



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:36 AM UTC

PDB ID : 9EVS / pdb_00009evs
EMDB ID : EMD-50011
Title : Structure of the flowering plant mitoribosome with P-site tRNA
Authors : Waltz, F.; Skaltsogiannis, V.; Giege, P.
Deposited on : 2024-04-02
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

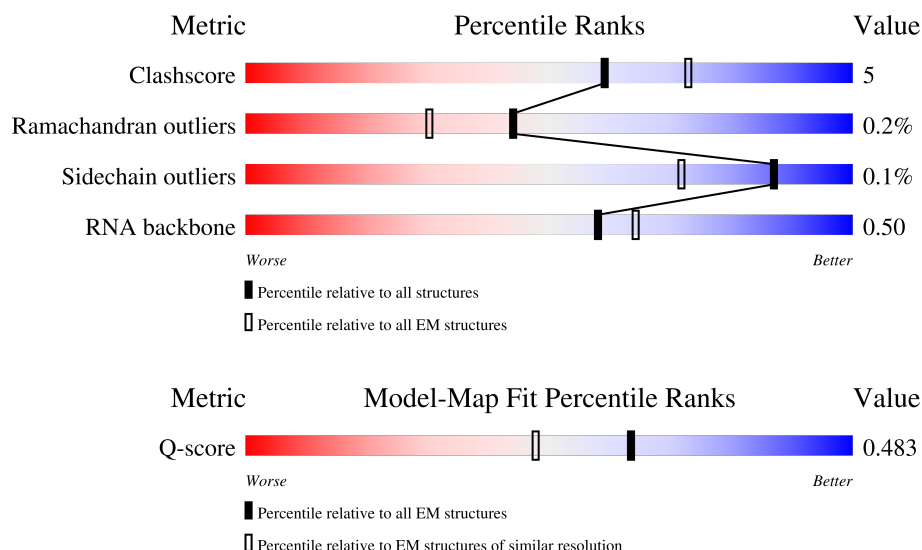
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 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.





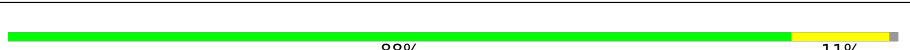
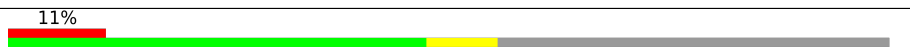
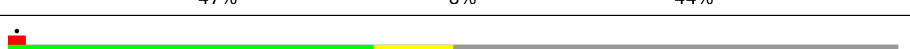
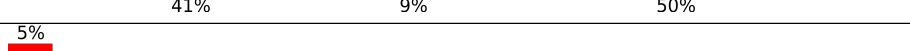
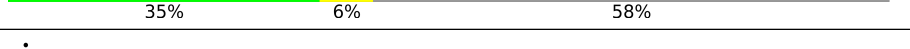





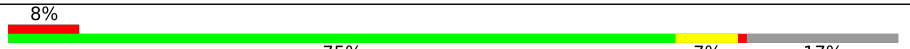


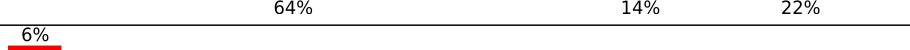


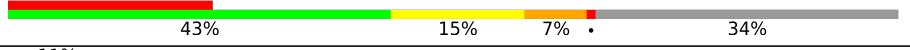





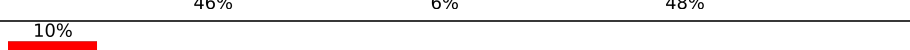
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	B	554	<div> <div>25%</div> <div>71%</div> <div>13%</div> <div>16%</div> </div>
2	C	362	<div> <div>9%</div> <div>81%</div> <div>10%</div> <div>8%</div> </div>
3	D	501	<div> <div>13%</div> <div>75%</div> <div>8%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	138	
5	F	157	
6	G	129	
7	H	383	
8	I	228	
9	J	304	
10	K	125	
11	L	154	
12	M	155	
13	N	414	
14	O	136	
15	P	110	
16	Q	237	
17	R	212	
18	S	100	
19	T	94	
20	U	192	
21	V	193	
22	W	483	
23	X	496	
24	Y	102	
25	Z	153	
26	1	2922	
27	3	118	
28	1B	220	








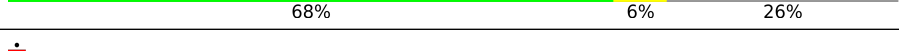
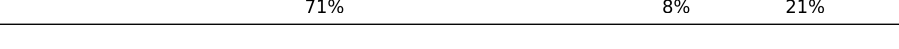
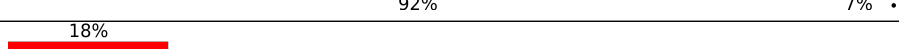


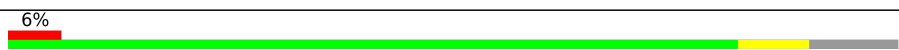

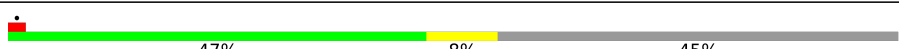




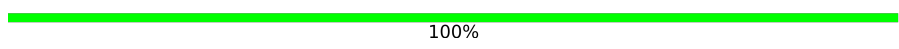
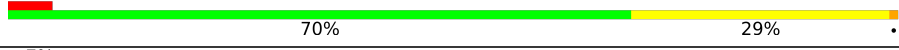
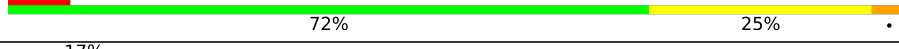



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Mol	Chain	Length	Quality of chain
29	1C	327	
30	1D	319	
31	1E	297	
32	1F	185	
33	1G	102	
34	1H	219	
35	1I	170	
36	1J	156	
37	1K	204	
38	1L	176	
39	1M	281	
40	1N	179	
41	1O	160	
42	1P	114	
43	1Q	233	
44	1R	126	
45	1S	270	
46	1T	264	
47	1U	180	
48	1V	159	
49	1W	249	
50	1X	271	
51	1Y	156	
52	1Z	212	
53	1a	144	

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Mol	Chain	Length	Quality of chain
54	1b	109	
55	1c	135	
56	1d	139	
57	1e	63	
58	1f	146	
59	1g	162	
60	1h	103	
61	1i	247	
62	1j	90	
63	1k	119	
64	1l	233	
65	1m	128	
66	1o	125	
67	1p	130	
68	1q	79	
69	1r	167	
70	1s	181	
71	1t	491	
72	1u	757	
73	1v	521	
74	1x	4	
75	5	76	
76	2	1591	
77	6	6	
78	a	424	

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Mol	Chain	Length	Quality of chain
79	b	80	
80	c	128	
81	d	110	
82	e	383	
83	f	410	
84	h	384	
85	i	725	
86	j	408	
87	k	155	
88	A	212	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 211395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	467	Total	C	N	O	S	0	0
			3877	2520	701	643	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 2 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	333	Total	C	N	O	S	0	0
			2811	1798	540	462	11		

- Molecule 3 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 4 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 5 is a protein called uS7m, Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 6 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 7 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	213	Total	C	N	O	S	0	0
			1682	1054	312	311	5		

- Molecule 8 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 9 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	127	Total	C	N	O	S	0	0
			988	608	195	181	4		

- Molecule 10 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	124	Total	C	N	O	S	0	0
			992	613	208	167	4		

- Molecule 11 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	119	Total	C	N	O	S	0	0
			940	572	200	163	5		

- Molecule 12 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 13 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 14 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 15 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 16 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

- Molecule 17 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 18 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 19 is a protein called bTHXm.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 20 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 21 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 22 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 23 is a protein called mS31/mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 24 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 25 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 26 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2922	Total	C	N	O	P	5	0
			62518	27942	11365	20289	2922		

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 28 is a protein called uL2m C-ter.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1B	177	Total	C	N	O	S	0	0
			1325	819	259	233	14		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2mz, N-terminal part.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1C	215	Total	C	N	O	S	0	0
			1696	1078	316	296	6		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	87	LYS	GLU	conflict	UNP P93311
1C	89	LEU	PHE	conflict	UNP P93311
1C	147	TYR	SER	conflict	UNP P93311
1C	155	SER	GLY	conflict	UNP P93311
1C	190	ASP	GLY	conflict	UNP P93311
1C	195	PRO	ALA	conflict	UNP P93311
1C	199	VAL	ALA	conflict	UNP P93311
1C	200	SER	LYS	conflict	UNP P93311
1C	201	THR	PRO	conflict	UNP P93311
1C	221	TYR	CYS	conflict	UNP P93311
1C	226	TRP	GLY	conflict	UNP P93311
1C	238	ASN	LYS	conflict	UNP P93311

- Molecule 30 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1D	264	Total	C	N	O	S	0	0
			2045	1309	367	358	11		

- Molecule 31 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1E	221	Total	C	N	O	S	0	0
			1753	1104	334	308	7		

- Molecule 32 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1F	158	Total	C	N	O	S	0	0
			1286	829	212	236	9		

- Molecule 33 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1G	98	Total	C	N	O	S	0	0
			779	508	136	130	5		

- Molecule 34 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1H	66	Total	C	N	O	S	0	0
			539	345	98	94	2		

- Molecule 35 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1I	130	Total	C	N	O	S	0	0
			1036	669	178	184	5		

- Molecule 36 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1J	147	Total	C	N	O	S	0	0
			1129	722	193	205	9		

- Molecule 37 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1K	189	Total	C	N	O	S	0	0
			1526	955	299	265	7		

- Molecule 38 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1L	127	Total	C	N	O	S	0	0
			966	609	184	168	5		

- Molecule 39 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1M	210	Total	C	N	O	S	0	0
			1649	1052	321	273	3		

- Molecule 40 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1N	148	Total	C	N	O	S	0	0
			1160	731	230	192	7		

- Molecule 41 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1O	151	Total	C	N	O	S	0	0
			1231	767	244	214	6		

- Molecule 42 is a protein called uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1P	113	Total	C	N	O	S	0	0
			878	564	160	149	5		

- Molecule 43 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1Q	122	Total	C	N	O	S	0	0
			1008	641	198	166	3		

- Molecule 44 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1R	110	Total	C	N	O	S	0	0
			915	572	184	154	5		

- Molecule 45 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1S	145	Total	C	N	O	S	0	0
			1170	750	207	211	2		

- Molecule 46 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1T	155	Total	C	N	O	S	0	0
			1241	782	249	205	5		

- Molecule 47 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1U	130	Total	C	N	O	S	0	0
			1048	675	190	181	2		

- Molecule 48 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1V	158	Total	C	N	O	S	0	0
			1223	770	229	220	4		

- Molecule 49 is a protein called bL25-2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1W	205	Total	C	N	O	S	0	0
			1588	1006	284	294	4		

- Molecule 50 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1X	216	Total	C	N	O	S	0	0
			1670	1069	298	302	1		

- Molecule 51 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1Y	98	Total	C	N	O	S	0	0
			768	484	152	131	1		

- Molecule 52 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1Z	177	Total	C	N	O	S	0	0
			1441	911	266	255	9		

- Molecule 53 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1a	110	Total	C	N	O	S	0	0
			928	588	172	158	10		

- Molecule 54 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1b	100	Total	C	N	O	S	0	0
			803	504	160	134	5		

- Molecule 55 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1c	59	Total	C	N	O	S	0	0
			489	313	98	73	5		

- Molecule 56 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1d	49	Total	C	N	O	S	0	0
			379	240	80	55	4		

- Molecule 57 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1e	54	Total	C	N	O	S	0	0
			459	300	85	72	2		

- Molecule 58 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	1f	44	Total	C	N	O	0	0
			364	224	88	52		

- Molecule 59 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	1g	91	Total	C	N	O	S	0	0
			770	496	152	119	3		

- Molecule 60 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	1h	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

- Molecule 61 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	1i	183	Total	C	N	O	S	0	0
			1424	885	255	274	10		

- Molecule 62 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	1j	71	Total	C	N	O	S	0	0
			570	369	102	97	2		

- Molecule 63 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	1k	118	Total	C	N	O	S	0	0
			952	599	184	165	4		

- Molecule 64 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	1l	211	Total	C	N	O	S	0	0
			1741	1131	286	316	8		

- Molecule 65 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	1m	122	Total	C	N	O	S	0	0
			970	610	170	184	6		

- Molecule 66 is a protein called mL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	1o	76	Total	C	N	O	0	0
			626	397	114	115		

- Molecule 67 is a protein called mL59/mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	1p	117	Total	C	N	O	S	0	0
			992	626	189	169	8		

- Molecule 68 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	1q	50	Total	C	N	O	S	0	0
			390	243	79	67	1		

- Molecule 69 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	1r	92	Total	C	N	O	S	0	0
			735	469	139	122	5		

- Molecule 70 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	1s	118	Total	C	N	O	S	0	0
			985	617	203	163	2		

- Molecule 71 is a protein called mL101 (rPPR4).

Mol	Chain	Residues	Atoms					AltConf	Trace
71	1t	484	Total	C	N	O	S	0	0
			3856	2433	665	733	25		

- Molecule 72 is a protein called mL102 (rPPR5).

Mol	Chain	Residues	Atoms					AltConf	Trace
72	1u	666	Total	C	N	O	S	0	0
			5264	3316	915	991	42		

- Molecule 73 is a protein called mL104 (rPPR9).

Mol	Chain	Residues	Atoms					AltConf	Trace
73	1v	433	Total	C	N	O	S	0	0
			3440	2173	599	640	28		

- Molecule 74 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	1x	4	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 75 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	5	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 76 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	2	1591	Total	C	N	O	P	0	0
			34081	15222	6213	11055	1591		

- Molecule 77 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	6	6	Total	C	N	O	P	0	0
			130	59	27	38	6		

- Molecule 78 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a	315	Total	C	N	O	S	0	0
			2487	1547	448	482	10		

- Molecule 79 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 80 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 81 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 82 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 83 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 84 is a protein called mS83 (rPPR10).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	h	310	Total	C	N	O	S	0	0
			2460	1551	436	458	15		

- Molecule 85 is a protein called mS77 (NFD5).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	i	306	Total	C	N	O	S	0	0
			2487	1567	419	487	14		

- Molecule 86 is a protein called mS76 (rPPR1).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	j	381	Total	C	N	O	S	0	0
			2984	1885	510	567	22		

- Molecule 87 is a protein called mS86.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	k	47	Total	C	N	O	S	0	0
			314	194	61	55	4		

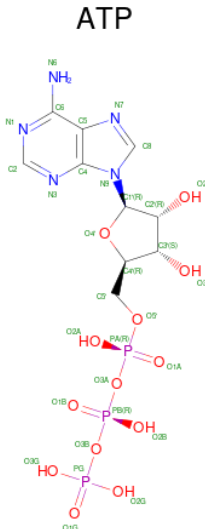
- Molecule 88 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	A	204	Total	C	N	O	S	0	0
			1611	1032	284	285	10		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

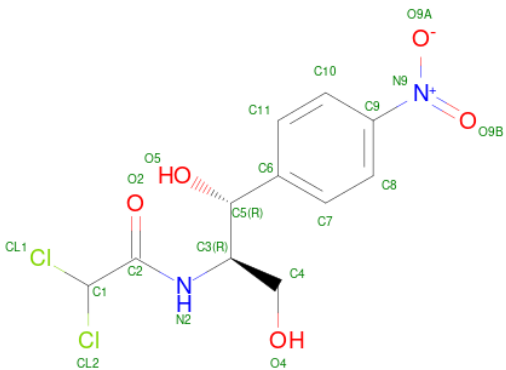
Mol	Chain	Residues	Atoms		AltConf
89	T	1	Total	Mg	0
			1	1	
89	W	1	Total	Mg	0
			1	1	
89	1	249	Total	Mg	0
			249	249	
89	3	3	Total	Mg	0
			3	3	
89	1D	1	Total	Mg	0
			1	1	
89	1h	1	Total	Mg	0
			1	1	
89	1j	1	Total	Mg	0
			1	1	
89	1q	2	Total	Mg	0
			2	2	
89	2	98	Total	Mg	0
			98	98	

- Molecule 90 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
90	W	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 91 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					AltConf
91	1	1	Total 20	C 11	Cl 2	N 2	O 5	0

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
92	1	56	Total 56	K 56	0
92	1B	3	Total 3	K 3	0
92	1E	1	Total 1	K 1	0
92	2	14	Total 14	K 14	0

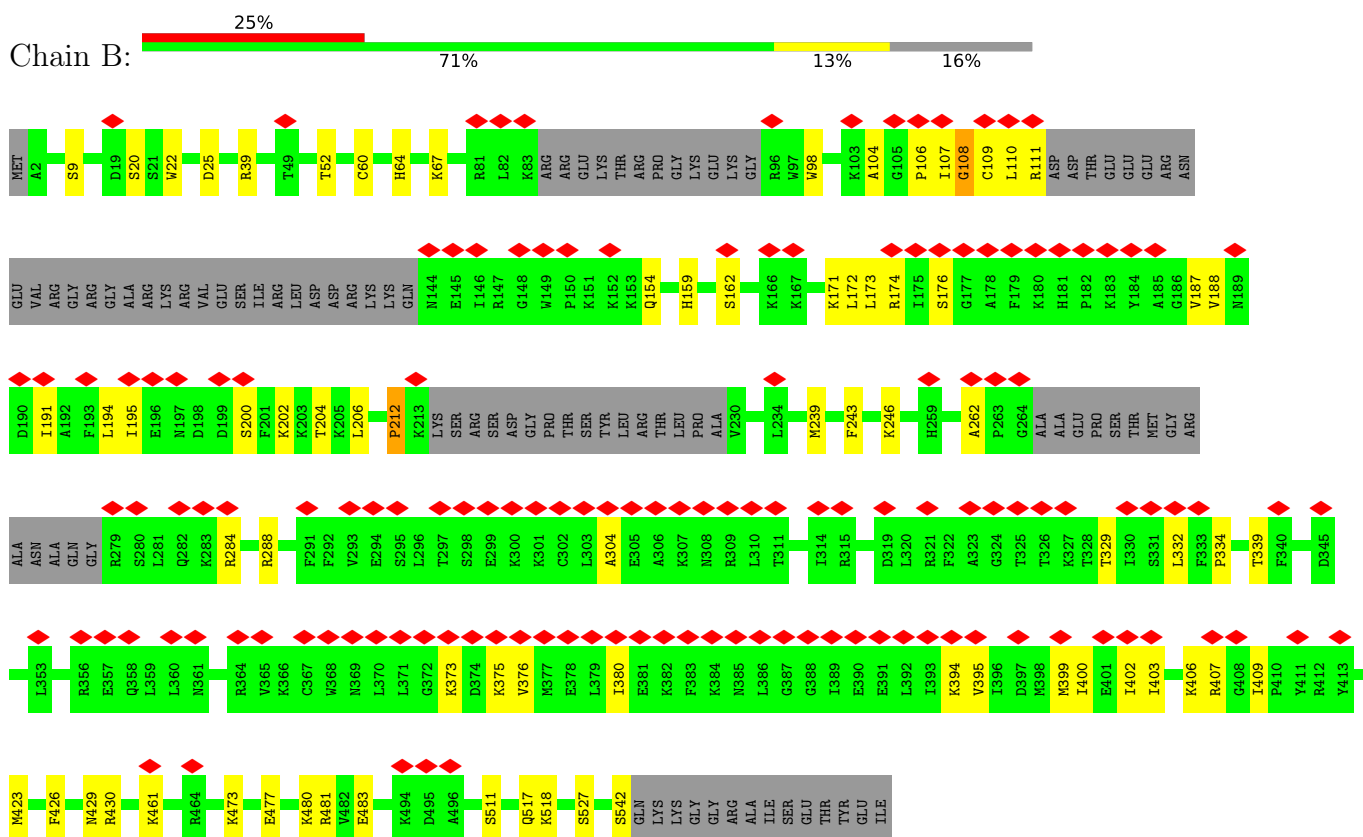
- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
93	1d	1	Total 1	Zn 1	0
93	1h	1	Total 1	Zn 1	0

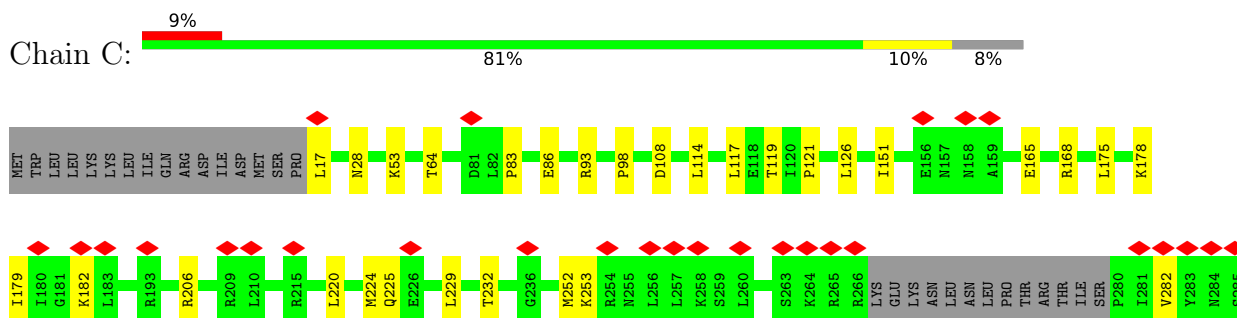
3 Residue-property plots

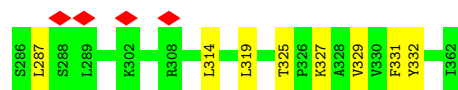
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Small ribosomal subunit protein uS3m

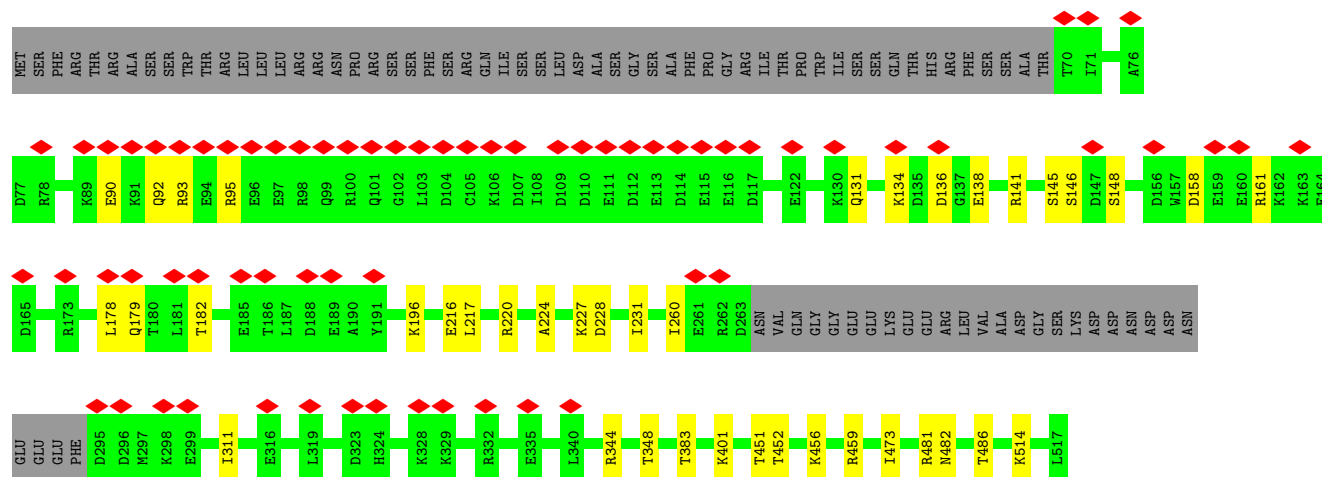
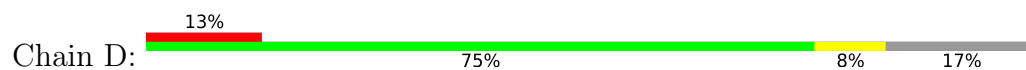


- Molecule 2: uS4m

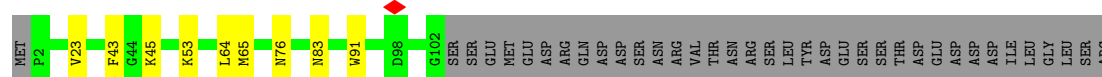




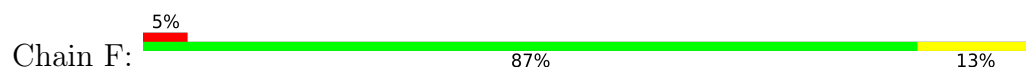
• Molecule 3: uS5m



• Molecule 4: bS6m



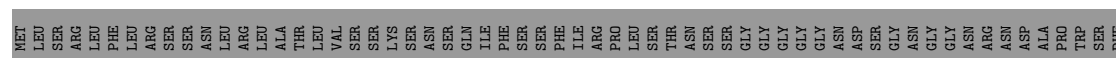
• Molecule 5: uS7m, Small ribosomal subunit protein uS7m

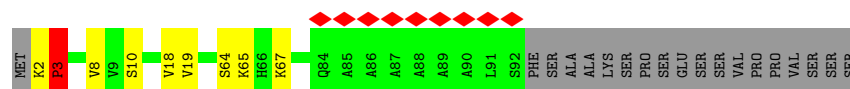
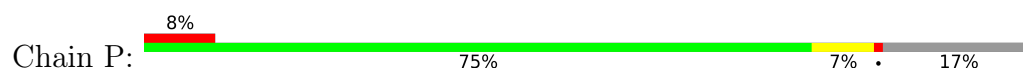


• Molecule 6: uS8m

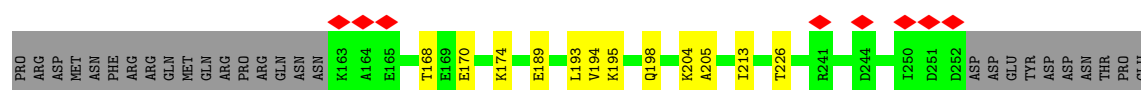
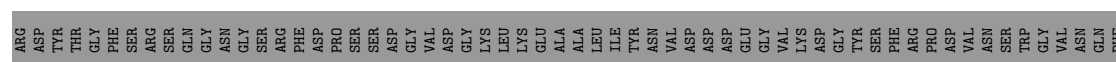
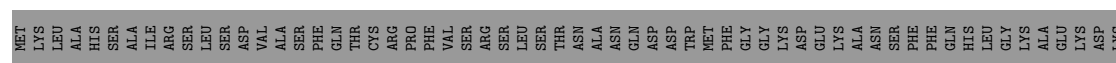


• Molecule 7: uS9m

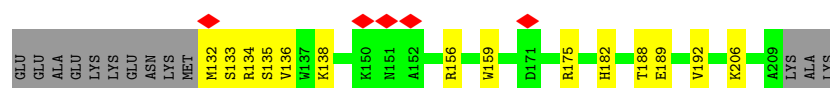
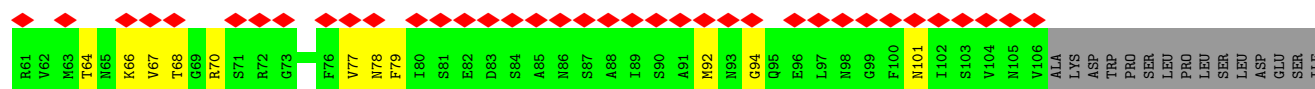
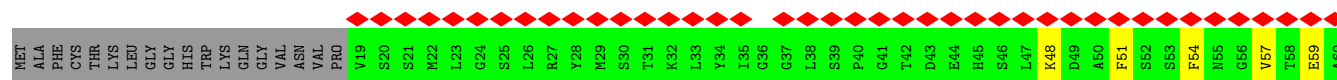
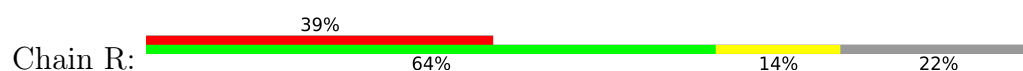




• Molecule 16: bS18m



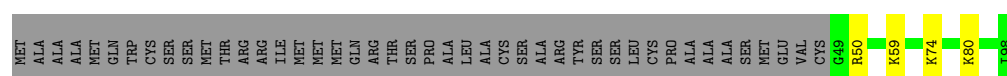
• Molecule 17: uS19m



• Molecule 18: bS21m

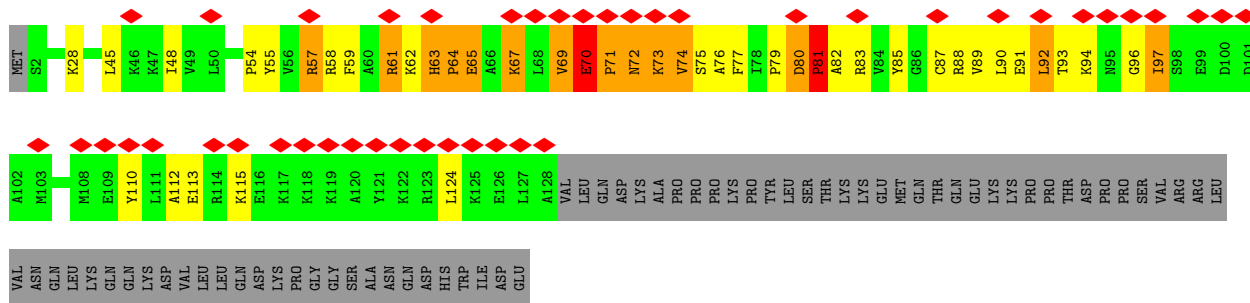


• Molecule 19: bTHXm

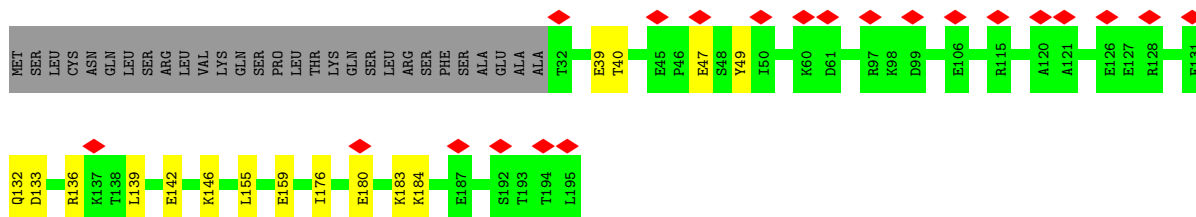
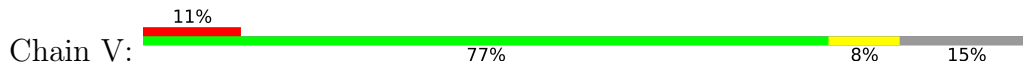


• Molecule 20: mS23

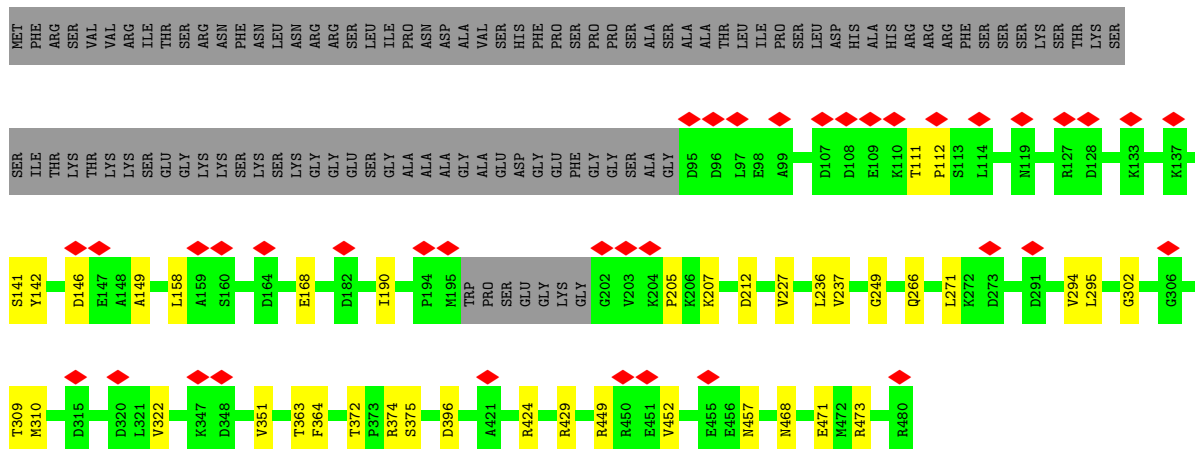




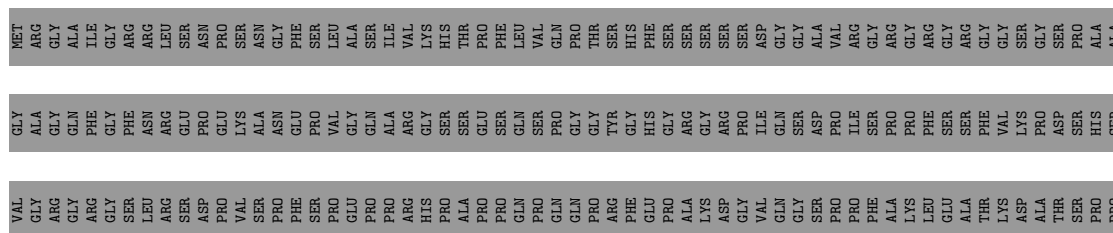
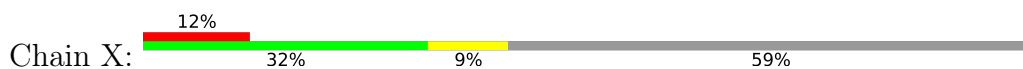
- Molecule 21: mS26

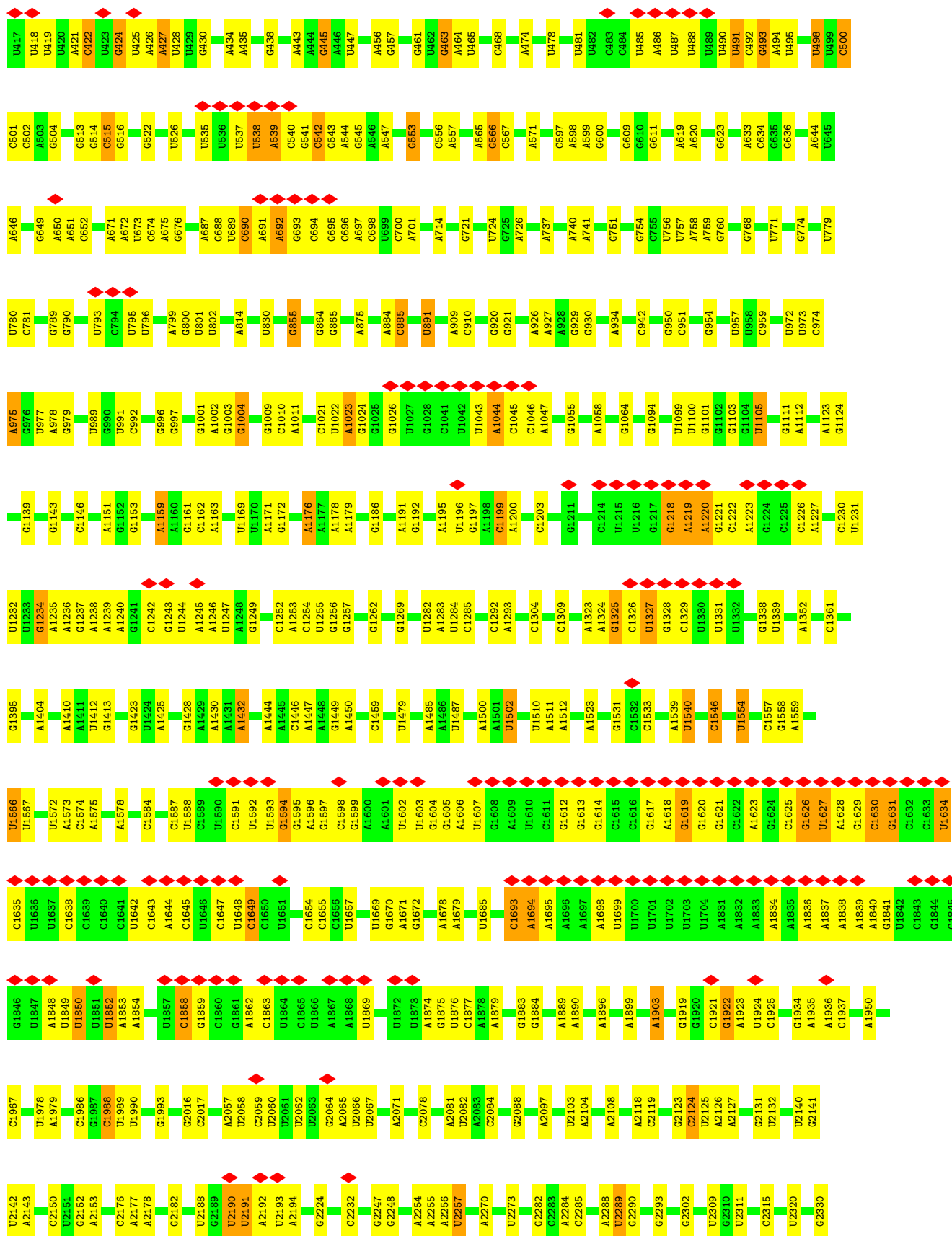


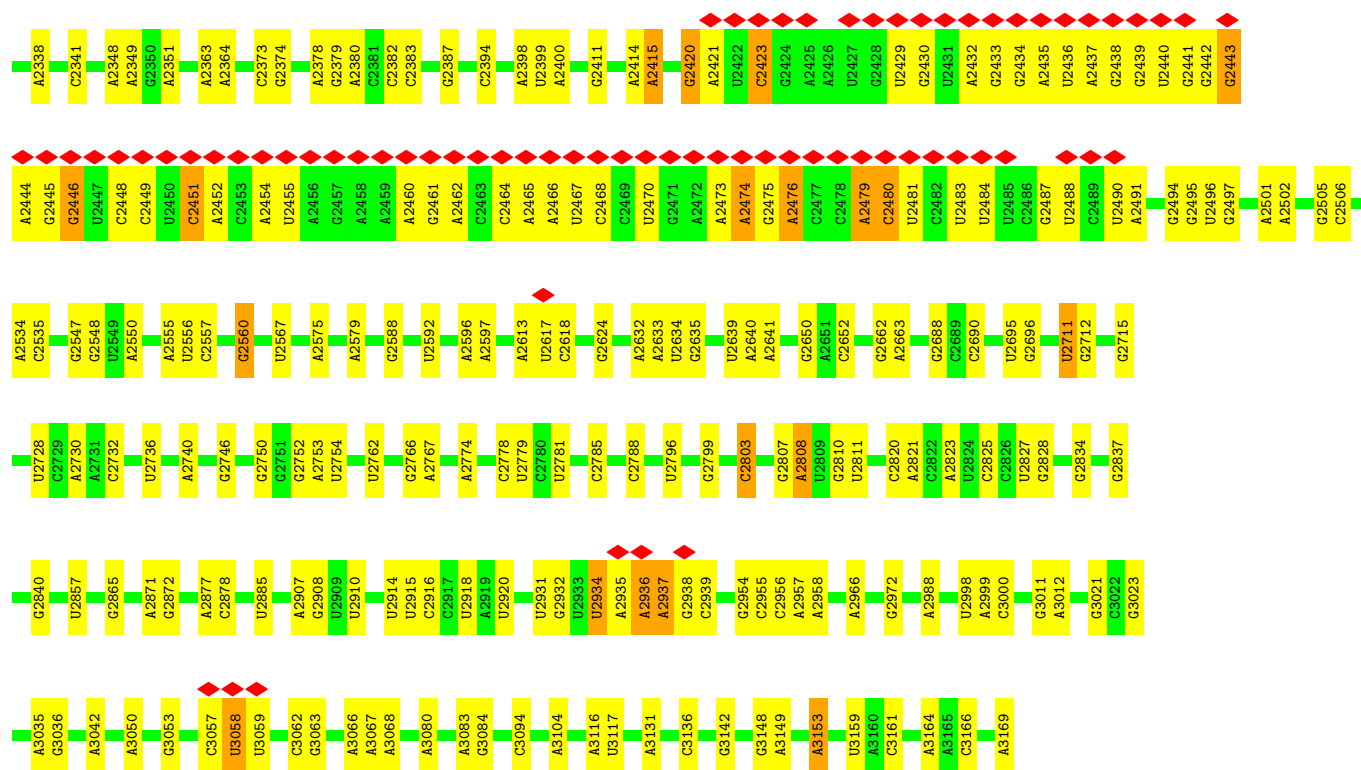
- Molecule 22: mS29



- Molecule 23: mS31/mS46

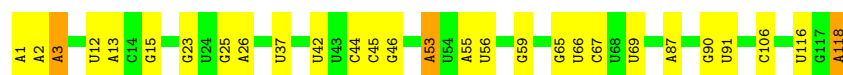






• Molecule 27: 5S rRNA

Chain 3: 76% 21% .



