



Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 03:45 PM EDT

PDB ID : 9Q1Q / pdb_00009q1q
EMDB ID : EMD-72136
Title : NediV IRES (A site) in complex with Rabbit 80S ribosome
Authors : De, S.; Altomare, C.G.; Abaeva, I.S.; Dadhwal, P.; Garg, P.; Acosta-Reyes, F.; Brown, Z.P.; Pestova, T.V.; Hellen, C.U.T.; Frank, J.
Deposited on : 2025-08-14
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

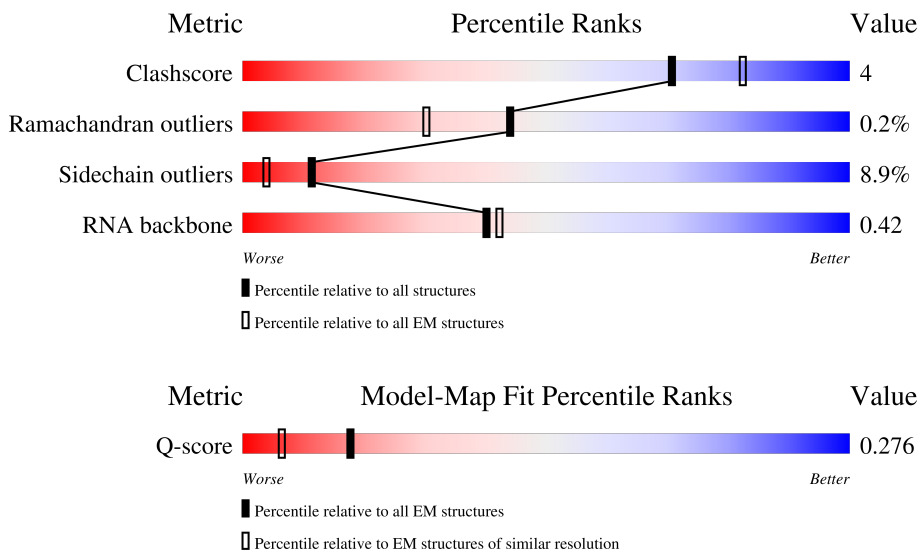
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.
























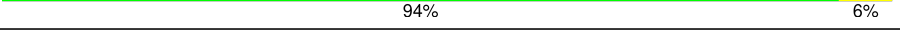



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	7	119	 82% 18%
2	A	248	 83% 15% •
3	B	394	 85% 14% •



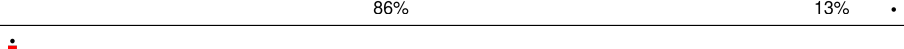
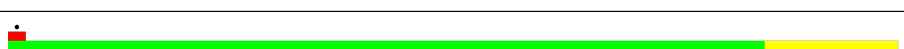



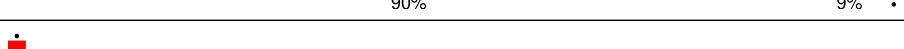



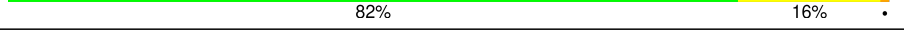

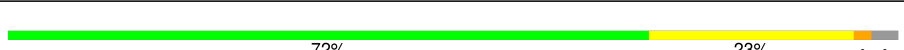










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Mol	Chain	Length	Quality of chain
4	C	362	 84% 15% .
5	D	293	 90% 10%
6	E	251	 73% 12% • 14%
7	F	225	 83% 16%
8	G	240	 84% 11% • •
9	H	190	 81% 18% •
10	I	213	 79% 15% • •
11	J	170	 88% 10% •
12	L	210	 89% 10% •
13	M	138	 89% 11%
14	N	203	 91% 9%
15	O	199	 87% 11% •
16	P	153	 90% 10% •
17	Q	187	 82% 17% •
18	R	180	 79% 21%
19	S	176	 82% 17% •
20	T	159	 77% 21% •
21	U	99	 89% 10% •
22	V	139	 79% 19% •
23	W	106	 14% 89% 10% •
24	X	118	 94% 6%
25	Y	134	 83% 15% •
26	Z	135	 82% 16% •
27	a	147	 82% 16% •
28	b	104	 5% 88% 10% ••

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Mol	Chain	Length	Quality of chain
29	c	98	
30	d	107	
31	e	128	
32	f	109	
33	g	114	
34	h	122	
35	i	102	
36	j	86	
37	k	69	
38	l	50	
39	m	52	
40	n	25	
41	o	104	
42	p	91	
43	r	124	
44	5	3603	
45	8	156	
46	DD	213	
47	FF	191	
48	KK	96	
49	MM	117	
50	PP	129	
51	QQ	142	
52	RR	132	
53	SS	144	

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Mol	Chain	Length	Quality of chain
54	TT	141	
55	UU	100	
56	ZZ	75	
57	cc	62	
58	dd	55	
59	ff	68	
60	gg	313	
61	9	1696	
62	AA	202	
63	BB	213	
64	CC	221	
65	EE	262	
66	GG	237	
67	HH	189	
68	II	206	
69	JJ	185	
70	LL	151	
71	NN	149	
72	OO	136	
73	VV	83	
74	WW	129	
75	XX	141	
76	YY	124	
77	aa	101	
78	bb	83	

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Mol	Chain	Length	Quality of chain
79	ee	57	<div><div></div><div>9%</div><div>81%</div><div>19%</div></div>
80	K	212	<div><div></div><div>10%</div><div>65%</div><div>24%</div><div>10%</div><div></div></div>
81	1	165	<div><div></div><div>8%</div><div>34%</div><div>58%</div><div>8%</div><div></div></div>
82	s	196	<div><div></div><div>5%</div><div></div><div>8%</div><div>88%</div></div>
83	t	153	<div><div></div><div>12%</div><div>9%</div><div>9%</div><div>5%</div><div>76%</div></div>

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 216047 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 2 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 4 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 5 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 6 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 7 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 8 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1872	1195	360	313	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 9 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 10 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	204	Total	C	N	O	S	0	0
			1660	1054	320	273	13		

- Molecule 11 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 12 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 13 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 14 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 16 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 17 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 18 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 19 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 20 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 21 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 23 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 25 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 27 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 28 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	103	Total	C	N	O	S	0	0
			841	522	188	128	3		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 30 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 31 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 32 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 35 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 36 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 37 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 39 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 40 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 41 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 43 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 44 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5	3603	Total	C	N	O	P	0	0
			77244	34401	14135	25105	3603		

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 46 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	DD	213	Total	C	N	O	S	0	0
			1653	1054	300	291	8		

- Molecule 47 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 48 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 49 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	MM	98	Total	C	N	O	S	0	0
			754	475	135	137	7		

- Molecule 50 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	PP	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 51 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 52 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RR	124	Total	C	N	O	S	0	0
			1002	628	190	180	4		

- Molecule 53 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 54 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 55 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 56 is a protein called 40S ribosomal protein S25.

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

- Molecule 57 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 58 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 59 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 61 is a RNA chain called 18S RNA (1696-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
61	9	1696	Total	C	N	O	P	0	0
			36209	16162	6504	11848	1695		

- Molecule 62 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AA	202	Total	C	N	O	S	0	0
			1586	1011	280	287	8		

- Molecule 63 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BB	206	Total	C	N	O	S	0	0
			1680	1068	300	298	14		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 65 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 66 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 67 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 68 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 70 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 71 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 72 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	28	ARG	CYS	conflict	UNP G1TFE8
aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	ee	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 80 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	K	212	Total	C	N	O	S	0	0
			1705	1091	306	300	8		

- Molecule 81 is a RNA chain called NediV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	1	165	Total	C	N	O	P	0	0
			3496	1564	608	1159	165		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1479	C	U	conflict	GB 403044781
1	1486	C	U	conflict	GB 403044781

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	s	23	Total	C	N	O	S	0	0
			173	106	35	29	3		

- Molecule 83 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	t	36	Total	C	N	O	S	0	0
			275	165	55	53	2		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	7	5	Total	Mg	0
			5	5	
84	P	1	Total	Mg	0
			1	1	
84	V	1	Total	Mg	0
			1	1	
84	a	1	Total	Mg	0
			1	1	
84	g	1	Total	Mg	0
			1	1	
84	j	1	Total	Mg	0
			1	1	
84	5	192	Total	Mg	0
			192	192	
84	8	3	Total	Mg	0
			3	3	
84	9	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total 1	Zn 1	0
85	m	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0
85	dd	1	Total 1	Zn 1	0
85	ff	1	Total 1	Zn 1	0
85	aa	1	Total 1	Zn 1	0

3 Residue-property plots


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.

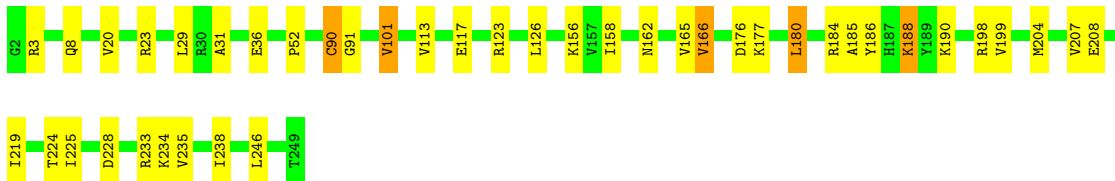
- Molecule 1: 5S rRNA

Chain 7:  82% 18%




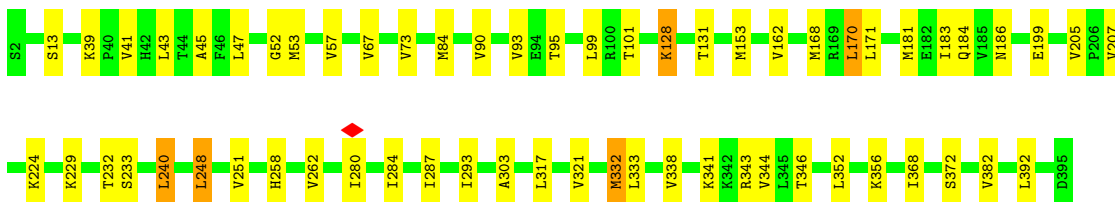
- Molecule 2: 60S ribosomal protein L8

Chain A:  83% 15% .




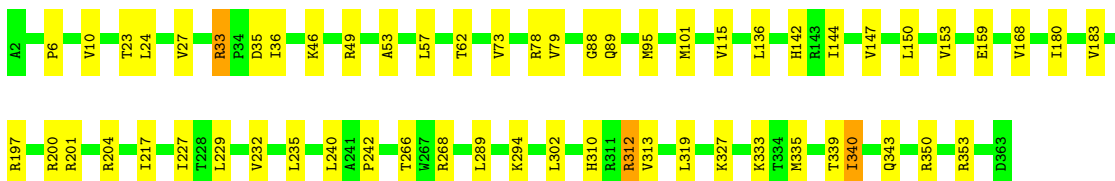
- Molecule 3: 60S ribosomal protein L3

Chain B:  85% 14% .



- Molecule 4: 60S ribosomal protein L4

Chain C:  84% 15% .

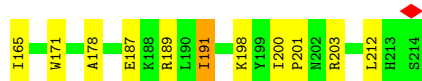
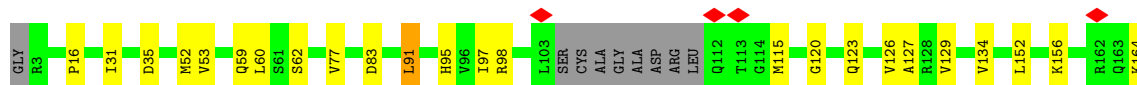


- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1 | I4 | N7 | I12 | V16 | I18 | V25 | V27 | V43 | L48 | K52 | R56 | V57 | D58 | K59 | N79 | R89 | R90 | K91 | N92 | R93 | S94 | V104 | I105 | Q106 | I114 | L118 | R124 | R125 | V126 | R127 | M128 | C134 | S135 | V136 | S137 | D142 | V145 | L146 |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



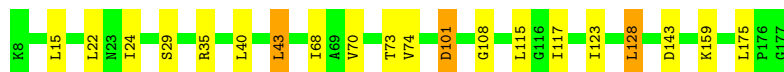
- Molecule 10: Ribosomal protein L10

Chain I: 79% 15% . .



- Molecule 11: 60S ribosomal protein L11

Chain J: 88% 10% .



- Molecule 12: Large ribosomal subunit protein eL13

Chain L: 89% 10% .



- Molecule 13: 60S ribosomal protein L14

Chain M: 89% 11%



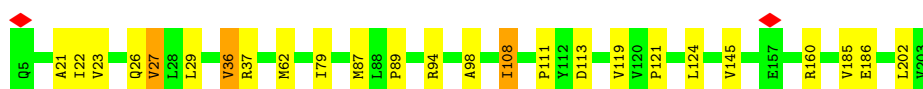
- Molecule 14: 60S ribosomal protein L15

Chain N: 91% 9%




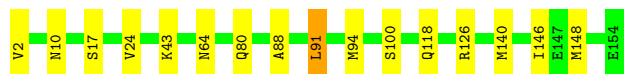
- Molecule 15: Large ribosomal subunit protein uL13

Chain O: 87% 11% .




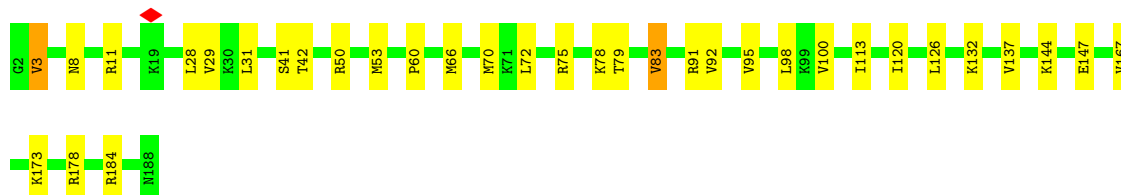
- Molecule 16: 60S ribosomal protein L17

Chain P:  90% 10%




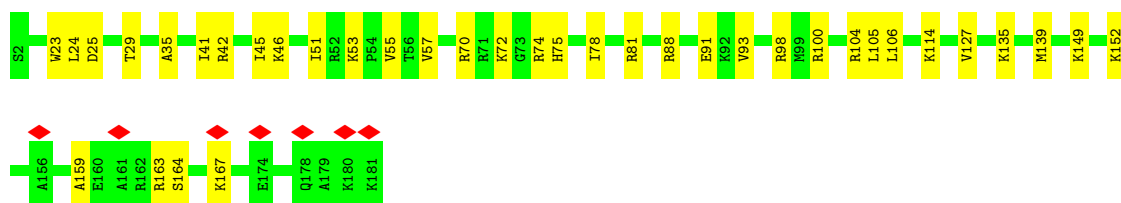
- Molecule 17: eL18

Chain Q:  82% 17%




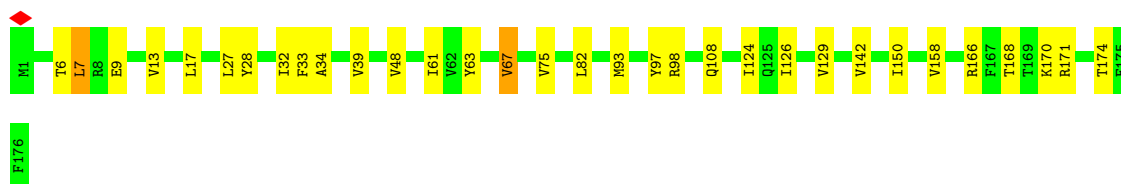
- Molecule 18: 60S ribosomal protein L19

Chain R:  79% 21%



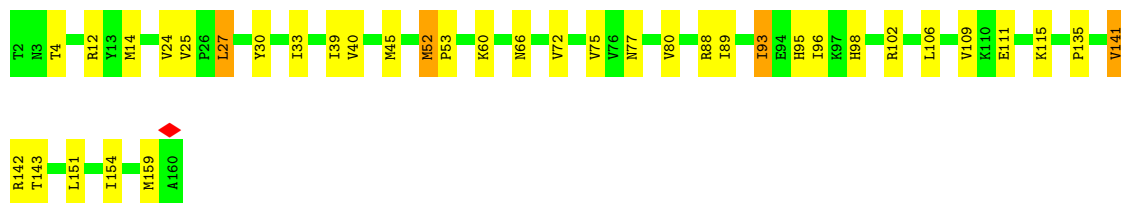
- Molecule 19: eL20

Chain S:  82% 17%




- Molecule 20: 60S ribosomal protein L21

Chain T:  77% 21%




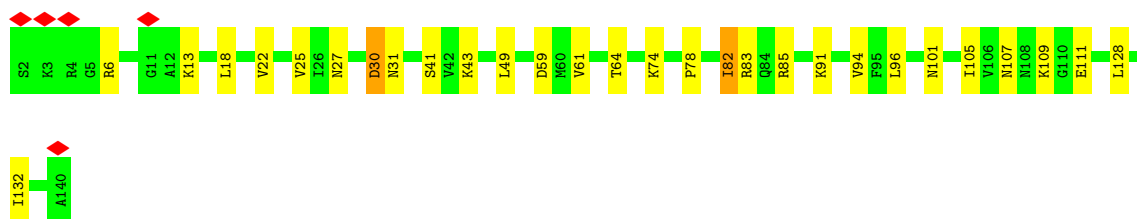
- Molecule 21: eL22

Chain U:  89% 10%



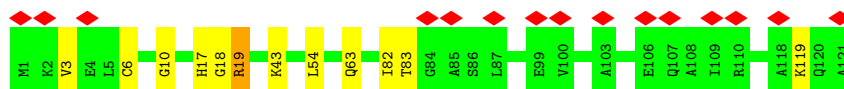
- Molecule 22: Large ribosomal subunit protein uL14

Chain V:  79% 19%



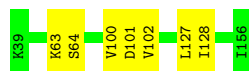
- Molecule 23: uL24

Chain W:  14% 89% 10%




- Molecule 24: Large ribosomal subunit protein uL23

Chain X:  94% 6%




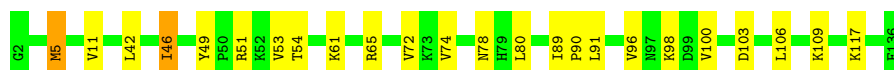
- Molecule 25: 60S ribosomal protein L26

Chain Y:  83% 15%




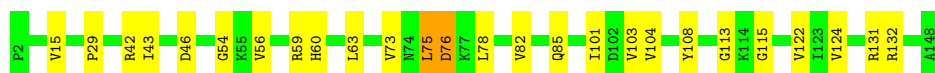
- Molecule 26: 60S ribosomal protein L27

Chain Z:  82% 16%

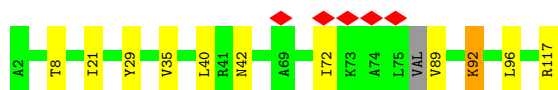
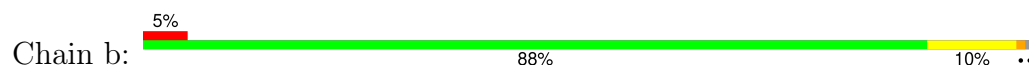


- Molecule 27: 60S ribosomal protein L27a

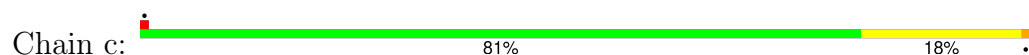
Chain a:  82% 16%



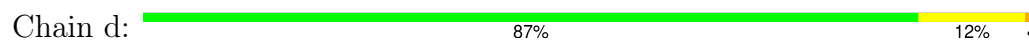
- Molecule 28: eL29



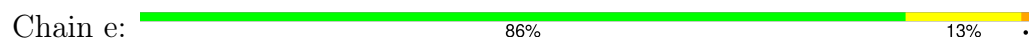
- Molecule 29: 60S ribosomal protein L30



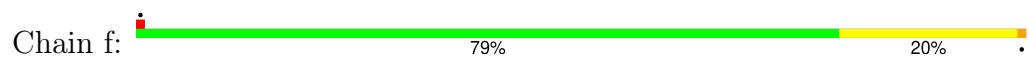
- Molecule 30: 60S ribosomal protein L31



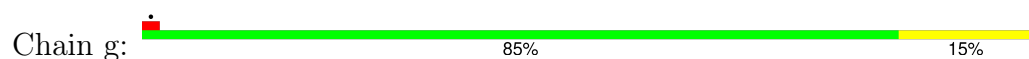
- Molecule 31: eL32



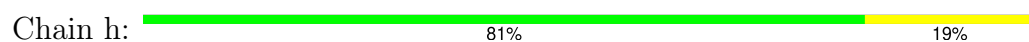
- Molecule 32: Large ribosomal subunit protein eL33



- Molecule 33: 60S ribosomal protein L34



- Molecule 34: 60S ribosomal protein L35





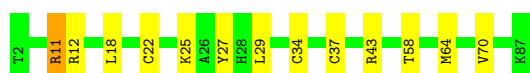
- Molecule 35: 60S ribosomal protein L36

Chain i: 85% 14%



- Molecule 36: 60S ribosomal protein L37

Chain j: 85% 14%



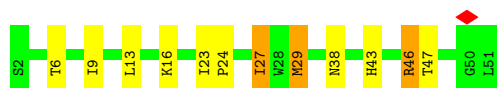
- Molecule 37: Large ribosomal subunit protein eL38

Chain k: 90% 9%



- Molecule 38: 60S ribosomal protein L39

Chain l: 76% 18% 6%



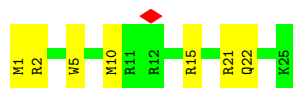
- Molecule 39: Large ribosomal subunit protein eL40

Chain m: 87% 13%



- Molecule 40: eL41

Chain n: 72% 28%

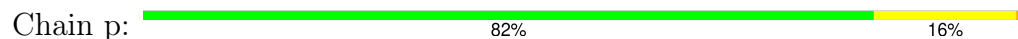


- Molecule 41: eL42

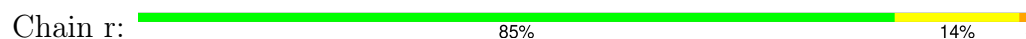
Chain o: 77% 21%



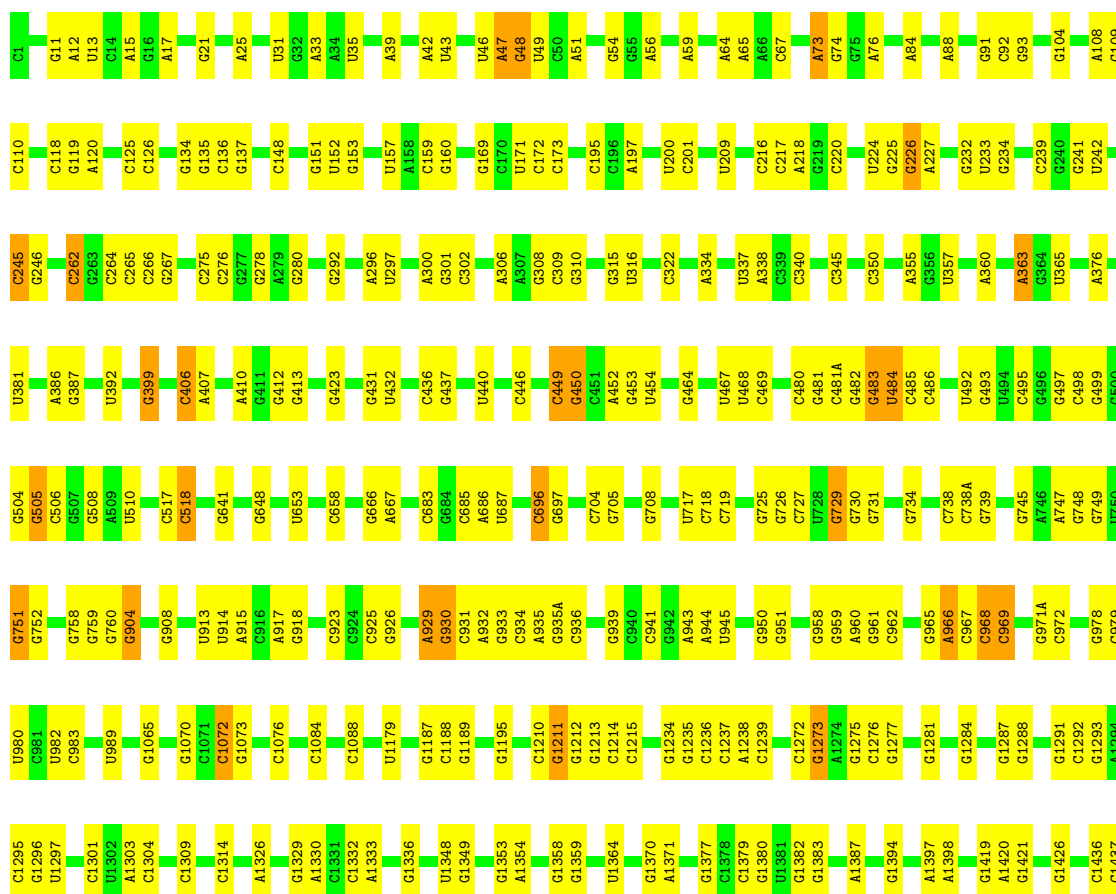
- Molecule 42: 60S ribosomal protein L37a



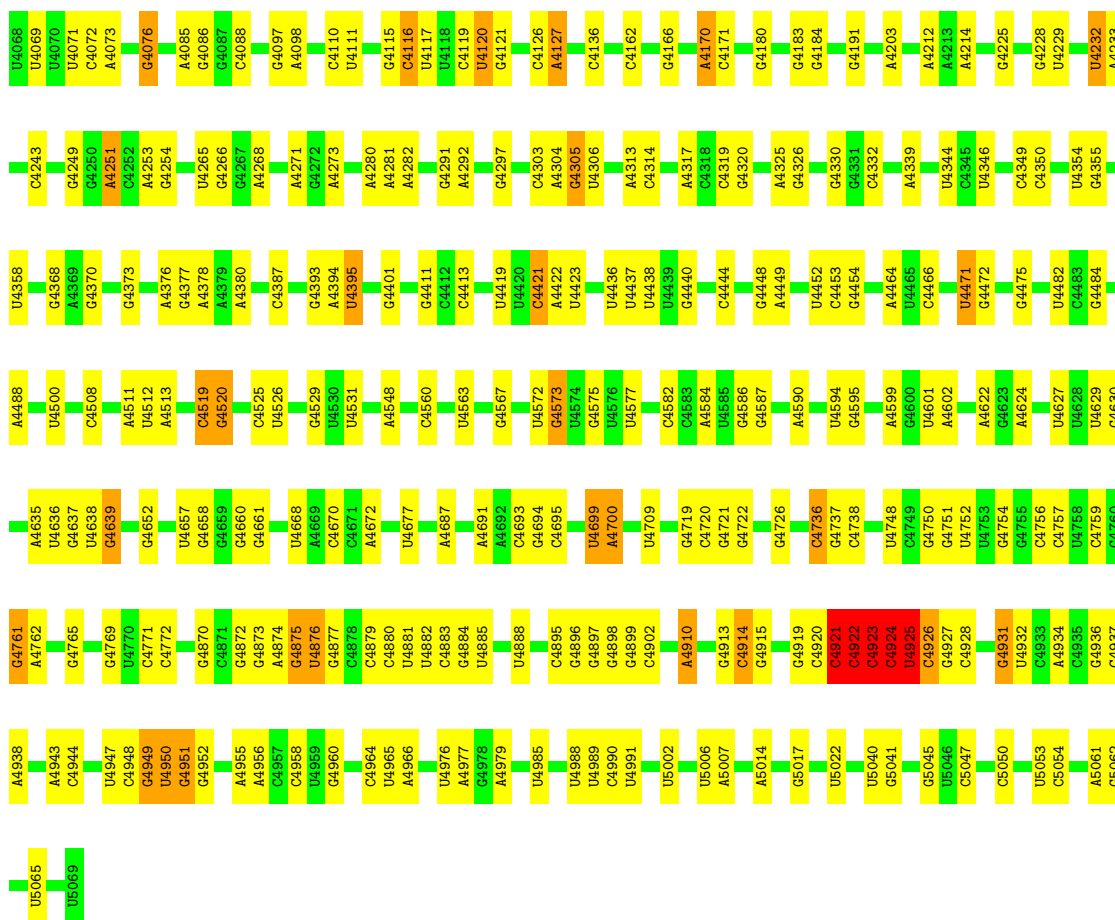
- Molecule 43: 60S ribosomal protein L28



- Molecule 44: 28S rRNA

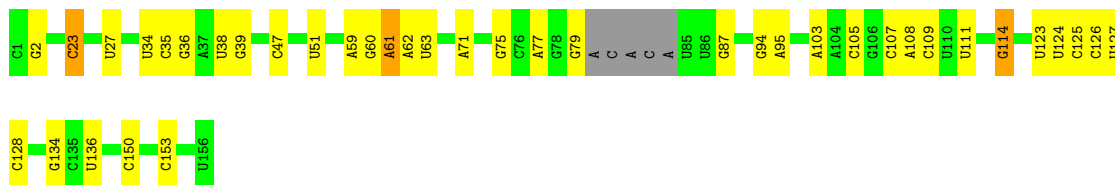


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G3938	G3813	C3673	G3678	G2711	C2572	G2448	G2306	C2081	U1980	A1858	U1754	C1441
G3939	U3814	G3679	G2826	G2712	A2573	G2450	G2309	C2084	A1983	G1869	U1756	G1444
U3940	A3817	U3679	U2826	C2713	G2574	A2451	G2313	G2085	A1984	C1884	U1757	U1445
G3941	U3818	U3680	U2827	G2714	U2575	G2452	A2313	A2088	G1985	G1885	G1758	C1446
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G3944	A3882	C2716	U2837	G2717	G2586	G2463	G2316	U2090	G1987	A1888	G1760	G1448
A3945	A3892	G2721	G2842	G2724	U2587	G2471	U2339	C2091	G1988	U1888	G1761	G1455
G3946	G3838	G2825	G2845	G2725	C2588	G2475	G2330	G2092	A1990	G1890	G1764	G1456
A3947	G3839	U3695	A2845	G2726	C2589	G2476	G2331	A2093	U1991	A1897	A1765	G1457
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G3968	G3876	G3755	C3605	U2765	A2647	G2515	A2382	G2262	G2023	G1933	U1649	G1502
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G3970	G3878	G3757	A3610	G2767	A2659	C2519	A2395	G2264	A2025	G1945	G1654	G1510
A3971	A3879	G3758	A3611	U2768	U2660	G2520	A2396	C2265	G2026	G1948	C1661	U1514
G3972	G3880	G3759	G3615	G2769	A2661	G2521	G2399	G2266	A2027	G1948	G1818	A1515
U3973	A3881	U2769	G3616	U2770	G2662	G2522	G2402	C2267	G2028	G1948	G1819	G1516
G3974	G3882	U2770	U3617	G2771	G2669	A2529	G2402	A2268	A2042	G1948	C1820	G1517
A3975	A3883	C3771	G3618	G2772	C2670	U2530	G2402	G2269	G2043	A1958	G1821	A1518
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G3977	A3885	G2773	G3620	U2774	G2672	G2537	C2411	G2275	G2045	A1960	G1822	A1520
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G3979	A3887	G2775	G3622	G2776	G2674	A2539	A2412	A2277	U2048	A1962	G1829	A1522
A3980	G3888	C2776	G3623	G2777	G2675	G2540	A2417	G2278	G2049	C1963	G1830	A1523
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G3982	G3890	U2779	G3625	U2779	U2677	A2542	C2422	C2280	G2051	G1969	G1832	A1525
A3983	A3891	G2780	G3626	G2780	G2678	G2543	C2422	C2281	G2052	G1970	G1833	A1526
U3984	G3892	G2781	G3627	G2781	U2679	A2544	U2425	C2282	G2053	C1971	G1834	A1527
G3985	A3893	U2782	G3628	G2782	U2680	G2545	U2426	C2283	G2054	G1972	U1835	A1528
A3986	G3894	G2783	G3629	G2783	A2677	G2546	A2426	A2284	G2055	G1973	G1836	A1529
U3987	A3895	C2784	G3630	U2784	U2678	G2547	U2427	C2285	G2056	U1974	C1837	A1530
G3988	A3896	G2785	G3631	G2785	G2679	G2548	U2428	C2286	G2057	G1975	G1838	A1531
U3989	A3897	U2786	G3632	G2786	U2681	G2549	U2429	C2287	G2058	G1976	C1839	A1532
A3990	G3898	U2787	G3633	U2787	U2682	A2550	A2429	A2288	G2059	G1977	G1840	A1533
U3991	A3899	G2788	A3653	G2788	U2683	G2551	A2430	C2289	G2060	G1978	C1841	A1534
G3992	G3899	G2789	G3634	G2789	G2684	G2552	A2431	C2290	G2061	G1979	G1842	A1535
A3993	A3900	C2790	G3635	G2790	U2685	G2553	U2432	C2291	G2062	G1980	G1843	A1536
U3994	A3901	U2791	G3636	G2791	U2686	G2554	U2433	C2292	G2063	G1981	C1844	A1537
G3995	A3902	G2792	G3637	G2792	U2687	G2555	A2434	A2293	G2064	U1979	G1845	A1538
A3996	A3903	G2793	G3638	G2793	G2688	G2556	U2435	C2294	G2065	G1980	C1846	A1539
U3997	A3904	C2794	G3639	G2794	U2689	G2557	U2436	A2295	G2066	G1981	G1847	A1540
G3998	A3905	U2795	G3640	G2795	U2690	G2558	A2437	C2296	G2067	G1982	C1848	A1541
A3999	A3906	G2796	U3637	G2796	G2691	G2559	U2438	C2297	G2068	U1982	G1849	A1542
U4000	A3907	C2797	G3641	G2797	U2692	G2560	U2439	A2298	G2069	G1983	C1850	A1543
G4001	A3908	U2798	G3642	G2798	U2693	G2561	A2440	C2299	G2070	G1984	G1851	A1544
A4002	A3909	G2799	G3643	G2799	U2694	G2562	U2441	A2300	G2071	G1985	C1852	A1545
U4003	A3910	C2799	G3644	G2800	U2695	G2563	A2442	C2301	G2072	G1986	G1853	A1546
G4004	A3911	U2800	A3657	G2800	G2696	G2564	U2443	A2302	G2073	G1987	G1854	A1547
A4005	A3912	G2801	U3658	G2801	A2697	G2565	U2444	C2303	G2074	G1988	C1855	A1548
U4006	A3913	U2802	G3659	G2802	G2698	G2566	U2445	A2304	G2075	G1989	G1856	A1549
G4007	A3914	C2803	G3660	G2803	U2699	G2567	A2446	C2305	G2076	G1990	C1857	A1550
A4008	A3915	U2804	A3661	G2804	U2700	G2568	U2447	A2306	G2077	G1991	G1858	A1551
U4009	A3916	G2805	G3662	G2805	G2699	G2569	A2448	C2307	G2078	G1992	G1859	A1552
G4010	A3917	C2806	A3663	G2806	A2701	G2570	U2449	A2308	G2079	G1993	C1860	A1553
A4011	A3918	U2807	G3664	G2807	U2702	G2571	A2450	C2309	G2080	G1994	G1861	A1554
U4012	A3919	G2808	G3665	G2808	G2703	G2572	U2451	A2310	G2081	G1995	C1862	A1555
G4013	A3920	C2809	A3666	G2809	U2704	G2573	A2452	C2311	G2082	G1996	G1863	A1556
A4014	A3921	U2810	A3667	U2810	A2705	G2574	U2453	A2312	G2083	G1997	C1864	A1557
U4015	A3922	G2811	G3668	G2811	U2706	G2575	A2454	C2313	G2084	G1998	G1865	A1558
G4016	A3923	C2812	G3669	G2812	U2707	G2576	U2455	A2314	G2085	G1999	C1866	A1559
A4017	A3924	U2813	A3670	G2813	U2708	G2577	A2456	C2315	G2086	G2000	G1867	A1560
U4018	A3925	G2814	G3671	G2814	U2709	G2578	U2457	A2316	G2087	G2001	C1868	A1561
G4019	A3926	C2815	G3672	G2815	G2710	G2579	A2458	C2317	G2088	G2002	G1869	A1562
A4020	A3927	U2816	A3671	G2816	U2711	G2580	U2459	A2318	G2089	G2003	G1870	A1563
U4021	A3928	G2817	G3673	G2817	U2712	G2581	A2460	C2319	G2090	G2004	C1871	A1564
G4022	A3929	C2818	G3674	G2818	U2713	G2582	A2461	A2320	U2091	U2005	G1872	A1565
A4023	A3930	U2819	A3672	G2819	U2714	G2583	U2462	C2321	G2092	G2006	G1873	A1566
U4024	A3931	G2820	G3673	G2820	U2715	G2584	U2463	A2322	A2093	G2007	C1874	A1567
G4025	A3932	C2821	G3674	G2821	G2716	G2585	A2464	C2323	G2094	G2008	G1875	A1568
A4026	A3933	U2821	A3673	G2821	U2717	G2586	U2465	A2324	U2095	U2009	C1876	A1569
U4027	A3934	G2822	G3675	G2822	U2718	G2587	U2466	C2325	G2096	G2010	G1877	A1570
G4028	A3935	C2823	G3676	G2823	U2719	G2588	A2467	A2326	G2097	G2011	C1878	A1571
A4029	A3936	U2824	A3674	G2824	U2720	G2589	U2468	C2327	U2098	G2012	G1879	A1572
U4030	A3937	G2825	G3675	G2825	U2721	G2590	A2469	A2328	G2099	A2013	A1794	A1573
G4031	A3938	C2826	G3676	G2826	U2722	G2591	U2470	C2329	A2104	G1920	G1637	A1574
A4032	A3939	U2827	A3675	G2827	U2723	G2592	A2471	A2330	G2105	G1921	A1638	A1575
U4033	A3940	G2828	G3676	G2828	U2724	G2593	U2472	C2331	U2106	G1922	G1639	A1576
G4034	A3941	C2829	G3677	G2829	U2725	G2594	A2473	A2332	U2107	A1923	C1637	A1577
A4035	A3942	U2830	A3676	G2830	U2726	G2595	U2474	C2333	G2108	G1924	G1638	A1578
U4036	A3943	G2831	G3677	G2831	U2727	G2596	A2475	A2334	A2109	G1925	A1639	A1579
G4037	A3944	C2832	G3678	G2832	U2728	G2597	A2476	C2335	G2110	G1926	G1640	A1580
A4038	A3945	U2833	A3677	G2833	U2729	G2598	U2477	A2336	G2111	G1927	C1641	A1581
U4039	A3946	G2834	G3678	G2834	U2730	G						



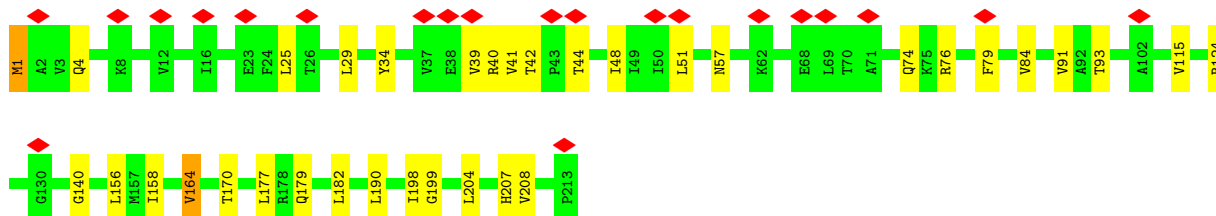
• Molecule 45: 5.8S rRNA

Chain 8: 72% 23%




• Molecule 46: Small ribosomal subunit protein uS3

Chain DD: 10% 84% 15%




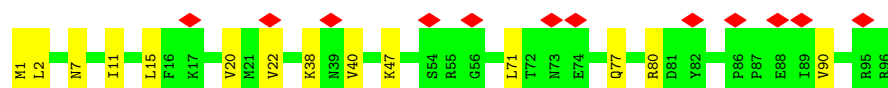
• Molecule 47: Small ribosomal subunit protein uS7

Chain FF:  85% 11% ..




