH1	2.34	0.42
6:A:624:A:C5	13:H:112:SER:HA	2.54	0.42
14:I:99:LEU:HD12	14:I:103:TRP:CZ2	2.54	0.42
30:a:325:G:H2'	30:a:326:G:C8	2.54	0.42
30:a:855:G:H2'	30:a:856:G:O4'	2.19	0.42
30:a:1859:C:O2	33:d:139:THR:HB	2.19	0.42
31:b:52:U:H1'	31:b:53:C:H5	1.83	0.42
7:B:58:LYS:HE2	7:B:58:LYS:HA	2.01	0.42
17:L:36:ARG:HB3	17:L:54:ARG:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:263:A:H2'	30:a:264:A:H8	1.82	0.42
30:a:273:G:N2	30:a:516:U:H1'	2.33	0.42
30:a:1014:G:H3'	30:a:1015:U:C6	2.54	0.42
30:a:2384:G:N2	30:a:2398:G:OP1	2.52	0.42
30:a:2500:G:H5''	30:a:2501:G:OP2	2.19	0.42
30:a:2766:U:H2'	30:a:2767:U:H2'	2.00	0.42
39:k:130:LYS:HB2	39:k:130:LYS:HE2	1.84	0.42
1:0:29:ASN:C	1:0:31:ARG:H	2.28	0.42
6:A:412:G:H21	6:A:434:A:H62	1.66	0.42
6:A:1332:A:H2'	14:I:10:ARG:HH21	1.84	0.42
46:r:4:THR:O	46:r:5:GLU:HG2	2.19	0.42
6:A:564:U:H2'	6:A:565:A:C8	2.55	0.42
6:A:920:C:C2	6:A:921:A:C8	3.07	0.42
7:B:218:ILE:HG13	7:B:219:ALA:N	2.33	0.42
8:C:23:C:H2'	8:C:24:U:C6	2.54	0.42
24:S:33:VAL:HG13	24:S:39:LEU:O	2.19	0.42
30:a:251:A:H2'	30:a:252:G:O4'	2.20	0.42
30:a:359:C:O2'	30:a:360:A:O4'	2.36	0.42
30:a:936:U:H2'	30:a:937:G:H8	1.85	0.42
30:a:1095:U:H5'	30:a:1096:G:H5''	2.01	0.42
30:a:1194:A:P	30:a:1194:A:H8	2.42	0.42
30:a:1750:A:OP2	32:c:84:TYR:OH	2.32	0.42
30:a:2185:U:H2'	30:a:2186:G:C8	2.55	0.42
30:a:3077:U:H2'	30:a:3078:U:C6	2.54	0.42
49:u:156:ASP:OD1	49:u:156:ASP:N	2.40	0.42
6:A:867:C:O2'	6:A:868:U:H5'	2.19	0.42
6:A:942:A:C2	26:U:55:ARG:HB3	2.54	0.42
6:A:1131:G:N2	6:A:1133:C:H41	2.18	0.42
14:I:88:PRO:HG3	14:I:149:ARG:HA	2.01	0.42
15:J:63:ILE:HD12	15:J:63:ILE:O	2.20	0.42
30:a:2584:G:OP2	30:a:2584:G:N2	2.34	0.42
30:a:2655:C:OP1	30:a:2657:C:N4	2.52	0.42
30:a:2719:U:H2'	30:a:2720:C:C6	2.55	0.42
30:a:2749:G:H2'	30:a:2750:C:C6	2.55	0.42
31:b:34:G:O2'	31:b:35:U:OP2	2.34	0.42
32:c:213:ARG:HD2	32:c:213:ARG:HA	1.70	0.42
35:f:14:LYS:HD3	35:f:106:TRP:CD1	2.55	0.42
35:f:78:LYS:HE2	35:f:78:LYS:HB2	1.71	0.42
38:j:64:ARG:O	38:j:82:ASN:HA	2.20	0.42
42:n:38:MET:HE2	42:n:102:PHE:CE1	2.55	0.42
45:q:57:LYS:HE3	45:q:57:LYS:HB3	1.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:59:THR:HG23	45:q:98:THR:OG1	2.18	0.42
47:s:5:LYS:HA	52:x:57:TYR:CZ	2.55	0.42
6:A:1340:C:H2'	6:A:1341:A:H8	1.84	0.42
7:B:72:THR:O	7:B:77:GLN:NE2	2.52	0.42
9:D:141:ARG:NH2	9:D:144:SER:HB3	2.31	0.42
9:D:147:LEU:HB3	9:D:150:ILE:HG13	2.01	0.42
12:G:72:PRO:HB3	12:G:102:ILE:HG21	2.02	0.42
21:P:120:ILE:HA	21:P:123:LYS:HG2	2.02	0.42
30:a:183:G:O2'	30:a:184:U:H5'	2.19	0.42
30:a:338:U:O2'	30:a:339:U:O5'	2.34	0.42
30:a:2474:U:H2'	30:a:2475:C:C6	2.53	0.42
30:a:2612:A:H2'	30:a:2612:A:N3	2.35	0.42
42:n:17:ALA:O	42:n:21:ARG:HG3	2.19	0.42
6:A:183:G:N2	6:A:226:G:O5'	2.53	0.42
6:A:1050:U:H4'	6:A:1051:C:O5'	2.20	0.42
6:A:1291:G:N2	6:A:1317:G:H1'	2.35	0.42
11:F:75:LEU:O	11:F:79:LEU:HG	2.20	0.42
12:G:149:ARG:HG2	12:G:168:ARG:HB3	2.01	0.42
24:S:37:PHE:CE1	24:S:44:LEU:HD22	2.55	0.42
30:a:38:C:H2'	30:a:39:C:C6	2.55	0.42
30:a:938:U:H2'	30:a:939:U:C6	2.54	0.42
31:b:7:G:O2'	42:n:41:THR:HG21	2.20	0.42
32:c:72:LYS:HE3	32:c:99:ASP:OD2	2.19	0.42
3:2:23:THR:HG22	3:2:49:VAL:HG22	2.01	0.42
3:2:25:ARG:HB3	39:k:61:PRO:HG2	2.01	0.42
6:A:1138:U:H4'	18:M:15:HIS:NE2	2.34	0.42
6:A:1356:C:H2'	6:A:1357:G:C8	2.55	0.42
16:K:112:GLU:H	16:K:112:GLU:HG3	1.71	0.42
17:L:68:PRO:O	17:L:99:ARG:NH1	2.49	0.42
19:N:4:LEU:HG	19:N:22:ILE:HD11	2.02	0.42
30:a:373:G:N2	30:a:437:G:H22	2.18	0.42
30:a:1036:G:O2'	30:a:2448:A:OP2	2.36	0.42
30:a:1050:U:H2'	30:a:1051:C:C6	2.54	0.42
30:a:1691:A:H2'	30:a:1691:A:N3	2.35	0.42
30:a:2284:G:N2	30:a:2370:C:C2	2.88	0.42
30:a:2415:U:H2'	30:a:2416:G:H8	1.85	0.42
30:a:2833:U:H2'	30:a:2834:U:C6	2.55	0.42
32:c:20:ASP:OD1	32:c:20:ASP:N	2.43	0.42
34:e:26:LEU:HD21	34:e:210:ARG:O	2.19	0.42
34:e:184:GLN:HE21	34:e:184:GLN:CA	2.30	0.42
36:g:52:LEU:HD12	36:g:52:LEU:HA	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:m:81:THR:HG22	41:m:82:GLU:OE2	2.19	0.42
6:A:45:G:H2'	6:A:46:G:C8	2.54	0.42
11:F:12:PRO:HA	11:F:59:ILE:HD11	2.01	0.42
24:S:16:PHE:HD2	24:S:19:ARG:HH11	1.68	0.42
30:a:373:G:N3	30:a:438:G:N2	2.68	0.42
30:a:474:C:O2'	30:a:477:G:N2	2.53	0.42
30:a:1052:G:H2'	30:a:1053:U:C6	2.54	0.42
30:a:1465:G:H2'	30:a:1466:U:C6	2.55	0.42
30:a:1984:G:C6	30:a:2385:U:H5''	2.55	0.42
30:a:2140:C:H2'	30:a:2141:C:C6	2.55	0.42
6:A:828:A:H4'	23:R:17:HIS:CD2	2.55	0.41
6:A:1345:C:OP2	24:S:35:ARG:NE	2.53	0.41
7:B:49:TYR:HD2	7:B:202:PRO:HD3	1.85	0.41
12:G:90:LEU:O	12:G:94:THR:HG23	2.19	0.41
14:I:113:GLU:CD	14:I:114:LYS:H	2.28	0.41
19:N:91:ARG:HB2	19:N:98:VAL:HG12	2.02	0.41
30:a:1092:A:N3	30:a:1237:C:O2'	2.50	0.41
30:a:1345:A:H2'	30:a:1346:G:O4'	2.20	0.41
30:a:1650:A:H2'	30:a:1651:A:H8	1.79	0.41
30:a:3026:G:H2'	30:a:3027:U:C6	2.55	0.41
31:b:25:A:H2'	31:b:26:A:C8	2.55	0.41
36:g:107:PHE:HB2	36:g:115:VAL:CG2	2.50	0.41
38:j:88:LYS:HD2	38:j:94:ARG:HA	2.01	0.41
49:u:62:SER:OG	49:u:64:GLU:OE2	2.30	0.41
53:y:11:LYS:HD2	53:y:11:LYS:HA	1.82	0.41
6:A:893:A:H2'	6:A:894:C:O4'	2.21	0.41
6:A:1138:U:H4'	18:M:15:HIS:CD2	2.55	0.41
6:A:1226:U:OP2	14:I:115:THR:HG23	2.20	0.41
6:A:1236:A:H2	6:A:1357:G:H1'	1.85	0.41
6:A:1341:A:H2'	6:A:1342:G:C8	2.54	0.41
11:F:82:ASP:HB3	11:F:85:ILE:HD12	2.02	0.41
21:P:6:ARG:NH1	21:P:25:SER:HA	2.35	0.41
24:S:6:LEU:HA	24:S:6:LEU:HD12	1.83	0.41
30:a:1992:A:H2'	30:a:1993:A:C8	2.55	0.41
30:a:2784:A:H4'	30:a:2785:G:C5'	2.50	0.41
30:a:2982:U:H5''	30:a:2983:C:H5	1.83	0.41
34:e:83:ALA:HB3	34:e:86:TRP:CD1	2.55	0.41
34:e:133:VAL:HA	34:e:141:LYS:NZ	2.35	0.41
39:k:88:LYS:HA	39:k:88:LYS:HD3	1.88	0.41
40:l:32:TYR:CE1	40:l:111:GLU:HG3	2.54	0.41
6:A:266:U:H2'	6:A:267:G:O4'	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:454:A:N1	21:P:93:LYS:HA	2.35	0.41
6:A:1053:G:N2	6:A:1093:G:H1'	2.34	0.41
6:A:1246:G:H2'	6:A:1247:A:H8	1.84	0.41
10:E:197:LYS:O	10:E:201:GLU:HG3	2.21	0.41
11:F:34:LYS:HE2	11:F:34:LYS:HB2	1.94	0.41
30:a:342:G:H2'	30:a:343:C:O4'	2.21	0.41
30:a:581:G:H2'	30:a:582:G:O4'	2.20	0.41
30:a:2287:G:N2	30:a:2367:G:C2	2.88	0.41
42:n:44:SER:O	42:n:77:LYS:NZ	2.52	0.41
6:A:1225:A:H62	6:A:1285:A:H61	1.68	0.41
7:B:82:GLU:HA	7:B:85:THR:HG22	2.02	0.41
9:D:145:LYS:CG	21:P:122:LYS:HE3	2.50	0.41
15:J:56:GLU:O	15:J:56:GLU:HG3	2.19	0.41
30:a:382:U:H2'	30:a:383:G:O4'	2.20	0.41
30:a:2094:PSU:H2'	30:a:2101:A:C2	2.56	0.41
30:a:2286:C:O5'	30:a:2286:C:H6	2.03	0.41
30:a:2561:G:H2'	30:a:2562:U:C6	2.55	0.41
30:a:2695:G:H2'	30:a:2696:U:C6	2.56	0.41
31:b:13:A:N1	31:b:69:G:O2'	2.44	0.41
33:d:20:LEU:O	33:d:27:LEU:HD12	2.21	0.41
35:f:161:MET:HE2	35:f:161:MET:HB3	1.91	0.41
48:t:40:GLY:HA2	48:t:43:ILE:HD11	2.02	0.41
48:t:117:LYS:O	48:t:118:LYS:HB3	2.20	0.41
6:A:476:A:HO2'	6:A:478:A:H8	1.67	0.41
6:A:655:G:H5''	11:F:87:ARG:NH1	2.35	0.41
6:A:1479:A:H4'	6:A:1480:A:C6	2.55	0.41
12:G:110:THR:O	12:G:201:ILE:HD13	2.20	0.41
15:J:47:PRO:HB3	15:J:64:THR:HA	2.02	0.41
15:J:83:ASN:HB2	15:J:85:VAL:HG23	2.02	0.41
18:M:34:ALA:HA	18:M:78:GLU:CB	2.50	0.41
30:a:2084:A:H2'	30:a:2085:C:C6	2.54	0.41
30:a:2598:C:OP1	39:k:64:GLY:HA3	2.20	0.41
30:a:2807:G:H2'	30:a:2808:C:C6	2.54	0.41
30:a:2830:G:H2'	30:a:2831:U:C6	2.55	0.41
31:b:28:C:H2'	31:b:29:A:O4'	2.20	0.41
38:j:67:LYS:O	38:j:68:SER:HB2	2.20	0.41
39:k:79:LEU:HD23	39:k:79:LEU:HA	1.88	0.41
41:m:5:THR:HG21	41:m:17:GLU:OE2	2.20	0.41
42:n:48:PHE:CD1	42:n:64:SER:HB3	2.52	0.41
45:q:47:THR:HG22	45:q:53:LEU:HD22	2.01	0.41
48:t:84:LYS:HA	48:t:84:LYS:HD3	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:y:22:GLU:OE1	53:y:25:ARG:NH2	2.51	0.41
6:A:482:G:H2'	6:A:483:C:C6	2.55	0.41
6:A:544:U:H1'	17:L:12:ARG:HB3	2.02	0.41
6:A:603:A:H2'	6:A:604:A:C8	2.56	0.41
6:A:1012:U:H3	6:A:1015:U:H3	1.66	0.41
6:A:1112:G:N2	6:A:1131:G:H1	2.19	0.41
6:A:1192:G:H2'	6:A:1193:C:O4'	2.21	0.41
6:A:1451:G:H2'	6:A:1452:U:H6	1.86	0.41
6:A:1505:MA6:H103	6:A:1506:MA6:H102	2.02	0.41
12:G:2:GLY:N	12:G:3:GLN:OE1	2.53	0.41
12:G:53:SER:C	12:G:54:ILE:HD13	2.46	0.41
14:I:27:VAL:HG21	14:I:40:GLN:HB3	2.02	0.41
14:I:72:SER:OG	14:I:73:LEU:HD12	2.21	0.41
16:K:35:ASN:HB3	16:K:63:LYS:HG3	2.02	0.41
23:R:34:SER:OG	23:R:35:GLU:N	2.52	0.41
30:a:357:G:N2	30:a:446:G:O6	2.53	0.41
30:a:504:A:H2'	30:a:505:C:C6	2.56	0.41
30:a:1125:G:H1	30:a:1196:U:H3	1.69	0.41
30:a:1133:A:C4	30:a:1134:A:C8	3.08	0.41
30:a:1224:U:OP2	37:i:68:LYS:NZ	2.53	0.41
30:a:1391:C:H2'	30:a:1392:A:H8	1.86	0.41
32:c:133:LEU:HD23	32:c:136:ILE:HD12	2.02	0.41
35:f:17:TYR:O	35:f:18:ARG:C	2.63	0.41
39:k:131:SER:O	39:k:135:LYS:HG3	2.21	0.41
41:m:72:ASP:OD2	41:m:75:ILE:HG12	2.20	0.41
4:3:22:ARG:CZ	4:3:35:ARG:HD3	2.51	0.41
6:A:78:G:H22	6:A:95:U:H3	1.66	0.41
6:A:339:G:H2'	6:A:340:A:C8	2.55	0.41
6:A:584:A:H2'	6:A:585:A:C8	2.55	0.41
6:A:1349:A:H5'	6:A:1350:A:H2'	2.03	0.41
7:B:19:GLN:H	7:B:19:GLN:HG2	1.73	0.41
9:D:57:ARG:HG2	9:D:67:PHE:CD1	2.56	0.41
9:D:102:LEU:HD12	9:D:150:ILE:HD13	2.02	0.41
10:E:172:GLU:HB3	10:E:175:GLU:CD	2.46	0.41
10:E:194:ARG:O	10:E:198:GLU:HG2	2.20	0.41
15:J:89:ILE:O	15:J:122:ARG:HB2	2.20	0.41
16:K:77:GLY:O	16:K:81:MET:HG2	2.20	0.41
30:a:130:G:H1	30:a:154:G:H1	1.69	0.41
30:a:659:U:H2'	30:a:660:G:C8	2.56	0.41
30:a:672:U:O2'	30:a:673:A:H5'	2.20	0.41
30:a:1147:C:H6	30:a:1147:C:O5'	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1491:C:C2	30:a:1492:C:H5	2.39	0.41
30:a:2128:G:H2'	30:a:2129:U:C6	2.56	0.41
31:b:113:G:H2'	31:b:114:C:C6	2.56	0.41
32:c:226:MET:HB3	32:c:230:ASP:HB2	2.03	0.41
33:d:8:LYS:HB2	33:d:8:LYS:HE2	1.89	0.41
34:e:137:LYS:H	34:e:137:LYS:CD	2.33	0.41
35:f:179:LEU:HG	35:f:184:PHE:CD1	2.55	0.41
46:r:101:ARG:HA	57:r:201:DXT:H612	2.01	0.41
48:t:82:ASP:O	48:t:84:LYS:HE2	2.20	0.41
1:0:7:ASP:OD1	1:0:7:ASP:N	2.54	0.41
6:A:942:A:N7	26:U:55:ARG:NH2	2.69	0.41
6:A:1236:A:H2'	6:A:1237:G:C8	2.55	0.41
15:J:70:TRP:CD1	15:J:105:VAL:HG21	2.56	0.41
17:L:73:ASN:OD1	17:L:105:GLN:HG2	2.21	0.41
22:Q:67:ARG:HH21	22:Q:86:ILE:HD11	1.86	0.41
23:R:18:ILE:HD11	23:R:21:VAL:HG12	2.03	0.41
30:a:663:C:H2'	30:a:664:C:H6	1.82	0.41
30:a:987:U:H2'	30:a:988:C:C6	2.56	0.41
30:a:1481:C:H2'	30:a:1482:G:H8	1.86	0.41
30:a:3009:G:H5''	33:d:83:ARG:NH1	2.36	0.41
31:b:66:A:N6	31:b:108:A:H2'	2.36	0.41
5:4:20:ASN:CG	5:4:40:LYS:HD2	2.46	0.41
6:A:95:U:O2	6:A:95:U:H2'	2.20	0.41
6:A:149:G:O2'	6:A:1433:A:N3	2.46	0.41
6:A:234:A:H2'	6:A:235:C:H6	1.86	0.41
6:A:454:A:N7	21:P:47:SER:HB3	2.36	0.41
6:A:739:U:H2'	6:A:740:G:O4'	2.20	0.41
6:A:843:U:H2'	6:A:844:A:C8	2.56	0.41
6:A:955:G:N1	6:A:1350:A:OP2	2.52	0.41
6:A:1333:G:O6	15:J:54:ARG:NH2	2.53	0.41
6:A:1387:5MC:O2'	6:A:1388:G:OP1	2.33	0.41
6:A:1428:G:H2'	6:A:1430:C:N4	2.36	0.41
14:I:24:SER:O	14:I:27:VAL:HG12	2.21	0.41
18:M:39:PRO:HG3	18:M:74:ILE:HD11	2.03	0.41
18:M:41:PRO:HA	18:M:72:ARG:HD3	2.02	0.41
19:N:40:SER:O	19:N:43:LEU:HD22	2.21	0.41
25:T:5:LYS:HA	25:T:8:ILE:HD12	2.01	0.41
30:a:11:G:O6	30:a:613:U:H2'	2.21	0.41
30:a:145:G:H2'	30:a:146:U:C6	2.55	0.41
30:a:437:G:H2'	30:a:438:G:C8	2.56	0.41
30:a:900:C:OP1	45:q:84:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1110:A:N1	30:a:1210:U:H5	2.19	0.41
30:a:1256:G:H2'	30:a:1257:U:O4'	2.21	0.41
30:a:1612:G:H2'	30:a:1613:U:C6	2.56	0.41
30:a:1862:A:H2'	30:a:1863:A:H8	1.82	0.41
30:a:2041:G:H2'	30:a:2042:A:C8	2.55	0.41
30:a:2098:3TD:H2'	30:a:2099:A:O4'	2.21	0.41
30:a:2200:U:O2'	30:a:2202:C:OP2	2.29	0.41
30:a:2429:A:H2'	30:a:2430:C:H6	1.85	0.41
30:a:2583:U:H2'	30:a:2584:G:O4'	2.21	0.41
30:a:2630:A:O2'	30:a:2631:H2U:H52	2.21	0.41
30:a:3075:C:H2'	30:a:3076:U:C6	2.56	0.41
30:a:3078:U:H2'	30:a:3079:C:H6	1.83	0.41
31:b:90:A:C2	31:b:91:U:H1'	2.55	0.41
34:e:137:LYS:HB2	34:e:170:SER:OG	2.20	0.41
34:e:174:LEU:HD23	34:e:174:LEU:HA	1.80	0.41
36:g:12:PRO:HD2	36:g:15:VAL:HG21	2.02	0.41
36:g:45:LYS:HD2	36:g:45:LYS:HA	1.77	0.41
38:j:64:ARG:HB2	38:j:83:ALA:HB3	2.02	0.41
53:y:45:ARG:HA	53:y:45:ARG:HD2	1.85	0.41
5:4:27:THR:O	5:4:28:SER:C	2.64	0.41
6:A:584:A:H2'	6:A:585:A:H8	1.85	0.41
6:A:1010:C:H2'	6:A:1011:C:C6	2.56	0.41
6:A:1271:G:H1'	6:A:1272:G:OP2	2.21	0.41
14:I:115:THR:HB	14:I:118:GLU:OE1	2.21	0.41
14:I:125:LEU:HD23	14:I:125:LEU:HA	1.91	0.41
16:K:22:VAL:O	16:K:24:ALA:N	2.53	0.41
22:Q:45:MET:HB3	22:Q:45:MET:HE3	1.73	0.41
23:R:12:PRO:O	23:R:14:LYS:HD2	2.21	0.41
30:a:784:A:H4'	30:a:1818:U:C4	2.56	0.41
30:a:1853:A:C8	38:j:5:GLU:HG3	2.56	0.41
30:a:1897:G:H3'	30:a:1898:C:H5''	2.01	0.41
30:a:2140:C:H2'	30:a:2141:C:H6	1.86	0.41
30:a:2651:A:N6	30:a:2663:G:H1'	2.35	0.41
30:a:2933:G:H4'	36:g:4:ILE:HD12	2.03	0.41
31:b:90:A:O2'	40:l:17:ARG:NE	2.53	0.41
34:e:13:LYS:HA	34:e:13:LYS:HD2	1.88	0.41
35:f:171:THR:HG22	35:f:173:GLU:OE2	2.21	0.41
39:k:130:LYS:O	39:k:134:GLU:HG3	2.21	0.41
41:m:118:ASP:OD1	41:m:118:ASP:N	2.53	0.41
48:t:103:ASP:OD1	48:t:105:SER:OG	2.33	0.41
49:u:100:LYS:HD2	49:u:100:LYS:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:27:THR:CG2	35:f:71:GLY:HA2	2.51	0.40
6:A:833:U:H2'	6:A:834:U:C6	2.56	0.40
6:A:1128:G:H3'	6:A:1129:G:C8	2.49	0.40
6:A:1360:G:P	15:J:115:THR:HG21	2.60	0.40
10:E:205:ALA:HA	10:E:208:MET:CE	2.37	0.40
16:K:29:ILE:HB	16:K:92:VAL:HG12	2.04	0.40
30:a:711:G:N7	39:k:104:ARG:NH2	2.65	0.40
30:a:751:C:H2'	30:a:752:U:C6	2.56	0.40
30:a:824:A:H1'	30:a:825:C:H5	1.87	0.40
30:a:838:U:H2'	30:a:839:G:C8	2.55	0.40
30:a:2119:A:OP1	30:a:2120:A:H5'	2.21	0.40
34:e:144:LYS:HA	34:e:147:LEU:HG	2.03	0.40
36:g:89:GLU:OE1	36:g:167:GLU:HA	2.22	0.40
53:y:2:MET:HE1	53:y:39:GLU:HG3	2.03	0.40
6:A:7:A:N1	10:E:192:MET:HG3	2.36	0.40
6:A:347:C:OP1	43:o:39:ARG:HD2	2.22	0.40
10:E:149:LYS:HA	10:E:149:LYS:HD2	1.90	0.40
17:L:36:ARG:HG2	17:L:38:TYR:CD1	2.57	0.40
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.86	0.40
30:a:631:G:H5'	30:a:632:U:H6	1.86	0.40
30:a:1867:C:H2'	30:a:1868:C:C6	2.56	0.40
37:i:4:TYR:CG	44:p:100:VAL:HG11	2.56	0.40
42:n:11:LEU:O	42:n:12:SER:C	2.64	0.40
6:A:1264:G:H4'	6:A:1265:A:O4'	2.22	0.40
6:A:1291:G:H22	6:A:1317:G:H1'	1.86	0.40
7:B:117:LEU:HD11	7:B:145:LEU:HD21	2.03	0.40
9:D:165:TRP:CE3	9:D:181:PRO:HD3	2.56	0.40
11:F:14:VAL:CG1	11:F:18:GLN:HB2	2.52	0.40
15:J:89:ILE:HG13	15:J:122:ARG:NH1	2.37	0.40
18:M:36:VAL:HG12	18:M:76:ILE:HA	2.02	0.40
30:a:643:C:H2'	30:a:644:G:O4'	2.21	0.40
30:a:2042:A:H2'	30:a:2043:A:O4'	2.21	0.40
30:a:2066:G:H2'	30:a:2067:A:C4	2.56	0.40
30:a:3035:U:H2'	30:a:3036:C:C6	2.57	0.40
34:e:155:LYS:NZ	34:e:190:VAL:HA	2.36	0.40
35:f:51:ASP:HB2	35:f:58:VAL:HG11	2.02	0.40
36:g:78:ILE:HA	36:g:81:THR:HG22	2.04	0.40
54:z:35:CYS:SG	54:z:48:CYS:CB	3.07	0.40
5:4:43:PRO:O	5:4:44:PHE:C	2.64	0.40
5:4:62:GLU:OE2	5:4:62:GLU:HA	2.20	0.40
6:A:94:G:N3	6:A:95:U:H3'	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:48:VAL:HG21	10:E:53:ARG:CZ	2.51	0.40
10:E:189:PRO:HG2	10:E:192:MET:HB2	2.03	0.40
11:F:9:ILE:HD12	11:F:87:ARG:HB3	2.03	0.40
12:G:123:LEU:HD23	12:G:195:ILE:HD11	2.02	0.40
14:I:57:ASP:HB3	14:I:60:GLN:CG	2.51	0.40
14:I:138:ARG:HH21	14:I:139:GLU:HG2	1.86	0.40
19:N:70:LEU:HD12	19:N:70:LEU:HA	1.89	0.40
26:U:27:THR:HG23	26:U:47:HIS:NE2	2.36	0.40
30:a:339:U:H5''	30:a:340:C:C5	2.56	0.40
30:a:356:G:HO2'	30:a:357:G:P	2.42	0.40
30:a:488:U:H2'	30:a:489:G:O4'	2.21	0.40
30:a:961:C:H2'	30:a:962:U:C6	2.57	0.40
30:a:1094:G:OP2	44:p:66:ASN:ND2	2.46	0.40
30:a:1232:U:H2'	30:a:1233:C:C6	2.57	0.40
30:a:1395:G:H2'	30:a:1396:U:C6	2.57	0.40
30:a:2289:U:H6	30:a:2289:U:P	2.45	0.40
30:a:2384:G:H4'	30:a:2385:U:OP2	2.22	0.40
30:a:2722:C:H2'	30:a:2723:A:O4'	2.20	0.40
32:c:261:LYS:HB3	32:c:261:LYS:HE2	1.70	0.40
35:f:189:LYS:HD2	35:f:190:ASP:O	2.21	0.40
38:j:17:LYS:HE2	38:j:45:ASP:OD2	2.21	0.40
45:q:89:ARG:HA	45:q:89:ARG:HD2	1.67	0.40
46:r:62:GLU:OE1	46:r:65:ARG:NH1	2.54	0.40
6:A:527:C:H2'	6:A:528:G:O4'	2.22	0.40
6:A:1392:G:O4'	6:A:1506:MA6:H4'	2.21	0.40
10:E:102:ARG:HA	10:E:102:ARG:HD3	1.84	0.40
15:J:84:LYS:HD2	15:J:84:LYS:N	2.36	0.40
21:P:4:LYS:HB2	21:P:6:ARG:HD2	2.03	0.40
23:R:25:ASP:OD1	23:R:25:ASP:C	2.65	0.40
30:a:348:G:C2	30:a:349:C:C4	3.10	0.40
30:a:933:U:H2'	30:a:934:C:H6	1.86	0.40
30:a:1139:G:H2'	30:a:1185:C:H41	1.87	0.40
30:a:1172:G:H22	30:a:1185:C:N4	2.19	0.40
30:a:1285:G:O2'	30:a:1314:A:N1	2.52	0.40
30:a:1688:U:O2	30:a:1690:A:H5''	2.21	0.40
30:a:2754:A:O2'	30:a:2757:C:OP1	2.30	0.40
30:a:2843:G:H2'	30:a:2844:A:C8	2.56	0.40
31:b:43:C:O2	35:f:101:ARG:NH1	2.53	0.40
36:g:55:ARG:NH2	36:g:58:ASP:OD1	2.54	0.40
38:j:4:GLN:HE21	38:j:5:GLU:HG2	1.87	0.40
47:s:4:LEU:HG	47:s:5:LYS:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
4	3	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
5	4	64/69 (93%)	54 (84%)	9 (14%)	1 (2%)	7	11
7	B	231/283 (82%)	207 (90%)	23 (10%)	1 (0%)	30	43
9	D	198/201 (98%)	185 (93%)	12 (6%)	1 (0%)	24	37
10	E	177/215 (82%)	168 (95%)	8 (4%)	1 (1%)	21	32
11	F	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	11	18
12	G	204/269 (76%)	195 (96%)	9 (4%)	0	100	100
13	H	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
14	I	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
15	J	132/173 (76%)	120 (91%)	12 (9%)	0	100	100
16	K	115/135 (85%)	105 (91%)	8 (7%)	2 (2%)	7	10
17	L	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
18	M	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	20
19	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
20	O	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
21	P	126/147 (86%)	113 (90%)	12 (10%)	1 (1%)	16	25
22	Q	88/90 (98%)	81 (92%)	7 (8%)	0	100	100
23	R	65/79 (82%)	61 (94%)	4 (6%)	0	100	100
24	S	58/61 (95%)	53 (91%)	5 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	76 (93%)	5 (6%)	1 (1%)	10	16
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
28	X	30/33 (91%)	28 (93%)	1 (3%)	1 (3%)	3	2
32	c	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
33	d	212/223 (95%)	202 (95%)	9 (4%)	1 (0%)	24	37
34	e	208/301 (69%)	179 (86%)	26 (12%)	3 (1%)	9	13
35	f	182/210 (87%)	174 (96%)	8 (4%)	0	100	100
36	g	175/180 (97%)	163 (93%)	12 (7%)	0	100	100
37	i	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
38	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
39	k	142/146 (97%)	119 (84%)	22 (16%)	1 (1%)	18	28
40	l	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
41	m	118/187 (63%)	111 (94%)	5 (4%)	2 (2%)	7	10
42	n	124/127 (98%)	118 (95%)	5 (4%)	1 (1%)	16	25
43	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
44	p	117/123 (95%)	114 (97%)	2 (2%)	1 (1%)	14	22
45	q	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
46	r	130/153 (85%)	126 (97%)	4 (3%)	0	100	100
47	s	93/102 (91%)	85 (91%)	7 (8%)	1 (1%)	11	18
48	t	103/122 (84%)	95 (92%)	7 (7%)	1 (1%)	12	20
49	u	177/205 (86%)	164 (93%)	13 (7%)	0	100	100
50	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
51	w	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	10
52	x	67/77 (87%)	63 (94%)	4 (6%)	0	100	100
53	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
54	z	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
All	All	5646/6322 (89%)	5302 (94%)	321 (6%)	23 (0%)	31	43