• Molecule 28: uL2m C-ter

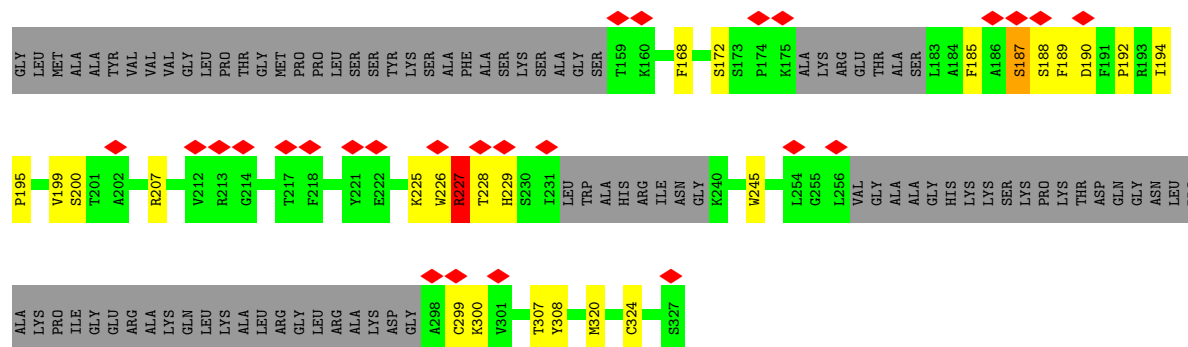
Chain 1B: 73% 7% 20%



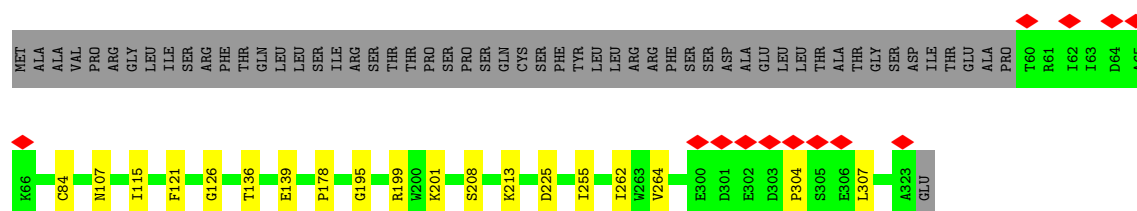
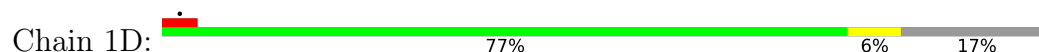
• Molecule 29: Large ribosomal subunit protein uL2mz, N-terminal part

Chain 1C: 12% 55% 10% 34%

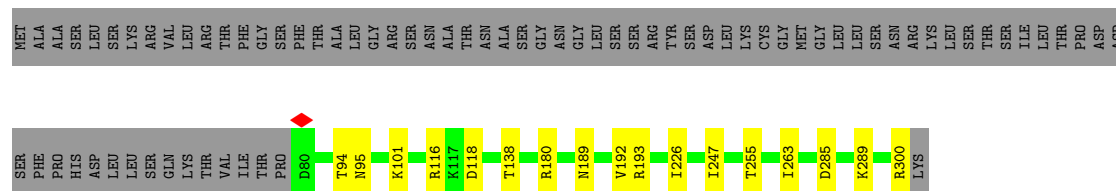




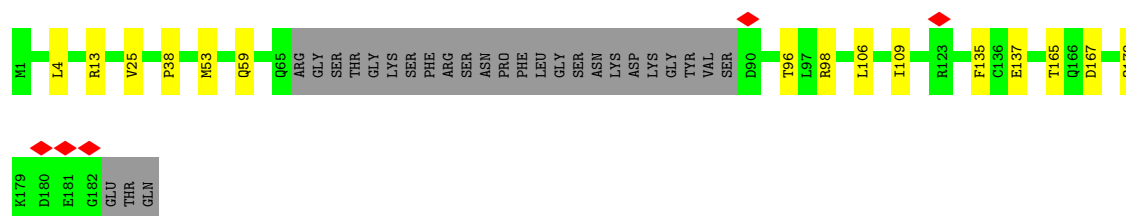
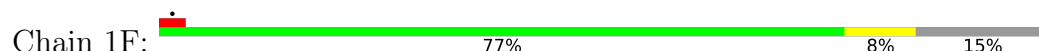
• Molecule 30: uL3m



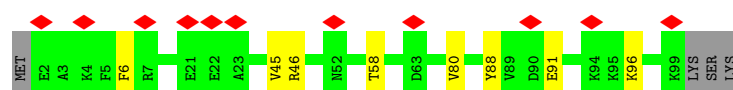
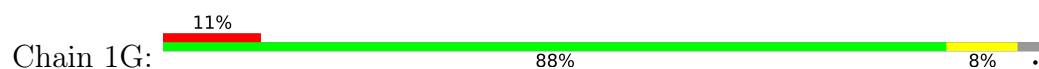
• Molecule 31: uL4m



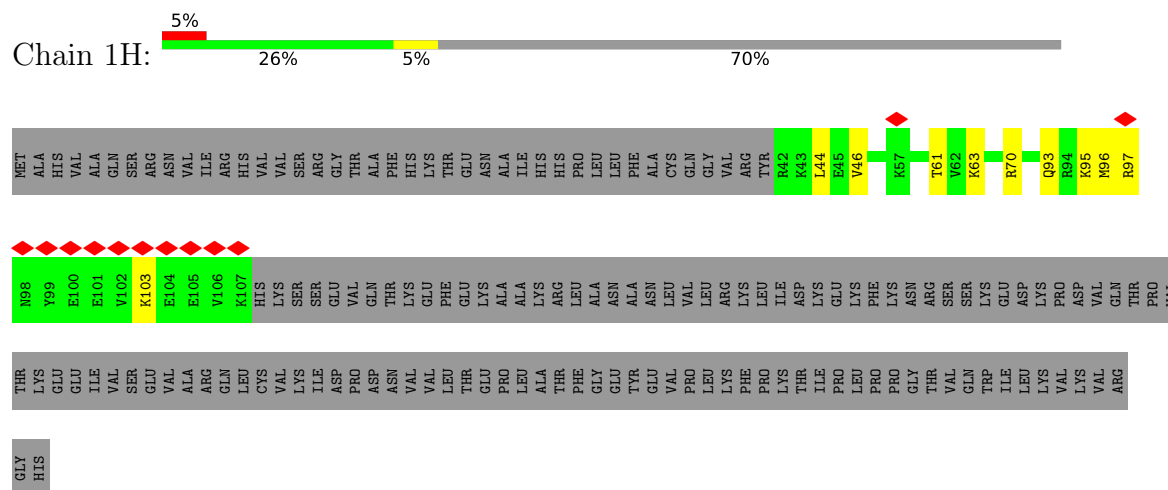
• Molecule 32: uL5m



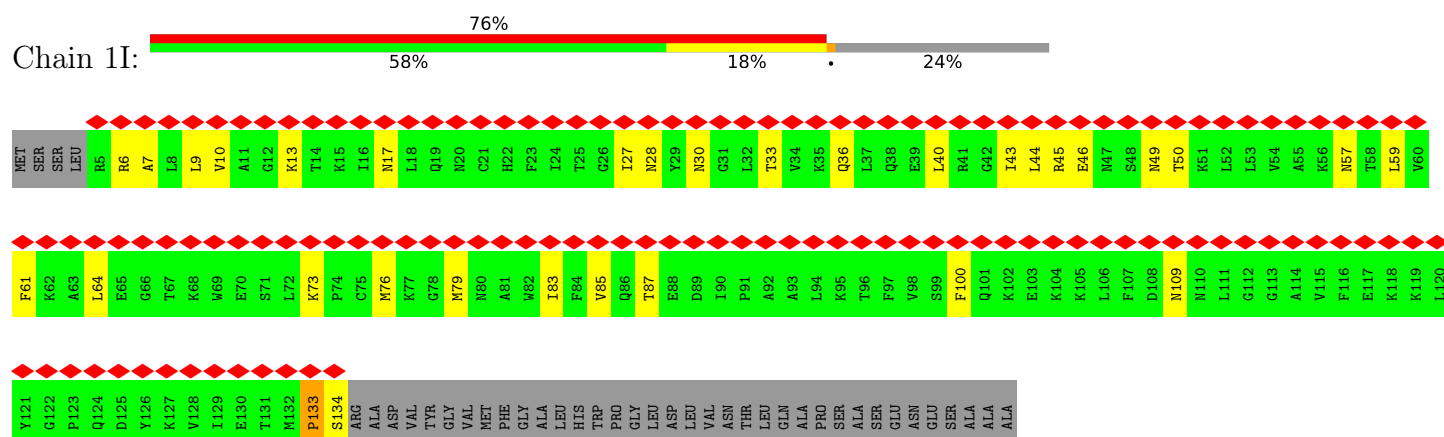
• Molecule 33: uL6m



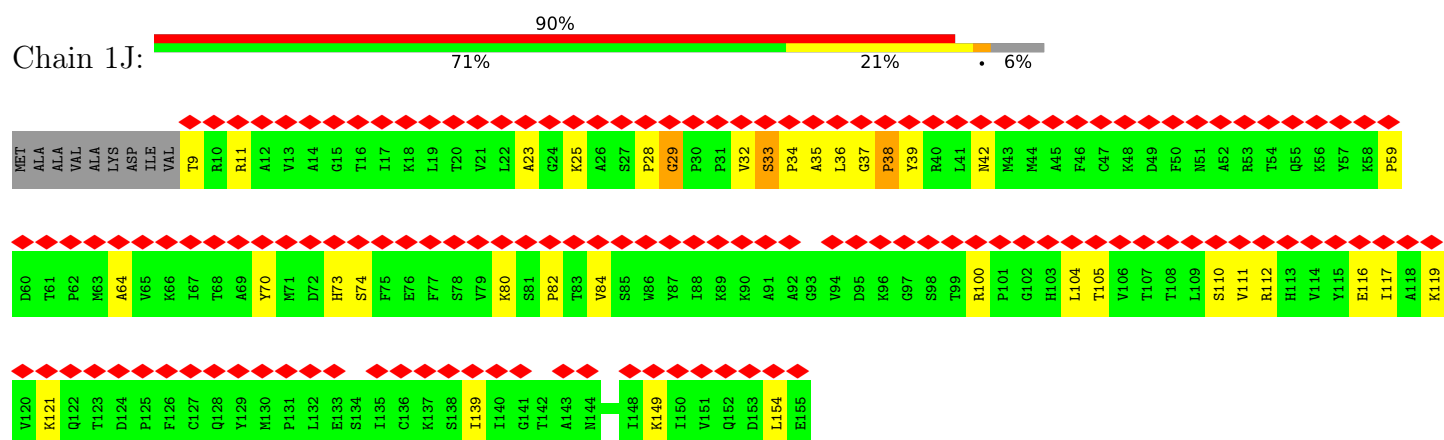
• Molecule 34: bL9m



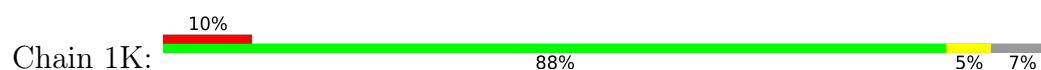
• Molecule 35: uL10m

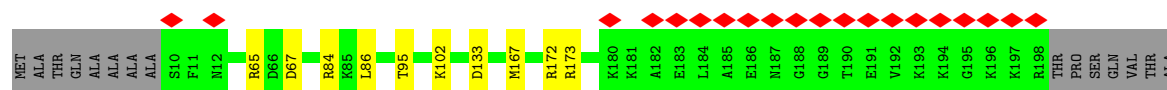


• Molecule 36: uL11m

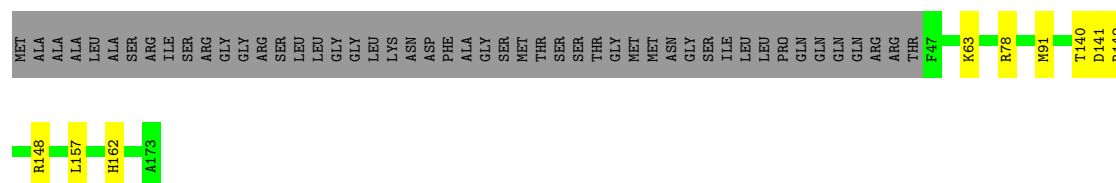


• Molecule 37: uL13m

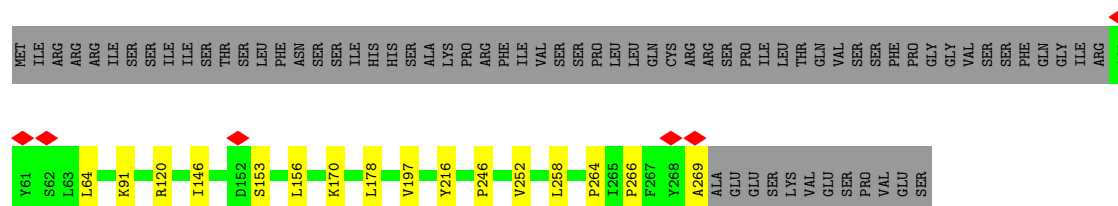




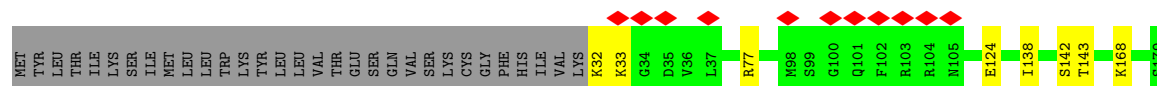
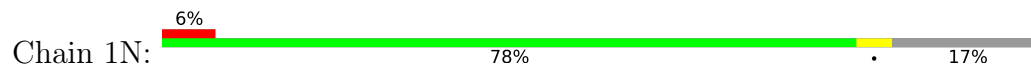
• Molecule 38: uL14m



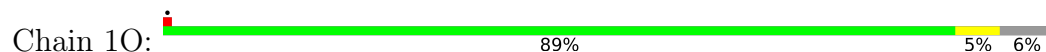
• Molecule 39: uL15m



• Molecule 40: uL16m



• Molecule 41: bL17m

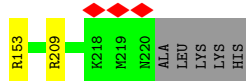


• Molecule 42: uL18m

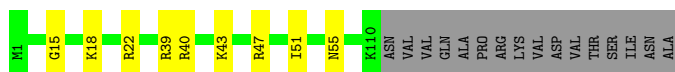


• Molecule 43: bL19m

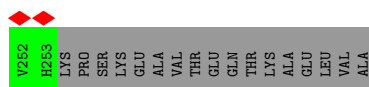
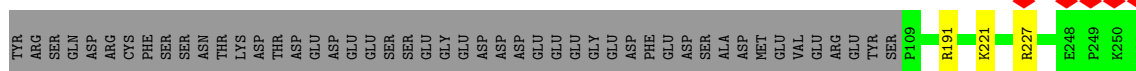




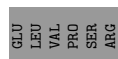
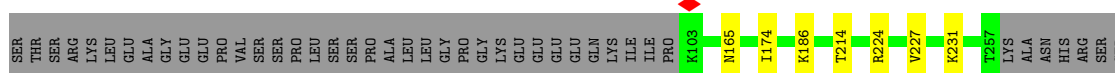
Chain 1R:



Chain 1S:  53% . 46%



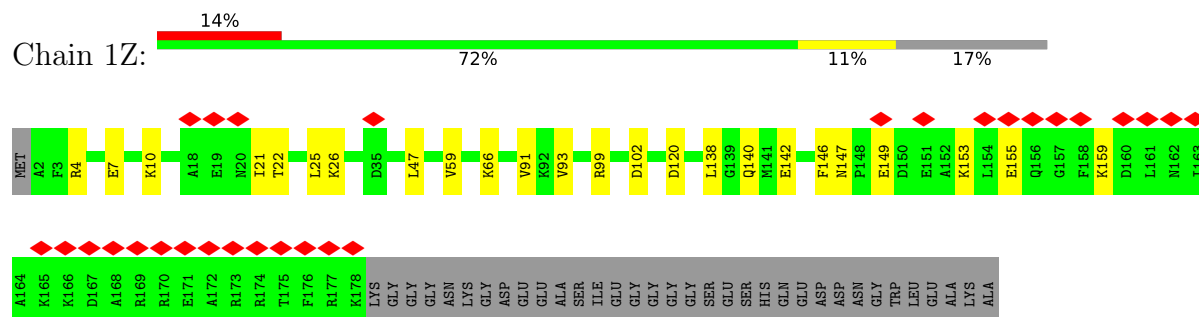
Chain 1T:  56% . 41%



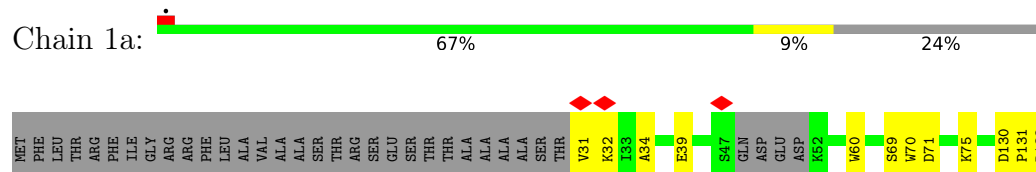
Chain 1U: 



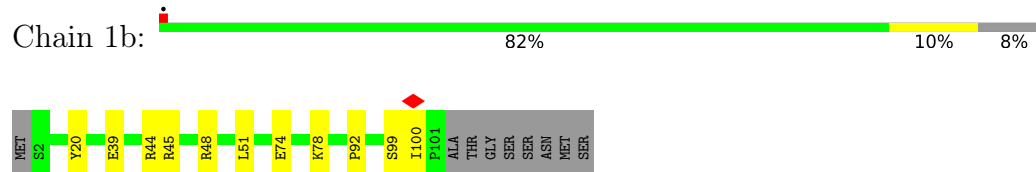
- Molecule 52: bL28m



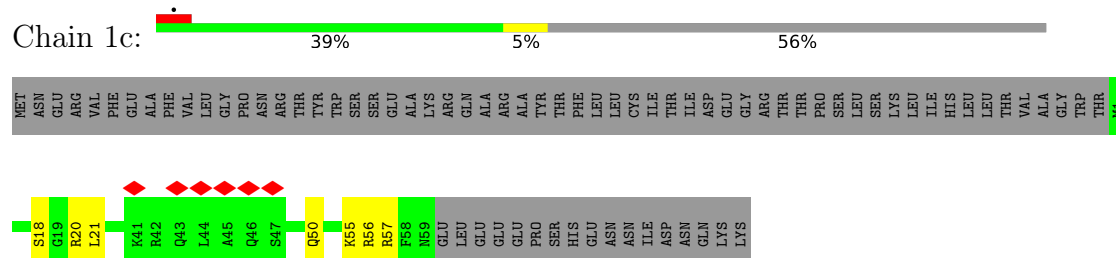
- Molecule 53: uL29m



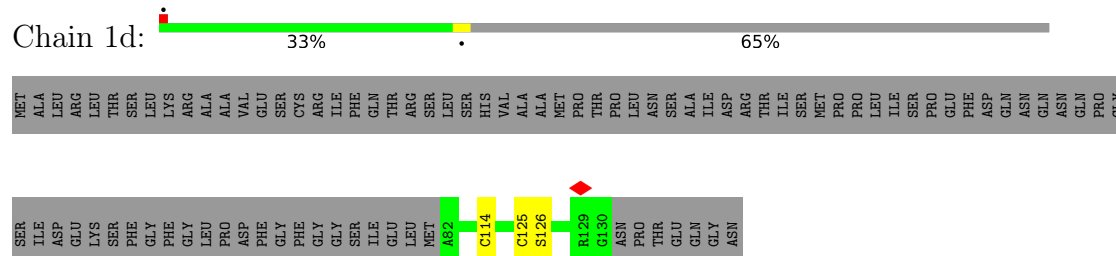
- Molecule 54: uL30m



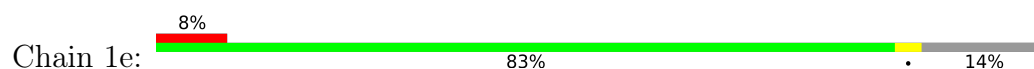
- Molecule 55: bL31m



- Molecule 56: bL32m

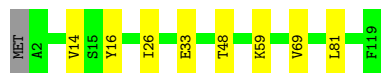


- Molecule 57: bL33m




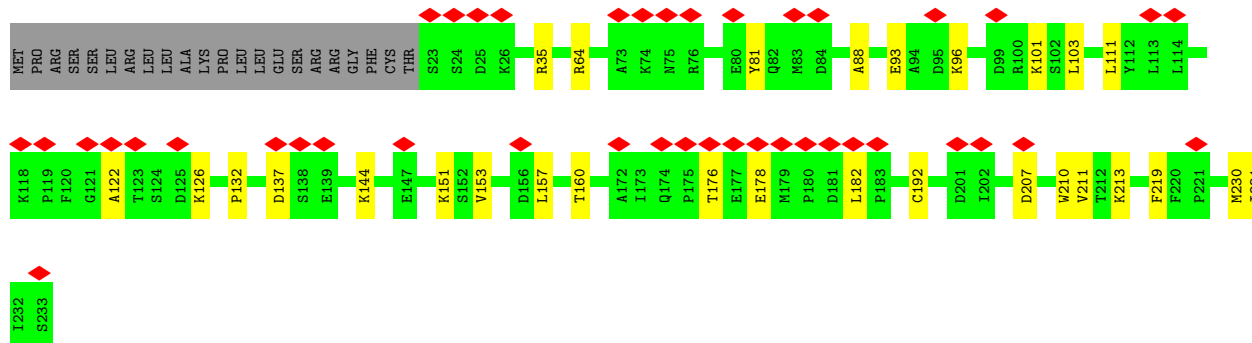
- Molecule 63: mL43

Chain 1k: 




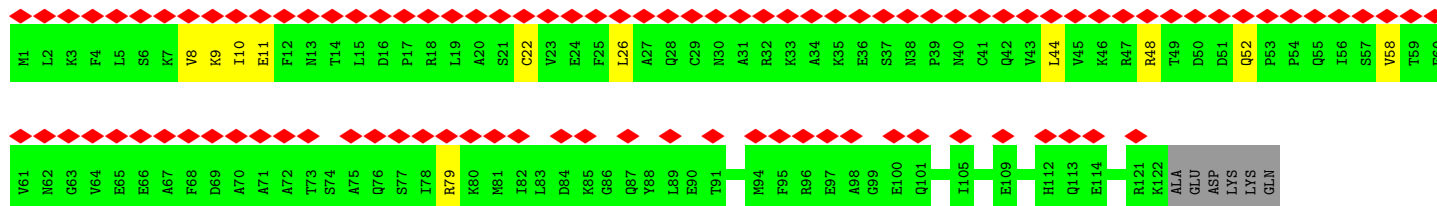
- Molecule 64: mL46

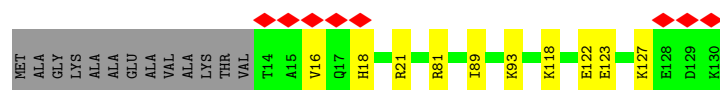
Chain 1l: 



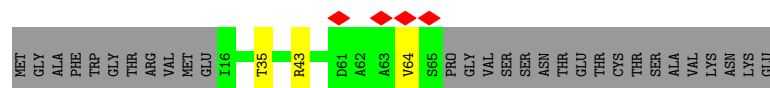
- Molecule 65: mL53

Chain 1m: 

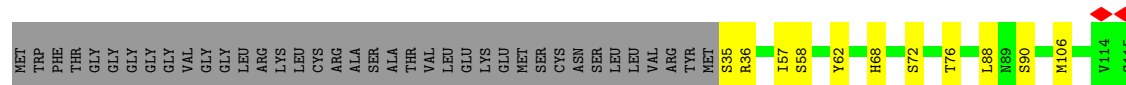




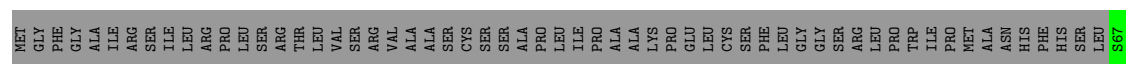
- Molecule 68: mL60



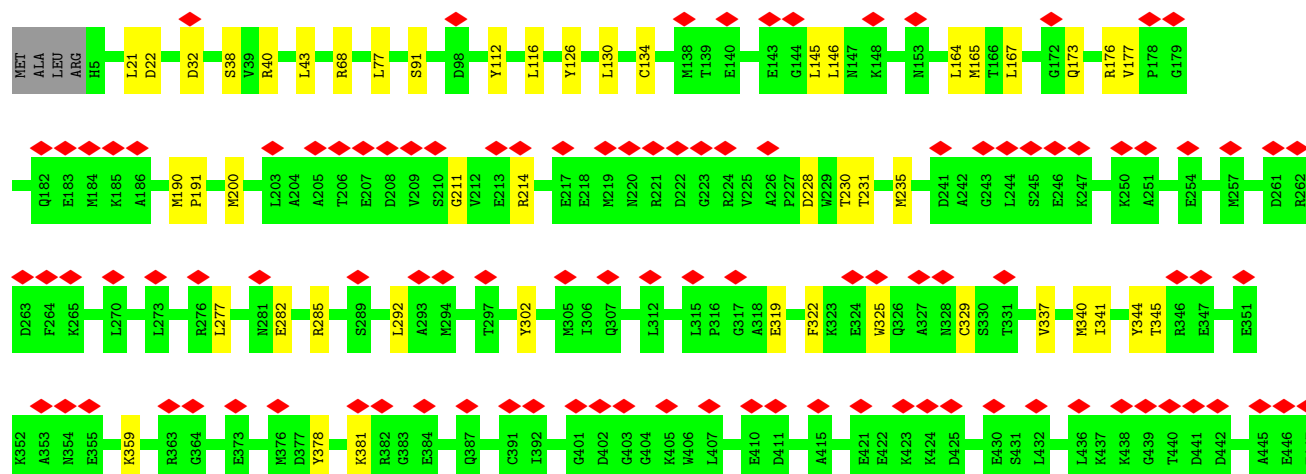
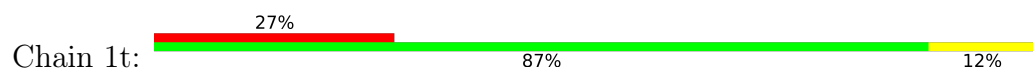
- Molecule 69: mL80

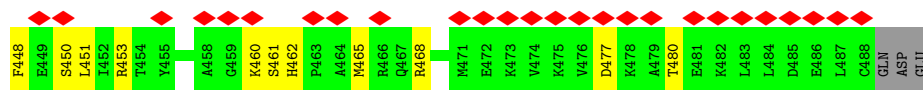


- Molecule 70: mL87

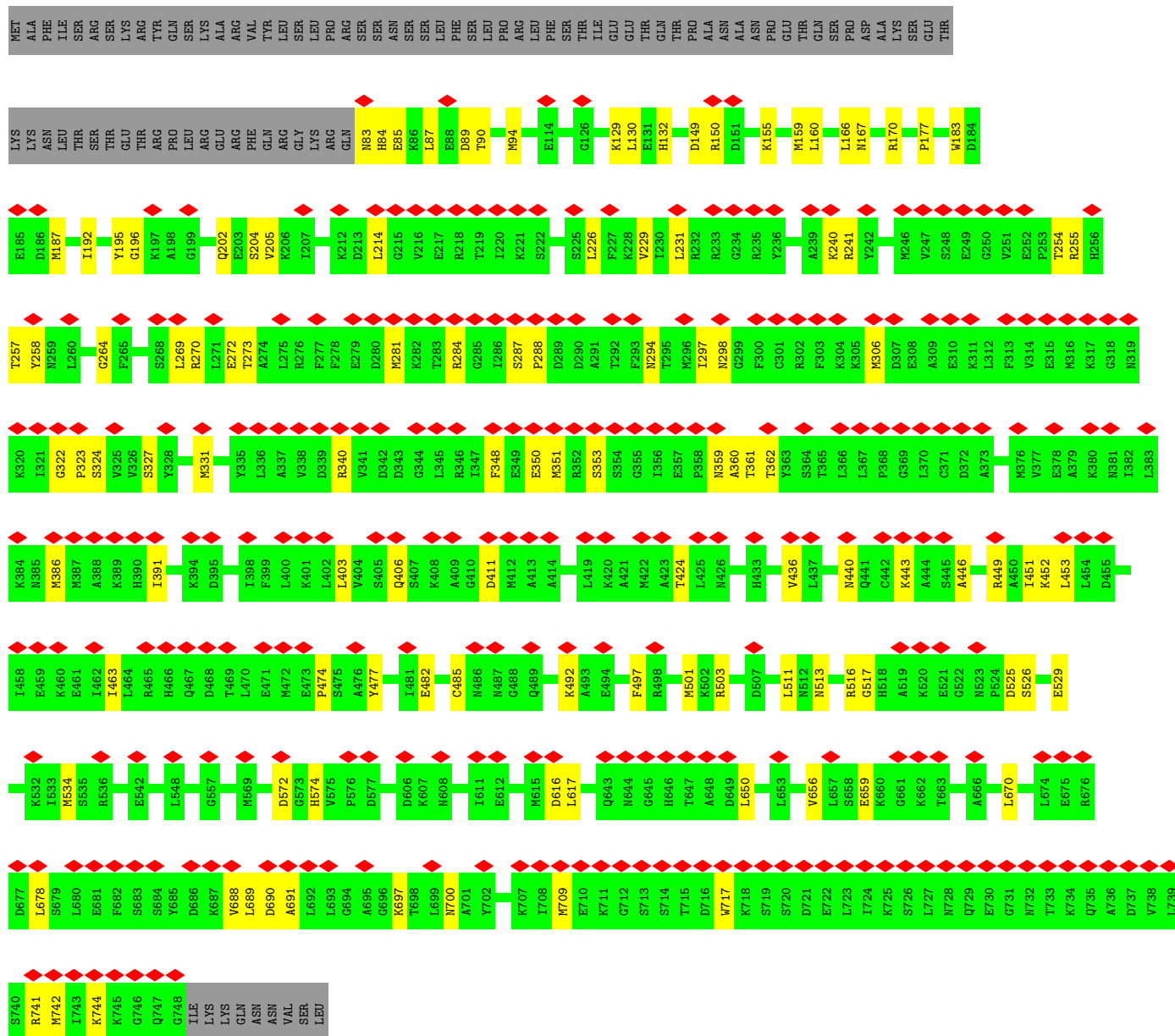
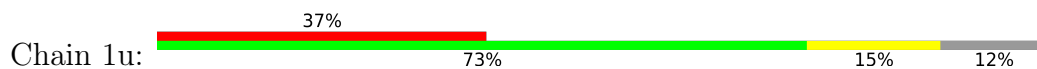


- Molecule 71: mL101 (rPPR4)

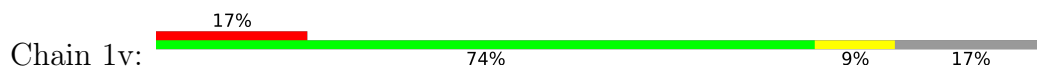


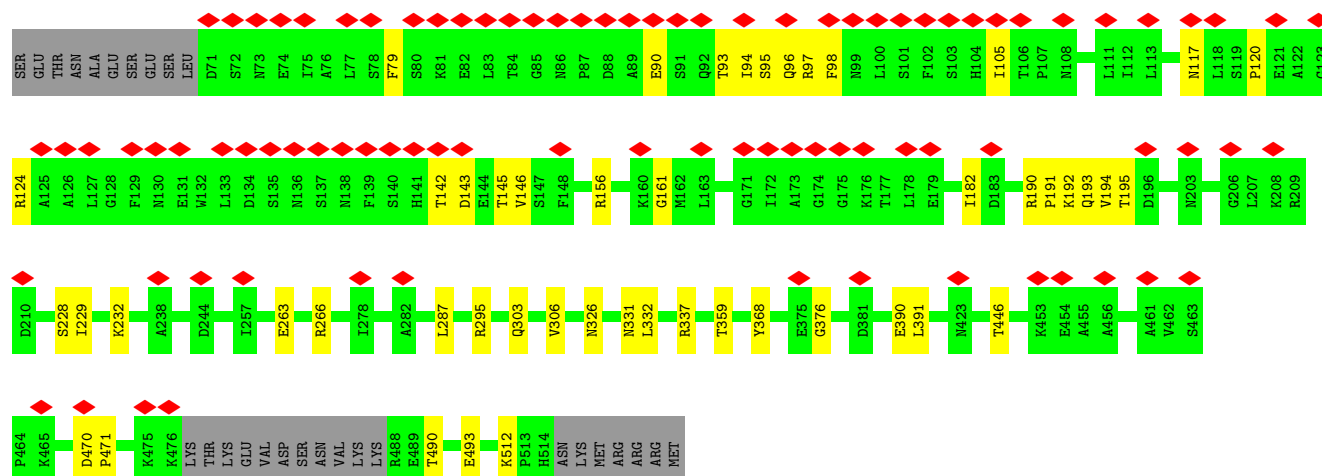


• Molecule 72: mL102 (rPPR5)



• Molecule 73: mL104 (rPPR9)





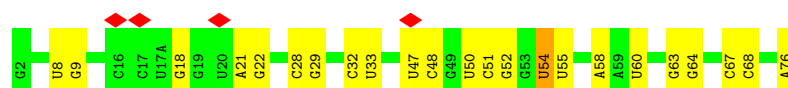
- Molecule 74: Nascent peptide

Chain 1x: 100%

There are no outlier residues recorded for this chain.

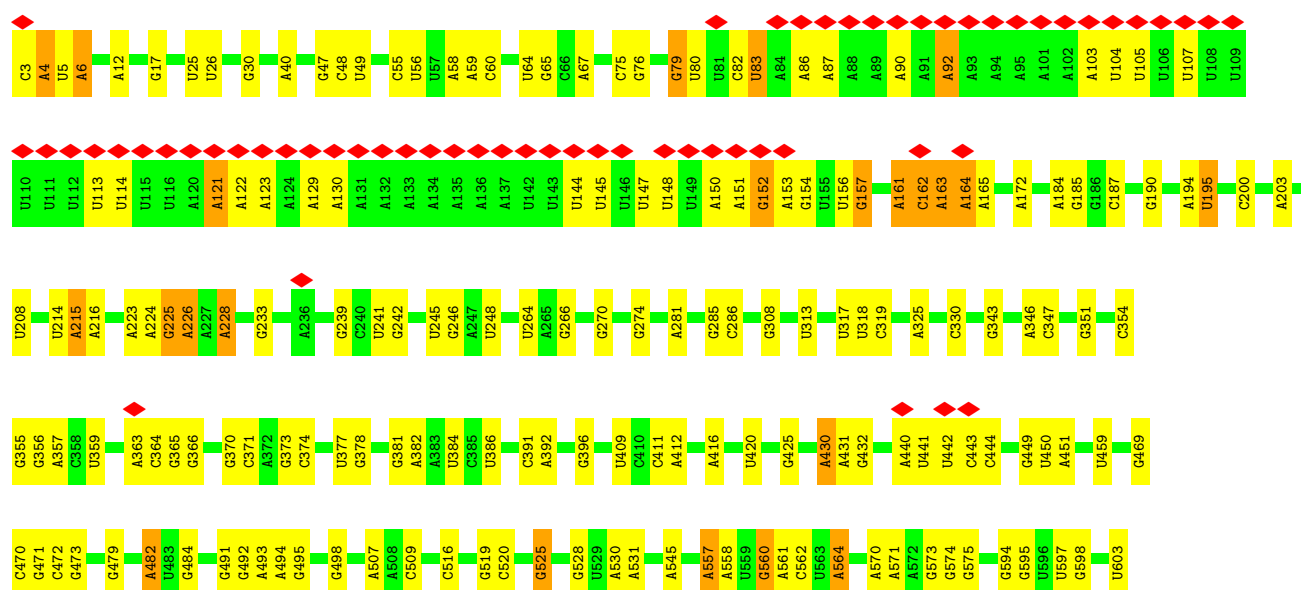
- Molecule 75: tRNA

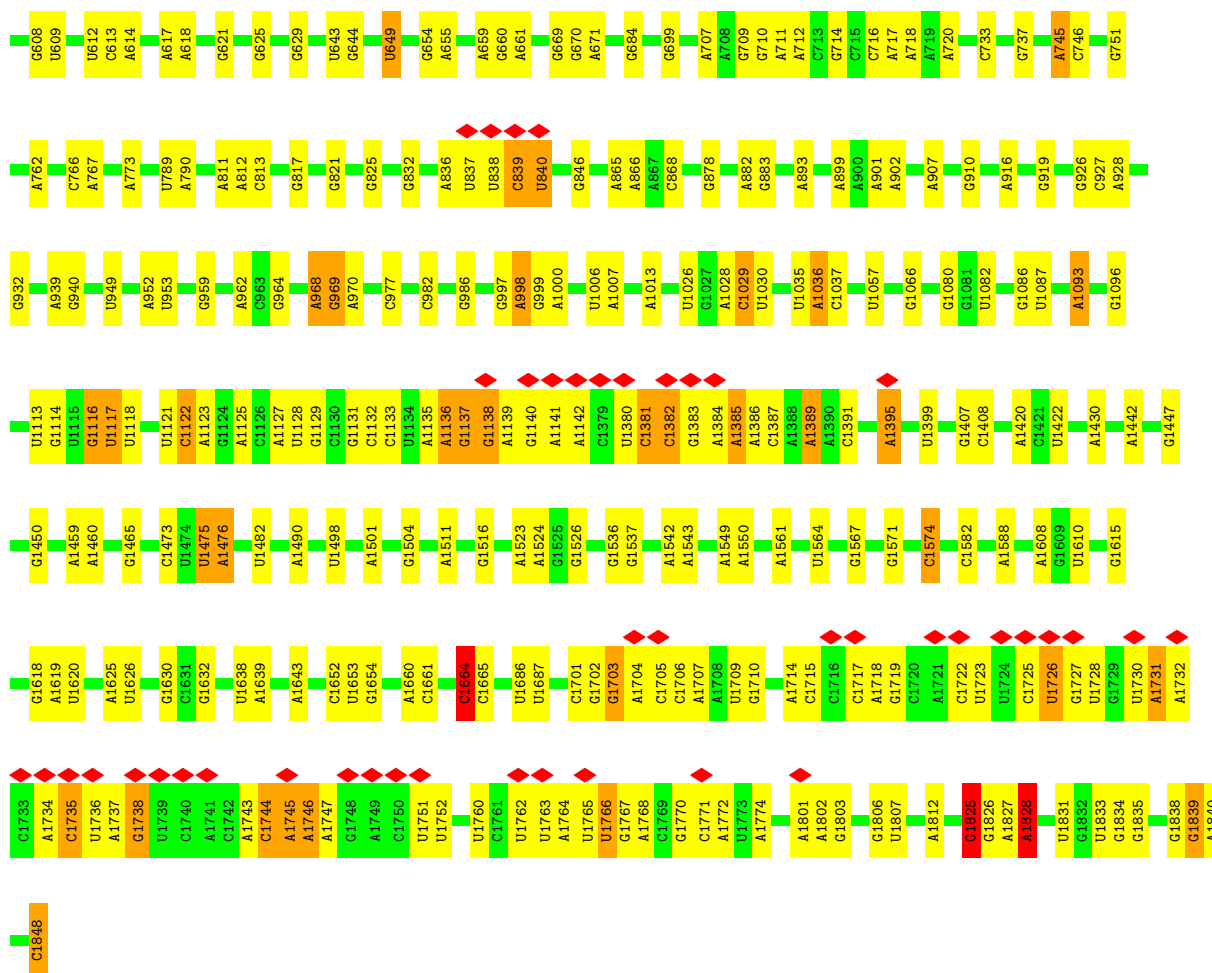
Chain 5: 5% 70% 29%



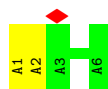
- Molecule 76: 18S rRNA

Chain 2: 7% 72% 25%

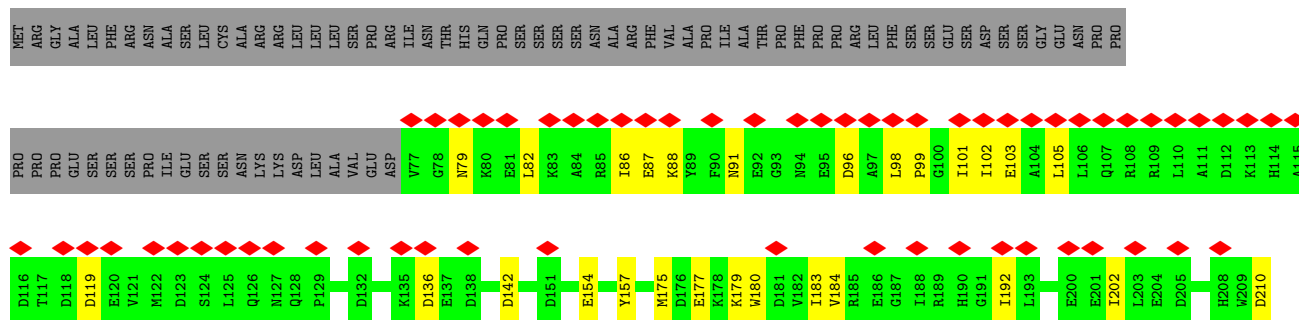


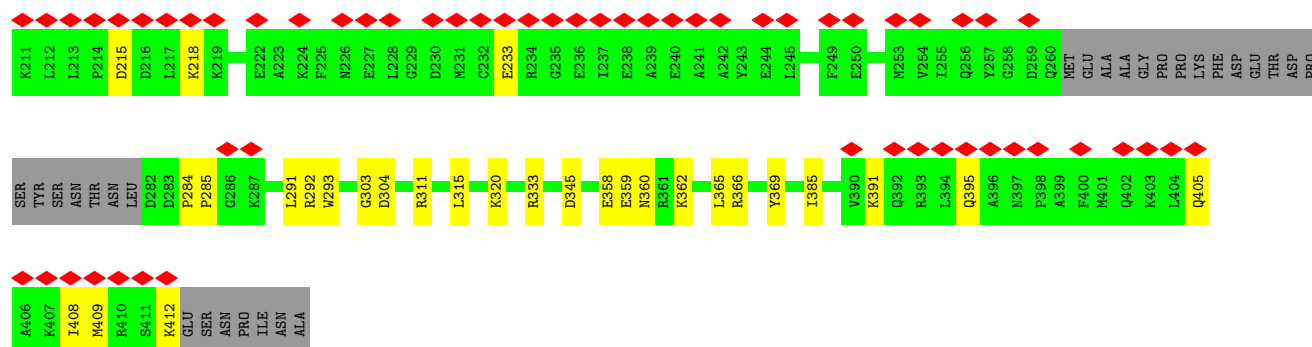


• Molecule 77: mRNA

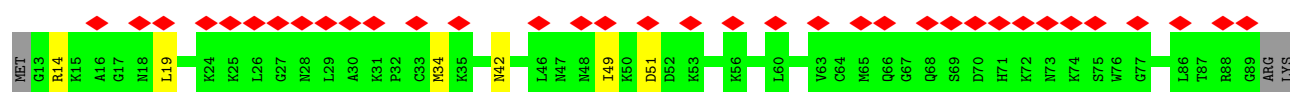
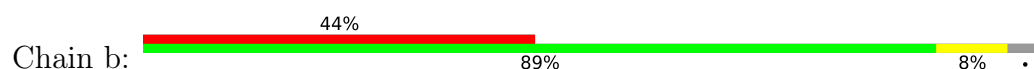


• Molecule 78: mS35

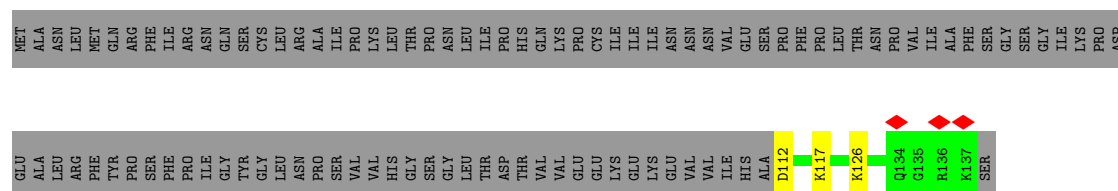




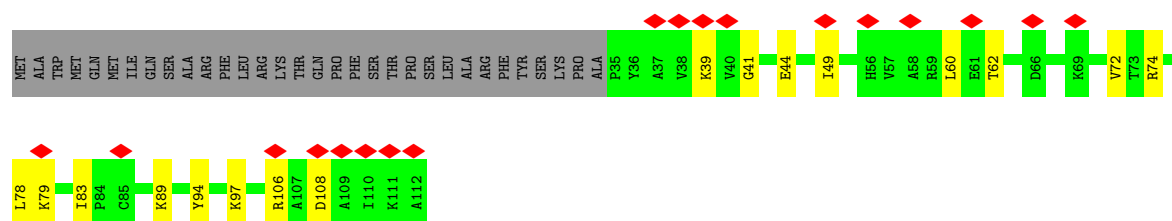
• Molecule 79: mS37



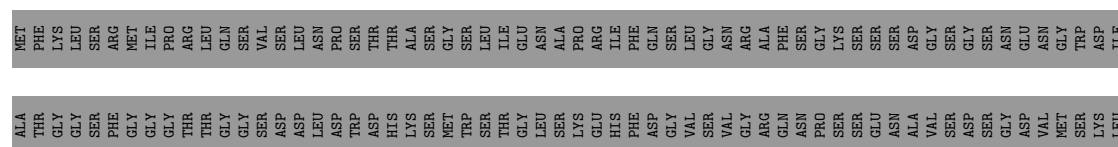
• Molecule 80: mS38

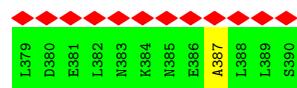


• Molecule 81: mS41

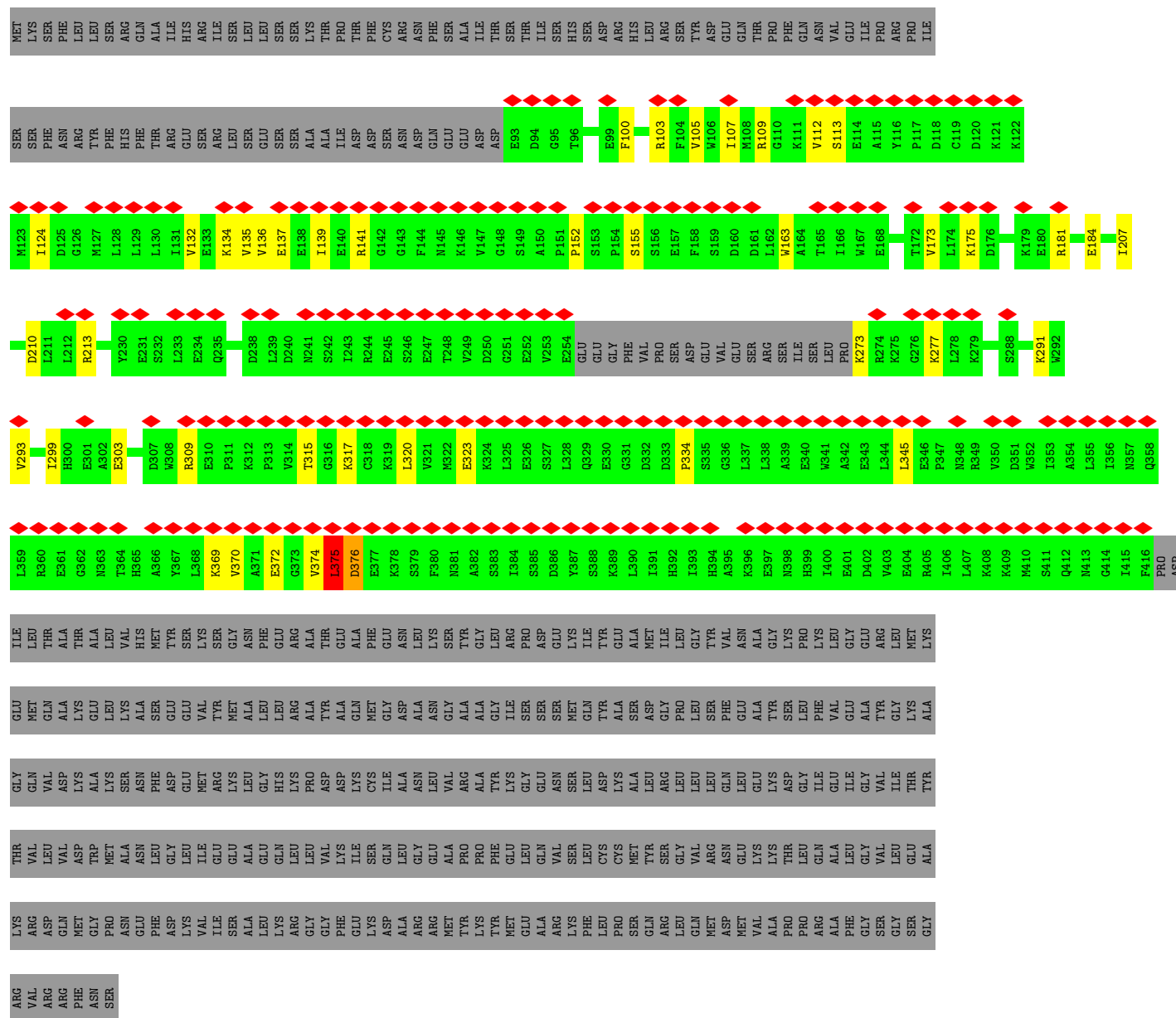
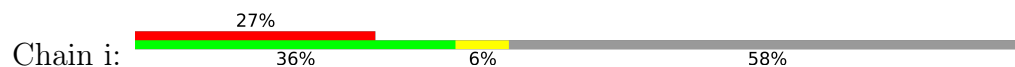


