



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:26 AM UTC

PDB ID : 7PKT / pdb_00007pkt
EMDB ID : EMD-13480
Title : Large subunit of the Chlamydomonas reinhardtii mitoribosome
Authors : Waltz, F.; Soufari, H.; Hashem, Y.
Deposited on : 2021-08-26
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

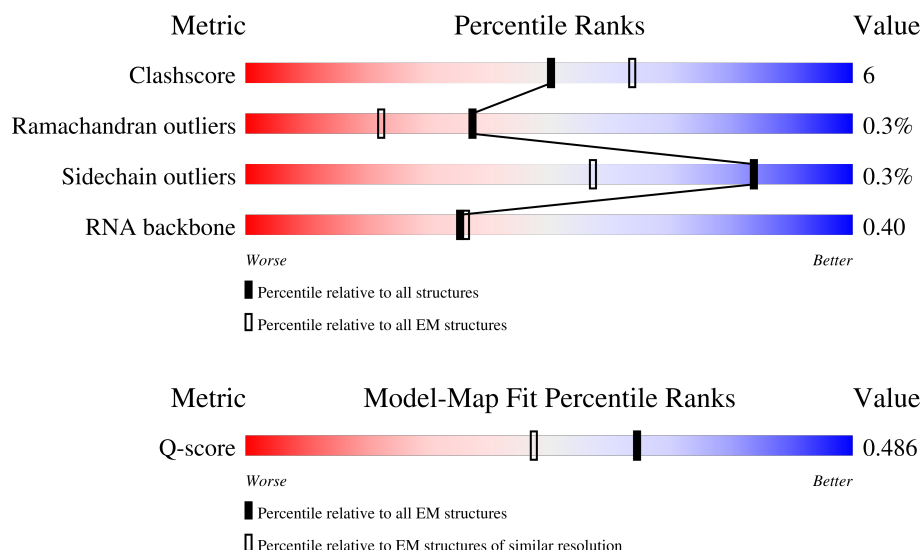
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	a	383	55% 55% 14% 31%
2	b	417	24% 58% 14% 27%
3	c	427	15% 63% 10% 26%

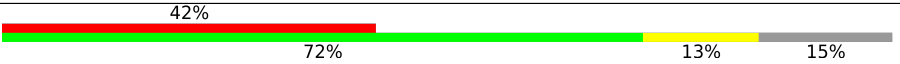
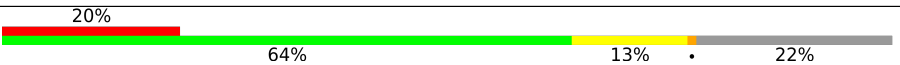
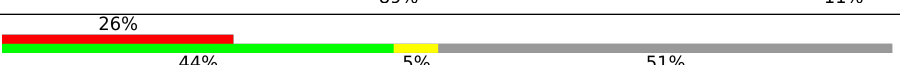
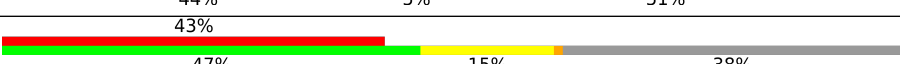
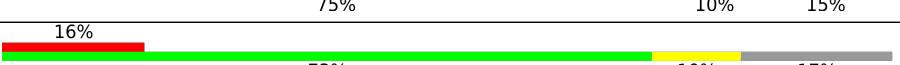
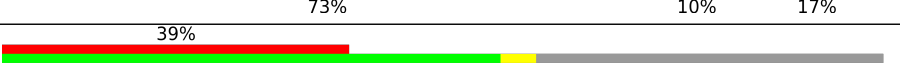
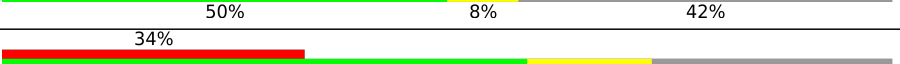
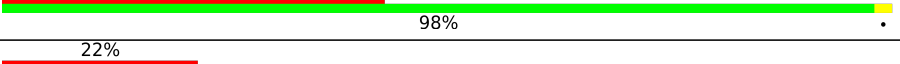
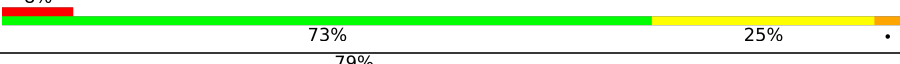
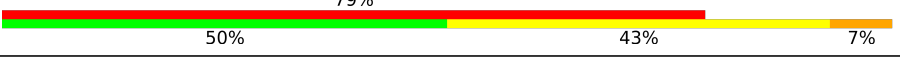
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Mol	Chain	Length	Quality of chain
4	d	216	
5	f	304	
6	i	277	
7	j	120	
8	k	337	
9	l	270	
10	m	183	
11	n	312	
12	o	115	
13	p	370	
14	q	377	
15	r	226	
16	s	309	
17	t	366	
18	u	173	
19	v	153	
20	w	127	
21	x	214	
22	y	123	
23	z	59	
24	A	280	
25	B	151	
26	e	207	
27	D	172	
28	E	112	