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	X	4	VAL
34	e	133	VAL
34	e	151	ALA
34	e	159	VAL
44	p	93	LYS
5	4	28	SER
26	U	84	VAL
41	m	37	THR
42	n	5	LEU
7	B	100	MET
9	D	26	PHE
10	E	113	ALA
11	F	16	GLU
18	M	6	ILE
51	w	8	CYS
21	P	97	GLU
33	d	215	LYS
39	k	124	VAL
47	s	93	ARG
48	t	64	ILE
16	K	23	VAL
41	m	70	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/51 (92%)	45 (96%)	2 (4%)	26	44
2	1	36/36 (100%)	33 (92%)	3 (8%)	10	17
3	2	54/55 (98%)	54 (100%)	0	100	100
4	3	35/35 (100%)	34 (97%)	1 (3%)	37	60
5	4	56/59 (95%)	48 (86%)	8 (14%)	3	4
7	B	197/234 (84%)	184 (93%)	13 (7%)	15	26
9	D	175/176 (99%)	169 (97%)	6 (3%)	32	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	E	130/155 (84%)	124 (95%)	6 (5%)	24	41
11	F	89/89 (100%)	86 (97%)	3 (3%)	32	54
12	G	160/200 (80%)	153 (96%)	7 (4%)	25	43
13	H	108/109 (99%)	103 (95%)	5 (5%)	24	41
14	I	132/133 (99%)	125 (95%)	7 (5%)	20	36
15	J	97/131 (74%)	89 (92%)	8 (8%)	10	18
16	K	88/101 (87%)	85 (97%)	3 (3%)	32	54
17	L	103/104 (99%)	98 (95%)	5 (5%)	22	39
18	M	89/93 (96%)	85 (96%)	4 (4%)	24	42
19	N	99/100 (99%)	94 (95%)	5 (5%)	21	37
20	O	74/74 (100%)	70 (95%)	4 (5%)	20	35
21	P	103/115 (90%)	93 (90%)	10 (10%)	8	12
22	Q	81/81 (100%)	77 (95%)	4 (5%)	22	39
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	52
24	S	48/49 (98%)	42 (88%)	6 (12%)	4	6
25	T	68/69 (99%)	65 (96%)	3 (4%)	25	43
26	U	72/80 (90%)	65 (90%)	7 (10%)	8	12
27	V	16/17 (94%)	15 (94%)	1 (6%)	16	29
28	X	28/29 (97%)	27 (96%)	1 (4%)	31	52
32	c	216/220 (98%)	210 (97%)	6 (3%)	38	60
33	d	166/172 (96%)	161 (97%)	5 (3%)	36	58
34	e	165/237 (70%)	150 (91%)	15 (9%)	9	14
35	f	154/175 (88%)	146 (95%)	8 (5%)	21	36
36	g	150/152 (99%)	142 (95%)	8 (5%)	20	36
37	i	118/120 (98%)	116 (98%)	2 (2%)	53	74
38	j	101/101 (100%)	96 (95%)	5 (5%)	22	38
39	k	111/113 (98%)	103 (93%)	8 (7%)	13	23
40	l	108/110 (98%)	101 (94%)	7 (6%)	15	27
41	m	100/142 (70%)	95 (95%)	5 (5%)	22	38
42	n	95/96 (99%)	91 (96%)	4 (4%)	26	45
43	o	97/99 (98%)	88 (91%)	9 (9%)	8	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	70
45	q	84/84 (100%)	78 (93%)	6 (7%)	13	23
46	r	105/118 (89%)	99 (94%)	6 (6%)	18	33
47	s	84/89 (94%)	81 (96%)	3 (4%)	31	52
48	t	91/103 (88%)	86 (94%)	5 (6%)	19	34
49	u	149/168 (89%)	144 (97%)	5 (3%)	32	54
50	v	60/67 (90%)	58 (97%)	2 (3%)	33	55
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	49
52	x	61/68 (90%)	58 (95%)	3 (5%)	22	39
53	y	53/55 (96%)	51 (96%)	2 (4%)	29	49
54	z	51/52 (98%)	49 (96%)	2 (4%)	28	48
All	All	4709/5133 (92%)	4465 (95%)	244 (5%)	22	36