• Molecule 82: mS45

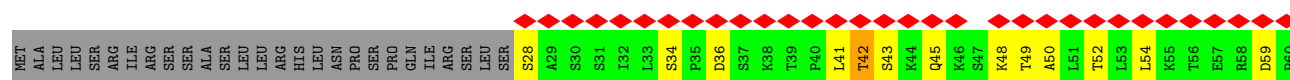


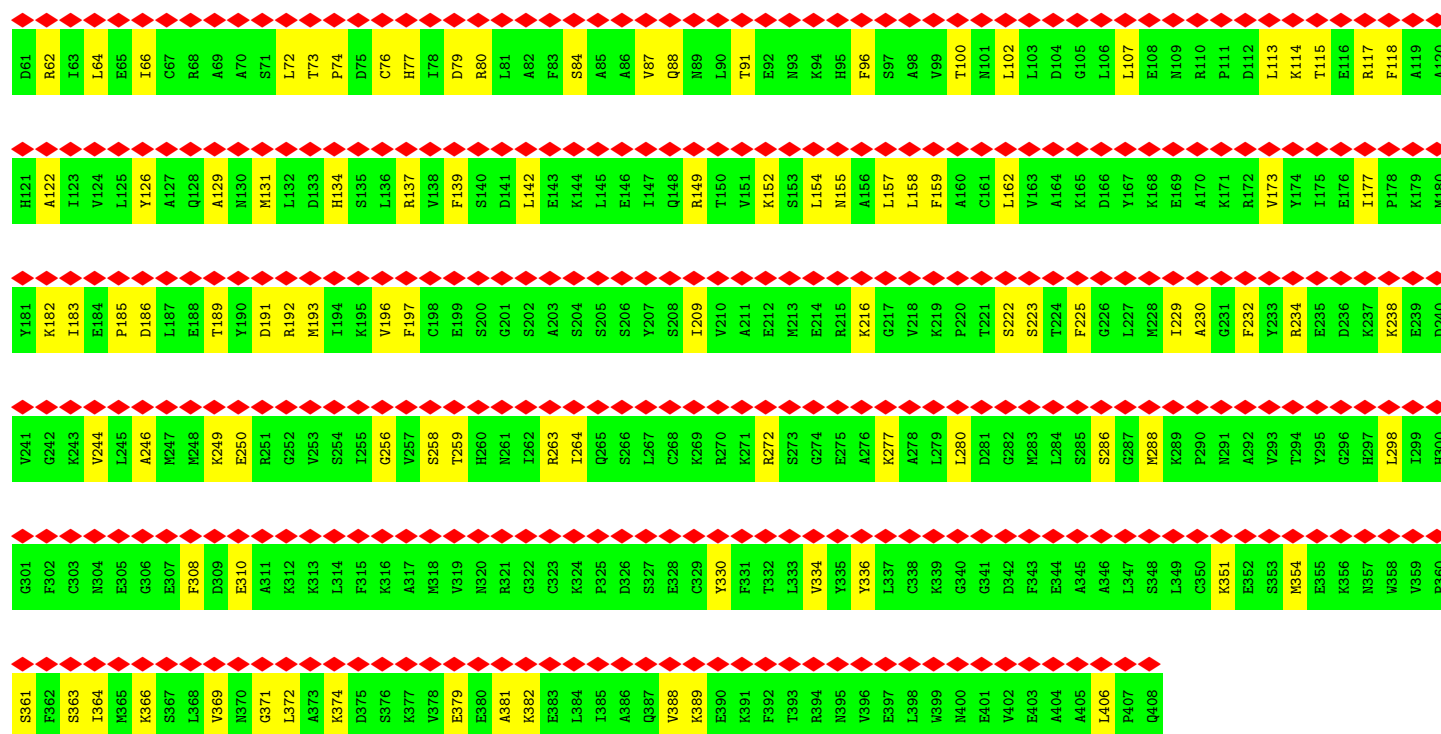


• Molecule 85: mS77 (NFD5)

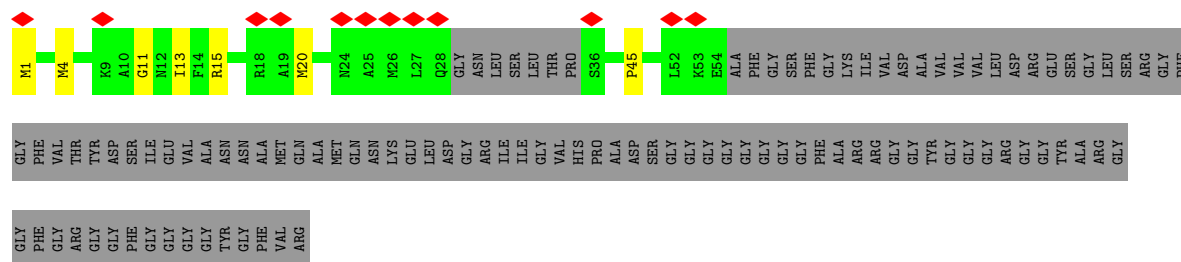


• Molecule 86: mS76 (rPPR1)

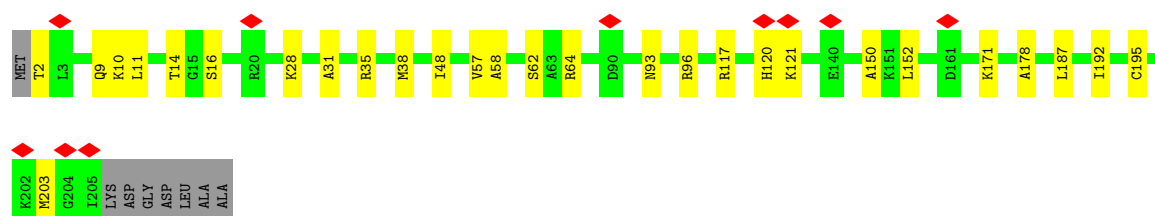
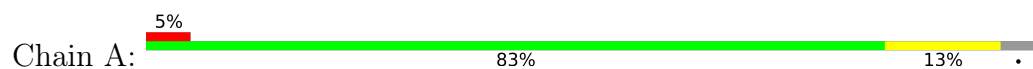




• Molecule 87: mS86



• Molecule 88: uS2m



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.541	Depositor
Minimum map value	-0.257	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0796	Depositor
Map size (Å)	596.712, 596.712, 596.712	wwPDB
Map dimensions	564, 564, 564	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, ZN, ATP, 2MG, 4OC, OMG, CLM, OMU, UR3, K, MA6, 5MU, G7M, PSU, OMC, H2U, MG, 2MA, 4SU

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	B	0.26	0/3969	0.54	2/5320 (0.0%)
2	C	0.27	0/2865	0.45	0/3836
3	D	0.27	0/3474	0.46	0/4647
4	E	0.27	0/838	0.41	0/1121
5	F	0.27	0/1225	0.53	0/1641
6	G	0.27	0/1054	0.44	0/1418
7	H	0.37	1/1707 (0.1%)	0.59	1/2287 (0.0%)
8	I	0.27	0/964	0.46	0/1293
9	J	0.38	0/1000	0.50	0/1340
10	K	0.24	0/1009	0.39	0/1345
11	L	0.32	0/950	0.52	0/1263
12	M	0.44	0/856	0.52	0/1134
13	N	0.26	0/958	0.41	0/1280
14	O	0.30	0/890	0.50	0/1196
15	P	0.28	0/730	0.48	1/984 (0.1%)
16	Q	0.23	0/733	0.41	0/978
17	R	0.24	0/1323	0.48	0/1772
18	S	0.27	0/614	0.41	0/809
19	T	0.28	0/416	0.40	0/547
20	U	0.51	1/1036 (0.1%)	0.90	8/1395 (0.6%)
21	V	0.19	0/1423	0.39	0/1895
22	W	0.22	0/3139	0.41	0/4250
23	X	0.27	0/1644	0.53	0/2216
24	Y	0.37	0/807	0.46	0/1077
25	Z	0.18	0/669	0.39	0/900
26	1	0.35	0/69733	0.40	1/108691 (0.0%)
27	3	0.31	0/2810	0.39	0/4378
28	1B	0.31	0/1347	0.43	0/1797
29	1C	0.38	0/1727	0.57	4/2311 (0.2%)
30	1D	0.32	0/2099	0.43	0/2836
31	1E	0.31	0/1786	0.41	0/2412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1F	0.26	0/1313	0.48	0/1772
33	1G	0.22	0/796	0.43	0/1067
34	1H	0.27	0/547	0.47	0/731
35	1I	0.24	0/1054	0.56	0/1417
36	1J	0.27	0/1155	0.61	1/1563 (0.1%)
37	1K	0.29	0/1553	0.36	0/2080
38	1L	0.30	0/976	0.47	0/1304
39	1M	0.32	0/1682	0.46	2/2248 (0.1%)
40	1N	0.28	0/1184	0.42	0/1580
41	1O	0.30	0/1255	0.43	0/1687
42	1P	0.28	0/895	0.47	0/1206
43	1Q	0.30	0/1022	0.39	0/1368
44	1R	0.37	0/930	0.41	0/1234
45	1S	0.31	0/1192	0.39	0/1602
46	1T	0.32	0/1259	0.41	0/1687
47	1U	0.28	0/1065	0.39	0/1421
48	1V	0.28	0/1247	0.37	0/1681
49	1W	0.24	0/1613	0.49	0/2180
50	1X	0.24	0/1703	0.41	0/2307
51	1Y	0.32	0/785	0.38	0/1051
52	1Z	0.31	0/1466	0.47	2/1954 (0.1%)
53	1a	0.32	0/946	0.43	0/1262
54	1b	0.30	0/818	0.47	0/1099
55	1c	0.29	0/501	0.44	0/666
56	1d	0.44	0/387	0.63	1/514 (0.2%)
57	1e	0.33	0/468	0.39	0/618
58	1f	0.40	0/370	0.43	0/486
59	1g	0.37	0/789	0.45	0/1048
60	1h	0.29	0/312	0.38	0/409
61	1i	0.24	0/1440	0.38	0/1927
62	1j	0.35	0/586	0.41	0/789
63	1k	0.32	0/970	0.45	0/1309
64	1l	0.26	0/1792	0.45	0/2423
65	1m	0.23	0/987	0.48	0/1331
66	1o	0.17	0/637	0.43	0/860
67	1p	0.26	0/1014	0.39	0/1349
68	1q	0.31	0/394	0.40	0/527
69	1r	0.26	0/750	0.45	0/1005
70	1s	0.27	0/1001	0.41	0/1327
71	1t	0.26	0/3919	0.48	0/5272
72	1u	0.24	0/5345	0.51	0/7180
73	1v	0.25	0/3497	0.46	0/4681
74	1x	0.19	0/18	0.26	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	5	0.24	0/1725	0.33	0/2689
76	2	0.29	0/37992	0.37	0/59224
77	6	0.19	0/146	0.22	0/225
78	a	0.25	0/2524	0.54	2/3387 (0.1%)
79	b	0.29	0/618	0.68	0/822
80	c	0.27	0/233	0.40	0/296
81	d	0.26	0/628	0.47	0/840
82	e	0.25	0/2118	0.48	0/2828
83	f	0.25	0/2981	0.50	0/4033
84	h	0.29	0/2507	0.54	0/3384
85	i	0.24	0/2532	0.49	1/3400 (0.0%)
86	j	0.24	0/3032	0.56	1/4073 (0.0%)
87	k	0.25	0/317	0.58	1/424 (0.2%)
88	A	0.25	0/1647	0.47	0/2227
All	All	0.31	2/224428 (0.0%)	0.43	28/325466 (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
7	H	0	1
11	L	0	1
30	1D	0	1
71	1t	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	404	LEU	CG-CD2	-5.93	1.32	1.52
20	U	81	PRO	N-CD	5.13	1.54	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	80	ASP	C-N-CD	-14.93	63.78	125.00
20	U	71	PRO	N-CA-C	-9.97	99.67	113.53
20	U	81	PRO	CA-N-CD	-9.66	98.47	112.00
36	1J	38	PRO	CA-N-CD	-9.01	99.39	112.00
20	U	61	ARG	N-CA-C	-8.98	101.90	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	3	PRO	CA-N-CD	-8.56	100.02	112.00
1	B	212	PRO	CA-N-CD	-8.47	100.14	112.00
56	1d	126	SER	N-CA-C	-8.01	97.20	109.85
78	a	284	PRO	N-CA-CB	7.28	110.14	103.08
29	1C	226	TRP	N-CA-C	-7.10	99.31	109.96
87	k	45	PRO	N-CA-CB	6.51	110.42	103.52
86	j	42	THR	CB-CA-C	-6.38	109.21	116.54
85	i	370	VAL	N-CA-C	6.37	116.53	110.42
78	a	285	PRO	N-CA-CB	5.83	110.03	102.86
29	1C	200	SER	CA-C-N	-5.77	113.50	122.16
29	1C	200	SER	C-N-CA	-5.77	113.50	122.16
20	U	93	THR	N-CA-C	-5.58	105.58	112.38
1	B	108	GLY	N-CA-C	-5.42	106.83	115.66
20	U	65	GLU	N-CA-C	-5.32	102.41	110.28
7	H	224	VAL	N-CA-C	-5.30	98.32	109.34
26	1	1566	U	P-O3'-C3'	5.29	128.13	120.20
39	1M	91	LYS	CA-C-N	5.26	131.58	121.54
39	1M	91	LYS	C-N-CA	5.26	131.58	121.54
29	1C	228	THR	N-CA-C	-5.26	107.53	114.31
20	U	72	ASN	N-CA-C	-5.07	101.32	109.39
20	U	67	LYS	N-CA-C	5.05	116.81	110.24
52	1Z	146	PHE	CA-C-N	5.05	128.36	120.68
52	1Z	146	PHE	C-N-CA	5.05	128.36	120.68

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	1D	225	ASP	Peptide
71	1t	462	HIS	Peptide
7	H	225	ILE	Peptide
11	L	136	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3877	0	4008	100	0
2	C	2811	0	2986	26	0
3	D	3425	0	3453	28	0
4	E	823	0	879	6	0
5	F	1254	0	1268	14	0
6	G	1037	0	1058	9	0
7	H	1682	0	1726	27	0
8	I	941	0	970	15	0
9	J	988	0	1022	13	0
10	K	992	0	1051	15	0
11	L	940	0	989	9	0
12	M	843	0	884	11	0
13	N	941	0	978	4	0
14	O	869	0	898	12	0
15	P	717	0	755	10	0
16	Q	724	0	744	10	0
17	R	1299	0	1307	21	0
18	S	611	0	687	7	0
19	T	408	0	444	4	0
20	U	1014	0	1061	62	0
21	V	1399	0	1427	10	0
22	W	3062	0	3030	23	0
23	X	1613	0	1559	57	0
24	Y	793	0	834	12	0
25	Z	649	0	662	5	0
26	1	62518	0	31499	260	0
27	3	2513	0	1275	4	0
28	1B	1325	0	1398	12	0
29	1C	1696	0	1745	51	0
30	1D	2045	0	2080	18	0
31	1E	1753	0	1815	19	0
32	1F	1286	0	1280	10	0
33	1G	779	0	810	5	0
34	1H	539	0	574	22	0
35	1I	1036	0	1084	40	0
36	1J	1129	0	1166	52	0
37	1K	1526	0	1586	8	0
38	1L	966	0	1048	6	0
39	1M	1649	0	1765	10	0
40	1N	1160	0	1206	6	0
41	1O	1231	0	1262	7	0
42	1P	878	0	939	3	0
43	1Q	1008	0	1101	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1R	915	0	946	6	0
45	1S	1170	0	1226	3	0
46	1T	1241	0	1346	5	0
47	1U	1048	0	1123	14	0
48	1V	1223	0	1278	12	0
49	1W	1588	0	1663	23	0
50	1X	1670	0	1751	10	0
51	1Y	768	0	792	7	0
52	1Z	1441	0	1485	17	0
53	1a	928	0	959	9	0
54	1b	803	0	845	12	0
55	1c	489	0	511	10	0
56	1d	379	0	416	1	0
57	1e	459	0	491	1	0
58	1f	364	0	398	1	0
59	1g	770	0	841	6	0
60	1h	309	0	337	0	0
61	1i	1424	0	1482	16	0
62	1j	570	0	593	9	0
63	1k	952	0	987	5	0
64	1l	1741	0	1707	19	0
65	1m	970	0	979	8	0
66	1o	626	0	657	11	0
67	1p	992	0	1027	8	0
68	1q	390	0	421	2	0
69	1r	735	0	781	16	0
70	1s	985	0	1072	8	0
71	1t	3856	0	3912	37	0
72	1u	5264	0	5353	74	0
73	1v	3440	0	3497	29	0
74	1x	19	0	14	0	0
75	5	1625	0	828	5	0
76	2	34081	0	17178	192	0
77	6	130	0	66	1	0
78	a	2487	0	2382	69	0
79	b	610	0	626	6	0
80	c	232	0	278	3	0
81	d	616	0	674	11	0
82	e	2074	0	2074	24	0
83	f	2922	0	2868	73	0
84	h	2460	0	2478	73	0
85	i	2487	0	2450	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	j	2984	0	3044	84	0
87	k	314	0	261	12	0
88	A	1611	0	1633	22	0
89	1	249	0	0	0	0
89	1D	1	0	0	0	0
89	1h	1	0	0	0	0
89	1j	1	0	0	0	0
89	1q	2	0	0	0	0
89	2	98	0	0	0	0
89	3	3	0	0	0	0
89	T	1	0	0	0	0
89	W	1	0	0	0	0
90	W	31	0	12	0	0
91	1	20	0	11	0	0
92	1	56	0	0	0	0
92	1B	3	0	0	0	0
92	1E	1	0	0	0	0
92	2	14	0	0	0	0
93	1d	1	0	0	0	0
93	1h	1	0	0	0	0
All	All	211395	0	164066	1717	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 5.