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Mol	Chain	Length	Quality of chain
29	F	141	
30	G	259	
31	I	132	
32	J	134	
33	K	249	
34	L	206	
35	C	36	
36	M	876	
37	N	455	
38	O	688	
39	P	530	
40	Q	820	
41	R	653	
42	S	334	
43	X	31	
44	Y	172	
45	Z	49	
46	1	162	
47	2	86	
48	0	75	
49	3	184	
50	4	118	
51	5	149	
52	6	136	
53	7	578	

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Mol	Chain	Length	Quality of chain
54	8	413	55% 51% 40% 9%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 103129 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 Ribosomal_L2_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	263	Total	C	N	O	S	0	0
			1993	1238	398	354	3		

- Molecule 2 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	304	Total	C	N	O	S	0	0
			2325	1481	430	403	11		

- Molecule 3 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	318	Total	C	N	O	S	0	0
			2497	1571	491	431	4		

- Molecule 4 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	184	Total	C	N	O	S	0	0
			1382	885	242	249	6		

- Molecule 5 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	60	Total	C	N	O	S	0	0
			464	289	92	81	2		

- Molecule 6 is a protein called Mitochondrial ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	152	Total	C	N	O	S	0	0
			1234	788	230	213	3		

- Molecule 7 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	120	Total	C	N	O	S	0	0
			941	604	173	161	3		

- Molecule 8 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	210	Total	C	N	O	S	0	0
			1620	1018	311	286	5		

- Molecule 9 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	136	Total	C	N	O	S	0	0
			1079	689	209	176	5		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L17,bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	177	Total	C	N	O	S	0	0
			1459	911	297	248	3		

- Molecule 11 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	173	Total	C	N	O	S	0	0
			1406	897	262	240	7		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	110	Total	C	N	O	S	0	0
			890	561	180	145	4		

- Molecule 13 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	204	Total	C	N	O	S	0	0
			1606	1022	301	281	2		

- Molecule 14 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	161	Total	C	N	O	S	0	0
			1270	795	246	221	8		

- Molecule 15 is a protein called Mitochondrial ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	158	Total	C	N	O	S	0	0
			1335	847	256	227	5		

- Molecule 16 is a protein called KOW domain-containing protein,uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	210	Total	C	N	O	S	0	0
			1565	983	284	294	4		

- Molecule 17 is a protein called Ribosomal_TL5_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	192	Total	C	N	O	S	0	0
			1489	942	282	257	8		

- Molecule 18 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	133	Total	C	N	O	S	0	0
			1007	633	194	177	3		

- Molecule 19 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	120	Total	C	N	O	S	0	0
			997	627	196	171	3		

- Molecule 20 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	120	Total	C	N	O	S	0	0
			974	611	185	173	5		

- Molecule 21 is a protein called Ribosomal_L30 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	x	167	Total	C	N	O	S	0	0
			1397	882	279	232	4		