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	VAL
1	0	13	THR
2	1	10	ARG
2	1	29	SER
2	1	39	ARG
4	3	14	CYS
5	4	14	VAL
5	4	23	THR
5	4	27	THR
5	4	40	LYS
5	4	41	CYS
5	4	52	LEU
5	4	57	ARG
5	4	58	VAL
7	B	19	GLN
7	B	30	PHE
7	B	57	VAL
7	B	89	MET
7	B	111	ILE
7	B	120	MET
7	B	130	LEU
7	B	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	B	162	VAL
7	B	188	LEU
7	B	197	VAL
7	B	208	ILE
7	B	227	MET
9	D	24	LYS
9	D	43	ASP
9	D	49	GLN
9	D	52	GLU
9	D	169	ARG
9	D	188	ILE
10	E	47	VAL
10	E	53	ARG
10	E	91	LYS
10	E	118	MET
10	E	133	SER
10	E	151	LEU
11	F	36	THR
11	F	81	ILE
11	F	91	MET
12	G	11	ARG
12	G	63	VAL
12	G	114	LEU
12	G	130	ARG
12	G	165	GLU
12	G	191	THR
12	G	192	PHE
13	H	23	ASP
13	H	25	THR
13	H	53	GLU
13	H	62	THR
13	H	66	THR
14	I	12	VAL
14	I	14	VAL
14	I	23	VAL
14	I	30	ILE
14	I	53	LYS
14	I	56	THR
14	I	80	VAL
15	J	63	ILE
15	J	72	ILE
15	J	104	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	J	117	GLN
15	J	130	ASN
15	J	138	ARG
15	J	146	MET
15	J	173	ARG
16	K	86	LYS
16	K	87	ARG
16	K	125	ASN
17	L	13	THR
17	L	18	LYS
17	L	64	THR
17	L	72	HIS
17	L	104	THR
18	M	16	GLU
18	M	44	THR
18	M	84	VAL
18	M	92	LEU
19	N	4	LEU
19	N	28	THR
19	N	42	ASP
19	N	49	THR
19	N	69	ASP
20	O	1	MET
20	O	7	LYS
20	O	15	THR
20	O	42	LYS
21	P	10	LEU
21	P	12	LYS
21	P	14	ARG
21	P	34	ILE
21	P	43	LYS
21	P	56	VAL
21	P	75	LYS
21	P	93	LYS
21	P	104	LEU
21	P	125	GLU
22	Q	1	MET
22	Q	14	VAL
22	Q	18	LEU
22	Q	83	VAL
23	R	35	GLU
23	R	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	S	6	LEU
24	S	18	VAL
24	S	37	PHE
24	S	42	ILE
24	S	53	LEU
24	S	57	THR
25	T	52	ARG
25	T	63	SER
25	T	77	SER
26	U	13	GLU
26	U	14	HIS
26	U	15	LEU
26	U	45	ILE
26	U	62	VAL
26	U	64	GLU
26	U	65	SER
27	V	3	LYS
28	X	30	ARG
32	c	71	ASP
32	c	73	ASP
32	c	83	GLU
32	c	122	GLU
32	c	166	VAL
32	c	264	SER
33	d	7	VAL
33	d	28	VAL
33	d	64	LYS
33	d	106	VAL
33	d	190	ARG
34	e	6	THR
34	e	7	ILE
34	e	13	LYS
34	e	26	LEU
34	e	61	SER
34	e	77	ARG
34	e	104	THR
34	e	114	ARG
34	e	134	ASP
34	e	142	GLN
34	e	154	ARG
34	e	157	LEU
34	e	176	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	e	184	GLN
34	e	185	LEU
35	f	10	MET
35	f	26	GLN
35	f	41	GLU
35	f	83	ILE
35	f	126	LEU
35	f	146	MET
35	f	153	ASP
35	f	180	LYS
36	g	4	ILE
36	g	19	LEU
36	g	32	THR
36	g	80	VAL
36	g	87	LYS
36	g	91	GLN
36	g	116	ILE
36	g	131	THR
37	i	55	VAL
37	i	98	ARG
38	j	9	LYS
38	j	47	ILE
38	j	81	GLU
38	j	116	SER
38	j	120	GLU
39	k	19	THR
39	k	36	THR
39	k	103	VAL
39	k	114	THR
39	k	118	THR
39	k	131	SER
39	k	142	SER
39	k	143	VAL
40	l	6	ARG
40	l	18	THR
40	l	89	THR
40	l	94	ILE
40	l	107	SER
40	l	113	VAL
40	l	118	MET
41	m	5	THR
41	m	37	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	m	56	LYS
41	m	57	THR
41	m	69	THR
42	n	5	LEU
42	n	14	ARG
42	n	51	VAL
42	n	101	VAL
43	o	10	LYS
43	o	16	ASP
43	o	27	LYS
43	o	49	SER
43	o	65	SER
43	o	76	LEU
43	o	87	ASP
43	o	109	LYS
43	o	115	SER
44	p	46	SER
44	p	59	SER
45	q	22	ILE
45	q	32	SER
45	q	35	LEU
45	q	65	GLU
45	q	84	LYS
45	q	95	VAL
46	r	16	ASP
46	r	28	ARG
46	r	41	VAL
46	r	48	ASP
46	r	79	GLU
46	r	103	ARG
47	s	75	VAL
47	s	81	THR
47	s	88	VAL
48	t	7	LYS
48	t	25	GLU
48	t	35	ARG
48	t	45	LYS
48	t	98	THR
49	u	64	GLU
49	u	77	ASP
49	u	126	ILE
49	u	138	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	u	147	GLU
50	v	38	VAL
50	v	83	VAL
51	w	8	CYS
51	w	54	LEU
52	x	32	ARG
52	x	40	LEU
52	x	43	THR
53	y	34	ASP
53	y	36	VAL
54	z	35	CYS
54	z	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	34	ASN
7	B	24	ASN
7	B	75	GLN
7	B	191	ASN
9	D	135	HIS
9	D	193	GLN
10	E	169	GLN
13	H	19	GLN
14	I	68	ASN
14	I	148	ASN
15	J	130	ASN
16	K	83	HIS
16	K	124	HIS
18	M	64	HIS
19	N	63	ASN
24	S	31	HIS
25	T	7	GLN
32	c	135	ASN
32	c	203	ASN
33	d	180	ASN
33	d	182	GLN
34	e	43	GLN
34	e	102	GLN
34	e	142	GLN
34	e	184	GLN
35	f	20	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	f	75	GLN
35	f	97	HIS
35	f	127	ASN
36	g	22	GLN
36	g	34	ASN
36	g	91	GLN
37	i	47	HIS
38	j	3	GLN
38	j	4	GLN
39	k	44	ASN
40	l	13	HIS
44	p	20	GLN
44	p	81	ASN
44	p	117	GLN
49	u	11	GLN
49	u	58	ASN
50	v	17	ASN
53	y	20	HIS
54	z	19	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	6 (66%)	0
30	a	2894/3086 (93%)	511 (17%)	0
31	b	117/120 (97%)	13 (11%)	0
6	A	1511/1537 (98%)	300 (19%)	27 (1%)
8	C	74/76 (97%)	10 (13%)	1 (1%)
All	All	4605/4841 (95%)	840 (18%)	28 (0%)

All (840) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	8	U
6	A	9	U
6	A	10	G
6	A	11	G
6	A	13	G
6	A	36	A
6	A	43	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	51	C
6	A	52	U
6	A	54	A
6	A	55	A
6	A	58	C
6	A	73	G
6	A	75	A
6	A	78	G
6	A	82	U
6	A	91	G
6	A	92	G
6	A	93	G
6	A	95	U
6	A	100	G
6	A	116	A
6	A	120	A
6	A	121	C
6	A	143	C
6	A	150	A
6	A	164	C
6	A	173	A
6	A	174	U
6	A	175	A
6	A	178	G
6	A	183	G
6	A	184	G
6	A	185	A
6	A	192	G
6	A	199	G
6	A	213	A
6	A	214	G
6	A	219	G
6	A	220	G
6	A	222	G
6	A	226	G
6	A	247	C
6	A	249	G
6	A	253	G
6	A	268	G
6	A	269	C
6	A	283	G
6	A	291	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	318	U
6	A	321	G
6	A	323	A
6	A	331	A
6	A	354	C
6	A	356	G
6	A	369	U
6	A	374	C
6	A	386	G
6	A	399	A
6	A	400	C
6	A	408	G
6	A	414	U
6	A	415	G
6	A	416	A
6	A	423	U
6	A	424	C
6	A	425	G
6	A	431	U
6	A	440	U
6	A	441	U
6	A	461	G
6	A	463	G
6	A	467	G
6	A	468	U
6	A	476	A
6	A	478	A
6	A	491	A
6	A	493	C
6	A	500	C
6	A	503	G
6	A	513	U
6	A	514	G
6	A	515	A
6	A	529	A
6	A	541	A
6	A	544	U
6	A	546	U
6	A	554	A
6	A	555	A
6	A	558	G
6	A	559	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	578	C
6	A	600	C
6	A	602	U
6	A	614	U
6	A	615	G
6	A	632	A
6	A	634	U
6	A	635	U
6	A	647	G
6	A	685	G
6	A	703	A
6	A	704	G
6	A	705	U
6	A	716	G
6	A	729	U
6	A	737	G
6	A	743	G
6	A	759	A
6	A	775	U
6	A	776	A
6	A	791	G
6	A	794	G
6	A	796	A
6	A	797	A
6	A	799	C
6	A	801	G
6	A	814	G
6	A	819	G
6	A	825	U
6	A	826	C
6	A	827	C
6	A	828	A
6	A	831	G
6	A	832	G
6	A	837	G
6	A	874	G
6	A	886	G
6	A	898	A
6	A	900	G
6	A	910	G
6	A	911	G
6	A	918	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	919	A
6	A	944	U
6	A	945	U
6	A	953	A
6	A	956	C
6	A	959	A
6	A	960	G
6	A	961	A
6	A	971	G
6	A	972	G
6	A	975	U
6	A	976	U
6	A	977	G
6	A	980	A
6	A	981	U
6	A	982	G
6	A	984	A
6	A	986	C
6	A	987	G
6	A	989	G
6	A	990	A
6	A	993	G
6	A	996	C
6	A	997	A
6	A	1003	G
6	A	1010	C
6	A	1012	U
6	A	1013	C
6	A	1014	U
6	A	1023	C
6	A	1024	G
6	A	1025	G
6	A	1026	U
6	A	1027	U
6	A	1029	A
6	A	1030	C
6	A	1031	A
6	A	1038	G
6	A	1040	A
6	A	1041	U
6	A	1043	G
6	A	1049	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1050	U
6	A	1051	C
6	A	1052	A
6	A	1053	G
6	A	1059	G
6	A	1066	G
6	A	1071	U
6	A	1074	G
6	A	1076	U
6	A	1077	A
6	A	1079	G
6	A	1080	U
6	A	1082	C
6	A	1083	C
6	A	1084	G
6	A	1086	A
6	A	1090	A
6	A	1093	G
6	A	1094	C
6	A	1107	C
6	A	1109	G
6	A	1110	U
6	A	1112	G
6	A	1113	C
6	A	1115	A
6	A	1116	G
6	A	1119	C
6	A	1120	G
6	A	1121	U
6	A	1122	U
6	A	1124	U
6	A	1125	G
6	A	1126	G
6	A	1127	U
6	A	1129	G
6	A	1130	G
6	A	1131	G
6	A	1132	A
6	A	1133	C
6	A	1134	U
6	A	1137	G
6	A	1138	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1139	G
6	A	1140	G
6	A	1145	C
6	A	1146	G
6	A	1147	C
6	A	1148	C
6	A	1150	G
6	A	1153	U
6	A	1154	C
6	A	1157	C
6	A	1160	G
6	A	1161	G
6	A	1165	A
6	A	1169	U
6	A	1170	G
6	A	1171	G
6	A	1173	G
6	A	1174	A
6	A	1182	A
6	A	1183	A
6	A	1186	C
6	A	1188	U
6	A	1199	A
6	A	1200	U
6	A	1210	U
6	A	1213	A
6	A	1222	A
6	A	1224	A
6	A	1227	G
6	A	1242	U
6	A	1243	G
6	A	1244	G
6	A	1246	G
6	A	1256	G
6	A	1261	A
6	A	1266	A
6	A	1272	G
6	A	1273	A
6	A	1286	G
6	A	1288	U
6	A	1291	G
6	A	1306	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1324	G
6	A	1332	A
6	A	1333	G
6	A	1339	G
6	A	1349	A
6	A	1351	C
6	A	1357	G
6	A	1365	C
6	A	1370	C
6	A	1382	C
6	A	1384	C
6	A	1385	A
6	A	1387	5MC
6	A	1388	G
6	A	1406	G
6	A	1415	A
6	A	1429	G
6	A	1433	A
6	A	1438	U
6	A	1440	G
6	A	1450	C
6	A	1474	G
6	A	1479	A
6	A	1480	A
6	A	1484	G
6	A	1490	A
6	A	1492	G
6	A	1493	U
6	A	1504	G
6	A	1516	G
6	A	1517	G
6	A	1518	A
6	A	1519	U
6	A	1521	A
6	A	1522	C
6	A	1523	C
6	A	1524	U
6	A	1526	C
6	A	1527	U
6	A	1528	U
8	C	9	G
8	C	17	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	18	G
8	C	19	G
8	C	21	A
8	C	46	G
8	C	47	U
8	C	69	C
8	C	75	C
8	C	76	A
29	Y	15	A
29	Y	16	A
29	Y	19	U
29	Y	20	U
29	Y	21	U
29	Y	22	U
30	a	11	G
30	a	12	U
30	a	34	G
30	a	42	G
30	a	50	G
30	a	57	G
30	a	62	G
30	a	70	A
30	a	73	A
30	a	74	G
30	a	82	G
30	a	83	A
30	a	93	C
30	a	95	A
30	a	96	G
30	a	101	G
30	a	117	A
30	a	118	A
30	a	119	U
30	a	132	A
30	a	133	A
30	a	135	G
30	a	136	U
30	a	137	C
30	a	147	G
30	a	166	A
30	a	169	G
30	a	171	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	180	U
30	a	188	A
30	a	203	A
30	a	206	A
30	a	222	G
30	a	223	A
30	a	229	A
30	a	230	A
30	a	236	U
30	a	240	A
30	a	255	G
30	a	272	A
30	a	273	G
30	a	274	G
30	a	279	A
30	a	283	U
30	a	284	G
30	a	285	U
30	a	286	G
30	a	287	U
30	a	288	G
30	a	289	U
30	a	290	G
30	a	291	U
30	a	304	G
30	a	305	U
30	a	307	U
30	a	309	G
30	a	310	C
30	a	311	A
30	a	312	U
30	a	313	G
30	a	322	U
30	a	323	G
30	a	324	U
30	a	325	G
30	a	331	C
30	a	332	U
30	a	336	G
30	a	337	G
30	a	338	U
30	a	339	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	345	G
30	a	346	C
30	a	347	C
30	a	348	G
30	a	353	A
30	a	354	U
30	a	355	U
30	a	356	G
30	a	359	C
30	a	360	A
30	a	366	A
30	a	367	A
30	a	369	U
30	a	370	G
30	a	371	U
30	a	372	U
30	a	379	A
30	a	380	G
30	a	384	A
30	a	385	A
30	a	386	G
30	a	387	C
30	a	389	U
30	a	393	G
30	a	396	A
30	a	402	A
30	a	408	G
30	a	415	A
30	a	419	U
30	a	423	G
30	a	427	C
30	a	431	A
30	a	432	A
30	a	433	G
30	a	434	C
30	a	435	G
30	a	447	U
30	a	449	G
30	a	453	U
30	a	454	G
30	a	460	A
30	a	475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	476	U
30	a	477	G
30	a	480	A
30	a	494	U
30	a	500	G
30	a	501	A
30	a	524	C
30	a	532	A
30	a	533	C
30	a	540	U
30	a	544	U
30	a	545	G
30	a	570	G
30	a	592	G
30	a	593	A
30	a	596	U
30	a	618	G
30	a	619	C
30	a	620	C
30	a	632	U
30	a	633	G
30	a	635	G
30	a	646	G
30	a	656	G
30	a	657	A
30	a	658	A
30	a	670	G
30	a	674	G
30	a	675	U
30	a	676	G
30	a	687	A
30	a	698	U
30	a	699	G
30	a	700	G
30	a	701	U
30	a	704	G
30	a	707	A
30	a	713	A
30	a	720	G
30	a	723	A
30	a	731	A
30	a	733	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	739	G
30	a	740	A
30	a	770	A
30	a	771	U
30	a	791	A
30	a	802	G
30	a	815	U
30	a	832	U
30	a	849	A
30	a	860	G
30	a	861	G
30	a	867	A
30	a	869	G
30	a	870	G
30	a	875	U
30	a	890	G
30	a	897	C
30	a	912	U
30	a	930	G
30	a	931	G
30	a	944	G
30	a	951	A
30	a	967	G
30	a	968	G
30	a	970	U
30	a	972	A
30	a	973	U
30	a	974	C
30	a	975	G
30	a	978	U
30	a	979	U
30	a	980	A
30	a	981	C
30	a	991	C
30	a	994	A
30	a	1014	G
30	a	1016	A
30	a	1026	U
30	a	1028	A
30	a	1029	G
30	a	1044	G
30	a	1057	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1066	A
30	a	1073	A
30	a	1079	A
30	a	1096	G
30	a	1105	G
30	a	1109	G
30	a	1116	U
30	a	1122	G
30	a	1128	U
30	a	1129	A
30	a	1130	G
30	a	1136	C
30	a	1144	U
30	a	1145	G
30	a	1147	C
30	a	1149	U
30	a	1150	G
30	a	1151	G
30	a	1152	A
30	a	1153	A
30	a	1154	G
30	a	1157	G
30	a	1159	C
30	a	1161	U
30	a	1165	U
30	a	1172	G
30	a	1174	G
30	a	1177	U
30	a	1178	A
30	a	1179	A
30	a	1181	A
30	a	1189	G
30	a	1191	U
30	a	1194	A
30	a	1195	G
30	a	1196	U
30	a	1211	A
30	a	1213	U
30	a	1215	U
30	a	1216	A
30	a	1218	C
30	a	1225	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1226	A
30	a	1227	A
30	a	1241	G
30	a	1254	G
30	a	1256	G
30	a	1258	G
30	a	1259	G
30	a	1297	G
30	a	1306	U
30	a	1307	G
30	a	1311	U
30	a	1314	A
30	a	1324	A
30	a	1330	A
30	a	1331	A
30	a	1333	G
30	a	1348	G
30	a	1349	U
30	a	1350	G
30	a	1351	U
30	a	1356	G
30	a	1376	A
30	a	1377	U
30	a	1397	C
30	a	1419	G
30	a	1426	C
30	a	1428	U
30	a	1441	A
30	a	1455	U
30	a	1460	A
30	a	1471	A
30	a	1472	U
30	a	1493	G
30	a	1595	A
30	a	1601	G
30	a	1607	A
30	a	1608	C
30	a	1609	G
30	a	1625	U
30	a	1626	C
30	a	1627	C
30	a	1630	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1633	G
30	a	1639	U
30	a	1641	U
30	a	1642	C
30	a	1657	U
30	a	1663	G
30	a	1673	U
30	a	1674	A
30	a	1675	A
30	a	1683	G
30	a	1688	U
30	a	1689	G
30	a	1690	A
30	a	1691	A
30	a	1692	G
30	a	1697	A
30	a	1698	G
30	a	1706	G
30	a	1710	A
30	a	1712	C
30	a	1714	C
30	a	1717	G
30	a	1718	G
30	a	1721	G
30	a	1723	G
30	a	1725	G
30	a	1726	U
30	a	1727	G
30	a	1728	A
30	a	1743	A
30	a	1749	G
30	a	1752	A
30	a	1761	G
30	a	1763	G
30	a	1769	G
30	a	1774	C
30	a	1787	A
30	a	1791	U
30	a	1792	A
30	a	1797	G
30	a	1818	U
30	a	1830	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1831	U
30	a	1832	C
30	a	1837	G
30	a	1838	A
30	a	1851	G
30	a	1858	G
30	a	1887	G
30	a	1898	C
30	a	1904	U
30	a	1905	G
30	a	1911	G
30	a	1912	U
30	a	1913	G
30	a	1915	G
30	a	1916	G
30	a	1920	G
30	a	1921	G
30	a	1923	G
30	a	1933	G
30	a	1939	G
30	a	1947	G
30	a	1956	A
30	a	1974	A
30	a	1983	C
30	a	1984	G
30	a	1985	A
30	a	1999	U
30	a	2012	A
30	a	2031	A
30	a	2041	G
30	a	2052	G
30	a	2053	U
30	a	2054	A
30	a	2055	U
30	a	2056	G
30	a	2066	G
30	a	2067	A
30	a	2068	A
30	a	2069	C
30	a	2089	G
30	a	2096	A
30	a	2098	3TD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2112	G
30	a	2113	G
30	a	2120	A
30	a	2121	A
30	a	2138	U
30	a	2150	C
30	a	2153	A
30	a	2154	U
30	a	2155	G
30	a	2174	U
30	a	2175	G
30	a	2176	U
30	a	2185	U
30	a	2199	U
30	a	2202	C
30	a	2203	A
30	a	2204	U
30	a	2206	A
30	a	2210	G
30	a	2214	A
30	a	2215	G
30	a	2216	A
30	a	2222	G
30	a	2226	C
30	a	2238	C
30	a	2239	G
30	a	2243	A
30	a	2244	G
30	a	2245	A
30	a	2280	U
30	a	2283	G
30	a	2287	G
30	a	2288	G
30	a	2289	U
30	a	2365	U
30	a	2366	U
30	a	2368	U
30	a	2384	G
30	a	2385	U
30	a	2386	G
30	a	2393	G
30	a	2394	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2407	A
30	a	2420	G
30	a	2421	G
30	a	2450	A
30	a	2451	G
30	a	2461	G
30	a	2465	C
30	a	2469	A
30	a	2487	U
30	a	2490	G
30	a	2501	G
30	a	2503	G
30	a	2504	A
30	a	2507	G
30	a	2517	A
30	a	2518	A
30	a	2529	C
30	a	2532	U
30	a	2536	A
30	a	2543	G
30	a	2565	G
30	a	2567	A
30	a	2573	G
30	a	2588	U
30	a	2589	G
30	a	2606	C
30	a	2607	A
30	a	2610	G
30	a	2611	G
30	a	2612	A
30	a	2613	U
30	a	2617	A
30	a	2623	C
30	a	2627	2MG
30	a	2630	A
30	a	2655	C
30	a	2656	U
30	a	2657	C
30	a	2658	A
30	a	2660	A
30	a	2661	G
30	a	2663	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2664	A
30	a	2673	U
30	a	2684	G
30	a	2687	G
30	a	2688	U
30	a	2700	A
30	a	2711	G
30	a	2712	G
30	a	2713	A
30	a	2714	G
30	a	2717	G
30	a	2719	U
30	a	2748	A
30	a	2749	G
30	a	2755	C
30	a	2763	G
30	a	2764	G
30	a	2765	G
30	a	2784	A
30	a	2791	U
30	a	2792	C
30	a	2793	C
30	a	2795	U
30	a	2811	A
30	a	2812	G
30	a	2816	U
30	a	2820	G
30	a	2827	G
30	a	2828	C
30	a	2843	G
30	a	2864	U
30	a	2871	U
30	a	2896	G
30	a	2908	C
30	a	2915	U
30	a	2917	G
30	a	2926	G
30	a	2930	A
30	a	2947	A
30	a	2948	G
30	a	2960	A
30	a	2961	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2962	A
30	a	2972	A
30	a	2978	G
30	a	2979	U
30	a	2980	G
30	a	2981	U
30	a	2982	U
30	a	2983	C
30	a	2988	U
30	a	3000	G
30	a	3015	A
30	a	3041	G
30	a	3047	G
30	a	3052	G
30	a	3053	A
30	a	3064	U
30	a	3066	G
30	a	3071	A
30	a	3073	G
30	a	3074	A
30	a	3075	C
31	b	24	G
31	b	25	A
31	b	30	C
31	b	35	U
31	b	42	C
31	b	56	U
31	b	57	A
31	b	84	C
31	b	91	U
31	b	100	A
31	b	106	A
31	b	109	C
31	b	110	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	9	U
6	A	90	U
6	A	94	G
6	A	146	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	289	U
6	A	418	G
6	A	467	G
6	A	514	G
6	A	591	A
6	A	869	G
6	A	918	C
6	A	955	G
6	A	975	U
6	A	1050	U
6	A	1051	C
6	A	1052	A
6	A	1070	U
6	A	1109	G
6	A	1114	C
6	A	1125	G
6	A	1186	C
6	A	1187	A
6	A	1271	G
6	A	1350	A
6	A	1387	5MC
6	A	1492	G
6	A	1523	C
8	C	74	C