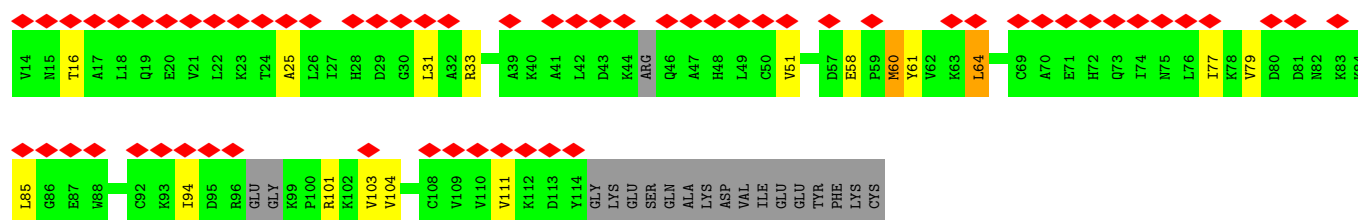
- Molecule 48: 40S ribosomal protein S10

Chain KK:  12% 85% 15%




- Molecule 49: 40S ribosomal protein S12

Chain MM:  53% 69% 13% 16%




- Molecule 50: Small ribosomal subunit protein uS19

Chain PP:  6% 76% 22%



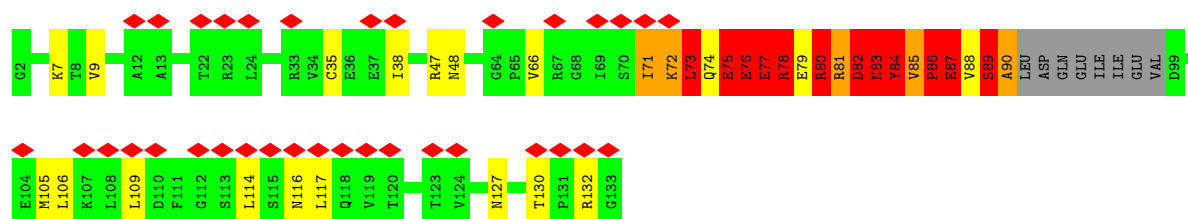
- Molecule 51: Small ribosomal subunit protein uS9

Chain QQ:  11% 87% 13%




- Molecule 52: 40S ribosomal protein S17

Chain RR:  26% 67% 14% 9% 6%




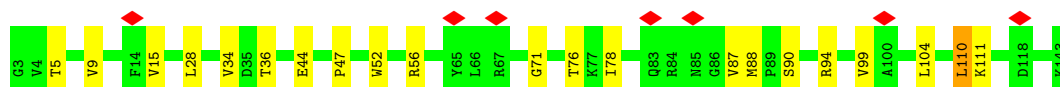
- Molecule 53: 40S ribosomal protein S18

Chain SS:  86% 13%




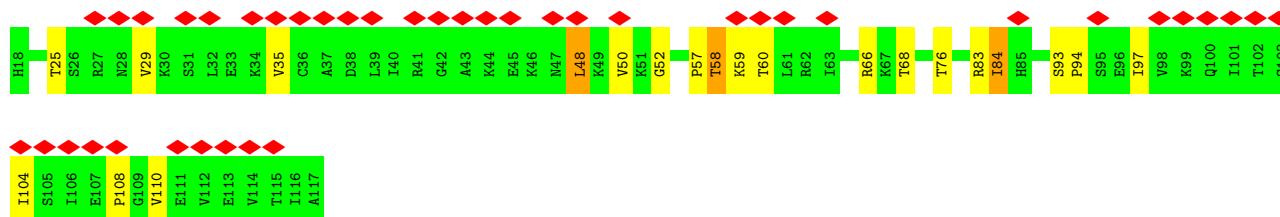
- Molecule 54: Small ribosomal subunit protein eS19

Chain TT:  5% 85% 14%




- Molecule 55: 40S ribosomal protein S20

Chain UU:  41% 79% 18%




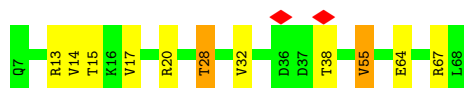
- Molecule 56: 40S ribosomal protein S25

Chain ZZ:  87% 13%




- Molecule 57: 40S ribosomal protein S28

Chain cc:  82% 15%

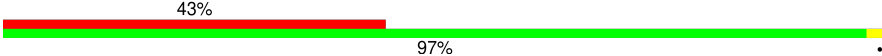


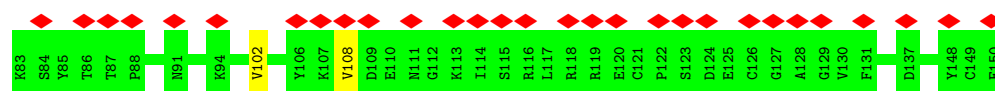
- Molecule 58: 40S ribosomal protein S29

Chain dd:  78% 20%




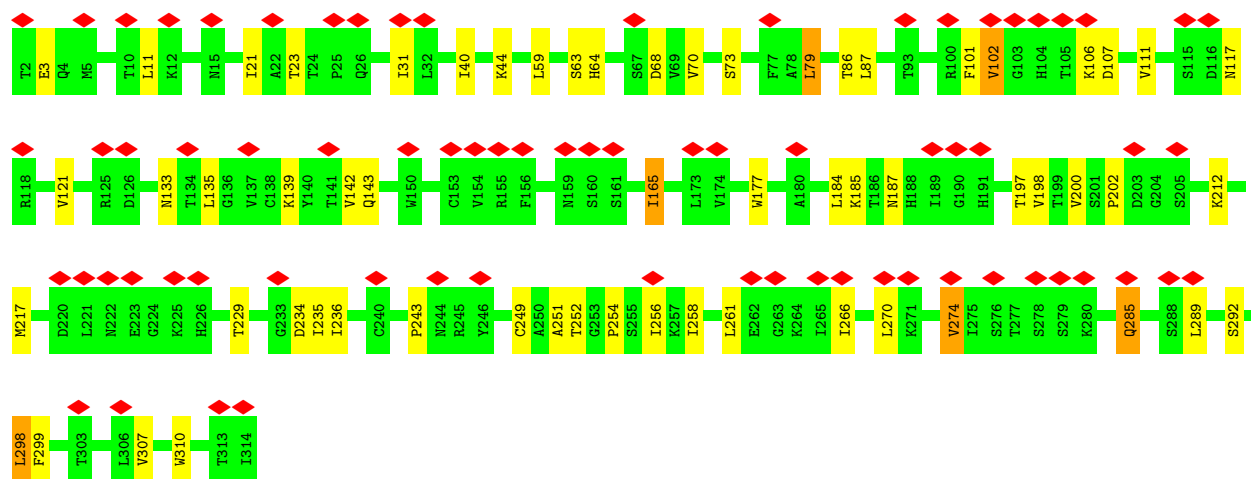
- Molecule 59: 40S ribosomal protein S27a

Chain ff: 



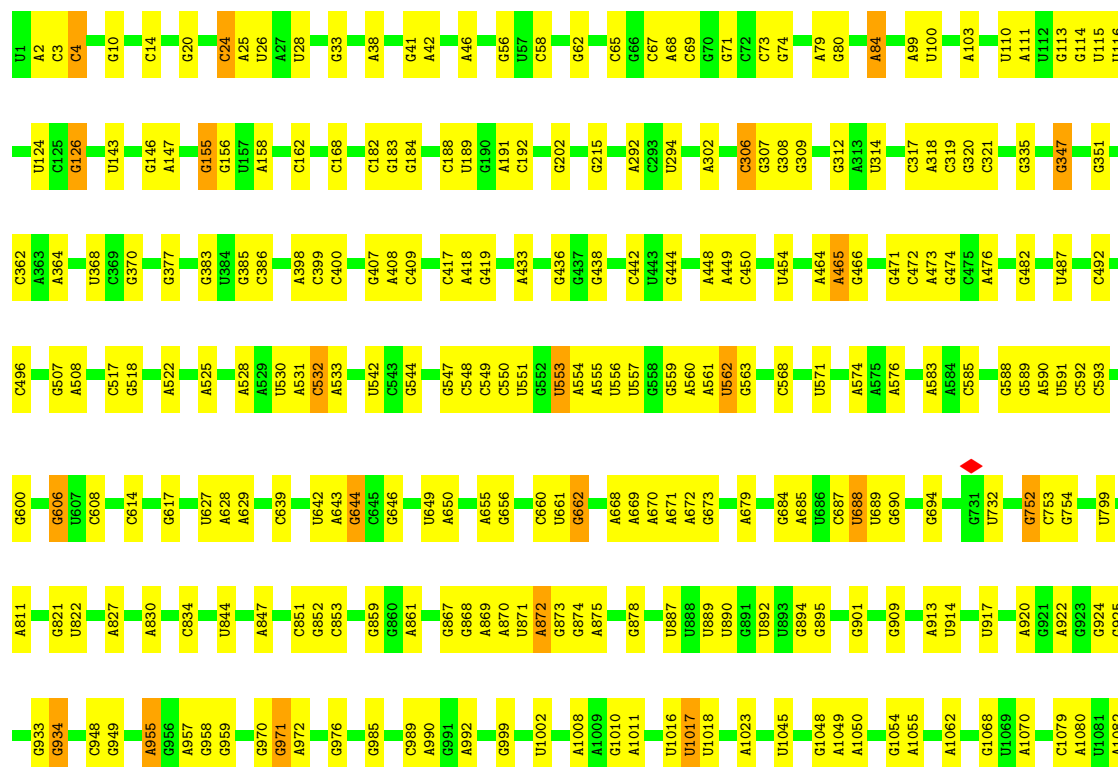
• Molecule 60: Receptor of activated protein C kinase 1

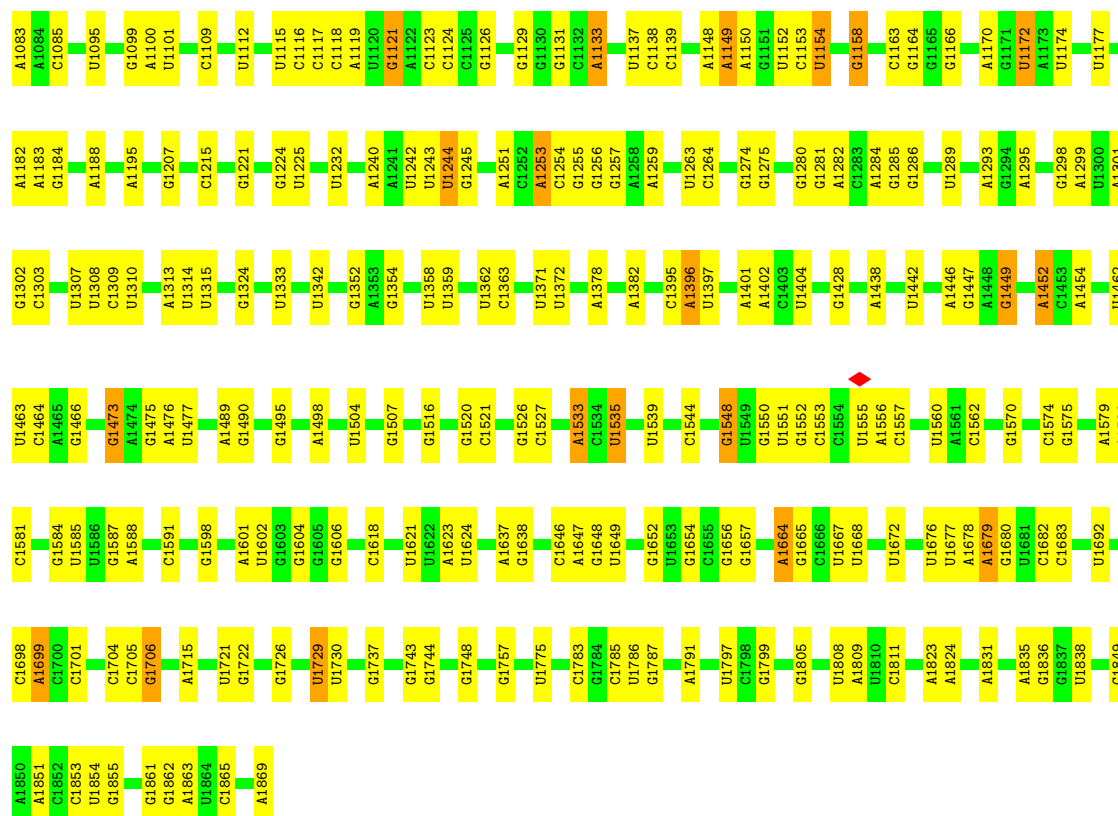
Chain gg: 



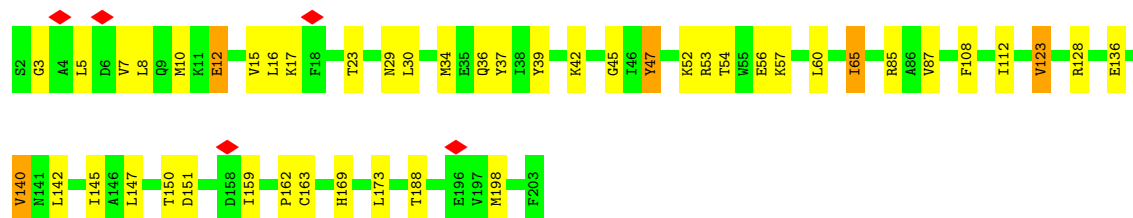
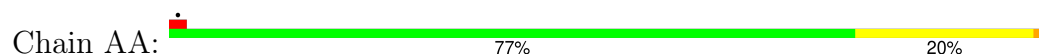
• Molecule 61: 18S RNA (1696-MER)

Chain 9: 

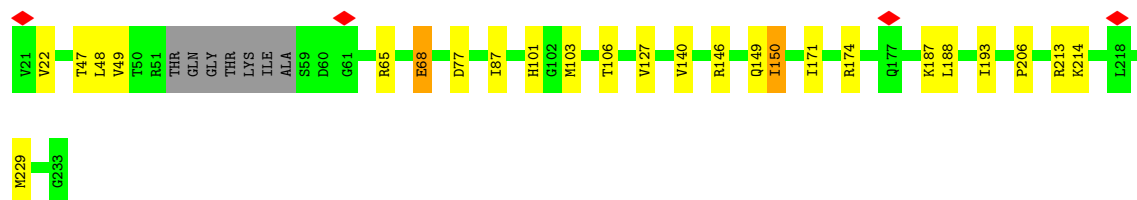
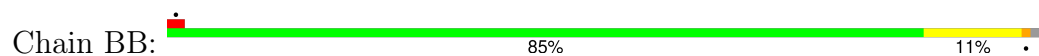




• Molecule 62: 40S ribosomal protein SA

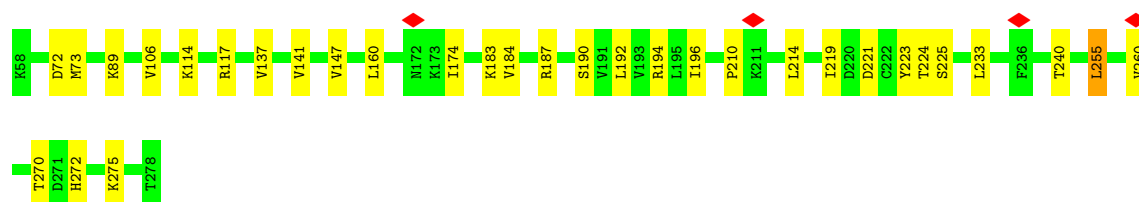


• Molecule 63: 40S ribosomal protein S3a



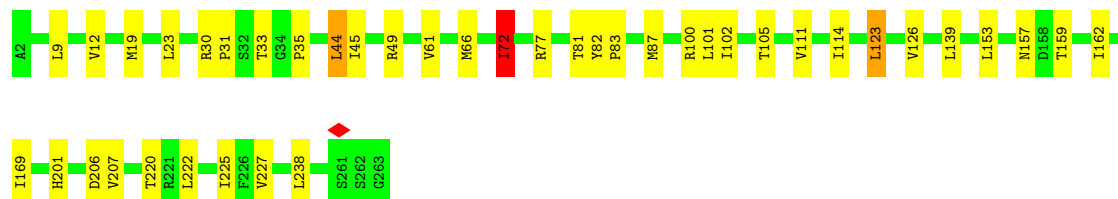
• Molecule 64: 40S ribosomal protein S2





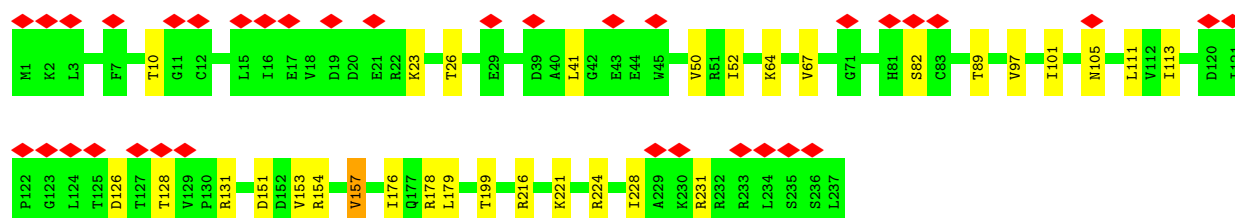
- Molecule 65: 40S ribosomal protein S4

Chain EE: 84% 15%



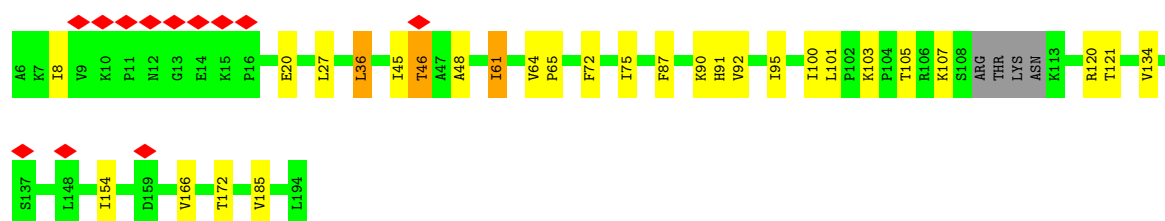
- Molecule 66: 40S ribosomal protein S6

Chain GG: 15% 87% 13%



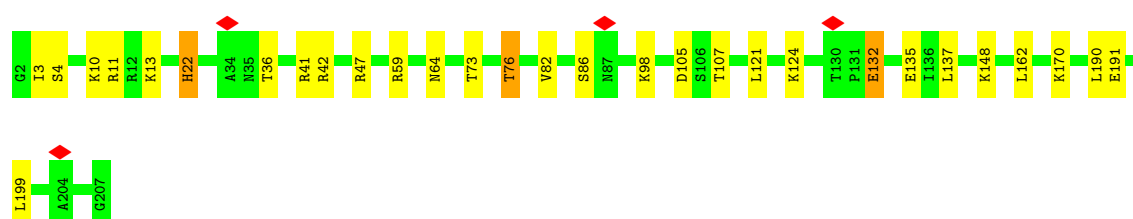
- Molecule 67: Small ribosomal subunit protein eS7

Chain HH: 6% 83% 14%



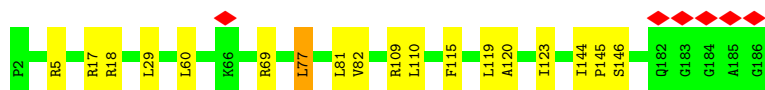
- Molecule 68: 40S ribosomal protein S8

Chain II: 85% 13%




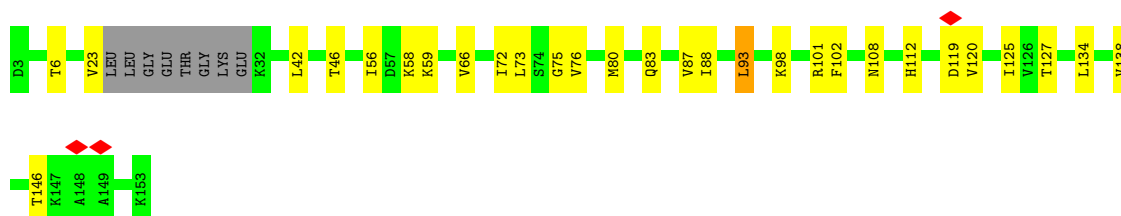
- Molecule 69: 40S ribosomal protein S9

Chain JJ:  90% 9%



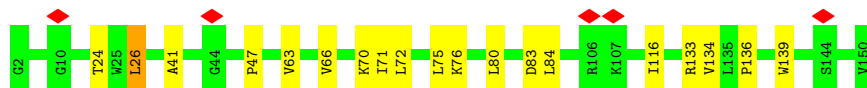
- Molecule 70: Small ribosomal subunit protein uS17

Chain LL:  75% 19% 5%



- Molecule 71: 40S ribosomal protein S13

Chain NN:  87% 12%




- Molecule 72: Small ribosomal subunit protein uS11

Chain OO:  86% 14%



- Molecule 73: eS21

Chain VV:  7% 81% 18%

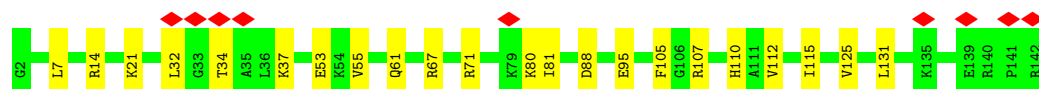
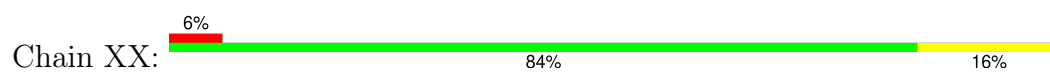


- Molecule 74: 40S ribosomal protein S15a

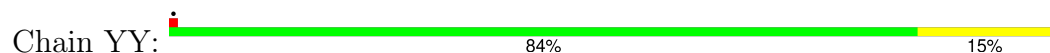
Chain WW:  87% 12%



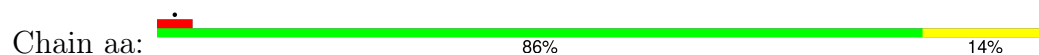
- Molecule 75: 40S ribosomal protein S23



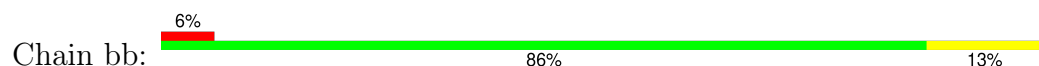
- Molecule 76: 40S ribosomal protein S24



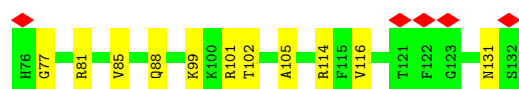
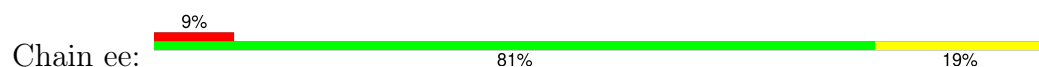
- Molecule 77: eS26



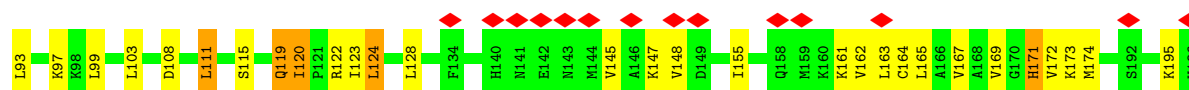
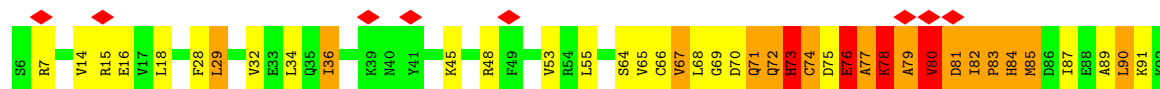
- Molecule 78: 40S ribosomal protein S27



- Molecule 79: Small ribosomal subunit protein eS30



- Molecule 80: Large ribosomal subunit protein uL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.798	Depositor
Minimum map value	-0.800	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	450.0, 450.0, 450.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.25, 1.25, 1.25	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	7	0.22	0/2836	0.39	0/4421
2	A	0.24	0/1936	0.59	0/2596
3	B	0.21	0/3240	0.52	0/4339
4	C	0.21	0/2937	0.54	0/3946
5	D	0.22	0/2437	0.49	0/3264
6	E	0.23	0/1762	0.56	2/2362 (0.1%)
7	F	0.26	0/1911	0.58	0/2549
8	G	0.24	0/1902	0.52	0/2556
9	H	0.25	0/1535	0.59	2/2063 (0.1%)
10	I	0.21	0/1698	0.47	0/2267
11	J	0.22	0/1385	0.51	0/1852
12	L	0.21	0/1733	0.50	0/2316
13	M	0.24	0/1158	0.58	0/1547
14	N	0.21	0/1746	0.50	0/2338
15	O	0.23	0/1662	0.54	0/2222
16	P	0.22	0/1268	0.52	0/1700
17	Q	0.21	0/1539	0.53	0/2054
18	R	0.24	0/1524	0.57	2/2013 (0.1%)
19	S	0.25	0/1501	0.49	0/2012
20	T	0.20	0/1326	0.51	0/1770
21	U	0.26	0/823	0.68	0/1104
22	V	0.21	0/1048	0.53	0/1402
23	W	0.21	0/873	0.51	0/1158
24	X	0.20	0/984	0.49	0/1323
25	Y	0.22	0/1132	0.52	0/1504
26	Z	0.23	0/1130	0.50	0/1507
27	a	0.21	0/1191	0.49	0/1590
28	b	0.20	0/854	0.48	0/1128
29	c	0.22	0/771	0.54	0/1034
30	d	0.24	0/903	0.60	0/1216
31	e	0.21	0/1071	0.57	0/1429
32	f	0.20	0/895	0.49	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.24	0/916	0.56	0/1220
34	h	0.23	0/1021	0.48	0/1348
35	i	0.23	0/841	0.51	0/1112
36	j	0.24	0/720	0.57	0/952
37	k	0.20	0/575	0.49	0/761
38	l	0.23	0/459	0.52	0/608
39	m	0.20	0/435	0.53	0/575
40	n	0.22	0/240	0.53	0/305
41	o	0.20	0/864	0.44	0/1140
42	p	0.25	0/718	0.65	0/953
43	r	0.24	0/1010	0.61	0/1354
44	5	0.25	9/86397 (0.0%)	0.47	33/134736 (0.0%)
45	8	0.25	0/3581	0.46	0/5577
46	DD	0.23	0/1679	0.54	0/2258
47	FF	0.21	0/1492	0.58	2/2005 (0.1%)
48	KK	0.20	0/834	0.54	2/1125 (0.2%)
49	MM	0.23	0/760	0.57	0/1021
50	PP	0.21	0/1079	0.53	0/1441
51	QQ	0.21	0/1146	0.53	2/1534 (0.1%)
52	RR	0.97	12/1015 (1.2%)	1.20	17/1359 (1.3%)
53	SS	0.22	0/1208	0.56	0/1618
54	TT	0.20	0/1115	0.47	0/1493
55	UU	0.20	0/805	0.48	0/1081
56	ZZ	0.23	0/604	0.56	0/810
57	cc	0.17	0/490	0.44	0/656
58	dd	0.22	0/470	0.54	0/623
59	ff	0.21	0/567	0.48	0/753
60	gg	0.21	0/2493	0.50	2/3394 (0.1%)
61	9	0.24	0/40486	0.47	11/63090 (0.0%)
62	AA	0.22	0/1621	0.57	0/2204
63	BB	0.21	0/1706	0.51	0/2281
64	CC	0.22	0/1753	0.49	0/2369
65	EE	0.21	0/2118	0.50	2/2849 (0.1%)
66	GG	0.19	0/1946	0.48	0/2590
67	HH	0.24	0/1510	0.53	1/2022 (0.0%)
68	II	0.23	0/1715	0.57	0/2287
69	JJ	0.21	0/1550	0.53	0/2069
70	LL	0.24	0/1195	0.55	0/1597
71	NN	0.20	0/1226	0.46	0/1649
72	OO	0.19	0/1029	0.45	0/1380
73	VV	0.20	0/643	0.54	0/860
74	WW	0.22	0/1051	0.52	0/1406
75	XX	0.25	0/1116	0.56	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.20	0/1028	0.49	0/1366
77	aa	0.22	0/828	0.51	0/1109
78	bb	0.22	0/665	0.45	0/891
79	ee	0.17	0/462	0.38	0/607
80	K	0.52	3/1733 (0.2%)	1.05	7/2324 (0.3%)
81	1	0.34	0/3904	0.78	12/6077 (0.2%)
82	s	0.54	0/172	0.92	0/225
83	t	0.71	0/275	1.04	1/367 (0.3%)
All	All	0.25	24/231977 (0.0%)	0.51	98/340701 (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
3	B	0	1
25	Y	0	1
32	f	0	1
52	RR	0	1
75	XX	0	1
81	1	1	0
All	All	1	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	RR	87	GLU	CA-C	8.27	1.63	1.52
52	RR	87	GLU	N-CA	7.39	1.55	1.46
52	RR	80	ARG	CA-C	-7.15	1.43	1.52
52	RR	84	TYR	CA-C	-7.02	1.43	1.52
52	RR	73	LEU	CA-C	-7.00	1.43	1.52
52	RR	89	SER	CA-C	-6.79	1.43	1.52
52	RR	84	TYR	N-CA	-6.70	1.37	1.46
80	K	85	MET	CA-C	-6.61	1.44	1.52
52	RR	78	ARG	N-CA	-6.42	1.38	1.46
44	5	2107	C	C1'-N1	6.32	1.57	1.48
44	5	4914	C	C1'-N1	6.18	1.57	1.48
44	5	262	C	C1'-N1	6.03	1.57	1.48
52	RR	83	ASN	CA-C	-5.97	1.44	1.52
80	K	80	VAL	N-CA	5.95	1.53	1.46
44	5	4876	U	C1'-N1	5.82	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	148	C	C1'-N1	5.73	1.57	1.48
44	5	1989	C	C1'-N1	5.70	1.56	1.48
80	K	80	VAL	CA-C	5.69	1.59	1.52
44	5	4136	C	C1'-N1	5.64	1.56	1.48
52	RR	86	PRO	CA-C	5.47	1.60	1.52
52	RR	82	ASP	CA-C	-5.41	1.45	1.52
44	5	904	G	C1'-N9	-5.24	1.40	1.48
52	RR	77	GLU	CA-C	-5.22	1.45	1.52
44	5	518	C	C1'-N1	5.21	1.56	1.48

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	K	77	ALA	N-CA-C	-23.05	80.91	112.25
80	K	72	GLN	N-CA-C	-18.34	73.50	107.98
52	RR	88	VAL	CB-CA-C	-12.57	90.68	111.29
44	5	4921	C	C1'-C2'-O2'	-11.42	94.67	111.80
52	RR	89	SER	N-CA-C	-11.09	87.17	110.80
52	RR	88	VAL	N-CA-C	10.89	132.00	109.34
52	RR	80	ARG	N-CA-C	-10.86	99.45	111.07
81	1	1435	G	O4'-C1'-N9	10.59	124.38	108.50
81	1	1435	G	N9-C1'-C2'	10.48	127.72	112.00
52	RR	87	GLU	N-CA-C	10.35	132.84	110.80
52	RR	83	ASN	N-CA-C	8.89	129.73	110.80
52	RR	77	GLU	N-CA-C	-8.84	102.40	113.01
44	5	4924	C	C2'-C3'-O3'	-8.18	101.43	113.70
52	RR	86	PRO	N-CA-C	8.00	128.94	112.47
80	K	74	CYS	N-CA-C	-7.87	98.50	110.70
52	RR	90	ALA	N-CA-C	-7.67	89.54	111.00
80	K	85	MET	CA-C-N	-7.66	107.03	120.97
80	K	85	MET	C-N-CA	-7.66	107.03	120.97
44	5	4923	C	C2'-C3'-O3'	-7.48	102.48	113.70
52	RR	83	ASN	N-CA-CB	-7.29	98.17	110.49
81	1	1433	U	P-O3'-C3'	7.27	131.10	120.20
52	RR	75	GLU	N-CA-C	-7.26	104.15	112.87
52	RR	86	PRO	CA-C-O	-7.23	107.44	120.60
44	5	2099	C	C1'-C2'-O2'	-7.07	101.20	111.80
81	1	1493	G	P-O3'-C3'	6.76	130.34	120.20
81	1	1392	G	P-O3'-C3'	6.75	130.33	120.20
44	5	4921	C	C3'-C2'-O2'	6.73	124.70	114.60
6	E	260	ILE	CA-C-N	6.63	129.33	120.58
6	E	260	ILE	C-N-CA	6.63	129.33	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	5	4923	C	C3'-C2'-O2'	-6.58	100.82	110.70
44	5	2046	G	P-O3'-C3'	6.54	130.01	120.20
52	RR	83	ASN	CB-CA-C	-6.53	97.44	110.42
61	9	553	U	P-O3'-C3'	6.30	129.65	120.20
61	9	752	G	P-O3'-C3'	6.05	129.28	120.20
44	5	2098	G	C2'-C3'-O3'	-5.98	104.72	113.70
44	5	1072	C	P-O3'-C3'	5.95	129.13	120.20
44	5	1477	C	C2'-C3'-O3'	5.81	122.41	113.70
61	9	1664	A	P-O3'-C3'	5.80	128.90	120.20
44	5	2695	A	P-O3'-C3'	5.75	128.83	120.20
61	9	532	C	P-O3'-C3'	5.67	128.71	120.20
44	5	4921	C	C4'-C3'-O3'	5.61	117.81	109.40
80	K	78	LYS	CB-CA-C	-5.60	99.28	110.42
81	1	1433	U	C2'-C3'-O3'	5.55	117.82	109.50
81	1	1341	U	C4'-C3'-O3'	5.53	117.69	109.40
61	9	24	C	C2'-C3'-O3'	5.52	121.97	113.70
44	5	696	C	P-O3'-C3'	5.51	128.47	120.20
44	5	2046	G	C2'-C3'-O3'	5.51	117.76	109.50
61	9	688	U	P-O3'-C3'	5.47	128.40	120.20
61	9	872	A	P-O3'-C3'	5.45	128.38	120.20
44	5	1477	C	P-O3'-C3'	5.43	128.35	120.20
52	RR	82	ASP	CA-C-N	-5.43	111.16	121.54
52	RR	82	ASP	C-N-CA	-5.43	111.16	121.54
81	1	1493	G	C2'-C3'-O3'	5.41	117.62	109.50
48	KK	2	LEU	CA-C-N	5.36	135.82	122.74
48	KK	2	LEU	C-N-CA	5.36	135.82	122.74
44	5	1211	G	C2'-C3'-O3'	5.35	121.73	113.70
44	5	4232	U	P-O3'-C3'	5.32	128.18	120.20
81	1	1408	C	P-O3'-C3'	5.32	128.18	120.20
44	5	406	C	P-O3'-C3'	5.29	128.13	120.20
44	5	245	C	P-O3'-C3'	5.28	128.12	120.20
44	5	2661	U	P-O3'-C3'	5.28	128.12	120.20
44	5	4922	C	C1'-C2'-O2'	-5.27	100.50	108.40
81	1	1379	U	P-O3'-C3'	5.24	128.06	120.20
44	5	930	G	C4'-C3'-O3'	5.23	117.25	109.40
60	gg	274	VAL	CA-C-N	5.23	131.39	121.97
60	gg	274	VAL	C-N-CA	5.23	131.39	121.97
65	EE	72	ILE	CA-C-N	5.22	129.82	122.46
65	EE	72	ILE	C-N-CA	5.22	129.82	122.46
44	5	4120	U	C2-N1-C1'	5.22	133.35	117.70
52	RR	76	GLU	N-CA-C	-5.20	99.73	110.80
67	HH	36	LEU	CA-CB-CG	5.18	134.42	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	5	48	G	P-O3'-C3'	5.16	127.94	120.20
44	5	1440	U	C2'-C3'-O3'	5.14	121.40	113.70
44	5	245	C	C2'-C3'-O3'	5.13	121.40	113.70
61	9	465	A	P-O3'-C3'	5.13	127.90	120.20
9	H	106	GLN	CA-C-N	5.11	131.30	121.54
9	H	106	GLN	C-N-CA	5.11	131.30	121.54
44	5	2502	G	P-O3'-C3'	5.11	127.86	120.20
44	5	4925	U	C2'-C3'-O3'	5.11	117.16	109.50
47	FF	42	LYS	CA-C-N	5.11	131.29	121.54
47	FF	42	LYS	C-N-CA	5.11	131.29	121.54
80	K	80	VAL	N-CA-C	5.11	119.96	109.34
44	5	3888	G	C2'-C3'-O3'	5.10	121.36	113.70
52	RR	73	LEU	N-CA-C	-5.10	99.94	110.80
44	5	4170	A	P-O3'-C3'	5.10	127.84	120.20
51	QQ	34	VAL	CA-C-N	5.09	129.35	122.07
51	QQ	34	VAL	C-N-CA	5.09	129.35	122.07
61	9	1535	U	C2-N1-C1'	5.07	132.90	117.70
81	1	1392	G	C2'-C3'-O3'	5.07	117.10	109.50
44	5	2100	G	C1'-C2'-O2'	-5.06	104.21	111.80
83	t	122	ALA	CB-CA-C	-5.05	110.36	117.23
18	R	35	ALA	CA-C-N	5.02	129.46	122.08
18	R	35	ALA	C-N-CA	5.02	129.46	122.08
61	9	1679	A	P-O3'-C3'	5.02	127.73	120.20
44	5	226	G	P-O3'-C3'	5.01	127.72	120.20
61	9	1253	A	P-O3'-C3'	5.01	127.72	120.20
81	1	1341	U	C2'-C3'-O3'	5.00	117.00	109.50
44	5	449	C	P-O3'-C3'	5.00	127.70	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
81	1	1435	G	C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	258	HIS	Peptide
52	RR	72	LYS	Mainchain
75	XX	61	GLN	Peptide
25	Y	121	ARG	Sidechain
32	f	106	TYR	Peptide

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	7	2538	0	1286	9	0
2	A	1898	0	1993	18	0
3	B	3172	0	3310	21	0
4	C	2883	0	3053	21	0
5	D	2391	0	2424	12	0
6	E	1729	0	1887	12	0
7	F	1875	0	1995	13	0
8	G	1872	0	2019	10	0
9	H	1516	0	1597	15	0
10	I	1660	0	1709	12	0
11	J	1362	0	1399	7	0
12	L	1702	0	1820	9	0
13	M	1137	0	1211	2	0
14	N	1701	0	1749	7	0
15	O	1630	0	1778	12	0
16	P	1242	0	1274	7	0
17	Q	1515	0	1634	16	0
18	R	1508	0	1664	13	0
19	S	1462	0	1508	12	0
20	T	1298	0	1366	14	0
21	U	809	0	833	5	0
22	V	1034	0	1097	10	0
23	W	860	0	903	5	0
24	X	967	0	1040	2	0
25	Y	1115	0	1205	9	0
26	Z	1107	0	1182	10	0
27	a	1162	0	1209	9	0
28	b	841	0	911	3	0
29	c	761	0	794	6	0
30	d	888	0	930	2	0
31	e	1053	0	1147	9	0
32	f	876	0	912	8	0
33	g	906	0	998	4	0
34	h	1013	0	1147	12	0
35	i	830	0	916	5	0
36	j	705	0	737	5	0
37	k	569	0	637	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	447	0	480	7	0
39	m	429	0	465	4	0
40	n	239	0	289	3	0
41	o	851	0	920	11	0
42	p	708	0	756	9	0
43	r	994	0	1051	11	0
44	5	77244	0	39022	418	0
45	8	3208	0	1629	6	0
46	DD	1653	0	1747	12	0
47	FF	1471	0	1522	7	0
48	KK	810	0	836	6	0
49	MM	754	0	790	6	0
50	PP	1058	0	1104	14	0
51	QQ	1128	0	1195	7	0
52	RR	1002	0	1054	74	0
53	SS	1190	0	1249	11	0
54	TT	1097	0	1132	7	0
55	UU	795	0	862	11	0
56	ZZ	598	0	656	3	0
57	cc	488	0	514	3	0
58	dd	459	0	448	6	0
59	ff	555	0	563	0	0
60	gg	2436	0	2393	24	0
61	9	36209	0	18290	113	0
62	AA	1586	0	1598	33	0
63	BB	1680	0	1748	12	0
64	CC	1716	0	1806	12	0
65	EE	2076	0	2177	15	0
66	GG	1923	0	2089	11	0
67	HH	1488	0	1582	8	0
68	II	1686	0	1772	12	0
69	JJ	1525	0	1640	10	0
70	LL	1175	0	1249	5	0
71	NN	1202	0	1289	8	0
72	OO	1016	0	1039	9	0
73	VV	636	0	637	8	0
74	WW	1034	0	1080	7	0
75	XX	1098	0	1167	8	0
76	YY	1011	0	1083	10	0
77	aa	814	0	863	3	0
78	bb	651	0	672	4	0
79	ee	457	0	502	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	K	1705	0	1810	99	0
81	1	3496	0	1771	15	0
82	s	173	0	192	46	0
83	t	275	0	283	57	0
84	5	192	0	0	0	0
84	7	5	0	0	0	0
84	8	3	0	0	0	0
84	9	1	0	0	0	0
84	P	1	0	0	0	0
84	V	1	0	0	0	0
84	a	1	0	0	0	0
84	g	1	0	0	0	0
84	j	1	0	0	0	0
85	aa	1	0	0	0	0
85	dd	1	0	0	0	0
85	ff	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
All	All	216047	0	160290	1291	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 4.