All (1717) 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)
75:5:54:5MU:C4	75:5:54:5MU:C5	1.82	1.65
36:1J:42:ASN:HB2	36:1J:73:HIS:CE1	1.37	1.60
29:1C:227:ARG:NH2	29:1C:229:HIS:HB2	1.21	1.44
36:1J:42:ASN:HB2	36:1J:73:HIS:NE2	1.33	1.41
29:1C:199:VAL:CG1	34:1H:97:ARG:HD2	1.53	1.39
16:Q:170:GLU:OE2	16:Q:174:LYS:CE	1.71	1.39
1:B:111:ARG:NH1	76:2:998:A:C2	1.96	1.32
83:f:323:GLY:N	83:f:334:ARG:HH22	1.27	1.31
29:1C:227:ARG:NH2	29:1C:229:HIS:CB	1.97	1.27
36:1J:42:ASN:CB	36:1J:73:HIS:CE1	2.17	1.27
12:M:150:LEU:HD22	12:M:155:GLU:OE1	1.36	1.25
36:1J:33:SER:CB	36:1J:34:PRO:HD3	1.67	1.22
1:B:243:PHE:CE2	23:X:393:LEU:HD21	1.75	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG22	1:B:109:CYS:H	1.06	1.17
29:1C:227:ARG:HH22	29:1C:229:HIS:CB	1.51	1.17
30:1D:115:ILE:CD1	30:1D:121:PHE:CE2	2.28	1.16
84:h:288:LEU:HD22	84:h:326:LEU:HD21	1.27	1.16
35:1I:49:ASN:HB2	35:1I:87:THR:CG2	1.74	1.16
83:f:323:GLY:CA	83:f:334:ARG:NH2	2.08	1.15
84:h:93:ILE:CG2	84:h:104:PRO:HG3	1.77	1.14
36:1J:33:SER:OG	36:1J:34:PRO:HD3	1.47	1.13
84:h:93:ILE:HG23	84:h:104:PRO:HG3	1.23	1.12
1:B:191:ILE:CD1	78:a:192:ILE:HD13	1.79	1.12
36:1J:42:ASN:N	36:1J:73:HIS:HE1	1.47	1.12
36:1J:33:SER:HB3	36:1J:34:PRO:CD	1.80	1.11
16:Q:170:GLU:OE2	16:Q:174:LYS:NZ	1.82	1.11
16:Q:170:GLU:OE2	16:Q:174:LYS:HE3	1.33	1.11
1:B:191:ILE:CD1	78:a:192:ILE:CD1	2.28	1.10
1:B:191:ILE:HD13	78:a:192:ILE:HD13	1.20	1.10
29:1C:199:VAL:HG11	34:1H:97:ARG:CD	1.82	1.09
29:1C:199:VAL:CG1	34:1H:97:ARG:CD	2.30	1.09
35:1I:49:ASN:HB2	35:1I:87:THR:HG21	1.17	1.09
36:1J:33:SER:CB	36:1J:34:PRO:CD	2.30	1.09
35:1I:49:ASN:CB	35:1I:87:THR:HG21	1.82	1.08
23:X:410:PRO:HG2	23:X:413:GLU:OE1	1.51	1.08
84:h:92:LYS:NZ	84:h:108:LEU:HD13	1.69	1.08
36:1J:42:ASN:H	36:1J:73:HIS:CE1	1.72	1.08
83:f:105:LEU:CD2	83:f:106:PRO:HD3	1.84	1.07
20:U:67:LYS:HB3	20:U:81:PRO:HG3	1.37	1.07
78:a:98:LEU:O	78:a:101:ILE:HG22	1.51	1.07
78:a:291:LEU:HB3	78:a:315:LEU:HD11	1.38	1.05
83:f:169:VAL:HG11	83:f:206:LYS:HE3	1.12	1.05
83:f:169:VAL:CG1	83:f:206:LYS:HE3	1.86	1.05
83:f:323:GLY:CA	83:f:334:ARG:HH22	1.64	1.04
83:f:323:GLY:N	83:f:334:ARG:NH2	2.04	1.03
83:f:169:VAL:HG11	83:f:206:LYS:CE	1.88	1.03
30:1D:115:ILE:HD12	30:1D:121:PHE:CE2	1.93	1.03
83:f:105:LEU:HD23	83:f:106:PRO:HD3	1.37	1.02
36:1J:33:SER:HB3	36:1J:34:PRO:HD3	1.38	1.01
69:1r:62:TYR:CE1	69:1r:124:VAL:HG13	1.94	1.00
35:1I:49:ASN:CB	35:1I:87:THR:CG2	2.37	1.00
12:M:150:LEU:CD2	12:M:155:GLU:OE1	2.09	1.00
54:1b:74:GLU:OE2	54:1b:78:LYS:HE3	1.60	1.00
86:j:173:VAL:HG13	86:j:177:ILE:HG13	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1J:38:PRO:HD2	36:1J:39:TYR:H	1.25	0.99
15:P:2:LYS:HB3	15:P:3:PRO:CD	1.91	0.99
31:1E:95:ASN:HB3	31:1E:101:LYS:HZ2	1.28	0.99
78:a:86:ILE:HD13	78:a:101:ILE:HD12	1.44	0.98
36:1J:42:ASN:N	36:1J:73:HIS:CE1	2.30	0.98
30:1D:115:ILE:HD11	30:1D:121:PHE:CE2	1.95	0.97
76:2:1726:U:H3	76:2:1744:C:H42	1.09	0.97
36:1J:42:ASN:CB	36:1J:73:HIS:NE2	2.19	0.96
84:h:288:LEU:CD2	84:h:326:LEU:HD21	1.96	0.95
26:1:1325:G:H1	26:1:1331:U:H3	1.12	0.94
83:f:42:GLN:CD	83:f:58:ARG:HH21	1.75	0.94
26:1:1594:G:H1	26:1:1657:U:H3	1.01	0.94
83:f:290:VAL:HG22	83:f:298:CYS:HB2	1.49	0.94
1:B:106:PRO:HD2	76:2:1028:A:N1	1.82	0.93
1:B:191:ILE:HD13	78:a:192:ILE:CD1	1.96	0.93
36:1J:36:LEU:C	36:1J:38:PRO:HD3	1.94	0.93
29:1C:227:ARG:CZ	29:1C:229:HIS:HB2	1.98	0.92
83:f:323:GLY:HA2	83:f:334:ARG:NH2	1.84	0.92
84:h:189:MET:SD	84:h:205:VAL:CG2	2.58	0.92
1:B:191:ILE:HD12	78:a:192:ILE:HD11	1.50	0.91
29:1C:199:VAL:HG21	34:1H:97:ARG:CB	2.00	0.91
1:B:107:ILE:HG22	1:B:109:CYS:N	1.84	0.91
36:1J:42:ASN:H	36:1J:73:HIS:HE1	0.96	0.90
78:a:86:ILE:HD13	78:a:101:ILE:CD1	2.02	0.90
83:f:105:LEU:CG	83:f:106:PRO:HD3	2.01	0.89
29:1C:199:VAL:HG11	34:1H:97:ARG:HD2	0.89	0.88
83:f:42:GLN:CD	83:f:58:ARG:NH2	2.30	0.88
86:j:48:LYS:O	86:j:52:THR:HG23	1.74	0.88
84:h:301:GLU:O	84:h:302:HIS:ND1	2.06	0.88
1:B:191:ILE:CD1	78:a:192:ILE:HD11	2.02	0.87
84:h:93:ILE:HG23	84:h:104:PRO:CG	2.04	0.86
78:a:98:LEU:C	78:a:101:ILE:HG22	2.00	0.86
83:f:206:LYS:NZ	85:i:315:THR:OG1	2.10	0.85
1:B:511:SER:O	1:B:517:GLN:OE1	1.92	0.85
84:h:189:MET:SD	84:h:205:VAL:HG22	2.17	0.85
23:X:410:PRO:CG	23:X:413:GLU:OE1	2.24	0.84
12:M:129:PHE:HE2	12:M:142:MET:SD	1.99	0.84
78:a:98:LEU:O	78:a:101:ILE:CG2	2.25	0.84
84:h:288:LEU:HD22	84:h:326:LEU:CD2	2.07	0.84
69:1r:62:TYR:HE1	69:1r:124:VAL:HG13	1.40	0.84
78:a:98:LEU:HA	78:a:101:ILE:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1J:42:ASN:CA	36:1J:73:HIS:HE1	1.91	0.84
83:f:389:THR:HG22	83:f:397:GLU:HB2	1.59	0.83
83:f:230:VAL:HG22	83:f:252:TYR:HB3	1.59	0.83
15:P:2:LYS:HB3	15:P:3:PRO:HD3	1.59	0.83
83:f:105:LEU:HD23	83:f:106:PRO:CD	2.09	0.83
29:1C:227:ARG:NH2	29:1C:229:HIS:CG	2.47	0.83
83:f:42:GLN:CG	83:f:58:ARG:HH21	1.91	0.82
36:1J:38:PRO:HD2	36:1J:39:TYR:N	1.94	0.82
87:k:20:MET:HE1	88:A:38:MET:CG	2.08	0.82
84:h:92:LYS:HZ1	84:h:108:LEU:HD13	1.44	0.81
78:a:98:LEU:CA	78:a:101:ILE:HG22	2.10	0.80
31:1E:95:ASN:CB	31:1E:101:LYS:HZ2	1.94	0.80
83:f:322:GLU:C	83:f:334:ARG:HH22	1.90	0.80
20:U:91:GLU:HA	20:U:94:LYS:HB2	1.65	0.79
12:M:129:PHE:CE2	12:M:142:MET:SD	2.76	0.79
35:1I:49:ASN:HD22	35:1I:87:THR:HG21	1.46	0.79
84:h:253:LYS:HG2	84:h:283:TYR:CE2	2.18	0.79
83:f:290:VAL:CG2	83:f:298:CYS:HB2	2.12	0.79
1:B:243:PHE:CE2	23:X:393:LEU:CD2	2.64	0.78
83:f:105:LEU:HG	83:f:106:PRO:HD3	1.64	0.78
86:j:264:ILE:HD11	86:j:298:LEU:HG	1.66	0.78
83:f:42:GLN:HG2	83:f:58:ARG:HH21	1.47	0.78
49:1W:31:HIS:NE2	49:1W:34:GLN:OE1	2.17	0.77
1:B:243:PHE:CZ	23:X:393:LEU:HD21	2.19	0.77
36:1J:37:GLY:N	36:1J:38:PRO:HD3	2.00	0.77
1:B:162:SER:OG	1:B:429:ASN:ND2	2.18	0.77
24:Y:7:LYS:O	24:Y:11:THR:HG23	1.85	0.77
36:1J:33:SER:HB3	36:1J:34:PRO:HD2	1.67	0.77
83:f:117:GLU:O	83:f:121:HIS:CD2	2.37	0.77
36:1J:29:GLY:O	36:1J:33:SER:HB2	1.84	0.77
84:h:330:LYS:HD3	84:h:375:VAL:HG21	1.67	0.77
53:1a:31:VAL:HG12	53:1a:32:LYS:HG3	1.66	0.77
29:1C:199:VAL:HG13	34:1H:97:ARG:CD	2.14	0.76
9:J:204:ASN:OD1	9:J:222:SER:HB2	1.84	0.76
76:2:26:U:H3	76:2:910:G:H1	1.33	0.76
85:i:372:GLU:O	85:i:375:LEU:HD22	1.85	0.76
86:j:96:PHE:O	86:j:100:THR:HG23	1.84	0.76
29:1C:199:VAL:CG2	34:1H:97:ARG:HD3	2.16	0.76
23:X:327:GLU:O	23:X:331:LEU:HG	1.84	0.76
29:1C:199:VAL:CG2	34:1H:97:ARG:CD	2.63	0.76
83:f:323:GLY:CA	83:f:334:ARG:HH21	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:1u:482:GLU:OE1	72:1u:513:ASN:ND2	2.19	0.75
36:1J:42:ASN:CB	36:1J:73:HIS:HE1	1.78	0.75
54:1b:100:ILE:O	54:1b:100:ILE:HG22	1.86	0.75
30:1D:115:ILE:HD12	30:1D:121:PHE:CZ	2.21	0.75
65:1m:11:GLU:HB2	65:1m:48:ARG:HH12	1.51	0.75
35:1I:49:ASN:HB2	35:1I:87:THR:HG23	1.69	0.75
20:U:67:LYS:HB3	20:U:81:PRO:CG	2.16	0.74
76:2:1726:U:H3	76:2:1744:C:N4	1.85	0.74
1:B:480:LYS:O	1:B:481:ARG:HB3	1.87	0.74
84:h:92:LYS:HZ3	84:h:108:LEU:HD13	1.52	0.74
35:1I:49:ASN:ND2	35:1I:87:THR:HG21	2.03	0.74
28:1B:43:VAL:HA	29:1C:53:MET:HE1	1.70	0.74
35:1I:49:ASN:CB	35:1I:87:THR:HG23	2.17	0.74
1:B:22:TRP:HB3	1:B:64:HIS:HB2	1.69	0.74
83:f:290:VAL:CG2	83:f:298:CYS:CB	2.66	0.74
5:F:143:ALA:O	5:F:144:HIS:ND1	2.21	0.73
35:1I:61:PHE:CE1	35:1I:73:LYS:HD3	2.24	0.73
36:1J:33:SER:OG	36:1J:34:PRO:CD	2.32	0.73
36:1J:33:SER:HG	36:1J:34:PRO:HD3	1.52	0.73
67:1p:16:VAL:O	67:1p:16:VAL:HG12	1.86	0.73
84:h:189:MET:SD	84:h:205:VAL:HG21	2.29	0.73
86:j:182:LYS:HG2	86:j:182:LYS:O	1.86	0.73
11:L:124:MET:SD	11:L:139:LYS:NZ	2.62	0.73
22:W:207:LYS:NZ	22:W:396:ASP:OD1	2.22	0.73
86:j:45:GLN:O	86:j:49:THR:HG23	1.88	0.72
7:H:236:ILE:HG12	88:A:9:GLN:HE22	1.55	0.72
9:J:199:LYS:HE2	9:J:201:LEU:HD21	1.72	0.72
36:1J:36:LEU:C	36:1J:38:PRO:CD	2.62	0.72
18:S:76:ASN:OD1	18:S:79:ARG:NH2	2.22	0.72
86:j:230:ALA:O	86:j:234:ARG:HG2	1.90	0.72
84:h:252:ARG:HG2	84:h:253:LYS:H	1.55	0.72
1:B:406:LYS:HD2	1:B:407:ARG:HH11	1.55	0.71
29:1C:225:LYS:HE3	29:1C:227:ARG:HA	1.72	0.71
83:f:42:GLN:OE1	83:f:58:ARG:NH2	2.23	0.71
36:1J:42:ASN:CA	36:1J:73:HIS:CE1	2.71	0.71
87:k:20:MET:HE1	88:A:38:MET:HG3	1.71	0.71
29:1C:199:VAL:HG21	34:1H:97:ARG:HB2	1.71	0.71
29:1C:199:VAL:HG22	34:1H:97:ARG:HD3	1.72	0.71
83:f:389:THR:CG2	83:f:397:GLU:HB2	2.20	0.71
29:1C:199:VAL:HG21	34:1H:97:ARG:CD	2.21	0.71
84:h:302:HIS:HA	84:h:360:ASP:OD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:246:LEU:HD13	88:A:10:LYS:HD2	1.74	0.70
84:h:301:GLU:C	84:h:302:HIS:ND1	2.50	0.70
83:f:169:VAL:CG1	83:f:206:LYS:CE	2.58	0.70
36:1J:38:PRO:CD	36:1J:39:TYR:H	2.04	0.69
69:1r:57:ILE:HG21	69:1r:88:LEU:HD21	1.75	0.69
69:1r:62:TYR:CE1	69:1r:124:VAL:CG1	2.73	0.69
83:f:269:MET:CE	83:f:273:TYR:CE1	2.75	0.69
84:h:301:GLU:O	84:h:302:HIS:CG	2.46	0.69
29:1C:227:ARG:HH22	29:1C:229:HIS:HB2	0.87	0.69
86:j:238:LYS:CE	86:j:272:ARG:HH12	2.06	0.68
49:1W:180:ILE:HG22	49:1W:181:ARG:HE	1.56	0.68
26:1:2432:A:N7	26:1:2433:G:N2	2.40	0.68
30:1D:115:ILE:CD1	30:1D:121:PHE:HE2	2.00	0.68
85:i:334:PRO:HG3	85:i:369:LYS:CG	2.24	0.68
7:H:245:MET:SD	85:i:291:LYS:NZ	2.67	0.68
27:3:53:A:OP2	42:1P:61:ARG:NH2	2.27	0.68
1:B:172:LEU:CD1	23:X:447:ARG:NH2	2.57	0.68
16:Q:170:GLU:OE2	16:Q:174:LYS:CD	2.42	0.68
86:j:158:LEU:HD22	86:j:192:ARG:HB3	1.75	0.68
86:j:154:LEU:HD21	86:j:177:ILE:HG21	1.76	0.68
87:k:20:MET:HE1	88:A:38:MET:HG2	1.76	0.68
81:d:72:VAL:O	81:d:74:ARG:NH1	2.27	0.67
20:U:62:LYS:O	20:U:63:HIS:C	2.37	0.67
7:H:395:ARG:NH2	76:2:1442:A:OP2	2.23	0.67
49:1W:209:LYS:HD2	49:1W:231:PRO:HG3	1.76	0.67
76:2:92:A:H61	86:j:192:ARG:HH22	1.42	0.67
78:a:292:ARG:O	78:a:315:LEU:HD12	1.95	0.67
35:1I:61:PHE:HE1	35:1I:73:LYS:HD3	1.57	0.67
47:1U:131:GLN:HE21	47:1U:134:ARG:HD2	1.60	0.67
78:a:98:LEU:HA	78:a:101:ILE:CG2	2.23	0.66
84:h:103:MET:HG2	84:h:140:LEU:HD11	1.76	0.66
26:1:338:A:N7	72:1u:241:ARG:NH1	2.43	0.66
69:1r:124:VAL:HG12	69:1r:125:LEU:N	2.09	0.66
76:2:163:A:H4'	76:2:164:A:H5'	1.78	0.66
26:1:1044:A:O2'	50:1X:250:ARG:NH2	2.27	0.66
2:C:182:LYS:HG3	2:C:220:LEU:HD22	1.77	0.66
84:h:342:LEU:HD13	84:h:387:ALA:O	1.95	0.66
86:j:87:VAL:O	86:j:91:THR:HG23	1.96	0.66
5:F:43:GLU:CD	5:F:44:ARG:H	2.04	0.66
26:1:1203:C:H5'	65:1m:79:ARG:HH12	1.60	0.66
31:1E:95:ASN:ND2	31:1E:101:LYS:NZ	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD12	23:X:447:ARG:NH2	2.11	0.65
1:B:243:PHE:HE2	23:X:393:LEU:HD21	1.53	0.65
26:1:463:G:OP1	48:1V:25:ARG:NH1	2.29	0.65
35:1I:30:ASN:ND2	35:1I:79:MET:SD	2.69	0.65
23:X:327:GLU:OE1	23:X:331:LEU:CD1	2.45	0.65
29:1C:168:PHE:O	29:1C:172:SER:HB3	1.97	0.65
29:1C:199:VAL:HG21	34:1H:97:ARG:HB3	1.76	0.65
85:i:334:PRO:HD3	85:i:369:LYS:HE2	1.77	0.65
62:1j:82:ILE:O	62:1j:83:GLU:HG3	1.97	0.65
11:L:135:ALA:HB3	11:L:139:LYS:HE2	1.77	0.65
15:P:2:LYS:CB	15:P:3:PRO:HD3	2.26	0.65
86:j:77:HIS:ND1	86:j:80:ARG:NH2	2.45	0.65
26:1:64:G:O2'	26:1:66:G:N7	2.28	0.65
86:j:91:THR:HG21	86:j:129:ALA:HB2	1.77	0.65
26:1:522:G:N7	52:1Z:99:ARG:NH2	2.45	0.65
84:h:168:LYS:HB3	84:h:189:MET:HE1	1.78	0.64
53:1a:130:ASP:OD1	53:1a:131:PRO:HD2	1.97	0.64
36:1J:34:PRO:O	36:1J:38:PRO:HG3	1.96	0.64
84:h:330:LYS:NZ	84:h:368:LEU:HD11	2.13	0.64
21:V:47:GLU:HG3	21:V:49:TYR:H	1.62	0.64
30:1D:195:GLY:O	30:1D:199:ARG:HB2	1.97	0.64
76:2:200:C:H5	76:2:246:G:H1	1.45	0.64
78:a:405:GLN:O	78:a:409:MET:HG2	1.97	0.64
1:B:480:LYS:O	1:B:481:ARG:CB	2.46	0.64
83:f:290:VAL:CG1	83:f:299:LYS:HZ3	2.10	0.64
84:h:93:ILE:HG21	84:h:104:PRO:HG3	1.73	0.64
35:1I:27:ILE:HD11	35:1I:83:ILE:HD12	1.80	0.64
84:h:113:ILE:HG22	84:h:125:LEU:HD11	1.79	0.63
23:X:345:ALA:HA	23:X:353:MET:HE1	1.79	0.63
35:1I:27:ILE:HD11	35:1I:83:ILE:CD1	2.28	0.63
9:J:205:THR:HG21	9:J:239:ALA:HA	1.79	0.63
7:H:357:THR:OG1	7:H:361:TRP:NE1	2.31	0.63
26:1:2446:G:N3	26:1:2476:A:O2'	2.31	0.63
35:1I:61:PHE:CD1	35:1I:73:LYS:NZ	2.61	0.63
49:1W:58:ILE:HG12	49:1W:140:ILE:HG23	1.80	0.63
9:J:251:LYS:HD3	9:J:282:TYR:CE1	2.34	0.63
26:1:2420:G:H1	26:1:2490:U:H3	1.44	0.62
72:1u:150:ARG:NH1	72:1u:187:MET:SD	2.71	0.62
31:1E:95:ASN:ND2	31:1E:101:LYS:HZ1	1.97	0.62
1:B:481:ARG:HD3	78:a:154:GLU:HB3	1.80	0.62
82:e:312:LEU:HD21	82:e:370:MET:HE1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:i:334:PRO:HG3	85:i:369:LYS:HG3	1.80	0.62
88:A:58:ALA:HB2	88:A:195:CYS:HB3	1.80	0.62
64:1l:151:LYS:HE2	64:1l:157:LEU:HD23	1.81	0.62
1:B:172:LEU:O	1:B:176:SER:HB3	2.00	0.62
21:V:155:LEU:O	21:V:159:GLU:HG3	1.99	0.62
1:B:111:ARG:NH1	76:2:998:A:N1	2.45	0.62
53:1a:34:ALA:HB1	53:1a:39:GLU:HB2	1.81	0.62
23:X:373:HIS:O	23:X:377:VAL:HG23	2.00	0.62
65:1m:9:LYS:HE2	65:1m:44:LEU:HD13	1.82	0.62
76:2:90:A:OP1	86:j:117:ARG:NH2	2.32	0.62
84:h:92:LYS:CE	84:h:108:LEU:HD13	2.30	0.62
71:1t:448:PHE:HA	71:1t:451:LEU:HB2	1.81	0.62
85:i:303:GLU:OE2	88:A:2:THR:N	2.33	0.62
86:j:107:LEU:CD2	86:j:118:PHE:CE2	2.83	0.62
26:1:1432:A:OP2	26:1:1988:C:N4	2.33	0.61
26:1:2078:C:H5	43:1Q:209:ARG:HH21	1.48	0.61
83:f:83:ASN:O	83:f:138:LYS:NZ	2.33	0.61
83:f:323:GLY:HA3	83:f:334:ARG:NH2	2.10	0.61
10:K:114:ARG:HB2	10:K:119:ALA:HB3	1.82	0.61
17:R:156:ARG:NH2	76:2:1013:A:OP1	2.32	0.61
9:J:191:THR:OG1	9:J:192:ASN:ND2	2.33	0.61
29:1C:189:PHE:O	29:1C:190:ASP:HB2	2.01	0.61
76:2:151:A:H5''	76:2:152:G:H5'	1.82	0.61
7:H:430:ARG:NH2	75:5:33:U:OP2	2.32	0.61
30:1D:115:ILE:HD11	30:1D:121:PHE:CD2	2.36	0.61
36:1J:82:PRO:O	36:1J:121:LYS:NZ	2.33	0.61
73:1v:295:ARG:NH1	73:1v:331:ASN:OD1	2.34	0.61
76:2:1731:A:OP1	84:h:219:GLY:N	2.32	0.61
83:f:249:LEU:O	83:f:253:SER:OG	2.10	0.61
28:1B:49:LYS:HA	28:1B:52:HIS:HD2	1.65	0.61
84:h:252:ARG:HG2	84:h:253:LYS:N	2.15	0.61
2:C:178:LYS:HE2	2:C:224:MET:HE1	1.83	0.61
49:1W:153:LYS:HA	49:1W:188:GLY:O	2.01	0.61
82:e:193:HIS:HB2	82:e:205:LEU:HD11	1.83	0.61
20:U:55:TYR:HA	20:U:58:ARG:HH21	1.66	0.61
29:1C:199:VAL:CB	34:1H:97:ARG:HD2	2.29	0.61
1:B:194:LEU:HD12	78:a:192:ILE:HD11	1.81	0.61
36:1J:111:VAL:HG23	36:1J:112:ARG:HG3	1.83	0.61
86:j:91:THR:HG21	86:j:129:ALA:CB	2.31	0.61
26:1:438:G:H1	26:1:447:U:H3	1.49	0.61
1:B:375:LYS:NZ	78:a:99:PRO:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1J:38:PRO:CD	36:1J:39:TYR:N	2.62	0.60
54:1b:74:GLU:OE2	54:1b:78:LYS:CE	2.43	0.60
83:f:269:MET:HE1	83:f:273:TYR:CE1	2.35	0.60
76:2:1734:A:H2'	76:2:1735:C:H4'	1.83	0.60
5:F:11:LEU:HD11	5:F:54:VAL:HG21	1.84	0.60
7:H:406:ARG:NH1	7:H:407:ASP:O	2.34	0.60
35:1I:49:ASN:CG	35:1I:87:THR:HG21	2.25	0.60
71:1t:450:SER:O	71:1t:453:ARG:NH1	2.34	0.60
84:h:330:LYS:HZ1	84:h:368:LEU:HD11	1.66	0.60
86:j:107:LEU:HD21	86:j:118:PHE:CD2	2.36	0.60
2:C:206:ARG:NH2	3:D:90:GLU:OE2	2.33	0.60
5:F:8:GLN:HB3	5:F:47:ILE:HD11	1.84	0.60
20:U:81:PRO:HD2	20:U:82:ALA:N	2.17	0.60
26:1:2142:U:O2'	28:1B:87:LEU:O	2.19	0.60
17:R:206:LYS:HD2	76:2:949:U:H1'	1.83	0.60
71:1t:322:PHE:HB2	71:1t:340:MET:HE1	1.83	0.60
73:1v:287:LEU:HD11	73:1v:306:VAL:HG23	1.84	0.60
1:B:481:ARG:CZ	78:a:154:GLU:OE1	2.49	0.60
10:K:44:LYS:HD3	76:2:1801:A:H5'	1.84	0.60
26:1:1257:G:OP1	35:1I:57:ASN:ND2	2.35	0.60
26:1:1649:C:OP1	49:1W:41:ARG:NH1	2.35	0.60
6:G:79:ASP:OD1	6:G:123:GLN:NE2	2.30	0.60
9:J:269:LYS:O	9:J:273:ASN:ND2	2.32	0.60
10:K:16:ARG:O	10:K:17:ARG:NH1	2.34	0.60
20:U:70:GLU:HB3	87:k:15:ARG:HH11	1.67	0.60
26:1:636:G:N3	46:1T:165:ASN:ND2	2.48	0.60
64:1l:101:LYS:NZ	64:1l:207:ASP:OD1	2.30	0.60
26:1:445:G:H21	26:1:465:U:H3'	1.67	0.60
26:1:926:A:OP1	28:1B:151:ARG:NH2	2.35	0.60
26:1:3000:C:H5'	26:1:3153:A:H5'	1.84	0.60
69:1r:35:SER:OG	69:1r:36:ARG:N	2.35	0.60
76:2:570:A:OP2	80:c:112:ASP:N	2.35	0.60
1:B:111:ARG:HH12	76:2:998:A:H2	1.42	0.59
26:1:891:PSU:HO2'	26:1:2916:C:HO2'	1.47	0.59
36:1J:105:THR:HG21	36:1J:149:LYS:HD3	1.84	0.59
71:1t:173:GLN:OE1	71:1t:176:ARG:NH1	2.34	0.59
84:h:93:ILE:CG2	84:h:104:PRO:CG	2.68	0.59
5:F:143:ALA:HB1	79:b:34:MET:HE3	1.84	0.59
84:h:323:LYS:O	84:h:327:GLU:HG3	2.02	0.59
2:C:64:THR:HG21	3:D:459:ARG:HG3	1.84	0.59
5:F:140:ARG:NH2	9:J:227:ASP:OD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1023:A:N6	26:1:1047:A:O2'	2.35	0.59
29:1C:194:ILE:O	29:1C:195:PRO:C	2.41	0.59
54:1b:39:GLU:HG3	54:1b:44:ARG:HH12	1.67	0.59
49:1W:204:LEU:HD22	49:1W:208:ASP:HB3	1.85	0.59
83:f:323:GLY:HA3	83:f:334:ARG:HH21	1.66	0.59
26:1:132:C:O2	53:1a:132:ARG:NH2	2.35	0.59
7:H:224:VAL:HG12	7:H:225:ILE:H	1.68	0.59
26:1:336:A:OP2	72:1u:240:LYS:NZ	2.36	0.59
26:1:2124:C:H5'	28:1B:79:MET:HE1	1.84	0.59
86:j:280:LEU:HD22	86:j:298:LEU:HD11	1.84	0.59
26:1:1169:U:OP2	37:1K:173:ARG:NH2	2.35	0.59
86:j:107:LEU:CD2	86:j:118:PHE:CD2	2.85	0.59
23:X:327:GLU:OE1	23:X:331:LEU:HD11	2.03	0.59
36:1J:37:GLY:N	36:1J:38:PRO:CD	2.66	0.59
55:1c:20:ARG:HB3	61:1i:225:THR:HG21	1.85	0.58
65:1m:10:ILE:HD11	65:1m:22:CYS:HB2	1.84	0.58
84:h:257:ASP:OD1	84:h:279:ARG:NH2	2.36	0.58
86:j:277:LYS:NZ	86:j:310:GLU:OE1	2.36	0.58
39:1M:246:PRO:O	67:1p:81:ARG:NH2	2.36	0.58
71:1t:146:LEU:HD11	71:1t:164:LEU:HD11	1.84	0.58
76:2:1129:G:H5''	78:a:320:LYS:HE3	1.84	0.58
1:B:109:CYS:SG	1:B:110:LEU:N	2.77	0.58
31:1E:95:ASN:HD22	31:1E:101:LYS:HZ1	1.51	0.58
20:U:76:ALA:O	87:k:13:ILE:HG22	2.03	0.58
26:1:334:A:H5'	72:1u:272:GLU:HG3	1.85	0.58
23:X:420:PRO:HB2	78:a:202:ILE:HD11	1.85	0.58
63:1k:33:GLU:HG2	63:1k:81:LEU:HD22	1.85	0.58
76:2:968:A:H4'	76:2:969:G:H5''	1.84	0.58
24:Y:40:LYS:NZ	76:2:1536:G:N7	2.52	0.58
67:1p:16:VAL:O	67:1p:16:VAL:CG1	2.52	0.58
71:1t:43:LEU:HD11	71:1t:77:LEU:HD13	1.85	0.58
1:B:399:MET:HE1	78:a:101:ILE:CG2	2.34	0.58
22:W:372:THR:HB	22:W:375:SER:HB3	1.85	0.58
28:1B:123:ARG:NH2	29:1C:324:CYS:O	2.36	0.58
29:1C:227:ARG:HH22	29:1C:229:HIS:HB3	1.59	0.58
61:1i:102:ARG:NH2	67:1p:123:GLU:OE2	2.34	0.58
76:2:79:G:H22	76:2:161:A:H2	1.52	0.58
1:B:39:ARG:NH1	1:B:60:CYS:O	2.31	0.58
10:K:81:LEU:HD23	10:K:98:ILE:HD12	1.86	0.58
27:3:45:C:O2	32:1F:98:ARG:NH1	2.36	0.58
35:1I:49:ASN:HB3	35:1I:87:THR:CG2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:1t:325:TRP:O	71:1t:329:CYS:HB3	2.03	0.58
1:B:481:ARG:CD	78:a:154:GLU:HB3	2.34	0.58
21:V:133:ASP:OD1	21:V:136:ARG:NH2	2.37	0.58
72:1u:572:ASP:OD2	72:1u:574:HIS:NE2	2.37	0.58
86:j:107:LEU:HD21	86:j:118:PHE:CE2	2.39	0.58
24:Y:95:ARG:HD2	76:2:1473:C:OP1	2.04	0.58
26:1:690:C:O2'	26:1:691:A:N7	2.37	0.58
26:1:2123:G:N7	28:1B:112:SER:OG	2.35	0.58
76:2:670:G:H2'	76:2:671:A:H8	1.68	0.58
86:j:73:THR:HG22	86:j:113:LEU:HD11	1.85	0.58
86:j:122:ALA:O	86:j:126:TYR:HB2	2.04	0.58
86:j:238:LYS:HE3	86:j:272:ARG:HH12	1.69	0.58
26:1:1594:G:O6	26:1:1657:U:O4	2.21	0.57
69:1r:62:TYR:CZ	69:1r:124:VAL:CG1	2.86	0.57
76:2:1131:G:OP1	78:a:333:ARG:NH2	2.36	0.57
84:h:330:LYS:CD	84:h:375:VAL:CG2	2.81	0.57
84:h:342:LEU:HD12	84:h:387:ALA:CB	2.34	0.57
64:1l:93:GLU:HA	64:1l:96:LYS:HG2	1.86	0.57
86:j:330:TYR:O	86:j:334:VAL:HG23	2.04	0.57
1:B:111:ARG:NH1	76:2:998:A:N3	2.48	0.57
20:U:80:ASP:O	20:U:81:PRO:C	2.46	0.57
26:1:1247:U:O2	36:1J:39:TYR:OH	2.22	0.57
61:1i:230:ILE:HB	61:1i:233:TYR:HB2	1.85	0.57
86:j:238:LYS:CE	86:j:272:ARG:NH1	2.66	0.57
1:B:423:MET:HA	1:B:426:PHE:CE2	2.39	0.57
20:U:81:PRO:HD2	20:U:82:ALA:H	1.69	0.57
26:1:1220:A:N7	26:1:1246:A:O2'	2.37	0.57
78:a:88:LYS:HZ1	78:a:96:ASP:HB3	1.69	0.57
86:j:149:ARG:HG2	86:j:183:ILE:HD11	1.86	0.57
1:B:461:LYS:NZ	1:B:527:SER:OG	2.38	0.57
15:P:3:PRO:HD2	15:P:3:PRO:O	2.04	0.57
67:1p:118:LYS:NZ	67:1p:122:GLU:OE2	2.36	0.57
9:J:237:TYR:OH	79:b:42:ASN:OD1	2.23	0.57
20:U:72:ASN:O	20:U:74:VAL:HG23	2.05	0.57
23:X:403:ILE:HG23	78:a:366:ARG:HE	1.69	0.57
26:1:855:G:H22	26:1:865:G:H22	1.53	0.57
26:1:1171:A:OP2	37:1K:84:ARG:NH2	2.37	0.57
86:j:173:VAL:HG13	86:j:177:ILE:CG1	2.27	0.57
72:1u:255:ARG:NH1	72:1u:287:SER:O	2.38	0.57
72:1u:406:GLN:NE2	72:1u:411:ASP:O	2.38	0.57
1:B:376:VAL:HG12	1:B:376:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:90:GLN:OE1	24:Y:93:HIS:HD2	1.87	0.57
38:1L:140:THR:HG22	38:1L:141:ASP:H	1.70	0.57
84:h:301:GLU:O	84:h:302:HIS:CE1	2.58	0.57
26:1:87:A:H5'	48:1V:39:ILE:HG23	1.87	0.57
29:1C:207:ARG:NH1	52:1Z:142:GLU:OE2	2.38	0.57
35:1I:28:ASN:O	35:1I:109:ASN:ND2	2.31	0.57
35:1I:49:ASN:HB3	35:1I:87:THR:HG23	1.87	0.57
54:1b:99:SER:OG	54:1b:100:ILE:N	2.38	0.57
78:a:293:TRP:CD2	78:a:315:LEU:HD13	2.40	0.57
84:h:278:LEU:HD23	84:h:281:GLU:OE1	2.05	0.57
85:i:334:PRO:CD	85:i:369:LYS:CE	2.82	0.57
29:1C:199:VAL:CG2	34:1H:97:ARG:HD2	2.34	0.56
55:1c:21:LEU:HD23	61:1i:147:LEU:HD21	1.86	0.56
61:1i:127:MET:O	64:1l:64:ARG:NH1	2.37	0.56
76:2:161:A:H2'	76:2:162:C:H4'	1.86	0.56
76:2:1391:C:OP2	76:2:1395:A:N6	2.37	0.56
83:f:269:MET:HE3	83:f:273:TYR:CE1	2.39	0.56
83:f:290:VAL:CG1	83:f:299:LYS:NZ	2.68	0.56
84:h:330:LYS:HD3	84:h:375:VAL:CG2	2.35	0.56
15:P:64:SER:OG	15:P:65:LYS:N	2.37	0.56
26:1:855:G:H1	26:1:865:G:H22	1.52	0.56
26:1:1143:G:OP2	44:1R:40:ARG:NH2	2.39	0.56
18:S:48:GLN:NE2	76:2:1848:C:OP2	2.38	0.56
20:U:80:ASP:O	20:U:82:ALA:N	2.38	0.56
21:V:39:GLU:HG3	21:V:40:THR:HG23	1.87	0.56
35:1I:50:THR:HG22	35:1I:85:VAL:HG13	1.88	0.56
78:a:101:ILE:HG23	78:a:102:ILE:N	2.20	0.56
84:h:168:LYS:CB	84:h:189:MET:HE1	2.36	0.56
7:H:231:ALA:HB1	7:H:234:ASP:HB2	1.87	0.56
72:1u:436:VAL:O	72:1u:440:ASN:ND2	2.38	0.56
76:2:1096:G:OP2	88:A:117:ARG:NH2	2.37	0.56
26:1:1625:C:O2'	26:1:1626:G:N7	2.39	0.56
52:1Z:147:ASN:ND2	52:1Z:149:GLU:OE1	2.32	0.56
71:1t:345:THR:HB	71:1t:378:TYR:HB2	1.88	0.56
80:c:112:ASP:O	80:c:117:LYS:NZ	2.37	0.56
84:h:203:GLU:OE2	84:h:236:LEU:HD21	2.06	0.56
23:X:477:VAL:HG13	23:X:478:PRO:HD2	1.88	0.56
26:1:87:A:N3	48:1V:37:ARG:NH2	2.54	0.56
38:1L:148:ARG:NH2	76:2:359:U:OP2	2.38	0.56
26:1:3117:U:OP2	43:1Q:110:LYS:NZ	2.38	0.56
61:1i:193:MET:HE1	64:1l:230:MET:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:1u:513:ASN:HA	72:1u:516:ARG:HE	1.71	0.56
85:i:334:PRO:HG3	85:i:369:LYS:HG2	1.88	0.56
20:U:63:HIS:O	20:U:64:PRO:C	2.48	0.56
52:1Z:59:VAL:HG22	52:1Z:66:LYS:HG2	1.88	0.56
83:f:290:VAL:CG2	83:f:298:CYS:HB3	2.35	0.56
1:B:172:LEU:HD13	23:X:447:ARG:NH2	2.21	0.56
1:B:187:VAL:HG21	1:B:329:THR:HG22	1.88	0.56
20:U:69:VAL:O	87:k:15:ARG:NH1	2.39	0.56
22:W:190:ILE:HG12	22:W:205:PRO:HB2	1.87	0.56
26:1:2788:C:N3	40:1N:168:LYS:NZ	2.53	0.56
32:1F:178:GLN:NE2	61:1i:221:ARG:O	2.37	0.56
35:1I:61:PHE:CE1	35:1I:73:LYS:CD	2.89	0.56
36:1J:28:PRO:HA	36:1J:32:VAL:HB	1.87	0.56
41:1O:140:ARG:NH2	43:1Q:104:LYS:O	2.39	0.56
73:1v:326:ASN:OD1	73:1v:359:THR:OG1	2.24	0.56
76:2:1000:A:H62	76:2:1026:U:H3	1.53	0.56
69:1r:124:VAL:CG1	69:1r:125:LEU:N	2.69	0.55
1:B:20:SER:OG	1:B:39:ARG:NH2	2.39	0.55
7:H:412:GLU:OE2	7:H:415:LYS:NZ	2.39	0.55
76:2:1524:A:H2	76:2:1537:G:H21	1.54	0.55
81:d:106:ARG:HE	81:d:108:ASP:HB3	1.71	0.55
15:P:8:VAL:HG22	15:P:19:VAL:HG22	1.88	0.55
26:1:3057:C:O2	26:1:3058:U:N3	2.38	0.55
50:1X:139:LEU:HD22	50:1X:166:LEU:HD13	1.88	0.55
7:H:241:ILE:HG13	7:H:245:MET:HE3	1.87	0.55
23:X:327:GLU:OE1	23:X:331:LEU:HD12	2.06	0.55
26:1:2190:U:O2'	26:1:2191:U:O4'	2.24	0.55
48:1V:38:VAL:HG22	48:1V:45:VAL:HG12	1.89	0.55
83:f:268:GLU:O	83:f:272:ARG:HG3	2.07	0.55
26:1:513:G:H21	26:1:515:C:H5'	1.71	0.55
26:1:1540:U:OP1	62:1j:33:ARG:NH2	2.40	0.55
53:1a:71:ASP:OD1	53:1a:75:LYS:NZ	2.38	0.55
76:2:411:C:H2'	76:2:412:A:H8	1.72	0.55
76:2:561:A:HO2'	76:2:564:A:HO2'	1.54	0.55
83:f:117:GLU:O	83:f:121:HIS:HD2	1.86	0.55
2:C:28:ASN:ND2	3:D:146:SER:O	2.40	0.55
3:D:131:GLN:NE2	76:2:430:A:OP1	2.38	0.55
17:R:94:GLY:O	17:R:101:ASN:ND2	2.37	0.55
26:1:757:U:OP2	31:1E:300:ARG:NH2	2.34	0.55
76:2:1137:G:H21	76:2:1389:A:H62	1.54	0.55
23:X:381:ASP:OD1	23:X:455:TYR:OH	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:2:83:U:H3	76:2:157:G:H1	1.54	0.55
76:2:354:C:H2'	76:2:355:G:H8	1.72	0.55
85:i:136:VAL:HA	85:i:139:ILE:HG12	1.89	0.55
20:U:70:GLU:H	20:U:71:PRO:HD2	1.72	0.55
26:1:1446:C:H2'	26:1:1447:A:H8	1.72	0.55
51:1Y:82:ILE:HG22	51:1Y:83:VAL:HG23	1.89	0.55
76:2:225:G:O2'	76:2:226:A:N7	2.37	0.55
78:a:180:TRP:O	78:a:184:VAL:HG23	2.07	0.55
86:j:246:ALA:O	86:j:250:GLU:HG3	2.07	0.55
3:D:344:ARG:NH1	3:D:348:THR:HB	2.22	0.55
20:U:58:ARG:HB2	20:U:62:LYS:HE3	1.89	0.55
75:5:50:U:H3	75:5:64:G:H1	1.55	0.55
6:G:18:ARG:NH2	76:2:868:C:O2'	2.38	0.55
22:W:302:GLY:HA3	64:1l:81:TYR:HE1	1.72	0.55
47:1U:127:HIS:ND1	71:1t:126:TYR:OH	2.40	0.55
26:1:3136:C:OP1	69:1r:90:SER:OG	2.24	0.54
35:1l:27:ILE:CD1	35:1l:83:ILE:CD1	2.85	0.54
76:2:669:G:H2'	76:2:670:G:C8	2.42	0.54
85:i:334:PRO:HD2	85:i:369:LYS:HE3	1.88	0.54
3:D:92:GLN:HG2	3:D:95:ARG:HH22	1.71	0.54
8:I:133:ALA:HB3	8:I:215:GLU:HB3	1.88	0.54
19:T:50:ARG:NH1	76:2:1498:U:OP1	2.40	0.54
23:X:401:PRO:HD2	78:a:365:LEU:HD22	1.89	0.54
26:1:1252:C:H2'	26:1:1253:A:H8	1.73	0.54
11:L:105:GLU:HA	11:L:108:ARG:HG2	1.89	0.54
26:1:1922:G:O6	73:1v:190:ARG:NH2	2.40	0.54
84:h:156:LYS:HA	84:h:159:VAL:HG12	1.89	0.54
85:i:134:LYS:NZ	85:i:155:SER:OG	2.41	0.54
1:B:98:TRP:CE2	23:X:331:LEU:CD2	2.90	0.54
26:1:2443:G:N1	26:1:2474:A:OP1	2.41	0.54
30:1D:178:PRO:HD3	30:1D:255:ILE:HD12	1.89	0.54
36:1J:70:TYR:HD2	36:1J:74:SER:O	1.91	0.54
48:1V:118:ARG:HE	48:1V:122:LEU:HD12	1.71	0.54
14:O:107:THR:HG23	14:O:109:ARG:H	1.71	0.54
20:U:91:GLU:CA	20:U:94:LYS:HB2	2.36	0.54
23:X:335:VAL:O	23:X:335:VAL:HG12	2.08	0.54
26:1:228:U:H3	26:1:240:A:H2	1.56	0.54
36:1J:100:ARG:HB3	36:1J:104:LEU:HD13	1.88	0.54
86:j:50:ALA:O	86:j:54:LEU:HB2	2.07	0.54
22:W:271:LEU:HD22	22:W:322:VAL:HG13	1.90	0.54
76:2:1745:A:OP2	84:h:147:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:135:ARG:HG2	8:I:185:LYS:HG3	1.90	0.54
8:I:224:LEU:HD11	78:a:369:TYR:HE1	1.73	0.54
15:P:10:SER:HB3	15:P:18:VAL:HB	1.90	0.54
26:1:2420:G:N2	26:1:2490:U:O2	2.37	0.54
59:1g:115:TYR:HD2	59:1g:118:TYR:CE2	2.26	0.54
72:1u:130:LEU:HD21	72:1u:160:LEU:HD23	1.90	0.54
76:2:241:U:H2'	76:2:242:G:H8	1.73	0.54
49:1W:177:LEU:HD11	49:1W:233:CYS:HB2	1.88	0.54
72:1u:192:ILE:HG23	72:1u:204:SER:HB3	1.88	0.54
76:2:1381:C:O2'	76:2:1382:C:O4'	2.21	0.54
2:C:119:THR:HB	2:C:121:PRO:HD2	1.88	0.54
26:1:1186:G:OP1	37:1K:173:ARG:NH1	2.39	0.54
26:1:1903:A:OP1	70:1s:85:LYS:NZ	2.40	0.54
37:1K:65:ARG:NH1	37:1K:67:ASP:OD2	2.41	0.54
67:1p:89:ILE:HG22	67:1p:93:LYS:HE2	1.90	0.54
73:1v:490:THR:OG1	73:1v:493:GLU:OE1	2.26	0.54
78:a:142:ASP:N	78:a:142:ASP:OD1	2.38	0.54
84:h:342:LEU:HD12	84:h:387:ALA:HB1	1.90	0.54
21:V:176:ILE:HG12	21:V:184:LYS:HD2	1.89	0.53
23:X:360:TYR:HA	23:X:363:ILE:HD12	1.89	0.53
72:1u:446:ALA:HB1	72:1u:449:ARG:HE	1.72	0.53
82:e:189:MET:HG3	82:e:205:LEU:HD22	1.89	0.53
85:i:374:VAL:O	85:i:376:ASP:N	2.41	0.53
86:j:185:PRO:O	86:j:216:LYS:NZ	2.31	0.53
1:B:154:GLN:NE2	78:a:304:ASP:OD2	2.38	0.53
26:1:978:A:H2'	26:1:979:G:H8	1.73	0.53
38:1L:63:LYS:HZ1	38:1L:91:MET:HE2	1.72	0.53
52:1Z:4:ARG:NH2	52:1Z:120:ASP:O	2.41	0.53
71:1t:460:LYS:NZ	71:1t:461:SER:O	2.33	0.53
72:1u:294:ASN:O	72:1u:298:ASN:ND2	2.42	0.53
72:1u:306:MET:HB3	72:1u:340:ARG:HH12	1.73	0.53
85:i:334:PRO:CD	85:i:369:LYS:HE3	2.39	0.53
22:W:295:LEU:HD21	22:W:310:MET:HG3	1.90	0.53
26:1:855:G:H1	26:1:865:G:H1	1.56	0.53
36:1J:36:LEU:CA	36:1J:38:PRO:HD3	2.37	0.53
82:e:228:GLU:OE1	82:e:232:LYS:NZ	2.38	0.53
32:1F:165:THR:HG22	32:1F:167:ASP:H	1.73	0.53
43:1Q:148:VAL:O	43:1Q:153:ARG:HA	2.08	0.53
69:1r:62:TYR:OH	69:1r:124:VAL:CG1	2.56	0.53
76:2:1828:MA6:OP1	80:c:126:LYS:NZ	2.42	0.53
84:h:94:LEU:HA	84:h:97:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:193:LEU:HD21	16:Q:213:ILE:HG21	1.90	0.53
29:1C:227:ARG:HH21	29:1C:229:HIS:CG	2.25	0.53
1:B:108:GLY:O	1:B:109:CYS:HB3	2.09	0.53
26:1:1255:U:H2'	26:1:1256:G:H8	1.74	0.53
29:1C:109:PHE:CZ	29:1C:195:PRO:HB3	2.44	0.53
52:1Z:21:ILE:HD12	52:1Z:26:LYS:HG2	1.89	0.53
61:1i:230:ILE:HD13	64:1l:88:ALA:HB2	1.91	0.53
78:a:291:LEU:CB	78:a:315:LEU:HD11	2.27	0.53
1:B:172:LEU:CD1	23:X:447:ARG:HH21	2.22	0.53
5:F:31:ILE:HD13	5:F:107:LEU:HD23	1.91	0.53
26:1:275:A:H2'	26:1:276:A:H8	1.73	0.53
49:1W:162:PHE:HE2	49:1W:165:LEU:HD11	1.74	0.53
85:i:334:PRO:CD	85:i:369:LYS:HE2	2.39	0.53
1:B:104:ALA:O	1:B:106:PRO:HD3	2.08	0.53
26:1:2150:C:O2'	26:1:2289:U:OP2	2.27	0.53
52:1Z:47:LEU:HB3	52:1Z:93:VAL:HG12	1.90	0.53
64:1l:213:LYS:NZ	64:1l:231:ILE:O	2.42	0.53
72:1u:440:ASN:HA	72:1u:443:LYS:HG2	1.91	0.53
20:U:87:CYS:O	20:U:91:GLU:HG2	2.09	0.53
26:1:2382:C:O2'	26:1:2560:OMG:N2	2.40	0.53
44:1R:15:GLY:O	44:1R:18:LYS:NZ	2.42	0.53
55:1c:21:LEU:O	61:1i:225:THR:OG1	2.27	0.53
1:B:399:MET:HE1	78:a:101:ILE:HG23	1.89	0.53
31:1E:285:ASP:OD2	31:1E:289:LYS:NZ	2.38	0.53
73:1v:93:THR:HG22	73:1v:96:GLN:HG2	1.91	0.53
78:a:183:ILE:HG22	78:a:183:ILE:O	2.09	0.53
9:J:246:ILE:O	9:J:250:VAL:HG23	2.08	0.52
26:1:338:A:H62	72:1u:241:ARG:HH22	1.56	0.52
26:1:1693:C:H2'	26:1:1694:A:C8	2.45	0.52
78:a:175:MET:HG3	78:a:179:LYS:HG2	1.90	0.52
78:a:293:TRP:CH2	78:a:315:LEU:HD22	2.44	0.52
83:f:290:VAL:HG13	83:f:299:LYS:NZ	2.25	0.52
85:i:152:PRO:HD2	85:i:163:TRP:HE1	1.74	0.52
17:R:132:MET:HE2	17:R:134:ARG:HG3	1.91	0.52
36:1J:25:LYS:O	36:1J:25:LYS:HG2	2.08	0.52
86:j:41:LEU:HD21	86:j:49:THR:OG1	2.09	0.52
86:j:84:SER:O	86:j:88:GLN:HG3	2.09	0.52
1:B:52:THR:HG21	78:a:136:ASP:HB2	1.92	0.52
20:U:74:VAL:HG12	20:U:75:SER:N	2.24	0.52
26:1:553:G:OP2	26:1:2711:U:O2'	2.24	0.52
26:1:2502:A:N1	26:1:2535:C:N4	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1I:6:ARG:HA	35:1I:9:LEU:HD12	1.91	0.52
72:1u:697:LYS:HB3	72:1u:700:ASN:HB2	1.90	0.52
76:2:710:G:H2'	76:2:711:A:C8	2.44	0.52
83:f:103:ASP:HB3	83:f:106:PRO:HG2	1.92	0.52
86:j:238:LYS:NZ	86:j:272:ARG:NH1	2.57	0.52
1:B:511:SER:HG	1:B:517:GLN:HE22	1.57	0.52
14:O:24:ASP:OD1	76:2:248:U:O2'	2.27	0.52
26:1:443:A:N3	26:1:463:G:O2'	2.43	0.52
26:1:1153:G:OP2	68:1q:35:THR:OG1	2.26	0.52
26:1:1619:G:N1	26:1:1634:U:N3	2.57	0.52
26:1:1693:C:H2'	26:1:1694:A:H8	1.75	0.52
72:1u:497:PHE:CE2	72:1u:501:MET:HE2	2.43	0.52
73:1v:182:ILE:HD12	73:1v:194:VAL:HG13	1.92	0.52
76:2:939:A:H2'	76:2:940:G:C8	2.44	0.52
88:A:57:VAL:HG11	88:A:192:ILE:HG23	1.90	0.52
23:X:488:PHE:O	23:X:492:VAL:HG23	2.09	0.52
26:1:1001:G:H2'	26:1:1002:A:C8	2.45	0.52
69:1r:62:TYR:CZ	69:1r:124:VAL:HG13	2.44	0.52
78:a:87:GLU:OE2	78:a:91:ASN:ND2	2.41	0.52
86:j:64:LEU:HD23	86:j:102:LEU:HD13	1.91	0.52
26:1:1309:C:OP1	54:1b:45:ARG:NH1	2.42	0.52
36:1J:64:ALA:HB3	36:1J:80:LYS:HB3	1.91	0.52
76:2:215:A:H2'	76:2:216:A:C8	2.45	0.52
8:I:131:CYS:HB2	8:I:217:GLN:HB2	1.92	0.52
64:1l:122:ALA:HB3	64:1l:182:LEU:HD21	1.92	0.52
1:B:172:LEU:HA	23:X:447:ARG:NH2	2.25	0.52
2:C:325:THR:HG21	2:C:327:LYS:HE2	1.92	0.52
7:H:388:GLN:HE22	7:H:395:ARG:HH11	1.56	0.52
12:M:126:ARG:NH1	12:M:131:GLY:O	2.43	0.52
20:U:63:HIS:HB3	20:U:110:TYR:CE2	2.45	0.52
26:1:2837:G:O2'	26:1:2966:A:N1	2.41	0.52
72:1u:616:ASP:OD1	72:1u:617:LEU:N	2.43	0.52
1:B:172:LEU:HA	23:X:447:ARG:CZ	2.40	0.52
8:I:215:GLU:HG3	8:I:217:GLN:HE21	1.74	0.52
11:L:36:ASN:ND2	32:1F:137:GLU:OE2	2.43	0.52
17:R:175:ARG:HB3	17:R:182:HIS:HB3	1.92	0.52
84:h:146:PHE:HB3	84:h:150:LEU:HD23	1.92	0.52
2:C:225:GLN:NE2	82:e:250:GLU:OE2	2.43	0.52
49:1W:69:ASP:O	49:1W:75:ARG:NH2	2.42	0.52
63:1k:59:LYS:HG3	63:1k:69:VAL:HG22	1.92	0.52
64:1l:35:ARG:HD3	64:1l:103:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:1u:451:ILE:HD12	72:1u:492:LYS:HZ1	1.74	0.52
86:j:134:HIS:CE1	86:j:137:ARG:HH21	2.27	0.52
9:J:204:ASN:HD21	9:J:221:THR:HB	1.74	0.51
26:1:1575:A:H5'	71:1t:91:SER:HB3	1.93	0.51
26:1:1978:U:O2'	26:1:2084:C:O2'	2.28	0.51
35:1I:27:ILE:CD1	35:1I:83:ILE:HD11	2.40	0.51
69:1r:72:SER:O	69:1r:76:THR:OG1	2.25	0.51
72:1u:89:ASP:N	72:1u:89:ASP:OD1	2.42	0.51
76:2:392:A:OP1	81:d:89:LYS:NZ	2.38	0.51
8:I:130:ILE:HD11	8:I:197:LEU:HD22	1.92	0.51
18:S:95:ILE:HA	18:S:98:VAL:HG12	1.92	0.51
24:Y:90:GLN:HB2	24:Y:93:HIS:HB2	1.91	0.51
59:1g:131:LEU:HD11	59:1g:155:PRO:HB2	1.91	0.51
71:1t:22:ASP:OD1	71:1t:22:ASP:N	2.43	0.51
14:O:6:ARG:NE	14:O:23:THR:OG1	2.43	0.51
26:1:1423:G:O2'	26:1:2330:G:O6	2.28	0.51
35:1I:7:ALA:HA	35:1I:59:LEU:HD21	1.91	0.51
52:1Z:4:ARG:HA	52:1Z:7:GLU:HG2	1.91	0.51
86:j:107:LEU:HD23	86:j:118:PHE:CE2	2.44	0.51
1:B:174:ARG:CZ	23:X:366:ARG:HD2	2.40	0.51
10:K:27:CYS:SG	76:2:382:A:N6	2.83	0.51
23:X:362:ASP:OD1	23:X:362:ASP:O	2.27	0.51
29:1C:192:PRO:HG2	29:1C:195:PRO:CG	2.41	0.51
66:1o:96:VAL:HA	66:1o:99:LEU:HD12	1.92	0.51
72:1u:183:TRP:HZ3	72:1u:214:LEU:HB3	1.76	0.51
7:H:388:GLN:HE22	7:H:395:ARG:NH1	2.08	0.51
20:U:58:ARG:O	20:U:61:ARG:N	2.43	0.51
20:U:59:PHE:HA	20:U:62:LYS:HB2	1.93	0.51
84:h:330:LYS:CD	84:h:375:VAL:HG21	2.37	0.51
86:j:152:LYS:HA	86:j:155:ASN:HB3	1.91	0.51
2:C:165:GLU:OE1	2:C:168:ARG:NH2	2.44	0.51
10:K:42:PRO:HB3	10:K:89:ASP:HB3	1.92	0.51
23:X:422:ILE:HD11	23:X:434:TRP:HH2	1.76	0.51
26:1:494:A:H5'	72:1u:167:ASN:HB2	1.92	0.51
26:1:2828:G:HO2'	26:1:3066:A:HO2'	1.58	0.51
29:1C:195:PRO:O	34:1H:93:GLN:NE2	2.37	0.51
62:1j:49:LYS:HE3	70:1s:78:PRO:HB3	1.92	0.51
64:1I:132:PRO:HB3	64:1I:153:VAL:HG21	1.91	0.51
69:1r:58:SER:OG	69:1r:106:MET:SD	2.67	0.51
73:1v:90:GLU:OE1	73:1v:97:ARG:NH2	2.44	0.51
76:2:1618:G:H2'	76:2:1619:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:k:1:MET:HE1	87:k:4:MET:HB3	1.92	0.51
1:B:400:ILE:HA	1:B:403:ILE:HG22	1.92	0.51
17:R:132:MET:HE3	17:R:133:SER:H	1.74	0.51
26:1:1993:G:H5'	41:1O:36:THR:HG21	1.92	0.51
17:R:48:LYS:NZ	17:R:57:VAL:O	2.44	0.51
26:1:539:A:OP2	72:1u:83:ASN:ND2	2.44	0.51
32:1F:4:LEU:HD21	32:1F:106:LEU:HD23	1.92	0.51
76:2:107:U:H5''	86:j:258:SER:HB3	1.93	0.51
76:2:377:U:H2'	76:2:378:G:H8	1.76	0.51
76:2:381:G:N2	76:2:384:U:OP2	2.42	0.51
83:f:228:GLY:HA2	83:f:231:GLU:HG2	1.92	0.51
86:j:351:LYS:HG3	86:j:354:MET:HE2	1.91	0.51
1:B:107:ILE:CG2	1:B:109:CYS:H	1.99	0.51
7:H:230:ARG:HD3	20:U:79:PRO:HG2	1.93	0.51
65:1m:8:VAL:HG23	65:1m:58:VAL:HG12	1.92	0.51
71:1t:134:CYS:HB2	71:1t:167:LEU:HB2	1.93	0.51
73:1v:263:GLU:OE1	73:1v:266:ARG:NH2	2.36	0.51
86:j:158:LEU:HD23	86:j:162:LEU:HD23	1.93	0.51
1:B:67:LYS:HD3	78:a:303:GLY:HA2	1.93	0.51
4:E:43:PHE:HB2	4:E:64:LEU:HB3	1.92	0.51
20:U:70:GLU:CD	87:k:15:ARG:HD3	2.36	0.51
26:1:691:A:H1'	26:1:692:A:H5'	1.93	0.51
26:1:1500:A:O2'	26:1:1502:U:OP1	2.29	0.51
26:1:2827:U:O2'	26:1:2956:C:OP1	2.25	0.51
29:1C:227:ARG:NH2	29:1C:229:HIS:CD2	2.79	0.51
76:2:1013:A:H2	76:2:1482:U:H1'	1.76	0.51
83:f:107:LEU:HD22	83:f:119:CYS:SG	2.51	0.51
2:C:17:LEU:HG	76:2:451:A:H4'	1.92	0.50
6:G:8:ASP:OD1	76:2:821:G:O2'	2.24	0.50
20:U:89:VAL:HA	20:U:92:LEU:HB2	1.93	0.50
24:Y:16:VAL:HG12	24:Y:17:GLY:N	2.26	0.50
25:Z:51:LYS:HB3	25:Z:55:GLU:HB2	1.91	0.50
29:1C:185:PHE:HE2	52:1Z:138:LEU:HD13	1.76	0.50
30:1D:115:ILE:CD1	30:1D:121:PHE:CZ	2.87	0.50
86:j:91:THR:CG2	86:j:129:ALA:HB2	2.40	0.50
86:j:91:THR:CG2	86:j:129:ALA:CB	2.88	0.50
2:C:151:ILE:HG12	2:C:329:VAL:HG22	1.93	0.50
76:2:195:U:O2'	76:2:281:A:N3	2.38	0.50
10:K:31:THR:OG1	76:2:382:A:H5'	2.11	0.50
26:1:1649:C:O3'	49:1W:53:ARG:NH2	2.44	0.50
26:1:2579:A:O2'	51:1Y:65:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:3159:U:OP1	41:1O:132:ARG:NH1	2.45	0.50
29:1C:227:ARG:CZ	29:1C:227:ARG:HB2	2.41	0.50
35:1I:13:LYS:O	35:1I:17:ASN:ND2	2.44	0.50
73:1v:79:PHE:HZ	73:1v:105:ILE:HG21	1.76	0.50
76:2:1080:G:OP1	79:b:14:ARG:NH2	2.42	0.50
85:i:375:LEU:O	85:i:376:ASP:HB3	2.10	0.50
20:U:54:PRO:O	20:U:57:ARG:HB2	2.11	0.50
8:I:199:ASN:OD1	78:a:177:GLU:HG3	2.12	0.50
12:M:142:MET:HE1	12:M:156:LEU:HD21	1.92	0.50
20:U:59:PHE:CD1	20:U:85:TYR:CD2	3.00	0.50
20:U:90:LEU:O	20:U:94:LYS:HB2	2.12	0.50
47:1U:21:MET:HG2	47:1U:104:ILE:HG21	1.93	0.50
76:2:1833:U:H2'	76:2:1834:G:C8	2.47	0.50
83:f:276:LEU:O	83:f:321:ARG:NH1	2.44	0.50
86:j:229:ILE:HG21	86:j:263:ARG:HD3	1.94	0.50
86:j:363:SER:HA	86:j:366:LYS:HD2	1.93	0.50
1:B:243:PHE:HE2	23:X:393:LEU:CD2	2.18	0.50
26:1:121:C:O2'	62:1j:37:LYS:O	2.26	0.50
26:1:160:U:O2'	26:1:161:U:O2	2.26	0.50
1:B:212:PRO:HD2	1:B:212:PRO:O	2.11	0.50
1:B:239:MET:HE3	23:X:448:MET:HE3	1.93	0.50
14:O:29:ARG:NH1	76:2:409:U:O2'	2.44	0.50
22:W:227:VAL:HG13	22:W:237:VAL:HG11	1.93	0.50
23:X:477:VAL:HG12	23:X:478:PRO:O	2.11	0.50
56:1d:114:CYS:HB3	56:1d:125:CYS:SG	2.51	0.50
57:1e:9:PHE:HD2	57:1e:27:ARG:HG3	1.77	0.50
65:1m:48:ARG:HD2	65:1m:52:GLN:HB2	1.92	0.50
83:f:171:ALA:HB2	83:f:206:LYS:HG2	1.94	0.50
86:j:129:ALA:HB3	86:j:131:MET:HE2	1.93	0.50
11:L:45:LEU:HD23	11:L:64:LEU:HD11	1.94	0.50
20:U:88:ARG:O	20:U:92:LEU:HD13	2.11	0.50
5:F:44:ARG:O	22:W:449:ARG:NH1	2.45	0.50
9:J:313:ARG:NH2	76:2:1831:U:OP1	2.44	0.50
26:1:345:A:H2'	26:1:346:A:C8	2.47	0.50
26:1:2820:C:H2'	26:1:2821:A:H8	1.77	0.50
69:1r:62:TYR:CZ	69:1r:124:VAL:HG11	2.47	0.50
81:d:49:ILE:HG12	81:d:94:TYR:HD2	1.77	0.50
86:j:369:VAL:HG22	86:j:406:LEU:HD21	1.94	0.50
11:L:105:GLU:OE2	76:2:1571:G:O2'	2.30	0.49
24:Y:43:ARG:NH1	76:2:1537:G:N7	2.59	0.49
26:1:1026:G:N2	26:1:1043:U:O2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1Y:117:ASN:HB2	51:1Y:124:TRP:HZ3	1.77	0.49
86:j:371:GLY:HA2	86:j:374:LYS:HG2	1.93	0.49
1:B:339:THR:OG1	23:X:383:ASN:ND2	2.38	0.49
26:1:1325:G:O6	26:1:1331:U:O4	2.30	0.49
54:1b:74:GLU:CD	54:1b:78:LYS:HE3	2.32	0.49
55:1c:20:ARG:NH1	61:1i:223:MET:O	2.46	0.49
72:1u:656:VAL:HA	72:1u:659:GLU:HG2	1.94	0.49
73:1v:193:GLN:N	73:1v:193:GLN:OE1	2.43	0.49
78:a:391:LYS:O	78:a:395:GLN:HG3	2.11	0.49
78:a:405:GLN:HA	78:a:408:ILE:HG12	1.94	0.49
3:D:136:ASP:OD1	3:D:136:ASP:N	2.44	0.49
20:U:70:GLU:H	20:U:71:PRO:CD	2.24	0.49
76:2:482:A:O2'	81:d:79:LYS:NZ	2.44	0.49
76:2:997:G:H1	76:2:1029:C:H41	1.59	0.49
76:2:1839:G:H2'	76:2:1840:A:C8	2.48	0.49
83:f:278:THR:OG1	83:f:280:GLU:OE1	2.24	0.49
2:C:229:LEU:O	2:C:232:THR:OG1	2.31	0.49
3:D:217:LEU:HD11	85:i:207:ILE:HD11	1.94	0.49
10:K:33:VAL:CG1	10:K:77:HIS:HA	2.43	0.49
26:1:1838:A:H3'	26:1:1839:A:H8	1.77	0.49
71:1t:302:TYR:HD2	71:1t:325:TRP:HD1	1.60	0.49
86:j:62:ARG:HH12	86:j:66:ILE:HG13	1.76	0.49
1:B:171:LYS:HG2	23:X:447:ARG:NH1	2.27	0.49
1:B:194:LEU:CD1	78:a:192:ILE:HD11	2.41	0.49
5:F:57:ILE:HD11	5:F:118:ALA:HB1	1.94	0.49
26:1:864:G:H2'	26:1:865:G:H8	1.78	0.49
26:1:2126:A:H2'	26:1:2127:A:C8	2.48	0.49
26:1:2188:U:OP1	26:1:2715:G:O2'	2.30	0.49
28:1B:75:HIS:ND1	28:1B:76:ASN:OD1	2.35	0.49
83:f:301:THR:O	83:f:305:VAL:HG23	2.12	0.49
86:j:107:LEU:CD2	86:j:118:PHE:HE2	2.26	0.49
86:j:259:THR:O	86:j:263:ARG:HG2	2.13	0.49
1:B:518:LYS:HE3	78:a:157:TYR:CD2	2.47	0.49
7:H:219:LYS:HZ2	20:U:124:LEU:HD23	1.77	0.49
23:X:505:ASP:N	23:X:505:ASP:OD1	2.43	0.49
3:D:311:ILE:HG21	3:D:344:ARG:HB2	1.94	0.49
8:I:178:GLN:NE2	76:2:1630:G:OP1	2.44	0.49
15:P:67:LYS:NZ	76:2:274:G:OP1	2.43	0.49
23:X:520:GLN:O	23:X:523:LYS:NZ	2.37	0.49
26:1:1546:C:N3	70:1s:76:ARG:NH2	2.56	0.49
26:1:1617:G:H2'	26:1:1618:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1V:14:LYS:O	48:1V:104:ARG:NH1	2.46	0.49
51:1Y:115:GLU:OE1	51:1Y:126:HIS:NE2	2.38	0.49
62:1j:82:ILE:C	62:1j:83:GLU:HG3	2.36	0.49
83:f:329:ASP:OD1	83:f:329:ASP:N	2.45	0.49
6:G:105:THR:OG1	6:G:108:GLY:O	2.29	0.49
16:Q:194:VAL:HG13	16:Q:198:GLN:NE2	2.28	0.49
26:1:435:A:H5''	48:1V:109:THR:HB	1.95	0.49
72:1u:650:LEU:HD13	72:1u:678:LEU:HD23	1.94	0.49
83:f:314:LYS:NZ	83:f:376:VAL:O	2.45	0.49
1:B:262:ALA:HB2	1:B:332:LEU:HD11	1.93	0.49
29:1C:187:SER:OG	29:1C:188:SER:N	2.44	0.49
31:1E:247:ILE:HG21	31:1E:263:ILE:HD12	1.95	0.49
76:2:129:A:H2'	76:2:130:A:H8	1.78	0.49
76:2:356:G:H2'	76:2:357:A:C8	2.48	0.49
76:2:660:G:H22	76:2:737:G:H1	1.61	0.49
76:2:1718:A:H2'	76:2:1719:G:H8	1.78	0.49
83:f:229:MET:HE1	88:A:48:ILE:HD12	1.95	0.49
17:R:159:TRP:HB2	76:2:1013:A:H1'	1.95	0.49
23:X:412:ARG:HH12	23:X:438:ILE:HG21	1.78	0.49
24:Y:39:HIS:NE2	76:2:1537:G:OP2	2.43	0.49
26:1:768:G:OP2	31:1E:193:ARG:NH1	2.45	0.49
49:1W:129:LEU:HD12	49:1W:130:LYS:HB2	1.95	0.49
72:1u:149:ASP:OD1	72:1u:149:ASP:N	2.44	0.49
75:5:58:A:O2'	75:5:60:U:OP2	2.26	0.49
76:2:709:G:H2'	76:2:710:G:C8	2.48	0.49
83:f:58:ARG:HB3	83:f:63:ASN:HA	1.94	0.49
84:h:152:GLN:HG2	84:h:184:ALA:HB3	1.94	0.49
1:B:200:SER:O	1:B:204:THR:OG1	2.25	0.48
26:1:2415:A:H61	26:1:2495:G:H1	1.61	0.48
65:1m:9:LYS:HG2	65:1m:44:LEU:HD13	1.94	0.48
76:2:997:G:H22	76:2:1029:C:H5	1.61	0.48
13:N:342:ASP:OD1	76:2:746:C:O2'	2.30	0.48
26:1:774:G:O6	39:1M:170:LYS:NZ	2.45	0.48
26:1:1840:A:H2'	26:1:1841:G:H8	1.79	0.48
26:1:2177:A:H2'	26:1:2178:A:C8	2.48	0.48
26:1:2799:G:H4'	40:1N:124:GLU:HG2	1.95	0.48
47:1U:56:VAL:HG13	47:1U:86:VAL:HG13	1.95	0.48
49:1W:132:HIS:HB3	49:1W:141:LEU:HB2	1.95	0.48
71:1t:337:VAL:O	71:1t:341:ILE:HG12	2.13	0.48
76:2:1719:G:H1	76:2:1752:U:H3	1.60	0.48
76:2:1730:U:H5''	84:h:187:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:j:49:THR:HA	86:j:52:THR:OG1	2.13	0.48
1:B:511:SER:OG	1:B:517:GLN:NE2	2.39	0.48
26:1:1176:A:OP1	26:1:1284:U:O2'	2.31	0.48
26:1:1619:G:O6	26:1:1634:U:O4	2.31	0.48
26:1:3131:A:N7	26:1:3149:A:O2'	2.41	0.48
41:1O:103:ASP:OD1	41:1O:103:ASP:N	2.44	0.48
71:1t:200:MET:HE1	71:1t:235:MET:HG2	1.95	0.48
83:f:290:VAL:HG23	83:f:298:CYS:HB3	1.95	0.48
86:j:76:CYS:SG	86:j:77:HIS:N	2.86	0.48
86:j:256:GLY:O	86:j:259:THR:OG1	2.30	0.48
3:D:514:LYS:NZ	82:e:270:PHE:O	2.47	0.48
26:1:1256:G:H2'	26:1:1257:G:H8	1.78	0.48
26:1:1630:C:N4	26:1:1631:G:O6	2.46	0.48
27:3:1:A:N6	27:3:118:A:O2'	2.38	0.48
36:1J:23:ALA:HB3	36:1J:59:PRO:HA	1.95	0.48
73:1v:120:PRO:O	73:1v:156:ARG:NH1	2.46	0.48
76:2:916:A:O2'	76:2:1661:C:OP2	2.30	0.48
72:1u:709:MET:HE3	72:1u:742:MET:HG2	1.96	0.48
84:h:181:PRO:HB2	84:h:214:LEU:HD11	1.95	0.48
26:1:2934:U:O2'	26:1:2936:A:N6	2.46	0.48
33:1G:88:TYR:HB2	33:1G:91:GLU:HB2	1.96	0.48
72:1u:359:ASN:HD21	72:1u:362:THR:HG23	1.79	0.48
78:a:79:ASN:HA	78:a:82:LEU:HB2	1.95	0.48
4:E:23:VAL:HG21	4:E:65:MET:HE2	1.95	0.48
8:I:204:LEU:HD23	8:I:207:TYR:CE2	2.49	0.48
19:T:80:LYS:NZ	76:2:1526:G:OP1	2.36	0.48
20:U:45:LEU:HD21	88:A:31:ALA:HB3	1.95	0.48