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

34 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	$\# Z > 2$
30	PSU	a	2762	30	18,21,22	0.94	1 (5%)	21,30,33	0.72	0
8	4SU	C	8	8	18,21,22	3.73	8 (44%)	25,30,33	2.27	5 (20%)
30	2MG	a	2627	30	23,26,27	2.98	8 (34%)	33,38,41	2.43	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	5MC	A	1387	6	19,22,23	4.38	8 (42%)	26,32,35	1.04	2 (7%)
8	PSU	C	55	8	18,21,22	0.95	1 (5%)	21,30,33	0.64	0
6	2MG	A	1503	6	23,26,27	0.33	0	33,38,41	0.55	0
8	5MU	C	54	8	19,22,23	0.25	0	27,32,35	0.27	0
30	PSU	a	2686	30	18,21,22	0.94	1 (5%)	21,30,33	0.76	1 (4%)
30	OMU	a	2734	30	19,22,23	0.27	0	25,31,34	0.46	0
6	4OC	A	1389	6	20,23,24	3.01	8 (40%)	25,32,35	0.94	1 (4%)
6	5MC	A	1391	6	19,22,23	4.29	8 (42%)	26,32,35	1.03	2 (7%)
30	PSU	a	1038	30	18,21,22	0.92	1 (5%)	21,30,33	0.75	0
30	5MU	a	2122	30	19,22,23	0.30	0	27,32,35	0.31	0
8	5MC	C	32	8	19,22,23	0.79	1 (5%)	26,32,35	0.48	0
30	5MC	a	2145	30	19,22,23	4.18	8 (42%)	26,32,35	1.14	2 (7%)
6	2MG	A	950	6	23,26,27	0.36	0	33,38,41	0.41	0
30	PSU	a	2787	30	18,21,22	0.94	1 (5%)	21,30,33	0.59	0
30	PSU	a	2094	30	18,21,22	0.94	1 (5%)	21,30,33	0.63	0
6	G7M	A	509	6	23,26,27	2.62	9 (39%)	34,39,42	1.70	7 (20%)
30	PSU	a	2639	30	18,21,22	0.93	1 (5%)	21,30,33	0.75	0
30	2MG	a	2018	30	23,26,27	3.01	8 (34%)	33,38,41	2.59	12 (36%)
6	UR3	A	1485	6	19,22,23	2.70	8 (42%)	26,32,35	1.66	3 (11%)
30	OMC	a	2680	56,30	19,22,23	3.11	8 (42%)	25,31,34	0.88	0
30	3TD	a	2098	30	19,22,23	4.15	7 (36%)	23,32,35	1.86	5 (21%)
6	MA6	A	1506	6	23,26,27	0.27	0	33,38,41	0.69	1 (3%)
30	PSU	a	2786	30	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
6	PSU	A	498	6	18,21,22	0.93	1 (5%)	21,30,33	0.61	0
30	H2U	a	2631	30	18,21,22	2.93	5 (27%)	19,30,33	1.52	4 (21%)
6	5MC	A	951	6	19,22,23	0.82	1 (5%)	26,32,35	0.48	0
6	MA6	A	1505	6	23,26,27	0.27	0	33,38,41	0.63	1 (3%)
30	PSU	a	2100	30	18,21,22	0.94	1 (5%)	21,30,33	0.66	0
30	OMG	a	2433	8,56,30	23,26,27	2.46	9 (39%)	32,38,41	2.31	11 (34%)
30	2MA	a	2685	56,30	22,25,26	3.46	8 (36%)	32,37,40	2.05	8 (25%)
6	5MC	A	1394	6	19,22,23	4.21	8 (42%)	26,32,35	0.97	2 (7%)

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
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	30	-	2/9/27/28	0/3/3/3
6	5MC	A	1387	6	-	3/7/25/26	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2686	30	-	0/7/25/26	0/2/2/2
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
6	4OC	A	1389	6	-	1/9/29/30	0/2/2/2
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
30	PSU	a	1038	30	-	0/7/25/26	0/2/2/2
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
6	2MG	A	950	6	-	0/9/27/28	0/3/3/3
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
6	G7M	A	509	6	-	2/7/25/26	0/3/3/3
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
30	OMC	a	2680	56,30	-	0/9/27/28	0/2/2/2
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
6	MA6	A	1506	6	-	0/11/29/30	0/3/3/3
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
6	PSU	A	498	6	-	0/7/25/26	0/2/2/2
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2433	8,56,30	-	0/9/27/28	0/3/3/3
30	2MA	a	2685	56,30	-	1/7/25/26	0/3/3/3
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2098	3TD	C6-C5	12.87	1.49	1.35
30	a	2685	2MA	C4-N3	10.46	1.47	1.34
6	A	1387	5MC	C6-C5	9.43	1.50	1.34
6	A	1394	5MC	C6-C5	9.15	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1391	5MC	C6-C5	9.14	1.49	1.34
30	a	2098	3TD	C2-N1	9.10	1.48	1.37
30	a	2145	5MC	C6-C5	9.08	1.49	1.34
6	A	1387	5MC	C5-C4	9.04	1.51	1.44
30	a	2631	H2U	C2-N1	8.90	1.48	1.35
6	A	1391	5MC	C5-C4	8.79	1.50	1.44
30	a	2145	5MC	C5-C4	8.48	1.50	1.44
6	A	1394	5MC	C5-C4	8.34	1.50	1.44
30	a	2018	2MG	C2-N3	7.83	1.46	1.32
30	a	2627	2MG	C2-N3	7.61	1.46	1.32
6	A	1387	5MC	C4-N3	7.34	1.45	1.34
6	A	1391	5MC	C4-N3	7.24	1.45	1.34
30	a	2145	5MC	C4-N3	7.18	1.45	1.34
6	A	1485	UR3	C2-N1	7.16	1.48	1.38
8	C	8	4SU	C2-N1	7.12	1.49	1.38
8	C	8	4SU	C2-N3	7.10	1.50	1.38
6	A	1394	5MC	C4-N3	7.10	1.45	1.34
30	a	2627	2MG	C4-N3	7.03	1.50	1.34
6	A	1387	5MC	C2-N3	6.96	1.50	1.36
30	a	2018	2MG	C4-N3	6.88	1.50	1.34
6	A	1394	5MC	C2-N3	6.84	1.49	1.36
6	A	1391	5MC	C2-N3	6.81	1.49	1.36
30	a	2145	5MC	C2-N3	6.76	1.49	1.36
6	A	1389	4OC	C4-N3	6.72	1.44	1.32
30	a	2680	OMC	C2-N3	6.68	1.49	1.36
8	C	8	4SU	C4-N3	6.65	1.44	1.37
6	A	509	G7M	C4-N3	6.52	1.49	1.34
30	a	2018	2MG	C2-N2	6.49	1.47	1.33
30	a	2433	OMG	C4-N3	6.39	1.48	1.34
30	a	2685	2MA	C2-N1	6.28	1.44	1.34
30	a	2685	2MA	C2-N3	6.27	1.44	1.34
6	A	1389	4OC	C6-C5	6.18	1.49	1.35
8	C	8	4SU	C5-C4	6.09	1.49	1.42
30	a	2627	2MG	C2-N2	6.00	1.46	1.33
6	A	1485	UR3	C6-C5	5.90	1.48	1.35
30	a	2098	3TD	C6-N1	5.83	1.45	1.36
30	a	2680	OMC	C6-C5	5.81	1.48	1.35
30	a	2631	H2U	C2-N3	5.79	1.48	1.38
6	A	1389	4OC	C2-N3	5.72	1.47	1.36
6	A	1387	5MC	C4-N4	5.65	1.48	1.34
8	C	8	4SU	C6-C5	5.63	1.48	1.35
6	A	1387	5MC	C6-N1	5.60	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1391	5MC	C4-N4	5.56	1.48	1.34
6	A	1394	5MC	C4-N4	5.51	1.48	1.34
6	A	1391	5MC	C6-N1	5.43	1.47	1.38
30	a	2145	5MC	C4-N4	5.42	1.48	1.34
6	A	1394	5MC	C6-N1	5.34	1.47	1.38
6	A	509	G7M	C2-N3	5.21	1.45	1.33
30	a	2433	OMG	C2-N3	5.16	1.45	1.33
30	a	2680	OMC	C4-N3	5.06	1.44	1.34
30	a	2145	5MC	C6-N1	5.04	1.46	1.38
30	a	2433	OMG	C2-N2	5.03	1.45	1.34
8	C	8	4SU	C4-S4	-4.88	1.60	1.68
6	A	509	G7M	C5-N7	-4.75	1.33	1.39
6	A	509	G7M	C2-N2	4.73	1.45	1.34
30	a	2680	OMC	C4-N4	4.70	1.45	1.33
30	a	2098	3TD	C2-N3	4.63	1.48	1.38
6	A	1485	UR3	C2-N3	4.61	1.48	1.39
30	a	2685	2MA	C5-C6	4.60	1.53	1.41
30	a	2018	2MG	C2-N1	4.58	1.44	1.36
30	a	2680	OMC	O2-C2	-4.57	1.15	1.23
30	a	2627	2MG	C2-N1	4.56	1.44	1.36
6	A	1391	5MC	C2-N1	4.51	1.49	1.40
6	A	1387	5MC	C2-N1	4.49	1.49	1.40
30	a	2631	H2U	C4-N3	4.38	1.44	1.37
6	A	1394	5MC	C2-N1	4.32	1.49	1.40
30	a	2680	OMC	C2-N1	4.26	1.49	1.40
30	a	2145	5MC	C2-N1	4.18	1.48	1.40
6	A	1389	4OC	C4-N4	4.12	1.44	1.36
30	a	2685	2MA	C6-N1	3.83	1.40	1.35
6	A	1389	4OC	C2-N1	3.79	1.48	1.40
6	A	509	G7M	C5-C6	3.77	1.53	1.43
30	a	2685	2MA	C6-N6	-3.75	1.24	1.34
8	C	55	PSU	C6-C5	3.72	1.39	1.35
30	a	2787	PSU	C6-C5	3.67	1.39	1.35
30	a	2100	PSU	C6-C5	3.67	1.39	1.35
30	a	2094	PSU	C6-C5	3.65	1.39	1.35
30	a	2762	PSU	C6-C5	3.65	1.39	1.35
6	A	498	PSU	C6-C5	3.62	1.39	1.35
6	A	1389	4OC	C5-C4	3.61	1.49	1.41
30	a	2639	PSU	C6-C5	3.61	1.39	1.35
30	a	2786	PSU	C6-C5	3.60	1.39	1.35
30	a	1038	PSU	C6-C5	3.56	1.39	1.35
30	a	2686	PSU	C6-C5	3.51	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2627	2MG	C5-N7	-3.49	1.32	1.39
30	a	2680	OMC	C6-N1	3.39	1.46	1.38
6	A	951	5MC	C5-C4	-3.30	1.41	1.44
30	a	2433	OMG	O6-C6	-3.30	1.17	1.23
6	A	1389	4OC	O2-C2	-3.27	1.17	1.23
30	a	2685	2MA	C5-N7	-3.17	1.33	1.39
30	a	2018	2MG	C5-N7	-3.15	1.32	1.39
8	C	32	5MC	C5-C4	-3.14	1.41	1.44
30	a	2631	H2U	O2-C2	-2.99	1.17	1.23
30	a	2627	2MG	O6-C6	-2.98	1.17	1.23
6	A	1389	4OC	C6-N1	2.93	1.45	1.38
6	A	1485	UR3	C6-N1	2.93	1.45	1.38
30	a	2018	2MG	O6-C6	-2.87	1.18	1.23
30	a	2018	2MG	C5-C6	2.76	1.54	1.44
30	a	2433	OMG	C5-C6	2.70	1.54	1.44
8	C	8	4SU	C6-N1	2.67	1.44	1.38
6	A	1394	5MC	O2-C2	-2.67	1.18	1.23
30	a	2145	5MC	O2-C2	-2.66	1.18	1.23
30	a	2631	H2U	O4-C4	-2.65	1.18	1.23
30	a	2627	2MG	C5-C6	2.64	1.54	1.44
6	A	509	G7M	O6-C6	-2.63	1.18	1.23
30	a	2098	3TD	C4-N3	2.63	1.45	1.40
6	A	1391	5MC	O2-C2	-2.62	1.18	1.23
6	A	509	G7M	C2-N1	2.62	1.44	1.37
30	a	2433	OMG	C2-N1	2.60	1.43	1.37
6	A	1387	5MC	O2-C2	-2.55	1.19	1.23
6	A	1485	UR3	O4-C4	-2.50	1.18	1.23
6	A	1485	UR3	O2-C2	-2.35	1.18	1.22
30	a	2433	OMG	C5-N7	-2.34	1.34	1.39
30	a	2680	OMC	C5-C4	2.32	1.48	1.42
30	a	2685	2MA	C8-N7	2.28	1.36	1.31
30	a	2433	OMG	C4-N9	-2.28	1.32	1.38
6	A	509	G7M	C6-N1	2.27	1.43	1.38
6	A	509	G7M	C4-N9	-2.26	1.32	1.38
30	a	2098	3TD	O4-C4	-2.22	1.18	1.23
30	a	2433	OMG	C6-N1	2.15	1.42	1.38
6	A	1485	UR3	C5-C4	2.13	1.49	1.43
8	C	8	4SU	O2-C2	-2.11	1.19	1.23
6	A	1485	UR3	C4-N3	2.09	1.44	1.40
30	a	2018	2MG	C6-N1	2.08	1.42	1.38
30	a	2098	3TD	O2-C2	-2.08	1.19	1.23
30	a	2627	2MG	C8-N9	-2.00	1.33	1.37