All (1291) 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)
80:K:65:VAL:HG23	80:K:81:ASP:OD1	1.37	1.18
80:K:74:CYS:SG	80:K:82:ILE:HD11	1.92	1.08
80:K:74:CYS:SG	80:K:84:HIS:HB3	1.94	1.06
44:5:169:G:N2	44:5:267:G:C6	2.23	1.04
52:RR:72:LYS:HA	52:RR:75:GLU:HB3	1.35	1.04
82:s:45:MET:HE1	83:t:117:ARG:HH22	1.22	1.02
44:5:759:G:O6	44:5:904:G:O6	1.77	1.00
61:9:1652:G:H1	61:9:1672:U:H3	1.05	0.98
44:5:989:U:H3	44:5:1065:G:H1	1.02	0.98
44:5:2573:A:H62	44:5:2761:U:H3	0.99	0.97
44:5:1993:C:H1'	83:t:138:SER:HB3	1.47	0.97
61:9:1743:G:H21	61:9:1791:A:H62	1.02	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:1656:G:H1	61:9:1668:U:H3	1.03	0.96
61:9:1533:A:H62	61:9:1602:U:H3	1.10	0.96
44:5:4454:G:H1	44:5:4526:U:H3	1.09	0.96
80:K:67:VAL:HG13	80:K:82:ILE:HA	1.45	0.95
61:9:1101:U:H3	61:9:1131:G:H1	1.12	0.95
81:1:1413:U:H3	81:1:1416:C:N4	1.66	0.94
52:RR:73:LEU:C	52:RR:77:GLU:HB3	1.93	0.94
80:K:78:LYS:HG2	80:K:82:ILE:HG21	1.50	0.93
61:9:1050:A:H62	61:9:1068:G:H21	0.96	0.93
44:5:4922:C:H2'	44:5:4923:C:C6	2.04	0.93
52:RR:90:ALA:HB2	62:AA:16:LEU:HB3	1.51	0.93
44:5:1998:A:H62	82:s:40:MET:HG3	1.32	0.92
52:RR:90:ALA:HB3	62:AA:17:LYS:HG3	1.52	0.92
80:K:74:CYS:HG	80:K:84:HIS:HB3	1.30	0.91
80:K:80:VAL:C	80:K:147:LYS:HZ3	1.78	0.91
1:7:77:A:H62	1:7:99:G:H21	1.14	0.90
44:5:2007:G:H21	44:5:2012:A:N6	1.70	0.90
44:5:3754:G:H1	44:5:3770:U:H3	0.95	0.90
61:9:1232:U:H3	61:9:1526:G:H1	0.93	0.90
44:5:2620:G:H1	44:5:2636:U:H3	0.93	0.90
52:RR:74:GLN:HA	52:RR:78:ARG:N	1.87	0.90
44:5:169:G:N2	44:5:267:G:O6	2.05	0.90
52:RR:73:LEU:HG	52:RR:77:GLU:HG2	1.55	0.89
44:5:2007:G:H21	44:5:2012:A:H62	1.20	0.88
61:9:924:G:H1	61:9:1018:U:H3	1.17	0.88
80:K:70:ASP:HA	80:K:73:HIS:HB3	1.54	0.88
44:5:1550:G:H1	44:5:1578:U:H3	1.22	0.88
80:K:85:MET:HE2	80:K:90:LEU:HD22	1.55	0.87
44:5:4888:U:H3	44:5:4931:G:H1	1.17	0.87
44:5:3944:G:H1	44:5:4069:U:H3	1.21	0.87
44:5:169:G:N2	44:5:267:G:N1	2.21	0.87
61:9:1050:A:H62	61:9:1068:G:N2	1.73	0.87
61:9:1743:G:N2	61:9:1791:A:H62	1.71	0.87
81:1:1413:U:H3	81:1:1416:C:H42	0.88	0.86
80:K:75:ASP:N	80:K:78:LYS:HB2	1.91	0.85
44:5:3930:U:H3	44:5:4180:G:H1	1.24	0.85
44:5:2573:A:N6	44:5:2761:U:H3	1.75	0.85
44:5:1973:G:N2	83:t:135:THR:HG23	1.92	0.85
44:5:392:U:H3	44:5:399:G:H1	1.24	0.84
44:5:4471:U:H3	44:5:4484:G:H1	1.24	0.84
44:5:2845:A:H61	44:5:3843:C:H42	1.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:K:67:VAL:CG1	80:K:82:ILE:HA	2.07	0.84
42:p:42:CYS:HB3	42:p:60:CYS:SG	2.18	0.83
61:9:1657:G:H1	61:9:1667:U:H3	1.23	0.83
44:5:505:G:H1	44:5:653:U:H3	1.26	0.83
44:5:4924:C:H2'	44:5:4925:U:C2	2.13	0.83
80:K:65:VAL:HG23	80:K:81:ASP:CG	2.03	0.83
80:K:76:GLU:C	80:K:78:LYS:H	1.87	0.82
44:5:2088:A:H5'	44:5:2268:A:H61	1.44	0.82
44:5:2007:G:N2	44:5:2012:A:H62	1.78	0.81
52:RR:79:GLU:HA	52:RR:82:ASP:CG	2.06	0.81
44:5:4923:C:H2'	44:5:4924:C:C5	2.15	0.81
52:RR:86:PRO:O	52:RR:87:GLU:HB2	1.79	0.81
44:5:4923:C:H2'	44:5:4924:C:C4	2.16	0.81
44:5:968:C:H42	44:5:2096:G:H1	1.27	0.80
82:s:47:LEU:HB3	82:s:51:ALA:HB3	1.65	0.79
44:5:1336:G:H21	44:5:2349:A:N6	1.79	0.79
80:K:74:CYS:SG	80:K:82:ILE:CD1	2.70	0.79
44:5:1973:G:C2	83:t:135:THR:HG23	2.18	0.79
44:5:4898:G:N2	44:5:4922:C:O2	2.17	0.78
52:RR:72:LYS:HA	52:RR:75:GLU:CB	2.12	0.77
44:5:1973:G:H4'	83:t:116:MET:SD	2.23	0.77
61:9:1743:G:H21	61:9:1791:A:N6	1.82	0.77
44:5:4896:G:N1	44:5:4924:C:C2	2.52	0.77
1:7:77:A:H62	1:7:99:G:N2	1.82	0.76
61:9:934:G:H1	61:9:1008:A:H2	1.29	0.76
80:K:65:VAL:CG2	80:K:81:ASP:OD1	2.28	0.76
44:5:4925:U:H4'	44:5:4926:C:H5'	1.68	0.76
44:5:1969:G:H4'	82:s:36:GLY:HA2	1.66	0.75
61:9:1050:A:N6	61:9:1068:G:H21	1.79	0.75
44:5:3946:G:H1	44:5:4067:U:H3	1.34	0.75
61:9:1352:G:H1	61:9:1359:U:H3	1.35	0.74
44:5:1336:G:H21	44:5:2349:A:H62	1.36	0.74
44:5:2095:A:H2'	44:5:2096:G:H8	1.50	0.74
80:K:71:GLN:C	80:K:73:HIS:N	2.38	0.74
44:5:1961:G:H1'	44:5:2025:A:H61	1.52	0.74
44:5:2100:G:H1'	44:5:2101:A:C4	2.22	0.74
44:5:3898:G:H1	44:5:4563:U:H3	1.34	0.74
61:9:1452:A:H61	61:9:1473:G:H21	1.34	0.74
52:RR:72:LYS:CA	52:RR:75:GLU:HB3	2.16	0.74
44:5:5002:U:H3	44:5:5045:G:H1	1.36	0.73
83:t:113:ALA:CB	83:t:129:ILE:HG13	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:1533:A:N6	61:9:1602:U:H3	1.85	0.73
45:8:114:G:H1	45:8:136:U:H3	1.34	0.73
52:RR:90:ALA:CB	62:AA:16:LEU:HB3	2.17	0.73
80:K:83:PRO:C	80:K:85:MET:H	1.95	0.73
82:s:45:MET:HE1	83:t:117:ARG:NH2	2.02	0.73
44:5:4638:U:H3	44:5:4661:G:H1	1.35	0.72
80:K:78:LYS:HE2	80:K:79:ALA:H	1.52	0.72
80:K:67:VAL:HG13	80:K:82:ILE:CA	2.18	0.72
52:RR:79:GLU:O	52:RR:82:ASP:HB2	1.88	0.72
52:RR:74:GLN:HA	52:RR:77:GLU:C	2.15	0.72
44:5:4899:G:N2	44:5:4921:C:C2	2.57	0.71
44:5:1969:G:O2'	82:s:37:SER:N	2.23	0.71
52:RR:77:GLU:O	52:RR:77:GLU:HG3	1.90	0.71
44:5:2095:A:H2'	44:5:2096:G:C8	2.25	0.71
80:K:80:VAL:HG23	80:K:147:LYS:HD3	1.70	0.71
83:t:109:ILE:HG23	83:t:132:ILE:HG22	1.71	0.70
81:1:1357:U:H3	81:1:1375:C:N4	1.89	0.70
44:5:2092:G:H1'	44:5:2095:A:H1'	1.71	0.70
44:5:4899:G:N1	44:5:4922:C:N3	2.40	0.70
44:5:2020:U:H4'	82:s:56:GLY:C	2.16	0.70
44:5:4421:C:H42	44:5:4475:G:H22	1.40	0.70
80:K:65:VAL:O	80:K:81:ASP:OD1	2.11	0.69
80:K:76:GLU:C	80:K:78:LYS:N	2.45	0.69
52:RR:85:VAL:HG23	62:AA:198:MET:HB3	1.75	0.69
52:RR:73:LEU:HG	52:RR:77:GLU:CG	2.21	0.69
44:5:969:C:N4	44:5:2095:A:H61	1.90	0.69
52:RR:85:VAL:CG2	62:AA:198:MET:HB3	2.23	0.69
61:9:1729:U:H3	61:9:1805:G:H1	1.39	0.69
44:5:1543:G:H1	44:5:1616:U:H3	1.41	0.69
44:5:1998:A:P	82:s:44:ARG:HH12	2.16	0.69
44:5:4923:C:H2'	44:5:4924:C:C6	2.27	0.68
80:K:80:VAL:C	80:K:147:LYS:NZ	2.50	0.68
44:5:1995:G:H4'	83:t:127:GLY:HA2	1.74	0.68
44:5:2098:G:H3'	44:5:2099:C:H6	1.57	0.68
44:5:2845:A:H61	44:5:3843:C:N4	1.91	0.68
44:5:4899:G:C2	44:5:4922:C:C2	2.82	0.68
52:RR:75:GLU:HG2	52:RR:76:GLU:HG3	1.75	0.68
52:RR:74:GLN:N	52:RR:77:GLU:HB3	2.09	0.68
52:RR:80:ARG:HG3	52:RR:81:ARG:N	2.08	0.68
44:5:4471:U:O2	44:5:4484:G:N2	2.26	0.67
44:5:759:G:C6	44:5:904:G:O6	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:1998:A:C5	82:s:55:MET:HB2	2.30	0.67
44:5:4926:C:H2'	44:5:4927:G:N9	2.09	0.67
7:F:242:LEU:O	7:F:246:MET:HB2	1.95	0.67
80:K:71:GLN:O	80:K:73:HIS:N	2.27	0.67
61:9:1452:A:N6	61:9:1473:G:H21	1.93	0.67
52:RR:90:ALA:HB2	62:AA:16:LEU:CB	2.26	0.66
83:t:128:THR:HA	83:t:131:GLU:OE2	1.96	0.66
44:5:3965:A:N6	44:5:4045:G:C6	2.63	0.66
44:5:966:A:C8	44:5:2096:G:C2	2.84	0.66
44:5:2845:A:N6	44:5:3843:C:H42	1.91	0.66
80:K:80:VAL:CA	80:K:147:LYS:HZ3	2.09	0.66
80:K:67:VAL:HG12	80:K:81:ASP:O	1.95	0.66
82:s:42:GLN:HA	82:s:45:MET:HB2	1.78	0.66
44:5:4897:G:H1	44:5:4923:C:H1'	1.61	0.65
80:K:79:ALA:O	80:K:81:ASP:N	2.30	0.65
44:5:1968:G:O2'	82:s:34:ASN:HA	1.96	0.65
44:5:2002:A:H62	83:t:135:THR:HG22	1.62	0.65
44:5:4924:C:H2'	44:5:4925:U:N3	2.11	0.64
52:RR:71:ILE:O	52:RR:75:GLU:HB3	1.96	0.64
80:K:74:CYS:SG	80:K:82:ILE:CG1	2.85	0.64
44:5:2100:G:H1'	44:5:2101:A:C2	2.32	0.64
61:9:116:U:H3	61:9:347:G:H1	1.45	0.64
44:5:982:U:H3	44:5:1273:G:H1	1.46	0.64
44:5:1968:G:H4'	82:s:34:ASN:HA	1.78	0.64
44:5:3965:A:C6	44:5:4045:G:C6	2.86	0.64
44:5:2098:G:H3'	44:5:2099:C:C6	2.33	0.63
44:5:2026:A:H2'	44:5:2027:U:O4'	1.98	0.63
44:5:4044:U:H3	44:5:4048:A:H62	1.46	0.63
44:5:4421:C:H42	44:5:4475:G:N2	1.96	0.63
44:5:4897:G:C6	44:5:4924:C:O2	2.52	0.63
82:s:48:ARG:NH2	83:t:122:ALA:O	2.32	0.63
80:K:67:VAL:O	80:K:82:ILE:HD12	1.99	0.63
80:K:67:VAL:H	80:K:83:PRO:HD2	1.62	0.63
40:n:5:TRP:HE1	61:9:1853:C:H41	1.47	0.63
61:9:1452:A:H61	61:9:1473:G:N2	1.97	0.63
44:5:2100:G:H1'	44:5:2101:A:C5	2.34	0.63
61:9:1324:G:H1	61:9:1504:U:H3	1.45	0.63
80:K:65:VAL:HG23	80:K:81:ASP:CB	2.28	0.63
80:K:83:PRO:C	80:K:85:MET:N	2.54	0.63
44:5:1336:G:N2	44:5:2349:A:H62	1.96	0.62
80:K:72:GLN:HB3	80:K:75:ASP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:4897:G:O6	44:5:4923:C:H1'	1.99	0.62
44:5:4920:C:C2	44:5:4921:C:H5	2.18	0.62
44:5:980:U:H3	44:5:1275:G:H1	1.46	0.62
61:9:1158:G:H21	74:WW:4:MET:HE1	1.65	0.62
52:RR:85:VAL:CG2	62:AA:198:MET:CB	2.78	0.62
44:5:4897:G:N1	44:5:4923:C:O2'	2.32	0.61
44:5:1993:C:H4'	83:t:137:GLN:NE2	2.16	0.61
44:5:4421:C:N4	44:5:4475:G:H22	1.97	0.61
44:5:2098:G:C6	44:5:2107:C:C2	2.88	0.61
44:5:1998:A:H5'	82:s:54:LEU:CD1	2.30	0.61
44:5:1996:C:H4'	82:s:48:ARG:HH12	1.65	0.61
52:RR:77:GLU:O	52:RR:80:ARG:HB3	2.00	0.61
61:9:955:A:N6	61:9:971:G:N2	2.49	0.61
44:5:4897:G:H1	44:5:4923:C:C1'	2.14	0.60
44:5:4924:C:H1'	44:5:4926:C:N4	2.17	0.60
44:5:1973:G:H5'	83:t:121:LEU:HD13	1.82	0.60
44:5:4926:C:H2'	44:5:4927:G:C4	2.35	0.60
44:5:2098:G:C6	44:5:2099:C:C2	2.90	0.60
44:5:2098:G:H2'	44:5:2099:C:O4'	2.01	0.60
44:5:4927:G:OP2	44:5:4927:G:C2	2.55	0.60
43:r:28:GLU:HB3	43:r:31:ASN:HB2	1.83	0.60
80:K:64:SER:H	80:K:108:ASP:HB2	1.66	0.60
44:5:1444:G:H21	44:5:2110:G:H1	1.49	0.60
52:RR:74:GLN:C	52:RR:76:GLU:N	2.57	0.59
80:K:85:MET:HE3	80:K:89:ALA:HB1	1.84	0.59
44:5:4926:C:H2'	44:5:4927:G:C8	2.37	0.59
44:5:4923:C:O2'	44:5:4924:C:C2	2.54	0.59
20:T:60:LYS:HE2	20:T:77:ASN:H	1.68	0.59
61:9:976:G:H21	72:OO:50:LYS:HE2	1.67	0.59
52:RR:73:LEU:C	52:RR:75:GLU:N	2.58	0.59
44:5:2088:A:H5'	44:5:2268:A:N6	2.16	0.59
46:DD:40:ARG:HA	55:UU:108:PRO:HB3	1.83	0.59
3:B:184:GLN:HE21	3:B:186:ASN:HD21	1.50	0.58
44:5:4920:C:O2	44:5:4921:C:H5	1.85	0.58
80:K:65:VAL:CG2	80:K:81:ASP:HB3	2.33	0.58
80:K:77:ALA:O	80:K:82:ILE:HD13	2.03	0.58
61:9:1099:G:H1	61:9:1133:A:H2	1.50	0.58
25:Y:66:GLN:HB2	25:Y:84:ARG:HH21	1.68	0.58
52:RR:90:ALA:CB	62:AA:17:LYS:HG3	2.29	0.58
81:1:1357:U:N3	81:1:1375:C:N4	2.49	0.58
83:t:110:VAL:HG22	83:t:129:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:7:LEU:HD13	19:S:33:PHE:HB3	1.86	0.58
44:5:1998:A:N6	82:s:40:MET:HG3	2.10	0.58
44:5:1998:A:C4	82:s:55:MET:HB2	2.39	0.58
44:5:4898:G:N2	44:5:4922:C:O2'	2.37	0.58
51:QQ:142:GLN:HE22	61:9:1225:U:H1'	1.69	0.58
15:O:89:PRO:HD3	44:5:1914:C:H4'	1.86	0.58
44:5:2095:A:N3	44:5:2096:G:C8	2.72	0.58
44:5:4922:C:H2'	44:5:4923:C:N1	2.19	0.58
61:9:442:C:H42	61:9:449:A:H62	1.50	0.58
25:Y:8:THR:HG23	25:Y:10:ASP:H	1.67	0.58
52:RR:73:LEU:HG	52:RR:77:GLU:CB	2.34	0.58
61:9:639:C:H5''	79:ee:114:ARG:HH21	1.68	0.58
44:5:2098:G:O2'	44:5:2099:C:H5'	2.04	0.58
60:gg:87:LEU:HB2	60:gg:101:PHE:HB2	1.86	0.58
80:K:74:CYS:SG	80:K:84:HIS:CB	2.84	0.58
44:5:4924:C:C2'	44:5:4925:U:C2	2.85	0.57
80:K:67:VAL:CG1	80:K:81:ASP:O	2.52	0.57
83:t:108:GLU:OE2	83:t:109:ILE:HG13	2.04	0.57
4:C:310:HIS:HB3	44:5:2100:G:O6	2.03	0.57
52:RR:73:LEU:HG	52:RR:77:GLU:HB3	1.86	0.57
80:K:83:PRO:O	80:K:85:MET:N	2.29	0.57
44:5:4922:C:H2'	44:5:4923:C:C5	2.38	0.57
44:5:3695:U:H3	44:5:3820:G:H1	1.53	0.57
44:5:4920:C:C2	44:5:4921:C:C5	2.92	0.57
44:5:4922:C:H6	44:5:4922:C:OP2	1.87	0.57
44:5:4924:C:C6	44:5:4924:C:OP2	2.58	0.57
44:5:4926:C:C2	44:5:4927:G:C5	2.93	0.57
2:A:184:ARG:HH12	44:5:2738:C:H4'	1.70	0.57
32:f:10:ILE:HB	32:f:29:LYS:HB3	1.87	0.57
17:Q:178:ARG:HH21	27:a:54:GLY:HA3	1.69	0.57
31:e:6:PRO:HG3	31:e:73:GLY:HA3	1.87	0.57
44:5:169:G:N2	44:5:267:G:H1	1.98	0.57
44:5:4897:G:N1	44:5:4923:C:H1'	2.20	0.57
31:e:104:SER:HB2	44:5:2303:C:H5''	1.86	0.57
44:5:2100:G:N3	44:5:2101:A:N6	2.53	0.57
18:R:70:ARG:HH22	44:5:2810:U:H5''	1.70	0.57
44:5:2092:G:H1'	44:5:2095:A:C1'	2.35	0.57
44:5:4923:C:C2'	44:5:4924:C:C2	2.88	0.57
52:RR:77:GLU:O	52:RR:78:ARG:C	2.45	0.57
80:K:72:GLN:CB	80:K:75:ASP:HB3	2.35	0.57
83:t:113:ALA:HB1	83:t:128:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:77:A:N6	1:7:99:G:H21	1.95	0.56
7:F:47:LYS:HG2	28:b:96:LEU:HD21	1.87	0.56
52:RR:90:ALA:HB3	62:AA:17:LYS:N	2.20	0.56
20:T:45:MET:H	20:T:95:HIS:HD2	1.51	0.56
44:5:1995:G:H4'	83:t:127:GLY:CA	2.35	0.56
61:9:1533:A:N6	61:9:1602:U:N3	2.46	0.56
17:Q:98:LEU:HB2	17:Q:113:ILE:HD11	1.87	0.56
28:b:117:ARG:HE	44:5:1273:G:H5''	1.70	0.56
44:5:450:G:H1	44:5:1297:U:H3	1.53	0.56
61:9:1095:U:H3	61:9:1149:A:H61	1.53	0.56
81:1:1404:A:C6	81:1:1433:U:O4	2.58	0.56
58:dd:17:GLY:HA2	58:dd:27:ARG:HG2	1.87	0.56
74:WW:91:ASN:HA	74:WW:97:ARG:HH12	1.71	0.56
80:K:85:MET:HE3	80:K:89:ALA:CB	2.36	0.56
4:C:53:ALA:HB3	45:8:27:U:H4'	1.87	0.56
44:5:3965:A:N6	44:5:4045:G:C5	2.74	0.56
52:RR:73:LEU:C	52:RR:75:GLU:H	2.13	0.56
3:B:99:LEU:HB3	44:5:4582:C:H4'	1.86	0.56
4:C:6:PRO:HD2	4:C:24:LEU:HD22	1.87	0.56
52:RR:76:GLU:C	52:RR:78:ARG:N	2.58	0.56
61:9:1533:A:N6	61:9:1602:U:C2	2.73	0.56
79:ee:101:ARG:HE	79:ee:105:ALA:HB1	1.71	0.56
80:K:78:LYS:CE	80:K:79:ALA:H	2.17	0.56
83:t:117:ARG:HH11	83:t:124:GLU:HA	1.71	0.56
8:G:233:PRO:HG2	8:G:272:VAL:HG13	1.87	0.56
44:5:4899:G:N2	44:5:4921:C:C6	2.74	0.56
80:K:73:HIS:C	80:K:75:ASP:H	2.14	0.56
20:T:75:VAL:HG22	20:T:88:ARG:HG2	1.87	0.56
44:5:4925:U:H6	44:5:4925:U:O5'	1.88	0.56
80:K:70:ASP:CA	80:K:73:HIS:HB3	2.31	0.56
19:S:34:ALA:HB1	19:S:39:VAL:HG23	1.87	0.56
36:j:22:CYS:HB3	36:j:37:CYS:SG	2.46	0.56
44:5:4897:G:C6	44:5:4923:C:H1'	2.41	0.56
17:Q:3:VAL:HG21	44:5:2277:C:H5''	1.88	0.56
44:5:1998:A:H5'	82:s:54:LEU:HD12	1.88	0.56
44:5:2089:G:H5'	44:5:2089:G:H8	1.69	0.56
44:5:4927:G:H2'	44:5:4927:G:N3	2.19	0.56
46:DD:190:LEU:HD23	46:DD:199:GLY:HA2	1.88	0.56
61:9:1177:U:H3	61:9:1184:G:H1	1.54	0.56
47:FF:88:MET:HE3	61:9:1591:C:H5''	1.88	0.55
44:5:4899:G:N1	44:5:4922:C:C2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:1973:G:H21	83:t:135:THR:HG23	1.68	0.55
60:gg:133:ASN:HD21	60:gg:139:LYS:HD3	1.71	0.55
43:r:6:GLN:O	43:r:10:VAL:HB	2.07	0.55
60:gg:256:ILE:HB	60:gg:270:LEU:HB2	1.88	0.55
2:A:186:TYR:O	2:A:190:LYS:HB2	2.07	0.55
52:RR:73:LEU:CG	52:RR:77:GLU:HG2	2.33	0.55
61:9:38:A:H5''	69:JJ:5:ARG:HB3	1.87	0.55
17:Q:50:ARG:HA	17:Q:53:MET:HG2	1.89	0.55
60:gg:177:TRP:HA	60:gg:184:LEU:HA	1.89	0.55
70:LL:98:LYS:HD3	75:XX:14:ARG:HH22	1.71	0.55
80:K:79:ALA:O	80:K:147:LYS:NZ	2.40	0.55
2:A:23:ARG:HA	2:A:52:PRO:HD2	1.89	0.55
2:A:31:ALA:HB2	2:A:123:ARG:HH21	1.72	0.55
2:A:224:THR:HG21	44:5:3705:G:H21	1.72	0.55
19:S:97:TYR:HB3	19:S:108:GLN:HE21	1.72	0.55
44:5:169:G:H21	44:5:267:G:H1	1.44	0.55
44:5:4897:G:O6	44:5:4924:C:N3	2.40	0.55
41:o:80:LYS:HE2	44:5:4346:U:H5''	1.89	0.55
44:5:2002:A:N6	83:t:135:THR:HG22	2.22	0.55
44:5:2659:A:H62	44:5:2675:G:N2	2.04	0.54
40:n:21:ARG:HH22	61:9:1174:U:H5''	1.72	0.54
15:O:119:VAL:HG11	19:S:171:ARG:HG2	1.89	0.54
26:Z:51:ARG:HB2	26:Z:65:ARG:HD2	1.89	0.54
44:5:1995:G:N3	83:t:122:ALA:HB2	2.21	0.54
44:5:2095:A:C2'	44:5:2096:G:H8	2.18	0.54
61:9:84:A:H5'	76:YY:122:LYS:HE2	1.88	0.54
75:XX:71:ARG:HD2	75:XX:80:LYS:HB3	1.89	0.54
52:RR:127:ASN:H	62:AA:45:GLY:H	1.55	0.54
60:gg:73:SER:H	60:gg:117:ASN:HD21	1.54	0.54
20:T:39:ILE:HD11	20:T:102:ARG:HB2	1.89	0.54
44:5:2395:A:N6	44:5:2820:C:O2	2.40	0.54
55:UU:58:THR:HG22	61:9:1446:A:H5''	1.89	0.54
61:9:1737:G:H1	61:9:1797:U:H3	1.55	0.54
80:K:66:CYS:SG	80:K:83:PRO:HD2	2.47	0.54
44:5:3697:U:H5''	44:5:3698:G:H5'	1.89	0.54
61:9:28:U:H3	61:9:646:G:H1	1.55	0.54
82:s:44:ARG:NH1	82:s:53:VAL:O	2.41	0.54
44:5:4899:G:N2	44:5:4921:C:N1	2.54	0.54
80:K:73:HIS:C	80:K:75:ASP:N	2.62	0.54
44:5:2092:G:O3'	44:5:2095:A:O4'	2.26	0.54
46:DD:74:GLN:HA	46:DD:79:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:1997:U:O3'	82:s:44:ARG:NH1	2.40	0.54
19:S:67:VAL:HA	44:5:729:G:H1	1.73	0.54
26:Z:103:ASP:HB3	26:Z:106:LEU:HB2	1.90	0.54
44:5:1973:G:C2	83:t:135:THR:CG2	2.91	0.54
44:5:1996:C:C4'	82:s:48:ARG:HH12	2.21	0.54
80:K:79:ALA:C	80:K:147:LYS:NZ	2.66	0.54
44:5:4923:C:OP2	44:5:4923:C:H3'	2.08	0.53
61:9:934:G:O6	61:9:1008:A:N1	2.41	0.53
9:H:128:MET:HE2	9:H:134:CYS:HB3	1.88	0.53
16:P:64:ASN:HD22	16:P:80:GLN:HE22	1.55	0.53
25:Y:46:SER:HB3	44:5:239:C:H5''	1.89	0.53
55:UU:94:PRO:HD2	55:UU:97:ILE:HD12	1.91	0.53
31:e:90:MET:HG2	43:r:33:LYS:HG2	1.91	0.53
44:5:2023:C:H2'	44:5:2024:G:H5''	1.90	0.53
44:5:4897:G:C6	44:5:4924:C:C2	2.96	0.53
72:OO:16:SER:HA	72:OO:88:LEU:HG	1.90	0.53
44:5:4577:U:H3	44:5:4726:G:H1	1.54	0.53
80:K:80:VAL:HG23	80:K:147:LYS:CD	2.39	0.53
44:5:1994:C:O2'	83:t:130:LYS:C	2.51	0.53
52:RR:84:TYR:CE2	62:AA:85:ARG:NH2	2.68	0.53
56:ZZ:47:LEU:HB2	56:ZZ:79:ILE:HG22	1.91	0.53
44:5:1971:C:O2	82:s:41:GLN:NE2	2.40	0.53
61:9:1099:G:O6	61:9:1133:A:N1	2.42	0.53
44:5:1995:G:H1'	83:t:131:GLU:CD	2.34	0.53
44:5:2095:A:C4	44:5:2096:G:C8	2.97	0.53
44:5:759:G:O6	44:5:904:G:C6	2.55	0.53
44:5:4761:G:H2'	44:5:4762:A:H8	1.74	0.53
80:K:80:VAL:CG2	80:K:147:LYS:HD3	2.39	0.53
9:H:89:ARG:HD3	9:H:91:LYS:HE3	1.89	0.53
12:L:63:THR:HG23	12:L:65:ARG:H	1.73	0.53
32:f:78:HIS:HB2	32:f:85:ARG:HG3	1.91	0.53
44:5:4924:C:H2'	44:5:4925:U:C4	2.44	0.53
52:RR:90:ALA:HB3	62:AA:17:LYS:CG	2.34	0.53
62:AA:123:VAL:HG13	62:AA:145:ILE:HB	1.91	0.53
3:B:95:THR:HG22	44:5:4910:A:H4'	1.91	0.53
30:d:50:ARG:HH21	44:5:2373:C:H5''	1.74	0.53
44:5:4898:G:C2	44:5:4922:C:O2	2.62	0.53
61:9:1152:U:H1'	74:WW:16:ASN:HD21	1.74	0.53
65:EE:31:PRO:HA	65:EE:81:THR:HB	1.91	0.53
71:NN:136:PRO:HG2	71:NN:139:TRP:HB2	1.91	0.53
52:RR:90:ALA:HB2	62:AA:16:LEU:CD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UU:60:THR:HG22	55:UU:83:ARG:HG2	1.91	0.52
19:S:98:ARG:HB2	19:S:142:VAL:HG13	1.91	0.52
26:Z:46:ILE:HD11	26:Z:49:TYR:HA	1.91	0.52
38:l:43:HIS:HE2	44:5:2429:A:H5''	1.73	0.52
44:5:4925:U:O5'	44:5:4925:U:C6	2.62	0.52
52:RR:79:GLU:HA	52:RR:82:ASP:OD2	2.08	0.52
61:9:851:C:H5''	61:9:852:G:H5'	1.92	0.52
22:V:82:ILE:HG22	22:V:83:ARG:HG3	1.89	0.52
44:5:1971:C:H4'	82:s:38:LYS:HB2	1.90	0.52
44:5:2447:U:H2'	44:5:2448:G:H8	1.74	0.52
44:5:2573:A:N7	44:5:2761:U:O4	2.42	0.52
53:SS:13:LEU:HB2	53:SS:20:ILE:HB	1.90	0.52
31:e:124:ASN:HB2	31:e:127:ALA:HB2	1.90	0.52
41:o:45:GLN:HE22	41:o:51:GLN:HA	1.74	0.52
44:5:4601:U:H2'	44:5:4602:A:H8	1.75	0.52
52:RR:73:LEU:O	52:RR:75:GLU:N	2.42	0.52
64:CC:196:ILE:HB	64:CC:223:TYR:HB2	1.90	0.52
44:5:2777:G:H5''	44:5:2778:G:H5'	1.92	0.52
11:J:43:LEU:HD22	11:J:117:ILE:HD12	1.91	0.52
37:k:12:LEU:HB3	37:k:16:ARG:HH21	1.75	0.52
44:5:1934:A:N1	44:5:2052:G:O6	2.42	0.52
44:5:4920:C:H2'	44:5:4921:C:H5'	1.91	0.52
44:5:4925:U:H4'	44:5:4926:C:C5'	2.37	0.52
65:EE:100:ARG:HB2	65:EE:114:ILE:HD13	1.92	0.52
2:A:234:LYS:HG2	2:A:238:ILE:HD12	1.92	0.52
29:c:36:LYS:HA	29:c:39:ARG:HD3	1.91	0.52
46:DD:51:LEU:HG	46:DD:91:VAL:HG22	1.91	0.52
52:RR:74:GLN:O	52:RR:78:ARG:HB3	2.09	0.52
80:K:70:ASP:HA	80:K:73:HIS:CB	2.31	0.52
81:1:1413:U:O2	81:1:1416:C:N3	2.42	0.52
44:5:1994:C:O2	83:t:131:GLU:HB2	2.10	0.52
44:5:4098:A:H61	44:5:4110:C:H42	1.58	0.52
3:B:317:LEU:HB2	3:B:372:SER:HB2	1.92	0.52
4:C:183:VAL:HG22	4:C:204:ARG:HB3	1.92	0.52
44:5:1962:A:H8	44:5:2024:G:H21	1.56	0.52
44:5:4923:C:H2'	44:5:4924:C:C2	2.44	0.52
58:dd:16:GLN:HG3	58:dd:27:ARG:HB3	1.92	0.52
62:AA:3:GLY:HA3	73:VV:80:SER:HB2	1.90	0.52
83:t:123:ARG:CB	83:t:127:GLY:HA3	2.39	0.52
44:5:2100:G:H1'	44:5:2101:A:C6	2.45	0.52
52:RR:82:ASP:O	52:RR:83:ASN:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:CYS:HB3	2:A:101:VAL:HG13	1.91	0.51
58:dd:27:ARG:HD3	61:9:1263:U:H4'	1.91	0.51
9:H:91:LYS:HG2	9:H:145:VAL:HG22	1.90	0.51
70:LL:58:LYS:HG3	70:LL:59:LYS:HG3	1.92	0.51
2:A:180:LEU:HB2	2:A:184:ARG:HG3	1.93	0.51
22:V:107:ASN:HD21	22:V:111:GLU:HB3	1.75	0.51
44:5:1973:G:N3	83:t:135:THR:HG23	2.26	0.51
52:RR:74:GLN:N	52:RR:74:GLN:OE1	2.43	0.51
44:5:760:G:H1'	44:5:904:G:N2	2.25	0.51
52:RR:74:GLN:HA	52:RR:78:ARG:H	1.74	0.51
52:RR:74:GLN:C	52:RR:76:GLU:H	2.16	0.51
3:B:128:LYS:HG2	3:B:131:THR:HG21	1.93	0.51
18:R:159:ALA:HB1	18:R:163:ARG:HH21	1.75	0.51
44:5:1998:A:C8	82:s:55:MET:HB2	2.46	0.51
44:5:2449:A:H62	44:5:2510:G:H21	1.57	0.51
44:5:3855:C:H2'	44:5:3856:A:H8	1.75	0.51
44:5:4736:C:H2'	44:5:4737:G:H8	1.74	0.51
62:AA:34:MET:HG2	62:AA:150:THR:HA	1.92	0.51
44:5:1999:A:H61	82:s:40:MET:HG3	1.75	0.51
34:h:70:ARG:HB3	34:h:83:LEU:HD22	1.93	0.51
41:o:64:LYS:HD2	44:5:4370:G:H5''	1.93	0.51
44:5:1993:C:O2'	83:t:137:GLN:HG3	2.10	0.51
53:SS:20:ILE:HD11	53:SS:33:ILE:HD11	1.92	0.51
63:BB:65:ARG:HE	72:OO:50:LYS:HD3	1.76	0.51
43:r:37:SER:HB3	43:r:40:TYR:H	1.75	0.51
44:5:4097:G:H22	44:5:4111:U:H3	1.59	0.51
80:K:85:MET:CE	80:K:90:LEU:HD22	2.36	0.51
29:c:38:ILE:HG21	29:c:63:TYR:HB3	1.93	0.51
44:5:4896:G:C6	44:5:4924:C:N3	2.79	0.51
61:9:1677:U:H2'	61:9:1678:A:H8	1.76	0.51
66:GG:154:ARG:HE	66:GG:179:LEU:HD21	1.76	0.51
6:E:156:LEU:HD11	6:E:198:ILE:HG13	1.92	0.50
41:o:55:ILE:HB	41:o:57:ARG:HH21	1.77	0.50
67:HH:101:LEU:HB2	67:HH:120:ARG:HB3	1.93	0.50
8:G:282:ARG:HG2	8:G:285:GLU:HB2	1.92	0.50
64:CC:214:LEU:HD22	64:CC:219:ILE:HD12	1.92	0.50
65:EE:222:LEU:HA	65:EE:225:ILE:HD12	1.92	0.50
5:D:40:ASP:HB2	5:D:43:LYS:HG2	1.94	0.50
9:H:7:ASN:HB2	9:H:56:ARG:HD3	1.94	0.50
43:r:10:VAL:HG22	43:r:14:SER:HB3	1.92	0.50
44:5:734:G:H22	44:5:929:A:H62	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:HH:154:ILE:HB	67:HH:185:VAL:HG22	1.93	0.50
81:1:1471:A:H3'	81:1:1472:A:H8	1.77	0.50
82:s:37:SER:HA	82:s:40:MET:HB2	1.92	0.50
4:C:200:ARG:HG2	4:C:201:ARG:HE	1.76	0.50
12:L:48:PRO:HB2	34:h:120:ALA:HB2	1.94	0.50
44:5:1972:G:N2	83:t:131:GLU:HB2	2.27	0.50
51:QQ:142:GLN:HB3	61:9:1527:C:H5''	1.93	0.50
80:K:71:GLN:HB2	80:K:77:ALA:HB2	1.93	0.50
81:1:1357:U:H3	81:1:1375:C:H42	1.49	0.50
4:C:312:ARG:HE	44:5:2274:C:H5'	1.76	0.50
44:5:1998:A:OP1	82:s:54:LEU:HA	2.11	0.50
80:K:65:VAL:HG23	80:K:81:ASP:HB3	1.91	0.50
10:I:16:PRO:HA	10:I:95:HIS:HD2	1.75	0.50
44:5:1996:C:H5'	83:t:123:ARG:HB2	1.93	0.50
44:5:2452:G:H21	44:5:2507:A:H62	1.59	0.50
44:5:3751:G:H21	44:5:3775:A:H8	1.60	0.50
60:gg:217:MET:HG2	60:gg:229:THR:HG23	1.93	0.50
43:r:39:ARG:HH22	44:5:2090:U:H3	1.59	0.50
44:5:2100:G:C4	44:5:2101:A:N6	2.80	0.50
61:9:655:A:H4'	61:9:656:G:H3'	1.92	0.50
83:t:109:ILE:HG21	83:t:133:LEU:HG	1.94	0.50
44:5:1084:C:H42	44:5:1213:G:H1	1.60	0.50
44:5:4899:G:N2	44:5:4921:C:C2'	2.74	0.50
61:9:1396:A:N7	61:9:1449:G:O6	2.45	0.50
11:J:108:GLY:HA3	44:5:4251:A:H5''	1.94	0.49
50:PP:18:ARG:HH21	50:PP:37:TYR:HA	1.77	0.49
82:s:48:ARG:HD3	83:t:123:ARG:CZ	2.42	0.49
4:C:33:ARG:HG2	4:C:36:ILE:HD12	1.94	0.49
26:Z:89:ILE:HG12	26:Z:91:LEU:HG	1.95	0.49
41:o:69:ARG:HH21	41:o:80:LYS:HE3	1.77	0.49
52:RR:73:LEU:O	52:RR:77:GLU:N	2.25	0.49
1:7:112:U:H2'	1:7:113:G:H8	1.76	0.49
11:J:35:ARG:HD2	11:J:123:ILE:HA	1.93	0.49
19:S:82:LEU:HB3	19:S:93:MET:HB2	1.94	0.49
44:5:1332:C:H2'	44:5:1333:A:H8	1.76	0.49
44:5:1972:G:N2	83:t:131:GLU:OE1	2.39	0.49
44:5:1998:A:H5'	82:s:54:LEU:HD11	1.94	0.49
44:5:4897:G:N1	44:5:4924:C:O2	2.45	0.49
44:5:4921:C:O2'	44:5:4922:C:O4'	2.20	0.49
52:RR:77:GLU:OE2	52:RR:80:ARG:HG2	2.12	0.49
60:gg:79:LEU:HD21	60:gg:87:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:955:A:N6	61:9:971:G:C2	2.81	0.49
66:GG:10:THR:HB	66:GG:128:THR:HA	1.94	0.49
67:HH:87:PHE:HB3	67:HH:90:LYS:HE2	1.94	0.49
9:H:12:ILE:HD12	9:H:16:VAL:HG23	1.94	0.49
44:5:1969:G:C4'	82:s:36:GLY:HA2	2.40	0.49
44:5:2638:G:H22	44:5:2697:A:H61	1.59	0.49
44:5:4899:G:N2	44:5:4921:C:O2'	2.46	0.49
80:K:81:ASP:O	80:K:147:LYS:NZ	2.42	0.49
83:t:113:ALA:HB3	83:t:129:ILE:HG13	1.93	0.49
17:Q:173:LYS:HD3	27:a:59:ARG:HH22	1.77	0.49
27:a:75:LEU:HA	27:a:78:LEU:HB2	1.94	0.49
44:5:1994:C:H2'	44:5:1995:G:H8	1.77	0.49
44:5:1995:G:O2'	83:t:123:ARG:HB2	2.12	0.49
44:5:1996:C:OP1	83:t:123:ARG:HG2	2.12	0.49
44:5:2096:G:H4'	44:5:2097:U:O4'	2.12	0.49
60:gg:11:LEU:HB2	60:gg:307:VAL:HB	1.93	0.49
68:II:42:ARG:HH21	68:II:59:ARG:HD2	1.77	0.49
8:G:112:ARG:O	8:G:116:LEU:HB2	2.13	0.49
17:Q:11:ARG:HB3	44:5:2081:C:H4'	1.94	0.49
23:W:18:GLY:HA2	23:W:19:ARG:HH21	1.77	0.49
44:5:300:A:H2'	44:5:301:G:H8	1.78	0.49
44:5:2557:G:H1	44:5:2570:U:H3	1.60	0.49
46:DD:204:LEU:HB3	46:DD:207:HIS:HB3	1.95	0.49
6:E:186:ARG:HG3	44:5:4938:A:H5'	1.94	0.49
6:E:257:ASP:O	6:E:261:LEU:HB2	2.12	0.49
39:m:94:ASN:HD21	44:5:4423:U:H5	1.61	0.49
44:5:2309:G:H1	44:5:2329:U:H3	1.59	0.49
44:5:4630:G:N2	44:5:4668:U:O2	2.45	0.49
52:RR:74:GLN:HA	52:RR:77:GLU:CA	2.43	0.49
52:RR:117:LEU:HG	62:AA:12:GLU:HG3	1.95	0.49
61:9:10:G:H21	64:CC:114:LYS:HA	1.77	0.49
3:B:13:SER:HB2	44:5:4622:A:H4'	1.95	0.48
44:5:4921:C:OP2	44:5:4922:C:C5	2.66	0.48
76:YY:10:ARG:HG2	76:YY:11:LYS:HG3	1.94	0.48
10:I:91:LEU:HD12	10:I:127:ALA:HB1	1.95	0.48
44:5:2335:C:H2'	44:5:2336:G:H8	1.78	0.48
45:8:47:C:H1'	45:8:61:A:H2'	1.95	0.48
58:dd:11:PRO:HB3	58:dd:13:LYS:HE2	1.95	0.48
83:t:109:ILE:HD13	83:t:133:LEU:HD21	1.95	0.48
10:I:152:LEU:HB3	10:I:165:ILE:HG12	1.94	0.48
33:g:66:ARG:HH22	44:5:2518:G:H5'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:2793:G:H5'	44:5:2794:C:H5''	1.95	0.48
52:RR:84:TYR:O	52:RR:85:VAL:HB	2.13	0.48
61:9:1550:G:H3'	61:9:1579:A:H61	1.78	0.48
4:C:339:THR:HB	4:C:343:GLN:HE21	1.78	0.48
32:f:36:ARG:HG3	32:f:80:ASN:HA	1.93	0.48
38:l:43:HIS:HB3	38:l:46:ARG:HB2	1.94	0.48
44:5:1998:A:C4	82:s:55:MET:CB	2.96	0.48
44:5:4926:C:C2	44:5:4927:G:N7	2.81	0.48
63:BB:171:ILE:HG12	63:BB:174:ARG:HH21	1.78	0.48
80:K:65:VAL:CG2	80:K:81:ASP:CB	2.92	0.48
10:I:97:ILE:HG13	10:I:123:GLN:HB2	1.94	0.48
10:I:98:ARG:HB3	10:I:120:GLY:HA3	1.95	0.48
44:5:4925:U:C4'	44:5:4926:C:H5'	2.41	0.48
50:PP:40:ARG:HH22	61:9:1624:U:H3	1.61	0.48
53:SS:28:PHE:HE1	53:SS:38:ARG:HE	1.61	0.48
60:gg:236:ILE:HG12	60:gg:252:THR:HG22	1.95	0.48
80:K:36:ILE:HG13	80:K:165:LEU:HB3	1.95	0.48
6:E:68:LYS:HE3	6:E:70:LEU:HD11	1.95	0.48
8:G:229:LYS:HG3	35:i:43:MET:HE2	1.94	0.48
44:5:3868:G:H22	44:5:3900:G:H1'	1.79	0.48
44:5:4949:G:H4'	44:5:4950:U:H5'	1.94	0.48
52:RR:72:LYS:HA	52:RR:75:GLU:CD	2.39	0.48
72:OO:98:ARG:HH21	72:OO:134:PRO:HG3	1.79	0.48
3:B:45:ALA:HB3	3:B:183:ILE:HG12	1.94	0.48
44:5:2096:G:H4'	44:5:2097:U:N1	2.29	0.48
44:5:4924:C:H1'	44:5:4926:C:H42	1.77	0.48
49:MM:31:LEU:HB2	49:MM:111:VAL:HA	1.94	0.48
52:RR:71:ILE:O	52:RR:75:GLU:N	2.47	0.48
52:RR:84:TYR:C	52:RR:84:TYR:CD2	2.91	0.48
7:F:161:ILE:HB	7:F:166:ILE:HD12	1.95	0.48
35:i:41:ARG:HH12	44:5:308:G:H2'	1.78	0.48
36:j:27:TYR:HA	36:j:34:CYS:HA	1.95	0.48
44:5:225:G:H21	44:5:242:U:H3	1.61	0.48
44:5:2002:A:N1	83:t:138:SER:OG	2.40	0.48
46:DD:158:ILE:HG13	46:DD:164:VAL:HG23	1.95	0.48
52:RR:72:LYS:HA	52:RR:75:GLU:CG	2.44	0.48
8:G:136:PHE:HB3	8:G:212:HIS:HB2	1.95	0.48
8:G:149:LEU:HD22	8:G:246:LEU:HD21	1.95	0.48
11:J:101:ASP:HA	11:J:159:LYS:HB2	1.95	0.48
44:5:1996:C:O2	82:s:41:GLN:HG2	2.14	0.48
44:5:2088:A:C6	44:5:2268:A:C5	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:2092:G:C2	44:5:2097:U:C5	3.02	0.48
44:5:2098:G:H2'	44:5:2098:G:N3	2.28	0.48
52:RR:74:GLN:CA	52:RR:78:ARG:N	2.67	0.48
62:AA:37:TYR:HD1	62:AA:53:ARG:HD3	1.79	0.48
72:OO:94:HIS:HD2	72:OO:128:ARG:H	1.61	0.48
78:bb:36:LYS:HD3	78:bb:43:ILE:HG12	1.96	0.48
80:K:78:LYS:O	80:K:82:ILE:HB	2.13	0.48
82:s:48:ARG:NH1	83:t:123:ARG:HD2	2.29	0.48
4:C:46:LYS:HB3	4:C:49:ARG:HH21	1.79	0.48
18:R:105:LEU:HD22	18:R:135:LYS:HG3	1.96	0.48
38:l:24:PRO:HG2	38:l:27:ILE:HG12	1.95	0.48
43:r:35:ARG:HH22	44:5:2265:G:H5''	1.78	0.48
52:RR:76:GLU:C	52:RR:78:ARG:H	2.21	0.48
26:Z:89:ILE:HD11	26:Z:117:LYS:HB3	1.96	0.47
44:5:2295:C:H2'	44:5:2296:G:H8	1.79	0.47
44:5:2449:A:H62	44:5:2510:G:N2	2.12	0.47
46:DD:76:ARG:HB2	48:KK:22:VAL:HG11	1.95	0.47
46:DD:140:GLY:HA3	46:DD:182:LEU:HG	1.95	0.47
51:QQ:86:GLN:HG2	51:QQ:90:LYS:HE2	1.96	0.47
61:9:694:G:H1	61:9:732:U:H3	1.61	0.47
61:9:1049:A:H3'	61:9:1050:A:H8	1.79	0.47
12:L:55:ILE:HB	12:L:116:ARG:HH12	1.79	0.47
44:5:2002:A:H61	83:t:135:THR:HA	1.79	0.47
57:cc:20:ARG:HE	57:cc:28:THR:HG23	1.79	0.47
4:C:242:PRO:HB2	44:5:2297:G:H5'	1.96	0.47
9:H:79:ASN:HB3	9:H:151:ILE:HG21	1.96	0.47
44:5:1857:C:H2'	44:5:1858:A:H8	1.79	0.47
44:5:1995:G:H1	82:s:41:GLN:NE2	2.12	0.47
15:O:36:VAL:HG13	15:O:37:ARG:HG3	1.97	0.47
18:R:81:ARG:HA	18:R:88:ARG:HH21	1.79	0.47
20:T:111:GLU:HG3	20:T:115:LYS:HE2	1.95	0.47
44:5:337:U:H2'	44:5:338:A:H8	1.79	0.47
44:5:1998:A:H1'	82:s:56:GLY:HA2	1.96	0.47
67:HH:46:THR:HG23	67:HH:65:PRO:HG3	1.97	0.47
68:II:132:GLU:HG3	68:II:135:GLU:HB3	1.96	0.47
81:l:1472:A:H4'	81:l:1486:C:H4'	1.96	0.47
14:N:159:ARG:HG2	14:N:164:LEU:HD12	1.95	0.47
34:h:31:LEU:HD22	34:h:43:LYS:HB3	1.95	0.47
41:o:57:ARG:HH11	44:5:4380:A:H5'	1.79	0.47
44:5:725:G:H2'	44:5:726:G:H8	1.79	0.47
44:5:1994:C:H1'	83:t:131:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:2095:A:C2	44:5:2096:G:C4	3.03	0.47
55:UU:59:LYS:HE3	61:9:1548:G:H5''	1.96	0.47
60:gg:254:PRO:HA	60:gg:285:GLN:HA	1.97	0.47
61:9:661:U:H3'	61:9:662:G:H2'	1.95	0.47
65:EE:45:ILE:HG12	65:EE:49:ARG:HH21	1.78	0.47
8:G:119:GLN:HA	8:G:122:ILE:HB	1.96	0.47
36:j:43:ARG:HG2	44:5:21:G:H5''	1.96	0.47
39:m:53:GLU:HB3	39:m:56:LEU:HB2	1.96	0.47
49:MM:58:GLU:HB3	49:MM:61:TYR:HB3	1.96	0.47
52:RR:79:GLU:O	52:RR:80:ARG:C	2.56	0.47
61:9:377:G:H5'	68:II:98:LYS:HG3	1.96	0.47
61:9:1079:C:H4'	61:9:1182:A:H61	1.79	0.47
78:bb:43:ILE:HD13	78:bb:80:ARG:HH12	1.79	0.47
2:A:156:LYS:HE2	2:A:158:ILE:HD11	1.96	0.47
4:C:333:LYS:HZ3	44:5:978:G:H5'	1.79	0.47
27:a:76:ASP:HB3	27:a:115:GLY:HA3	1.96	0.47
44:5:1968:G:H4'	82:s:34:ASN:CA	2.45	0.47
44:5:2522:G:H21	44:5:2711:G:H1	1.62	0.47
44:5:4303:C:H2'	44:5:4305:G:H8	1.80	0.47
47:FF:135:ARG:HH12	72:OO:71:PRO:HG2	1.79	0.47
80:K:120:ILE:HG13	80:K:122:ARG:H	1.80	0.47
9:H:89:ARG:HG3	9:H:145:VAL:HG13	1.97	0.47
17:Q:178:ARG:HH12	17:Q:184:ARG:HD3	1.80	0.47
38:l:29:MET:HE2	38:l:29:MET:HB2	1.85	0.47
44:5:1884:C:H2'	44:5:1885:G:H8	1.80	0.47
44:5:4924:C:O2'	44:5:4926:C:N3	2.45	0.47
17:Q:41:SER:HB3	17:Q:132:LYS:HG2	1.97	0.47
18:R:149:LYS:HA	18:R:152:LYS:HG2	1.97	0.47
25:Y:80:ILE:HD11	25:Y:104:VAL:HG21	1.96	0.47
44:5:1973:G:C4'	83:t:116:MET:SD	3.00	0.47
44:5:2002:A:N1	83:t:138:SER:CB	2.77	0.47
53:SS:36:VAL:HG23	53:SS:40:TYR:HB3	1.97	0.47
61:9:957:A:H3'	61:9:958:G:H21	1.80	0.47
4:C:78:ARG:HB3	4:C:88:GLY:HA2	1.96	0.46
44:5:2095:A:C4	44:5:2096:G:N7	2.83	0.46
52:RR:79:GLU:C	52:RR:82:ASP:H	2.23	0.46
52:RR:80:ARG:C	52:RR:80:ARG:HE	2.22	0.46
60:gg:23:THR:HG21	60:gg:292:SER:HA	1.97	0.46
61:9:306:C:H5	68:II:41:ARG:HH21	1.63	0.46
61:9:522:A:H5''	69:JJ:145:PRO:HD2	1.96	0.46
61:9:1112:U:O2	61:9:1121:G:O6	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:235:LEU:HD22	4:C:240:LEU:HD11	1.98	0.46
17:Q:144:LYS:HG2	44:5:1460:C:H5''	1.97	0.46
44:5:1993:C:C1'	83:t:138:SER:HB3	2.30	0.46
44:5:2868:G:H21	44:5:2882:A:H62	1.61	0.46
44:5:4899:G:H21	44:5:4921:C:C2'	2.29	0.46
80:K:78:LYS:O	80:K:147:LYS:NZ	2.39	0.46
33:g:8:ARG:HH22	44:5:2520:C:H5'	1.78	0.46
44:5:950:G:H2'	44:5:951:G:H8	1.80	0.46
44:5:1794:A:H5''	44:5:4214:A:H61	1.79	0.46
44:5:2096:G:H4'	44:5:2097:U:C2	2.51	0.46
54:TT:28:LEU:HD23	54:TT:110:LEU:HD21	1.96	0.46
80:K:79:ALA:C	80:K:147:LYS:HZ2	2.24	0.46
83:t:108:GLU:H	83:t:108:GLU:HG3	1.19	0.46
6:E:195:LYS:HG2	32:f:107:PRO:HA	1.98	0.46
18:R:100:ARG:HB3	18:R:104:ARG:HH21	1.81	0.46
43:r:63:VAL:HG22	43:r:79:ARG:HH22	1.80	0.46
44:5:4573:G:H22	44:5:4722:G:H21	1.63	0.46
61:9:1652:G:O6	61:9:1672:U:O4	2.34	0.46
80:K:207:LYS:HE2	80:K:209:THR:HA	1.98	0.46
7:F:107:VAL:HG21	7:F:134:ILE:HD11	1.98	0.46
10:I:203:ARG:HA	10:I:203:ARG:HD2	1.83	0.46
29:c:38:ILE:HD11	29:c:46:VAL:HG11	1.97	0.46
44:5:2100:G:C4	44:5:2101:A:C6	3.03	0.46
44:5:4344:U:H3	44:5:4368:G:H1	1.62	0.46
52:RR:90:ALA:HB2	62:AA:16:LEU:C	2.41	0.46
61:9:642:U:H4'	61:9:644:G:H4'	1.97	0.46
80:K:15:ARG:HB3	80:K:16:GLU:H	1.62	0.46
83:t:123:ARG:HB3	83:t:127:GLY:HA3	1.98	0.46
44:5:1188:C:H2'	44:5:1189:G:H8	1.80	0.46
51:QQ:109:LYS:HA	51:QQ:112:LEU:HB2	1.97	0.46
61:9:1124:C:H5''	63:BB:150:ILE:HG13	1.97	0.46
64:CC:183:LYS:HE2	64:CC:196:ILE:HG23	1.98	0.46