26:1:213:C:N4	26:1:2712:G:N3	2.60	0.48
72:1u:350:GLU:O	72:1u:353:SER:OG	2.30	0.48
83:f:191:ARG:NH2	83:f:326:GLN:O	2.47	0.48
84:h:301:GLU:C	84:h:302:HIS:CG	2.91	0.48
85:i:112:VAL:HG12	85:i:124:ILE:HG12	1.96	0.48
85:i:181:ARG:HA	85:i:184:GLU:HG2	1.96	0.48
85:i:334:PRO:HD3	85:i:369:LYS:CE	2.42	0.48
3:D:481:ARG:NH2	76:2:557:A:OP1	2.47	0.48
7:H:415:LYS:HE3	76:2:1450:G:H5'	1.96	0.48
17:R:67:VAL:HG23	17:R:68:THR:HG23	1.95	0.48
22:W:249:GLY:O	22:W:266:GLN:NE2	2.40	0.48
26:1:153:U:H2'	26:1:154:U:H6	1.79	0.48
26:1:434:A:OP2	48:1V:107:ARG:NH1	2.46	0.48
26:1:1231:U:H2'	26:1:1232:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:3:A:H61	27:3:116:U:H3	1.62	0.48
36:1J:112:ARG:HG2	66:1o:74:TYR:HE2	1.78	0.48
76:2:1825:2MG:N2	76:2:1828:MA6:OP2	2.45	0.48
81:d:62:THR:HA	86:j:28:SER:HB3	1.95	0.48
26:1:538:U:H3'	72:1u:83:ASN:HD22	1.79	0.48
26:1:1554:U:OP1	70:1s:110:ASN:N	2.42	0.48
49:1W:130:LYS:HB3	49:1W:144:VAL:HB	1.95	0.48
88:A:120:HIS:CG	88:A:121:LYS:H	2.31	0.48
1:B:195:ILE:O	1:B:202:LYS:NZ	2.36	0.48
2:C:83:PRO:HB2	2:C:86:GLU:HB2	1.96	0.48
22:W:302:GLY:HA3	64:1l:81:TYR:CE1	2.49	0.48
26:1:1879:A:O2'	71:1t:40:ARG:NH2	2.47	0.48
28:1B:70:ILE:HD11	28:1B:100:GLU:HG2	1.95	0.48
35:1I:49:ASN:HD22	35:1I:87:THR:CG2	2.22	0.48
86:j:232:PHE:HE2	86:j:244:VAL:HG11	1.79	0.48
5:F:29:ARG:NE	7:H:343:ASP:OD2	2.47	0.47
12:M:163:SER:O	12:M:164:TRP:HB3	2.14	0.47
24:Y:91:LYS:NZ	76:2:1475:U:OP2	2.40	0.47
76:2:1717:C:H4'	84:h:105:PRO:HG3	1.96	0.47
9:J:207:VAL:HB	9:J:246:ILE:HG13	1.96	0.47
17:R:51:PHE:HD2	17:R:77:VAL:HG11	1.79	0.47
26:1:544:A:H2'	26:1:545:G:C8	2.50	0.47
32:1F:59:GLN:NE2	32:1F:96:THR:O	2.47	0.47
34:1H:44:LEU:O	34:1H:63:LYS:HA	2.14	0.47
36:1J:116:GLU:HA	36:1J:119:LYS:HD2	1.95	0.47
48:1V:3:TRP:HB2	73:1v:512:LYS:HG3	1.96	0.47
76:2:1121:U:H5''	76:2:1122:C:H5'	1.95	0.47
8:I:156:MET:HB2	8:I:185:LYS:HB3	1.96	0.47
10:K:31:THR:OG1	76:2:382:A:C5'	2.63	0.47
12:M:65:GLN:NE2	12:M:67:VAL:O	2.46	0.47
20:U:58:ARG:O	20:U:62:LYS:N	2.29	0.47
23:X:348:MET:HB3	23:X:348:MET:HE3	1.66	0.47
62:1j:82:ILE:O	62:1j:83:GLU:CG	2.62	0.47
71:1t:465:MET:HA	71:1t:468:ARG:HD3	1.95	0.47
20:U:96:GLY:O	20:U:97:ILE:C	2.57	0.47
22:W:236:LEU:HB3	22:W:351:VAL:HG22	1.96	0.47
29:1C:109:PHE:HB3	29:1C:112:LEU:HD12	1.96	0.47
34:1H:70:ARG:NH1	52:1Z:102:ASP:OD2	2.47	0.47
65:1m:10:ILE:HG21	65:1m:26:LEU:HD21	1.97	0.47
76:2:107:U:HO2'	86:j:223:SER:HG	1.63	0.47
76:2:1839:G:H2'	76:2:1840:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:j:142:LEU:HD11	86:j:149:ARG:HG3	1.95	0.47
1:B:98:TRP:HB2	23:X:330:ALA:HB1	1.97	0.47
3:D:158:ASP:OD1	3:D:161:ARG:NH1	2.46	0.47
14:O:4:ARG:NE	76:2:396:G:OP1	2.48	0.47
26:1:1558:G:H2'	26:1:1559:A:C8	2.49	0.47
35:1I:27:ILE:HD12	35:1I:83:ILE:HD11	1.95	0.47
54:1b:45:ARG:HH21	54:1b:48:ARG:HH22	1.62	0.47
76:2:939:A:H2'	76:2:940:G:H8	1.79	0.47
76:2:1737:A:H3'	76:2:1738:G:H21	1.79	0.47
88:A:62:SER:O	88:A:64:ARG:NH1	2.45	0.47
20:U:92:LEU:C	20:U:94:LYS:N	2.68	0.47
26:1:71:A:OP2	47:1U:14:ASN:ND2	2.48	0.47
34:1H:46:VAL:O	34:1H:61:THR:HA	2.13	0.47
76:2:609:U:H3	76:2:625:G:H22	1.61	0.47
1:B:98:TRP:CE2	23:X:331:LEU:HD23	2.49	0.47
2:C:117:LEU:HD11	2:C:126:LEU:HD12	1.96	0.47
7:H:352:LEU:HD23	7:H:387:LEU:HD11	1.96	0.47
7:H:422:ARG:HG3	76:2:1610:U:H4'	1.97	0.47
14:O:79:ARG:HE	82:e:334:ILE:HD12	1.79	0.47
20:U:58:ARG:HB2	20:U:62:LYS:HZ2	1.79	0.47
23:X:348:MET:HE1	23:X:352:ILE:HB	1.96	0.47
26:1:422:C:O2'	26:1:424:G:O5'	2.32	0.47
26:1:977:U:H2'	26:1:978:A:C8	2.50	0.47
26:1:977:U:H2'	26:1:978:A:H8	1.79	0.47
26:1:2414:A:H2'	26:1:2415:A:C8	2.50	0.47
29:1C:119:ARG:HD2	52:1Z:140:GLN:HG3	1.96	0.47
71:1t:211:GLY:HA2	71:1t:214:ARG:HE	1.80	0.47
73:1v:142:THR:H	73:1v:145:THR:HG22	1.80	0.47
76:2:1746:A:H2'	76:2:1747:A:C8	2.50	0.47
81:d:41:GLY:N	81:d:44:GLU:OE2	2.48	0.47
83:f:286:MET:HG2	83:f:298:CYS:HB3	1.95	0.47
85:i:109:ARG:NH1	85:i:113:SER:OG	2.48	0.47
6:G:56:ARG:NH2	21:V:142:GLU:OE1	2.46	0.47
28:1B:176:SER:HB2	28:1B:180:GLY:HA3	1.97	0.47
72:1u:670:LEU:HD22	72:1u:688:VAL:HG21	1.97	0.47
76:2:969:G:H22	76:2:1625:A:H5'	1.80	0.47
84:h:224:VAL:HA	84:h:227:ILE:HG22	1.96	0.47
1:B:376:VAL:HG12	1:B:380:ILE:HG23	1.96	0.47
26:1:751:G:OP1	31:1E:116:ARG:NH1	2.39	0.47
63:1k:14:VAL:HG13	63:1k:26:ILE:HD11	1.96	0.47
67:1p:18:HIS:HB3	67:1p:21:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:1u:254:THR:O	72:1u:257:THR:OG1	2.28	0.47
81:d:78:LEU:HB3	81:d:83:ILE:HD11	1.97	0.47
82:e:328:SER:OG	82:e:329:SER:N	2.48	0.47
22:W:363:THR:OG1	22:W:364:PHE:N	2.45	0.47
72:1u:449:ARG:HA	72:1u:452:LYS:HD3	1.97	0.47
73:1v:303:GLN:HA	73:1v:306:VAL:HG12	1.97	0.47
76:2:356:G:H2'	76:2:357:A:H8	1.80	0.47
76:2:1116:G:O2'	76:2:1408:C:N3	2.43	0.47
76:2:1137:G:H2'	76:2:1138:G:C2	2.50	0.47
86:j:186:ASP:O	86:j:189:THR:OG1	2.33	0.47
1:B:174:ARG:HH22	23:X:366:ARG:HH11	1.62	0.46
1:B:406:LYS:HD2	1:B:407:ARG:NH1	2.28	0.46
4:E:76:ASN:HD22	76:2:733:C:H1'	1.80	0.46
5:F:11:LEU:HD12	5:F:89:ILE:HD11	1.96	0.46
7:H:235:LEU:HD12	85:i:299:ILE:HG12	1.97	0.46
20:U:48:ILE:HG23	88:A:35:ARG:HD2	1.96	0.46
20:U:72:ASN:O	20:U:73:LYS:C	2.57	0.46
26:1:978:A:H2'	26:1:979:G:C8	2.51	0.46
26:1:1558:G:H2'	26:1:1559:A:H8	1.80	0.46
55:1c:18:SER:HB2	61:1i:229:PRO:HB3	1.98	0.46
13:N:315:HIS:HD2	13:N:316:PRO:HD2	1.80	0.46
26:1:1978:U:H2'	26:1:1979:A:C8	2.50	0.46
26:1:2141:G:OP1	29:1C:65:ARG:NH2	2.48	0.46
30:1D:115:ILE:HD11	30:1D:121:PHE:HE2	1.64	0.46
36:1J:35:ALA:O	36:1J:38:PRO:CG	2.63	0.46
73:1v:368:TYR:CE1	73:1v:376:GLY:HA3	2.50	0.46
76:2:190:G:OP1	76:2:603:U:O2'	2.28	0.46
84:h:252:ARG:CG	84:h:253:LYS:H	2.26	0.46
86:j:197:PHE:HD2	86:j:209:ILE:HD11	1.81	0.46
26:1:153:U:H2'	26:1:154:U:C6	2.50	0.46
39:1M:120:ARG:NH2	59:1g:135:GLU:OE2	2.45	0.46
64:1l:126:LYS:H	64:1l:126:LYS:HG2	1.55	0.46
3:D:451:THR:HG23	3:D:452:THR:HG23	1.97	0.46
20:U:81:PRO:CD	20:U:82:ALA:N	2.79	0.46
21:V:146:LYS:NZ	76:2:745:A:OP1	2.48	0.46
23:X:493:ALA:HB2	23:X:511:MET:HE2	1.97	0.46
26:1:346:A:H2'	26:1:347:A:C8	2.49	0.46
49:1W:130:LYS:NZ	49:1W:132:HIS:HB2	2.30	0.46
26:1:1191:A:H2'	26:1:1192:G:H8	1.81	0.46
29:1C:119:ARG:HH11	52:1Z:140:GLN:HG3	1.80	0.46
61:1i:202:PRO:HD2	61:1i:205:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:e:188:GLU:O	82:e:192:LEU:HB2	2.15	0.46
5:F:82:ASP:OD1	5:F:83:ARG:N	2.48	0.46
19:T:59:LYS:NZ	76:2:1588:A:OP1	2.49	0.46
26:1:76:C:H2'	26:1:77:A:H8	1.81	0.46
26:1:2490:U:H2'	26:1:2491:A:C8	2.50	0.46
31:1E:95:ASN:CG	31:1E:101:LYS:NZ	2.74	0.46
31:1E:118:ASP:OD1	31:1E:118:ASP:N	2.48	0.46
39:1M:178:LEU:HB3	39:1M:197:VAL:HG23	1.98	0.46
66:1o:81:LEU:HG	66:1o:82:LEU:HG	1.98	0.46
76:2:1709:U:H2'	76:2:1710:G:H8	1.80	0.46
83:f:159:GLY:O	83:f:162:ARG:NH1	2.47	0.46
84:h:110:TRP:CE3	84:h:113:ILE:HD11	2.51	0.46
84:h:356:SER:O	84:h:359:SER:OG	2.28	0.46
20:U:62:LYS:C	20:U:64:PRO:N	2.69	0.46
32:1F:38:PRO:HD3	32:1F:53:MET:HE1	1.98	0.46
69:1r:62:TYR:OH	69:1r:124:VAL:HG11	2.15	0.46
72:1u:183:TRP:CZ3	72:1u:214:LEU:HB3	2.51	0.46
76:2:883:G:O2'	76:2:899:A:N6	2.47	0.46
76:2:1129:G:O2'	78:a:345:ASP:OD1	2.34	0.46
82:e:312:LEU:HA	82:e:315:LYS:HD3	1.97	0.46
86:j:191:ASP:OD1	86:j:191:ASP:O	2.34	0.46
86:j:388:VAL:HG12	86:j:389:LYS:HD2	1.97	0.46
1:B:304:ALA:HB1	78:a:233:GLU:HG3	1.97	0.46
33:1G:6:PHE:CE1	33:1G:58:THR:HG23	2.51	0.46
42:1P:76:ARG:HG2	42:1P:79:MET:HE2	1.98	0.46
76:2:812:A:OP1	76:2:1835:G:O2'	2.31	0.46
76:2:1738:G:OP2	76:2:1738:G:N2	2.45	0.46
86:j:114:LYS:C	86:j:115:THR:HG23	2.41	0.46
17:R:132:MET:HG3	17:R:134:ARG:H	1.81	0.46
22:W:452:VAL:O	22:W:457:ASN:ND2	2.48	0.46
26:1:138:G:H1'	26:1:139:G:H5'	1.97	0.46
26:1:358:A:H2'	26:1:359:A:H8	1.80	0.46
26:1:1607:U:H5'	49:1W:68:LEU:HD13	1.98	0.46
26:1:2624:G:OP2	26:1:2624:G:N2	2.37	0.46
36:1J:110:SER:OG	36:1J:154:LEU:N	2.49	0.46
49:1W:67:LEU:HA	49:1W:75:ARG:HG3	1.97	0.46
76:2:223:A:H2'	76:2:224:A:C8	2.51	0.46
10:K:50:ARG:NH2	10:K:89:ASP:OD2	2.48	0.46
14:O:8:SER:OG	14:O:21:MET:SD	2.61	0.46
26:1:959:C:O3'	45:1S:227:ARG:NH2	2.49	0.46
26:1:1123:A:H5''	45:1S:221:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2828:G:O2'	26:1:3066:A:O2'	2.32	0.46
39:1M:258:LEU:HD23	39:1M:258:LEU:HA	1.75	0.46
59:1g:90:MET:HG3	59:1g:94:LYS:HE2	1.97	0.46
71:1t:228:ASP:OD1	71:1t:231:THR:OG1	2.31	0.46
26:1:342:A:O4'	72:1u:202:GLN:NE2	2.47	0.45
26:1:513:G:N2	26:1:515:C:H5'	2.31	0.45
26:1:1967:C:OP1	70:1s:128:ARG:NH2	2.42	0.45
30:1D:136:THR:OG1	30:1D:139:GLU:OE1	2.32	0.45
72:1u:231:LEU:HD13	72:1u:264:GLY:HA3	1.98	0.45
72:1u:525:ASP:OD1	72:1u:525:ASP:N	2.49	0.45
76:2:164:A:H2'	76:2:165:A:H8	1.80	0.45
76:2:654:G:H2'	76:2:655:A:C8	2.51	0.45
78:a:311:ARG:O	78:a:360:ASN:ND2	2.49	0.45
83:f:105:LEU:HG	83:f:106:PRO:CD	2.39	0.45
84:h:93:ILE:HG23	84:h:104:PRO:CB	2.46	0.45
1:B:174:ARG:NH1	23:X:366:ARG:HD2	2.31	0.45
4:E:83:ASN:OD1	4:E:91:TRP:NE1	2.43	0.45
7:H:395:ARG:HE	7:H:399:ARG:HD3	1.81	0.45
20:U:59:PHE:CD1	20:U:63:HIS:CD2	3.03	0.45
26:1:2634:U:H2'	26:1:2635:G:C8	2.51	0.45
66:1o:100:PRO:HD2	66:1o:103:ASP:HB2	1.97	0.45
67:1p:127:LYS:HE3	67:1p:127:LYS:HB3	1.83	0.45
86:j:77:HIS:CE1	86:j:80:ARG:NH2	2.84	0.45
1:B:174:ARG:HH22	23:X:366:ARG:NH1	2.14	0.45
26:1:358:A:H2'	26:1:359:A:C8	2.52	0.45
29:1C:299:CYS:SG	29:1C:300:LYS:N	2.89	0.45
72:1u:129:LYS:HB2	72:1u:132:HIS:CD2	2.51	0.45
10:K:66:TYR:OH	76:2:520:C:OP2	2.33	0.45
26:1:951:C:OP1	26:1:975:A:O2'	2.31	0.45
36:1J:73:HIS:CG	36:1J:73:HIS:O	2.68	0.45
41:1O:93:ARG:HH22	41:1O:122:SER:HB3	1.80	0.45
82:e:214:GLN:OE1	82:e:300:TYR:HD1	1.98	0.45
83:f:42:GLN:HB3	83:f:69:MET:HE2	1.99	0.45
84:h:153:GLN:HA	84:h:156:LYS:HG2	1.98	0.45
7:H:355:THR:HG23	7:H:357:THR:HG22	1.99	0.45
26:1:1218:G:N2	26:1:1245:A:O2'	2.39	0.45
26:1:1612:G:H2'	26:1:1613:G:C8	2.51	0.45
72:1u:270:ARG:HB3	72:1u:273:THR:HB	1.97	0.45
76:2:654:G:H2'	76:2:655:A:H8	1.80	0.45
76:2:1113:U:H2'	76:2:1114:G:C8	2.51	0.45
83:f:58:ARG:HB2	83:f:69:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:GLU:HB2	3:D:141:ARG:HB2	1.98	0.45
3:D:482:ASN:O	3:D:486:THR:OG1	2.30	0.45
10:K:83:ARG:NH1	10:K:84:GLY:O	2.48	0.45
26:1:565:A:H5''	26:1:566:G:H5''	1.98	0.45
26:1:1326:C:O2'	26:1:1327:U:O4'	2.33	0.45
39:1M:266:PRO:HB2	39:1M:269:ALA:HB3	1.99	0.45
76:2:122:A:H2'	76:2:123:A:C8	2.51	0.45
76:2:670:G:H2'	76:2:671:A:C8	2.50	0.45
83:f:312:SER:HA	83:f:315:ILE:HD12	1.99	0.45
85:i:132:VAL:HA	85:i:135:VAL:HG12	1.98	0.45
88:A:93:ASN:HB3	88:A:96:ARG:HB3	1.98	0.45
59:1g:92:LYS:HE3	59:1g:92:LYS:HB3	1.72	0.45
66:1o:115:LYS:HA	66:1o:118:GLU:HG2	1.99	0.45
84:h:256:PHE:HZ	84:h:275:VAL:O	1.98	0.45
85:i:317:LYS:HD2	85:i:320:LEU:HD21	1.99	0.45
1:B:376:VAL:O	1:B:376:VAL:CG1	2.65	0.45
18:S:80:LYS:O	18:S:84:ILE:HG12	2.17	0.45
36:1J:70:TYR:CD2	36:1J:74:SER:O	2.69	0.45
46:1T:231:LYS:HD2	46:1T:231:LYS:HA	1.73	0.45
49:1W:161:VAL:HG21	49:1W:196:LYS:HE3	1.99	0.45
71:1t:32:ASP:HB3	71:1t:38:SER:HB3	1.98	0.45
72:1u:690:ASP:OD1	72:1u:691:ALA:N	2.50	0.45
76:2:6:A:OP2	82:e:373:LYS:NZ	2.36	0.45
76:2:711:A:H2'	76:2:712:A:C8	2.52	0.45
85:i:375:LEU:O	85:i:376:ASP:CB	2.64	0.45
1:B:334:PRO:HG3	78:a:180:TRP:CE2	2.52	0.45
3:D:383:THR:HG22	3:D:401:LYS:HB2	1.99	0.45
20:U:70:GLU:HG3	20:U:71:PRO:HD3	1.99	0.45
22:W:468:ASN:HB3	22:W:471:GLU:HB2	1.99	0.45
26:1:1840:A:H2'	26:1:1841:G:C8	2.52	0.45
1:B:98:TRP:CE2	23:X:331:LEU:HD21	2.52	0.45
26:1:1591:C:H5'	71:1t:68:ARG:HH22	1.82	0.45
44:1R:39:ARG:O	44:1R:43:LYS:NZ	2.49	0.45
64:1l:176:THR:HG23	64:1l:178:GLU:HG3	1.99	0.45
72:1u:403:LEU:HD23	72:1u:403:LEU:HA	1.83	0.45
72:1u:741:ARG:HH12	72:1u:744:LYS:HD2	1.82	0.45
76:2:147:U:H2'	76:2:148:U:C6	2.52	0.45
76:2:1549:A:H2'	76:2:1550:A:C8	2.52	0.45
83:f:62:LEU:HB3	83:f:97:THR:HG21	1.99	0.45
26:1:1159:A:N3	26:1:1304:C:O2'	2.44	0.44
26:1:1323:A:H2'	26:1:1324:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1K:133:ASP:OD1	37:1K:133:ASP:N	2.49	0.44
84:h:263:ALA:HB3	84:h:272:LEU:HD13	1.99	0.44
18:S:53:GLU:HA	18:S:56:ILE:HG22	1.98	0.44
26:1:134:C:O2	47:1U:4:ARG:NH1	2.50	0.44
26:1:1219:A:H4'	26:1:1220:A:C8	2.53	0.44
26:1:1235:A:H2'	26:1:1236:A:C4	2.52	0.44
26:1:2479:A:H2'	26:1:2480:C:H5	1.82	0.44
26:1:2956:C:H2'	26:1:2957:A:H8	1.83	0.44
76:2:121:A:H2'	76:2:122:A:C8	2.52	0.44
76:2:164:A:H2'	76:2:165:A:C8	2.52	0.44
84:h:82:PRO:HG3	84:h:124:PHE:CE2	2.52	0.44
1:B:171:LYS:HG2	23:X:447:ARG:HH11	1.83	0.44
17:R:135:SER:HB3	55:1c:57:ARG:HG2	1.99	0.44
26:1:740:A:H2'	26:1:741:A:C8	2.52	0.44
26:1:1178:A:H2'	26:1:1179:A:C8	2.53	0.44
35:1I:64:LEU:HD23	35:1I:64:LEU:HA	1.87	0.44
50:1X:124:ARG:HG2	50:1X:132:VAL:HG22	1.99	0.44
50:1X:237:ARG:HD3	50:1X:238:PRO:HD2	1.99	0.44
55:1c:56:ARG:NH2	76:2:1574:C:OP1	2.43	0.44
59:1g:131:LEU:HD12	59:1g:156:GLY:O	2.18	0.44
69:1r:57:ILE:CG2	69:1r:88:LEU:HD21	2.45	0.44
71:1t:130:LEU:HD13	71:1t:145:LEU:HD22	2.00	0.44
73:1v:390:GLU:HG2	73:1v:391:LEU:HD22	2.00	0.44
86:j:74:PRO:HG3	86:j:118:PHE:HD1	1.81	0.44
1:B:481:ARG:HG2	1:B:481:ARG:O	2.16	0.44
18:S:89:LYS:HD2	79:b:19:LEU:HD11	1.99	0.44
26:1:737:A:N1	26:1:954:G:O2'	2.41	0.44
29:1C:74:TRP:NE1	29:1C:307:THR:OG1	2.39	0.44
35:1I:10:VAL:HA	35:1I:13:LYS:HB2	1.99	0.44
49:1W:62:VAL:HA	49:1W:145:PHE:O	2.17	0.44
71:1t:282:GLU:HA	71:1t:285:ARG:HB3	1.98	0.44
76:2:92:A:H61	86:j:192:ARG:NH2	2.12	0.44
78:a:215:ASP:HA	78:a:218:LYS:HB2	1.98	0.44
86:j:59:ASP:HB2	86:j:62:ARG:HB2	1.99	0.44
86:j:372:LEU:HG	86:j:381:ALA:HB2	2.00	0.44
20:U:80:ASP:HB3	20:U:81:PRO:HD3	1.59	0.44
26:1:542:C:H2'	26:1:543:G:H8	1.82	0.44
26:1:2441:G:H2'	26:1:2442:G:H8	1.82	0.44
29:1C:107:PHE:HB2	34:1H:96:MET:HE1	1.99	0.44
30:1D:304:PRO:HA	30:1D:307:LEU:HD12	2.00	0.44
45:1S:191:ARG:NH2	54:1b:92:PRO:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:1u:297:ILE:HD12	72:1u:331:MET:HE3	1.99	0.44
86:j:361:SER:HB2	86:j:364:ILE:HD12	2.00	0.44
88:A:11:LEU:O	88:A:14:THR:OG1	2.35	0.44
2:C:252:MET:HB3	2:C:252:MET:HE2	1.76	0.44
17:R:64:THR:OG1	17:R:70:ARG:O	2.33	0.44
26:1:136:G:O2'	26:1:137:U:O2	2.34	0.44
26:1:891:PSU:O2'	26:1:2916:C:O2'	2.30	0.44
26:1:1026:G:H1	26:1:1043:U:H3	1.63	0.44
39:1M:146:ILE:HD12	39:1M:153:SER:HB2	1.98	0.44
40:1N:77:ARG:HG2	40:1N:138:ILE:HD12	1.99	0.44
72:1u:258:TYR:OH	72:1u:284:ARG:NH1	2.44	0.44
72:1u:281:MET:HE1	72:1u:288:PRO:HG3	2.00	0.44
76:2:144:U:H2'	76:2:145:U:H6	1.82	0.44
76:2:187:C:OP1	76:2:330:C:O2'	2.31	0.44
76:2:597:U:H2'	76:2:598:G:H8	1.81	0.44
3:D:224:ALA:HB1	3:D:228:ASP:HB3	1.99	0.44
6:G:9:ALA:HB1	6:G:26:LEU:HD13	1.99	0.44
8:I:170:HIS:CE1	8:I:171:VAL:HG22	2.53	0.44
14:O:79:ARG:HH12	82:e:357:PRO:HA	1.82	0.44
36:1J:111:VAL:HB	66:1o:78:LEU:HG	2.00	0.44
47:1U:40:THR:HB	47:1U:43:GLU:HG3	2.00	0.44
48:1V:62:ASP:OD1	48:1V:62:ASP:N	2.51	0.44
71:1t:277:LEU:HD23	71:1t:277:LEU:HA	1.88	0.44
83:f:115:ASN:ND2	83:f:118:GLU:OE2	2.50	0.44
84:h:285:GLN:NE2	84:h:286:HIS:O	2.50	0.44
1:B:399:MET:CE	78:a:101:ILE:HG23	2.47	0.44
4:E:53:LYS:NZ	76:2:707:A:OP1	2.49	0.44
17:R:54:PHE:CE2	17:R:92:MET:HE1	2.53	0.44
26:1:275:A:H5'	72:1u:424:THR:HG21	1.99	0.44
26:1:721:G:H2'	26:1:2348:A:N7	2.33	0.44
26:1:1234:G:H2'	26:1:1235:A:C8	2.53	0.44
26:1:1862:A:H2'	26:1:1863:C:C6	2.53	0.44
33:1G:6:PHE:HE1	33:1G:58:THR:HG23	1.82	0.44
71:1t:165:MET:HG2	71:1t:177:VAL:HG13	2.00	0.44
71:1t:381:LYS:HD2	71:1t:381:LYS:HA	1.84	0.44
86:j:193:MET:HA	86:j:196:VAL:HG12	2.00	0.44
3:D:134:LYS:NZ	76:2:431:A:OP1	2.38	0.44
26:1:1410:A:H5'	44:1R:22:ARG:HH12	1.83	0.44
63:1k:33:GLU:HB3	63:1k:81:LEU:HD13	1.99	0.44
71:1t:477:ASP:O	71:1t:480:THR:OG1	2.28	0.44
72:1u:196:GLY:HA3	72:1u:229:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:h:203:GLU:HG2	84:h:236:LEU:HD21	2.00	0.44
86:j:34:SER:OG	86:j:36:ASP:OD1	2.33	0.44
1:B:107:ILE:HG22	1:B:109:CYS:CA	2.48	0.43
2:C:93:ARG:HD2	2:C:98:PRO:HG2	1.99	0.43
17:R:136:VAL:HG12	17:R:138:LYS:H	1.82	0.43
26:1:259:A:H2	72:1u:129:LYS:HD3	1.82	0.43
26:1:309:A:H2'	72:1u:361:THR:HG21	1.99	0.43
26:1:2270:A:N3	26:1:2865:G:O2'	2.47	0.43
26:1:2363:A:H2'	26:1:2364:A:C8	2.52	0.43
36:1J:35:ALA:C	36:1J:38:PRO:HD3	2.43	0.43
44:1R:47:ARG:O	44:1R:51:ILE:HG12	2.18	0.43
52:1Z:155:GLU:HG3	52:1Z:159:LYS:HE3	1.99	0.43
72:1u:177:PRO:HD3	72:1u:183:TRP:HE1	1.83	0.43
72:1u:446:ALA:HA	72:1u:449:ARG:HH21	1.82	0.43
2:C:108:ASP:N	2:C:108:ASP:OD1	2.51	0.43
2:C:332:TYR:OH	82:e:260:HIS:ND1	2.38	0.43
7:H:226:LYS:HD3	20:U:113:GLU:HG2	1.99	0.43
20:U:115:LYS:HB2	20:U:115:LYS:HE3	1.84	0.43
26:1:1654:C:H2'	26:1:1655:C:H6	1.82	0.43
33:1G:80:VAL:HG22	33:1G:96:LYS:HG2	2.00	0.43
37:1K:95:THR:HG21	37:1K:102:LYS:HE2	2.00	0.43
47:1U:101:VAL:O	47:1U:105:GLU:HG2	2.18	0.43
50:1X:141:ARG:NH2	50:1X:167:LYS:O	2.50	0.43
62:1j:34:ASP:OD1	62:1j:34:ASP:N	2.47	0.43
76:2:612:U:H2'	76:2:613:C:C6	2.54	0.43
76:2:643:U:H2'	76:2:644:G:H8	1.83	0.43
76:2:1746:A:H2'	76:2:1747:A:H8	1.83	0.43
78:a:183:ILE:O	78:a:183:ILE:CG2	2.66	0.43
82:e:214:GLN:HG3	82:e:303:PHE:CD2	2.53	0.43
83:f:290:VAL:HG23	83:f:298:CYS:CB	2.47	0.43
2:C:114:LEU:HD21	2:C:319:LEU:HD22	1.99	0.43
9:J:296:GLU:HG3	18:S:28:ARG:HB3	2.01	0.43
26:1:2766:G:H2'	26:1:2767:A:C8	2.54	0.43
35:1I:33:THR:OG1	35:1I:36:GLN:HG3	2.18	0.43
36:1J:9:THR:OG1	36:1J:11:ARG:NE	2.51	0.43
46:1T:186:LYS:HB2	46:1T:186:LYS:HE2	1.81	0.43
61:1i:203:GLU:O	61:1i:207:MET:HG2	2.19	0.43
72:1u:324:SER:O	72:1u:327:SER:OG	2.30	0.43
1:B:9:SER:HB3	12:M:152:ASN:O	2.18	0.43
20:U:80:ASP:O	20:U:83:ARG:N	2.43	0.43
21:V:180:GLU:HG3	21:V:183:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:372:THR:HG22	22:W:374:ARG:H	1.82	0.43
32:1F:106:LEU:HA	32:1F:109:ILE:HG22	2.01	0.43
42:1P:14:ASP:OD1	42:1P:14:ASP:N	2.50	0.43
49:1W:51:ARG:NE	71:1t:292:LEU:O	2.51	0.43
64:1l:137:ASP:OD1	64:1l:137:ASP:N	2.51	0.43
73:1v:124:ARG:HH12	73:1v:161:GLY:HA3	1.83	0.43
85:i:345:LEU:HD23	85:i:345:LEU:HA	1.86	0.43
3:D:145:SER:HB2	3:D:148:SER:HB2	1.99	0.43
10:K:13:GLU:O	76:2:560:G:O2'	2.34	0.43
14:O:50:LYS:NZ	76:2:473:G:OP1	2.37	0.43
26:1:427:A:H2'	26:1:430:G:C8	2.54	0.43
26:1:864:G:H2'	26:1:865:G:C8	2.53	0.43
26:1:1850:U:O2'	26:1:1852:U:O2	2.32	0.43
26:1:2633:A:H2'	26:1:2634:U:C6	2.53	0.43
29:1C:227:ARG:HH11	29:1C:227:ARG:H	1.65	0.43
35:1I:61:PHE:HA	35:1I:73:LYS:NZ	2.33	0.43
49:1W:80:LYS:HE3	49:1W:80:LYS:HB3	1.79	0.43
71:1t:228:ASP:OD2	71:1t:230:THR:OG1	2.31	0.43
76:2:969:G:OP2	76:2:1620:U:O2'	2.36	0.43
78:a:119:ASP:OD1	78:a:119:ASP:N	2.50	0.43
81:d:60:LEU:HD12	81:d:60:LEU:HA	1.82	0.43
86:j:107:LEU:HD23	86:j:118:PHE:CD2	2.53	0.43
14:O:52:MET:SD	14:O:76:LEU:HD12	2.58	0.43
16:Q:195:LYS:NZ	76:2:716:C:OP1	2.44	0.43
24:Y:10:VAL:HA	78:a:385:ILE:HD11	2.01	0.43
40:1N:32:LYS:HA	40:1N:32:LYS:HD3	1.83	0.43
46:1T:224:ARG:O	46:1T:227:VAL:HG12	2.19	0.43
76:2:228:A:N1	76:2:239:G:O2'	2.39	0.43
76:2:613:C:H2'	76:2:614:A:C8	2.54	0.43
76:2:1128:U:H2'	76:2:1129:G:H8	1.83	0.43
82:e:168:LEU:HA	82:e:171:VAL:HG12	2.00	0.43
82:e:198:GLU:HG2	82:e:199:VAL:HG23	2.01	0.43
85:i:105:VAL:HG11	85:i:273:LYS:HE3	1.99	0.43
86:j:249:LYS:HD3	86:j:249:LYS:HA	1.89	0.43
1:B:394:LYS:HD3	1:B:394:LYS:HA	1.73	0.43
15:P:3:PRO:CD	15:P:3:PRO:O	2.66	0.43
22:W:168:GLU:HG3	22:W:473:ARG:HD3	2.00	0.43
26:1:76:C:H2'	26:1:77:A:C8	2.52	0.43
26:1:360:A:H2'	26:1:361:A:C8	2.53	0.43
26:1:1591:C:H2'	26:1:1592:U:C2	2.53	0.43
72:1u:485:CYS:HB3	72:1u:517:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:A:16:SER:HB2	88:A:178:ALA:HB1	2.00	0.43
2:C:287:LEU:HD22	3:D:178:LEU:HD13	2.00	0.43
10:K:121:LYS:HE2	76:2:498:G:H5'	2.01	0.43
16:Q:168:THR:HG23	16:Q:205:ALA:HB2	2.01	0.43
22:W:111:THR:HA	22:W:112:PRO:HD3	1.84	0.43
26:1:198:A:OP1	52:1Z:10:LYS:NZ	2.42	0.43
26:1:456:A:H5'	26:1:474:A:H1'	1.99	0.43
26:1:1839:A:H4'	71:1t:359:LYS:HG2	2.01	0.43
28:1B:46:MET:HG3	29:1C:320:MET:HG2	2.01	0.43
66:1o:82:LEU:HD23	66:1o:82:LEU:HA	1.90	0.43
78:a:98:LEU:CA	78:a:101:ILE:CG2	2.88	0.43
84:h:203:GLU:OE2	84:h:236:LEU:HD11	2.19	0.43
2:C:175:LEU:O	2:C:179:ILE:HG22	2.19	0.43
2:C:282:VAL:HG21	82:e:143:ILE:HD12	2.00	0.43
3:D:179:GLN:HA	3:D:182:THR:HG22	1.99	0.43
24:Y:16:VAL:CG1	24:Y:17:GLY:N	2.81	0.43
29:1C:227:ARG:HB2	29:1C:227:ARG:NH1	2.34	0.43
30:1D:213:LYS:HB3	30:1D:213:LYS:HE2	1.86	0.43
50:1X:216:LEU:HD11	50:1X:222:LEU:HG	2.00	0.43
63:1k:16:TYR:HE1	63:1k:48:THR:HG23	1.84	0.43
76:2:64:U:H2'	76:2:65:G:C8	2.53	0.43
76:2:65:G:H1	76:2:374:C:H5	1.67	0.43
76:2:1770:G:H3'	76:2:1771:C:H4'	2.00	0.43
78:a:412:LYS:HD2	78:a:412:LYS:HA	1.76	0.43
85:i:334:PRO:HD2	85:i:369:LYS:CE	2.46	0.43
86:j:139:PHE:O	86:j:142:LEU:HD22	2.19	0.43
86:j:379:GLU:HA	86:j:382:LYS:HZ3	1.82	0.43
23:X:389:GLU:HG2	23:X:391:GLU:H	1.84	0.43
26:1:1199:C:H2'	26:1:1200:A:H8	1.83	0.43
26:1:1858:C:H2'	26:1:1859:G:C8	2.54	0.43
26:1:2103:U:OP2	26:1:2108:A:N6	2.42	0.43
26:1:2399:U:H2'	26:1:2400:A:H8	1.84	0.43
32:1F:109:ILE:HG13	32:1F:135:PHE:CZ	2.54	0.43
39:1M:156:LEU:HD13	39:1M:264:PRO:HB3	2.01	0.43
39:1M:216:TYR:HB2	39:1M:252:VAL:HG11	2.01	0.43
54:1b:20:TYR:CZ	54:1b:51:LEU:HD13	2.53	0.43
85:i:100:PHE:HD1	85:i:173:VAL:HG11	1.83	0.43
1:B:483:GLU:HG3	1:B:542:SER:HB3	2.01	0.42
23:X:335:VAL:O	23:X:335:VAL:CG1	2.67	0.42
26:1:248:U:O2'	26:1:571:A:N3	2.47	0.42
26:1:274:A:H2'	26:1:275:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1613:G:H2'	26:1:1614:G:C8	2.53	0.42
76:2:472:C:H2'	76:2:473:G:C8	2.54	0.42
76:2:839:C:O2'	76:2:840:U:O4'	2.34	0.42
76:2:952:A:O2'	76:2:977:C:O2'	2.31	0.42
76:2:1730:U:H5''	84:h:187:HIS:HE1	1.83	0.42
82:e:144:GLU:O	82:e:148:ARG:HG2	2.19	0.42
84:h:163:ALA:HB1	84:h:166:HIS:HD2	1.82	0.42
84:h:168:LYS:CA	84:h:189:MET:HE1	2.49	0.42
1:B:191:ILE:HD11	78:a:192:ILE:CD1	2.38	0.42
1:B:473:LYS:NZ	1:B:477:GLU:OE2	2.40	0.42
2:C:331:PHE:HB2	82:e:214:GLN:HB3	2.02	0.42
17:R:66:LYS:N	76:2:1136:A:OP1	2.52	0.42
20:U:70:GLU:CB	87:k:15:ARG:HH11	2.32	0.42
20:U:76:ALA:HB1	87:k:13:ILE:HA	2.02	0.42
26:1:1009:G:H2'	26:1:1010:C:C6	2.54	0.42
26:1:1255:U:H2'	26:1:1256:G:C8	2.54	0.42
26:1:2382:C:H2'	26:1:2383:C:C6	2.54	0.42
26:1:2496:U:H2'	26:1:2497:G:H8	1.84	0.42
34:1H:95:LYS:HB2	34:1H:95:LYS:HE3	1.77	0.42
62:1j:82:ILE:HG22	62:1j:83:GLU:HG3	2.00	0.42
73:1v:95:SER:HA	73:1v:98:PHE:CD2	2.54	0.42
83:f:280:GLU:HA	83:f:283:ILE:HG12	2.01	0.42
17:R:192:VAL:O	55:1c:50:GLN:NE2	2.49	0.42
20:U:67:LYS:HE3	20:U:69:VAL:HG13	2.01	0.42
22:W:294:VAL:HA	22:W:309:THR:HG22	2.00	0.42
26:1:361:A:H5'	73:1v:446:THR:HB	2.00	0.42
26:1:461:G:H5'	48:1V:5:ALA:HB1	2.02	0.42
26:1:756:U:C5	31:1E:300:ARG:HD3	2.55	0.42
26:1:801:U:H2'	26:1:802:U:C6	2.54	0.42
26:1:2957:A:H2'	26:1:2958:A:H8	1.84	0.42
26:1:3083:A:H5''	26:1:3084:G:H5'	2.01	0.42
35:1I:43:ILE:HG22	35:1I:44:LEU:HD12	2.00	0.42
50:1X:192:ILE:HD12	50:1X:242:PRO:HB2	2.01	0.42
72:1u:350:GLU:OE2	72:1u:353:SER:OG	2.38	0.42
76:2:313:U:OP1	76:2:608:G:O2'	2.31	0.42
76:2:1138:G:N2	76:2:1383:G:H1	2.17	0.42
76:2:1703:G:H3'	76:2:1704:A:H8	1.85	0.42
85:i:175:LYS:HA	85:i:175:LYS:HD3	1.92	0.42
1:B:375:LYS:NZ	78:a:103:GLU:HB2	2.34	0.42
7:H:336:ASP:OD2	22:W:429:ARG:NH1	2.51	0.42
19:T:74:LYS:HD3	19:T:74:LYS:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:88:ARG:O	20:U:92:LEU:N	2.52	0.42
26:1:346:A:H2'	26:1:347:A:H8	1.85	0.42
26:1:498:U:O2'	26:1:500:C:OP2	2.32	0.42
26:1:1449:G:H2'	26:1:1450:A:C8	2.55	0.42
26:1:1449:G:H2'	26:1:1450:A:H8	1.84	0.42
31:1E:226:ILE:HG21	31:1E:255:THR:HG22	2.02	0.42
35:1I:61:PHE:HA	35:1I:73:LYS:HZ1	1.85	0.42
66:1o:60:LEU:HD23	66:1o:60:LEU:HA	1.90	0.42
76:2:144:U:H2'	76:2:145:U:C6	2.54	0.42
76:2:1653:U:H2'	76:2:1654:G:C8	2.55	0.42
1:B:174:ARG:NH2	23:X:366:ARG:HD2	2.34	0.42
11:L:40:PRO:HG2	11:L:43:LYS:HD3	2.02	0.42
17:R:59:GLU:HB2	17:R:78:ASN:HB3	2.00	0.42
26:1:556:C:H2'	26:1:557:A:H8	1.84	0.42
29:1C:9:LEU:HD12	70:1s:108:SER:HA	2.00	0.42
31:1E:94:THR:OG1	31:1E:95:ASN:N	2.53	0.42
54:1b:74:GLU:CG	54:1b:78:LYS:HE3	2.49	0.42
75:5:28:C:H2'	75:5:29:G:H8	1.85	0.42
84:h:330:LYS:CD	84:h:375:VAL:HG23	2.48	0.42
87:k:1:MET:HE3	87:k:1:MET:HB3	1.71	0.42
11:L:90:GLY:O	61:1i:249:LYS:NZ	2.38	0.42
21:V:132:GLN:HG3	21:V:136:ARG:HH12	1.84	0.42
25:Z:89:ASP:OD2	25:Z:92:HIS:ND1	2.39	0.42
26:1:2957:A:H2'	26:1:2958:A:C8	2.54	0.42
26:1:3062:C:H2'	26:1:3063:G:H8	1.84	0.42
35:1I:27:ILE:CD1	35:1I:83:ILE:HD12	2.46	0.42
47:1U:14:ASN:HD21	53:1a:144:MET:HE2	1.83	0.42
64:1l:211:VAL:HG11	64:1l:219:PHE:CE2	2.54	0.42
66:1o:102:ASP:OD1	66:1o:102:ASP:N	2.52	0.42
72:1u:87:LEU:HA	72:1u:90:THR:HG22	2.00	0.42
76:2:343:G:N1	76:2:346:A:OP2	2.52	0.42
76:2:1066:G:O2'	76:2:1093:A:N1	2.45	0.42
77:6:1:A:H2'	77:6:2:A:H8	1.85	0.42
83:f:141:ILE:HG13	83:f:161:PHE:HB2	2.00	0.42
83:f:269:MET:HE1	83:f:273:TYR:CZ	2.55	0.42
1:B:399:MET:HE1	78:a:101:ILE:HG21	2.01	0.42
8:I:201:LEU:HD13	8:I:218:PHE:HZ	1.84	0.42
31:1E:95:ASN:CG	31:1E:101:LYS:HE3	2.45	0.42
40:1N:142:SER:OG	40:1N:143:THR:N	2.52	0.42
55:1c:55:LYS:HD2	55:1c:55:LYS:HA	1.83	0.42
72:1u:453:LEU:HD23	72:1u:453:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:1v:143:ASP:HA	73:1v:146:VAL:HG22	2.01	0.42
76:2:90:A:H5''	86:j:117:ARG:HH12	1.84	0.42
88:A:152:LEU:HD23	88:A:152:LEU:HA	1.88	0.42
3:D:196:LYS:HE2	3:D:196:LYS:HB2	1.93	0.42
15:P:2:LYS:NZ	76:2:595:G:OP1	2.40	0.42
26:1:1222:C:N4	26:1:1249:G:O6	2.52	0.42
26:1:1617:G:H2'	26:1:1618:A:C8	2.54	0.42
35:1I:44:LEU:O	35:1I:50:THR:OG1	2.30	0.42
37:1K:167:MET:HE3	37:1K:172:ARG:HG3	2.02	0.42
47:1U:110:SER:HA	47:1U:113:LYS:HE2	2.01	0.42
72:1u:511:LEU:HD13	72:1u:534:MET:HG2	2.02	0.42
73:1v:94:ILE:HG22	73:1v:98:PHE:CZ	2.55	0.42
78:a:210:ASP:OD1	78:a:210:ASP:N	2.50	0.42
83:f:257:TYR:CE2	85:i:293:VAL:HG12	2.54	0.42
1:B:284:ARG:HH11	1:B:288:ARG:NH2	2.17	0.42
4:E:45:LYS:HE3	4:E:45:LYS:HB3	1.78	0.42
7:H:208:ARG:HA	7:H:211:LYS:HD2	2.02	0.42
11:L:138:LYS:HA	11:L:138:LYS:HD2	1.85	0.42
21:V:139:LEU:HA	21:V:142:GLU:HG2	2.02	0.42
26:1:2451:C:H2'	26:1:2460:A:N1	2.35	0.42
30:1D:107:ASN:HA	30:1D:126:GLY:O	2.20	0.42
30:1D:201:LYS:HA	30:1D:201:LYS:HD2	1.89	0.42
38:1L:140:THR:O	38:1L:142:ARG:HD2	2.20	0.42
50:1X:72:LYS:HE2	50:1X:72:LYS:HB3	1.88	0.42
64:1l:144:LYS:HA	64:1l:144:LYS:HD3	1.88	0.42
71:1t:228:ASP:OD1	71:1t:228:ASP:N	2.52	0.42
76:2:75:C:O2'	76:2:216:A:N3	2.47	0.42
76:2:113:U:H2'	76:2:114:U:C6	2.54	0.42
76:2:557:A:H4'	76:2:558:A:H3'	2.01	0.42
76:2:1113:U:H2'	76:2:1114:G:H8	1.85	0.42
76:2:1638:U:H2'	76:2:1639:A:C8	2.55	0.42
83:f:63:ASN:ND2	83:f:97:THR:O	2.53	0.42
85:i:309:ARG:HA	85:i:309:ARG:HD3	1.87	0.42
1:B:159:HIS:O	1:B:430:ARG:NH1	2.50	0.42
6:G:28:PRO:HB3	76:2:649:U:H5	1.84	0.42
8:I:156:MET:HE1	76:2:1117:U:C2	2.55	0.42
20:U:112:ALA:HA	20:U:115:LYS:HE3	2.01	0.42
26:1:1161:G:OP2	44:1R:55:ASN:ND2	2.52	0.42
30:1D:84:CYS:HA	43:1Q:112:ALA:HB1	2.00	0.42
36:1J:34:PRO:O	36:1J:38:PRO:CG	2.65	0.42
49:1W:148:ALA:HB1	49:1W:190:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1X:54:ILE:HA	50:1X:101:GLN:HE22	1.84	0.42
81:d:94:TYR:HA	81:d:97:LYS:HB2	2.01	0.42
86:j:222:SER:HA	86:j:225:PHE:HB2	2.02	0.42
2:C:53:LYS:HE3	2:C:53:LYS:HB3	1.88	0.41
20:U:59:PHE:N	20:U:62:LYS:HZ2	2.18	0.41
23:X:348:MET:CE	23:X:352:ILE:HB	2.50	0.41
26:1:1105:PSU:HN3	26:1:1112:A:H62	1.68	0.41
29:1C:192:PRO:O	29:1C:195:PRO:HD2	2.19	0.41
47:1U:134:ARG:HG2	47:1U:135:ARG:N	2.35	0.41
51:1Y:64:LYS:HA	51:1Y:64:LYS:HD3	1.87	0.41
51:1Y:104:LEU:HD12	51:1Y:125:ILE:HD12	2.01	0.41
64:1l:111:LEU:HD13	64:1l:210:TRP:HB3	2.02	0.41
72:1u:463:ILE:O	72:1u:503:ARG:NH1	2.53	0.41
76:2:25:U:H2'	76:2:26:U:C6	2.55	0.41
1:B:395:VAL:HG13	78:a:105:LEU:HD11	2.02	0.41
12:M:99:LEU:HD22	12:M:104:ARG:HG3	2.02	0.41
22:W:146:ASP:HB3	22:W:149:ALA:HB3	2.02	0.41
23:X:322:LYS:HD2	23:X:322:LYS:HA	1.89	0.41
26:1:1151:A:OP1	68:1q:43:ARG:NH1	2.53	0.41
26:1:1226:C:H2'	26:1:1227:A:H8	1.84	0.41
26:1:2441:G:H2'	26:1:2442:G:C8	2.55	0.41
26:1:2560:OMG:HM23	26:1:2560:OMG:H1'	1.70	0.41
26:1:3011:G:H2'	26:1:3012:A:H8	1.85	0.41
26:1:3036:G:OP1	38:1L:78:ARG:NH2	2.48	0.41
32:1F:13:ARG:NH2	32:1F:25:VAL:O	2.53	0.41
41:1O:78:THR:HB	70:1s:168:TRP:CE2	2.55	0.41
72:1u:269:LEU:O	72:1u:270:ARG:NH1	2.45	0.41
83:f:327:THR:OG1	83:f:329:ASP:OD1	2.30	0.41
86:j:286:SER:OG	86:j:288:MET:CE	2.68	0.41
5:F:100:ARG:NE	5:F:105:ILE:O	2.53	0.41
16:Q:189:GLU:O	16:Q:226:THR:OG1	2.35	0.41
20:U:59:PHE:CE1	20:U:63:HIS:CD2	3.08	0.41
20:U:77:PHE:O	87:k:11:GLY:HA3	2.20	0.41
23:X:423:VAL:HA	23:X:428:ILE:HD13	2.01	0.41
23:X:523:LYS:HE2	23:X:523:LYS:HB2	1.95	0.41
72:1u:526:SER:HA	72:1u:529:GLU:HG2	2.02	0.41
76:2:86:A:H2'	76:2:87:A:H8	1.86	0.41
82:e:183:ASP:HA	82:e:186:LYS:HD2	2.02	0.41
82:e:192:LEU:HG	82:e:200:TYR:HD2	1.83	0.41
83:f:206:LYS:NZ	85:i:315:THR:HG1	2.15	0.41
86:j:159:PHE:HA	86:j:162:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:C	1:B:109:CYS:H	2.29	0.41
3:D:216:GLU:O	3:D:220:ARG:HG2	2.20	0.41
20:U:70:GLU:C	20:U:72:ASN:N	2.73	0.41
25:Z:50:LYS:HB2	25:Z:119:ARG:HB3	2.02	0.41
26:1:1967:C:H4'	70:1s:132:ILE:HG12	2.02	0.41
35:1I:133:PRO:HB2	35:1I:134:SER:H	1.69	0.41
37:1K:86:LEU:HD23	37:1K:86:LEU:HA	1.90	0.41
51:1Y:77:ILE:HA	51:1Y:109:GLU:HG3	2.02	0.41
52:1Z:22:THR:HG23	52:1Z:25:LEU:H	1.85	0.41
71:1t:112:TYR:O	71:1t:116:LEU:HG	2.20	0.41
76:2:129:A:H2'	76:2:130:A:C8	2.54	0.41
76:2:1664:4OC:H2'	76:2:1665:C:O4'	2.19	0.41
83:f:105:LEU:N	83:f:106:PRO:CD	2.84	0.41
83:f:165:THR:HA	83:f:222:CYS:O	2.19	0.41
84:h:203:GLU:O	84:h:207:LYS:HG3	2.20	0.41
88:A:14:THR:HG21	88:A:187:LEU:HD22	2.03	0.41
88:A:64:ARG:HH22	88:A:203:MET:HG2	1.85	0.41
1:B:173:LEU:HD21	23:X:376:LEU:HD23	2.03	0.41
1:B:188:VAL:HA	1:B:191:ILE:HG22	2.02	0.41
3:D:456:LYS:HD3	3:D:456:LYS:HA	1.86	0.41
13:N:331:LYS:HD2	13:N:331:LYS:HA	1.77	0.41
23:X:463:ALA:N	78:a:359:GLU:OE1	2.50	0.41
26:1:1230:C:H2'	26:1:1231:U:H6	1.85	0.41
26:1:1254:C:H2'	26:1:1255:U:H6	1.85	0.41
26:1:1836:A:H2'	26:1:1837:A:C8	2.55	0.41
29:1C:245:TRP:HB2	52:1Z:91:VAL:HG12	2.02	0.41
30:1D:262:ILE:HG12	30:1D:264:VAL:HG23	2.03	0.41
47:1U:125:LYS:HB3	47:1U:125:LYS:HE2	1.87	0.41
52:1Z:153:LYS:HE2	52:1Z:153:LYS:HB3	1.88	0.41
76:2:3:C:O2'	76:2:4:A:O5'	2.39	0.41
76:2:1141:A:H61	76:2:1381:C:H4'	1.85	0.41
84:h:129:LEU:HG	84:h:177:HIS:HB3	2.02	0.41
85:i:277:LYS:HE3	85:i:277:LYS:HB2	1.79	0.41
86:j:72:LEU:HB3	86:j:79:ASP:HB3	2.02	0.41
86:j:157:LEU:HD23	86:j:173:VAL:HG11	2.02	0.41
3:D:473:ILE:HD13	3:D:473:ILE:HG21	1.85	0.41
20:U:28:LYS:HA	20:U:28:LYS:HD2	1.89	0.41
20:U:91:GLU:O	20:U:94:LYS:HB3	2.21	0.41
22:W:141:SER:OG	22:W:142:TYR:N	2.54	0.41
26:1:2017:C:O2	30:1D:208:SER:OG	2.38	0.41
26:1:2936:A:H5''	26:1:2937:A:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1E:95:ASN:CB	31:1E:101:LYS:NZ	2.76	0.41
35:1I:57:ASN:HB2	35:1I:76:MET:HE2	2.02	0.41
71:1t:190:MET:HA	71:1t:191:PRO:HD3	1.88	0.41
72:1u:90:THR:O	72:1u:94:MET:HG2	2.20	0.41
72:1u:155:LYS:HG3	72:1u:159:MET:HE3	2.02	0.41
76:2:64:U:H2'	76:2:65:G:H8	1.85	0.41
76:2:1766:U:H2'	76:2:1767:G:C8	2.56	0.41
84:h:266:ARG:HA	84:h:266:ARG:HD2	1.94	0.41
6:G:114:GLU:OE2	6:G:118:ARG:NH1	2.53	0.41
17:R:54:PHE:CZ	17:R:92:MET:HE1	2.55	0.41
25:Z:62:ASN:OD1	84:h:145:ASN:ND2	2.54	0.41
26:1:141:U:N3	73:1v:117:ASN:O	2.51	0.41
26:1:292:U:H2'	26:1:293:U:C6	2.56	0.41
47:1U:131:GLN:NE2	47:1U:134:ARG:HD2	2.33	0.41
55:1c:20:ARG:HE	61:1i:229:PRO:HG3	1.85	0.41
72:1u:474:PRO:HA	72:1u:477:TYR:CZ	2.55	0.41
73:1v:191:PRO:HG2	73:1v:229:ILE:HD11	2.03	0.41
73:1v:332:LEU:HD22	73:1v:337:ARG:HB2	2.01	0.41
76:2:1686:U:H2'	76:2:1687:U:C6	2.56	0.41
76:2:1709:U:H2'	76:2:1710:G:C8	2.56	0.41
86:j:42:THR:OG1	86:j:43:SER:N	2.52	0.41
1:B:25:ASP:OD1	1:B:25:ASP:N	2.53	0.41
2:C:314:LEU:HD11	82:e:245:LEU:HD22	2.03	0.41
17:R:57:VAL:HG22	17:R:79:PHE:CE1	2.55	0.41
20:U:63:HIS:O	20:U:64:PRO:O	2.39	0.41
26:1:740:A:H2'	26:1:741:A:H8	1.86	0.41
26:1:2494:G:H2'	26:1:2495:G:C8	2.56	0.41
29:1C:71:LEU:HD13	29:1C:308:TYR:HE1	1.86	0.41
29:1C:199:VAL:HG21	34:1H:97:ARG:CG	2.50	0.41
36:1J:84:VAL:HG21	36:1J:139:ILE:HG12	2.03	0.41
71:1t:21:LEU:HD23	71:1t:21:LEU:HA	1.90	0.41
72:1u:166:LEU:HB3	72:1u:195:TYR:CE1	2.55	0.41
72:1u:205:VAL:HG22	72:1u:226:LEU:HD11	2.03	0.41
73:1v:332:LEU:HD23	73:1v:332:LEU:HA	1.88	0.41
88:A:150:ALA:HB2	88:A:171:LYS:HB3	2.02	0.41
1:B:204:THR:HG22	1:B:206:LEU:H	1.84	0.41
1:B:373:LYS:H	1:B:375:LYS:HG2	1.84	0.41
3:D:227:LYS:O	3:D:231:ILE:HG12	2.21	0.41
6:G:103:VAL:HG12	6:G:124:VAL:HA	2.02	0.41
7:H:254:ASP:OD1	7:H:254:ASP:N	2.53	0.41
8:I:168:SER:HB3	8:I:172:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:129:PHE:CD2	12:M:142:MET:SD	3.12	0.41
16:Q:204:LYS:HD2	76:2:659:A:H5''	2.02	0.41
20:U:45:LEU:HG	88:A:28:LYS:HD3	2.03	0.41
22:W:212:ASP:OD2	22:W:424:ARG:NH1	2.54	0.41
25:Z:71:LYS:HB2	25:Z:74:TRP:CG	2.55	0.41
26:1:272:A:H2'	26:1:273:A:H8	1.86	0.41
26:1:609:G:OP2	58:1f:191:ARG:HD3	2.21	0.41
26:1:758:A:H2'	26:1:759:A:C8	2.56	0.41
26:1:1004:G:O2'	26:1:1064:G:O6	2.30	0.41
26:1:1219:A:N7	26:1:1223:A:N6	2.69	0.41
26:1:1511:A:H2'	26:1:1512:A:C8	2.56	0.41
26:1:2556:U:H2'	26:1:2557:C:H6	1.86	0.41
31:1E:138:THR:O	31:1E:180:ARG:NH1	2.54	0.41
41:1O:3:LYS:HE3	41:1O:3:LYS:HB2	1.86	0.41
53:1a:60:TRP:HH2	62:1j:73:LEU:HD22	1.84	0.41
54:1b:74:GLU:HG3	54:1b:78:LYS:HE3	2.03	0.41
66:1o:88:LEU:HD12	66:1o:88:LEU:HA	1.95	0.41
73:1v:192:LYS:O	73:1v:195:THR:OG1	2.31	0.41
76:2:48:C:H2'	76:2:49:U:C6	2.55	0.41
76:2:1035:U:O2'	76:2:1036:A:O5'	2.35	0.41
85:i:320:LEU:HA	85:i:323:GLU:HB2	2.02	0.41
8:I:170:HIS:ND1	8:I:171:VAL:HG22	2.36	0.41
13:N:329:LEU:HA	13:N:332:VAL:HG22	2.02	0.41
26:1:337:A:H2'	26:1:338:A:C8	2.56	0.41
26:1:2662:G:O2'	26:1:2663:A:H5''	2.21	0.41
34:1H:103:LYS:HE2	34:1H:103:LYS:HB3	1.78	0.41
49:1W:34:GLN:HB2	49:1W:107:PHE:HD1	1.85	0.41
81:d:39:LYS:HZ2	81:d:39:LYS:HG2	1.67	0.41
84:h:110:TRP:O	84:h:114:GLU:HG2	2.21	0.41
84:h:256:PHE:CE2	84:h:279:ARG:HB2	2.55	0.41
84:h:286:HIS:HB3	84:h:291:ALA:HB2	2.04	0.41
85:i:210:ASP:OD1	85:i:213:ARG:NH1	2.50	0.41
1:B:162:SER:HG	1:B:429:ASN:HD21	1.55	0.40
5:F:134:GLY:HA2	79:b:49:ILE:HD13	2.02	0.40
10:K:88:LYS:HE3	10:K:88:LYS:HB3	1.88	0.40
20:U:94:LYS:HA	20:U:94:LYS:HD2	1.84	0.40
26:1:600:G:O2'	26:1:611:G:O6	2.36	0.40
28:1B:64:PRO:HA	28:1B:123:ARG:HA	2.03	0.40
39:1M:64:LEU:HD23	39:1M:64:LEU:HA	1.94	0.40
50:1X:209:ILE:HG21	50:1X:227:LEU:HD22	2.03	0.40
53:1a:69:SER:OG	53:1a:70:TRP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1a:130:ASP:OD1	53:1a:131:PRO:CD	2.66	0.40
79:b:51:ASP:OD1	79:b:51:ASP:N	2.53	0.40
85:i:137:GLU:OE1	85:i:141:ARG:NH2	2.54	0.40
1:B:246:LYS:HB3	1:B:246:LYS:HE3	1.87	0.40
2:C:253:LYS:HB3	2:C:253:LYS:HE2	1.87	0.40
3:D:90:GLU:HA	3:D:93:ARG:HG2	2.02	0.40
26:1:412:U:H2'	26:1:413:U:C6	2.56	0.40
26:1:490:U:H2'	26:1:491:U:C6	2.56	0.40
26:1:493:G:OP2	72:1u:170:ARG:NH2	2.54	0.40
26:1:556:C:H2'	26:1:557:A:C8	2.56	0.40
26:1:996:G:H2'	26:1:997:G:H8	1.85	0.40
26:1:2931:U:H2'	26:1:2932:G:C8	2.56	0.40
40:1N:33:LYS:HE3	40:1N:33:LYS:HB3	1.79	0.40
46:1T:174:ILE:HB	46:1T:214:THR:HG22	2.01	0.40
72:1u:84:HIS:HB3	72:1u:85:GLU:H	1.65	0.40
76:2:901:A:H2'	76:2:902:A:H8	1.86	0.40
76:2:1141:A:N6	76:2:1381:C:O3'	2.54	0.40
76:2:1384:A:H2'	76:2:1385:A:C8	2.57	0.40
85:i:103:ARG:O	85:i:107:ILE:HG22	2.21	0.40
14:O:98:ARG:NH2	82:e:327:ARG:O	2.40	0.40
22:W:158:LEU:HD23	22:W:158:LEU:HA	1.92	0.40
26:1:151:U:H1'	26:1:152:C:H5'	2.04	0.40
26:1:1613:G:H2'	26:1:1614:G:H8	1.85	0.40
26:1:1627:U:H2'	26:1:1628:A:C5	2.56	0.40
26:1:2555:A:H2'	26:1:2556:U:C6	2.57	0.40
48:1V:159:LEU:HD23	48:1V:159:LEU:HA	1.91	0.40
64:1l:160:THR:HB	64:1l:192:CYS:SG	2.60	0.40
71:1t:465:MET:H	71:1t:468:ARG:NH1	2.19	0.40
72:1u:360:ALA:HA	72:1u:391:ILE:HD11	2.02	0.40
76:2:411:C:H2'	76:2:412:A:C8	2.55	0.40
76:2:613:C:H2'	76:2:614:A:H8	1.86	0.40
76:2:1664:4OC:H6	76:2:1664:4OC:O5'	2.21	0.40
78:a:358:GLU:HG3	78:a:362:LYS:HE3	2.02	0.40
86:j:308:PHE:HZ	86:j:336:TYR:HB3	1.87	0.40
1:B:402:ILE:HD12	78:a:86:ILE:HD11	2.04	0.40
3:D:158:ASP:HA	3:D:161:ARG:HG2	2.03	0.40
7:H:230:ARG:HD3	20:U:79:PRO:CG	2.52	0.40
24:Y:96:ARG:HH21	76:2:1476:A:H4'	1.86	0.40
26:1:884:A:H1'	26:1:885:C:H5	1.86	0.40
26:1:2567:U:O2'	26:1:2732:C:OP2	2.37	0.40
31:1E:189:ASN:HB2	31:1E:192:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1G:45:VAL:O	33:1G:46:ARG:NH1	2.46	0.40
35:1I:40:LEU:HD13	35:1I:100:PHE:CD2	2.56	0.40
36:1J:117:ILE:HG22	36:1J:139:ILE:HD13	2.04	0.40
47:1U:31:PHE:HE1	47:1U:88:LEU:HD21	1.85	0.40
66:1o:122:ILE:HD13	66:1o:122:ILE:HA	1.95	0.40
71:1t:319:GLU:OE2	71:1t:344:TYR:OH	2.39	0.40
72:1u:348:PHE:HA	72:1u:351:MET:HB2	2.03	0.40
72:1u:689:LEU:HB3	72:1u:717:TRP:CH2	2.57	0.40
73:1v:228:SER:O	73:1v:232:LYS:HG2	2.21	0.40
14:O:26:ARG:HE	14:O:26:ARG:HB2	1.69	0.40
17:R:188:THR:HG22	17:R:189:GLU:H	1.86	0.40
20:U:58:ARG:HB2	20:U:62:LYS:CE	2.51	0.40
26:1:272:A:H2'	26:1:273:A:C8	2.57	0.40
26:1:2118:A:H2'	26:1:2119:C:H6	1.87	0.40
26:1:2423:C:N4	26:1:2487:G:O2'	2.55	0.40
35:1I:45:ARG:NH2	35:1I:46:GLU:OE2	2.54	0.40
38:1L:157:LEU:HB3	38:1L:162:HIS:HB2	2.03	0.40
61:1i:193:MET:HE2	61:1i:193:MET:HB3	1.91	0.40
72:1u:322:GLY:HA2	72:1u:323:PRO:HD3	1.88	0.40
72:1u:386:MET:O	72:1u:391:ILE:HG22	2.21	0.40
73:1v:470:ASP:HA	73:1v:471:PRO:HD3	1.94	0.40
76:2:766:C:H2'	76:2:767:A:H8	1.86	0.40
78:a:101:ILE:CG2	78:a:102:ILE:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	457/554 (82%)	425 (93%)	31 (7%)	1 (0%)	43	70
2	C	329/362 (91%)	317 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	413/501 (82%)	397 (96%)	15 (4%)	1 (0%)	43	70
4	E	99/138 (72%)	96 (97%)	3 (3%)	0	100	100
5	F	146/157 (93%)	140 (96%)	6 (4%)	0	100	100
6	G	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
7	H	209/383 (55%)	197 (94%)	11 (5%)	1 (0%)	24	52
8	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
9	J	125/304 (41%)	121 (97%)	4 (3%)	0	100	100
10	K	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
11	L	117/154 (76%)	110 (94%)	7 (6%)	0	100	100
12	M	99/155 (64%)	96 (97%)	3 (3%)	0	100	100
13	N	114/414 (28%)	113 (99%)	1 (1%)	0	100	100
14	O	108/136 (79%)	104 (96%)	4 (4%)	0	100	100
15	P	89/110 (81%)	84 (94%)	4 (4%)	1 (1%)	11	34
16	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100
17	R	162/212 (76%)	152 (94%)	10 (6%)	0	100	100
18	S	73/100 (73%)	72 (99%)	1 (1%)	0	100	100
19	T	48/94 (51%)	44 (92%)	4 (8%)	0	100	100
20	U	125/192 (65%)	109 (87%)	9 (7%)	7 (6%)	1	7
21	V	162/193 (84%)	160 (99%)	2 (1%)	0	100	100
22	W	376/483 (78%)	368 (98%)	8 (2%)	0	100	100
23	X	202/496 (41%)	191 (95%)	8 (4%)	3 (2%)	8	28
24	Y	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
25	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100	100
28	1B	175/220 (80%)	171 (98%)	4 (2%)	0	100	100
29	1C	203/327 (62%)	194 (96%)	7 (3%)	2 (1%)	12	37
30	1D	262/319 (82%)	257 (98%)	5 (2%)	0	100	100
31	1E	219/297 (74%)	217 (99%)	2 (1%)	0	100	100
32	1F	154/185 (83%)	148 (96%)	6 (4%)	0	100	100
33	1G	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
34	1H	64/219 (29%)	63 (98%)	1 (2%)	0	100	100
35	1I	128/170 (75%)	119 (93%)	8 (6%)	1 (1%)	16	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1J	145/156 (93%)	132 (91%)	11 (8%)	2 (1%)	9	29
37	1K	187/204 (92%)	184 (98%)	3 (2%)	0	100	100
38	1L	125/176 (71%)	119 (95%)	6 (5%)	0	100	100
39	1M	208/281 (74%)	195 (94%)	13 (6%)	0	100	100
40	1N	146/179 (82%)	143 (98%)	3 (2%)	0	100	100
41	1O	149/160 (93%)	141 (95%)	8 (5%)	0	100	100
42	1P	111/114 (97%)	102 (92%)	9 (8%)	0	100	100
43	1Q	120/233 (52%)	116 (97%)	4 (3%)	0	100	100
44	1R	108/126 (86%)	107 (99%)	1 (1%)	0	100	100
45	1S	143/270 (53%)	139 (97%)	4 (3%)	0	100	100
46	1T	153/264 (58%)	148 (97%)	5 (3%)	0	100	100
47	1U	126/180 (70%)	120 (95%)	6 (5%)	0	100	100
48	1V	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
49	1W	203/249 (82%)	192 (95%)	11 (5%)	0	100	100
50	1X	214/271 (79%)	209 (98%)	5 (2%)	0	100	100
51	1Y	96/156 (62%)	94 (98%)	2 (2%)	0	100	100
52	1Z	175/212 (82%)	174 (99%)	1 (1%)	0	100	100
53	1a	106/144 (74%)	104 (98%)	2 (2%)	0	100	100
54	1b	98/109 (90%)	94 (96%)	4 (4%)	0	100	100
55	1c	57/135 (42%)	54 (95%)	3 (5%)	0	100	100
56	1d	47/139 (34%)	47 (100%)	0	0	100	100
57	1e	52/63 (82%)	51 (98%)	1 (2%)	0	100	100
58	1f	42/146 (29%)	42 (100%)	0	0	100	100
59	1g	89/162 (55%)	89 (100%)	0	0	100	100
60	1h	36/103 (35%)	34 (94%)	2 (6%)	0	100	100
61	1i	181/247 (73%)	176 (97%)	5 (3%)	0	100	100
62	1j	69/90 (77%)	68 (99%)	1 (1%)	0	100	100
63	1k	116/119 (98%)	111 (96%)	5 (4%)	0	100	100
64	1l	209/233 (90%)	198 (95%)	11 (5%)	0	100	100
65	1m	120/128 (94%)	119 (99%)	1 (1%)	0	100	100
66	1o	74/125 (59%)	70 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	1p	115/130 (88%)	112 (97%)	3 (3%)	0	100	100
68	1q	48/79 (61%)	47 (98%)	0	1 (2%)	5	21
69	1r	90/167 (54%)	84 (93%)	6 (7%)	0	100	100
70	1s	116/181 (64%)	113 (97%)	3 (3%)	0	100	100
71	1t	482/491 (98%)	468 (97%)	14 (3%)	0	100	100
72	1u	664/757 (88%)	624 (94%)	40 (6%)	0	100	100
73	1v	429/521 (82%)	412 (96%)	17 (4%)	0	100	100
74	1x	2/4 (50%)	2 (100%)	0	0	100	100
78	a	311/424 (73%)	305 (98%)	6 (2%)	0	100	100
79	b	75/80 (94%)	68 (91%)	7 (9%)	0	100	100
80	c	24/128 (19%)	23 (96%)	1 (4%)	0	100	100
81	d	76/110 (69%)	74 (97%)	2 (3%)	0	100	100
82	e	244/383 (64%)	236 (97%)	8 (3%)	0	100	100
83	f	375/410 (92%)	361 (96%)	14 (4%)	0	100	100
84	h	308/384 (80%)	301 (98%)	7 (2%)	0	100	100
85	i	302/725 (42%)	290 (96%)	10 (3%)	2 (1%)	18	45
86	j	379/408 (93%)	365 (96%)	14 (4%)	0	100	100
87	k	43/155 (28%)	37 (86%)	6 (14%)	0	100	100
88	A	202/212 (95%)	196 (97%)	6 (3%)	0	100	100
All	All	13521/19033 (71%)	13005 (96%)	494 (4%)	22 (0%)	44	70