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	8	4SU	C4-N3-C2	-7.87	119.78	127.31
30	a	2018	2MG	C2-N3-C4	7.44	121.30	112.00
30	a	2627	2MG	C2-N3-C4	6.59	120.25	112.00
30	a	2685	2MA	C5-C4-N3	-6.37	120.47	127.18
30	a	2018	2MG	C5-C4-N3	-6.31	118.35	128.39
6	A	1485	UR3	C4-N3-C2	-5.96	119.78	124.58
30	a	2433	OMG	C1'-N9-C8	-5.91	109.94	126.73
30	a	2627	2MG	C5-C4-N3	-5.89	119.01	128.39
30	a	2098	3TD	N1-C2-N3	5.84	120.37	116.13
30	a	2018	2MG	C2-N1-C6	-5.01	118.49	124.55
8	C	8	4SU	C5-C4-N3	4.98	119.39	114.75
30	a	2627	2MG	C2-N1-C6	-4.65	118.93	124.55
30	a	2433	OMG	C1'-N9-C4	4.62	140.14	126.49
30	a	2685	2MA	N9-C8-N7	-4.54	107.49	113.94
30	a	2433	OMG	C2-N3-C4	4.48	120.02	112.30
30	a	2627	2MG	C1'-N9-C4	-4.26	113.91	126.49
6	A	509	G7M	C2-N3-C4	4.25	119.62	112.30
30	a	2018	2MG	C1'-N9-C8	4.24	138.78	126.73
30	a	2433	OMG	C5-C4-N3	-4.24	121.64	128.39
8	C	8	4SU	N3-C2-N1	4.21	120.37	114.89
30	a	2018	2MG	C1'-N9-C4	-4.16	114.19	126.49
30	a	2627	2MG	C1'-N9-C8	4.08	138.32	126.73
30	a	2018	2MG	N9-C4-N3	3.99	133.94	125.95
6	A	509	G7M	C5-C6-N1	3.93	119.96	111.84
30	a	2098	3TD	C4-N3-C2	-3.92	120.46	124.61
30	a	2433	OMG	N9-C8-N7	-3.90	106.17	113.40
30	a	2627	2MG	N9-C4-N3	3.88	133.70	125.95
30	a	2631	H2U	N3-C2-N1	3.82	120.49	116.65
6	A	1485	UR3	C5-C4-N3	3.80	120.04	115.04
30	a	2685	2MA	N3-C4-N9	3.70	131.69	126.99
6	A	509	G7M	C5-C4-N3	-3.69	121.18	128.15
30	a	2145	5MC	C5-C6-N1	-3.67	119.33	123.31
30	a	2685	2MA	N3-C2-N1	-3.44	119.71	125.77
8	C	8	4SU	C5-C4-S4	-3.37	120.45	124.31
6	A	1391	5MC	C5-C6-N1	-3.36	119.66	123.31
6	A	1387	5MC	C5-C6-N1	-3.34	119.69	123.31
30	a	2018	2MG	N1-C2-N2	3.27	119.90	116.56
6	A	1394	5MC	C5-C6-N1	-3.22	119.81	123.31
6	A	509	G7M	O6-C6-C5	-3.14	120.99	128.01
30	a	2685	2MA	C5-N7-C8	3.11	108.33	103.45
30	a	2631	H2U	C5-C4-N3	3.09	119.97	116.69
30	a	2098	3TD	C1'-C5-C4	3.07	122.27	117.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2433	OMG	C2-N1-C6	-3.06	119.56	125.11
6	A	509	G7M	N9-C4-N3	3.06	132.07	125.95
30	a	2018	2MG	C5-C6-N1	3.01	120.92	113.25
30	a	2433	OMG	C5-C6-N1	2.91	120.67	113.25
6	A	509	G7M	C2-N1-C6	-2.83	119.98	125.11
30	a	2627	2MG	C5-C6-N1	2.82	120.42	113.25
6	A	1505	MA6	C2-N1-C6	2.80	118.67	111.83
6	A	1506	MA6	C2-N1-C6	2.78	118.62	111.83
30	a	2631	H2U	C5-C6-N1	2.76	119.86	111.52
6	A	509	G7M	N9-C8-N7	-2.70	105.92	112.48
30	a	2631	H2U	O2-C2-N1	-2.68	119.88	123.10
30	a	2627	2MG	N9-C8-N7	-2.60	108.58	113.40
30	a	2145	5MC	CM5-C5-C6	-2.58	119.36	122.85
30	a	2685	2MA	C4-N9-C8	2.52	108.39	105.74
30	a	2018	2MG	O6-C6-C5	-2.52	119.87	126.53
30	a	2433	OMG	N9-C4-N3	2.44	130.83	125.95
30	a	2433	OMG	C8-N7-C5	2.43	108.59	104.26
30	a	2627	2MG	O6-C6-C5	-2.38	120.25	126.53
30	a	2098	3TD	C6-C5-C4	2.37	119.78	118.19
30	a	2433	OMG	O6-C6-C5	-2.37	120.29	126.53
30	a	2685	2MA	C4-C5-N7	-2.31	107.95	110.58
30	a	2018	2MG	N9-C8-N7	-2.28	109.18	113.40
30	a	2686	PSU	C2'-C3'-C4'	-2.26	98.23	102.61
6	A	1485	UR3	C6-N1-C2	-2.22	119.99	121.80
30	a	2627	2MG	CM2-N2-C2	-2.21	118.91	123.65
6	A	1391	5MC	CM5-C5-C6	-2.20	119.88	122.85
30	a	2018	2MG	CM2-N2-C2	-2.15	119.03	123.65
30	a	2627	2MG	N1-C2-N2	2.15	118.75	116.56
6	A	1389	4OC	C6-C5-C4	2.15	119.58	117.00
30	a	2098	3TD	O4'-C1'-C2'	2.10	108.06	105.15
30	a	2627	2MG	C8-N7-C5	2.09	107.99	104.26
30	a	2685	2MA	CM2-C2-N1	2.09	120.25	117.13
30	a	2433	OMG	C8-N9-C4	2.06	109.89	106.03
6	A	1387	5MC	CM5-C5-C6	-2.05	120.07	122.85
6	A	1394	5MC	CM5-C5-C6	-2.04	120.09	122.85
8	C	8	4SU	O2-C2-N1	-2.04	120.14	122.80
30	a	2018	2MG	N1-C2-N3	-2.02	120.28	123.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1387	5MC	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
30	a	2098	3TD	C3'-C4'-C5'-O5'
6	A	509	G7M	C3'-C4'-C5'-O5'
6	A	1387	5MC	C3'-C4'-C5'-O5'
30	a	2627	2MG	C3'-C4'-C5'-O5'
30	a	2018	2MG	O4'-C4'-C5'-O5'
30	a	2018	2MG	C3'-C4'-C5'-O5'
6	A	509	G7M	O4'-C4'-C5'-O5'
6	A	1387	5MC	C4'-C5'-O5'-P
30	a	2685	2MA	O4'-C4'-C5'-O5'
30	a	2627	2MG	O4'-C4'-C5'-O5'
6	A	1389	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	2627	2MG	1	0
6	A	1387	5MC	2	0
6	A	1503	2MG	1	0
30	a	2094	PSU	2	0
6	A	509	G7M	2	0
6	A	1485	UR3	2	0
30	a	2098	3TD	2	0
6	A	1506	MA6	7	0
30	a	2631	H2U	1	0
6	A	1505	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 300 ligands modelled in this entry, 293 are monoatomic - leaving 7 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	$\# Z > 2$
57	DXT	a	3130	56	34,35,35	1.12	2 (5%)	42,57,57	1.38	6 (14%)
57	DXT	s	201	56	34,35,35	1.11	2 (5%)	42,57,57	0.88	1 (2%)
57	DXT	a	3123	56	34,35,35	1.12	2 (5%)	42,57,57	0.95	2 (4%)
57	DXT	r	201	56	34,35,35	1.11	2 (5%)	42,57,57	1.08	3 (7%)
57	DXT	a	3146	56	34,35,35	1.13	2 (5%)	42,57,57	0.95	2 (4%)
57	DXT	A	1615	56	34,35,35	1.11	2 (5%)	42,57,57	1.04	2 (4%)
57	DXT	a	3138	56	34,35,35	1.13	2 (5%)	42,57,57	0.97	1 (2%)

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
57	DXT	a	3130	56	-	7/8/74/74	0/4/4/4
57	DXT	s	201	56	-	4/8/74/74	0/4/4/4
57	DXT	a	3123	56	-	1/8/74/74	0/4/4/4
57	DXT	r	201	56	-	8/8/74/74	0/4/4/4
57	DXT	a	3146	56	-	1/8/74/74	0/4/4/4
57	DXT	A	1615	56	-	2/8/74/74	0/4/4/4
57	DXT	a	3138	56	-	3/8/74/74	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3138	DXT	C21-N21	5.02	1.47	1.33
57	a	3130	DXT	C21-N21	4.99	1.47	1.33
57	a	3123	DXT	C21-N21	4.96	1.47	1.33
57	a	3146	DXT	C21-N21	4.96	1.47	1.33
57	s	201	DXT	C21-N21	4.94	1.47	1.33
57	A	1615	DXT	C21-N21	4.94	1.47	1.33
57	r	201	DXT	C21-N21	4.93	1.47	1.33
57	r	201	DXT	O11-C11	2.22	1.27	1.23
57	a	3130	DXT	O11-C11	2.22	1.27	1.23
57	a	3123	DXT	O11-C11	2.21	1.27	1.23
57	a	3146	DXT	O11-C11	2.21	1.27	1.23
57	A	1615	DXT	O11-C11	2.21	1.27	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3138	DXT	O11-C11	2.20	1.27	1.23
57	s	201	DXT	O11-C11	2.16	1.27	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	a	3130	DXT	C4B-C1-C2	3.79	121.77	115.75
57	A	1615	DXT	C21-C2-C1	3.10	124.64	120.97
57	a	3130	DXT	C4B-C12-C5B	2.99	126.10	123.06
57	a	3130	DXT	O13-C4B-C12	-2.96	105.41	110.14
57	r	201	DXT	C4B-C1-C2	2.80	120.19	115.75
57	a	3130	DXT	C42-N4-C4	2.75	120.37	114.10
57	s	201	DXT	C4B-C1-C2	2.56	119.83	115.75
57	a	3130	DXT	O12-C12-C5B	-2.56	118.55	123.52
57	a	3138	DXT	C4B-C1-C2	2.35	119.49	115.75
57	a	3123	DXT	O10-C10-C6B	-2.23	117.02	121.14
57	a	3123	DXT	C4B-C1-C2	2.21	119.26	115.75
57	a	3146	DXT	O3-C3-C2	-2.20	119.24	122.93
57	a	3146	DXT	C4B-C1-C2	2.14	119.16	115.75
57	r	201	DXT	C11-C5B-C12	2.14	120.49	118.80
57	A	1615	DXT	O3-C3-C2	-2.12	119.39	122.93
57	r	201	DXT	C5A-C5-C4A	2.11	114.07	110.55
57	a	3130	DXT	C6A-C6B-C11	2.05	121.00	119.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1615	DXT	C4A-C4-N4-C42
57	a	3123	DXT	C4A-C4-N4-C41
57	a	3130	DXT	C1-C2-C21-O21
57	a	3130	DXT	C1-C2-C21-N21
57	a	3130	DXT	C3-C2-C21-O21
57	a	3130	DXT	C3-C2-C21-N21
57	a	3130	DXT	C4A-C4-N4-C41
57	a	3138	DXT	C3-C2-C21-N21
57	a	3146	DXT	C4A-C4-N4-C41
57	r	201	DXT	C1-C2-C21-O21
57	r	201	DXT	C1-C2-C21-N21
57	r	201	DXT	C3-C2-C21-O21
57	r	201	DXT	C3-C2-C21-N21
57	r	201	DXT	C3-C4-N4-C42

Continued on next page...

Continued from previous page...

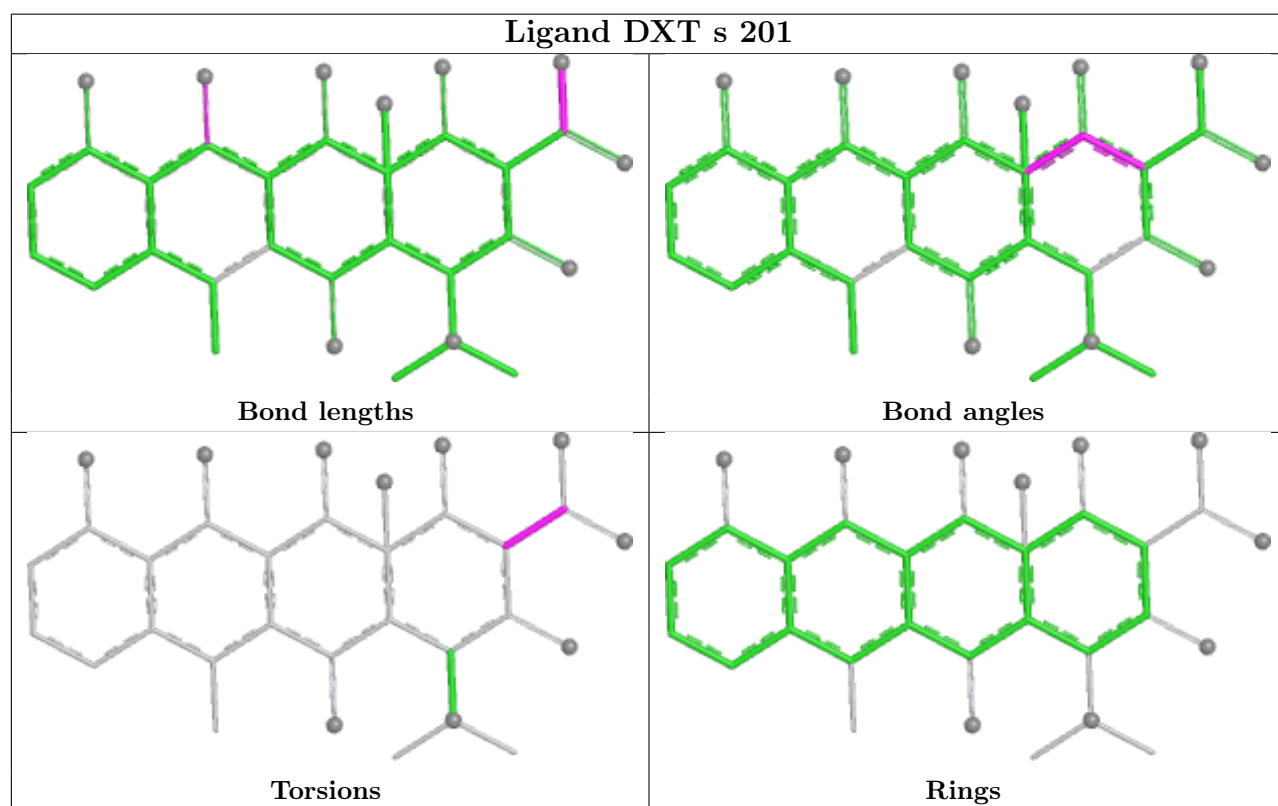
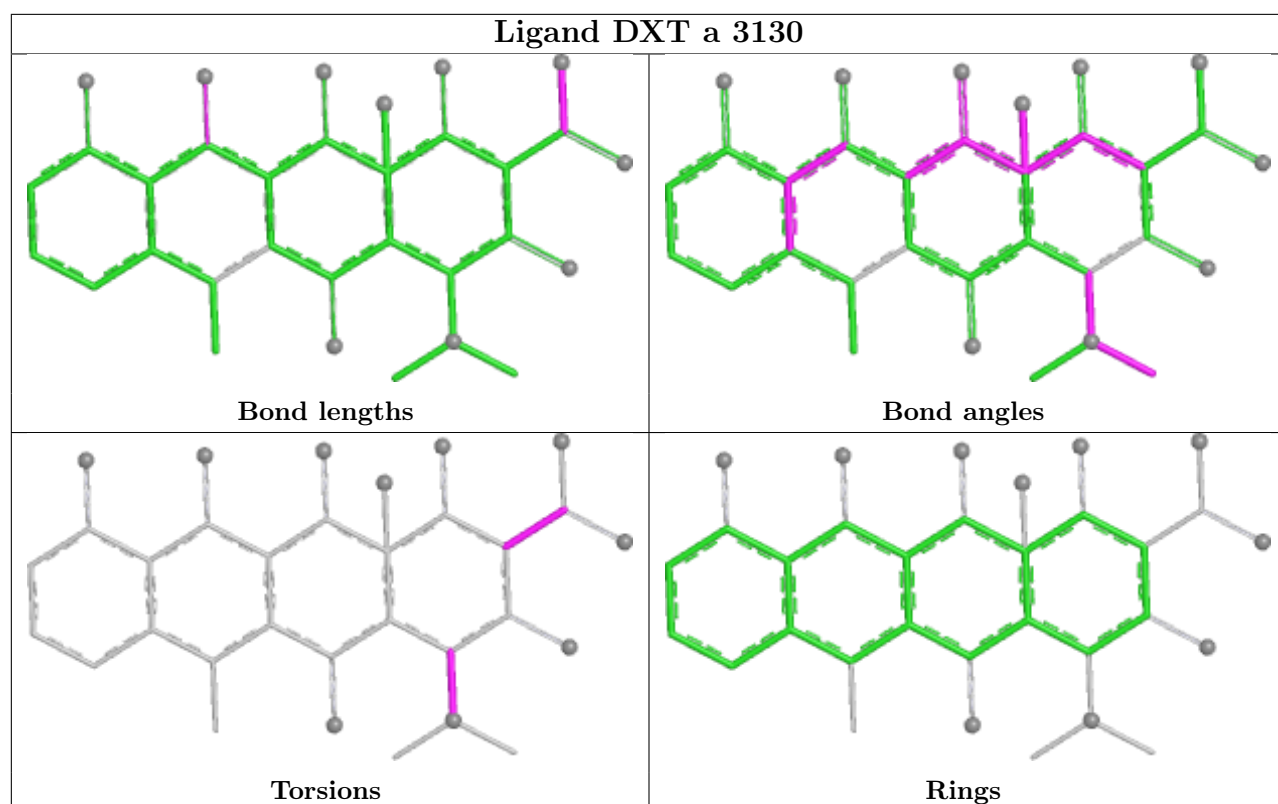
Mol	Chain	Res	Type	Atoms
57	s	201	DXT	C1-C2-C21-O21
57	s	201	DXT	C1-C2-C21-N21
57	s	201	DXT	C3-C2-C21-O21
57	s	201	DXT	C3-C2-C21-N21
57	A	1615	DXT	C3-C4-N4-C42
57	a	3130	DXT	C3-C4-N4-C42
57	a	3130	DXT	C4A-C4-N4-C42
57	r	201	DXT	C3-C4-N4-C41
57	r	201	DXT	C4A-C4-N4-C41
57	r	201	DXT	C4A-C4-N4-C42
57	a	3138	DXT	C3-C2-C21-O21
57	a	3138	DXT	C1-C2-C21-O21