7:F:156:ARG:HD2	7:F:212:LEU:HD23	1.97	0.46
12:L:36:ARG:HH22	44:5:1364:U:H5''	1.80	0.46
18:R:70:ARG:HE	18:R:75:HIS:HB3	1.81	0.46
44:5:1998:A:P	82:s:44:ARG:HH22	2.38	0.46
47:FF:82:ASN:HA	47:FF:85:LYS:HD2	1.98	0.46
63:BB:213:ARG:HD2	63:BB:214:LYS:HB2	1.98	0.46
64:CC:73:MET:HE2	64:CC:73:MET:HB2	1.86	0.46
69:JJ:109:ARG:HE	69:JJ:146:SER:HA	1.81	0.46
83:t:108:GLU:CD	83:t:109:ILE:HG13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:85:GLU:HB2	20:T:135:PRO:HB3	1.98	0.46
19:S:13:VAL:HG12	19:S:63:TYR:HB3	1.97	0.46
22:V:43:LYS:HA	44:5:4508:C:H4'	1.96	0.46
13:M:91:TRP:HA	13:M:94:LYS:HE2	1.98	0.46
41:o:41:TYR:O	41:o:45:GLN:HB2	2.16	0.46
52:RR:90:ALA:CB	62:AA:17:LYS:N	2.78	0.46
60:gg:79:LEU:HD22	60:gg:111:VAL:HG21	1.97	0.46
69:JJ:17:ARG:HG2	69:JJ:18:ARG:HG2	1.97	0.46
9:H:94:SER:H	9:H:142:ASP:HB3	1.81	0.46
32:f:58:VAL:HG12	32:f:64:PRO:HG3	1.97	0.46
39:m:68:MET:HG2	39:m:79:PRO:HA	1.98	0.46
44:5:2100:G:C2	44:5:2101:A:N6	2.84	0.46
44:5:2411:C:H2'	44:5:2412:A:H8	1.81	0.46
61:9:959:G:H1	72:OO:65:ASP:HB3	1.81	0.46
73:VV:51:LYS:HE3	73:VV:76:ASP:HB3	1.98	0.46
3:B:168:MET:HA	3:B:171:LEU:HD23	1.97	0.45
5:D:30:TYR:HA	5:D:33:ARG:HB3	1.98	0.45
16:P:126:ARG:HG2	16:P:140:MET:HE1	1.97	0.45
25:Y:86:GLN:HB3	25:Y:96:HIS:HD2	1.81	0.45
44:5:517:C:H2'	44:5:518:C:C6	2.50	0.45
61:9:948:C:H2'	61:9:949:G:H8	1.80	0.45
9:H:92:MET:HB3	9:H:181:VAL:HA	1.99	0.45
31:e:6:PRO:HG2	31:e:9:LYS:HG2	1.98	0.45
35:i:97:MET:HE3	35:i:97:MET:HB3	1.88	0.45
44:5:1538:U:H2'	44:5:1539:G:H8	1.81	0.45
44:5:1995:G:H1'	83:t:131:GLU:OE1	2.16	0.45
44:5:4519:C:H5''	44:5:4520:G:H5''	1.96	0.45
50:PP:73:PRO:HG2	50:PP:92:SER:HA	1.97	0.45
80:K:66:CYS:HA	80:K:83:PRO:CD	2.46	0.45
80:K:67:VAL:HG23	80:K:111:LEU:HD22	1.98	0.45
80:K:76:GLU:N	80:K:78:LYS:HB2	2.30	0.45
38:l:23:ILE:HG23	38:l:38:ASN:HB2	1.98	0.45
44:5:2098:G:C5	44:5:2099:C:C4	3.04	0.45
63:BB:187:LYS:HD3	63:BB:193:ILE:HD11	1.98	0.45
64:CC:194:ARG:HB3	64:CC:225:SER:HB3	1.99	0.45
65:EE:35:PRO:HD2	65:EE:83:PRO:HG2	1.97	0.45
66:GG:157:VAL:HB	66:GG:176:ILE:HD11	1.99	0.45
80:K:78:LYS:HA	80:K:82:ILE:HD13	1.98	0.45
81:1:1357:U:C4	81:1:1375:C:N4	2.84	0.45
1:7:15:C:H2'	1:7:16:A:H8	1.82	0.45
18:R:74:ARG:HH12	44:5:2891:U:H5	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:6:ALA:HA	34:h:9:LEU:HD12	1.98	0.45
48:KK:1:MET:HE1	48:KK:47:LYS:HD2	1.99	0.45
60:gg:86:THR:HG22	60:gg:102:VAL:HG23	1.98	0.45
63:BB:49:VAL:HG13	63:BB:65:ARG:HH12	1.81	0.45
65:EE:72:ILE:HD11	65:EE:77:ARG:HB2	1.98	0.45
80:K:73:HIS:CD2	80:K:74:CYS:H	2.34	0.45
3:B:53:MET:HE2	3:B:53:MET:HB2	1.84	0.45
44:5:1906:U:H2'	44:5:1907:A:H8	1.81	0.45
44:5:2093:A:H4'	44:5:2094:C:H5'	1.99	0.45
48:KK:15:LEU:HG	48:KK:71:LEU:HD22	1.97	0.45
60:gg:165:ILE:HG13	60:gg:177:TRP:HB2	1.97	0.45
62:AA:17:LYS:HB3	62:AA:173:LEU:HD21	1.99	0.45
80:K:162:VAL:HG13	80:K:164:CYS:H	1.81	0.45
44:5:4896:G:O6	44:5:4924:C:N3	2.50	0.45
47:FF:49:LEU:HD12	51:QQ:50:LYS:HG2	1.98	0.45
61:9:1699:A:H2'	64:CC:117:ARG:HH22	1.81	0.45
80:K:48:ARG:HH21	80:K:195:LYS:HG2	1.81	0.45
2:A:3:ARG:H	2:A:207:VAL:HG22	1.82	0.45
2:A:20:VAL:HG12	2:A:23:ARG:HD2	1.98	0.45
2:A:177:LYS:HB2	42:p:29:ILE:HG21	1.99	0.45
6:E:64:MET:HG3	6:E:68:LYS:HE2	1.99	0.45
12:L:46:ILE:HB	12:L:49:ARG:HB2	1.98	0.45
14:N:184:ILE:HG23	14:N:194:ARG:HH22	1.81	0.45
21:U:21:PHE:HB2	21:U:72:VAL:HG13	1.98	0.45
32:f:54:LYS:HE3	44:5:4748:U:H5''	1.99	0.45
44:5:2100:G:H1'	44:5:2101:A:N3	2.31	0.45
47:FF:55:ARG:HH22	51:QQ:125:ARG:HG3	1.81	0.45
50:PP:47:ARG:HH21	61:9:1618:C:H5''	1.82	0.45
51:QQ:58:LEU:HD21	51:QQ:108:ILE:HG23	1.98	0.45
78:bb:51:GLN:HE21	78:bb:51:GLN:HB3	1.68	0.45
83:t:123:ARG:HD2	83:t:123:ARG:HA	1.76	0.45
25:Y:49:ILE:HD11	25:Y:101:PRO:HB3	1.99	0.45
42:p:57:CYS:SG	42:p:60:CYS:HB2	2.57	0.45
50:PP:39:ALA:HA	50:PP:42:ARG:HG3	1.98	0.45
52:RR:106:LEU:HD21	62:AA:10:MET:HE2	1.99	0.45
1:7:117:G:H5'	5:D:256:LYS:HD2	1.99	0.45
3:B:343:ARG:HH22	44:5:4977:A:H5'	1.82	0.45
7:F:178:LEU:HB3	7:F:183:ILE:HB	1.99	0.45
20:T:52:MET:HE3	20:T:53:PRO:HD2	1.99	0.45
42:p:48:LYS:HD2	42:p:48:LYS:HA	1.83	0.45
44:5:2097:U:H2'	44:5:2097:U:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:4319:C:H2'	44:5:4320:G:H8	1.80	0.45
44:5:4923:C:H2'	44:5:4924:C:N3	2.32	0.45
61:9:1172:U:O2	61:9:1188:A:N7	2.50	0.45
80:K:74:CYS:C	80:K:78:LYS:HG3	2.41	0.45
80:K:85:MET:HE1	80:K:93:LEU:CD1	2.46	0.45
10:I:60:LEU:HD13	10:I:129:VAL:HG21	1.99	0.45
21:U:19:LEU:HD22	21:U:78:PHE:H	1.82	0.45
44:5:4922:C:O2'	44:5:4923:C:H5'	2.17	0.45
44:5:4924:C:H2'	44:5:4925:U:N1	2.32	0.45
44:5:4951:G:H2'	44:5:4952:G:H8	1.82	0.45
60:gg:21:ILE:HG21	60:gg:299:PHE:HB2	1.99	0.45
76:YY:99:LYS:HD2	76:YY:99:LYS:HA	1.83	0.45
80:K:78:LYS:HB3	80:K:79:ALA:H	1.34	0.45
21:U:49:VAL:HB	21:U:57:GLY:HA3	1.99	0.44
34:h:42:SER:O	34:h:46:LYS:HB2	2.17	0.44
44:5:1348:U:H2'	44:5:1349:G:H8	1.82	0.44
53:SS:4:VAL:HA	56:ZZ:50:PHE:HB2	1.98	0.44
66:GG:221:LYS:HA	66:GG:224:ARG:HG2	1.99	0.44
80:K:78:LYS:HA	80:K:82:ILE:HB	1.99	0.44
18:R:46:LYS:HE3	18:R:46:LYS:HB3	1.84	0.44
36:j:18:LEU:HA	36:j:25:LYS:HA	1.99	0.44
44:5:1382:G:H2'	44:5:1383:G:H8	1.83	0.44
44:5:3664:G:H2'	44:5:3665:G:H8	1.82	0.44
50:PP:93:MET:HE3	50:PP:104:GLN:HB3	1.99	0.44
61:9:4:C:H1'	69:JJ:18:ARG:HH22	1.82	0.44
80:K:76:GLU:N	80:K:78:LYS:CB	2.81	0.44
6:E:49:ASN:H	6:E:64:MET:HE1	1.83	0.44
10:I:52:MET:HE1	10:I:156:LYS:HG2	1.99	0.44
14:N:108:ARG:HH22	44:5:54:G:H4'	1.82	0.44
29:c:48:LEU:HD13	29:c:57:LYS:HG3	1.99	0.44
44:5:717:U:H3	44:5:951:G:H1	1.64	0.44
50:PP:122:THR:HG21	61:9:1516:G:H4'	1.98	0.44
63:BB:87:ILE:HG12	63:BB:101:HIS:HB2	1.99	0.44
80:K:69:GLY:O	80:K:84:HIS:ND1	2.50	0.44
80:K:78:LYS:HE2	80:K:78:LYS:HB3	1.39	0.44
81:1:1404:A:N1	81:1:1433:U:C4	2.85	0.44
1:7:6:C:H4'	5:D:52:ILE:HD13	1.99	0.44
5:D:160:PHE:HA	5:D:163:LEU:HB3	1.99	0.44
6:E:115:MET:HE2	6:E:115:MET:HB2	1.82	0.44
44:5:1973:G:H5'	83:t:121:LEU:CD1	2.48	0.44
61:9:444:G:H3'	68:II:47:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:9:955:A:C6	61:9:971:G:N2	2.85	0.44
61:9:955:A:H62	61:9:971:G:N2	2.14	0.44
83:t:114:ARG:HD2	83:t:114:ARG:HA	1.85	0.44
27:a:75:LEU:HD22	27:a:113:GLY:HA2	1.99	0.44
44:5:2096:G:C8	44:5:2096:G:O5'	2.70	0.44
44:5:2098:G:C2'	44:5:2099:C:H5'	2.47	0.44
44:5:4897:G:C6	44:5:4924:C:N3	2.86	0.44
47:FF:101:HIS:HB2	47:FF:108:PRO:HG3	1.98	0.44
49:MM:25:ALA:HB1	49:MM:31:LEU:HB3	1.98	0.44
61:9:894:G:H2'	61:9:895:G:H8	1.82	0.44
71:NN:63:VAL:HG11	71:NN:71:ILE:HG13	1.99	0.44
77:aa:22:ARG:HH21	77:aa:27:ALA:HB1	1.82	0.44
79:ee:77:GLY:HA2	79:ee:81:ARG:HD2	1.98	0.44
80:K:36:ILE:HG22	80:K:204:LEU:HA	2.00	0.44
34:h:80:PRO:HD2	34:h:83:LEU:HD12	1.99	0.44
54:TT:71:GLY:HA3	61:9:1562:C:H5''	1.99	0.44
69:JJ:115:PHE:HA	69:JJ:120:ALA:HB3	2.00	0.44
5:D:104:LEU:HG	5:D:247:ILE:HG12	1.99	0.44
42:p:9:GLY:H	42:p:27:LYS:HE2	1.83	0.44
44:5:1758:G:H2'	44:5:1759:G:H8	1.83	0.44
44:5:1998:A:P	82:s:54:LEU:HD12	2.57	0.44
44:5:2026:A:O2'	44:5:2027:U:H5'	2.18	0.44
44:5:2098:G:N7	44:5:2099:C:C4	2.86	0.44
44:5:4897:G:H1	44:5:4923:C:C2'	2.31	0.44
61:9:1054:G:H2'	61:9:1055:A:H8	1.81	0.44
82:s:44:ARG:N	82:s:44:ARG:HD3	2.32	0.44
12:L:184:MET:HE1	44:5:1487:G:H1'	2.00	0.44
25:Y:51:LYS:HG2	25:Y:72:GLN:HA	1.98	0.44
44:5:751:G:H3'	44:5:752:G:H8	1.83	0.44
44:5:966:A:C8	44:5:2096:G:N2	2.85	0.44
44:5:1616:U:H2'	44:5:1617:G:H8	1.83	0.44
46:DD:177:LEU:HD22	46:DD:179:GLN:HE22	1.82	0.44
61:9:1656:G:O6	61:9:1668:U:O4	2.35	0.44
18:R:164:SER:HA	18:R:167:LYS:HG2	2.00	0.44
34:h:28:LEU:HD12	34:h:50:VAL:HG23	2.00	0.44
37:k:67:LYS:HZ2	37:k:69:LEU:HG	1.82	0.44
44:5:4899:G:N3	44:5:4921:C:N3	2.66	0.44
50:PP:98:ASN:HD21	50:PP:120:SER:HB2	1.83	0.44
60:gg:68:ASP:HB3	60:gg:111:VAL:HG12	2.00	0.44
62:AA:108:PHE:HB2	62:AA:136:GLU:HG2	1.99	0.44
80:K:67:VAL:CG1	80:K:82:ILE:CA	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:K:78:LYS:CG	80:K:79:ALA:N	2.79	0.44
24:X:64:SER:HB2	34:h:69:LEU:HD22	1.99	0.43
38:l:23:ILE:HB	38:l:27:ILE:HD11	1.99	0.43
44:5:1968:G:C4'	82:s:34:ASN:HA	2.44	0.43
44:5:3970:G:H1	44:5:4051:C:H2'	1.83	0.43
49:MM:94:ILE:HD12	49:MM:101:ARG:HD3	2.00	0.43
61:9:617:G:H4'	75:XX:88:ASP:HB2	2.00	0.43
75:XX:53:GLU:HG2	75:XX:71:ARG:HB3	1.99	0.43
80:K:65:VAL:HG21	80:K:81:ASP:HB3	1.99	0.43
4:C:197:ARG:HH12	44:5:350:C:H3'	1.83	0.43
44:5:2647:A:H62	44:5:2686:G:H8	1.66	0.43
46:DD:1:MET:H3	46:DD:4:GLN:HA	1.82	0.43
50:PP:37:TYR:HB2	50:PP:38:SER:H	1.62	0.43
52:RR:84:TYR:HB2	52:RR:85:VAL:H	1.41	0.43
52:RR:109:LEU:HD23	73:VV:82:ASN:HB3	2.00	0.43
72:OO:75:MET:HE3	72:OO:75:MET:HB3	1.93	0.43
80:K:67:VAL:N	80:K:83:PRO:HD2	2.30	0.43
80:K:85:MET:HE1	80:K:93:LEU:HD12	1.99	0.43
83:t:113:ALA:HB2	83:t:129:ILE:HG13	1.97	0.43
3:B:52:GLY:HA2	3:B:341:LYS:HE3	2.00	0.43
9:H:114:ILE:HG22	9:H:124:ARG:HB2	1.99	0.43
10:I:189:ARG:HH12	10:I:201:PRO:HA	1.83	0.43
15:O:121:PRO:HA	15:O:124:LEU:HB2	2.01	0.43
16:P:88:ALA:HA	16:P:91:LEU:HD23	2.00	0.43
44:5:3610:A:H2'	44:5:3611:A:H8	1.83	0.43
61:9:1244:U:H2'	61:9:1245:G:H8	1.83	0.43
80:K:79:ALA:O	80:K:82:ILE:HG22	2.18	0.43
2:A:113:VAL:HG12	2:A:166:VAL:HG13	2.00	0.43
16:P:148:MET:HE3	16:P:148:MET:HB3	1.93	0.43
44:5:1494:U:H2'	44:5:1495:G:H8	1.83	0.43
44:5:2098:G:C3'	44:5:2099:C:H6	2.28	0.43
53:SS:85:ASN:HD21	53:SS:98:VAL:HG12	1.83	0.43
61:9:562:U:H2'	61:9:563:G:H8	1.83	0.43
62:AA:65:ILE:H	62:AA:65:ILE:HG12	1.60	0.43
73:VV:11:LEU:HD12	73:VV:12:TYR:HB3	2.00	0.43
80:K:67:VAL:HG22	80:K:77:ALA:O	2.17	0.43
3:B:356:LYS:HA	3:B:356:LYS:HD2	1.81	0.43
5:D:9:ASN:H	5:D:12:TYR:HB3	1.83	0.43
8:G:217:ILE:HD11	14:N:22:LEU:HD11	2.00	0.43
9:H:1:MET:HE2	9:H:1:MET:HB2	1.94	0.43
11:J:22:LEU:HB3	11:J:128:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:61:VAL:HB	43:r:79:ARG:HH21	1.82	0.43
43:r:64:MET:HB3	43:r:78:VAL:HG12	2.00	0.43
44:5:2751:G:H2'	44:5:2752:G:H8	1.83	0.43
53:SS:132:ARG:HB2	53:SS:134:GLN:HE22	1.83	0.43
64:CC:210:PRO:HB3	64:CC:240:THR:HG21	2.00	0.43
72:OO:95:ILE:HB	72:OO:129:ILE:HG12	2.00	0.43
80:K:73:HIS:O	80:K:75:ASP:N	2.44	0.43
3:B:224:LYS:HB3	3:B:224:LYS:HE2	1.83	0.43
3:B:240:LEU:HB2	3:B:248:LEU:HA	1.99	0.43
6:E:153:LEU:HD13	6:E:197:VAL:HG11	2.01	0.43
15:O:27:VAL:HG13	15:O:98:ALA:HB1	2.01	0.43
15:O:94:ARG:HD2	44:5:1309:C:H5''	2.01	0.43
44:5:2095:A:C2'	44:5:2096:G:C8	2.97	0.43
44:5:4115:G:H5''	44:5:4116:C:H5'	2.00	0.43
58:dd:39:CYS:SG	58:dd:42:CYS:HB2	2.59	0.43
61:9:971:G:H4'	61:9:972:A:H5'	2.00	0.43
76:YY:55:ILE:HG12	76:YY:75:ILE:HG12	2.00	0.43
77:aa:38:LYS:HD3	77:aa:83:VAL:HG11	1.99	0.43
2:A:185:ALA:HA	2:A:188:LYS:HB2	2.01	0.43
11:J:43:LEU:HD11	11:J:115:LEU:HD13	2.00	0.43
15:O:22:ILE:HG22	15:O:26:GLN:HE21	1.83	0.43
18:R:139:MET:HE2	18:R:139:MET:HB2	1.88	0.43
22:V:74:LYS:HB3	22:V:74:LYS:HE3	1.80	0.43
41:o:26:TYR:HB3	41:o:67:VAL:HB	1.99	0.43
54:TT:56:ARG:HH22	54:TT:99:VAL:HB	1.84	0.43
60:gg:202:PRO:HG2	60:gg:243:PRO:HA	2.01	0.43
6:E:204:ILE:HD12	6:E:204:ILE:HA	1.91	0.43
7:F:227:VAL:HA	19:S:39:VAL:HG12	2.01	0.43
22:V:78:PRO:HG2	22:V:107:ASN:HA	1.99	0.43
42:p:37:TYR:H	42:p:47:MET:HB2	1.82	0.43
44:5:2023:C:H2'	44:5:2024:G:C5'	2.48	0.43
44:5:3805:U:H2'	44:5:3806:G:H8	1.83	0.43
44:5:3939:G:H1'	44:5:4076:G:H22	1.84	0.43
50:PP:108:LYS:HG3	50:PP:111:MET:HG3	2.00	0.43
56:ZZ:91:LEU:HD23	56:ZZ:94:LYS:HE2	2.01	0.43
61:9:593:C:H1'	79:ee:99:LYS:HD2	2.01	0.43
63:BB:146:ARG:HB2	63:BB:149:GLN:HB2	2.00	0.43
71:NN:47:PRO:HG2	71:NN:72:LEU:HD13	2.00	0.43
23:W:6:CYS:HB3	23:W:10:GLY:H	1.82	0.43
44:5:2098:G:C5	44:5:2107:C:N3	2.87	0.43
52:RR:89:SER:HB2	52:RR:90:ALA:H	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UU:35:VAL:HG11	55:UU:110:VAL:HG11	2.01	0.43
66:GG:221:LYS:HE3	66:GG:224:ARG:HH21	1.83	0.43
82:s:55:MET:HE3	82:s:55:MET:HB3	1.95	0.43
3:B:332:MET:HE2	3:B:332:MET:HB2	1.81	0.43
15:O:186:GLU:H	15:O:186:GLU:HG3	1.72	0.43
17:Q:50:ARG:HB3	17:Q:83:VAL:HG11	2.01	0.43
44:5:4926:C:C2	44:5:4927:G:C6	3.07	0.43
44:5:4927:G:N3	44:5:4927:G:O5'	2.52	0.43
60:gg:21:ILE:HG23	60:gg:31:ILE:HD11	1.99	0.43
61:9:1692:U:H5'	77:aa:88:SER:HA	2.00	0.43
62:AA:54:THR:HG22	62:AA:162:PRO:HG2	2.01	0.43
70:LL:93:LEU:HD12	70:LL:102:PHE:HB3	2.01	0.43
20:T:27:LEU:HA	20:T:30:TYR:HD2	1.84	0.42
33:g:8:ARG:HB2	33:g:34:TYR:HE2	1.84	0.42
44:5:3848:U:H2'	44:5:3849:A:H8	1.84	0.42
44:5:3870:C:H2'	44:5:3871:A:H8	1.84	0.42
44:5:4920:C:C2'	44:5:4921:C:H5'	2.49	0.42
50:PP:52:LYS:HE2	50:PP:52:LYS:HB2	1.90	0.42
61:9:433:A:H5''	68:II:22:HIS:HB3	2.00	0.42
61:9:924:G:N2	61:9:1018:U:O2	2.37	0.42
4:C:73:VAL:HB	4:C:78:ARG:HH21	1.85	0.42
7:F:93:ARG:HD2	7:F:108:LEU:HD12	2.02	0.42
44:5:483:G:H5''	44:5:484:U:H2'	2.01	0.42
44:5:1998:A:C5	82:s:55:MET:CB	3.00	0.42
44:5:2025:A:OP2	44:5:2025:A:H8	2.02	0.42
44:5:4896:G:O6	44:5:4924:C:C4	2.71	0.42
52:RR:47:ARG:HH21	52:RR:48:ASN:HD21	1.67	0.42
52:RR:77:GLU:O	52:RR:80:ARG:N	2.49	0.42
53:SS:46:ARG:HH12	54:TT:52:TRP:HE1	1.66	0.42
55:UU:57:PRO:HA	61:9:1446:A:H5'	2.00	0.42
60:gg:251:ALA:HB2	60:gg:289:LEU:HD22	2.00	0.42
61:9:684:G:H2'	61:9:685:A:H8	1.84	0.42
73:VV:15:ARG:HB3	73:VV:24:ILE:HD12	2.01	0.42
3:B:303:ALA:HA	3:B:368:ILE:HD12	2.00	0.42
22:V:91:LYS:HA	22:V:91:LYS:HD3	1.83	0.42
26:Z:109:LYS:HE2	44:5:2556:G:H4'	2.02	0.42
29:c:26:LYS:HB3	29:c:97:ILE:HB	2.01	0.42
52:RR:77:GLU:HG3	52:RR:80:ARG:HB3	2.02	0.42
61:9:126:G:H2'	66:GG:199:THR:HG21	2.01	0.42
61:9:1121:G:H21	63:BB:206:PRO:HD3	1.83	0.42
61:9:1811:C:H5''	75:XX:37:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:GG:64:LYS:HE2	66:GG:82:SER:HB3	2.01	0.42
71:NN:76:LYS:HE3	71:NN:76:LYS:HB3	1.87	0.42
74:WW:30:CYS:HA	74:WW:34:ILE:HD11	2.01	0.42
4:C:266:THR:HG23	4:C:268:ARG:H	1.85	0.42
19:S:170:LYS:HE2	44:5:4875:G:H5'	2.02	0.42
21:U:67:LYS:HB2	21:U:67:LYS:HE2	1.86	0.42
34:h:91:MET:HE2	34:h:91:MET:HB2	1.83	0.42
60:gg:121:VAL:HG21	60:gg:165:ILE:HD13	2.01	0.42
65:EE:45:ILE:HA	65:EE:61:VAL:HG11	2.01	0.42
76:YY:91:LEU:HD22	76:YY:96:LEU:HD11	2.01	0.42
80:K:34:LEU:HD12	80:K:206:ILE:HA	2.02	0.42
10:I:171:TRP:HB2	10:I:178:ALA:HA	2.01	0.42
15:O:87:MET:HE3	15:O:87:MET:HB3	1.91	0.42
17:Q:113:ILE:HD12	17:Q:113:ILE:HA	1.96	0.42
20:T:12:ARG:HH22	44:5:1789:C:H5'	1.84	0.42
41:o:9:ARG:HA	41:o:20:PRO:HA	2.02	0.42
44:5:965:G:N2	44:5:2096:G:O2'	2.52	0.42
44:5:4639:G:O6	44:5:4660:G:O6	2.37	0.42
62:AA:57:LYS:HD3	62:AA:60:LEU:HD12	2.01	0.42
62:AA:140:VAL:HB	62:AA:142:LEU:HG	2.01	0.42
80:K:67:VAL:HG13	80:K:82:ILE:CB	2.50	0.42
3:B:168:MET:HE2	3:B:168:MET:HB2	1.97	0.42
9:H:118:LEU:HD11	9:H:167:VAL:HG22	2.01	0.42
11:J:24:ILE:HG23	44:5:4251:A:H61	1.84	0.42
26:Z:61:LYS:HB2	26:Z:61:LYS:HE2	1.80	0.42
27:a:131:ARG:HH21	27:a:132:ARG:HH21	1.68	0.42
33:g:26:PRO:HD2	44:5:2521:G:H4'	2.02	0.42
39:m:100:LYS:HE2	39:m:100:LYS:HB2	1.90	0.42
44:5:1993:C:H1'	83:t:138:SER:CB	2.34	0.42
44:5:4594:U:H2'	44:5:4595:G:H8	1.84	0.42
44:5:4699:U:H1'	44:5:4700:A:H5''	2.02	0.42
60:gg:106:LYS:HB3	60:gg:107:ASP:H	1.69	0.42
67:HH:105:THR:HG23	67:HH:107:LYS:H	1.83	0.42
68:II:13:LYS:H	68:II:13:LYS:HG3	1.65	0.42
75:XX:21:LYS:HA	75:XX:21:LYS:HD2	1.84	0.42
75:XX:107:ARG:HB3	75:XX:110:HIS:HB3	2.01	0.42
76:YY:38:THR:HA	76:YY:41:ARG:HD3	2.00	0.42
2:A:36:GLU:HA	2:A:91:GLY:HA2	2.02	0.42
12:L:197:LYS:HD2	44:5:4358:U:H4'	2.01	0.42
15:O:29:LEU:HG	32:f:10:ILE:HG21	2.00	0.42
27:a:29:PRO:HA	44:5:1654:G:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:p:8:VAL:HG23	42:p:11:VAL:HG23	2.01	0.42
43:r:63:VAL:HG13	43:r:79:ARG:HH12	1.85	0.42
44:5:2088:A:O2'	44:5:2089:G:P	2.78	0.42
44:5:2098:G:C6	44:5:2099:C:N3	2.88	0.42
52:RR:74:GLN:CA	52:RR:77:GLU:HB3	2.50	0.42
4:C:350:ARG:HD3	4:C:353:ARG:HH21	1.85	0.42
26:Z:5:MET:HE3	26:Z:5:MET:HB3	1.90	0.42
44:5:1446:C:H42	44:5:2108:G:H1	1.68	0.42
44:5:1995:G:N3	83:t:122:ALA:CB	2.82	0.42
44:5:2089:G:H5'	44:5:2089:G:C8	2.53	0.42
44:5:4896:G:H2'	44:5:4897:G:H8	1.84	0.42
46:DD:124:ARG:HA	46:DD:124:ARG:HD2	1.88	0.42
49:MM:60:MET:HE2	49:MM:60:MET:HB2	1.93	0.42
50:PP:75:VAL:HG11	50:PP:104:GLN:HE22	1.85	0.42
61:9:1786:U:H2'	61:9:1787:G:H8	1.85	0.42
65:EE:126:VAL:HG11	65:EE:139:LEU:HD13	2.01	0.42
74:WW:105:THR:HB	74:WW:110:ILE:HG22	2.01	0.42
76:YY:74:MET:HE2	76:YY:74:MET:HB2	1.86	0.42
81:1:1404:A:N1	81:1:1433:U:O4	2.52	0.42
1:7:36:C:H5'	5:D:155:THR:HB	2.02	0.42
2:A:204:MET:HE3	2:A:208:GLU:HG3	2.02	0.42
2:A:233:ARG:HD2	2:A:233:ARG:HA	1.88	0.42
12:L:8:MET:HE2	12:L:8:MET:HB2	1.96	0.42
17:Q:70:MET:HE3	17:Q:70:MET:HB3	1.94	0.42
18:R:23:TRP:HB2	18:R:53:LYS:HG3	2.01	0.42
26:Z:98:LYS:HE2	26:Z:98:LYS:HB3	1.88	0.42
28:b:92:LYS:HB2	28:b:92:LYS:HE2	1.76	0.42
30:d:43:PRO:HG3	44:5:2372:U:H5'	2.02	0.42
31:e:109:LYS:HA	31:e:109:LYS:HD3	1.80	0.42
44:5:2624:G:H1	44:5:2632:U:H3	1.68	0.42
48:KK:77:GLN:HA	48:KK:80:ARG:HD2	2.01	0.42
65:EE:44:LEU:HD23	65:EE:82:TYR:HB3	2.01	0.42
79:ee:85:VAL:HA	79:ee:88:GLN:HG2	2.02	0.42
14:N:135:ILE:HD13	14:N:151:ILE:HG21	2.01	0.42
19:S:9:GLU:HG3	19:S:67:VAL:HG13	2.02	0.42
22:V:13:LYS:HB2	22:V:128:LEU:HD11	2.01	0.42
35:i:61:LEU:HB3	35:i:94:LEU:HD22	2.02	0.42
55:UU:25:THR:HB	55:UU:84:ILE:HD11	2.01	0.42
65:EE:162:ILE:HG22	65:EE:169:ILE:HG22	2.02	0.42
66:GG:23:LYS:HB3	66:GG:41:LEU:HD12	2.02	0.42
80:K:66:CYS:SG	80:K:83:PRO:HG2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:K:171:HIS:HB3	80:K:173:LYS:H	1.85	0.42
4:C:340:ILE:HD13	4:C:340:ILE:HA	1.95	0.41
6:E:163:LYS:HE3	6:E:163:LYS:HB2	1.93	0.41
8:G:210:ILE:HG22	8:G:254:THR:HG22	2.02	0.41
9:H:43:VAL:HG12	9:H:59:LYS:HE2	2.01	0.41
19:S:28:TYR:HB3	20:T:151:LEU:HD22	2.02	0.41
36:j:11:ARG:HH22	44:5:1535:C:H5'	1.85	0.41
44:5:31:U:H3	44:5:51:A:H61	1.68	0.41
44:5:2096:G:H8	44:5:2096:G:O5'	2.03	0.41
44:5:4924:C:H2'	44:5:4925:U:C6	2.56	0.41
61:9:606:G:H8	79:ee:131:ASN:HD21	1.67	0.41
65:EE:153:LEU:HD13	66:GG:216:ARG:HH11	1.84	0.41
67:HH:61:ILE:HD11	67:HH:95:ILE:HB	2.02	0.41
71:NN:41:ALA:HB3	71:NN:80:LEU:HD23	2.01	0.41
2:A:29:LEU:H	2:A:123:ARG:HB3	1.85	0.41
3:B:84:MET:HE2	3:B:84:MET:HB2	1.89	0.41
5:D:41:LYS:HA	5:D:41:LYS:HD3	1.78	0.41
16:P:17:SER:HB2	16:P:94:MET:HE2	2.01	0.41
17:Q:60:PRO:HG3	44:5:1353:G:H22	1.84	0.41
17:Q:98:LEU:HD23	17:Q:98:LEU:HA	1.94	0.41
25:Y:16:LYS:HG2	45:8:23:C:H4'	2.02	0.41
29:c:11:LEU:HA	29:c:14:ILE:HD12	2.03	0.41
34:h:87:LYS:HE2	34:h:87:LYS:HB3	1.94	0.41
40:n:1:MET:HG2	61:9:1706:G:H4'	2.02	0.41
53:SS:26:ILE:HD11	53:SS:54:LYS:HB2	2.02	0.41
61:9:1048:G:H21	61:9:1070:A:H62	1.68	0.41
62:AA:30:LEU:HB2	62:AA:47:TYR:HE2	1.86	0.41
62:AA:56:GLU:H	62:AA:56:GLU:HG2	1.74	0.41
65:EE:45:ILE:HG12	65:EE:49:ARG:HE	1.84	0.41
73:VV:7:GLU:H	73:VV:7:GLU:HG3	1.73	0.41
74:WW:48:GLY:HA3	74:WW:64:ASN:HD22	1.85	0.41
80:K:73:HIS:O	80:K:77:ALA:HB3	2.20	0.41
80:K:78:LYS:O	80:K:79:ALA:O	2.37	0.41
9:H:52:LYS:HB3	9:H:52:LYS:HE2	1.88	0.41
16:P:43:LYS:HE2	44:5:5065:U:H5''	2.02	0.41
16:P:118:GLN:HE22	44:5:423:G:H21	1.68	0.41
20:T:14:MET:HE3	20:T:14:MET:HB3	1.81	0.41
44:5:33:A:H3'	44:5:47:A:H61	1.85	0.41
46:DD:29:LEU:HB2	46:DD:34:TYR:HB2	2.02	0.41
52:RR:105:MET:HE3	62:AA:52:LYS:H	1.85	0.41
54:TT:47:PRO:HA	61:9:1539:U:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:TT:111:LYS:HD3	54:TT:111:LYS:HA	1.92	0.41
61:9:649:U:H2'	61:9:650:A:H8	1.85	0.41
61:9:925:G:H1	61:9:1017:U:H3	1.68	0.41
63:BB:103:MET:HE3	63:BB:103:MET:HB3	1.81	0.41
64:CC:272:HIS:HA	64:CC:275:LYS:HE2	2.02	0.41
73:VV:68:SER:HA	73:VV:71:ARG:HE	1.85	0.41
76:YY:37:LYS:HB2	76:YY:37:LYS:HE3	1.90	0.41
81:1:1393:U:H2'	81:1:1394:A:C8	2.56	0.41
83:t:110:VAL:HA	83:t:129:ILE:HD11	2.02	0.41
3:B:47:LEU:HD22	3:B:181:MET:HG2	2.03	0.41
5:D:36:LEU:HD23	44:5:4325:A:H1'	2.03	0.41
17:Q:78:LYS:HG2	17:Q:137:VAL:HG23	2.03	0.41
23:W:82:ILE:HG12	66:GG:131:ARG:HE	1.85	0.41
27:a:103:VAL:HG12	27:a:108:TYR:HB2	2.03	0.41
44:5:2098:G:C3'	44:5:2099:C:C6	3.03	0.41
52:RR:74:GLN:HA	52:RR:77:GLU:N	2.36	0.41
55:UU:48:LEU:HD13	55:UU:93:SER:HB2	2.02	0.41
55:UU:66:ARG:HD2	55:UU:66:ARG:HA	1.92	0.41
61:9:1808:U:H2'	61:9:1809:A:H8	1.85	0.41
65:EE:9:LEU:HD13	65:EE:30:ARG:HE	1.85	0.41
3:B:229:LYS:HB3	3:B:233:SER:HB2	2.02	0.41
5:D:197:LYS:HD2	5:D:202:GLN:HG2	2.03	0.41
5:D:211:LEU:HB3	5:D:219:TYR:HB2	2.02	0.41
38:l:9:ILE:O	38:l:13:LEU:HB2	2.19	0.41
44:5:2088:A:C5	44:5:2268:A:C6	3.09	0.41
44:5:2543:A:H2	44:5:2773:G:H1	1.67	0.41
44:5:4921:C:O2'	44:5:4922:C:C1'	2.69	0.41
52:RR:7:LYS:HD2	52:RR:7:LYS:HA	1.88	0.41
58:dd:31:ILE:HB	58:dd:36:LEU:HD23	2.03	0.41
61:9:155:G:H2'	61:9:156:G:H8	1.85	0.41
61:9:1579:A:H4'	61:9:1581:C:H5	1.84	0.41
61:9:1652:G:N2	61:9:1672:U:O2	2.44	0.41
80:K:90:LEU:HB3	80:K:124:LEU:HG	2.02	0.41
81:1:1410:C:H2'	81:1:1411:A:H8	1.85	0.41
4:C:327:LYS:HE3	4:C:327:LYS:HB3	1.95	0.41
7:F:180:LYS:HG3	7:F:181:TYR:HD1	1.85	0.41
10:I:191:ILE:HG23	10:I:198:LYS:HB2	2.01	0.41
22:V:30:ASP:HB2	22:V:31:ASN:H	1.70	0.41
44:5:1999:A:H61	82:s:40:MET:CB	2.33	0.41
44:5:2098:G:C5	44:5:2099:C:C2	3.09	0.41
61:9:1757:G:O6	61:9:1775:U:O2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:II:162:LEU:HD11	68:II:191:GLU:HG2	2.03	0.41
71:NN:133:ARG:HD2	71:NN:133:ARG:HA	1.89	0.41
7:F:110:LEU:HD13	44:5:1840:G:H1'	2.03	0.41
14:N:114:ARG:HE	14:N:137:PRO:HG3	1.86	0.41
15:O:21:ALA:HA	15:O:87:MET:HE2	2.03	0.41
31:e:4:LEU:H	31:e:121:ARG:HD2	1.86	0.41
44:5:152:U:H2'	44:5:153:G:H8	1.86	0.41
47:FF:86:LYS:HA	47:FF:89:THR:HG22	2.02	0.41
48:KK:11:ILE:HD13	48:KK:11:ILE:HA	1.98	0.41
49:MM:64:LEU:HD13	49:MM:64:LEU:HA	1.97	0.41
54:TT:76:THR:HB	54:TT:94:ARG:HB3	2.03	0.41
63:BB:68:GLU:H	63:BB:68:GLU:HG3	1.62	0.41
1:7:92:C:H2'	1:7:93:G:H8	1.85	0.41
3:B:170:LEU:H	3:B:170:LEU:HG	1.71	0.41
13:M:89:THR:HG22	13:M:91:TRP:H	1.85	0.41
17:Q:75:ARG:HH21	44:5:1456:C:H2'	1.86	0.41
20:T:159:MET:HE3	20:T:159:MET:HB3	1.94	0.41
31:e:99:ILE:H	31:e:99:ILE:HG13	1.63	0.41
34:h:54:ILE:HA	34:h:57:VAL:HG22	2.02	0.41
44:5:969:C:N4	44:5:2095:A:N6	2.62	0.41
44:5:1509:C:H2'	44:5:1510:G:H8	1.85	0.41
44:5:4126:C:H5''	44:5:4127:A:H5''	2.02	0.41
44:5:4920:C:O2	44:5:4921:C:C5	2.71	0.41
70:LL:75:GLY:HA3	70:LL:88:ILE:HD12	2.03	0.41
76:YY:44:LEU:HD23	76:YY:75:ILE:HD11	2.01	0.41
80:K:28:PHE:HB2	80:K:29:LEU:H	1.63	0.41
9:H:105:ILE:HD13	9:H:135:SER:HA	2.02	0.41
15:O:108:ILE:HG12	15:O:113:ASP:HB3	2.01	0.41
20:T:93:ILE:H	20:T:93:ILE:HG13	1.60	0.41
22:V:109:LYS:HE3	22:V:111:GLU:HB2	2.02	0.41
41:o:70:LEU:HD11	41:o:81:ARG:HG2	2.02	0.41
44:5:363:A:H61	44:5:376:A:H5''	1.86	0.41
44:5:1961:G:N2	44:5:2024:G:O2'	2.54	0.41
44:5:1977:C:H42	44:5:1990:A:H61	1.68	0.41
44:5:2620:G:O6	44:5:2636:U:O4	2.38	0.41
48:KK:7:ASN:HA	48:KK:38:LYS:HZ3	1.85	0.41
50:PP:127:LYS:HA	50:PP:127:LYS:HD2	1.89	0.41
55:UU:52:GLY:HA3	61:9:1401:A:H4'	2.02	0.41
57:cc:64:GLU:HG2	57:cc:67:ARG:HH12	1.86	0.41
62:AA:128:ARG:HH22	62:AA:151:ASP:HB3	1.86	0.41
66:GG:228:ILE:HG23	66:GG:231:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:II:124:LYS:HD2	68:II:124:LYS:HA	1.94	0.41
69:JJ:18:ARG:HA	69:JJ:18:ARG:HD3	1.90	0.41
70:LL:112:HIS:HB2	70:LL:138:VAL:HG11	2.03	0.41
71:NN:116:ILE:HD12	71:NN:116:ILE:HA	1.98	0.41
10:I:53:VAL:HG22	10:I:134:VAL:HG22	2.02	0.41
12:L:16:LYS:HG2	44:5:46:U:H5''	2.02	0.41
24:X:63:LYS:HD2	45:8:134:G:H5''	2.03	0.41
31:e:21:ILE:HD12	31:e:21:ILE:HA	1.95	0.41
32:f:93:PRO:HB2	32:f:95:LYS:HG2	2.03	0.41
42:p:31:ILE:HD12	42:p:31:ILE:HA	1.93	0.41
44:5:2098:G:O4'	44:5:2098:G:P	2.79	0.41
44:5:2573:A:N6	44:5:2761:U:C2	2.89	0.41
44:5:4926:C:O2	44:5:4926:C:H3'	2.21	0.41
50:PP:50:ARG:HH21	61:9:1618:C:H4'	1.86	0.41
60:gg:298:LEU:HG	60:gg:310:TRP:HB2	2.03	0.41
61:9:1163:C:H2'	61:9:1164:G:H8	1.86	0.41
75:XX:67:ARG:HG3	75:XX:115:ILE:HG12	2.03	0.41
80:K:66:CYS:SG	80:K:83:PRO:CG	3.09	0.41
81:1:1416:C:H2'	81:1:1417:A:C8	2.56	0.41
4:C:294:LYS:HE2	4:C:294:LYS:HB3	1.89	0.40
22:V:85:ARG:HB3	44:5:2846:G:H4'	2.04	0.40
23:W:43:LYS:HA	23:W:43:LYS:HD2	1.88	0.40
44:5:1999:A:H61	82:s:40:MET:CG	2.34	0.40
44:5:2095:A:H3'	44:5:2096:G:C8	2.57	0.40
63:BB:229:MET:HE2	63:BB:229:MET:HB2	1.98	0.40
68:II:105:ASP:HA	68:II:170:LYS:HE2	2.02	0.40
71:NN:26:LEU:H	71:NN:26:LEU:HG	1.74	0.40
7:F:102:PRO:HB3	7:F:105:ARG:HH21	1.87	0.40
8:G:242:ARG:H	8:G:242:ARG:HG2	1.67	0.40
25:Y:124:LYS:HD2	25:Y:124:LYS:HA	1.89	0.40
27:a:85:GLN:HE22	44:5:508:G:H21	1.69	0.40
37:k:26:LYS:HD3	37:k:69:LEU:HD22	2.02	0.40
42:p:61:MET:HE2	42:p:61:MET:HB2	1.88	0.40
44:5:73:A:H2'	44:5:74:G:H8	1.86	0.40
44:5:436:C:H2'	44:5:437:G:H8	1.85	0.40
44:5:2095:A:C8	44:5:2095:A:H5'	2.56	0.40
44:5:2610:G:H2'	44:5:2611:A:H8	1.87	0.40
44:5:4923:C:C2'	44:5:4924:C:C6	3.03	0.40
60:gg:44:LYS:HD3	60:gg:44:LYS:HA	1.92	0.40
64:CC:89:LYS:HE2	64:CC:89:LYS:HB2	1.95	0.40
65:EE:87:MET:HG2	65:EE:123:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:EE:201:HIS:HD2	65:EE:206:ASP:HA	1.86	0.40
68:II:10:LYS:HB3	68:II:11:ARG:H	1.69	0.40
69:JJ:144:ILE:HG22	69:JJ:146:SER:H	1.85	0.40
80:K:119:GLN:HE21	80:K:119:GLN:HB2	1.71	0.40
82:s:47:LEU:HD22	82:s:51:ALA:HB3	2.03	0.40
6:E:257:ASP:O	6:E:261:LEU:CB	2.68	0.40
14:N:96:ARG:HH21	14:N:100:SER:HB2	1.86	0.40
18:R:42:ARG:HA	18:R:45:ILE:HG12	2.03	0.40
34:h:89:ARG:HD2	45:8:36:G:H3'	2.04	0.40
41:o:12:CYS:HB3	41:o:15:CYS:HB2	2.03	0.40
44:5:1996:C:H5'	83:t:123:ARG:CB	2.51	0.40
44:5:2099:C:H6	44:5:2099:C:OP2	2.04	0.40
44:5:2349:A:H5''	44:5:2350:U:H5''	2.04	0.40
44:5:3911:C:H1'	44:5:4395:U:H3	1.86	0.40
44:5:4044:U:O4	44:5:4048:A:N7	2.54	0.40
44:5:4454:G:O6	44:5:4526:U:O4	2.40	0.40
44:5:4899:G:C2	44:5:4922:C:O2	2.75	0.40
44:5:4926:C:N3	44:5:4927:G:O6	2.55	0.40
60:gg:212:LYS:HE3	60:gg:212:LYS:HB2	1.91	0.40
61:9:1154:U:H6	64:CC:194:ARG:HD2	1.84	0.40
64:CC:255:LEU:HD11	73:VV:14:PRO:HD2	2.04	0.40
67:HH:91:HIS:HB2	67:HH:172:THR:HG21	2.04	0.40
76:YY:101:LYS:HA	76:YY:101:LYS:HD2	1.84	0.40
80:K:67:VAL:H	80:K:83:PRO:CD	2.30	0.40
80:K:78:LYS:C	80:K:147:LYS:HD2	2.46	0.40
7:F:80:PHE:HB3	20:T:141:VAL:HG23	2.04	0.40
21:U:48:LYS:HA	21:U:53:ALA:HA	2.04	0.40
23:W:119:LYS:HE3	23:W:119:LYS:HB3	1.98	0.40
26:Z:11:VAL:HG11	26:Z:80:LEU:HD13	2.03	0.40
35:i:76:ARG:HA	35:i:76:ARG:HD2	1.91	0.40
44:5:1996:C:O3'	82:s:44:ARG:HB3	2.22	0.40
53:SS:14:ARG:HD2	53:SS:14:ARG:HA	1.83	0.40
53:SS:18:THR:HG21	53:SS:33:ILE:HA	2.03	0.40
57:cc:13:ARG:HA	57:cc:55:VAL:HA	2.04	0.40
62:AA:36:GLN:HE21	62:AA:36:GLN:HB3	1.77	0.40
62:AA:52:LYS:HA	62:AA:52:LYS:HD2	1.90	0.40
67:HH:20:GLU:HG2	67:HH:48:ALA:HB3	2.03	0.40
68:II:76:THR:HG22	68:II:105:ASP:HB2	2.03	0.40
69:JJ:77:LEU:H	69:JJ:77:LEU:HG	1.74	0.40
74:WW:23:ARG:HG3	78:bb:4:ALA:HB2	2.03	0.40
4:C:159:GLU:HA	4:C:217:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:1494:U:H2'	44:5:1495:G:C8	2.57	0.40
44:5:2098:G:C5	44:5:2099:C:N3	2.90	0.40
52:RR:35:CYS:HA	52:RR:38:ILE:HG12	2.03	0.40
52:RR:80:ARG:C	52:RR:82:ASP:H	2.28	0.40
61:9:934:G:C6	61:9:1008:A:N1	2.90	0.40
61:9:1010:G:H2'	61:9:1011:A:H8	1.87	0.40
61:9:1854:U:H2'	61:9:1855:G:H8	1.87	0.40
69:JJ:81:LEU:HD12	69:JJ:81:LEU:HA	1.95	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	
2	A	246/248 (99%)	226 (92%)	20 (8%)	0	100	100
3	B	392/394 (100%)	370 (94%)	22 (6%)	0	100	100
4	C	360/362 (99%)	343 (95%)	17 (5%)	0	100	100
5	D	291/293 (99%)	276 (95%)	14 (5%)	1 (0%)	36	67
6	E	208/251 (83%)	197 (95%)	11 (5%)	0	100	100
7	F	223/225 (99%)	210 (94%)	12 (5%)	1 (0%)	30	62
8	G	226/240 (94%)	212 (94%)	14 (6%)	0	100	100
9	H	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
10	I	200/213 (94%)	184 (92%)	16 (8%)	0	100	100
11	J	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
12	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
13	M	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
14	N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
16	P	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
17	Q	185/187 (99%)	178 (96%)	7 (4%)	0	100	100
18	R	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
19	S	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	21	54
20	T	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
21	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
22	V	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
23	W	102/106 (96%)	95 (93%)	7 (7%)	0	100	100
24	X	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
25	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
26	Z	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	16	49
27	a	145/147 (99%)	131 (90%)	14 (10%)	0	100	100
28	b	99/104 (95%)	94 (95%)	4 (4%)	1 (1%)	12	44
29	c	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
30	d	105/107 (98%)	97 (92%)	7 (7%)	1 (1%)	12	44
31	e	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
32	f	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	47
33	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
34	h	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
35	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
36	j	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
37	k	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
38	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
39	m	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
40	n	23/25 (92%)	23 (100%)	0	0	100	100
41	o	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
42	p	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
43	r	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
46	DD	211/213 (99%)	205 (97%)	4 (2%)	2 (1%)	14	47
47	FF	181/191 (95%)	169 (93%)	11 (6%)	1 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	KK	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
49	MM	92/117 (79%)	84 (91%)	8 (9%)	0	100	100
50	PP	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
51	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
52	RR	120/132 (91%)	98 (82%)	15 (12%)	7 (6%)	1	13
53	SS	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
54	TT	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
55	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
56	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
57	cc	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
58	dd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
59	ff	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
60	gg	311/313 (99%)	281 (90%)	30 (10%)	0	100	100
62	AA	200/202 (99%)	185 (92%)	15 (8%)	0	100	100
63	BB	202/213 (95%)	193 (96%)	9 (4%)	0	100	100
64	CC	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
65	EE	260/262 (99%)	237 (91%)	23 (9%)	0	100	100
66	GG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
67	HH	181/189 (96%)	173 (96%)	8 (4%)	0	100	100
68	II	204/206 (99%)	187 (92%)	17 (8%)	0	100	100
69	JJ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
70	LL	139/151 (92%)	129 (93%)	10 (7%)	0	100	100
71	NN	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
72	OO	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
73	VV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
74	WW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
75	XX	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
76	YY	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
77	aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
78	bb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
79	ee	55/57 (96%)	52 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	K	210/212 (99%)	168 (80%)	32 (15%)	10 (5%)	2	16
82	s	21/196 (11%)	18 (86%)	3 (14%)	0	100	100
83	t	34/153 (22%)	30 (88%)	3 (9%)	1 (3%)	3	26
All	All	11381/11962 (95%)	10661 (94%)	692 (6%)	28 (0%)	44	74