- Molecule 22 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	71	Total	C	N	O	S	0	0
			542	335	105	97	5		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	53	Total	C	N	O	S	0	0
			439	290	77	71	1		

- Molecule 24 is a protein called bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	50	Total	C	N	O		0	0
			427	259	100	68			

- Molecule 25 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	128	Total	C	N	O	S	0	0
			1058	664	218	175	1		

- Molecule 26 is a protein called Plastid ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	164	Total	C	N	O	S	0	0
			1238	785	223	226	4		

- Molecule 27 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	94	Total	C	N	O	S	0	0
			740	467	135	134	4		

- Molecule 28 is a protein called mL41.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	79	Total	C	N	O	0	0
			636	409	119	108		

- Molecule 29 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	129	Total	C	N	O	S	0	0
			1036	650	199	182	5		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	199	Total	C	N	O	S	0	0
			1482	924	268	286	4		

- Molecule 31 is a protein called mL63/57/60.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	97	Total	C	N	O	S	0	0
			780	490	152	133	5		

- Molecule 32 is a protein called mL59/64.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	114	Total	C	N	O	S	0	0
			842	529	156	154	3		

- Molecule 33 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	195	Total	C	N	O	S	0	0
			1571	987	305	276	3		

- Molecule 34 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	137	Total	C	N	O	S	0	0
			1167	735	234	195	3		

- Molecule 35 is a protein called bL36m.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	C	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 36 is a protein called mL113.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	430	Total	C	N	O	S	0	0
			3152	1965	617	561	9		

- Molecule 37 is a protein called mL114.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	283	Total	C	N	O	S	0	0
			2116	1337	397	377	5		

- Molecule 38 is a protein called mL115.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	584	Total	C	N	O	S	0	0
			4260	2671	792	778	19		

- Molecule 39 is a protein called mL116.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	438	Total	C	N	O	S	0	0
			3151	1979	602	564	6		

- Molecule 40 is a protein called mL117.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	498	Total	C	N	O	S	0	0
			3073	1893	581	587	12		

- Molecule 41 is a protein called mL118.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	376	Total	C	N	O	S	0	0
			2594	1616	511	461	6		

- Molecule 42 is a protein called mL119.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S	244	Total	C	N	O	S	0	0
			1967	1211	376	362	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	257	THR	GLY	conflict	UNP A0A2K3D424

- Molecule 43 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	X	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 44 is a protein called PPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Y	149	Total	C	N	O	0	0
			745	447	149	149		

- Molecule 45 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Z	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 46 is a RNA chain called L1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	162	Total	C	N	O	P	0	0
			3440	1541	607	1130	162		

- Molecule 47 is a RNA chain called L2a rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	86	Total	C	N	O	P	0	0
			1821	816	311	608	86		

- Molecule 48 is a RNA chain called L3a rRNA (5S).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	75	Total	C	N	O	P	0	0
			1592	713	280	524	75		

- Molecule 49 is a RNA chain called L3b rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	184	Total	C	N	O	P	0	0
			3933	1757	709	1283	184		

- Molecule 50 is a RNA chain called L4 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	118	Total	C	N	O	P	0	0
			2538	1135	478	807	118		

- Molecule 51 is a RNA chain called L5 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5	149	Total	C	N	O	P	0	0
			3156	1412	545	1050	149		

- Molecule 52 is a RNA chain called L6 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	136	Total	C	N	O	P	0	0
			2913	1306	542	929	136		

- Molecule 53 is a RNA chain called L7 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	7	578	Total	C	N	O	P	0	0
			12344	5521	2237	4008	578		

- Molecule 54 is a RNA chain called L8 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	8	413	Total	C	N	O	P	0	0
			8792	3931	1558	2890	413		