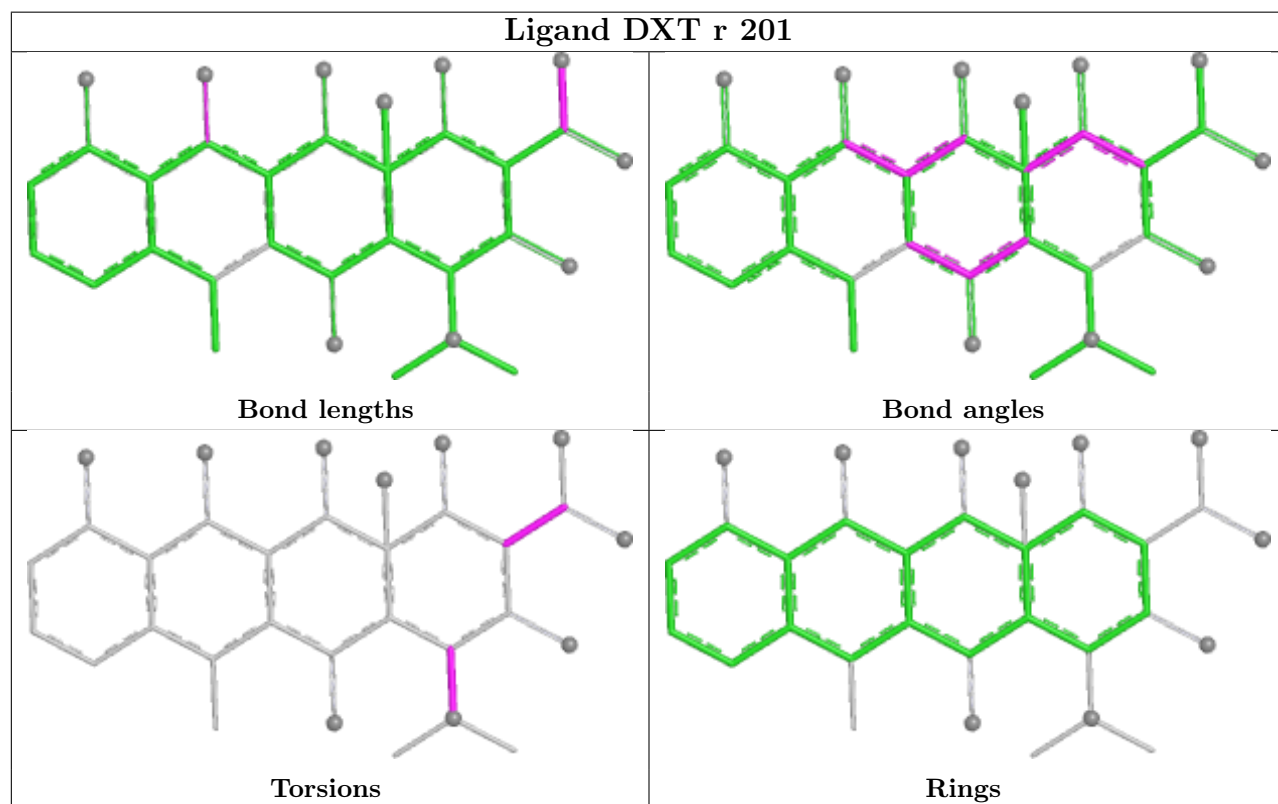
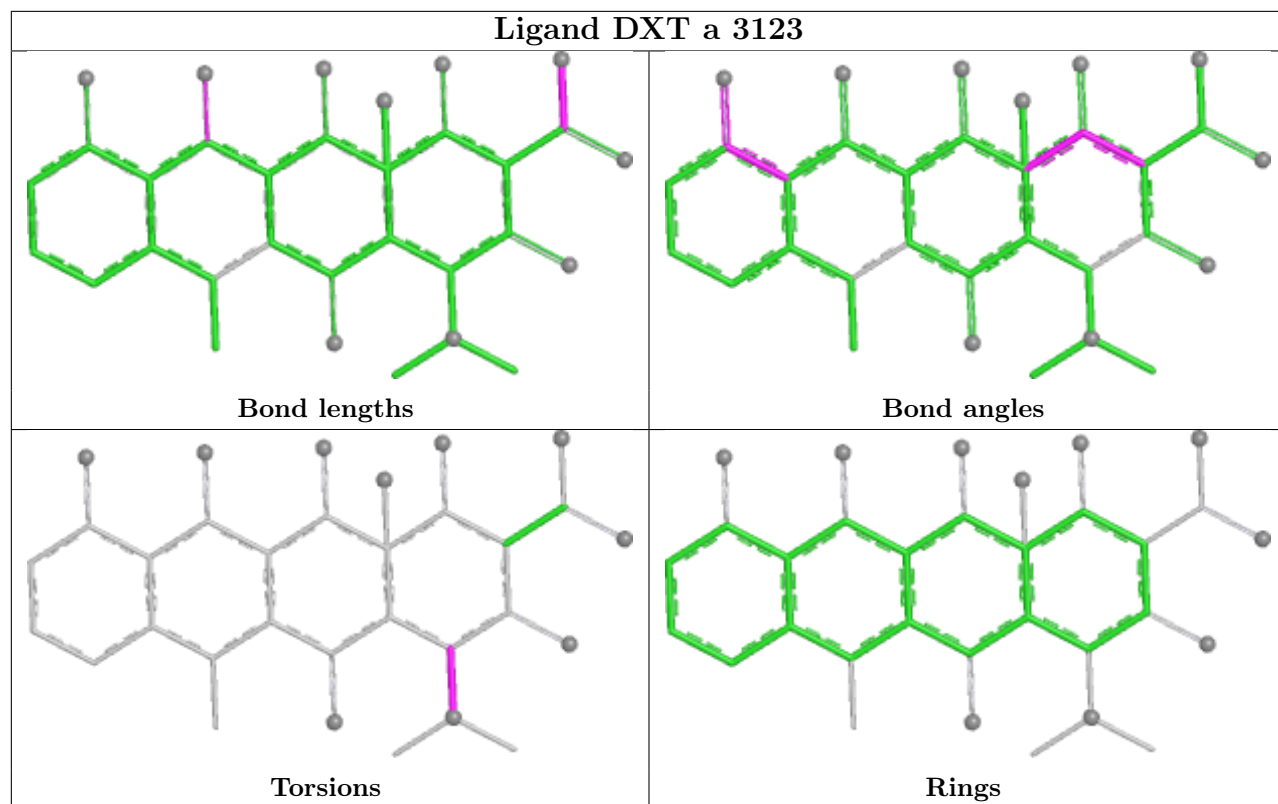
There are no ring outliers.

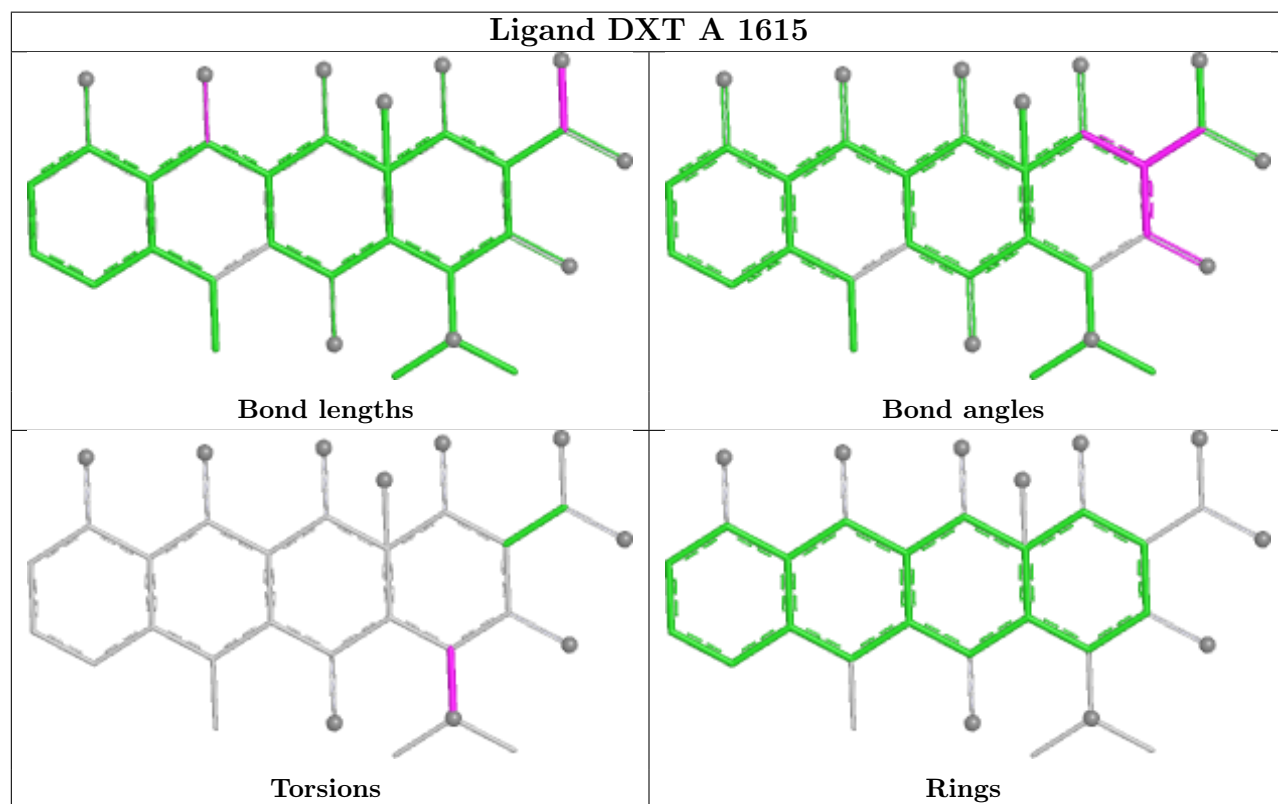
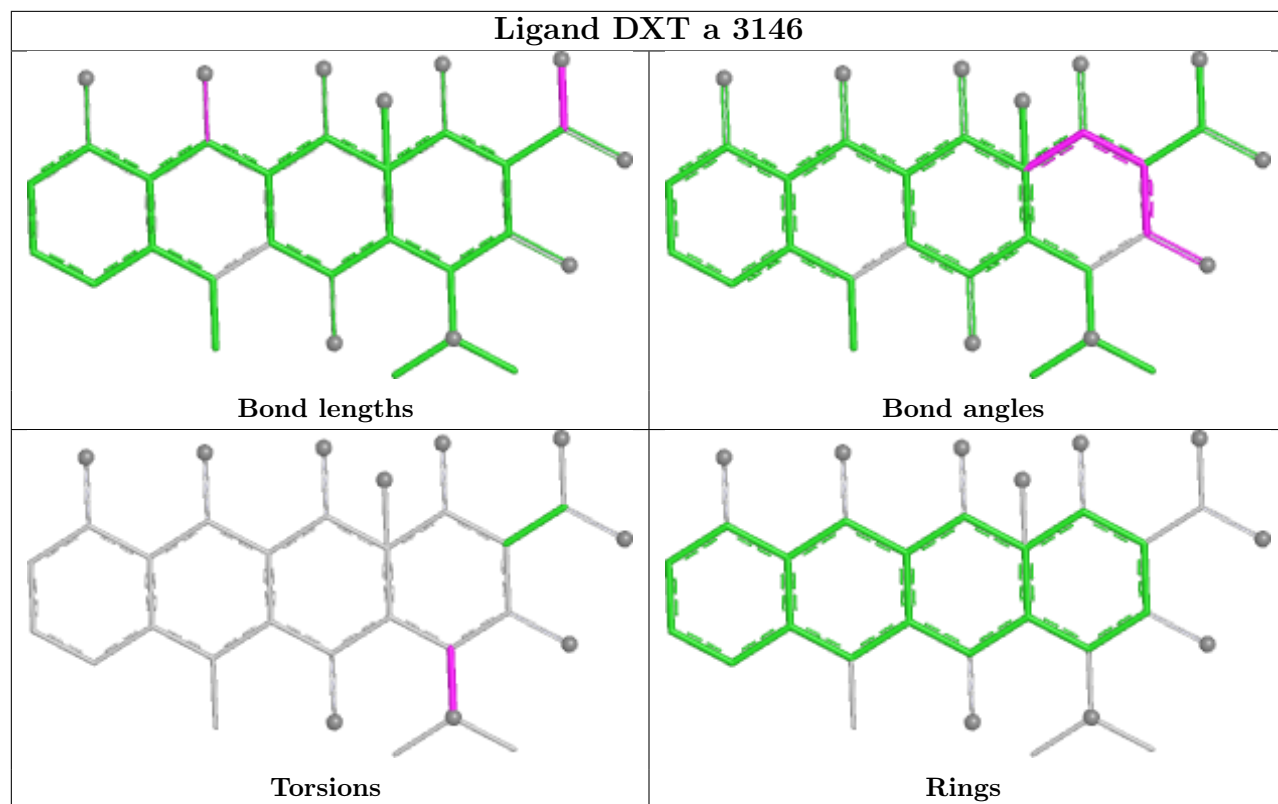
5 monomers are involved in 6 short contacts:

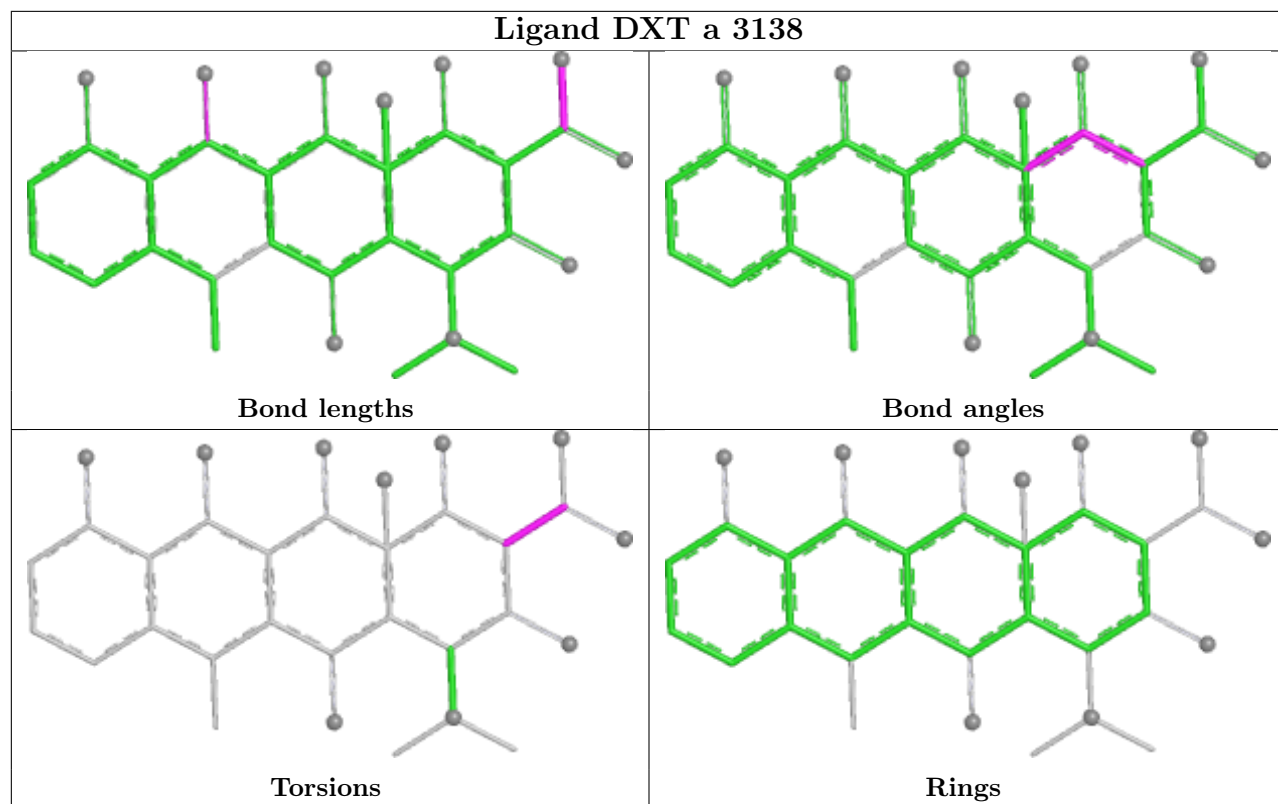
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	a	3123	DXT	2	0
57	r	201	DXT	1	0
57	a	3146	DXT	1	0
57	A	1615	DXT	1	0
57	a	3138	DXT	1	0

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](#)

There are no chain breaks in this entry.

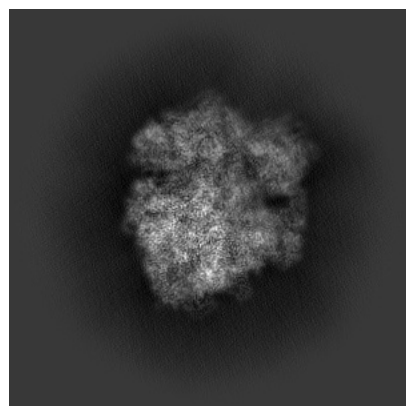
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71682. These allow visual inspection of the internal detail of the map and identification of artifacts.

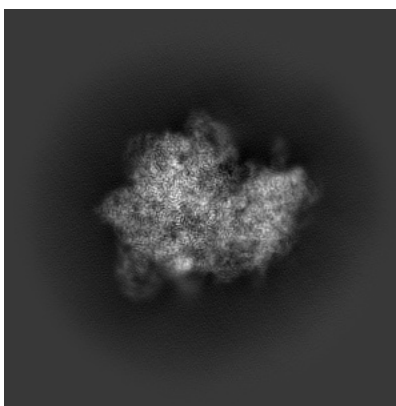
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

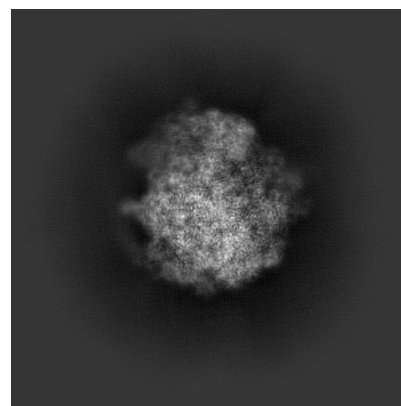
6.1.1 Primary map



X

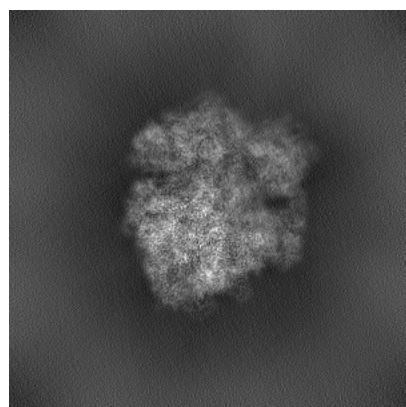


Y

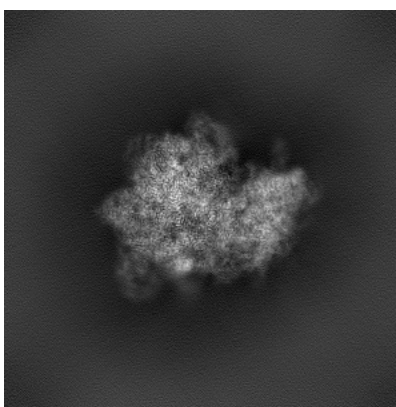


Z

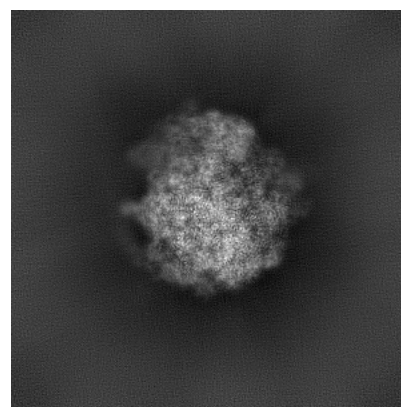
6.1.2 Raw map



X



Y

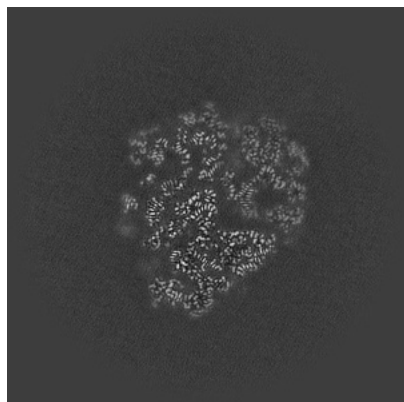


Z

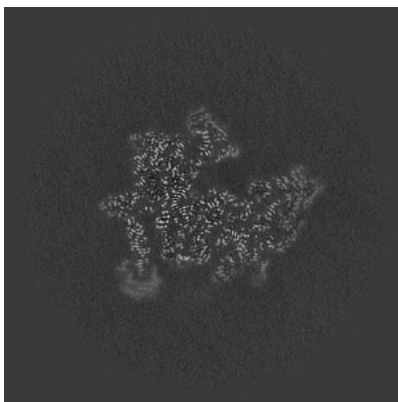
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