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	d	96	GLU
46	DD	93	THR
52	RR	83	ASN
52	RR	86	PRO
52	RR	87	GLU
52	RR	89	SER
80	K	73	HIS
80	K	76	GLU
80	K	79	ALA
80	K	80	VAL
80	K	83	PRO
47	FF	43	GLU
52	RR	82	ASP
80	K	84	HIS
26	Z	90	PRO
52	RR	85	VAL
80	K	81	ASP
80	K	115	SER
80	K	174	MET
5	D	125	VAL
83	t	124	GLU
19	S	166	ARG
28	b	29	TYR
46	DD	44	THR
52	RR	84	TYR
80	K	71	GLN
7	F	196	VAL
32	f	106	TYR

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	
2	A	190/190 (100%)	172 (90%)	18 (10%)	8	31
3	B	342/342 (100%)	308 (90%)	34 (10%)	7	29
4	C	302/302 (100%)	272 (90%)	30 (10%)	7	29
5	D	247/247 (100%)	237 (96%)	10 (4%)	28	54
6	E	190/223 (85%)	171 (90%)	19 (10%)	7	28
7	F	196/196 (100%)	179 (91%)	17 (9%)	9	33
8	G	199/205 (97%)	181 (91%)	18 (9%)	9	32
9	H	169/169 (100%)	158 (94%)	11 (6%)	15	42
10	I	175/180 (97%)	161 (92%)	14 (8%)	11	35
11	J	143/143 (100%)	131 (92%)	12 (8%)	10	34
12	L	175/175 (100%)	161 (92%)	14 (8%)	11	35
13	M	117/117 (100%)	105 (90%)	12 (10%)	7	28
14	N	171/171 (100%)	164 (96%)	7 (4%)	27	53
15	O	171/171 (100%)	160 (94%)	11 (6%)	16	42
16	P	134/134 (100%)	128 (96%)	6 (4%)	24	50
17	Q	164/164 (100%)	146 (89%)	18 (11%)	6	26
18	R	159/159 (100%)	144 (91%)	15 (9%)	8	31
19	S	157/157 (100%)	141 (90%)	16 (10%)	7	28
20	T	139/139 (100%)	119 (86%)	20 (14%)	3	18
21	U	89/89 (100%)	86 (97%)	3 (3%)	32	57
22	V	106/106 (100%)	89 (84%)	17 (16%)	2	14
23	W	86/86 (100%)	80 (93%)	6 (7%)	14	39
24	X	106/106 (100%)	101 (95%)	5 (5%)	23	49
25	Y	124/124 (100%)	114 (92%)	10 (8%)	11	35
26	Z	117/117 (100%)	107 (92%)	10 (8%)	10	34
27	a	119/119 (100%)	104 (87%)	15 (13%)	4	21
28	b	83/84 (99%)	75 (90%)	8 (10%)	8	30
29	c	84/84 (100%)	75 (89%)	9 (11%)	6	27
30	d	98/98 (100%)	86 (88%)	12 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	e	114/114 (100%)	107 (94%)	7 (6%)	17	43
32	f	88/88 (100%)	78 (89%)	10 (11%)	5	24
33	g	98/98 (100%)	85 (87%)	13 (13%)	4	20
34	h	109/109 (100%)	104 (95%)	5 (5%)	24	50
35	i	86/86 (100%)	76 (88%)	10 (12%)	5	24
36	j	73/73 (100%)	67 (92%)	6 (8%)	10	34
37	k	64/64 (100%)	61 (95%)	3 (5%)	23	49
38	l	47/47 (100%)	41 (87%)	6 (13%)	4	21
39	m	48/48 (100%)	47 (98%)	1 (2%)	47	66
40	n	24/24 (100%)	20 (83%)	4 (17%)	2	13
41	o	92/92 (100%)	82 (89%)	10 (11%)	6	26
42	p	74/74 (100%)	70 (95%)	4 (5%)	20	46
43	r	108/108 (100%)	102 (94%)	6 (6%)	19	46
46	DD	176/176 (100%)	162 (92%)	14 (8%)	11	35
47	FF	158/161 (98%)	147 (93%)	11 (7%)	14	39
48	KK	87/87 (100%)	84 (97%)	3 (3%)	32	57
49	MM	83/99 (84%)	73 (88%)	10 (12%)	5	23
50	PP	115/115 (100%)	102 (89%)	13 (11%)	5	25
51	QQ	117/117 (100%)	107 (92%)	10 (8%)	10	34
52	RR	111/119 (93%)	96 (86%)	15 (14%)	4	20
53	SS	125/125 (100%)	121 (97%)	4 (3%)	34	59
54	TT	111/111 (100%)	99 (89%)	12 (11%)	6	26
55	UU	92/92 (100%)	84 (91%)	8 (9%)	9	33
56	ZZ	66/66 (100%)	61 (92%)	5 (8%)	12	37
57	cc	55/55 (100%)	48 (87%)	7 (13%)	4	21
58	dd	48/48 (100%)	44 (92%)	4 (8%)	10	34
59	ff	61/61 (100%)	59 (97%)	2 (3%)	33	58
60	gg	272/272 (100%)	246 (90%)	26 (10%)	8	30
62	AA	168/169 (99%)	148 (88%)	20 (12%)	5	23
63	BB	189/194 (97%)	179 (95%)	10 (5%)	20	47
64	CC	187/187 (100%)	170 (91%)	17 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	EE	224/224 (100%)	206 (92%)	18 (8%)	11	35
66	GG	207/207 (100%)	192 (93%)	15 (7%)	13	38
67	HH	165/169 (98%)	150 (91%)	15 (9%)	9	32
68	II	178/178 (100%)	162 (91%)	16 (9%)	9	32
69	JJ	161/161 (100%)	153 (95%)	8 (5%)	22	48
70	LL	130/136 (96%)	109 (84%)	21 (16%)	2	14
71	NN	130/130 (100%)	122 (94%)	8 (6%)	16	43
72	OO	106/106 (100%)	99 (93%)	7 (7%)	15	41
73	VV	67/67 (100%)	62 (92%)	5 (8%)	12	37
74	WW	112/112 (100%)	104 (93%)	8 (7%)	13	38
75	XX	113/113 (100%)	103 (91%)	10 (9%)	9	32
76	YY	107/107 (100%)	100 (94%)	7 (6%)	15	42
77	aa	88/88 (100%)	79 (90%)	9 (10%)	7	28
78	bb	75/75 (100%)	67 (89%)	8 (11%)	6	27
79	ee	47/47 (100%)	45 (96%)	2 (4%)	26	51
80	K	190/191 (100%)	149 (78%)	41 (22%)	1	6
82	s	19/164 (12%)	15 (79%)	4 (21%)	1	6
83	t	30/126 (24%)	23 (77%)	7 (23%)	1	5
All	All	9947/10277 (97%)	9065 (91%)	882 (9%)	11	32