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	225	ILE
20	U	64	PRO
20	U	81	PRO
29	1C	227	ARG
35	1I	133	PRO
36	1J	33	SER
85	i	375	LEU
85	i	376	ASP
20	U	97	ILE
15	P	3	PRO
20	U	57	ARG

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Mol	Chain	Res	Type
20	U	73	LYS
20	U	74	VAL
29	1C	187	SER
36	1J	29	GLY
20	U	70	GLU
23	X	428	ILE
23	X	461	VAL
68	1q	64	VAL
3	D	260	ILE
1	B	409	ILE
23	X	458	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	421/492 (86%)	421 (100%)	0	100	100
2	C	314/343 (92%)	314 (100%)	0	100	100
3	D	370/444 (83%)	370 (100%)	0	100	100
4	E	90/126 (71%)	90 (100%)	0	100	100
5	F	124/124 (100%)	124 (100%)	0	100	100
6	G	112/113 (99%)	112 (100%)	0	100	100
7	H	176/320 (55%)	175 (99%)	1 (1%)	78	81
8	I	104/197 (53%)	104 (100%)	0	100	100
9	J	108/256 (42%)	107 (99%)	1 (1%)	70	78
10	K	107/108 (99%)	107 (100%)	0	100	100
11	L	99/128 (77%)	99 (100%)	0	100	100
12	M	90/137 (66%)	90 (100%)	0	100	100
13	N	107/362 (30%)	107 (100%)	0	100	100
14	O	93/117 (80%)	93 (100%)	0	100	100
15	P	78/95 (82%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	75/203 (37%)	75 (100%)	0	100	100
17	R	141/180 (78%)	141 (100%)	0	100	100
18	S	68/90 (76%)	68 (100%)	0	100	100
19	T	44/79 (56%)	44 (100%)	0	100	100
20	U	109/170 (64%)	104 (95%)	5 (5%)	24	52
21	V	147/173 (85%)	147 (100%)	0	100	100
22	W	328/410 (80%)	328 (100%)	0	100	100
23	X	174/395 (44%)	174 (100%)	0	100	100
24	Y	84/86 (98%)	84 (100%)	0	100	100
25	Z	65/119 (55%)	65 (100%)	0	100	100
28	1B	141/176 (80%)	141 (100%)	0	100	100
29	1C	184/268 (69%)	183 (100%)	1 (0%)	81	82
30	1D	216/264 (82%)	216 (100%)	0	100	100
31	1E	192/257 (75%)	192 (100%)	0	100	100
32	1F	145/168 (86%)	145 (100%)	0	100	100
33	1G	82/86 (95%)	82 (100%)	0	100	100
34	1H	58/195 (30%)	58 (100%)	0	100	100
35	1I	113/143 (79%)	113 (100%)	0	100	100
36	1J	125/131 (95%)	125 (100%)	0	100	100
37	1K	161/170 (95%)	161 (100%)	0	100	100
38	1L	103/140 (74%)	103 (100%)	0	100	100
39	1M	169/235 (72%)	169 (100%)	0	100	100
40	1N	116/146 (80%)	116 (100%)	0	100	100
41	1O	129/139 (93%)	129 (100%)	0	100	100
42	1P	94/95 (99%)	94 (100%)	0	100	100
43	1Q	110/208 (53%)	110 (100%)	0	100	100
44	1R	96/110 (87%)	96 (100%)	0	100	100
45	1S	130/244 (53%)	130 (100%)	0	100	100
46	1T	133/229 (58%)	133 (100%)	0	100	100
47	1U	114/147 (78%)	114 (100%)	0	100	100
48	1V	132/133 (99%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	1W	181/216 (84%)	181 (100%)	0	100	100
50	1X	186/235 (79%)	186 (100%)	0	100	100
51	1Y	80/127 (63%)	80 (100%)	0	100	100
52	1Z	150/173 (87%)	150 (100%)	0	100	100
53	1a	102/128 (80%)	102 (100%)	0	100	100
54	1b	88/95 (93%)	88 (100%)	0	100	100
55	1c	51/119 (43%)	51 (100%)	0	100	100
56	1d	42/119 (35%)	42 (100%)	0	100	100
57	1e	49/57 (86%)	49 (100%)	0	100	100
58	1f	35/129 (27%)	35 (100%)	0	100	100
59	1g	84/152 (55%)	84 (100%)	0	100	100
60	1h	36/87 (41%)	36 (100%)	0	100	100
61	1i	152/203 (75%)	152 (100%)	0	100	100
62	1j	64/79 (81%)	64 (100%)	0	100	100
63	1k	105/106 (99%)	105 (100%)	0	100	100
64	1l	189/209 (90%)	189 (100%)	0	100	100
65	1m	107/112 (96%)	107 (100%)	0	100	100
66	1o	71/105 (68%)	71 (100%)	0	100	100
67	1p	101/108 (94%)	101 (100%)	0	100	100
68	1q	41/65 (63%)	41 (100%)	0	100	100
69	1r	83/138 (60%)	82 (99%)	1 (1%)	63	75
70	1s	103/155 (66%)	103 (100%)	0	100	100
71	1t	417/423 (99%)	417 (100%)	0	100	100
72	1u	578/663 (87%)	578 (100%)	0	100	100
73	1v	374/461 (81%)	374 (100%)	0	100	100
78	a	252/374 (67%)	252 (100%)	0	100	100
79	b	68/71 (96%)	68 (100%)	0	100	100
80	c	25/116 (22%)	25 (100%)	0	100	100
81	d	65/93 (70%)	65 (100%)	0	100	100
82	e	226/339 (67%)	226 (100%)	0	100	100
83	f	321/351 (92%)	321 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	h	271/337 (80%)	271 (100%)	0	100	100
85	i	272/629 (43%)	271 (100%)	1 (0%)	84	84
86	j	330/355 (93%)	330 (100%)	0	100	100
87	k	22/106 (21%)	22 (100%)	0	100	100
88	A	177/182 (97%)	177 (100%)	0	100	100
All	All	11869/16368 (72%)	11859 (100%)	10 (0%)	87	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	368	THR
9	J	205	THR
20	U	63	HIS
20	U	65	GLU
20	U	69	VAL
20	U	70	GLU
20	U	92	LEU
29	1C	227	ARG
69	1r	68	HIS
85	i	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	432	ASN
1	B	507	HIS
1	B	517	GLN
2	C	301	HIS
4	E	63	GLN
4	E	76	ASN
4	E	96	HIS
5	F	139	ASN
7	H	388	GLN
9	J	192	ASN
9	J	304	ASN
11	L	36	ASN
13	N	359	HIS
15	P	27	ASN
17	R	45	HIS

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Mol	Chain	Res	Type
18	S	62	HIS
20	U	63	HIS
22	W	327	ASN
24	Y	93	HIS
28	1B	83	GLN
29	1C	32	HIS
29	1C	229	HIS
30	1D	279	ASN
31	1E	95	ASN
32	1F	104	ASN
32	1F	145	HIS
34	1H	88	HIS
35	1I	20	ASN
35	1I	30	ASN
35	1I	49	ASN
35	1I	57	ASN
35	1I	80	ASN
36	1J	73	HIS
37	1K	187	ASN
38	1L	143	GLN
39	1M	97	HIS
39	1M	191	HIS
40	1N	105	ASN
42	1P	24	HIS
45	1S	253	HIS
46	1T	116	GLN
46	1T	141	GLN
46	1T	156	HIS
47	1U	11	HIS
47	1U	29	HIS
48	1V	20	ASN
49	1W	218	HIS
50	1X	98	GLN
50	1X	101	GLN
50	1X	108	HIS
52	1Z	20	ASN
61	1i	119	GLN
63	1k	10	GLN
63	1k	55	HIS
64	1l	51	GLN
64	1l	59	GLN
64	1l	130	HIS

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Mol	Chain	Res	Type
65	1m	13	ASN
65	1m	55	GLN
68	1q	49	GLN
69	1r	68	HIS
71	1t	162	ASN
71	1t	299	ASN
71	1t	326	GLN
71	1t	419	GLN
72	1u	83	ASN
72	1u	298	ASN
72	1u	359	ASN
72	1u	732	ASN
73	1v	99	ASN
73	1v	141	HIS
73	1v	330	ASN
78	a	126	GLN
78	a	208	HIS
78	a	356	HIS
78	a	397	ASN
79	b	68	GLN
80	c	125	HIS
83	f	121	HIS
83	f	251	GLN
83	f	288	ASN
84	h	145	ASN
84	h	286	HIS
85	i	358	GLN
85	i	412	GLN
86	j	260	HIS
86	j	265	GLN
86	j	297	HIS
88	A	9	GLN
88	A	93	ASN
88	A	94	HIS
88	A	163	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2910/2922 (99%)	539 (18%)	28 (0%)
27	3	117/118 (99%)	24 (20%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
75	5	75/76 (98%)	12 (16%)	0
76	2	1583/1591 (99%)	267 (16%)	11 (0%)
77	6	5/6 (83%)	0	0
All	All	4690/4713 (99%)	842 (17%)	40 (0%)

All (842) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	49	G
26	1	50	G
26	1	51	A
26	1	54	G
26	1	63	A
26	1	64	G
26	1	65	A
26	1	70	A
26	1	74	G
26	1	87	A
26	1	88	C
26	1	96	G
26	1	113	U
26	1	126	U
26	1	127	C
26	1	128	C
26	1	129	A
26	1	131	G
26	1	132	C
26	1	136	G
26	1	137	U
26	1	138	G
26	1	139	G
26	1	141	U
26	1	142	A
26	1	144	U
26	1	147	G
26	1	148	C
26	1	150	C
26	1	151	U
26	1	152	C
26	1	153	U
26	1	157	G
26	1	158	A

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Mol	Chain	Res	Type
26	1	159	C
26	1	161	U
26	1	163	G
26	1	164	A
26	1	181	A
26	1	184	A
26	1	201	A
26	1	206	A
26	1	207	A
26	1	233	G
26	1	249	U
26	1	251	G
26	1	257	U
26	1	259	A
26	1	276	A
26	1	308	A
26	1	309	A
26	1	311	A
26	1	312	A
26	1	313	U
26	1	331	A
26	1	332	A
26	1	333	A
26	1	334	A
26	1	337	A
26	1	339	A
26	1	342	A
26	1	344	A
26	1	345	A
26	1	351	A
26	1	352	A
26	1	353	A
26	1	354	A
26	1	357	A
26	1	416	U
26	1	418	U
26	1	419	U
26	1	421	A
26	1	422	C
26	1	424	G
26	1	425	U
26	1	426	A

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Mol	Chain	Res	Type
26	1	427	A
26	1	428	U
26	1	445	G
26	1	457	G
26	1	463	G
26	1	464	A
26	1	468	C
26	1	478	U
26	1	481	U
26	1	485	U
26	1	486	A
26	1	487	U
26	1	488	U
26	1	491	U
26	1	493	G
26	1	495	U
26	1	498	U
26	1	500	C
26	1	501	C
26	1	502	C
26	1	504	G
26	1	514	G
26	1	515	C
26	1	516	G
26	1	526	U
26	1	535	U
26	1	537	U
26	1	538	U
26	1	539	A
26	1	540	C
26	1	541	G
26	1	542	C
26	1	547	A
26	1	553	G
26	1	566	G
26	1	567	C
26	1	597	C
26	1	598	A
26	1	599	A
26	1	620	A
26	1	623	G
26	1	633	A

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Mol	Chain	Res	Type
26	1	634	C
26	1	644	A
26	1	646	A
26	1	649	G
26	1	650	A
26	1	651	A
26	1	652	C
26	1	671	A
26	1	672	A
26	1	673	U
26	1	674	C
26	1	675	A
26	1	676	G
26	1	687	A
26	1	689	U
26	1	690	C
26	1	692	A
26	1	693	G
26	1	694	C
26	1	695	G
26	1	696	C
26	1	697	A
26	1	698	C
26	1	700	C
26	1	701	A
26	1	714	A
26	1	724	U
26	1	726	A
26	1	754	G
26	1	760	G
26	1	771	U
26	1	779	U
26	1	780	U
26	1	781	C
26	1	789	G
26	1	790	G
26	1	793	U
26	1	795	U
26	1	796	U
26	1	799	A
26	1	800	G
26	1	814	A

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Mol	Chain	Res	Type
26	1	830	U
26	1	855	G
26	1	875	A
26	1	885	C
26	1	909	A
26	1	910	C
26	1	920	G
26	1	921	G
26	1	927	A
26	1	929	G
26	1	930	G
26	1	934	A
26	1	942	C
26	1	950	G
26	1	957	U
26	1	972	U
26	1	973	U
26	1	974	C
26	1	975	A
26	1	989	U
26	1	992	C
26	1	1003	G
26	1	1004	G
26	1	1011	A
26	1	1021	C
26	1	1022	U
26	1	1023	A
26	1	1024	G
26	1	1044	A
26	1	1045	C
26	1	1046	C
26	1	1055	G
26	1	1058	A
26	1	1094	G
26	1	1099	U
26	1	1101	G
26	1	1103	G
26	1	1111	G
26	1	1124	G
26	1	1139	G
26	1	1146	C
26	1	1159	A

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Mol	Chain	Res	Type
26	1	1162	C
26	1	1163	A
26	1	1172	G
26	1	1176	A
26	1	1195	A
26	1	1196	U
26	1	1197	G
26	1	1199	C
26	1	1218	G
26	1	1219	A
26	1	1220	A
26	1	1221	G
26	1	1234	G
26	1	1237	G
26	1	1238	A
26	1	1239	A
26	1	1240	A
26	1	1242	C
26	1	1243	G
26	1	1244	U
26	1	1262	G
26	1	1269	G
26	1	1282	U
26	1	1283	A
26	1	1285	C
26	1	1292	C
26	1	1293	A
26	1	1325	G
26	1	1327	U
26	1	1328	G
26	1	1329	C
26	1	1338	G
26	1	1339	U
26	1	1352	A
26	1	1361	C
26	1	1395	G
26	1	1404	A
26	1	1412	U
26	1	1413	G
26	1	1425	A
26	1	1428	G
26	1	1430	A

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Mol	Chain	Res	Type
26	1	1432	A
26	1	1444	A
26	1	1459	C
26	1	1479	U
26	1	1485	A
26	1	1487	U
26	1	1502	U
26	1	1510	U
26	1	1523	A
26	1	1531	G
26	1	1533	C
26	1	1539	A
26	1	1540	U
26	1	1546	C
26	1	1554	U
26	1	1557	C
26	1	1566	U
26	1	1567	U
26	1	1572	U
26	1	1573	A
26	1	1574	C
26	1	1578	A
26	1	1584	C
26	1	1587	C
26	1	1588	U
26	1	1593	U
26	1	1594	G
26	1	1595	G
26	1	1596	A
26	1	1597	G
26	1	1598	C
26	1	1599	G
26	1	1602	U
26	1	1603	U
26	1	1604	G
26	1	1605	G
26	1	1606	A
26	1	1619	G
26	1	1620	G
26	1	1621	G
26	1	1623	A
26	1	1626	G