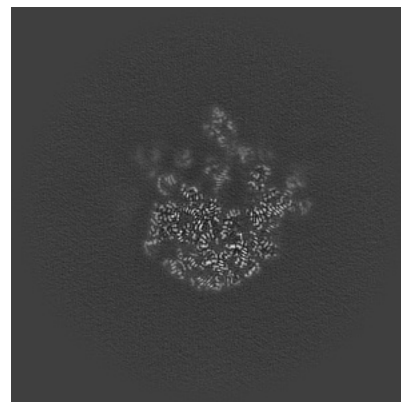
6.2.1 Primary map



X Index: 220

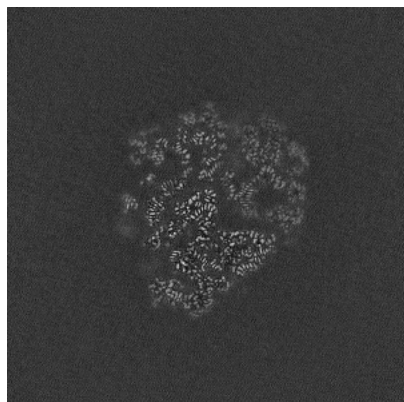


Y Index: 220

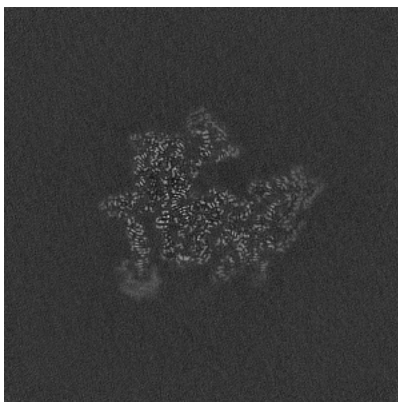


Z Index: 220

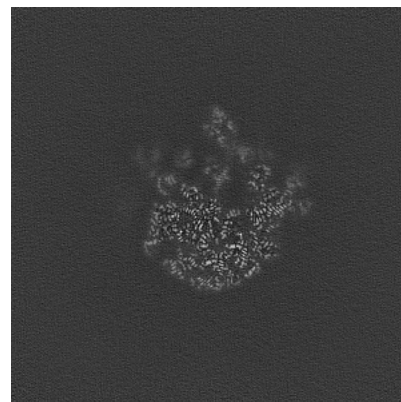
6.2.2 Raw map



X Index: 220



Y Index: 220

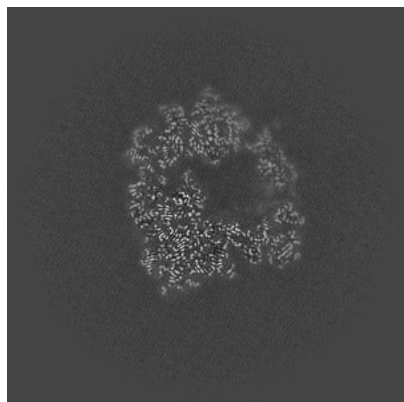


Z Index: 220

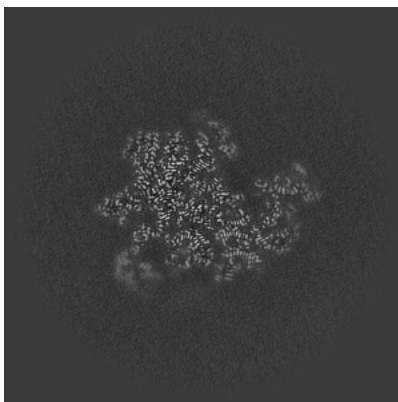
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

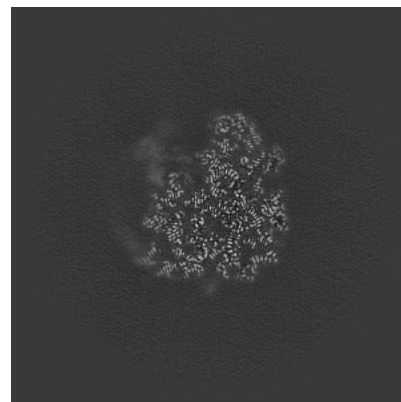
6.3.1 Primary map



X Index: 242

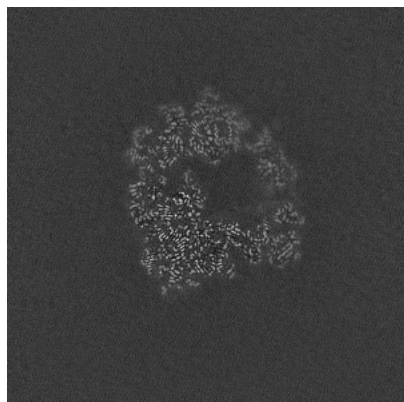


Y Index: 211

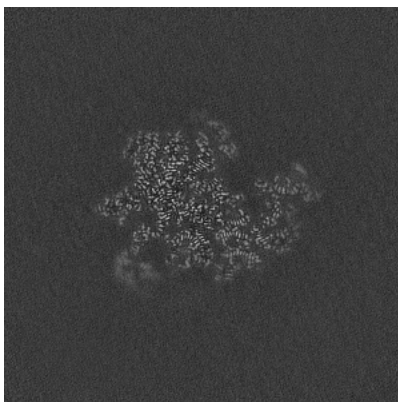


Z Index: 190

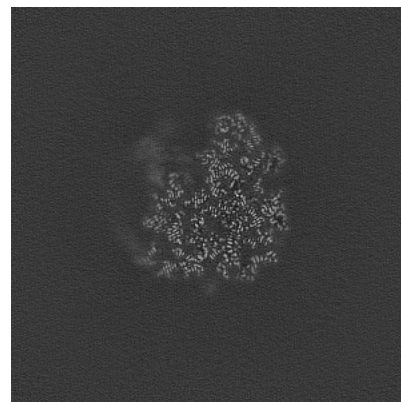
6.3.2 Raw map



X Index: 242



Y Index: 211

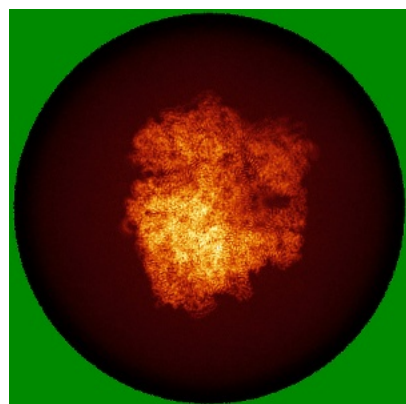


Z Index: 190

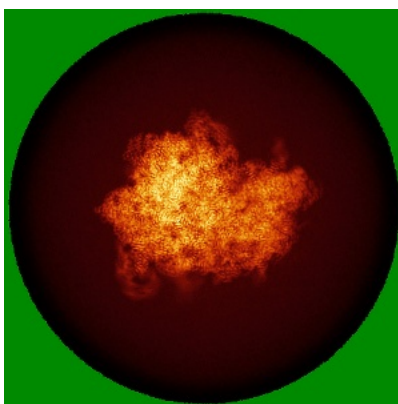
The images above show the largest variance slices of the map in three orthogonal directions.

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

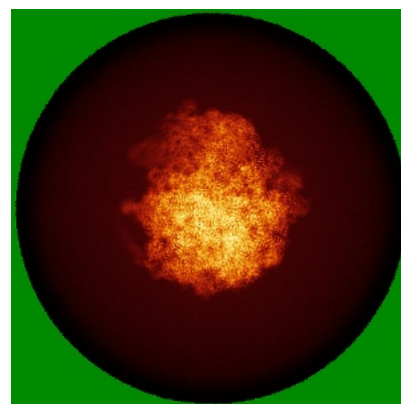
6.4.1 Primary map



X

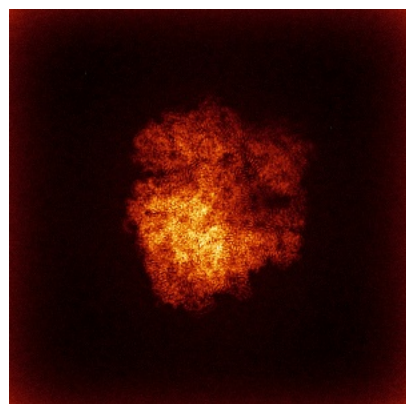


Y

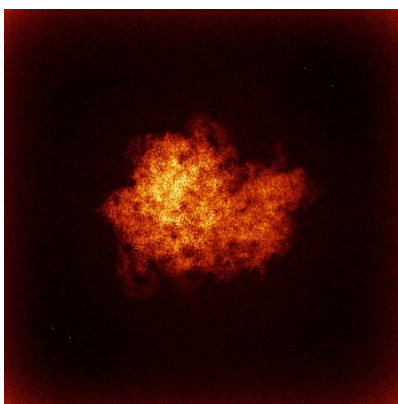


Z

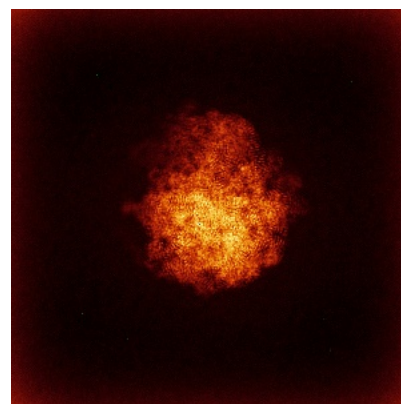
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



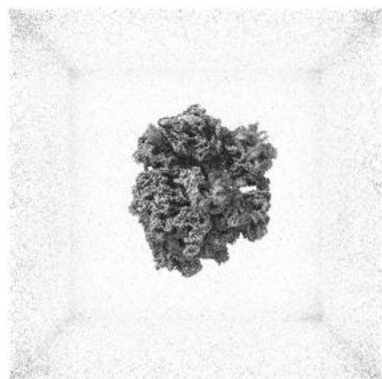
Y



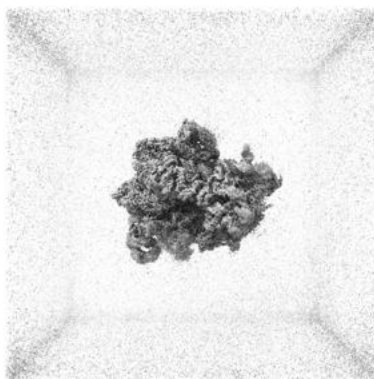
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

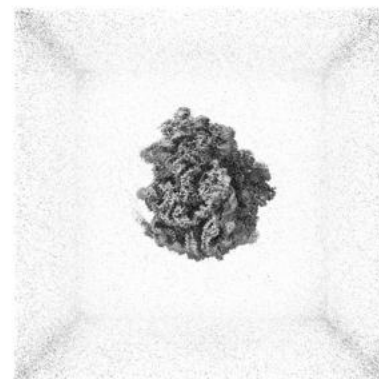
6.5.2 Raw map



X



Y



Z

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

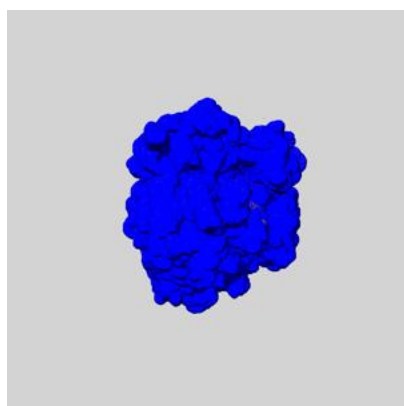
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

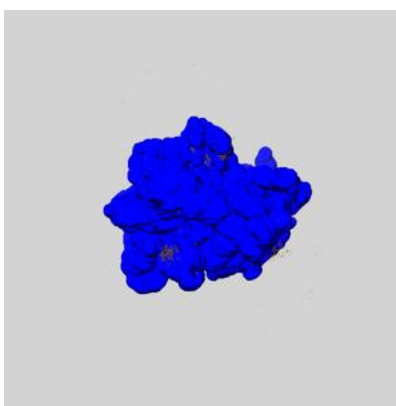
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

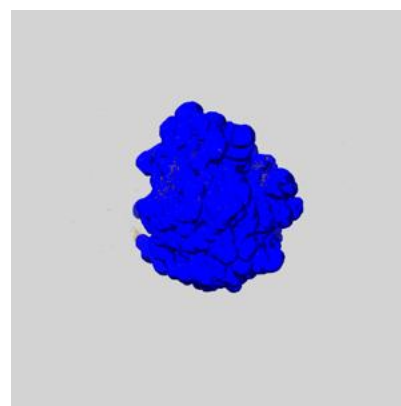
6.6.1 emd_71682_msk_1.map [i](#)



X



Y

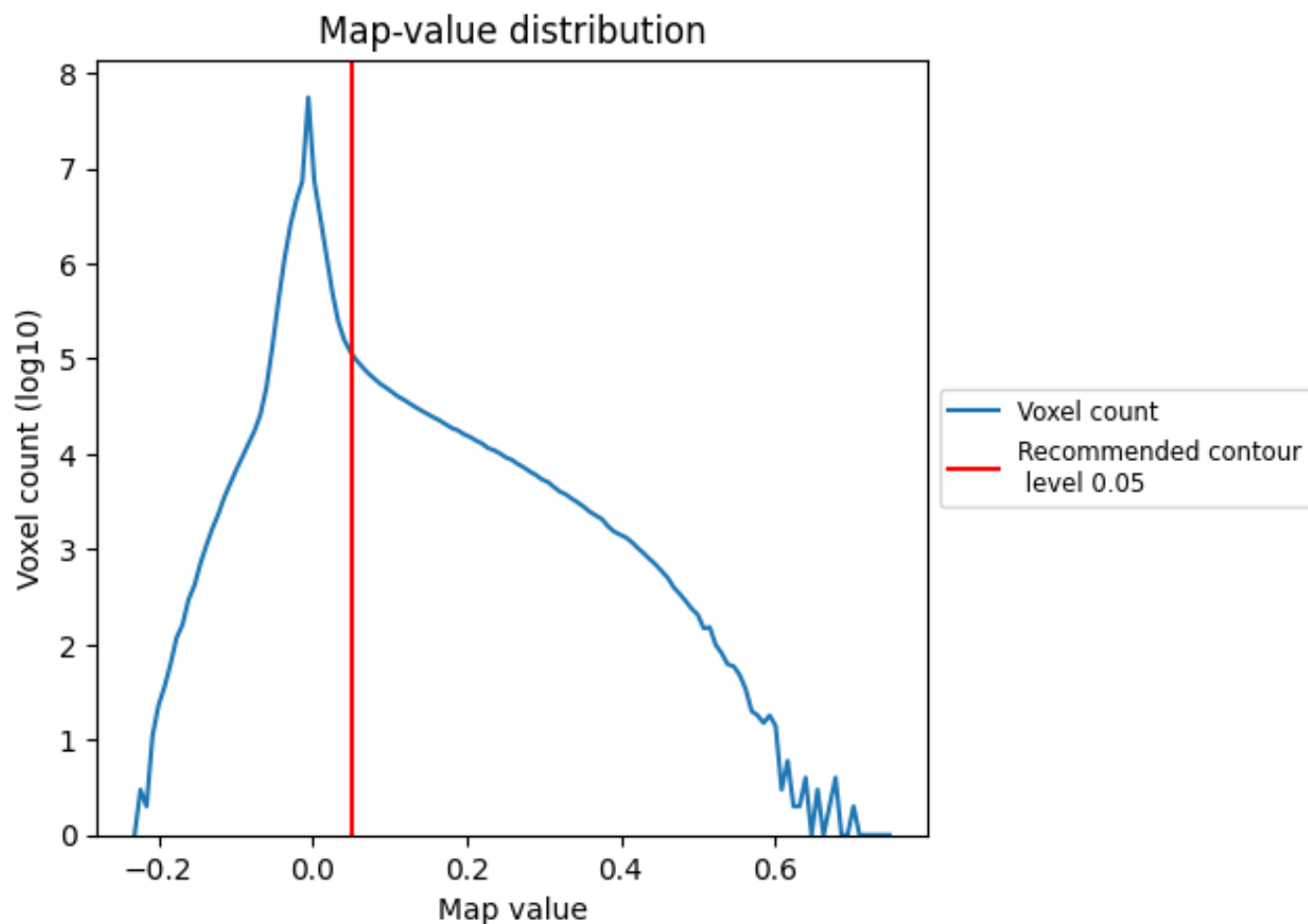


Z

7 Map analysis [i](#)

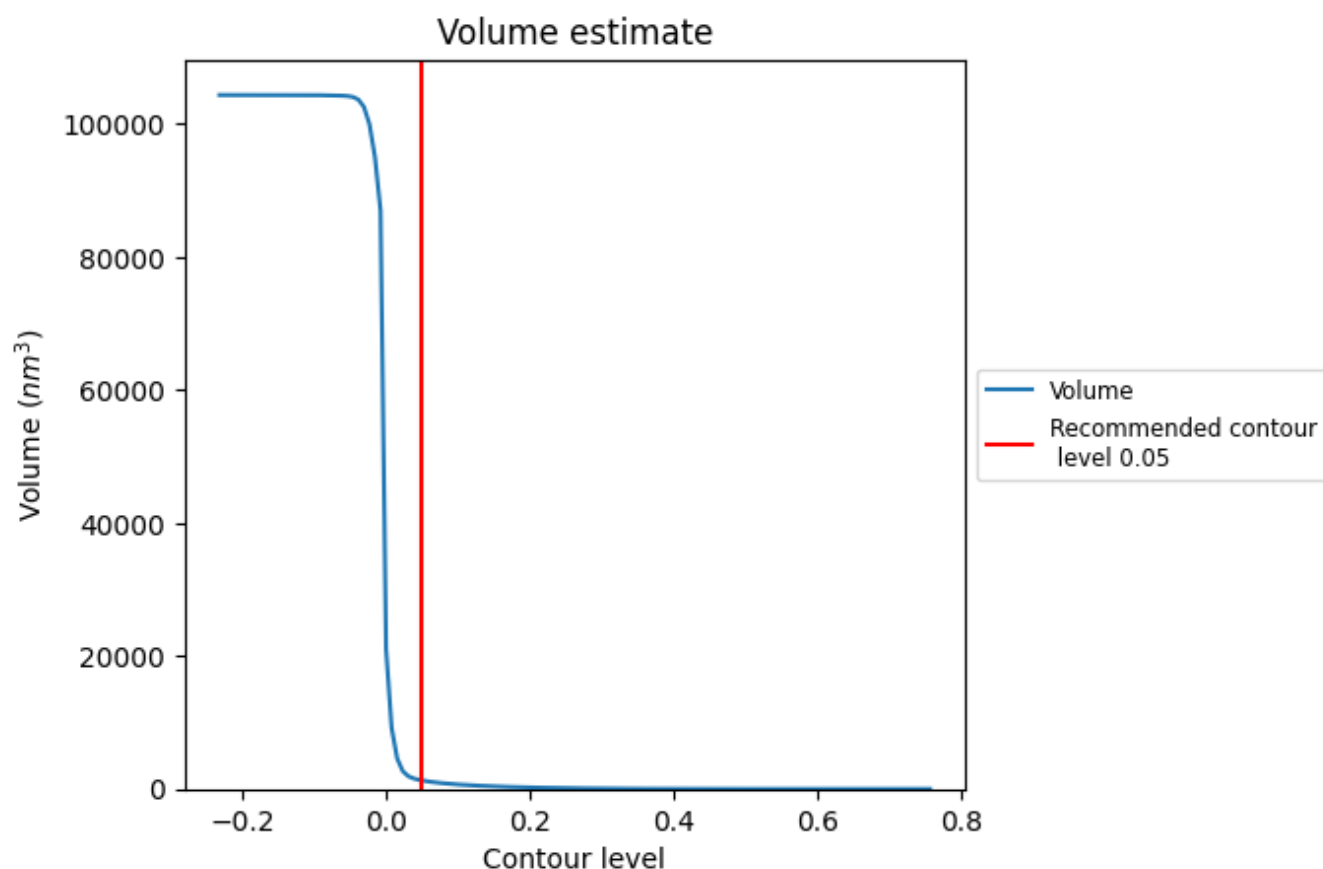
This section contains the results of statistical analysis of the map.