All (882) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	GLN
2	A	90	CYS
2	A	101	VAL
2	A	117	GLU
2	A	126	LEU
2	A	162	ASN
2	A	165	VAL
2	A	166	VAL
2	A	176	ASP
2	A	180	LEU
2	A	188	LYS
2	A	198	ARG
2	A	199	VAL

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Mol	Chain	Res	Type
2	A	219	ILE
2	A	225	ILE
2	A	228	ASP
2	A	235	VAL
2	A	246	LEU
3	B	39	LYS
3	B	41	VAL
3	B	43	LEU
3	B	57	VAL
3	B	67	VAL
3	B	73	VAL
3	B	90	VAL
3	B	93	VAL
3	B	101	THR
3	B	128	LYS
3	B	153	MET
3	B	162	VAL
3	B	170	LEU
3	B	199	GLU
3	B	205	VAL
3	B	207	VAL
3	B	232	THR
3	B	240	LEU
3	B	248	LEU
3	B	251	VAL
3	B	262	VAL
3	B	280	ILE
3	B	284	ILE
3	B	287	ILE
3	B	293	ILE
3	B	321	VAL
3	B	332	MET
3	B	333	LEU
3	B	338	VAL
3	B	344	VAL
3	B	346	THR
3	B	352	LEU
3	B	382	VAL
3	B	392	LEU
4	C	10	VAL
4	C	23	THR
4	C	27	VAL

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Mol	Chain	Res	Type
4	C	33	ARG
4	C	35	ASP
4	C	57	LEU
4	C	62	THR
4	C	79	VAL
4	C	89	GLN
4	C	95	MET
4	C	101	MET
4	C	115	VAL
4	C	136	LEU
4	C	142	HIS
4	C	144	ILE
4	C	147	VAL
4	C	150	LEU
4	C	153	VAL
4	C	168	VAL
4	C	180	ILE
4	C	227	ILE
4	C	229	LEU
4	C	232	VAL
4	C	289	LEU
4	C	302	LEU
4	C	312	ARG
4	C	313	VAL
4	C	319	LEU
4	C	335	MET
4	C	340	ILE
5	D	72	ASP
5	D	75	VAL
5	D	92	LEU
5	D	104	LEU
5	D	118	ILE
5	D	123	VAL
5	D	143	THR
5	D	146	LEU
5	D	189	GLU
5	D	252	VAL
6	E	53	VAL
6	E	112	LEU
6	E	115	MET
6	E	124	VAL
6	E	140	VAL

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Mol	Chain	Res	Type
6	E	155	ILE
6	E	157	THR
6	E	165	VAL
6	E	166	VAL
6	E	178	VAL
6	E	192	THR
6	E	197	VAL
6	E	200	THR
6	E	213	LYS
6	E	215	LEU
6	E	259	GLN
6	E	277	VAL
6	E	289	LEU
6	E	290	VAL
7	F	41	LEU
7	F	70	MET
7	F	73	MET
7	F	82	VAL
7	F	87	LYS
7	F	94	ILE
7	F	110	LEU
7	F	116	ILE
7	F	120	THR
7	F	146	LEU
7	F	153	ILE
7	F	186	MET
7	F	189	LEU
7	F	219	MET
7	F	231	ASP
7	F	235	ARG
7	F	239	ILE
8	G	84	LEU
8	G	105	THR
8	G	107	PHE
8	G	108	VAL
8	G	122	ILE
8	G	123	LEU
8	G	139	VAL
8	G	151	LEU
8	G	159	THR
8	G	200	VAL
8	G	207	LEU

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Mol	Chain	Res	Type
8	G	217	ILE
8	G	220	VAL
8	G	224	PRO
8	G	254	THR
8	G	258	THR
8	G	272	VAL
8	G	275	ILE
9	H	4	ILE
9	H	18	ILE
9	H	25	VAL
9	H	27	VAL
9	H	48	LEU
9	H	57	VAL
9	H	104	VAL
9	H	126	VAL
9	H	137	SER
9	H	146	LEU
9	H	151	ILE
10	I	31	ILE
10	I	35	ASP
10	I	59	GLN
10	I	62	SER
10	I	77	VAL
10	I	83	ASP
10	I	91	LEU
10	I	115	MET
10	I	126	VAL
10	I	164	LYS
10	I	187	GLU
10	I	191	ILE
10	I	200	ILE
10	I	212	LEU
11	J	15	LEU
11	J	29	SER
11	J	40	LEU
11	J	43	LEU
11	J	68	ILE
11	J	70	VAL
11	J	73	THR
11	J	74	VAL
11	J	101	ASP
11	J	128	LEU

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Mol	Chain	Res	Type
11	J	143	ASP
11	J	175	LEU
12	L	9	ILE
12	L	22	VAL
12	L	46	ILE
12	L	63	THR
12	L	64	VAL
12	L	90	VAL
12	L	107	THR
12	L	110	LEU
12	L	124	LEU
12	L	154	VAL
12	L	160	VAL
12	L	182	LEU
12	L	184	MET
12	L	204	GLU
13	M	2	VAL
13	M	25	VAL
13	M	38	VAL
13	M	43	THR
13	M	50	MET
13	M	54	CYS
13	M	56	GLN
13	M	59	ASP
13	M	61	ILE
13	M	78	GLU
13	M	112	VAL
13	M	127	VAL
14	N	32	GLN
14	N	60	VAL
14	N	89	VAL
14	N	155	VAL
14	N	161	MET
14	N	174	LEU
14	N	200	LEU
15	O	23	VAL
15	O	27	VAL
15	O	36	VAL
15	O	62	MET
15	O	79	ILE
15	O	108	ILE
15	O	111	PRO

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Mol	Chain	Res	Type
15	O	145	VAL
15	O	160	ARG
15	O	185	VAL
15	O	202	LEU
16	P	2	VAL
16	P	10	ASN
16	P	24	VAL
16	P	91	LEU
16	P	100	SER
16	P	146	ILE
17	Q	3	VAL
17	Q	8	ASN
17	Q	28	LEU
17	Q	29	VAL
17	Q	31	LEU
17	Q	42	THR
17	Q	66	MET
17	Q	72	LEU
17	Q	79	THR
17	Q	83	VAL
17	Q	91	ARG
17	Q	92	VAL
17	Q	95	VAL
17	Q	100	VAL
17	Q	120	ILE
17	Q	126	LEU
17	Q	147	GLU
17	Q	167	VAL
18	R	24	LEU
18	R	25	ASP
18	R	29	THR
18	R	41	ILE
18	R	51	ILE
18	R	55	VAL
18	R	57	VAL
18	R	72	LYS
18	R	78	ILE
18	R	91	GLU
18	R	93	VAL
18	R	98	ARG
18	R	106	LEU
18	R	114	LYS

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Mol	Chain	Res	Type
18	R	127	VAL
19	S	6	THR
19	S	7	LEU
19	S	17	LEU
19	S	27	LEU
19	S	32	ILE
19	S	48	VAL
19	S	61	ILE
19	S	67	VAL
19	S	75	VAL
19	S	124	ILE
19	S	126	ILE
19	S	129	VAL
19	S	150	ILE
19	S	158	VAL
19	S	168	THR
19	S	174	THR
20	T	4	THR
20	T	24	VAL
20	T	25	VAL
20	T	27	LEU
20	T	33	ILE
20	T	40	VAL
20	T	52	MET
20	T	66	ASN
20	T	72	VAL
20	T	80	VAL
20	T	89	ILE
20	T	93	ILE
20	T	96	ILE
20	T	98	HIS
20	T	106	LEU
20	T	109	VAL
20	T	141	VAL
20	T	142	ARG
20	T	143	THR
20	T	154	ILE
21	U	61	VAL
21	U	63	LEU
21	U	72	VAL
22	V	6	ARG
22	V	18	LEU

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Mol	Chain	Res	Type
22	V	22	VAL
22	V	25	VAL
22	V	27	ASN
22	V	30	ASP
22	V	41	SER
22	V	49	LEU
22	V	59	ASP
22	V	61	VAL
22	V	64	THR
22	V	82	ILE
22	V	94	VAL
22	V	96	LEU
22	V	101	ASN
22	V	105	ILE
22	V	132	ILE
23	W	3	VAL
23	W	17	HIS
23	W	19	ARG
23	W	54	LEU
23	W	63	GLN
23	W	83	THR
24	X	100	VAL
24	X	101	ASP
24	X	102	VAL
24	X	127	LEU
24	X	128	ILE
25	Y	2	LYS
25	Y	8	THR
25	Y	32	SER
25	Y	49	ILE
25	Y	55	VAL
25	Y	79	VAL
25	Y	104	VAL
25	Y	107	THR
25	Y	111	LEU
25	Y	112	ASP
26	Z	5	MET
26	Z	42	LEU
26	Z	46	ILE
26	Z	53	VAL
26	Z	54	THR
26	Z	72	VAL

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Mol	Chain	Res	Type
26	Z	74	VAL
26	Z	78	ASN
26	Z	96	VAL
26	Z	100	VAL
27	a	15	VAL
27	a	42	ARG
27	a	43	ILE
27	a	46	ASP
27	a	56	VAL
27	a	60	HIS
27	a	63	LEU
27	a	73	VAL
27	a	75	LEU
27	a	76	ASP
27	a	82	VAL
27	a	101	ILE
27	a	104	VAL
27	a	122	VAL
27	a	124	VAL
28	b	8	THR
28	b	21	ILE
28	b	35	VAL
28	b	40	LEU
28	b	42	ASN
28	b	72	ILE
28	b	89	VAL
28	b	92	LYS
29	c	12	GLU
29	c	18	LEU
29	c	28	VAL
29	c	39	ARG
29	c	50	ASN
29	c	71	VAL
29	c	81	LEU
29	c	91	VAL
29	c	94	LEU
30	d	20	VAL
30	d	26	THR
30	d	38	PHE
30	d	46	LEU
30	d	64	ILE
30	d	80	VAL

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Mol	Chain	Res	Type
30	d	86	VAL
30	d	96	GLU
30	d	105	LEU
30	d	106	VAL
30	d	107	THR
30	d	113	THR
31	e	26	ASP
31	e	29	VAL
31	e	70	LEU
31	e	84	GLU
31	e	89	LEU
31	e	99	ILE
31	e	122	VAL
32	f	23	GLU
32	f	30	ILE
32	f	31	GLU
32	f	33	VAL
32	f	43	LEU
32	f	67	THR
32	f	84	VAL
32	f	100	ARG
32	f	101	ILE
32	f	103	VAL
33	g	5	LEU
33	g	11	LEU
33	g	22	LEU
33	g	31	VAL
33	g	32	TYR
33	g	33	LEU
33	g	48	VAL
33	g	54	ARG
33	g	56	VAL
33	g	63	VAL
33	g	64	LEU
33	g	74	VAL
33	g	98	GLU
34	h	63	GLN
34	h	82	ASP
34	h	88	THR
34	h	94	ARG
34	h	102	LEU
35	i	3	LEU

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Mol	Chain	Res	Type
35	i	9	VAL
35	i	12	ASN
35	i	17	VAL
35	i	18	THR
35	i	30	ARG
35	i	34	THR
35	i	37	THR
35	i	43	MET
35	i	77	VAL
36	j	11	ARG
36	j	12	ARG
36	j	29	LEU
36	j	58	THR
36	j	64	MET
36	j	70	VAL
37	k	35	LYS
37	k	36	VAL
37	k	69	LEU
38	l	6	THR
38	l	16	LYS
38	l	27	ILE
38	l	29	MET
38	l	46	ARG
38	l	47	THR
39	m	92	THR
40	n	2	ARG
40	n	10	MET
40	n	15	ARG
40	n	22	GLN
41	o	2	VAL
41	o	4	VAL
41	o	8	ARG
41	o	10	THR
41	o	18	HIS
41	o	67	VAL
41	o	70	LEU
41	o	73	VAL
41	o	77	CYS
41	o	85	ILE
42	p	8	VAL
42	p	26	VAL
42	p	54	ILE

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Mol	Chain	Res	Type
42	p	88	GLU
43	r	10	VAL
43	r	24	THR
43	r	78	VAL
43	r	80	THR
43	r	82	ILE
43	r	96	MET
46	DD	1	MET
46	DD	25	LEU
46	DD	39	VAL
46	DD	41	VAL
46	DD	42	THR
46	DD	48	ILE
46	DD	57	ASN
46	DD	84	VAL
46	DD	115	VAL
46	DD	156	LEU
46	DD	164	VAL
46	DD	170	THR
46	DD	198	ILE
46	DD	208	VAL
47	FF	14	THR
47	FF	41	VAL
47	FF	43	GLU
47	FF	56	TYR
47	FF	71	ARG
47	FF	72	LEU
47	FF	77	MET
47	FF	154	LEU
47	FF	160	GLU
47	FF	166	ILE
47	FF	198	ARG
48	KK	20	VAL
48	KK	40	VAL
48	KK	90	VAL
49	MM	16	THR
49	MM	33	ARG
49	MM	51	VAL
49	MM	60	MET
49	MM	64	LEU
49	MM	77	ILE
49	MM	79	VAL

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Mol	Chain	Res	Type
49	MM	85	LEU
49	MM	103	VAL
49	MM	104	VAL
50	PP	12	PHE
50	PP	22	LEU
50	PP	37	TYR
50	PP	41	GLN
50	PP	70	MET
50	PP	76	VAL
50	PP	78	THR
50	PP	94	VAL
50	PP	107	ILE
50	PP	108	LYS
50	PP	110	GLU
50	PP	121	ILE
50	PP	126	VAL
51	QQ	18	THR
51	QQ	31	LEU
51	QQ	41	MET
51	QQ	47	LEU
51	QQ	66	VAL
51	QQ	67	ASP
51	QQ	102	GLU
51	QQ	109	LYS
51	QQ	118	THR
51	QQ	119	LEU
52	RR	9	VAL
52	RR	66	VAL
52	RR	71	ILE
52	RR	73	LEU
52	RR	75	GLU
52	RR	76	GLU
52	RR	77	GLU
52	RR	78	ARG
52	RR	80	ARG
52	RR	81	ARG
52	RR	89	SER
52	RR	114	LEU
52	RR	116	ASN
52	RR	130	THR
52	RR	132	ARG
53	SS	36	VAL

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Mol	Chain	Res	Type
53	SS	52	LEU
53	SS	73	ASN
53	SS	131	VAL
54	TT	5	THR
54	TT	9	VAL
54	TT	15	VAL
54	TT	34	VAL
54	TT	36	THR
54	TT	44	GLU
54	TT	78	ILE
54	TT	87	VAL
54	TT	88	MET
54	TT	90	SER
54	TT	104	LEU
54	TT	110	LEU
55	UU	29	VAL
55	UU	48	LEU
55	UU	50	VAL
55	UU	58	THR
55	UU	68	THR
55	UU	76	THR
55	UU	84	ILE
55	UU	104	ILE
56	ZZ	44	LEU
56	ZZ	102	LYS
56	ZZ	104	ARG
56	ZZ	107	VAL
56	ZZ	110	THR
57	cc	14	VAL
57	cc	15	THR
57	cc	17	VAL
57	cc	28	THR
57	cc	32	VAL
57	cc	38	THR
57	cc	55	VAL
58	dd	25	SER
58	dd	31	ILE
58	dd	53	ILE
58	dd	54	LYS
59	ff	102	VAL
59	ff	108	VAL
60	gg	3	GLU

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Mol	Chain	Res	Type
60	gg	40	ILE
60	gg	59	LEU
60	gg	63	SER
60	gg	64	HIS
60	gg	70	VAL
60	gg	79	LEU
60	gg	102	VAL
60	gg	135	LEU
60	gg	142	VAL
60	gg	143	GLN
60	gg	165	ILE
60	gg	185	LYS
60	gg	187	ASN
60	gg	197	THR
60	gg	198	VAL
60	gg	200	VAL
60	gg	234	ASP
60	gg	235	ILE
60	gg	249	CYS
60	gg	258	ILE
60	gg	261	LEU
60	gg	266	ILE
60	gg	274	VAL
60	gg	285	GLN
60	gg	298	LEU
62	AA	5	LEU
62	AA	7	VAL
62	AA	8	LEU
62	AA	12	GLU
62	AA	15	VAL
62	AA	23	THR
62	AA	29	ASN
62	AA	39	TYR
62	AA	42	LYS
62	AA	47	TYR
62	AA	65	ILE
62	AA	87	VAL
62	AA	112	ILE
62	AA	123	VAL
62	AA	140	VAL
62	AA	147	LEU
62	AA	159	ILE

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Mol	Chain	Res	Type
62	AA	163	CYS
62	AA	169	HIS
62	AA	188	THR
63	BB	22	VAL
63	BB	47	THR
63	BB	48	LEU
63	BB	68	GLU
63	BB	77	ASP
63	BB	106	THR
63	BB	127	VAL
63	BB	140	VAL
63	BB	150	ILE
63	BB	188	LEU
64	CC	72	ASP
64	CC	106	VAL
64	CC	137	VAL
64	CC	141	VAL
64	CC	147	VAL
64	CC	160	LEU
64	CC	174	ILE
64	CC	184	VAL
64	CC	187	ARG
64	CC	190	SER
64	CC	192	LEU
64	CC	221	ASP
64	CC	224	THR
64	CC	233	LEU
64	CC	255	LEU
64	CC	260	VAL
64	CC	270	THR
65	EE	12	VAL
65	EE	19	MET
65	EE	23	LEU
65	EE	33	THR
65	EE	44	LEU
65	EE	66	MET
65	EE	72	ILE
65	EE	101	LEU
65	EE	102	ILE
65	EE	105	THR
65	EE	111	VAL
65	EE	123	LEU

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Mol	Chain	Res	Type
65	EE	157	ASN
65	EE	159	THR
65	EE	207	VAL
65	EE	220	THR
65	EE	227	VAL
65	EE	238	LEU
66	GG	26	THR
66	GG	50	VAL
66	GG	52	ILE
66	GG	67	VAL
66	GG	89	THR
66	GG	97	VAL
66	GG	101	ILE
66	GG	105	ASN
66	GG	111	LEU
66	GG	113	ILE
66	GG	126	ASP
66	GG	151	ASP
66	GG	153	VAL
66	GG	157	VAL
66	GG	178	ARG
67	HH	8	ILE
67	HH	27	LEU
67	HH	36	LEU
67	HH	45	ILE
67	HH	46	THR
67	HH	61	ILE
67	HH	64	VAL
67	HH	72	PHE
67	HH	75	ILE
67	HH	92	VAL
67	HH	100	ILE
67	HH	103	LYS
67	HH	121	THR
67	HH	134	VAL
67	HH	166	VAL
68	II	3	ILE
68	II	4	SER
68	II	22	HIS
68	II	36	THR
68	II	64	ASN
68	II	73	THR

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Mol	Chain	Res	Type
68	II	76	THR
68	II	82	VAL
68	II	86	SER
68	II	107	THR
68	II	121	LEU
68	II	132	GLU
68	II	137	LEU
68	II	148	LYS
68	II	190	LEU
68	II	199	LEU
69	JJ	29	LEU
69	JJ	60	LEU
69	JJ	69	ARG
69	JJ	77	LEU
69	JJ	82	VAL
69	JJ	110	LEU
69	JJ	119	LEU
69	JJ	123	ILE
70	LL	6	THR
70	LL	23	VAL
70	LL	42	LEU
70	LL	46	THR
70	LL	56	ILE
70	LL	66	VAL
70	LL	72	ILE
70	LL	73	LEU
70	LL	76	VAL
70	LL	80	MET
70	LL	83	GLN
70	LL	87	VAL
70	LL	93	LEU
70	LL	101	ARG
70	LL	108	ASN
70	LL	119	ASP
70	LL	120	VAL
70	LL	125	ILE
70	LL	127	THR
70	LL	134	LEU
70	LL	146	THR
71	NN	24	THR
71	NN	26	LEU
71	NN	66	VAL

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Mol	Chain	Res	Type
71	NN	70	LYS
71	NN	75	LEU
71	NN	83	ASP
71	NN	84	LEU
71	NN	134	VAL
72	OO	21	VAL
72	OO	47	LEU
72	OO	56	VAL
72	OO	67	ASP
72	OO	116	LEU
72	OO	119	LEU
72	OO	135	ILE
73	VV	11	LEU
73	VV	42	VAL
73	VV	43	THR
73	VV	52	THR
73	VV	66	ASP
74	WW	7	LEU
74	WW	25	VAL
74	WW	28	ARG
74	WW	74	VAL
74	WW	93	LEU
74	WW	105	THR
74	WW	110	ILE
74	WW	115	GLU
75	XX	7	LEU
75	XX	32	LEU
75	XX	34	THR
75	XX	55	VAL
75	XX	81	ILE
75	XX	95	GLU
75	XX	105	PHE
75	XX	112	VAL
75	XX	125	VAL
75	XX	131	LEU
76	YY	17	LEU
76	YY	28	LEU
76	YY	57	VAL
76	YY	69	THR
76	YY	102	THR
76	YY	120	THR
76	YY	122	LYS

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Mol	Chain	Res	Type
77	aa	18	VAL
77	aa	30	VAL
77	aa	41	ILE
77	aa	46	GLU
77	aa	60	ASP
77	aa	63	VAL
77	aa	67	LEU
77	aa	69	VAL
77	aa	77	CYS
78	bb	9	HIS
78	bb	11	SER
78	bb	46	VAL
78	bb	51	GLN
78	bb	57	VAL
78	bb	62	VAL
78	bb	72	ARG
78	bb	74	THR
79	ee	102	THR
79	ee	116	VAL
80	K	7	ARG
80	K	14	VAL
80	K	18	LEU
80	K	29	LEU
80	K	32	VAL
80	K	36	ILE
80	K	45	LYS
80	K	53	VAL
80	K	55	LEU
80	K	67	VAL
80	K	68	LEU
80	K	73	HIS
80	K	76	GLU
80	K	78	LYS
80	K	80	VAL
80	K	82	ILE
80	K	87	ILE
80	K	90	LEU
80	K	91	LYS
80	K	97	LYS
80	K	99	LEU
80	K	103	LEU
80	K	111	LEU

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Mol	Chain	Res	Type
80	K	119	GLN
80	K	120	ILE
80	K	123	ILE
80	K	124	LEU
80	K	128	LEU
80	K	145	VAL
80	K	148	VAL
80	K	155	ILE
80	K	161	LYS
80	K	163	LEU
80	K	167	VAL
80	K	169	VAL
80	K	171	HIS
80	K	172	VAL
80	K	201	VAL
80	K	204	LEU
80	K	206	ILE
80	K	216	LEU
82	s	35	VAL
82	s	38	LYS
82	s	44	ARG
82	s	50	LYS
83	t	108	GLU
83	t	119	ARG
83	t	123	ARG
83	t	129	ILE
83	t	130	LYS
83	t	132	ILE
83	t	137	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	100	ASN
2	A	132	ASN
2	A	218	HIS
3	B	3	HIS
3	B	11	HIS
3	B	55	HIS
3	B	138	GLN
3	B	186	ASN
3	B	236	HIS

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Mol	Chain	Res	Type
3	B	301	ASN
3	B	354	GLN
4	C	50	GLN
4	C	60	HIS
4	C	187	GLN
4	C	236	ASN
4	C	317	ASN
4	C	329	ASN
4	C	343	GLN
4	C	347	HIS
5	D	9	ASN
5	D	131	ASN
5	D	202	GLN
5	D	230	ASN
5	D	282	GLN
6	E	131	HIS
6	E	170	GLN
6	E	194	GLN
7	F	55	HIS
7	F	79	ASN
7	F	118	ASN
7	F	234	ASN
7	F	240	ASN
8	G	91	ASN
8	G	119	GLN
8	G	134	ASN
8	G	153	HIS
8	G	161	GLN
8	G	259	GLN
8	G	278	ASN
9	H	15	ASN
9	H	39	ASN
9	H	98	HIS
9	H	106	GLN
9	H	140	GLN
9	H	156	ASN
9	H	188	GLN
10	I	59	GLN
10	I	95	HIS
10	I	100	ASN
10	I	147	HIS
13	M	34	ASN

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Mol	Chain	Res	Type
13	M	70	GLN
13	M	125	ASN
14	N	15	GLN
14	N	145	ASN
14	N	199	GLN
15	O	14	HIS
15	O	26	GLN
15	O	42	ASN
15	O	50	ASN
15	O	65	ASN
16	P	56	GLN
16	P	64	ASN
16	P	75	GLN
16	P	97	ASN
16	P	116	HIS
16	P	118	GLN
16	P	120	ASN
17	Q	57	ASN
18	R	58	HIS
19	S	50	GLN
19	S	77	ASN
19	S	108	GLN
19	S	117	HIS
20	T	3	ASN
20	T	69	GLN
20	T	95	HIS
21	U	44	GLN
21	U	50	ASN
22	V	27	ASN
22	V	107	ASN
23	W	48	GLN
23	W	59	HIS
24	X	94	ASN
24	X	105	ASN
24	X	107	HIS
24	X	111	GLN
25	Y	56	GLN
25	Y	96	HIS
27	a	17	HIS
27	a	39	HIS
27	a	60	HIS
27	a	120	GLN

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Mol	Chain	Res	Type
28	b	7	HIS
28	b	10	HIS
28	b	42	ASN
28	b	50	ASN
28	b	60	ASN
28	b	101	HIS
29	c	50	ASN
29	c	51	ASN
30	d	79	ASN
31	e	23	HIS
31	e	80	HIS
31	e	81	ASN
31	e	101	HIS
31	e	102	ASN
33	g	114	GLN
34	h	65	GLN
34	h	98	HIS
34	h	107	GLN
35	i	15	HIS
35	i	36	HIS
38	l	4	HIS
38	l	17	GLN
38	l	19	GLN
39	m	83	ASN
39	m	94	ASN
41	o	36	GLN
41	o	45	GLN
41	o	90	HIS
41	o	102	GLN
43	r	6	GLN
43	r	12	ASN
43	r	21	ASN
43	r	31	ASN
43	r	100	ASN
46	DD	56	GLN
46	DD	145	GLN
46	DD	179	GLN
46	DD	207	HIS
47	FF	137	GLN
47	FF	149	GLN
48	KK	42	ASN
48	KK	61	GLN

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Mol	Chain	Res	Type
48	KK	84	HIS
49	MM	15	ASN
49	MM	73	GLN
49	MM	82	ASN
50	PP	53	GLN
50	PP	98	ASN
50	PP	104	GLN
51	QQ	35	ASN
51	QQ	142	GLN
52	RR	31	ASN
52	RR	116	ASN
54	TT	10	ASN
54	TT	11	GLN
54	TT	12	GLN
54	TT	51	ASN
54	TT	83	GLN
54	TT	105	GLN
54	TT	117	GLN
56	ZZ	64	ASN
57	cc	7	GLN
58	dd	3	HIS
58	dd	16	GLN
58	dd	37	ASN
59	ff	91	ASN
60	gg	20	GLN
60	gg	117	ASN
60	gg	119	GLN
60	gg	133	ASN
60	gg	187	ASN
60	gg	285	GLN
60	gg	305	ASN
62	AA	36	GLN
62	AA	113	GLN
62	AA	169	HIS
63	BB	124	HIS
63	BB	163	GLN
63	BB	177	GLN
63	BB	179	ASN
63	BB	202	GLN
64	CC	113	GLN
64	CC	120	GLN
64	CC	172	ASN

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Mol	Chain	Res	Type
64	CC	272	HIS
65	EE	8	HIS
65	EE	36	HIS
65	EE	67	GLN
65	EE	112	HIS
65	EE	161	GLN
65	EE	201	HIS
65	EE	209	HIS
65	EE	260	GLN
66	GG	56	ASN
66	GG	81	HIS
66	GG	186	GLN
66	GG	197	GLN
67	HH	97	GLN
67	HH	165	ASN
68	II	35	ASN
68	II	146	GLN
69	JJ	140	GLN
69	JJ	154	GLN
69	JJ	156	HIS
71	NN	49	GLN
72	OO	26	ASN
72	OO	83	GLN
72	OO	94	HIS
73	VV	35	ASN
73	VV	47	ASN
74	WW	16	ASN
74	WW	64	ASN
74	WW	92	ASN
75	XX	39	ASN
75	XX	92	ASN
75	XX	97	ASN
76	YY	19	GLN
76	YY	22	GLN
76	YY	63	HIS
76	YY	85	ASN
77	aa	8	ASN
77	aa	17	HIS
78	bb	29	ASN
78	bb	49	HIS
78	bb	51	GLN
79	ee	95	GLN

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Mol	Chain	Res	Type
79	ee	110	GLN
79	ee	131	ASN
80	K	119	GLN
80	K	129	ASN
80	K	199	GLN
83	t	118	HIS
83	t	137	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	7	118/119 (99%)	11 (9%)	0
44	5	3580/3603 (99%)	872 (24%)	60 (1%)
45	8	149/156 (95%)	33 (22%)	1 (0%)
61	9	1684/1696 (99%)	380 (22%)	16 (0%)
81	1	164/165 (99%)	101 (61%)	10 (6%)
All	All	5695/5739 (99%)	1397 (24%)	87 (1%)

All (1397) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	7	3	C
1	7	11	A
1	7	22	A
1	7	53	U
1	7	54	A
1	7	63	C
1	7	64	G
1	7	97	G
1	7	100	A
1	7	102	U
1	7	110	G
44	5	11	G
44	5	12	A
44	5	13	U
44	5	15	A
44	5	17	A
44	5	25	A
44	5	35	U
44	5	39	A
44	5	42	A

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Mol	Chain	Res	Type
44	5	43	U
44	5	47	A
44	5	48	G
44	5	49	U
44	5	56	A
44	5	59	A
44	5	64	A
44	5	65	A
44	5	67	C
44	5	73	A
44	5	76	A
44	5	84	A
44	5	88	A
44	5	91	G
44	5	92	C
44	5	93	G
44	5	104	G
44	5	108	A
44	5	109	G
44	5	110	C
44	5	118	C
44	5	119	G
44	5	120	A
44	5	126	C
44	5	134	G
44	5	135	G
44	5	136	C
44	5	137	G
44	5	151	G
44	5	157	U
44	5	159	C
44	5	160	G
44	5	171	U
44	5	172	C
44	5	173	C
44	5	195	C
44	5	197	A
44	5	200	U
44	5	201	C
44	5	209	U
44	5	216	C
44	5	218	A

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Mol	Chain	Res	Type
44	5	220	C
44	5	224	U
44	5	227	A
44	5	232	G
44	5	233	U
44	5	234	G
44	5	241	G
44	5	246	G
44	5	262	C
44	5	264	C
44	5	265	C
44	5	266	C
44	5	276	C
44	5	278	G
44	5	280	G
44	5	292	G
44	5	296	A
44	5	297	U
44	5	302	C
44	5	306	A
44	5	309	C
44	5	310	G
44	5	315	G
44	5	316	U
44	5	322	C
44	5	334	A
44	5	340	C
44	5	345	C
44	5	355	A
44	5	357	U
44	5	360	A
44	5	363	A
44	5	365	U
44	5	381	U
44	5	386	A
44	5	387	G
44	5	399	G
44	5	407	A
44	5	410	A
44	5	412	G
44	5	413	G
44	5	431	G

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Mol	Chain	Res	Type
44	5	432	U
44	5	440	U
44	5	446	C
44	5	449	C
44	5	450	G
44	5	452	A
44	5	453	G
44	5	454	U
44	5	464	G
44	5	467	U
44	5	468	U
44	5	469	C
44	5	481	G
44	5	481(A)	C
44	5	482	G
44	5	483	G
44	5	484	U
44	5	485	C
44	5	486	C
44	5	492	U
44	5	493	G
44	5	495	C
44	5	497	G
44	5	498	C
44	5	499	G
44	5	505	G
44	5	506	C
44	5	510	U
44	5	641	G
44	5	648	G
44	5	658	C
44	5	666	G
44	5	667	A
44	5	683	C
44	5	685	C
44	5	686	A
44	5	687	U
44	5	696	C
44	5	697	G
44	5	704	C
44	5	705	G
44	5	708	G