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Mol	Chain	Res	Type
26	1	1627	U
26	1	1629	G
26	1	1630	C
26	1	1631	G
26	1	1634	U
26	1	1635	C
26	1	1638	C
26	1	1643	C
26	1	1644	A
26	1	1645	C
26	1	1647	C
26	1	1648	U
26	1	1649	C
26	1	1669	U
26	1	1670	G
26	1	1671	A
26	1	1672	G
26	1	1678	A
26	1	1679	A
26	1	1685	U
26	1	1693	C
26	1	1694	A
26	1	1695	A
26	1	1698	A
26	1	1699	U
26	1	1834	A
26	1	1848	A
26	1	1849	U
26	1	1850	U
26	1	1852	U
26	1	1853	A
26	1	1854	A
26	1	1858	C
26	1	1869	U
26	1	1874	A
26	1	1875	G
26	1	1876	U
26	1	1877	C
26	1	1883	G
26	1	1884	G
26	1	1889	A
26	1	1890	A

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Mol	Chain	Res	Type
26	1	1896	A
26	1	1899	A
26	1	1903	A
26	1	1919	G
26	1	1921	C
26	1	1922	G
26	1	1923	A
26	1	1924	U
26	1	1925	C
26	1	1934	G
26	1	1935	A
26	1	1936	A
26	1	1937	C
26	1	1950	A
26	1	1986	C
26	1	1988	C
26	1	1989	U
26	1	1990	U
26	1	2016	G
26	1	2058	U
26	1	2060	U
26	1	2062	U
26	1	2064	G
26	1	2065	A
26	1	2066	U
26	1	2067	U
26	1	2071	A
26	1	2081	A
26	1	2082	U
26	1	2088	G
26	1	2097	A
26	1	2104	A
26	1	2124	C
26	1	2125	U
26	1	2131	G
26	1	2132	U
26	1	2140	U
26	1	2143	A
26	1	2152	G
26	1	2153	A
26	1	2176	C
26	1	2182	G

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Mol	Chain	Res	Type
26	1	2190	U
26	1	2191	U
26	1	2192	A
26	1	2193	U
26	1	2194	A
26	1	2224	G
26	1	2232	C
26	1	2247	G
26	1	2248	G
26	1	2254	A
26	1	2255	A
26	1	2256	A
26	1	2257	5MU
26	1	2273	U
26	1	2282	G
26	1	2284	A
26	1	2285	C
26	1	2288	A
26	1	2289	U
26	1	2290	G
26	1	2293	G
26	1	2302	G
26	1	2309	U
26	1	2311	U
26	1	2315	C
26	1	2320	U
26	1	2338	A
26	1	2341	C
26	1	2349	A
26	1	2351	A
26	1	2373	C
26	1	2374	G
26	1	2378	A
26	1	2379	G
26	1	2380	A
26	1	2387	G
26	1	2394	C
26	1	2398	A
26	1	2411	G
26	1	2415	A
26	1	2420	G
26	1	2421	A

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Mol	Chain	Res	Type
26	1	2423	C
26	1	2429	U
26	1	2430	G
26	1	2434	G
26	1	2435	A
26	1	2436	U
26	1	2437	A
26	1	2438	G
26	1	2439	G
26	1	2440	U
26	1	2443	G
26	1	2444	A
26	1	2445	G
26	1	2446	G
26	1	2448	C
26	1	2449	C
26	1	2451	C
26	1	2452	A
26	1	2454	A
26	1	2455	U
26	1	2461	G
26	1	2462	A
26	1	2464	C
26	1	2465	A
26	1	2466	A
26	1	2467	U
26	1	2468	C
26	1	2470	U
26	1	2473	A
26	1	2474	A
26	1	2475	G
26	1	2476	A
26	1	2479	A
26	1	2480	C
26	1	2481	U
26	1	2483	U
26	1	2484	U
26	1	2488	U
26	1	2501	A
26	1	2506	C
26	1	2534	A
26	1	2547	G

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Mol	Chain	Res	Type
26	1	2548	G
26	1	2550	A
26	1	2575	A
26	1	2588	G
26	1	2592	U
26	1	2596	A
26	1	2597	A
26	1	2613	A
26	1	2618	C
26	1	2632	A
26	1	2639	U
26	1	2640	A
26	1	2641	A
26	1	2650	G
26	1	2652	C
26	1	2688	G
26	1	2690	C
26	1	2695	U
26	1	2696	G
26	1	2711	U
26	1	2728	U
26	1	2730	A
26	1	2736	U
26	1	2740	A
26	1	2746	G
26	1	2750	G
26	1	2752	G
26	1	2753	A
26	1	2774	A
26	1	2779	U
26	1	2781	U
26	1	2785	C
26	1	2796	U
26	1	2803	OMC
26	1	2807	G
26	1	2808	2MA
26	1	2810	G
26	1	2811	U
26	1	2823	A
26	1	2825	C
26	1	2834	G
26	1	2840	G

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Mol	Chain	Res	Type
26	1	2871	A
26	1	2872	G
26	1	2877	A
26	1	2878	C
26	1	2907	A
26	1	2908	G
26	1	2914	U
26	1	2915	U
26	1	2918	U
26	1	2920	U
26	1	2934	U
26	1	2935	A
26	1	2936	A
26	1	2937	A
26	1	2938	G
26	1	2939	C
26	1	2954	G
26	1	2955	C
26	1	2972	G
26	1	2988	A
26	1	2998	U
26	1	2999	A
26	1	3021	G
26	1	3023	G
26	1	3035	A
26	1	3042	A
26	1	3050	A
26	1	3053	G
26	1	3058	U
26	1	3059	U
26	1	3067	A
26	1	3068	A
26	1	3080	A
26	1	3094	C
26	1	3104	A
26	1	3116	A
26	1	3142	G
26	1	3148	G
26	1	3153	A
26	1	3161	C
26	1	3164	A
26	1	3166[A]	C

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Mol	Chain	Res	Type
26	1	3169	A
27	3	2	A
27	3	3	A
27	3	13	A
27	3	15	G
27	3	23	G
27	3	25	G
27	3	26	A
27	3	37	U
27	3	42	U
27	3	44	C
27	3	46	G
27	3	53	A
27	3	55	A
27	3	56	U
27	3	59	G
27	3	65	G
27	3	66	U
27	3	67	C
27	3	69	U
27	3	87	A
27	3	90	G
27	3	91	U
27	3	106	C
27	3	118	A
75	5	9	G
75	5	18	G
75	5	21	A
75	5	22	G
75	5	47	U
75	5	48	C
75	5	51	C
75	5	52	G
75	5	63	G
75	5	67	C
75	5	68	C
75	5	76	A
76	2	4	A
76	2	5	U
76	2	6	A
76	2	12	A
76	2	17	G

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Mol	Chain	Res	Type
76	2	30	G
76	2	40	A
76	2	47	G
76	2	55	C
76	2	56	U
76	2	58	A
76	2	59	A
76	2	60	C
76	2	67	A
76	2	76	G
76	2	79	G
76	2	80	U
76	2	82	C
76	2	83	U
76	2	92	A
76	2	104	U
76	2	105	U
76	2	121	A
76	2	150	A
76	2	152	G
76	2	153	A
76	2	154	G
76	2	156	U
76	2	157	G
76	2	161	A
76	2	162	C
76	2	163	A
76	2	164	A
76	2	172	A
76	2	184	A
76	2	185	G
76	2	194	A
76	2	195	U
76	2	203	A
76	2	208	U
76	2	214	U
76	2	215	A
76	2	225	G
76	2	226	A
76	2	228	A
76	2	233	G
76	2	245	U

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Mol	Chain	Res	Type
76	2	264	U
76	2	266	G
76	2	270	G
76	2	285	G
76	2	286	C
76	2	308	G
76	2	317	U
76	2	318	U
76	2	319	C
76	2	325	A
76	2	347	C
76	2	351	G
76	2	363	A
76	2	364	C
76	2	365	G
76	2	366	G
76	2	370	G
76	2	371	C
76	2	373	G
76	2	386	U
76	2	391	C
76	2	416	A
76	2	420	U
76	2	425	G
76	2	430	A
76	2	432	G
76	2	440	A
76	2	441	U
76	2	442	U
76	2	443	C
76	2	444	C
76	2	449	G
76	2	450	U
76	2	459	U
76	2	469	G
76	2	470	C
76	2	471	G
76	2	479	G
76	2	482	A
76	2	484	G
76	2	492	G
76	2	493	A

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Mol	Chain	Res	Type
76	2	494	A
76	2	495	G
76	2	507	A
76	2	509	C
76	2	516	C
76	2	519	G
76	2	525	G7M
76	2	528	G
76	2	530	A
76	2	531	A
76	2	545	A
76	2	557	A
76	2	560	G
76	2	562	C
76	2	564	A
76	2	571	A
76	2	573	G
76	2	574	G
76	2	575	G
76	2	594	G
76	2	617	A
76	2	618	A
76	2	621	G
76	2	629	G
76	2	649	U
76	2	661	A
76	2	684	G
76	2	699	G
76	2	714	G
76	2	717	A
76	2	718	A
76	2	720	A
76	2	745	A
76	2	751	G
76	2	762	A
76	2	773	A
76	2	789	U
76	2	790	A
76	2	811	A
76	2	813	C
76	2	817	G
76	2	825	G

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Mol	Chain	Res	Type
76	2	832	G
76	2	836	A
76	2	837	U
76	2	838	U
76	2	839	C
76	2	840	U
76	2	846	G
76	2	865	A
76	2	866	A
76	2	878	G
76	2	882	A
76	2	893	A
76	2	907	A
76	2	919	G
76	2	926	G
76	2	927	C
76	2	928	A
76	2	932	G
76	2	953	U
76	2	959	G
76	2	962	A
76	2	964	G
76	2	968	A
76	2	969	G
76	2	970	A
76	2	982	C
76	2	986	G
76	2	998	A
76	2	999	G
76	2	1006	U
76	2	1007	A
76	2	1029	C
76	2	1030	U
76	2	1036	A
76	2	1037	C
76	2	1057	U
76	2	1082	U
76	2	1086	G
76	2	1087	U
76	2	1093	A
76	2	1116	G
76	2	1117	U

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Mol	Chain	Res	Type
76	2	1118	U
76	2	1122	C
76	2	1123	A
76	2	1125	A
76	2	1127	A
76	2	1132	C
76	2	1133	C
76	2	1135	A
76	2	1136	A
76	2	1137	G
76	2	1138	G
76	2	1139	A
76	2	1140	G
76	2	1142	A
76	2	1380	U
76	2	1381	C
76	2	1382	C
76	2	1385	A
76	2	1386	A
76	2	1387	C
76	2	1389	A
76	2	1395	A
76	2	1399	U
76	2	1407	G
76	2	1420	A
76	2	1422	U
76	2	1430	A
76	2	1447	G
76	2	1459	A
76	2	1460	A
76	2	1465	G
76	2	1475	U
76	2	1476	A
76	2	1490	A
76	2	1501	A
76	2	1504	G
76	2	1511	A
76	2	1516	G
76	2	1523	A
76	2	1542	A
76	2	1543	A
76	2	1561	A

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Mol	Chain	Res	Type
76	2	1564	U
76	2	1567	G
76	2	1574	C
76	2	1582	C
76	2	1608	A
76	2	1615	G
76	2	1626	U
76	2	1632	G
76	2	1643	A
76	2	1652	C
76	2	1660	A
76	2	1664	4OC
76	2	1702	G
76	2	1703	G
76	2	1706	C
76	2	1707	A
76	2	1714	A
76	2	1715	C
76	2	1722	C
76	2	1723	U
76	2	1725	C
76	2	1727	G
76	2	1728	U
76	2	1731	A
76	2	1732	A
76	2	1735	C
76	2	1736	U
76	2	1738	G
76	2	1743	A
76	2	1744	C
76	2	1745	A
76	2	1746	A
76	2	1751	U
76	2	1760	U
76	2	1762	U
76	2	1763	U
76	2	1764	A
76	2	1765	U
76	2	1766	U
76	2	1768	A
76	2	1772	A
76	2	1774	A

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Mol	Chain	Res	Type
76	2	1802	A
76	2	1803	G
76	2	1806	G
76	2	1812	A
76	2	1825	2MG
76	2	1826	G
76	2	1828	MA6
76	2	1838	G
76	2	1839	G
76	2	1848	C

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	131	G
26	1	163	G
26	1	308	A
26	1	312	A
26	1	421	A
26	1	427	A
26	1	487	U
26	1	492	C
26	1	540	C
26	1	566	G
26	1	619	A
26	1	688	G
26	1	929	G
26	1	991	U
26	1	1100	U
26	1	1566	U
26	1	1598	C
26	1	1642	U
26	1	1923	A
26	1	2057	A
26	1	2059	C
26	1	2257	5MU
26	1	2445	G
26	1	2461	G
26	1	2505	G
26	1	2617	U
26	1	2778	C
26	1	2998	U

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Mol	Chain	Res	Type
27	3	12	U
76	2	103	A
76	2	225	G
76	2	491	G
76	2	493	A
76	2	998	A
76	2	1117	U
76	2	1701	C
76	2	1705	C
76	2	1706	C
76	2	1726	U
76	2	1802	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	PSU	1	2885	92,26	18,21,22	1.07	3 (16%)	21,30,33	1.97	5 (23%)
26	OMG	1	2560	92,75,26	23,26,27	2.38	7 (30%)	32,38,41	2.29	8 (25%)
75	4SU	5	8	75	18,21,22	4.12	7 (38%)	25,30,33	2.44	4 (16%)
76	2MG	2	1825	76	23,26,27	2.83	6 (26%)	33,38,41	3.05	14 (42%)
26	5MU	1	2257	92,26	19,22,23	1.47	4 (21%)	27,32,35	2.41	6 (22%)
26	PSU	1	2762	26	18,21,22	1.00	2 (11%)	21,30,33	1.89	4 (19%)
26	PSU	1	1105	26	18,21,22	1.04	2 (11%)	21,30,33	1.92	3 (14%)
76	MA6	2	1827	76	23,26,27	1.83	6 (26%)	33,38,41	3.39	13 (39%)
26	PSU	1	891	26,89	18,21,22	1.09	2 (11%)	21,30,33	1.98	4 (19%)
76	UR3	2	1807	76	19,22,23	2.62	7 (36%)	26,32,35	1.68	2 (7%)
75	5MU	5	54	75	19,22,23	7.76	9 (47%)	27,32,35	3.50	10 (37%)
26	OMC	1	2803	26,89	19,22,23	2.74	7 (36%)	25,31,34	1.00	1 (4%)
26	PSU	1	2910	26	18,21,22	1.02	2 (11%)	21,30,33	1.83	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	G7M	2	525	76	23,26,27	2.32	7 (30%)	34,39,42	3.11	10 (29%)
26	OMU	1	2857	26,89	19,22,23	3.01	8 (42%)	25,31,34	1.83	4 (16%)
76	MA6	2	1828	76	23,26,27	1.81	5 (21%)	33,38,41	3.41	12 (36%)
75	5MC	5	32	75	19,22,23	3.55	8 (42%)	26,32,35	1.15	2 (7%)
26	H2U	1	2754	26	18,21,22	0.69	0	19,30,33	1.19	1 (5%)
76	4OC	2	1664	76	20,23,24	3.19	8 (40%)	25,32,35	0.90	1 (4%)
26	2MA	1	2808	26,89	22,25,26	3.90	7 (31%)	32,37,40	2.45	10 (31%)
75	PSU	5	55	75	18,21,22	1.14	1 (5%)	21,30,33	1.92	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	1	2885	92,26	-	1/7/25/26	0/2/2/2
26	OMG	1	2560	92,75,26	-	1/9/27/28	0/3/3/3
75	4SU	5	8	75	-	0/7/25/26	0/2/2/2
76	2MG	2	1825	76	-	2/9/27/28	0/3/3/3
26	5MU	1	2257	92,26	-	1/7/25/26	0/2/2/2
26	PSU	1	2762	26	-	0/7/25/26	0/2/2/2
26	PSU	1	1105	26	-	0/7/25/26	0/2/2/2
76	MA6	2	1827	76	-	0/11/29/30	0/3/3/3
26	PSU	1	891	26,89	-	1/7/25/26	0/2/2/2
76	UR3	2	1807	76	-	0/7/25/26	0/2/2/2
75	5MU	5	54	75	-	0/7/25/26	0/2/2/2
26	OMC	1	2803	26,89	-	0/9/27/28	0/2/2/2
26	PSU	1	2910	26	-	0/7/25/26	0/2/2/2
76	G7M	2	525	76	-	3/7/25/26	0/3/3/3
26	OMU	1	2857	26,89	-	0/9/27/28	0/2/2/2
76	MA6	2	1828	76	-	0/11/29/30	0/3/3/3
75	5MC	5	32	75	-	0/7/25/26	0/2/2/2
26	H2U	1	2754	26	-	0/7/38/39	0/2/2/2
76	4OC	2	1664	76	-	2/9/29/30	0/2/2/2
26	2MA	1	2808	26,89	-	2/7/25/26	0/3/3/3
75	PSU	5	55	75	-	0/7/25/26	0/2/2/2

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	5	54	5MU	C4-C5	22.99	1.82	1.44
75	5	54	5MU	C6-N1	15.66	1.64	1.38
75	5	54	5MU	C6-C5	-12.21	1.14	1.34
26	1	2808	2MA	C4-N3	12.21	1.50	1.34
75	5	54	5MU	C4-N3	-12.02	1.16	1.38
75	5	32	5MC	C6-C5	8.26	1.48	1.34
75	5	8	4SU	C2-N3	7.83	1.51	1.38
75	5	8	4SU	C5-C4	7.77	1.51	1.42
76	2	1825	2MG	C2-N2	7.71	1.49	1.33
75	5	8	4SU	C4-N3	7.60	1.45	1.37
75	5	8	4SU	C2-N1	7.55	1.50	1.38
26	1	2808	2MA	C2-N3	7.31	1.46	1.34
76	2	1825	2MG	C2-N3	7.24	1.45	1.32
76	2	1664	4OC	C4-N3	7.13	1.44	1.32
75	5	32	5MC	C4-N3	7.09	1.45	1.34
26	1	2857	OMU	C2-N1	6.98	1.49	1.38
26	1	2808	2MA	C6-N1	6.77	1.44	1.35
76	2	1807	UR3	C2-N1	6.62	1.47	1.38
26	1	2857	OMU	C2-N3	6.62	1.49	1.38
76	2	525	G7M	C4-N3	6.52	1.49	1.34
26	1	2560	OMG	C4-N3	6.36	1.48	1.34
76	2	1664	4OC	C6-C5	6.34	1.49	1.35
76	2	1664	4OC	C2-N3	6.27	1.48	1.36
75	5	32	5MC	C2-N3	6.10	1.48	1.36
76	2	1807	UR3	C6-C5	5.98	1.48	1.35
26	1	2803	OMC	C2-N3	5.93	1.48	1.36
76	2	1825	2MG	C4-N3	5.74	1.47	1.34
75	5	8	4SU	C6-C5	5.72	1.48	1.35
76	2	1664	4OC	C4-N4	5.57	1.47	1.36
26	1	2803	OMC	C6-C5	5.56	1.48	1.35
75	5	54	5MU	C2-N3	5.53	1.47	1.38
26	1	2857	OMU	C6-C5	5.47	1.47	1.35
26	1	2808	2MA	C2-N1	5.47	1.43	1.34
26	1	2560	OMG	C2-N3	5.21	1.45	1.33
76	2	1828	MA6	C6-N6	5.06	1.50	1.36
76	2	1827	MA6	C6-N6	4.97	1.50	1.36
75	5	32	5MC	C6-N1	4.85	1.46	1.38
75	5	8	4SU	C4-S4	-4.81	1.60	1.68
76	2	525	G7M	C5-N7	-4.68	1.33	1.39
26	1	2808	2MA	C5-C6	4.68	1.54	1.41
75	5	54	5MU	C2-N1	4.58	1.45	1.38
75	5	32	5MC	C5-C4	4.52	1.47	1.44
26	1	2560	OMG	C2-N2	4.48	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	2803	OMC	C4-N3	4.46	1.43	1.34
26	1	2803	OMC	C4-N4	4.38	1.44	1.33
76	2	1807	UR3	C2-N3	4.37	1.47	1.39
76	2	525	G7M	C2-N2	4.23	1.44	1.34
26	1	2803	OMC	C2-N1	4.12	1.48	1.40
75	5	32	5MC	C4-N4	4.07	1.44	1.34
76	2	525	G7M	C2-N3	4.00	1.42	1.33
76	2	1825	2MG	C2-N1	3.95	1.43	1.36
75	5	55	PSU	C6-C5	3.94	1.39	1.35
26	1	2857	OMU	C4-N3	3.94	1.45	1.38
26	1	2560	OMG	C5-N7	-3.78	1.31	1.39
75	5	32	5MC	C2-N1	3.59	1.47	1.40
26	1	2808	2MA	C6-N6	-3.54	1.25	1.34
76	2	1827	MA6	C5-C4	-3.51	1.32	1.39
76	2	1828	MA6	C5-N7	-3.41	1.32	1.39
76	2	1828	MA6	C5-C4	-3.36	1.33	1.39
75	5	54	5MU	O4-C4	-3.33	1.17	1.23
76	2	1664	4OC	C2-N1	3.31	1.47	1.40
76	2	1664	4OC	C5-C4	3.30	1.48	1.41
75	5	8	4SU	C6-N1	3.26	1.45	1.38
26	1	2257	5MU	C4-N3	-3.13	1.33	1.38
26	1	2857	OMU	O4-C4	-3.07	1.18	1.24
76	2	1664	4OC	O2-C2	-3.05	1.18	1.23
76	2	1827	MA6	C5-N7	-3.04	1.33	1.39
26	1	2257	5MU	C6-N1	-2.99	1.32	1.38
26	1	2857	OMU	O2-C2	-2.96	1.17	1.23
26	1	2803	OMC	O2-C2	-2.94	1.18	1.23
26	1	2857	OMU	C6-N1	2.93	1.45	1.38
76	2	1664	4OC	C6-N1	2.83	1.44	1.38
76	2	1827	MA6	C8-N9	-2.83	1.32	1.37
75	5	32	5MC	O2-C2	-2.80	1.18	1.23
26	1	2257	5MU	C2-N3	-2.77	1.33	1.38
26	1	2808	2MA	C5-N7	-2.77	1.34	1.39
26	1	891	PSU	C6-C5	2.73	1.38	1.35
75	5	54	5MU	O2-C2	-2.71	1.18	1.23
76	2	1807	UR3	O4-C4	-2.66	1.17	1.23
76	2	1807	UR3	C6-N1	2.66	1.44	1.38
26	1	2560	OMG	O6-C6	-2.63	1.18	1.23
76	2	1807	UR3	O2-C2	-2.61	1.17	1.22
76	2	525	G7M	C5-C6	2.60	1.50	1.43
26	1	2910	PSU	C6-C5	2.60	1.38	1.35
26	1	2803	OMC	C6-N1	2.59	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	2	1828	MA6	C8-N9	-2.54	1.33	1.37
76	2	1825	2MG	C5-C6	2.53	1.53	1.44
26	1	2885	PSU	C6-C5	2.52	1.38	1.35
76	2	1828	MA6	C10-N6	2.45	1.51	1.45
26	1	2857	OMU	C5-C4	2.42	1.48	1.43
26	1	1105	PSU	C6-C5	2.41	1.38	1.35
76	2	1827	MA6	C10-N6	2.40	1.51	1.45
26	1	2885	PSU	O4'-C1'	-2.39	1.40	1.43
76	2	1827	MA6	C4-N9	-2.33	1.32	1.37
76	2	525	G7M	C6-N1	2.30	1.43	1.38
26	1	2762	PSU	C6-C5	2.28	1.37	1.35
26	1	891	PSU	C4-C5	-2.27	1.38	1.44
26	1	2910	PSU	C4-C5	-2.23	1.38	1.44
76	2	525	G7M	C2-N1	2.20	1.43	1.37
26	1	1105	PSU	C4-C5	-2.20	1.38	1.44
26	1	2257	5MU	C6-C5	2.18	1.38	1.34
75	5	54	5MU	C5M-C5	2.17	1.55	1.50
26	1	2762	PSU	C4-C5	-2.16	1.38	1.44
76	2	1825	2MG	C5-N7	-2.13	1.34	1.39
26	1	2560	OMG	C2-N1	2.13	1.42	1.37
26	1	2885	PSU	C4-C5	-2.12	1.38	1.44
26	1	2560	OMG	C5-C6	2.03	1.52	1.44
76	2	1807	UR3	C5-C4	2.01	1.48	1.43

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	2	1828	MA6	N1-C6-N6	-11.92	102.33	116.86
76	2	1827	MA6	N1-C6-N6	-11.92	102.34	116.86
75	5	54	5MU	C5-C4-N3	10.84	124.75	115.32
76	2	525	G7M	CN7-N7-C5	9.01	138.03	126.80
75	5	8	4SU	C4-N3-C2	-8.30	119.36	127.31
76	2	1828	MA6	C5-C6-N6	8.08	138.12	125.33
76	2	1827	MA6	C5-C6-N6	7.93	137.88	125.33
26	1	2808	2MA	C5-C4-N3	-7.92	118.84	127.18
75	5	54	5MU	C5-C6-N1	-7.42	115.25	123.31
76	2	1825	2MG	C1'-N9-C8	-7.37	105.81	126.73
76	2	525	G7M	C1'-N9-C4	7.31	148.08	126.49
76	2	1825	2MG	C1'-N9-C4	7.28	147.98	126.49
75	5	54	5MU	C4-N3-C2	-7.21	117.88	127.34
76	2	525	G7M	CN7-N7-C8	-7.02	114.16	124.79
26	1	2560	OMG	C5-C4-N3	-6.51	118.03	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	2	525	G7M	C1'-N9-C8	-6.44	104.98	126.74
76	2	1825	2MG	C2-N3-C4	6.37	119.97	112.00
76	2	1825	2MG	N1-C2-N2	6.03	122.72	116.56
76	2	1827	MA6	N1-C2-N3	-6.01	119.48	128.58
26	1	2257	5MU	C4-N3-C2	-5.98	119.50	127.34
76	2	1807	UR3	C4-N3-C2	-5.91	119.83	124.58
75	5	8	4SU	C5-C4-N3	5.76	120.11	114.75
26	1	2857	OMU	C4-N3-C2	-5.72	119.51	126.61
76	2	1828	MA6	N1-C2-N3	-5.70	119.95	128.58
75	5	54	5MU	O4-C4-C5	-5.54	118.58	124.92
76	2	1828	MA6	C5-C4-N3	-5.48	119.17	126.72
26	1	2257	5MU	N3-C2-N1	5.42	121.95	114.89
76	2	1827	MA6	N9-C8-N7	-5.21	106.54	113.94
26	1	891	PSU	C4-N3-C2	-5.19	119.22	126.37
26	1	2560	OMG	C2-N3-C4	5.16	121.19	112.30
26	1	1105	PSU	C4-N3-C2	-5.08	119.37	126.37
26	1	2257	5MU	C5-C4-N3	5.03	119.70	115.32
26	1	2910	PSU	C4-N3-C2	-4.98	119.51	126.37
26	1	891	PSU	N1-C2-N3	4.98	120.42	115.17
26	1	2885	PSU	N1-C2-N3	4.95	120.39	115.17
26	1	2762	PSU	C4-N3-C2	-4.95	119.55	126.37
26	1	2808	2MA	N3-C4-N9	4.93	133.25	126.99
75	5	55	PSU	N1-C2-N3	4.93	120.36	115.17
76	2	1825	2MG	C5-C4-N3	-4.90	120.60	128.39
76	2	1828	MA6	C4-C5-C6	4.76	120.83	115.91
26	1	2885	PSU	C4-N3-C2	-4.76	119.81	126.37
26	1	1105	PSU	N1-C2-N3	4.74	120.16	115.17
76	2	525	G7M	C2-N3-C4	4.71	120.41	112.30
75	5	55	PSU	C4-N3-C2	-4.67	119.94	126.37
76	2	1828	MA6	N9-C8-N7	-4.64	107.36	113.94
26	1	2257	5MU	C5-C6-N1	-4.63	118.29	123.31
76	2	1827	MA6	C5-C4-N3	-4.50	120.52	126.72
26	1	2762	PSU	N1-C2-N3	4.47	119.88	115.17
76	2	1825	2MG	C2-N1-C6	-4.46	119.16	124.55
26	1	2910	PSU	N1-C2-N3	4.44	119.85	115.17
26	1	2560	OMG	C1'-N9-C8	4.40	139.22	126.73
76	2	525	G7M	C5-C4-N3	-4.40	119.84	128.15
26	1	2257	5MU	O4-C4-C5	-4.39	119.89	124.92
75	5	54	5MU	N3-C2-N1	4.39	120.60	114.89
26	1	2560	OMG	C1'-N9-C4	-4.26	113.91	126.49
75	5	8	4SU	C5-C4-S4	-4.21	119.50	124.31
26	1	2560	OMG	N9-C4-N3	4.18	134.32	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	2	525	G7M	C5-C6-N1	4.16	120.44	111.84
75	5	8	4SU	N3-C2-N1	4.14	120.28	114.89
26	1	2857	OMU	N3-C2-N1	4.11	120.24	114.89
75	5	54	5MU	C5M-C5-C6	-4.08	117.33	122.85
76	2	1807	UR3	C5-C4-N3	4.05	120.37	115.04
76	2	1825	2MG	CM2-N2-C2	-3.99	115.07	123.65
26	1	2754	H2U	C5-C4-N3	-3.98	112.46	116.69
26	1	2808	2MA	C4-N9-C1'	-3.87	117.57	126.63
26	1	2808	2MA	N9-C8-N7	-3.82	108.51	113.94
76	2	1827	MA6	C4-N9-C8	3.79	109.72	105.74
26	1	2857	OMU	C5-C4-N3	3.77	120.07	114.80
76	2	1827	MA6	C4-C5-C6	3.71	119.74	115.91
26	1	2808	2MA	N3-C2-N1	-3.61	119.39	125.77
26	1	2808	2MA	C1'-N9-C8	3.58	135.04	127.09
76	2	1828	MA6	C2-N3-C4	3.57	120.55	111.83
76	2	1827	MA6	C2-N1-C6	3.51	120.40	111.83
76	2	1828	MA6	N3-C4-N9	3.49	133.11	127.17
76	2	525	G7M	O6-C6-C5	-3.44	120.33	128.01
76	2	1827	MA6	C2-N3-C4	3.38	120.08	111.83
26	1	2257	5MU	O2-C2-N1	-3.37	118.41	122.80
75	5	54	5MU	C5M-C5-C4	3.36	122.37	118.78
76	2	1828	MA6	C5-N7-C8	3.35	108.72	103.45
76	2	1828	MA6	C2-N1-C6	3.32	119.94	111.83
26	1	2560	OMG	C2-N1-C6	-3.30	119.12	125.11
76	2	525	G7M	C2-N1-C6	-3.26	119.20	125.11
76	2	1827	MA6	C5-N7-C8	3.23	108.53	103.45
26	1	2885	PSU	O2-C2-N1	-3.06	119.64	122.79
76	2	1825	2MG	N2-C2-N3	-3.05	116.62	120.51
26	1	891	PSU	O2-C2-N1	-3.05	119.64	122.79
76	2	1827	MA6	N3-C4-N9	3.04	132.34	127.17
26	1	2762	PSU	O2-C2-N1	-2.92	119.78	122.79
75	5	55	PSU	C6-N1-C2	-2.88	120.02	122.69
75	5	55	PSU	O2-C2-N1	-2.83	119.87	122.79
26	1	2885	PSU	C6-N1-C2	-2.78	120.11	122.69
26	1	2808	2MA	C5-N7-C8	2.78	107.82	103.45
75	5	54	5MU	C6-C5-C4	2.76	120.30	118.02
26	1	2857	OMU	O4-C4-C5	-2.76	120.41	125.16
26	1	2560	OMG	O6-C6-C5	-2.74	119.29	126.53
75	5	32	5MC	C5-C6-N1	-2.74	120.34	123.31
76	2	1825	2MG	C5-C6-N1	2.70	120.12	113.25
26	1	2560	OMG	C5-C6-N1	2.68	120.07	113.25
76	2	1825	2MG	N9-C8-N7	-2.67	108.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	891	PSU	C6-N1-C2	-2.63	120.25	122.69
76	2	1825	2MG	C5-C4-N9	2.60	110.31	105.66
26	1	2808	2MA	CM2-C2-N1	2.54	120.93	117.13
76	2	525	G7M	N9-C4-N3	2.52	130.99	125.95
26	1	2803	OMC	O2-C2-N3	-2.51	118.37	122.33
76	2	1827	MA6	C4-N9-C1'	-2.49	120.81	126.63
26	1	2885	PSU	O4'-C1'-C2'	2.46	108.55	105.15
76	2	1828	MA6	C4-N9-C8	2.43	108.29	105.74
75	5	54	5MU	C1'-N1-C6	-2.34	117.30	121.15
76	2	1828	MA6	C4-C5-N7	-2.33	107.92	110.58
26	1	1105	PSU	O2-C2-N1	-2.31	120.41	122.79
76	2	1825	2MG	C4-C5-N7	-2.29	107.04	110.67
26	1	2808	2MA	C6-C5-C4	2.29	120.30	117.18
75	5	32	5MC	O2-C2-N3	-2.25	118.79	122.33
26	1	2808	2MA	N6-C6-N1	2.20	120.00	117.03
76	2	1827	MA6	C4-C5-N7	-2.20	108.07	110.58
76	2	1664	4OC	C6-C5-C4	2.19	119.64	117.00
26	1	2762	PSU	O4'-C1'-C2'	2.19	108.18	105.15
75	5	54	5MU	C1'-N1-C2	2.16	121.48	117.59
76	2	1825	2MG	C8-N7-C5	2.12	108.04	104.26
76	2	1825	2MG	O6-C6-C5	-2.10	120.98	126.53
26	1	2910	PSU	C6-N1-C2	-2.09	120.75	122.69
26	1	2910	PSU	O2-C2-N1	-2.05	120.67	122.79
26	1	2910	PSU	C5-C4-N3	2.01	120.98	116.55

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	2560	OMG	C1'-C2'-O2'-CM2
76	2	1664	4OC	O4'-C4'-C5'-O5'
76	2	1825	2MG	O4'-C4'-C5'-O5'
76	2	525	G7M	C3'-C4'-C5'-O5'
26	1	2808	2MA	O4'-C4'-C5'-O5'
76	2	525	G7M	O4'-C4'-C5'-O5'
76	2	1664	4OC	C3'-C4'-C5'-O5'
76	2	1825	2MG	C3'-C4'-C5'-O5'
26	1	2808	2MA	C3'-C4'-C5'-O5'
26	1	2257	5MU	O4'-C4'-C5'-O5'
26	1	2885	PSU	O4'-C4'-C5'-O5'
26	1	891	PSU	O4'-C1'-C5-C6
76	2	525	G7M	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	2560	OMG	2	0
76	2	1825	2MG	1	0
26	1	1105	PSU	1	0
26	1	891	PSU	2	0
75	5	54	5MU	1	0
76	2	1828	MA6	2	0
76	2	1664	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 435 ligands modelled in this entry, 433 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
90	ATP	W	501	89	32,33,33	1.33	4 (12%)	48,52,52	1.80	11 (22%)
91	CLM	1	3201	-	20,20,20	1.64	3 (15%)	23,27,27	1.16	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	ATP	W	501	89	-	0/22/38/38	0/3/3/3
91	CLM	1	3201	-	-	2/20/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	1	3201	CLM	C2-N2	4.75	1.44	1.34
90	W	501	ATP	C5-C4	4.32	1.46	1.39
91	1	3201	CLM	O9B-N9	-3.11	1.17	1.22
91	1	3201	CLM	O2-C2	-3.00	1.17	1.23
90	W	501	ATP	C5-C6	2.56	1.48	1.41
90	W	501	ATP	C5-N7	-2.41	1.34	1.39
90	W	501	ATP	C8-N7	2.20	1.35	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	W	501	ATP	C5-C4-N3	-5.95	118.53	126.72
90	W	501	ATP	N3-C4-N9	4.81	135.34	127.17
90	W	501	ATP	C2-N3-C4	3.76	121.02	111.83
90	W	501	ATP	C4-C5-N7	-3.39	106.70	110.58
90	W	501	ATP	N3-C2-N1	-3.21	123.72	128.58
91	1	3201	CLM	C5-C3-N2	-3.05	104.52	110.03
90	W	501	ATP	C4-N9-C8	2.93	108.81	105.74
90	W	501	ATP	C5-N7-C8	2.66	107.62	103.45
90	W	501	ATP	C3'-C2'-C1'	2.55	106.28	101.46
91	1	3201	CLM	O5-C5-C6	-2.34	106.11	111.20
90	W	501	ATP	C2'-C1'-N9	-2.29	107.62	113.30
90	W	501	ATP	N9-C8-N7	-2.26	110.73	113.94
90	W	501	ATP	C6-C5-N7	2.06	136.07	132.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

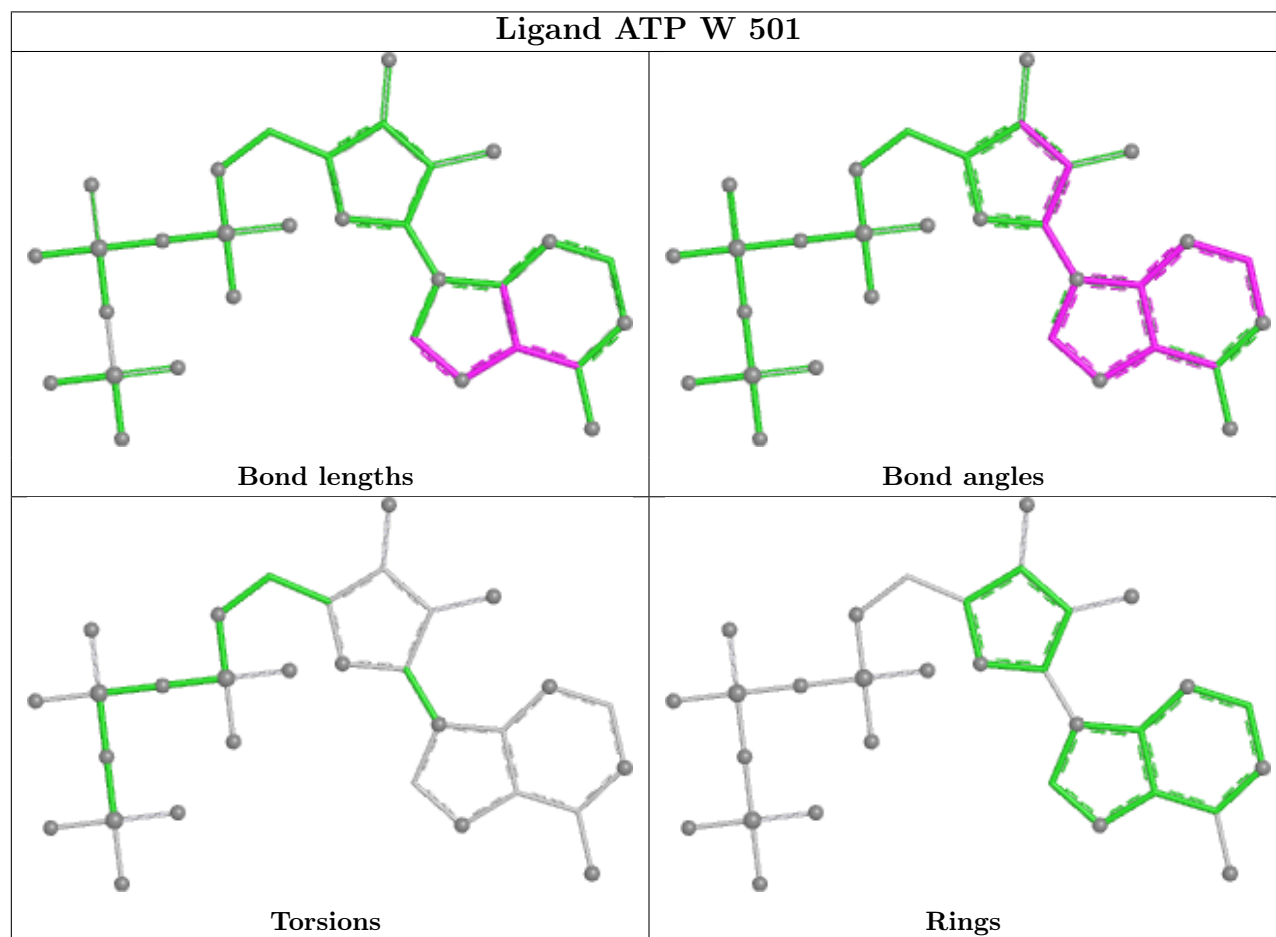
Mol	Chain	Res	Type	Atoms
91	1	3201	CLM	N2-C3-C4-O4
91	1	3201	CLM	C5-C3-C4-O4

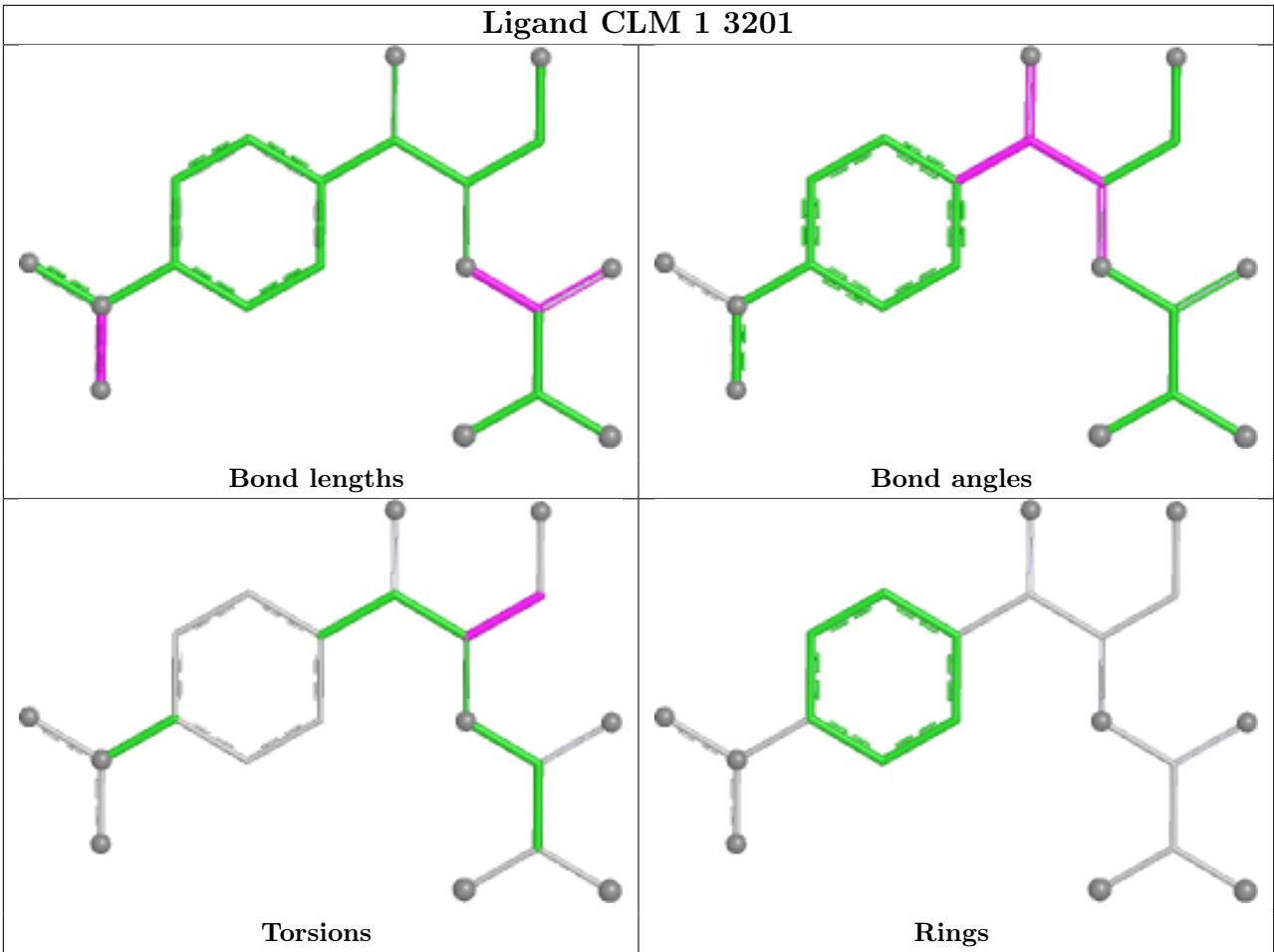
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	1	11
76	2	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	295:U	O3'	307:A	P	27.62
1	1	261:G	O3'	270:A	P	26.81
1	2	95:A	O3'	101:A	P	23.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1704:U	O3'	1831:A	P	17.44
1	1	363:A	O3'	405:U	P	17.26
1	1	1028:G	O3'	1041:C	P	17.01
1	1	283:A	O3'	288:U	P	16.63
1	1	323:U	O3'	330:A	P	15.74
1	1	2613:A	O3'	2617:U	P	15.52
1	2	124:A	O3'	129:A	P	15.35
1	2	116:U	O3'	120:A	P	15.02
1	2	137:A	O3'	142:U	P	14.96
1	2	1142:A	O3'	1379:C	P	14.23
1	1	1664:A	O3'	1667:C	P	12.07
1	1	2509:C	O3'	2528:G	P	9.64
1	2	84:A	O3'	86:A	P	8.48
1	2	1842:U	O3'	1845:A	P	8.37
1	1	859:U	O3'	861:A	P	3.88

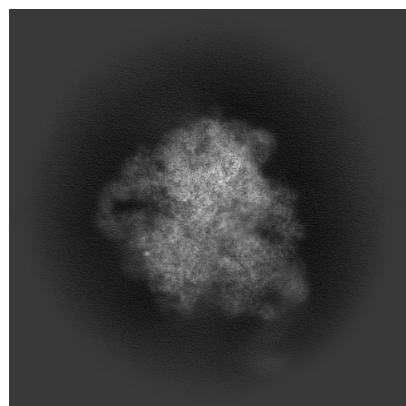
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50011. These allow visual inspection of the internal detail of the map and identification of artifacts.