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.

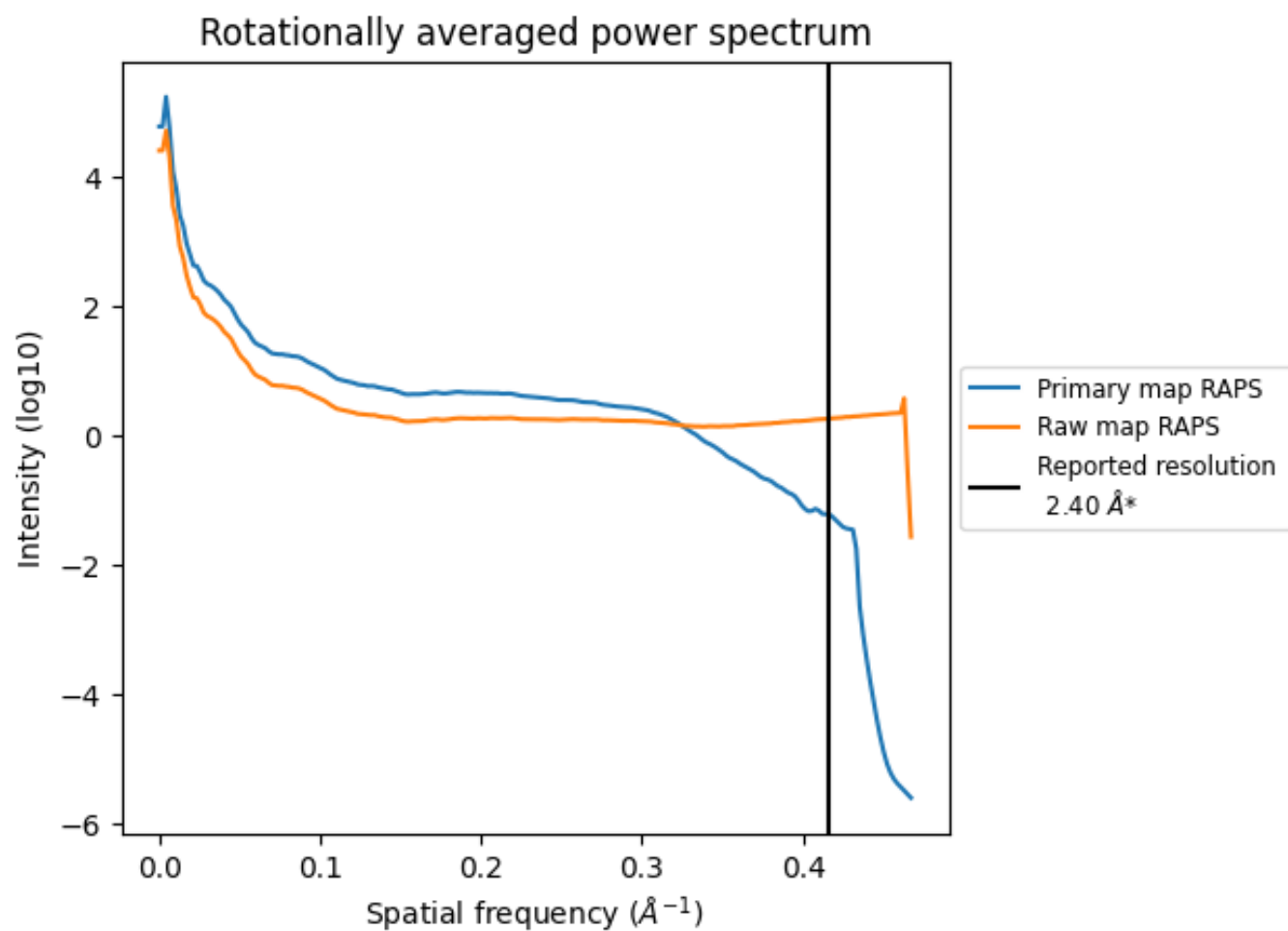
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1284 nm^3 ; this corresponds to an approximate mass of 1160 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 ⓘ

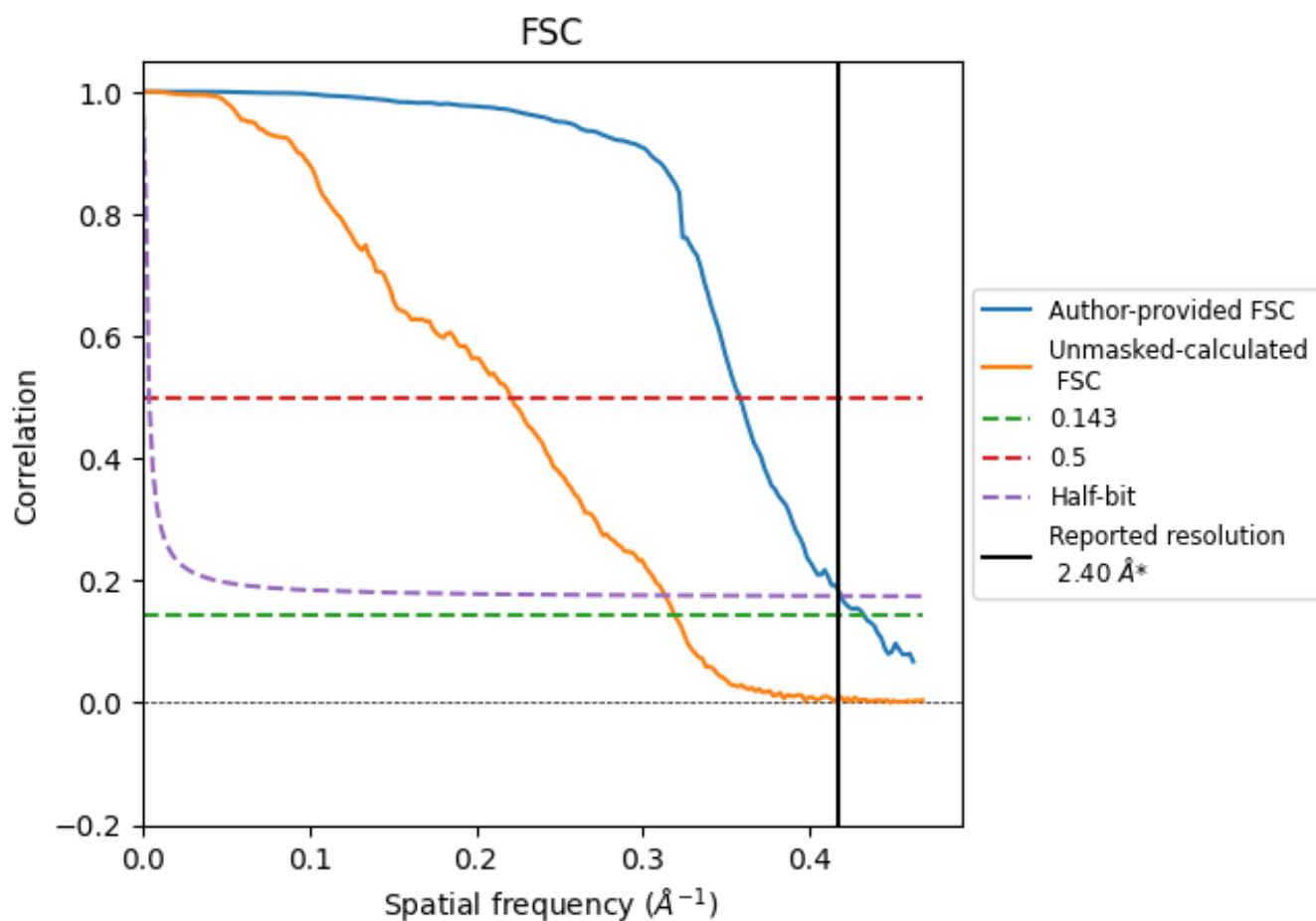


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

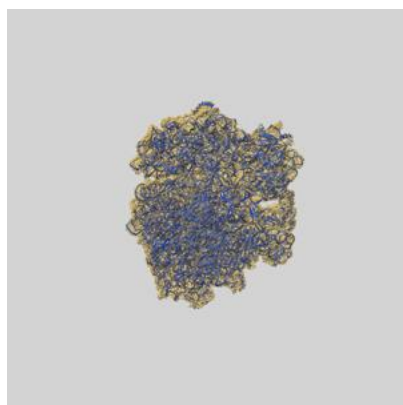
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.31	2.79	2.39
Unmasked-calculated*	3.14	4.52	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.4 by more than 10 %

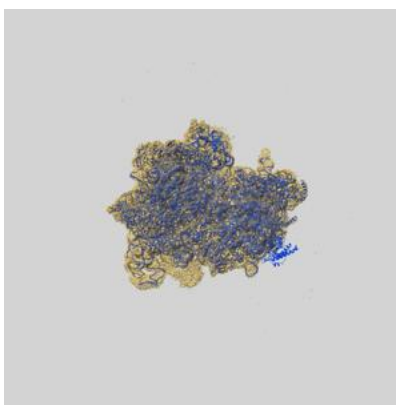
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71682 and PDB model 9PJ7. Per-residue inclusion information can be found in section [3](#) on page [17](#).

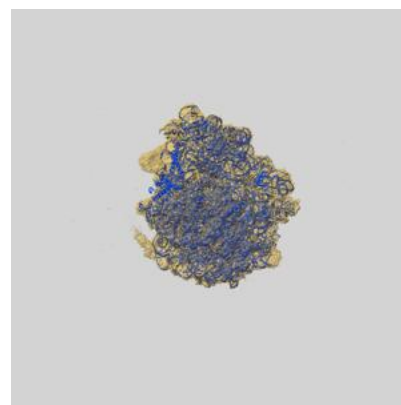
9.1 Map-model overlay [i](#)



X



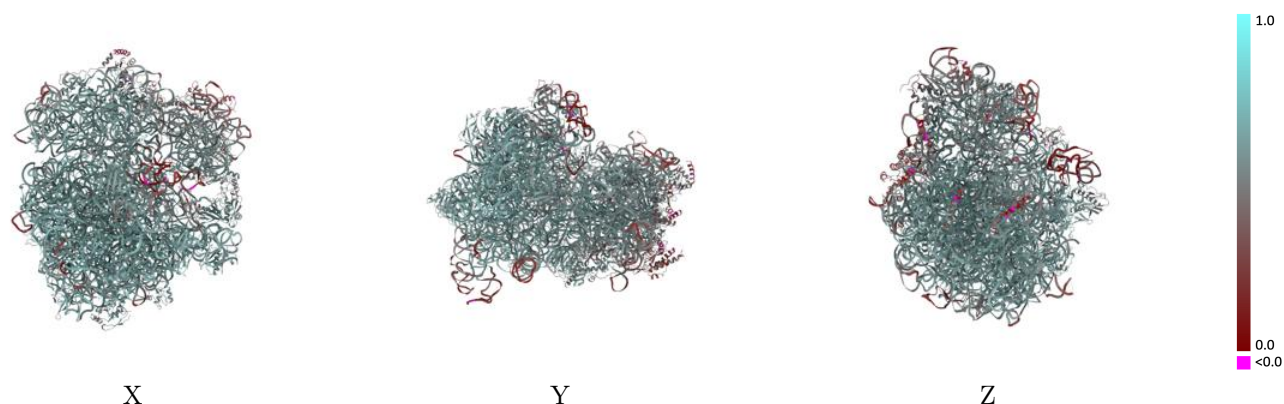
Y



Z

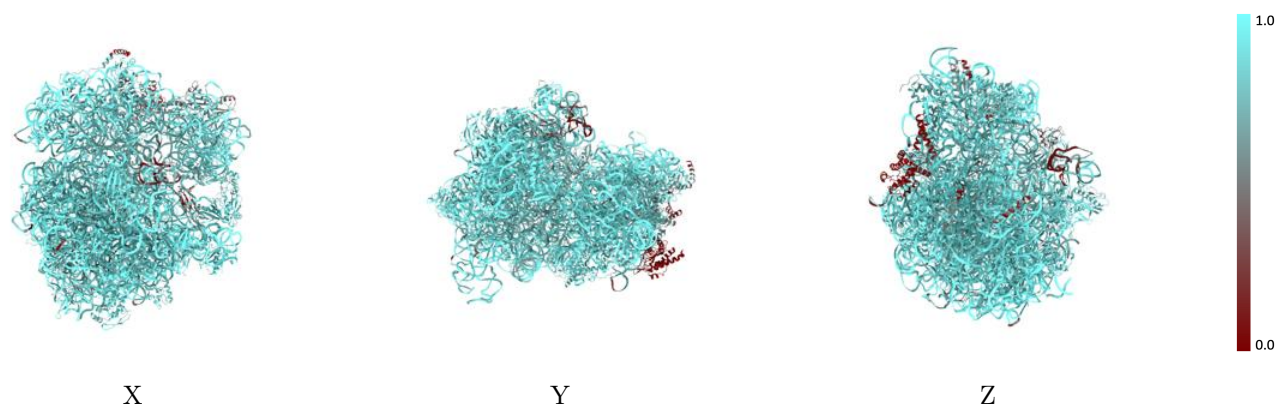
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



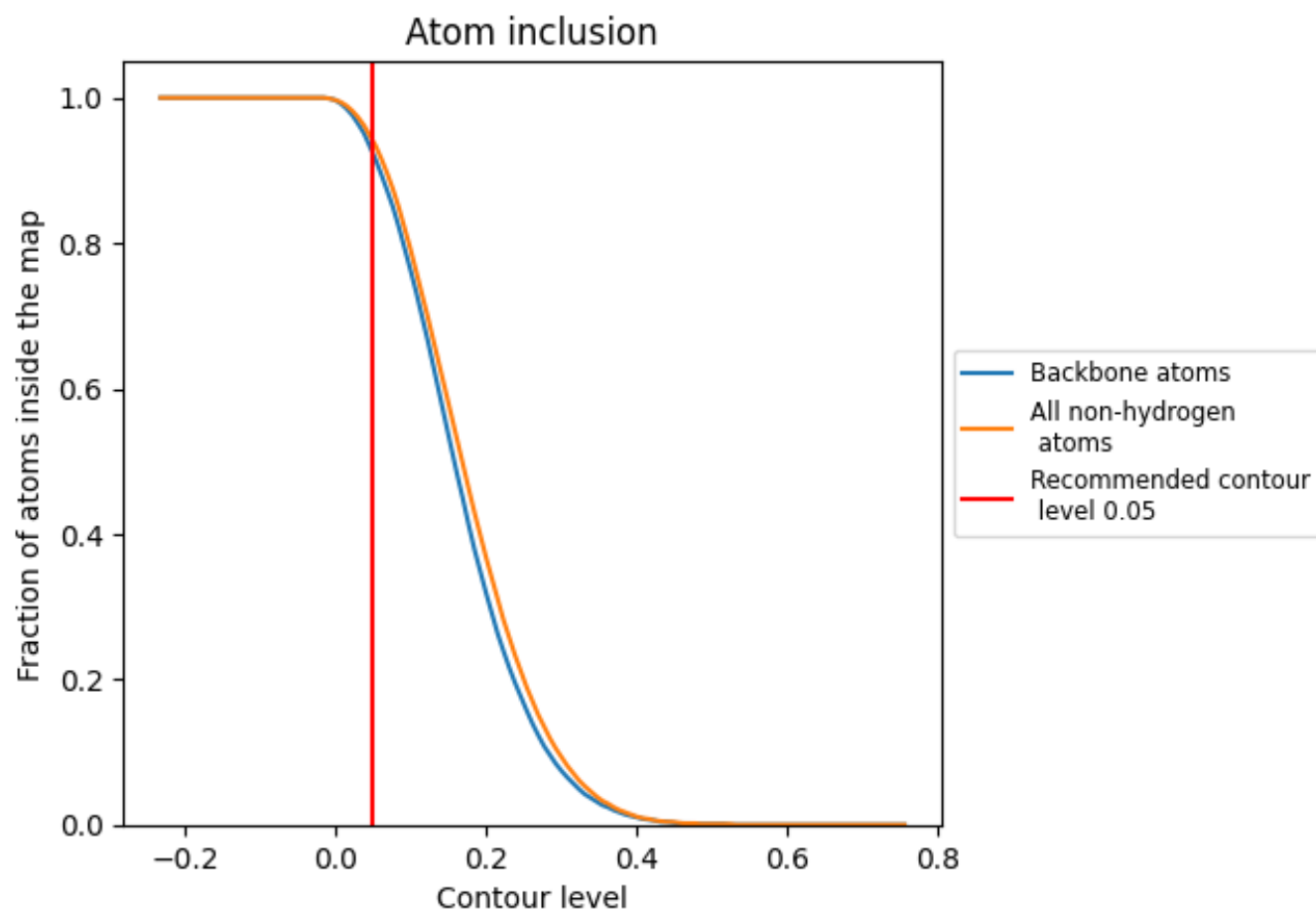
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.5810
0	 0.9580	 0.6150
1	 0.9910	 0.6610
2	 0.9700	 0.6420
3	 0.9560	 0.6240
4	 0.8590	 0.5050
A	 0.9830	 0.5710
B	 0.0430	 0.3090
C	 0.9600	 0.5800
D	 0.8910	 0.5340
E	 0.8340	 0.5490
F	 0.8920	 0.5300
G	 0.7750	 0.4970
H	 0.9440	 0.5860
I	 0.8960	 0.5260
J	 0.8600	 0.4820
K	 0.9320	 0.5650
L	 0.9360	 0.6020
M	 0.6470	 0.4270
N	 0.8800	 0.5360
O	 0.9360	 0.5710
P	 0.8370	 0.4950
Q	 0.8720	 0.5580
R	 0.8450	 0.5280
S	 0.8840	 0.5550
T	 0.9290	 0.5730
U	 0.9180	 0.5210
V	 0.9770	 0.6560
X	 0.9270	 0.6150
Y	 0.7680	 0.4690
a	 0.9690	 0.5980
b	 0.9950	 0.6110
c	 0.9710	 0.6390
d	 0.9700	 0.6280
e	 0.9380	 0.5870



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.9430	 0.5750
g	 0.9120	 0.5240
i	 0.9730	 0.6380
j	 0.9490	 0.6170
k	 0.9590	 0.6140
l	 0.9650	 0.6280
m	 0.9620	 0.6230
n	 0.9720	 0.5940
o	 0.9450	 0.6270
p	 0.9600	 0.6350
q	 0.9490	 0.6150
r	 0.9530	 0.6240
s	 0.9490	 0.6010
t	 0.9370	 0.5940
u	 0.6770	 0.4910
v	 0.9540	 0.6360
w	 0.9720	 0.6380
x	 0.9270	 0.5780
y	 0.9470	 0.6150
z	 0.9630	 0.6280