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Mol	Chain	Res	Type
44	5	718	C
44	5	719	C
44	5	727	C
44	5	729	G
44	5	730	G
44	5	731	G
44	5	738	C
44	5	738(A)	C
44	5	739	G
44	5	745	G
44	5	747	A
44	5	748	G
44	5	749	G
44	5	751	G
44	5	758	G
44	5	908	G
44	5	913	U
44	5	914	U
44	5	915	A
44	5	917	A
44	5	918	G
44	5	923	C
44	5	925	C
44	5	926	G
44	5	929	A
44	5	930	G
44	5	931	C
44	5	932	A
44	5	933	G
44	5	934	C
44	5	935	A
44	5	935(A)	G
44	5	936	C
44	5	939	G
44	5	941	C
44	5	943	A
44	5	944	A
44	5	945	U
44	5	958	G
44	5	959	G
44	5	960	A
44	5	961	G

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Mol	Chain	Res	Type
44	5	962	C
44	5	966	A
44	5	967	C
44	5	968	C
44	5	969	C
44	5	972	C
44	5	979	C
44	5	983	C
44	5	1070	G
44	5	1072	C
44	5	1073	G
44	5	1076	C
44	5	1088	C
44	5	1179	U
44	5	1187	G
44	5	1195	G
44	5	1210	C
44	5	1211	G
44	5	1212	G
44	5	1214	C
44	5	1215	C
44	5	1234	G
44	5	1235	G
44	5	1236	C
44	5	1237	C
44	5	1238	A
44	5	1239	C
44	5	1272	C
44	5	1273	G
44	5	1276	C
44	5	1277	G
44	5	1281	G
44	5	1284	G
44	5	1287	G
44	5	1288	G
44	5	1292	C
44	5	1293	G
44	5	1295	C
44	5	1296	G
44	5	1301	C
44	5	1303	A
44	5	1304	C

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Mol	Chain	Res	Type
44	5	1314	C
44	5	1326	A
44	5	1330	A
44	5	1354	A
44	5	1358	G
44	5	1359	G
44	5	1370	G
44	5	1371	A
44	5	1377	G
44	5	1379	C
44	5	1380	G
44	5	1387	A
44	5	1394	G
44	5	1397	A
44	5	1398	A
44	5	1419	G
44	5	1420	A
44	5	1421	G
44	5	1426	G
44	5	1436	C
44	5	1437	C
44	5	1438	U
44	5	1440	U
44	5	1441	C
44	5	1445	U
44	5	1446	C
44	5	1448	G
44	5	1456	C
44	5	1457	G
44	5	1458	C
44	5	1465	G
44	5	1477	C
44	5	1478	C
44	5	1482	G
44	5	1483	C
44	5	1484	G
44	5	1497	A
44	5	1498	G
44	5	1501	C
44	5	1502	G
44	5	1514	U
44	5	1516	G

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Mol	Chain	Res	Type
44	5	1518	A
44	5	1523	A
44	5	1534	A
44	5	1543	G
44	5	1547	A
44	5	1563	A
44	5	1566	C
44	5	1574	G
44	5	1578	U
44	5	1591	U
44	5	1596	U
44	5	1597	G
44	5	1602	U
44	5	1607	C
44	5	1612	G
44	5	1613	A
44	5	1624	G
44	5	1625	G
44	5	1631	A
44	5	1633	G
44	5	1634	A
44	5	1637	A
44	5	1638	A
44	5	1641	G
44	5	1649	U
44	5	1650	A
44	5	1654	G
44	5	1661	C
44	5	1676	C
44	5	1679	A
44	5	1724	G
44	5	1731	C
44	5	1733	G
44	5	1734	G
44	5	1740	C
44	5	1741	G
44	5	1742	A
44	5	1750	G
44	5	1751	A
44	5	1752	G
44	5	1754	U
44	5	1755	C

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Mol	Chain	Res	Type
44	5	1756	U
44	5	1757	U
44	5	1761	G
44	5	1764	G
44	5	1768	C
44	5	1769	G
44	5	1772	C
44	5	1773	U
44	5	1776	A
44	5	1777	C
44	5	1781	U
44	5	1787	A
44	5	1797	G
44	5	1803	G
44	5	1804	A
44	5	1805	A
44	5	1806	G
44	5	1815	G
44	5	1819	G
44	5	1821	G
44	5	1822	U
44	5	1828	C
44	5	1830	G
44	5	1834	U
44	5	1835	G
44	5	1836	G
44	5	1837	A
44	5	1842	G
44	5	1855	G
44	5	1869	G
44	5	1888	A
44	5	1890	G
44	5	1897	A
44	5	1898	C
44	5	1899	G
44	5	1910	G
44	5	1915	C
44	5	1916	G
44	5	1917	A
44	5	1918	U
44	5	1920	C
44	5	1921	C

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Mol	Chain	Res	Type
44	5	1922	G
44	5	1923	A
44	5	1930	U
44	5	1931	C
44	5	1933	G
44	5	1945	G
44	5	1948	G
44	5	1958	A
44	5	1959	U
44	5	1961	G
44	5	1962	A
44	5	1963	C
44	5	1969	G
44	5	1974	U
44	5	1976	G
44	5	1977	C
44	5	1978	C
44	5	1979	A
44	5	1980	U
44	5	1981	G
44	5	1982	G
44	5	1984	A
44	5	1985	G
44	5	1986	U
44	5	1987	C
44	5	1991	A
44	5	1992	U
44	5	1997	U
44	5	2001	G
44	5	2002	A
44	5	2003	G
44	5	2004	U
44	5	2008	U
44	5	2011	C
44	5	2024	G
44	5	2025	A
44	5	2026	A
44	5	2042	A
44	5	2044	U
44	5	2046	G
44	5	2047	A
44	5	2048	U

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Mol	Chain	Res	Type
44	5	2052	G
44	5	2055	G
44	5	2056	G
44	5	2062	C
44	5	2063	G
44	5	2064	G
44	5	2069	A
44	5	2070	C
44	5	2084	C
44	5	2085	G
44	5	2088	A
44	5	2089	G
44	5	2090	U
44	5	2091	C
44	5	2092	G
44	5	2093	A
44	5	2094	C
44	5	2095	A
44	5	2096	G
44	5	2097	U
44	5	2098	G
44	5	2099	C
44	5	2100	G
44	5	2102	G
44	5	2104	A
44	5	2105	A
44	5	2106	G
44	5	2107	C
44	5	2108	G
44	5	2109	A
44	5	2259	G
44	5	2260	C
44	5	2262	G
44	5	2264	C
44	5	2266	C
44	5	2267	U
44	5	2268	A
44	5	2269	C
44	5	2270	G
44	5	2275	G
44	5	2279	A
44	5	2289	C

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Mol	Chain	Res	Type
44	5	2297	G
44	5	2300	A
44	5	2301	G
44	5	2306	G
44	5	2313	A
44	5	2316	G
44	5	2331	G
44	5	2332	A
44	5	2333	G
44	5	2345	G
44	5	2347	A
44	5	2348	G
44	5	2350	U
44	5	2351	C
44	5	2360	A
44	5	2369	U
44	5	2370	A
44	5	2382	A
44	5	2395	A
44	5	2396	A
44	5	2399	G
44	5	2402	G
44	5	2410	C
44	5	2417	A
44	5	2422	C
44	5	2425	U
44	5	2426	U
44	5	2433	G
44	5	2441	C
44	5	2450	G
44	5	2453	A
44	5	2463	G
44	5	2471	G
44	5	2475	G
44	5	2476	G
44	5	2488	C
44	5	2489	C
44	5	2490	U
44	5	2491	C
44	5	2503	G
44	5	2504	C
44	5	2505	C

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Mol	Chain	Res	Type
44	5	2506	G
44	5	2511	A
44	5	2512	A
44	5	2513	A
44	5	2515	G
44	5	2529	A
44	5	2530	U
44	5	2537	A
44	5	2546	G
44	5	2547	G
44	5	2549	G
44	5	2553	A
44	5	2554	U
44	5	2566	G
44	5	2572	C
44	5	2575	U
44	5	2583	C
44	5	2586	G
44	5	2587	A
44	5	2589	C
44	5	2600	A
44	5	2601	A
44	5	2612	G
44	5	2618	G
44	5	2620	G
44	5	2638	G
44	5	2658	G
44	5	2661	U
44	5	2662	G
44	5	2669	C
44	5	2670	C
44	5	2673	G
44	5	2675	G
44	5	2676	A
44	5	2681	G
44	5	2686	G
44	5	2687	U
44	5	2694	G
44	5	2695	A
44	5	2696	A
44	5	2708	U
44	5	2710	C

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Mol	Chain	Res	Type
44	5	2711	G
44	5	2712	G
44	5	2714	G
44	5	2715	G
44	5	2716	C
44	5	2721	G
44	5	2724	G
44	5	2725	A
44	5	2726	G
44	5	2739	C
44	5	2740	U
44	5	2743	A
44	5	2753	G
44	5	2754	G
44	5	2759	G
44	5	2760	G
44	5	2761	U
44	5	2763	U
44	5	2764	A
44	5	2769	U
44	5	2772	C
44	5	2787	A
44	5	2788	U
44	5	2789	A
44	5	2790	U
44	5	2794	C
44	5	2795	A
44	5	2796	G
44	5	2798	A
44	5	2806	A
44	5	2807	A
44	5	2808	G
44	5	2814	C
44	5	2825	A
44	5	2826	U
44	5	2827	G
44	5	2828	U
44	5	2837	U
44	5	2842	G
44	5	2855	G
44	5	2875	C
44	5	2880	U

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Mol	Chain	Res	Type
44	5	2897	G
44	5	2898	G
44	5	3598	C
44	5	3604	A
44	5	3605	C
44	5	3606	U
44	5	3615	G
44	5	3616	U
44	5	3620	G
44	5	3625	G
44	5	3626	G
44	5	3635	A
44	5	3636	C
44	5	3638	G
44	5	3653	A
44	5	3657	U
44	5	3662	A
44	5	3664	G
44	5	3673	C
44	5	3678	G
44	5	3679	U
44	5	3680	U
44	5	3682	A
44	5	3692	A
44	5	3705	G
44	5	3711	A
44	5	3714	G
44	5	3729	U
44	5	3742	G
44	5	3747	A
44	5	3753	G
44	5	3756	A
44	5	3759	A
44	5	3760	A
44	5	3765	G
44	5	3772	U
44	5	3773	U
44	5	3774	A
44	5	3776	G
44	5	3777	G
44	5	3778	U
44	5	3784	A

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Mol	Chain	Res	Type
44	5	3786	U
44	5	3798	U
44	5	3810	C
44	5	3812	C
44	5	3814	U
44	5	3817	A
44	5	3819	G
44	5	3838	U
44	5	3839	G
44	5	3840	U
44	5	3843	C
44	5	3861	A
44	5	3876	A
44	5	3877	A
44	5	3878	C
44	5	3879	G
44	5	3882	C
44	5	3889	G
44	5	3892	U
44	5	3897	G
44	5	3901	A
44	5	3905	A
44	5	3906	A
44	5	3907	G
44	5	3908	A
44	5	3915	U
44	5	3916	G
44	5	3917	A
44	5	3918	G
44	5	3938	G
44	5	3939	G
44	5	3941	G
44	5	3944	G
44	5	3947	A
44	5	3950	U
44	5	3952	A
44	5	3954	A
44	5	3956	G
44	5	3957	U
44	5	3958	G
44	5	3960	A
44	5	3965	A

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Mol	Chain	Res	Type
44	5	3966	A
44	5	3969	G
44	5	3970	G
44	5	3971	G
44	5	3972	A
44	5	3973	G
44	5	4039	G
44	5	4040	C
44	5	4042	G
44	5	4043	G
44	5	4044	U
44	5	4045	G
44	5	4046	A
44	5	4047	A
44	5	4048	A
44	5	4049	U
44	5	4050	A
44	5	4052	C
44	5	4053	A
44	5	4054	C
44	5	4055	U
44	5	4056	A
44	5	4062	A
44	5	4063	U
44	5	4064	C
44	5	4065	G
44	5	4067	U
44	5	4071	U
44	5	4072	C
44	5	4073	A
44	5	4076	G
44	5	4085	A
44	5	4086	G
44	5	4088	C
44	5	4116	C
44	5	4117	U
44	5	4119	C
44	5	4120	U
44	5	4121	G
44	5	4127	A
44	5	4162	C
44	5	4166	G

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Mol	Chain	Res	Type
44	5	4170	A
44	5	4171	C
44	5	4183	G
44	5	4184	G
44	5	4191	G
44	5	4203	A
44	5	4212	A
44	5	4225	G
44	5	4228	G
44	5	4229	U
44	5	4233	A
44	5	4243	C
44	5	4249	G
44	5	4251	A
44	5	4253	A
44	5	4254	G
44	5	4265	U
44	5	4266	G
44	5	4268	A
44	5	4271	A
44	5	4273	A
44	5	4280	A
44	5	4281	A
44	5	4282	A
44	5	4291	G
44	5	4292	A
44	5	4297	G
44	5	4304	A
44	5	4305	G
44	5	4306	U
44	5	4313	A
44	5	4314	C
44	5	4317	A
44	5	4326	G
44	5	4330	G
44	5	4332	C
44	5	4339	A
44	5	4349	C
44	5	4350	C
44	5	4354	U
44	5	4355	G
44	5	4373	G

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Mol	Chain	Res	Type
44	5	4376	A
44	5	4377	G
44	5	4378	A
44	5	4387	C
44	5	4393	G
44	5	4394	A
44	5	4395	U
44	5	4401	G
44	5	4411	G
44	5	4413	C
44	5	4419	U
44	5	4421	C
44	5	4422	A
44	5	4436	U
44	5	4437	U
44	5	4438	U
44	5	4440	G
44	5	4444	C
44	5	4448	G
44	5	4449	A
44	5	4452	U
44	5	4453	C
44	5	4464	A
44	5	4466	C
44	5	4471	U
44	5	4472	G
44	5	4482	U
44	5	4488	A
44	5	4500	U
44	5	4511	A
44	5	4512	U
44	5	4513	A
44	5	4519	C
44	5	4520	G
44	5	4525	C
44	5	4529	G
44	5	4531	U
44	5	4548	A
44	5	4560	C
44	5	4567	G
44	5	4572	U
44	5	4573	G

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Mol	Chain	Res	Type
44	5	4575	G
44	5	4584	A
44	5	4586	G
44	5	4587	G
44	5	4590	A
44	5	4599	A
44	5	4624	A
44	5	4627	U
44	5	4629	U
44	5	4635	A
44	5	4636	U
44	5	4637	G
44	5	4639	G
44	5	4652	G
44	5	4657	U
44	5	4658	G
44	5	4670	C
44	5	4672	A
44	5	4677	U
44	5	4687	A
44	5	4691	A
44	5	4693	C
44	5	4694	G
44	5	4695	C
44	5	4700	A
44	5	4709	U
44	5	4720	C
44	5	4721	G
44	5	4736	C
44	5	4738	C
44	5	4750	G
44	5	4751	G
44	5	4752	U
44	5	4754	G
44	5	4756	C
44	5	4757	C
44	5	4759	C
44	5	4761	G
44	5	4765	G
44	5	4769	G
44	5	4771	C
44	5	4772	C

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Mol	Chain	Res	Type
44	5	4870	G
44	5	4872	G
44	5	4873	G
44	5	4874	A
44	5	4875	G
44	5	4876	U
44	5	4877	G
44	5	4879	C
44	5	4880	C
44	5	4881	U
44	5	4882	U
44	5	4883	C
44	5	4885	U
44	5	4895	C
44	5	4902	C
44	5	4910	A
44	5	4913	G
44	5	4914	C
44	5	4915	G
44	5	4919	G
44	5	4921	C
44	5	4922	C
44	5	4923	C
44	5	4924	C
44	5	4925	U
44	5	4926	C
44	5	4928	C
44	5	4931	G
44	5	4932	U
44	5	4934	A
44	5	4937	C
44	5	4943	A
44	5	4944	C
44	5	4947	U
44	5	4948	C
44	5	4949	G
44	5	4950	U
44	5	4951	G
44	5	4955	A
44	5	4956	A
44	5	4958	C
44	5	4960	G

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Mol	Chain	Res	Type
44	5	4964	C
44	5	4965	U
44	5	4966	A
44	5	4976	U
44	5	4979	A
44	5	4985	U
44	5	4988	U
44	5	4989	U
44	5	4990	C
44	5	4991	U
44	5	5006	U
44	5	5007	A
44	5	5014	A
44	5	5017	G
44	5	5022	U
44	5	5040	U
44	5	5041	G
44	5	5047	C
44	5	5050	C
44	5	5053	U
44	5	5054	C
44	5	5061	A
44	5	5062	G
45	8	2	G
45	8	23	C
45	8	34	U
45	8	35	C
45	8	38	U
45	8	39	G
45	8	51	U
45	8	59	A
45	8	60	G
45	8	61	A
45	8	62	A
45	8	63	U
45	8	71	A
45	8	75	G
45	8	77	A
45	8	79	G
45	8	87	G
45	8	94	G
45	8	95	A

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Mol	Chain	Res	Type
45	8	103	A
45	8	105	C
45	8	107	C
45	8	108	A
45	8	109	C
45	8	111	U
45	8	114	G
45	8	123	U
45	8	125	C
45	8	126	C
45	8	127	U
45	8	128	C
45	8	150	C
45	8	153	C
61	9	2	A
61	9	3	C
61	9	4	C
61	9	14	C
61	9	20	G
61	9	25	A
61	9	26	U
61	9	33	G
61	9	41	G
61	9	42	A
61	9	46	A
61	9	56	G
61	9	58	C
61	9	62	G
61	9	65	C
61	9	67	C
61	9	68	A
61	9	69	C
61	9	71	G
61	9	73	C
61	9	74	G
61	9	79	A
61	9	80	G
61	9	84	A
61	9	99	A
61	9	100	U
61	9	103	A
61	9	110	U

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Mol	Chain	Res	Type
61	9	111	A
61	9	113	G
61	9	114	G
61	9	115	U
61	9	124	U
61	9	126	G
61	9	143	U
61	9	146	G
61	9	147	A
61	9	155	G
61	9	158	A
61	9	162	C
61	9	168	C
61	9	182	C
61	9	183	G
61	9	184	G
61	9	188	C
61	9	189	U
61	9	191	A
61	9	192	C
61	9	202	G
61	9	215	G
61	9	292	A
61	9	294	U
61	9	302	A
61	9	306	C
61	9	307	G
61	9	308	G
61	9	309	G
61	9	312	G
61	9	314	U
61	9	317	C
61	9	318	A
61	9	319	C
61	9	320	G
61	9	321	C
61	9	335	G
61	9	347	G
61	9	351	G
61	9	362	C
61	9	364	A
61	9	368	U

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Mol	Chain	Res	Type
61	9	370	G
61	9	383	G
61	9	385	G
61	9	386	C
61	9	398	A
61	9	399	C
61	9	400	C
61	9	407	G
61	9	408	A
61	9	409	C
61	9	417	C
61	9	418	A
61	9	419	G
61	9	436	G
61	9	438	G
61	9	448	A
61	9	450	C
61	9	454	U
61	9	464	A
61	9	465	A
61	9	466	G
61	9	471	G
61	9	472	C
61	9	473	A
61	9	474	G
61	9	476	A
61	9	482	G
61	9	487	U
61	9	492	C
61	9	496	C
61	9	507	G
61	9	508	A
61	9	517	C
61	9	518	G
61	9	525	A
61	9	528	A
61	9	530	U
61	9	531	A
61	9	532	C
61	9	533	A
61	9	542	U
61	9	544	G

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Mol	Chain	Res	Type
61	9	547	G
61	9	548	C
61	9	549	C
61	9	550	C
61	9	551	U
61	9	554	A
61	9	555	A
61	9	556	U
61	9	557	U
61	9	559	G
61	9	560	A
61	9	562	U
61	9	568	C
61	9	571	U
61	9	574	A
61	9	576	A
61	9	583	A
61	9	585	C
61	9	588	G
61	9	589	G
61	9	590	A
61	9	591	U
61	9	592	C
61	9	600	G
61	9	606	G
61	9	608	C
61	9	614	C
61	9	627	U
61	9	628	A
61	9	629	A
61	9	643	A
61	9	644	G
61	9	660	C
61	9	662	G
61	9	668	A
61	9	669	A
61	9	670	A
61	9	671	A
61	9	672	A
61	9	673	G
61	9	679	A
61	9	687	C

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Mol	Chain	Res	Type
61	9	689	U
61	9	690	G
61	9	752	G
61	9	753	C
61	9	754	G
61	9	799	U
61	9	811	A
61	9	821	G
61	9	822	U
61	9	827	A
61	9	830	A
61	9	834	C
61	9	844	U
61	9	847	A
61	9	853	C
61	9	859	G
61	9	861	A
61	9	867	G
61	9	868	G
61	9	869	A
61	9	870	A
61	9	871	U
61	9	872	A
61	9	873	G
61	9	874	G
61	9	875	A
61	9	878	G
61	9	887	U
61	9	889	U
61	9	890	U
61	9	892	U
61	9	901	G
61	9	909	G
61	9	913	A
61	9	914	U
61	9	917	U
61	9	920	A
61	9	922	A
61	9	933	G
61	9	934	G
61	9	955	A
61	9	970	G

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Mol	Chain	Res	Type
61	9	971	G
61	9	985	G
61	9	989	C
61	9	990	A
61	9	992	A
61	9	999	G
61	9	1002	U
61	9	1016	U
61	9	1017	U
61	9	1023	A
61	9	1045	U
61	9	1062	A
61	9	1080	A
61	9	1082	A
61	9	1083	A
61	9	1085	C
61	9	1100	A
61	9	1109	C
61	9	1115	U
61	9	1116	C
61	9	1117	C
61	9	1118	C
61	9	1119	A
61	9	1121	G
61	9	1123	C
61	9	1126	G
61	9	1129	G
61	9	1133	A
61	9	1137	U
61	9	1138	C
61	9	1139	C
61	9	1148	A
61	9	1149	A
61	9	1150	A
61	9	1153	C
61	9	1154	U
61	9	1158	G
61	9	1166	G
61	9	1170	A
61	9	1172	U
61	9	1183	A
61	9	1195	A

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Mol	Chain	Res	Type
61	9	1207	G
61	9	1215	C
61	9	1221	G
61	9	1224	G
61	9	1240	A
61	9	1242	U
61	9	1243	U
61	9	1244	U
61	9	1251	A
61	9	1253	A
61	9	1254	C
61	9	1255	G
61	9	1256	G
61	9	1257	G
61	9	1259	A
61	9	1264	C
61	9	1274	G
61	9	1275	G
61	9	1280	G
61	9	1281	G
61	9	1282	A
61	9	1284	A
61	9	1285	G
61	9	1286	G
61	9	1289	U
61	9	1293	A
61	9	1295	A
61	9	1298	G
61	9	1299	A
61	9	1301	A
61	9	1302	G
61	9	1303	C
61	9	1307	U
61	9	1308	U
61	9	1309	C
61	9	1310	U
61	9	1313	A
61	9	1314	U
61	9	1315	U
61	9	1333	U
61	9	1342	U
61	9	1354	G

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Mol	Chain	Res	Type
61	9	1358	U
61	9	1362	U
61	9	1363	C
61	9	1371	U
61	9	1372	U
61	9	1378	A
61	9	1382	A
61	9	1396	A
61	9	1397	U
61	9	1402	A
61	9	1404	U
61	9	1428	G
61	9	1438	A
61	9	1442	U
61	9	1447	G
61	9	1449	G
61	9	1452	A
61	9	1454	A
61	9	1462	U
61	9	1463	U
61	9	1464	C
61	9	1466	G
61	9	1473	G
61	9	1475	G
61	9	1476	A
61	9	1477	U
61	9	1489	A
61	9	1490	G
61	9	1495	G
61	9	1498	A
61	9	1507	G
61	9	1520	G
61	9	1521	C
61	9	1533	A
61	9	1535	U
61	9	1544	C
61	9	1548	G
61	9	1551	U
61	9	1552	G
61	9	1553	C
61	9	1555	U
61	9	1556	A

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Mol	Chain	Res	Type
61	9	1557	C
61	9	1560	U
61	9	1570	G
61	9	1574	C
61	9	1575	G
61	9	1580	A
61	9	1584	G
61	9	1585	U
61	9	1587	G
61	9	1588	A
61	9	1598	G
61	9	1601	A
61	9	1604	G
61	9	1606	G
61	9	1621	U
61	9	1623	A
61	9	1637	A
61	9	1638	G
61	9	1646	C
61	9	1647	A
61	9	1648	G
61	9	1649	U
61	9	1654	G
61	9	1665	G
61	9	1676	U
61	9	1680	G
61	9	1682	C
61	9	1683	C
61	9	1698	C
61	9	1699	A
61	9	1701	C
61	9	1704	C
61	9	1705	C
61	9	1706	G
61	9	1715	A
61	9	1721	U
61	9	1722	G
61	9	1726	G
61	9	1729	U
61	9	1730	U
61	9	1744	G
61	9	1748	G

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Mol	Chain	Res	Type
61	9	1783	C
61	9	1785	C
61	9	1799	G
61	9	1823	A
61	9	1824	A
61	9	1831	A
61	9	1835	A
61	9	1836	G
61	9	1838	U
61	9	1849	G
61	9	1851	A
61	9	1861	G
61	9	1862	G
61	9	1863	A
61	9	1865	C
61	9	1869	A
81	1	1332	G
81	1	1335	U
81	1	1336	G
81	1	1337	U
81	1	1338	A
81	1	1340	A
81	1	1341	U
81	1	1342	A
81	1	1343	C
81	1	1352	U
81	1	1353	U
81	1	1354	U
81	1	1356	G
81	1	1358	A
81	1	1360	A
81	1	1361	U
81	1	1362	A
81	1	1364	U
81	1	1365	U
81	1	1366	G
81	1	1367	G
81	1	1369	A
81	1	1371	U
81	1	1372	C
81	1	1375	C
81	1	1378	A

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Mol	Chain	Res	Type
81	1	1379	U
81	1	1380	G
81	1	1381	G
81	1	1387	G
81	1	1388	A
81	1	1389	C
81	1	1390	A
81	1	1391	G
81	1	1392	G
81	1	1393	U
81	1	1398	C
81	1	1399	A
81	1	1400	U
81	1	1401	U
81	1	1402	U
81	1	1403	C
81	1	1404	A
81	1	1405	C
81	1	1407	C
81	1	1408	C
81	1	1409	C
81	1	1410	C
81	1	1412	U
81	1	1414	U
81	1	1415	U
81	1	1416	C
81	1	1421	U
81	1	1422	A
81	1	1423	C
81	1	1424	U
81	1	1426	C
81	1	1429	A
81	1	1433	U
81	1	1434	G
81	1	1435	G
81	1	1436	A
81	1	1437	C
81	1	1439	A
81	1	1445	G
81	1	1446	G
81	1	1448	U
81	1	1449	U

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Mol	Chain	Res	Type
81	1	1451	C
81	1	1452	C
81	1	1453	C
81	1	1454	A
81	1	1457	G
81	1	1458	C
81	1	1461	C
81	1	1462	C
81	1	1463	U
81	1	1464	U
81	1	1465	U
81	1	1467	G
81	1	1470	C
81	1	1471	A
81	1	1473	A
81	1	1474	G
81	1	1475	C
81	1	1476	A
81	1	1477	G
81	1	1478	C
81	1	1481	G
81	1	1482	U
81	1	1483	A
81	1	1484	U
81	1	1485	A
81	1	1486	C
81	1	1487	A
81	1	1488	G
81	1	1491	C
81	1	1492	C
81	1	1493	G
81	1	1494	C
81	1	1495	U

All (87) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	5	48	G
44	5	125	C
44	5	217	C
44	5	226	G
44	5	245	C

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Mol	Chain	Res	Type
44	5	275	C
44	5	406	C
44	5	449	C
44	5	480	C
44	5	485	C
44	5	492	U
44	5	504	G
44	5	696	C
44	5	930	G
44	5	959	G
44	5	971(A)	G
44	5	1072	C
44	5	1211	G
44	5	1236	C
44	5	1238	A
44	5	1291	G
44	5	1329	G
44	5	1370	G
44	5	1440	U
44	5	1445	U
44	5	1455	G
44	5	1477	C
44	5	1633	G
44	5	1804	A
44	5	1818	G
44	5	1921	C
44	5	1979	A
44	5	2024	G
44	5	2025	A
44	5	2046	G
44	5	2068	C
44	5	2088	A
44	5	2089	G
44	5	2095	A
44	5	2097	U
44	5	2099	C
44	5	2265	G
44	5	2266	C
44	5	2502	G
44	5	2546	G
44	5	2587	A
44	5	2661	U

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Mol	Chain	Res	Type
44	5	2695	A
44	5	3625	G
44	5	3888	G
44	5	3904	G
44	5	4170	A
44	5	4232	U
44	5	4448	G
44	5	4699	U
44	5	4719	G
44	5	4884	G
44	5	4925	U
44	5	4936	G
44	5	4947	U
45	8	124	U
61	9	24	C
61	9	110	U
61	9	465	A
61	9	532	C
61	9	553	U
61	9	555	A
61	9	561	A
61	9	688	U
61	9	752	G
61	9	870	A
61	9	872	A
61	9	1137	U
61	9	1253	A
61	9	1395	C
61	9	1664	A
61	9	1679	A
81	1	1334	U
81	1	1341	U
81	1	1379	U
81	1	1391	G
81	1	1392	G
81	1	1397	C
81	1	1408	C
81	1	1433	U
81	1	1435	G
81	1	1493	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 214 ligands modelled in this entry, 214 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
44	5	26
61	9	12
23	W	1
6	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.18
1	W	63:GLN	C	79:GLN	N	40.60
1	5	1252:C	O3'	1271:G	P	36.81
1	5	1219:G	O3'	1233:G	P	19.65

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	130:G	O3'	141:A	P	18.46
1	9	697:G	O3'	729:C	P	18.12
1	9	1761:U	O3'	1771:G	P	17.58
1	5	523:C	O3'	638:G	P	17.15
1	5	4101:C	O3'	4107:G	P	17.11
1	9	323:C	O3'	329:G	P	17.11
1	5	1406(C):G	O3'	1411:C	P	16.96
1	5	4138:C	O3'	4146:G	P	16.95
1	9	756:C	O3'	788:G	P	16.88
1	5	990:C	O3'	1064:G	P	16.65
1	9	834:C	O3'	841:G	P	16.33
1	5	3977:C	O3'	4034:G	P	16.12
1	9	1417:C	O3'	1423:C	P	15.75
1	5	4777:C	O3'	4859:C	P	15.20
1	5	1696:C	O3'	1720:C	P	15.19
1	5	760:G	O3'	904:G	P	14.98
1	5	5022:U	O3'	5028:G	P	13.60
1	5	2901:G	O3'	3597:G	P	13.43
1	5	1364:U	O3'	1368:A	P	13.16
1	5	182:G	O3'	189:G	P	12.32
1	5	4729:A	O3'	4735:G	P	10.23
1	9	225:G	O3'	287:U	P	8.39
1	5	1180:C	O3'	1183:C	P	8.02
1	5	512:U	O3'	515:C	P	7.04
1	9	736:C	O3'	743:U	P	6.18
1	E	100:GLY	C	105:GLY	N	6.15
1	5	500:G	O3'	504:G	P	5.76
1	5	1239:C	O3'	1244:G	P	5.65
1	9	745:C	O3'	749:U	P	5.42
1	9	1690:U	O3'	1692:U	P	4.83
1	5	1100:U	O3'	1168:G	P	4.61
1	5	4740:G	O3'	4743:G	P	4.38
1	5	3940:U	O3'	3941:G	P	3.39
1	5	1438:U	O3'	1440:U	P	3.34
1	9	1432:U	O3'	1438:A	P	3.33
1	5	4899:G	O3'	4902:C	P	3.32

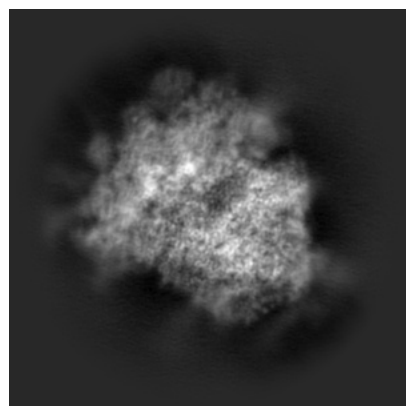
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72136. These allow visual inspection of the internal detail of the map and identification of artifacts.

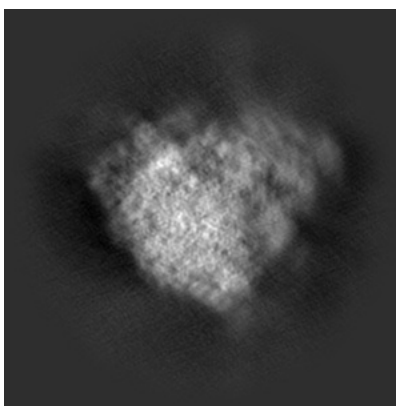
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

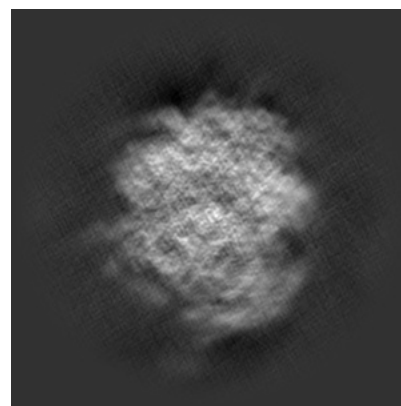
6.1.1 Primary map



X

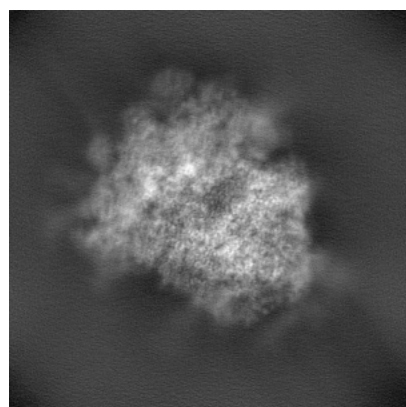


Y

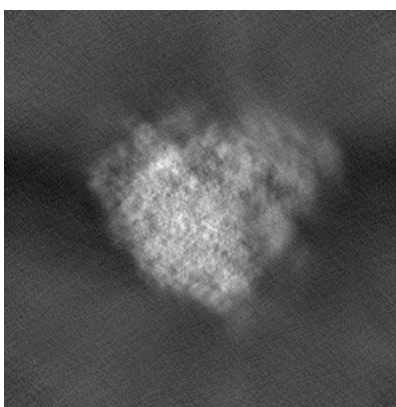


Z

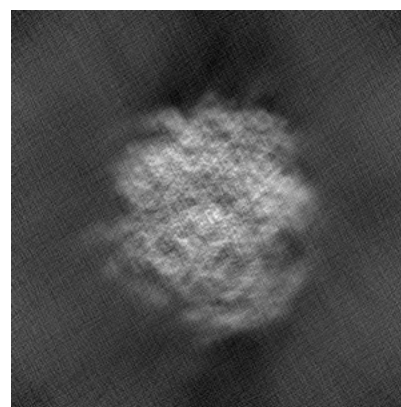
6.1.2 Raw map



X



Y

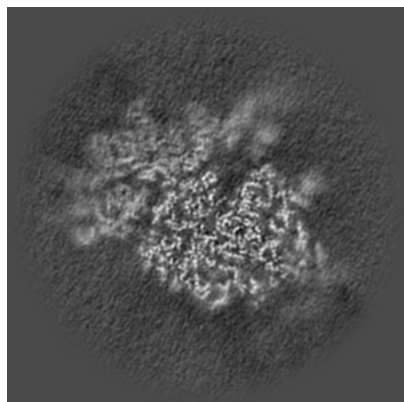


Z

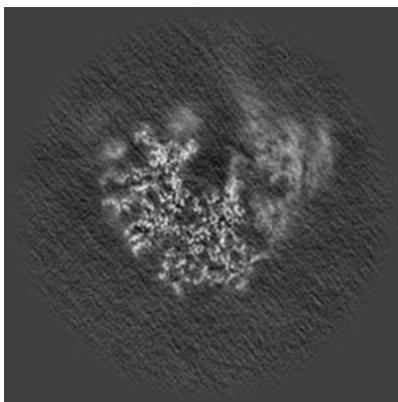
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

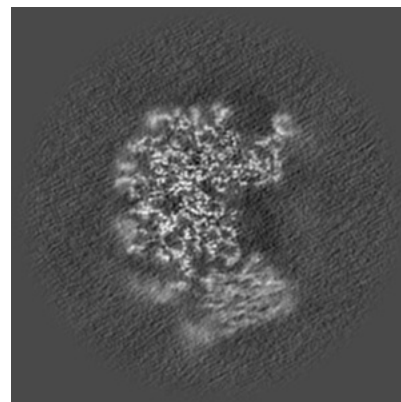
6.2.1 Primary map



X Index: 180

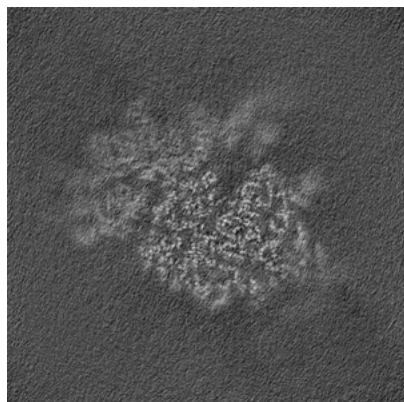


Y Index: 180

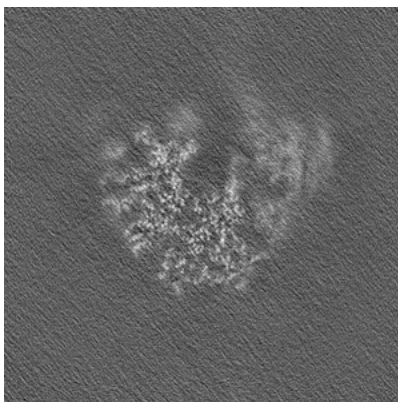


Z Index: 180

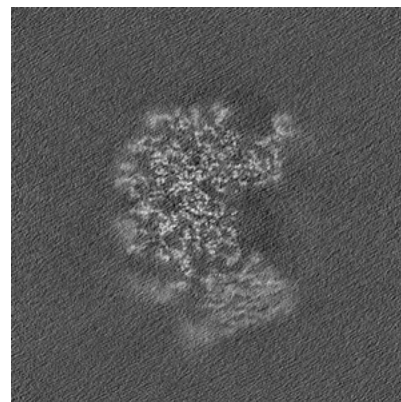
6.2.2 Raw map



X Index: 180



Y Index: 180

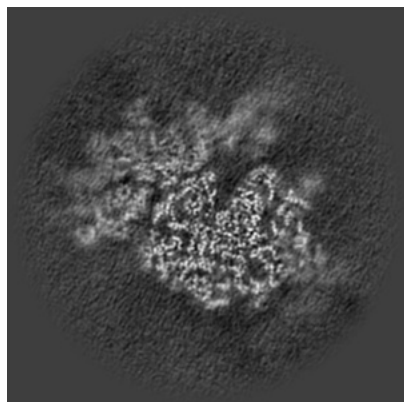


Z Index: 180

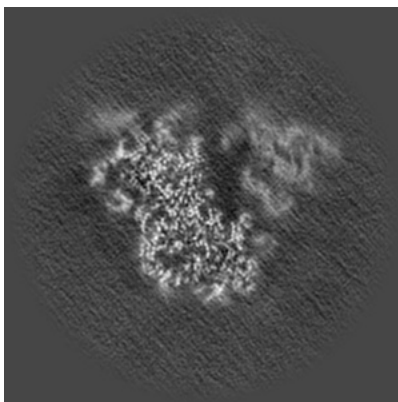
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

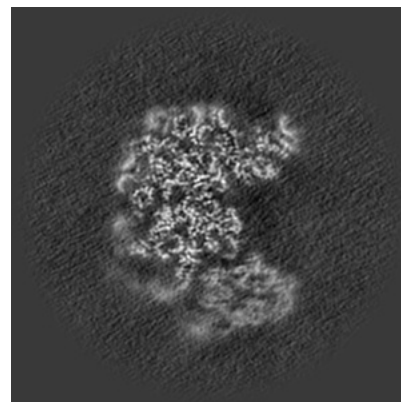
6.3.1 Primary map



X Index: 182

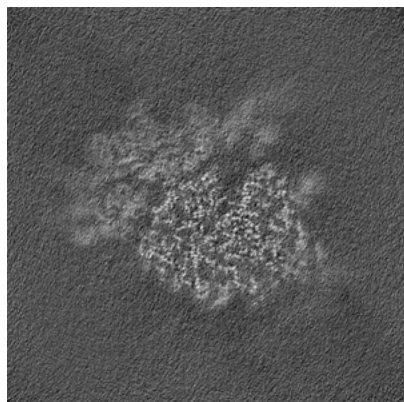


Y Index: 198

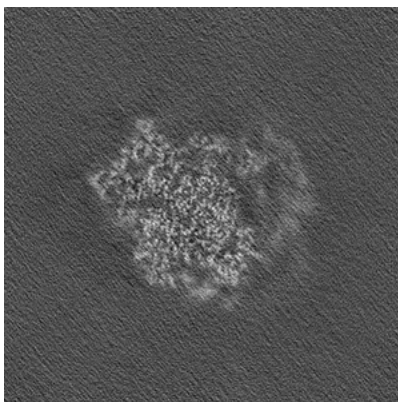


Z Index: 184

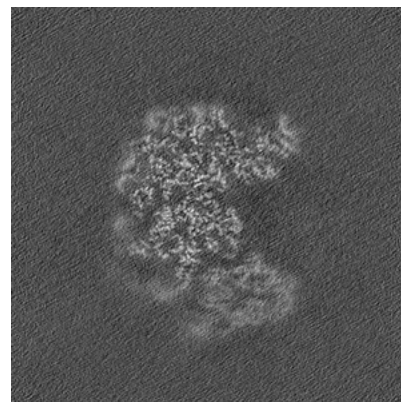
6.3.2 Raw map



X Index: 179



Y Index: 217

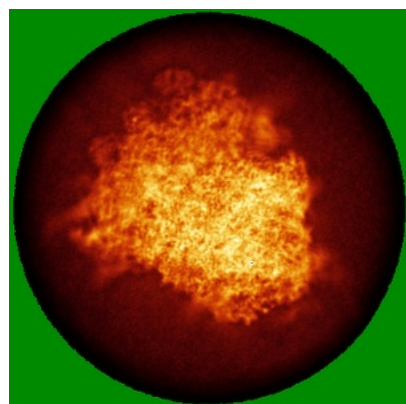


Z Index: 184

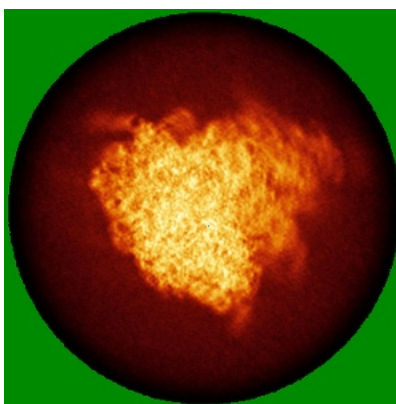
The images above show the largest variance slices of the map in three orthogonal directions.