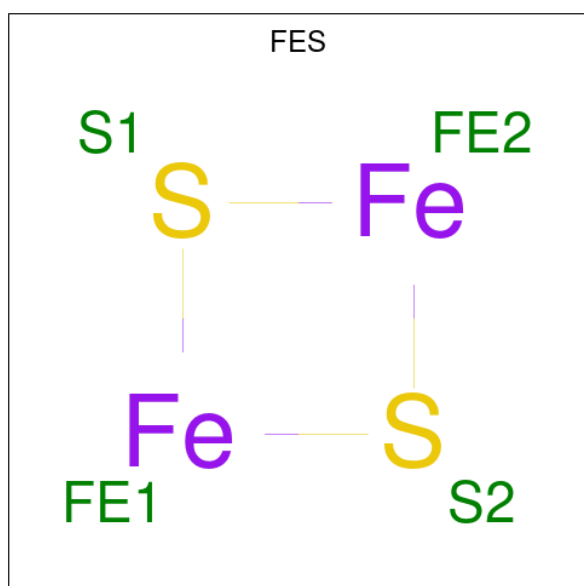
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	y	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
56	Q	1	Total	Mg	0
			1	1	
56	1	6	Total	Mg	0
			6	6	
56	2	7	Total	Mg	0
			7	7	
56	0	1	Total	Mg	0
			1	1	
56	3	12	Total	Mg	0
			12	12	
56	4	8	Total	Mg	0
			8	8	
56	5	3	Total	Mg	0
			3	3	
56	6	6	Total	Mg	0
			6	6	
56	7	18	Total	Mg	0
			18	18	
56	8	7	Total	Mg	0
			7	7	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