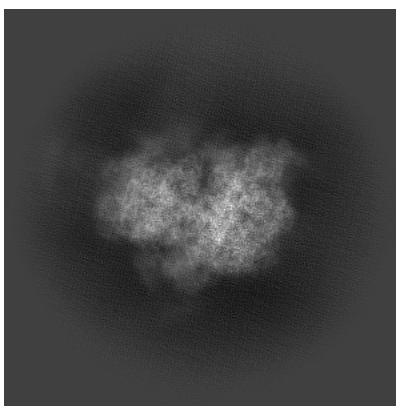
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

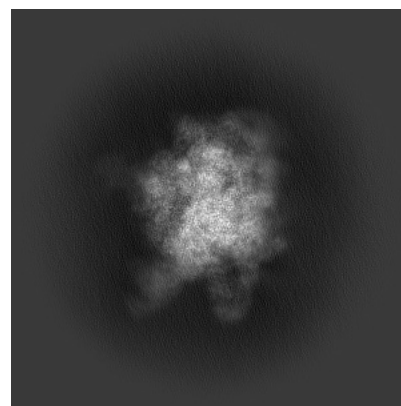
6.1.1 Primary map



X

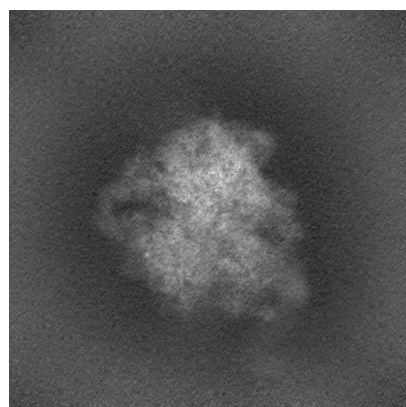


Y

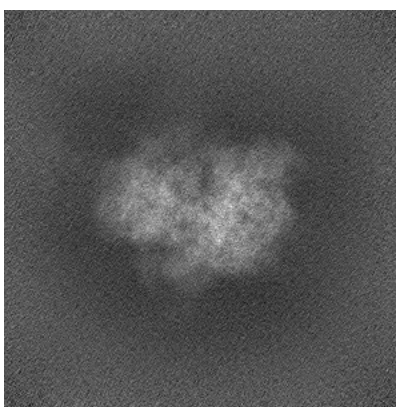


Z

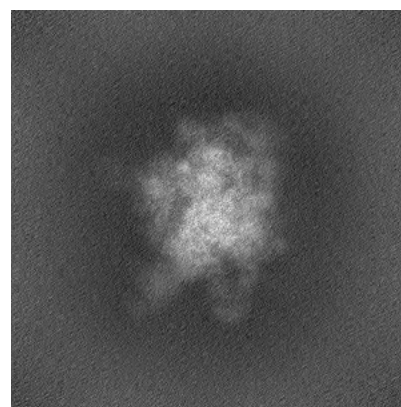
6.1.2 Raw map



X



Y

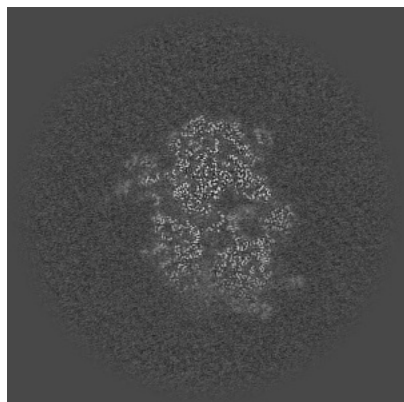


Z

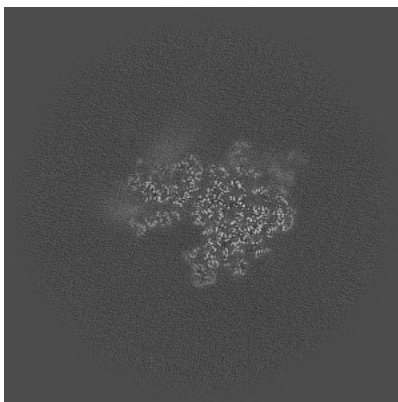
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

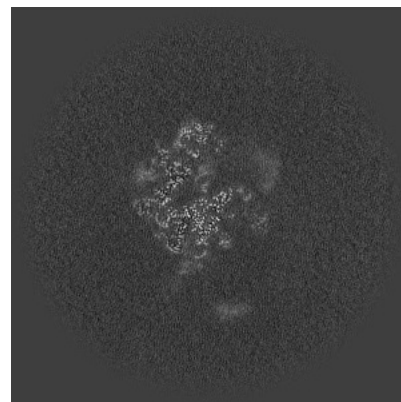
6.2.1 Primary map



X Index: 282

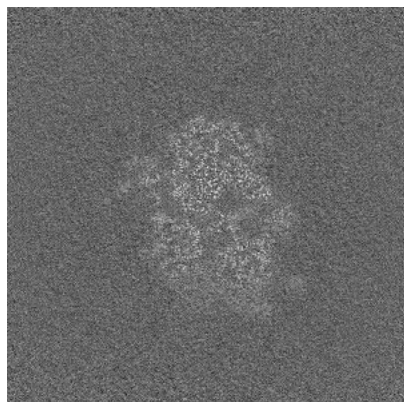


Y Index: 282

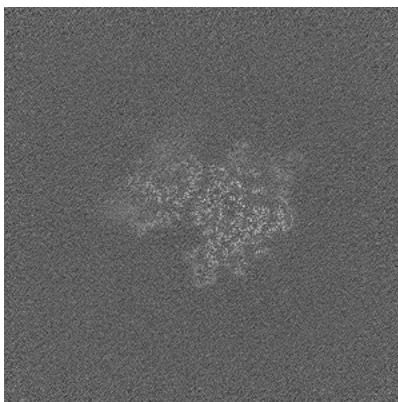


Z Index: 282

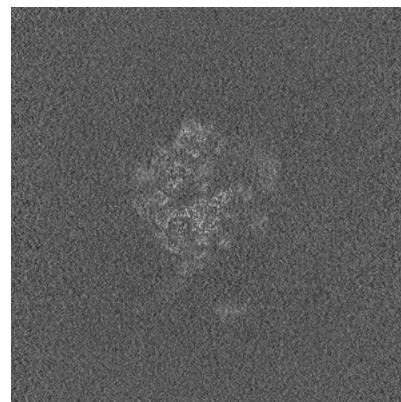
6.2.2 Raw map



X Index: 282



Y Index: 282

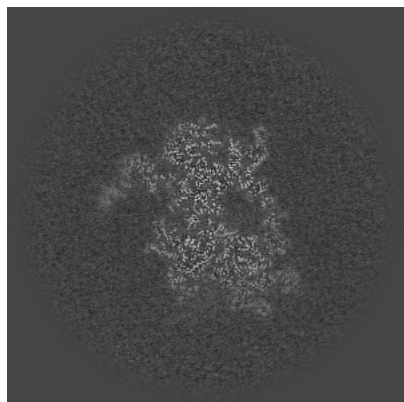


Z Index: 282

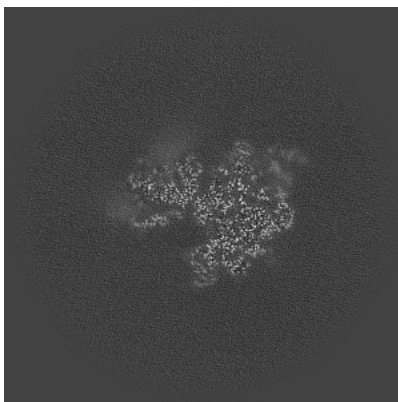
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

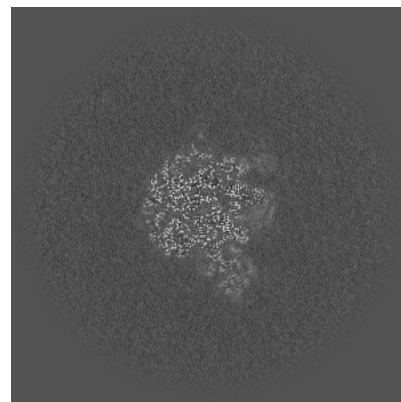
6.3.1 Primary map



X Index: 293

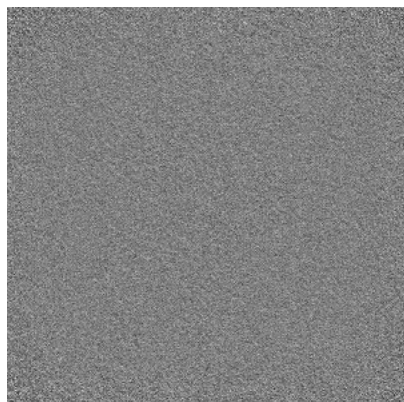


Y Index: 285

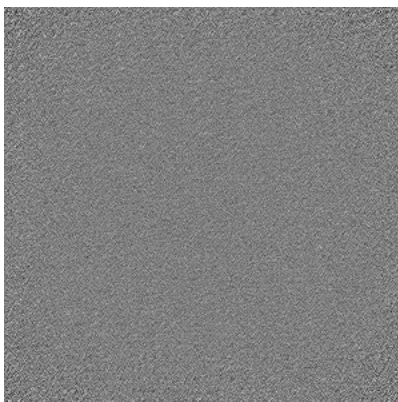


Z Index: 325

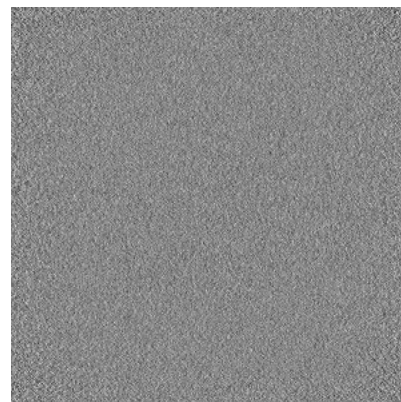
6.3.2 Raw map



X Index: 0



Y Index: 0

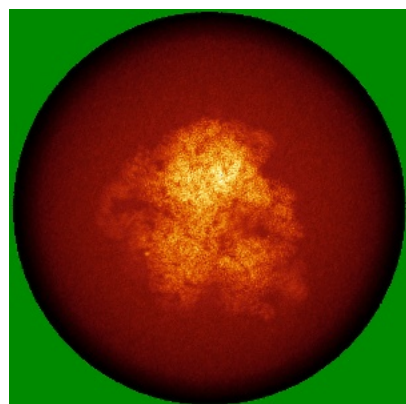


Z Index: 0

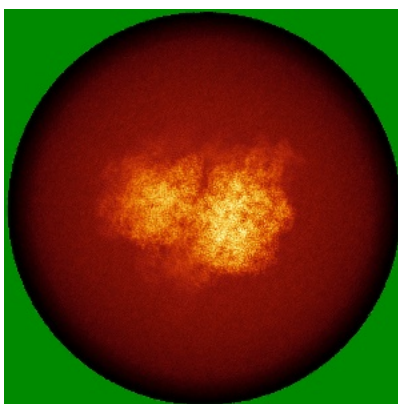
The images above show the largest variance slices of the map in three orthogonal directions.

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

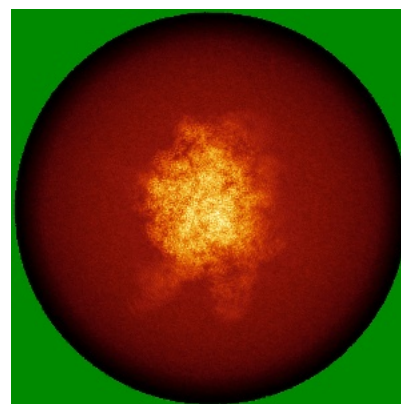
6.4.1 Primary map



X

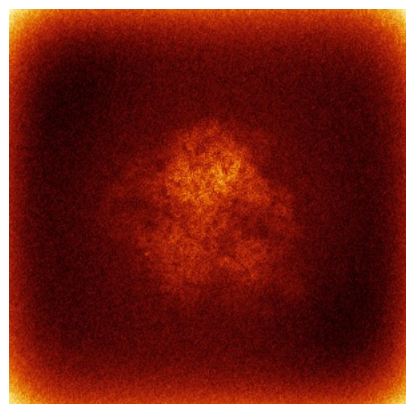


Y

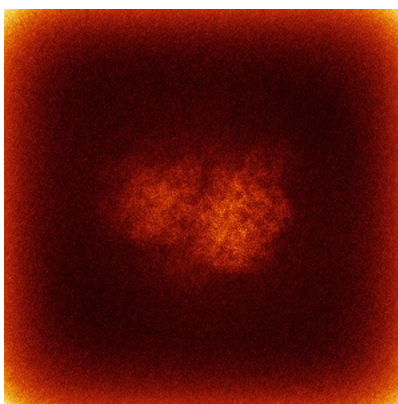


Z

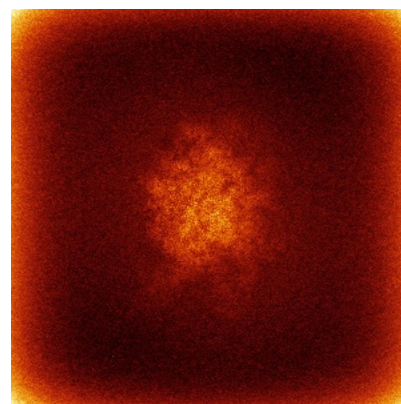
6.4.2 Raw map



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.

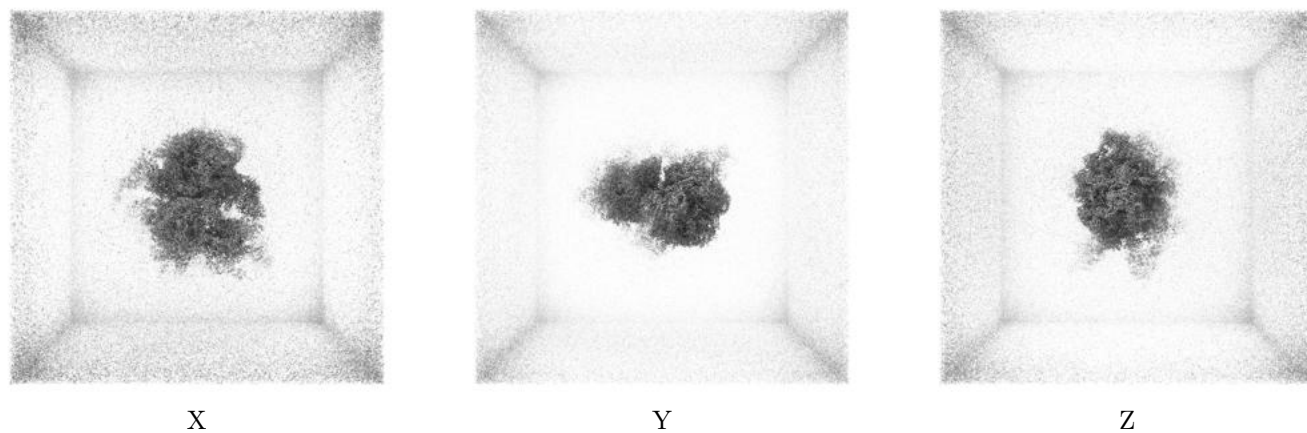
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0796. 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.

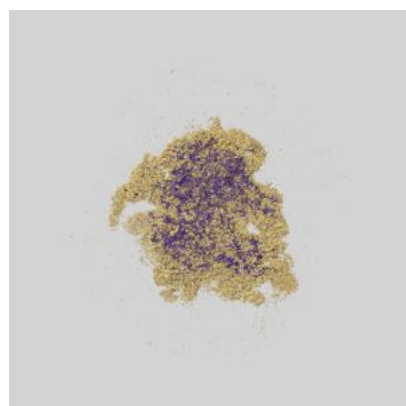
6.6 Mask visualisation [i](#)

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

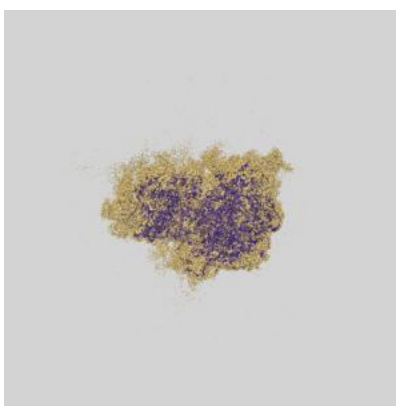
A mask typically either:

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

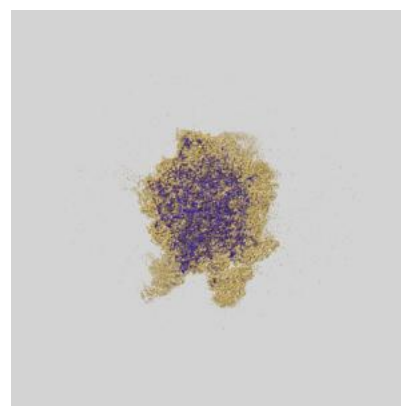
6.6.1 emd_50011_msk_1.map [i](#)



X



Y

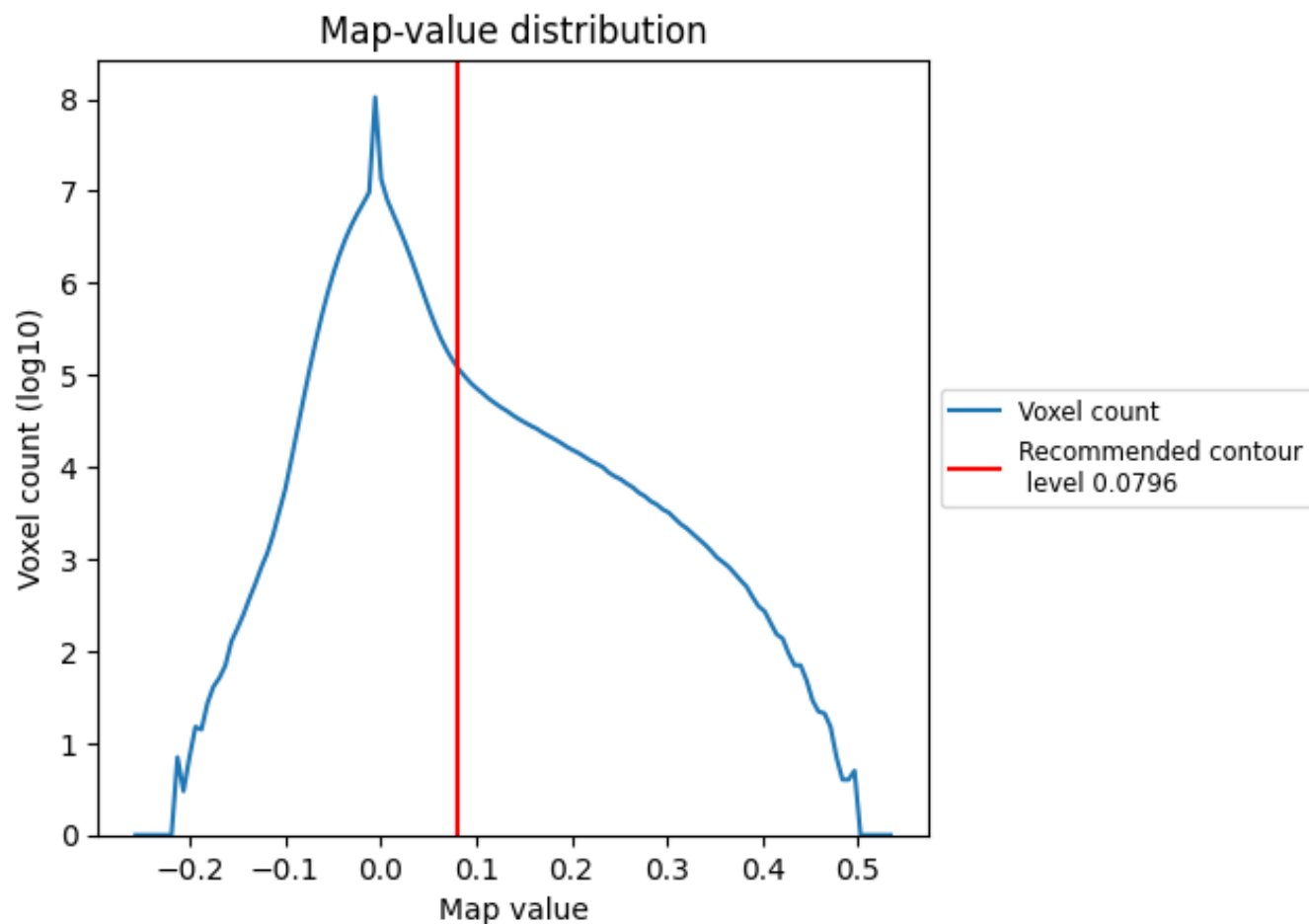


Z

7 Map analysis [i](#)

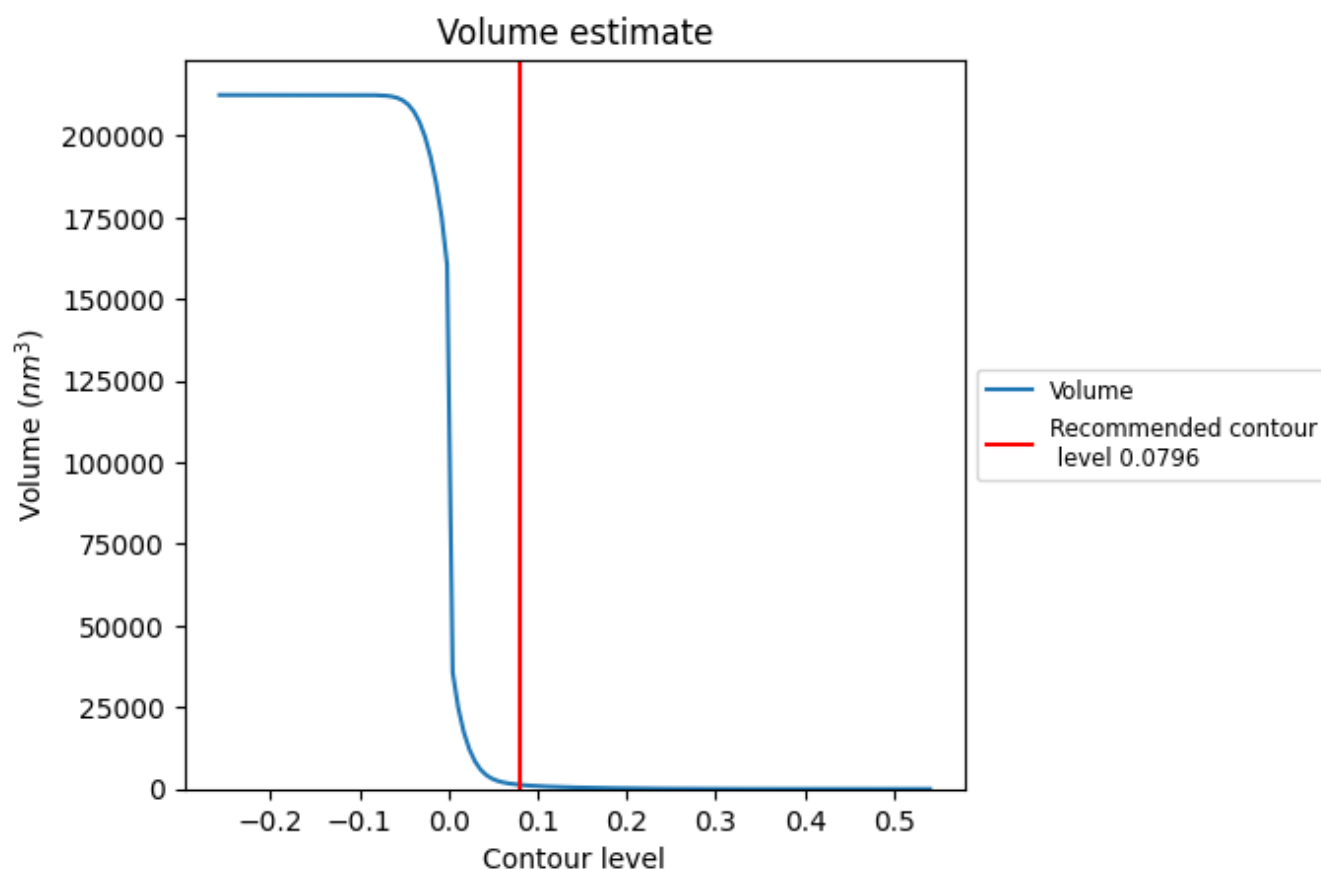
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

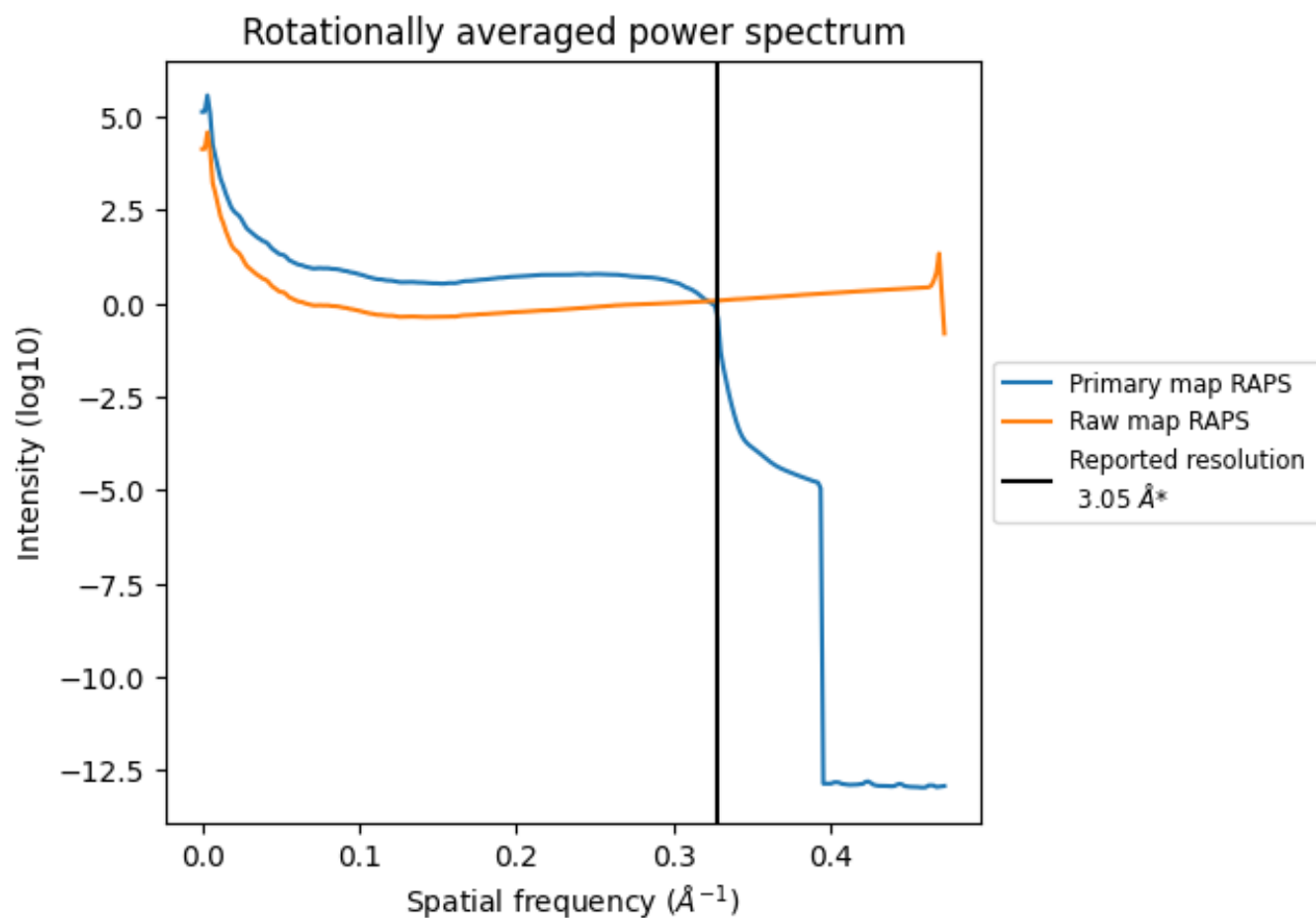
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1277 nm^3 ; this corresponds to an approximate mass of 1154 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 ⓘ

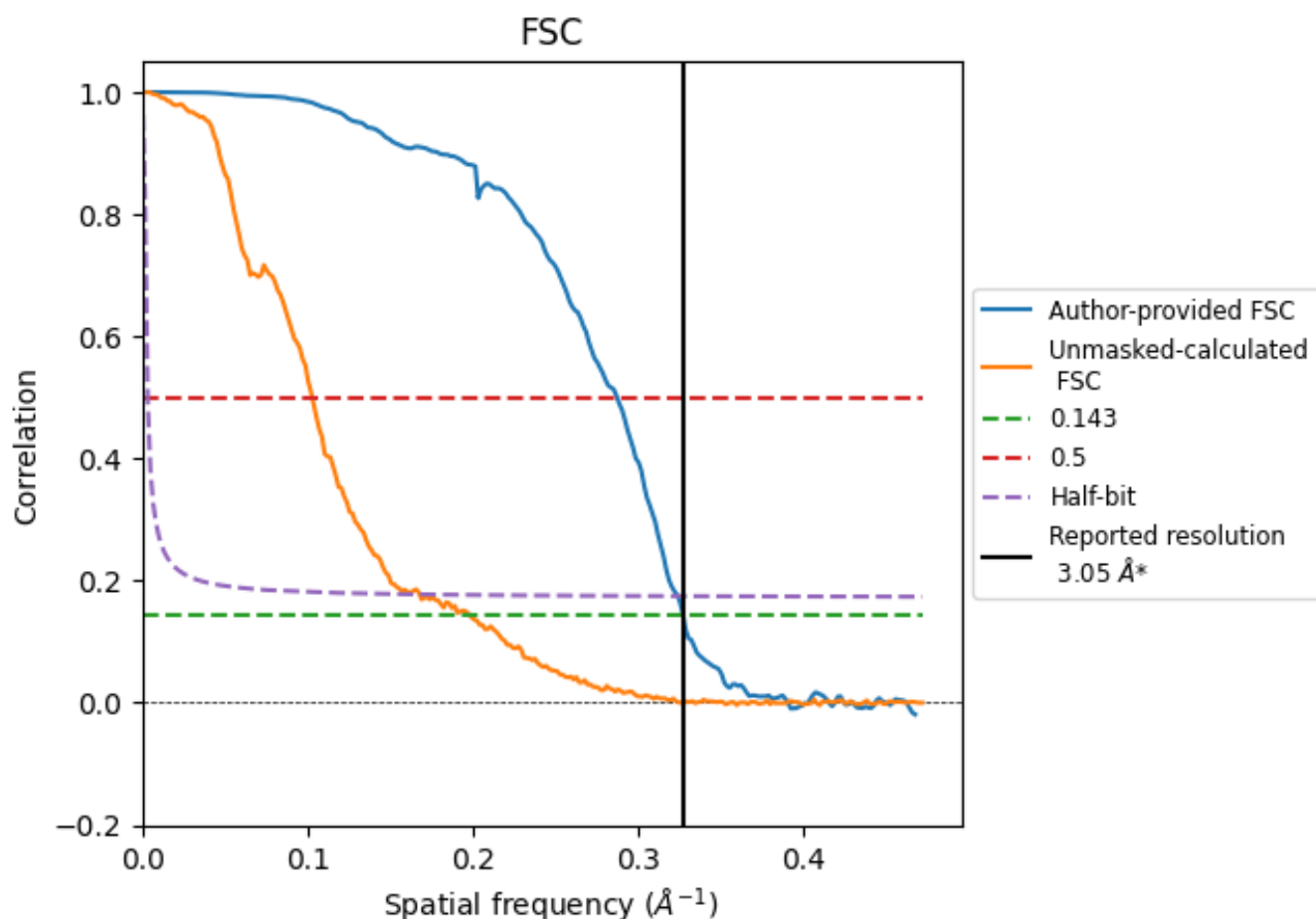


*Reported resolution corresponds to spatial frequency of 0.328 \AA^{-1}

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 0.328 \AA^{-1}

8.2 Resolution estimates [i](#)

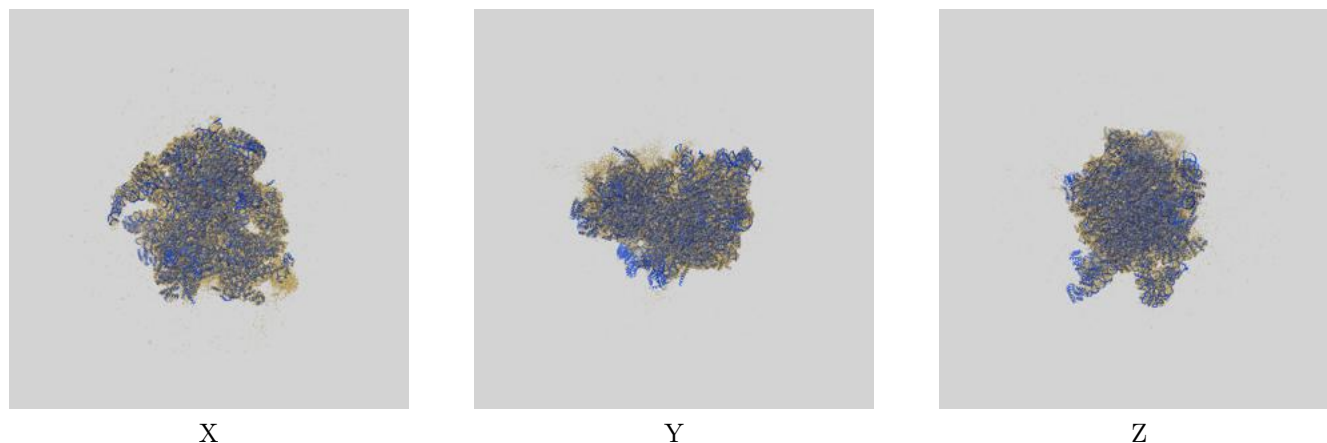
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.05	3.48	3.08
Unmasked-calculated*	5.04	9.71	5.95

*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 5.04 differs from the reported value 3.05 by more than 10 %

9 Map-model fit [i](#)

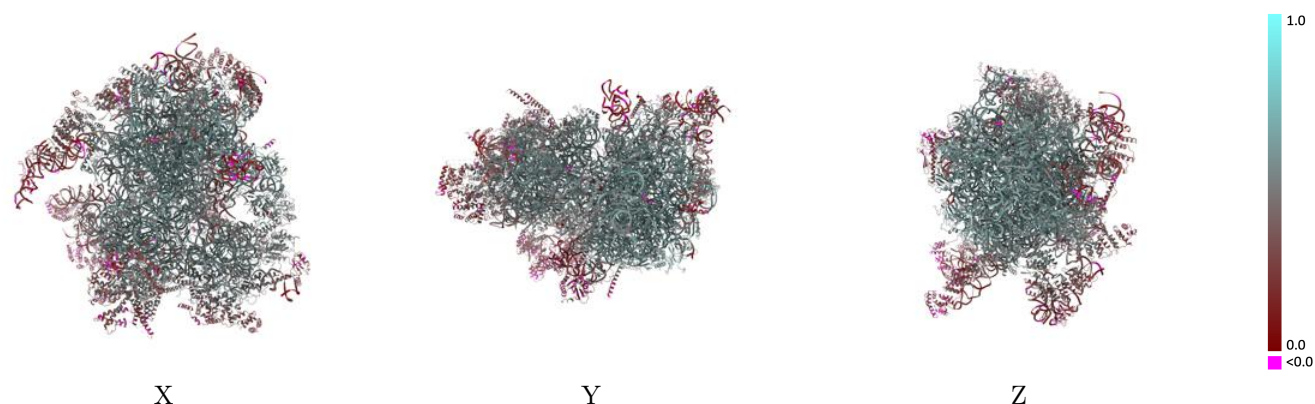
This section contains information regarding the fit between EMDB map EMD-50011 and PDB model 9EVS. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



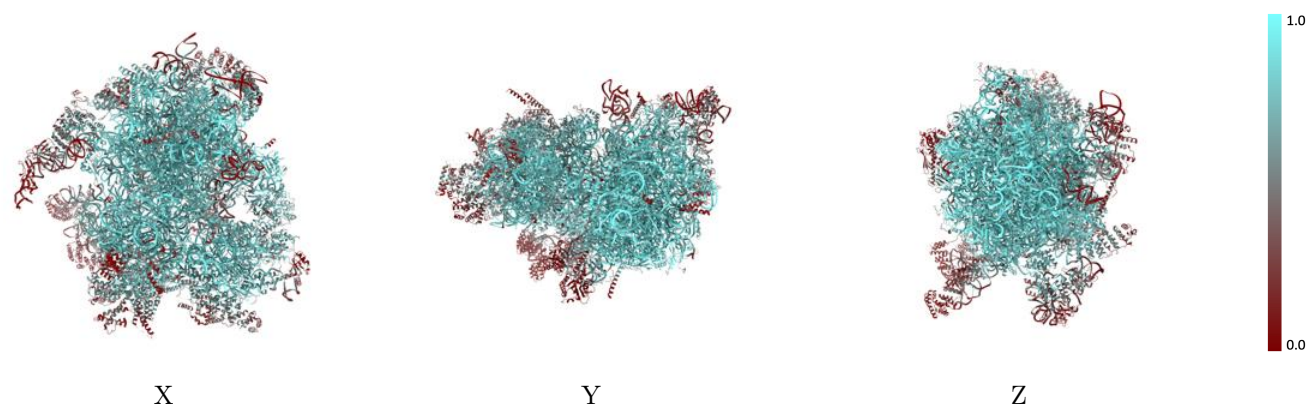
The images above show the 3D surface view of the map at the recommended contour level 0.0796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



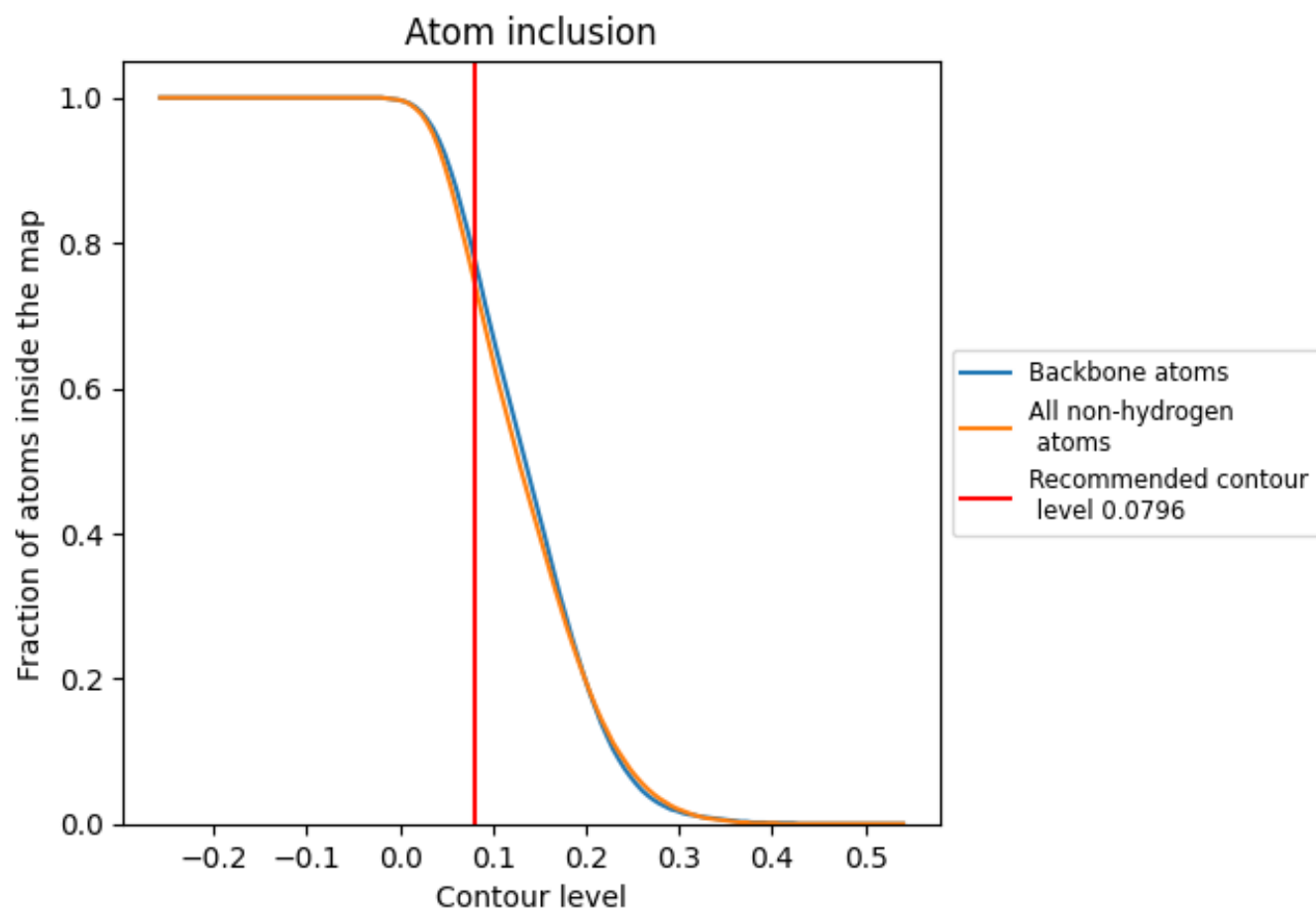
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0796).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.0796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.4830
1	 0.8610	 0.5200
1B	 0.8510	 0.5650
1C	 0.7010	 0.5050
1D	 0.8610	 0.5710
1E	 0.8800	 0.5720
1F	 0.7420	 0.5240
1G	 0.6510	 0.4930
1H	 0.6770	 0.4830
1I	 0.0220	 0.1690
1J	 0.0920	 0.1880
1K	 0.8180	 0.5400
1L	 0.8220	 0.5680
1M	 0.8570	 0.5660
1N	 0.7890	 0.5350
1O	 0.8840	 0.5740
1P	 0.8430	 0.5530
1Q	 0.8110	 0.5530
1R	 0.9310	 0.5900
1S	 0.8270	 0.5670
1T	 0.8840	 0.5750
1U	 0.8200	 0.5590
1V	 0.8360	 0.5640
1W	 0.2130	 0.2470
1X	 0.7670	 0.5210
1Y	 0.8280	 0.5540
1Z	 0.7440	 0.5130
1a	 0.8600	 0.5550
1b	 0.8710	 0.5680
1c	 0.8050	 0.5300
1d	 0.9210	 0.5750
1e	 0.8200	 0.5520
1f	 0.9770	 0.6090
1g	 0.8910	 0.5810
1h	 0.8770	 0.5720



























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Chain	Atom inclusion	Q-score
1i	 0.6960	 0.5070
1j	 0.8940	 0.5730
1k	 0.8810	 0.5730
1l	 0.6310	 0.4620
1m	 0.2300	 0.2880
1o	 0.1180	 0.2320
1p	 0.7760	 0.5430
1q	 0.8400	 0.5550
1r	 0.8000	 0.5250
1s	 0.7830	 0.5280
1t	 0.5730	 0.4040
1u	 0.4600	 0.3640
1v	 0.6100	 0.4180
1x	 0.8950	 0.6300
2	 0.8760	 0.5060
3	 0.9400	 0.5490
5	 0.7550	 0.4260
6	 0.6610	 0.5240
A	 0.7660	 0.5170
B	 0.5750	 0.4150
C	 0.7130	 0.4830
D	 0.6730	 0.4740
E	 0.7820	 0.5330
F	 0.7040	 0.4850
G	 0.8330	 0.5470
H	 0.6380	 0.4690
I	 0.8060	 0.5270
J	 0.7400	 0.5030
K	 0.7660	 0.5340
L	 0.7530	 0.5200
M	 0.8250	 0.5460
N	 0.7780	 0.5340
O	 0.8180	 0.5280
P	 0.7660	 0.5260
Q	 0.7350	 0.5030
R	 0.4240	 0.3540
S	 0.6830	 0.5110
T	 0.8410	 0.5580
U	 0.5330	 0.3830
V	 0.6440	 0.4420
W	 0.7000	 0.4850
X	 0.5160	 0.3830

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Chain	Atom inclusion	Q-score
Y	 0.6910	 0.4800
Z	 0.5970	 0.3770
a	 0.5220	 0.3680
b	 0.4680	 0.3790
c	 0.8340	 0.5570
d	 0.5750	 0.4190
e	 0.6980	 0.4680
f	 0.5830	 0.4150
h	 0.1910	 0.2040
i	 0.2840	 0.2850
j	 0.0290	 0.1450
k	 0.5630	 0.4150