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

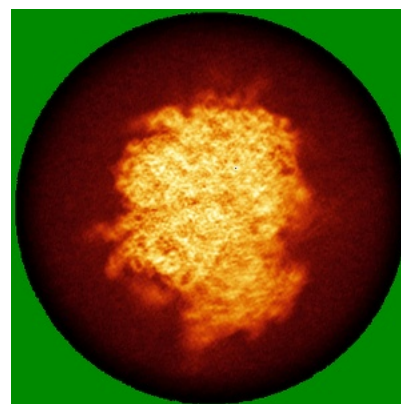
6.4.1 Primary map



X

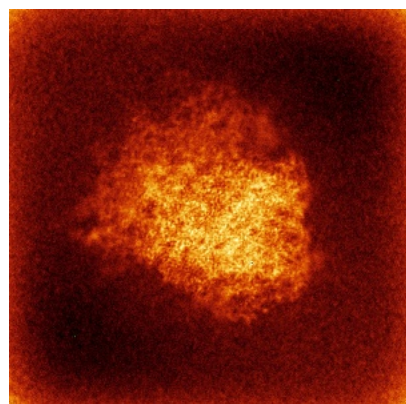


Y

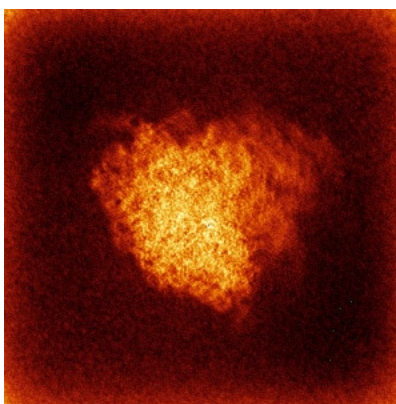


Z

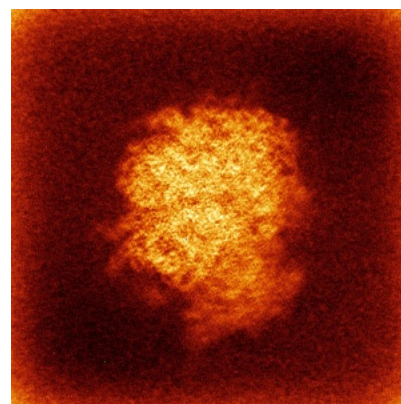
6.4.2 Raw map



X



Y

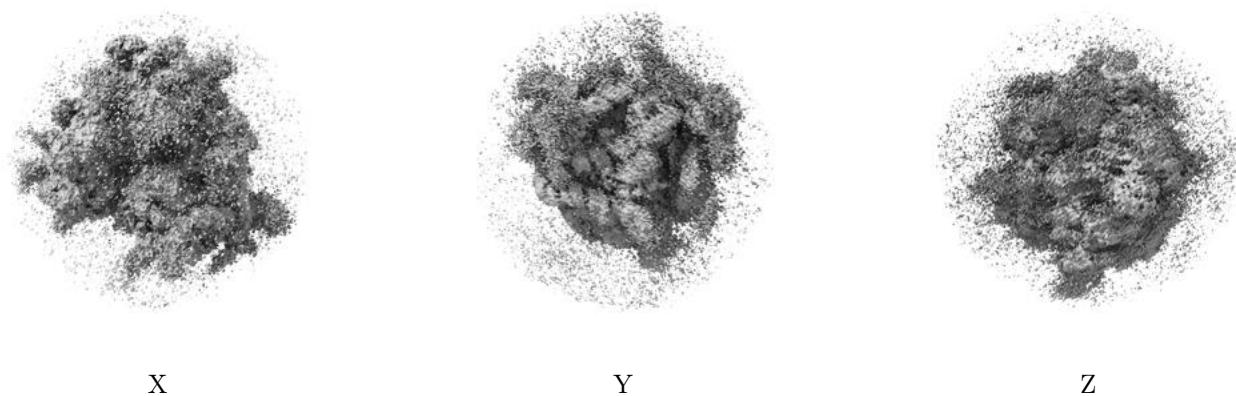


Z

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

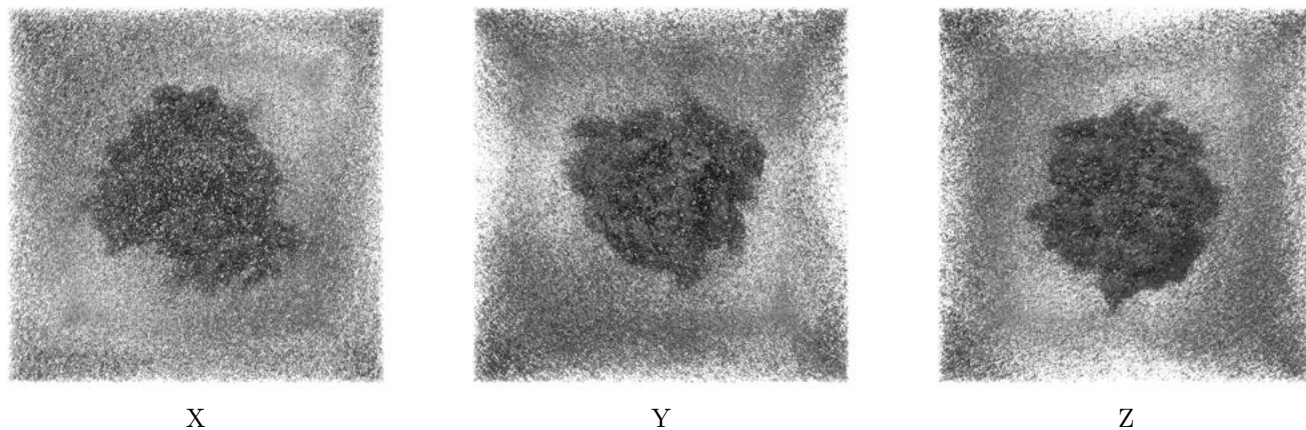
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

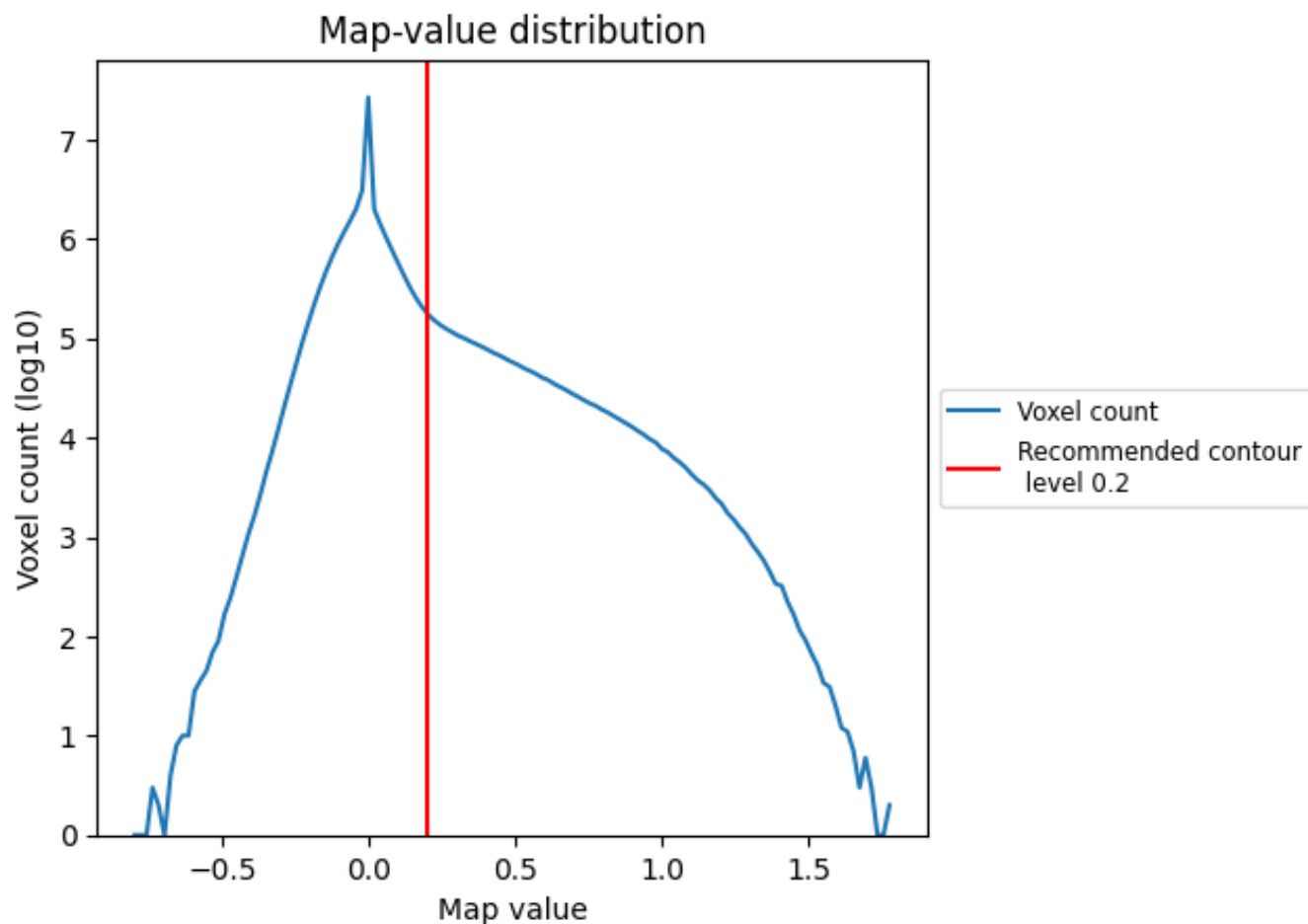
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

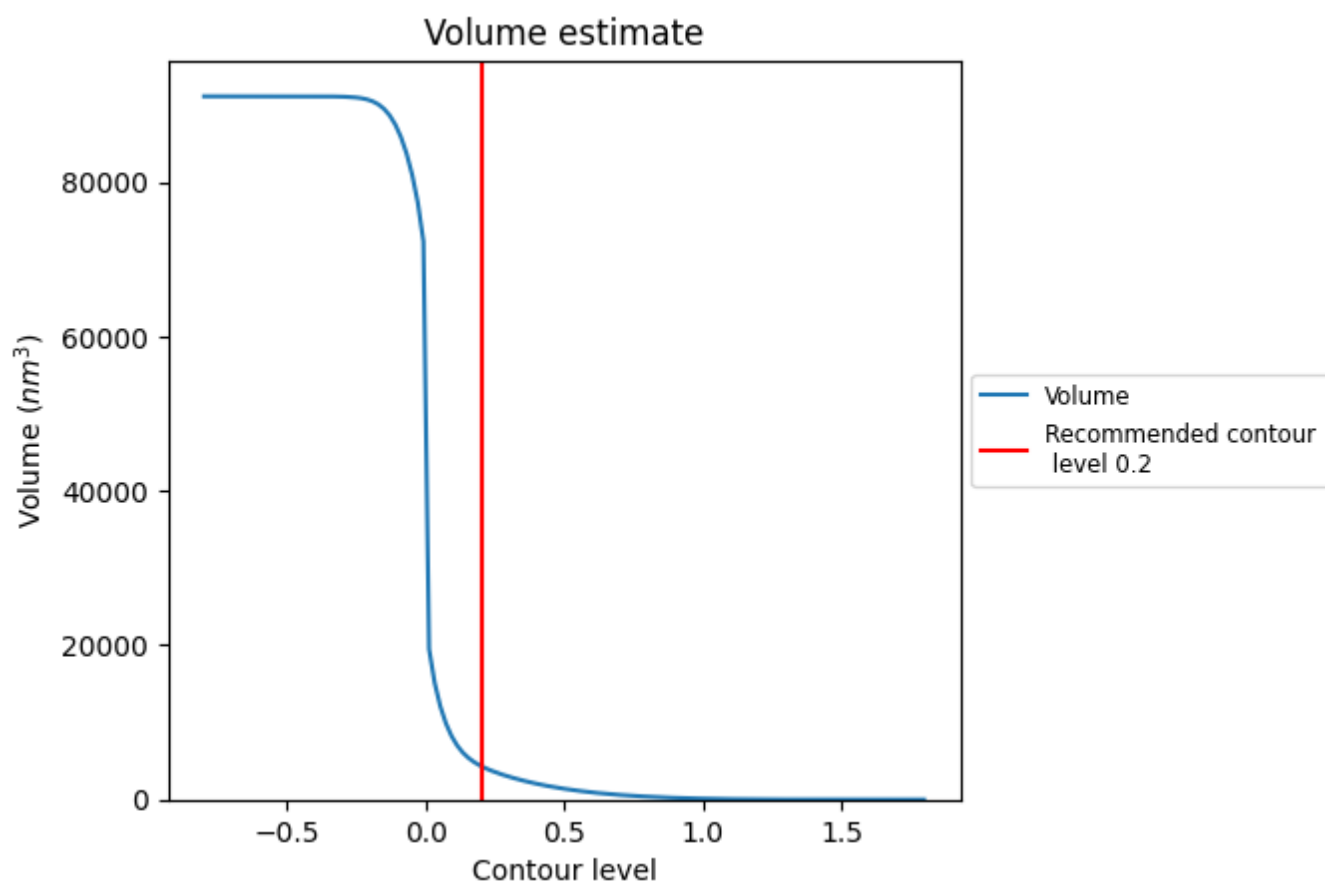
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

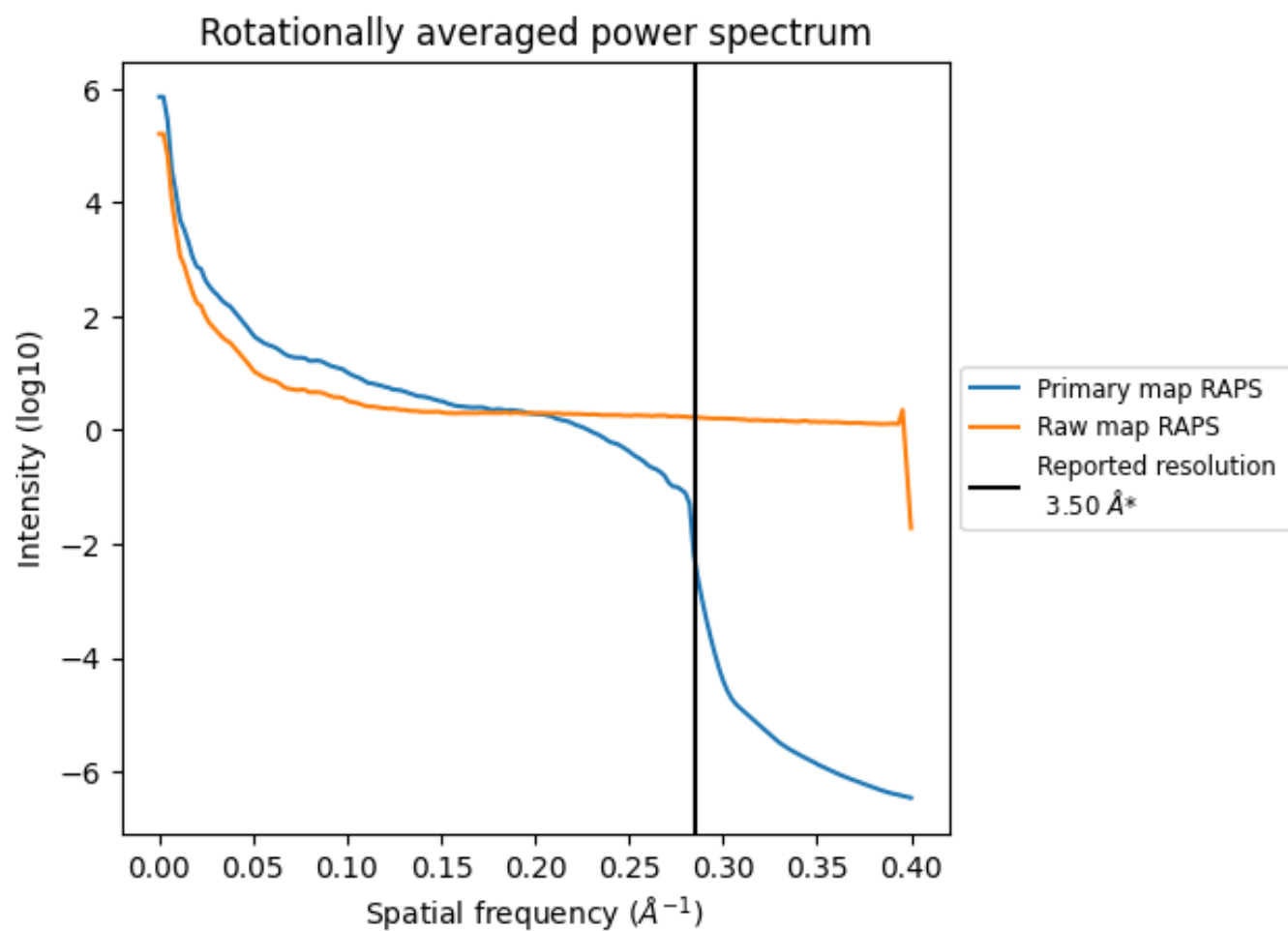
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4338 nm³; this corresponds to an approximate mass of 3918 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 ⓘ

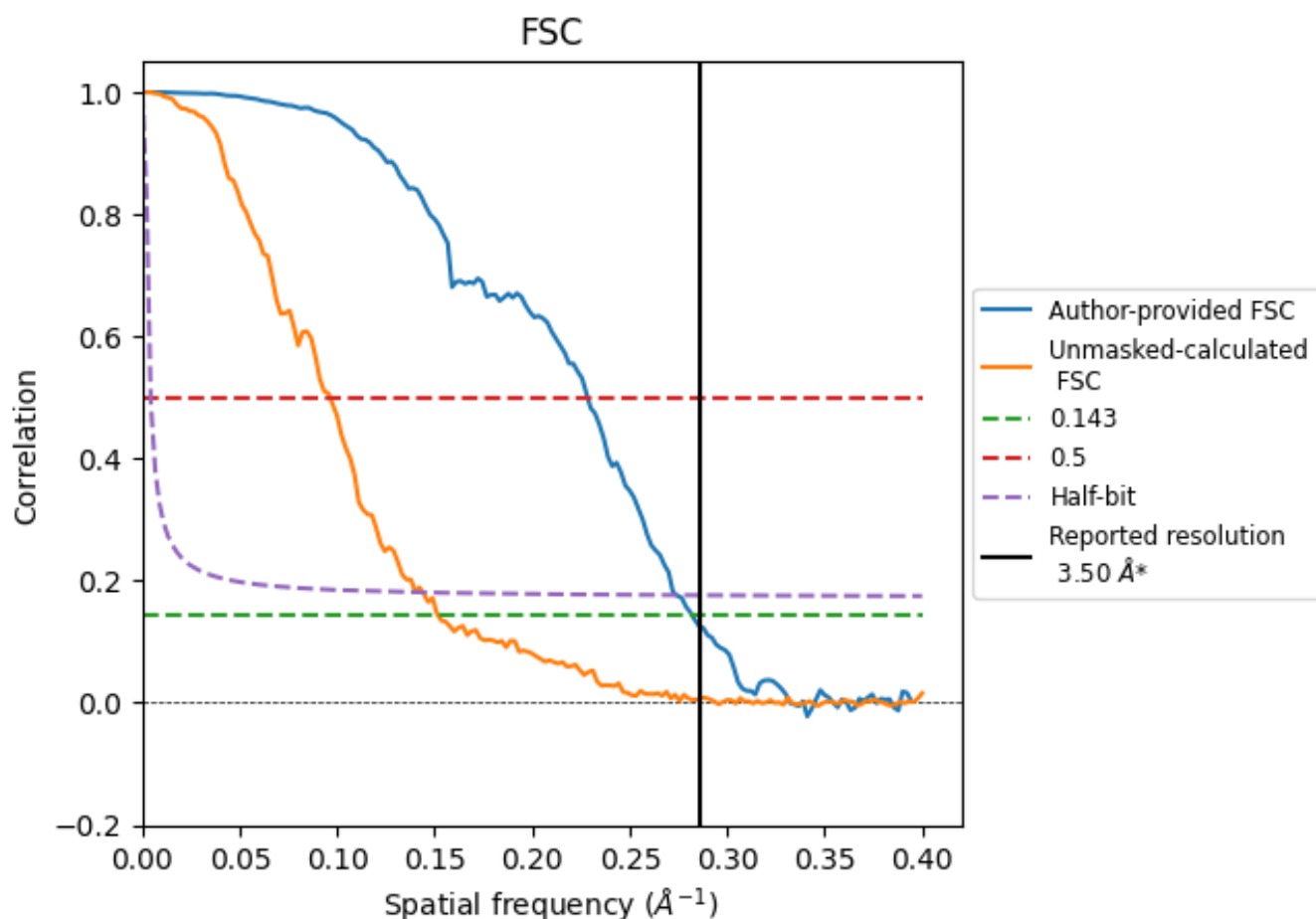


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

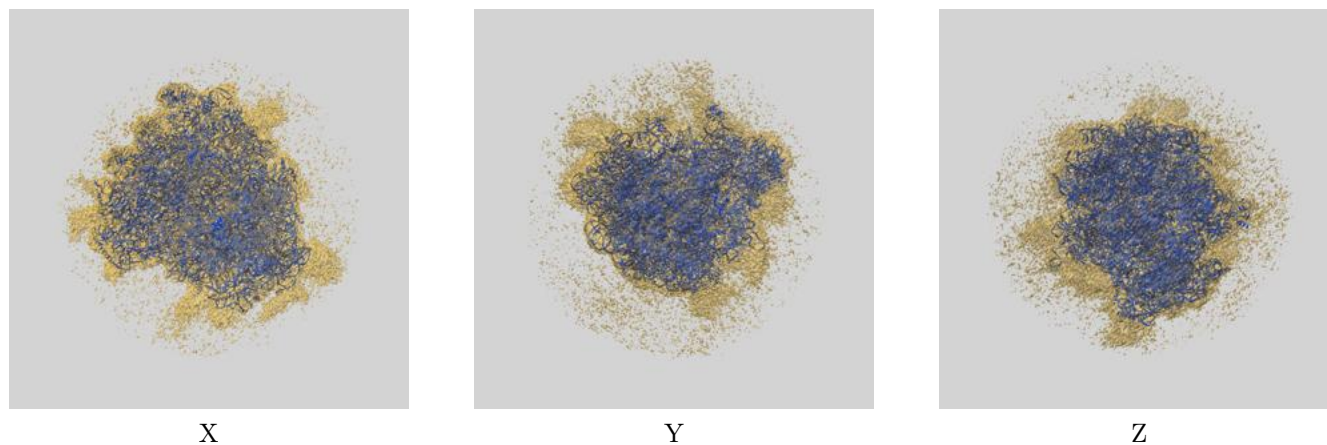
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.54	4.38	3.65
Unmasked-calculated*	6.59	10.38	6.94

*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 6.59 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

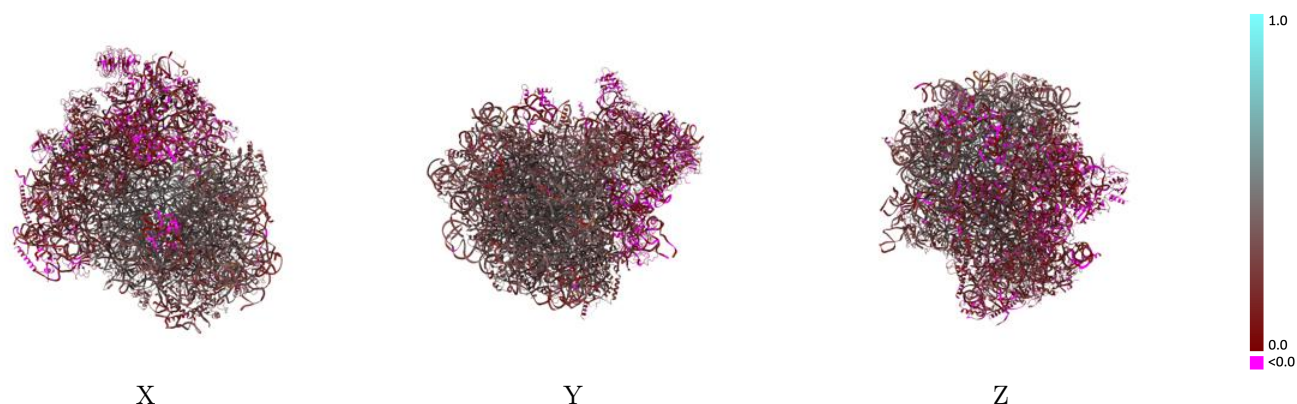
This section contains information regarding the fit between EMDB map EMD-72136 and PDB model 9Q1Q. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



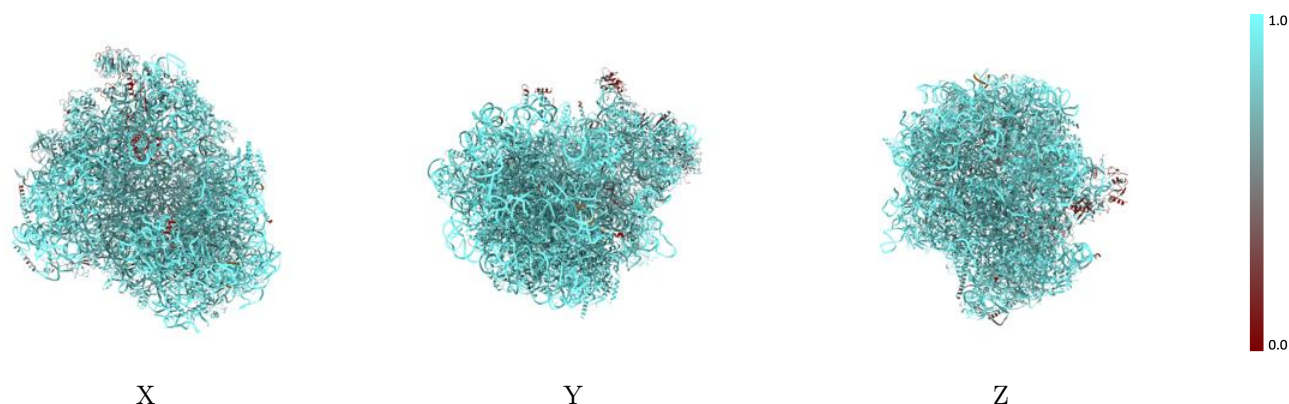
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



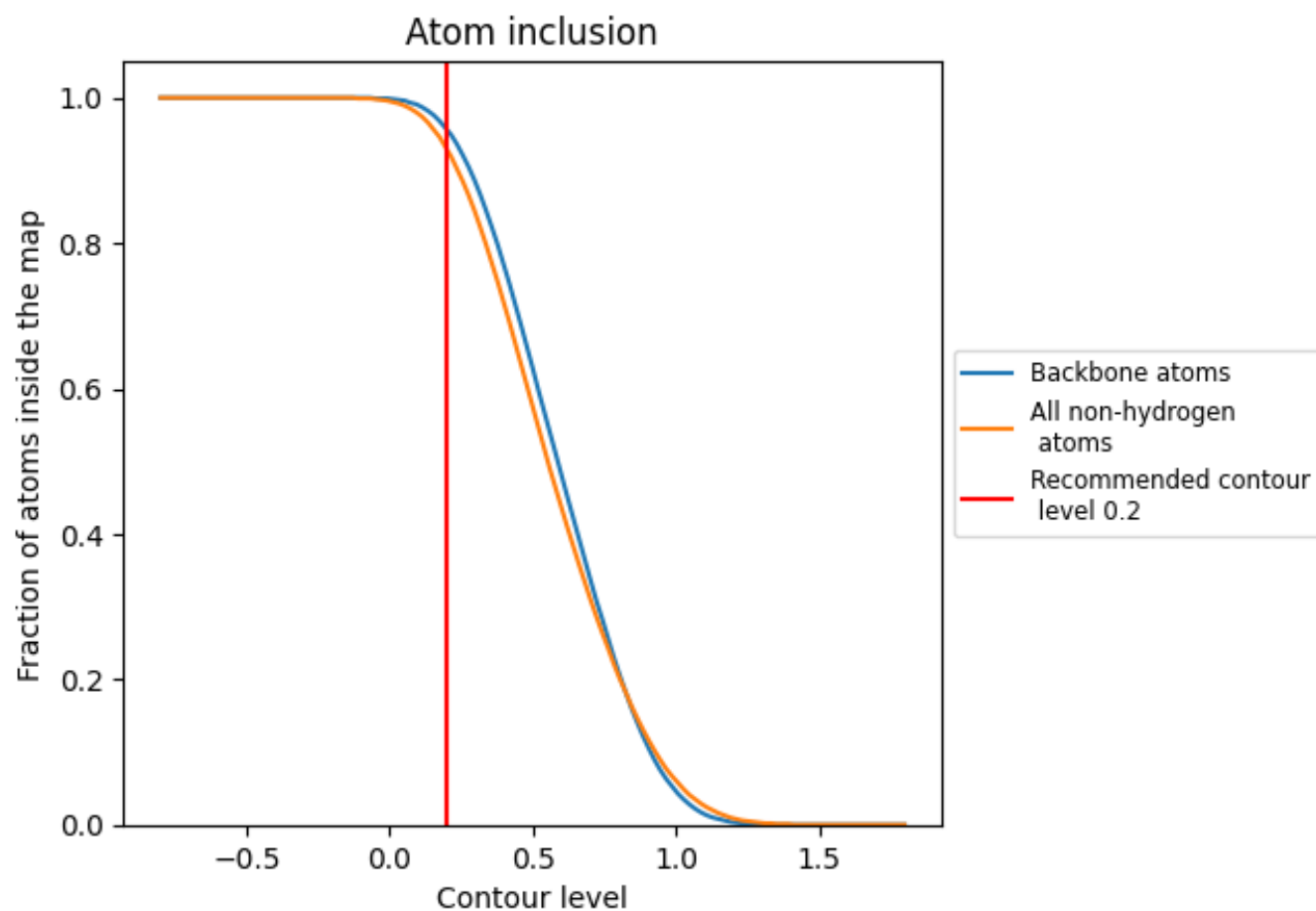
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.2760
1	 0.8170	 0.0860
5	 0.9850	 0.3420
7	 0.9950	 0.3480
8	 0.9860	 0.3510
9	 0.9660	 0.2200
A	 0.8910	 0.3490
AA	 0.8280	 0.1810
B	 0.8740	 0.3680
BB	 0.8870	 0.1390
C	 0.9260	 0.3540
CC	 0.9020	 0.2060
D	 0.9610	 0.2930
DD	 0.7740	 0.1070
E	 0.8990	 0.2990
EE	 0.9270	 0.1970
F	 0.8810	 0.3140
FF	 0.8810	 0.1390
G	 0.9190	 0.2740
GG	 0.7820	 0.1220
H	 0.9380	 0.2960
HH	 0.8010	 0.1720
I	 0.9060	 0.3140
II	 0.9170	 0.1630
J	 0.8870	 0.2640
JJ	 0.9190	 0.1630
K	 0.8360	 0.0470
KK	 0.7410	 0.0890
L	 0.9220	 0.3260
LL	 0.8680	 0.2420
M	 0.9400	 0.2780
MM	 0.3140	 0.0320
N	 0.9200	 0.3520
NN	 0.8610	 0.2070
O	 0.8690	 0.3280

















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Chain	Atom inclusion	Q-score
OO	 0.8770	 0.1340
P	 0.9500	 0.3740
PP	 0.8880	 0.1630
Q	 0.9200	 0.3620
QQ	 0.8040	 0.1110
R	 0.9070	 0.3000
RR	 0.6170	 0.1300
S	 0.9200	 0.3130
SS	 0.8530	 0.1670
T	 0.8910	 0.3380
TT	 0.8380	 0.1250
U	 0.9620	 0.2780
UU	 0.5180	 0.0690
V	 0.8040	 0.3380
VV	 0.8200	 0.2190
W	 0.7170	 0.1760
WW	 0.8470	 0.2580
X	 0.8960	 0.3190
XX	 0.8080	 0.2120
Y	 0.9490	 0.3210
YY	 0.9460	 0.1280
Z	 0.9580	 0.2540
ZZ	 0.9430	 0.1640
a	 0.9580	 0.3800
aa	 0.8630	 0.1850
b	 0.8860	 0.2790
bb	 0.8890	 0.1590
c	 0.9490	 0.2840
cc	 0.8910	 0.1220
d	 0.9360	 0.3520
dd	 0.8620	 0.1230
e	 0.8920	 0.3660
ee	 0.8480	 0.1400
f	 0.8730	 0.3450
ff	 0.4750	 0.0360
g	 0.9120	 0.3050
gg	 0.6530	 0.0810
h	 0.9410	 0.3030
i	 0.9250	 0.3190
j	 0.9210	 0.3620
k	 0.9370	 0.2830
l	 0.8780	 0.3170

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Chain	Atom inclusion	Q-score
m	 0.9450	 0.3130
n	 0.8300	 0.2910
o	 0.8680	 0.3320
p	 0.9140	 0.3300
r	 0.9160	 0.3500
s	 0.5090	 0.0270
t	 0.4160	 0.0220