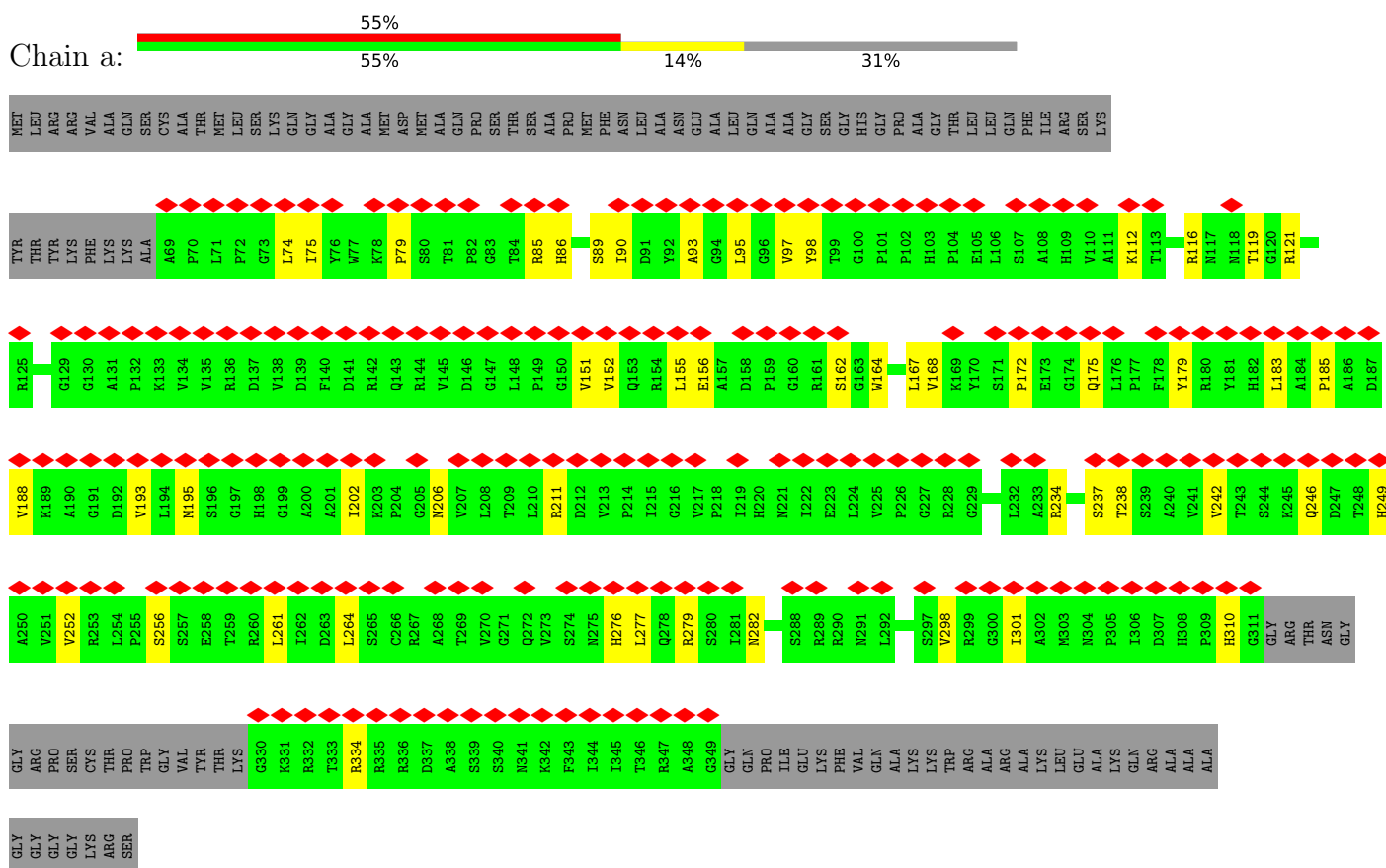


Mol	Chain	Residues	Atoms			AltConf
57	S	1	Total	Fe	S	0
			4	2	2	

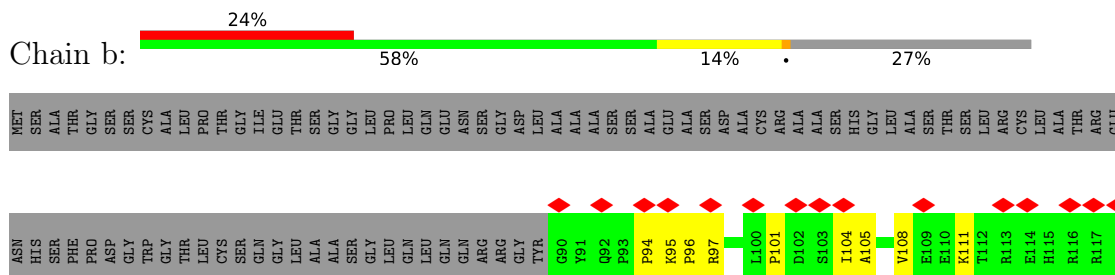
3 Residue-property plots

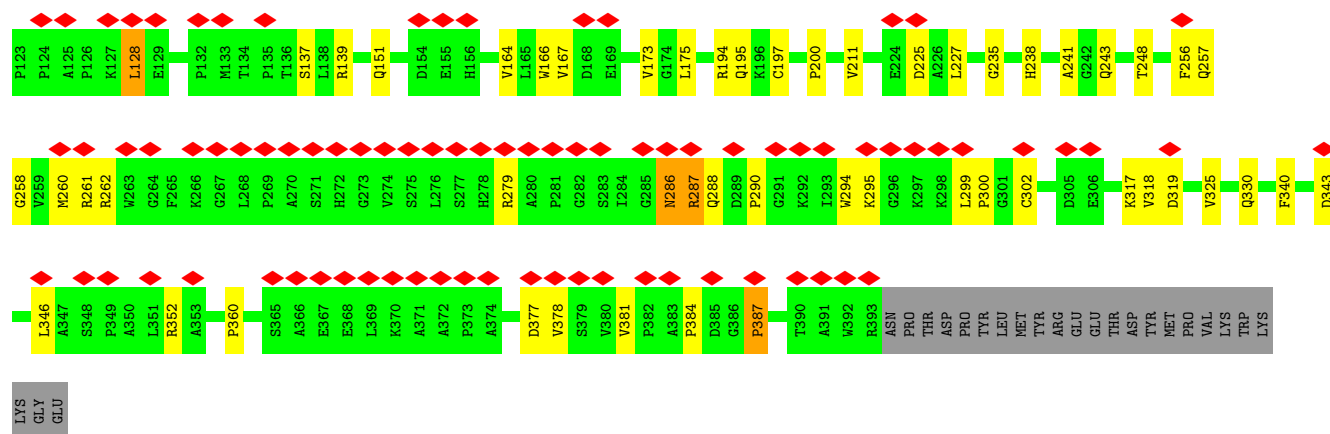
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribosomal_L2_C domain-containing protein

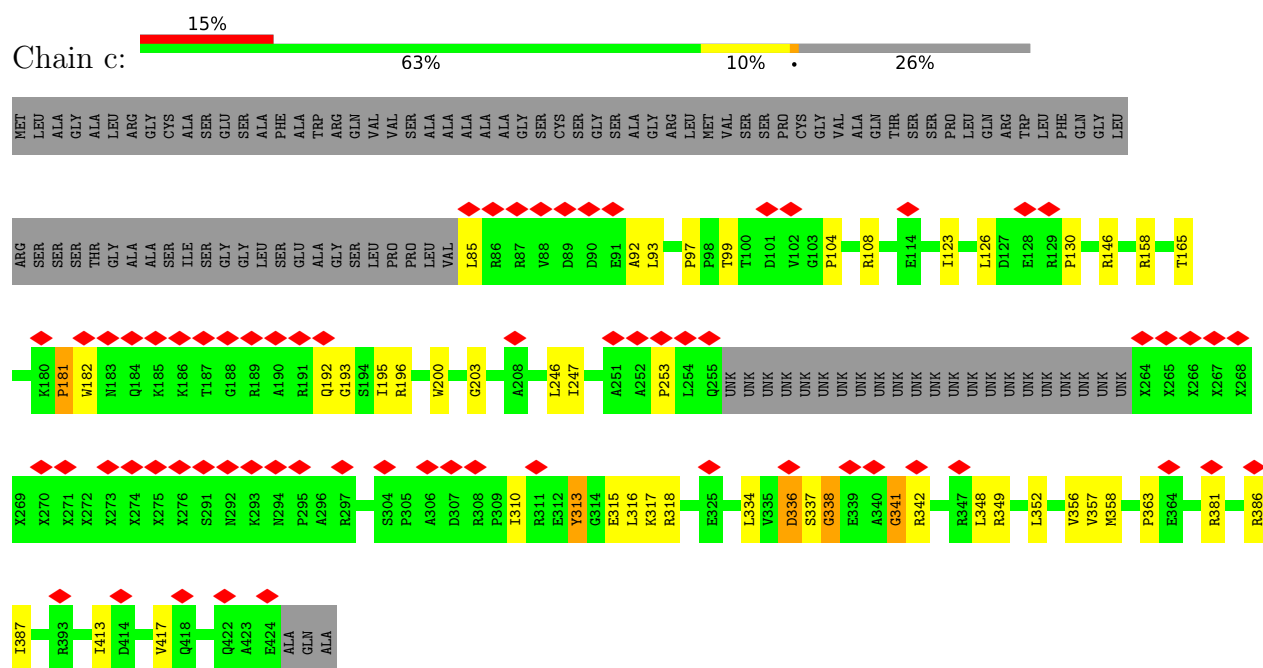


• Molecule 2: uL3m

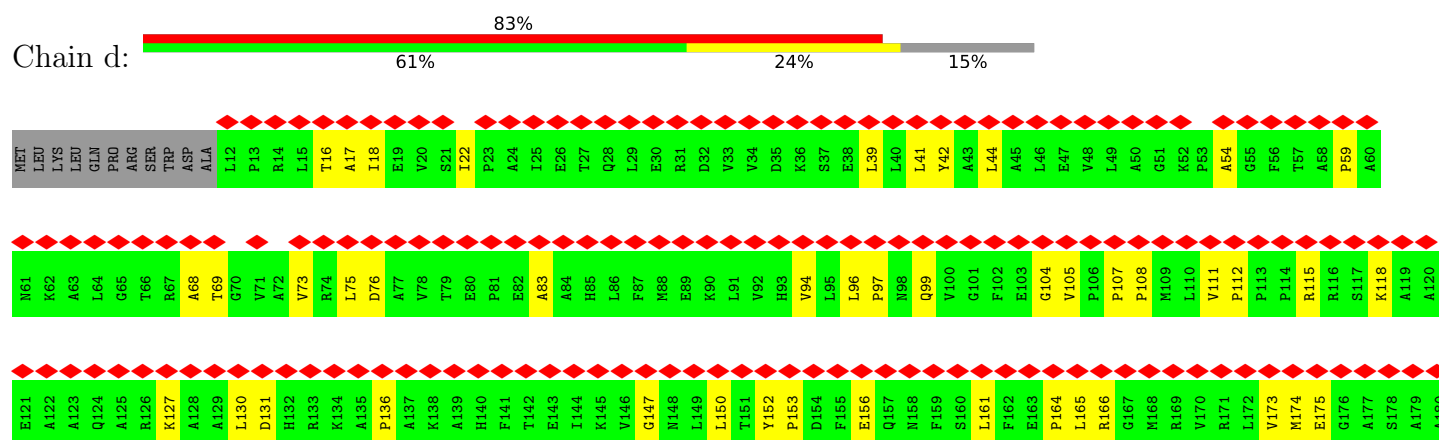


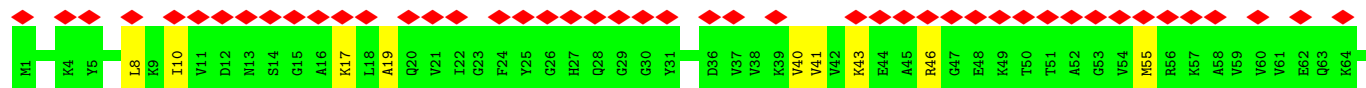


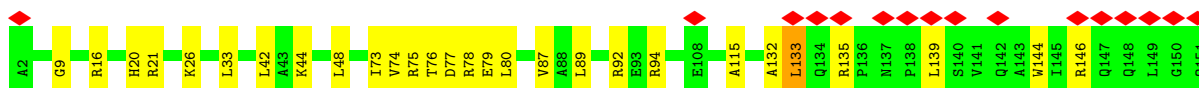
• Molecule 3: uL4m

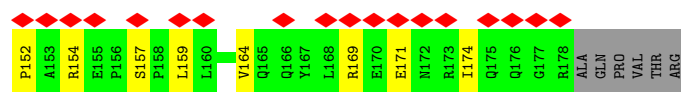


• Molecule 4: uL5m

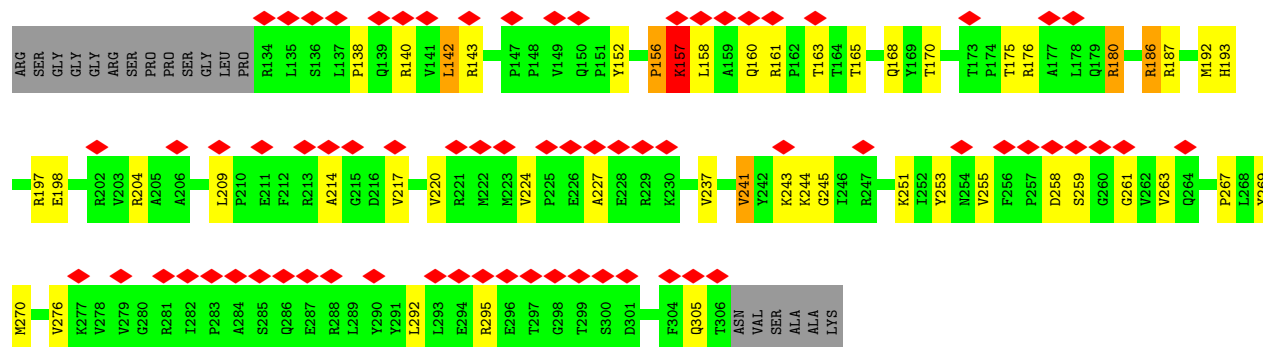
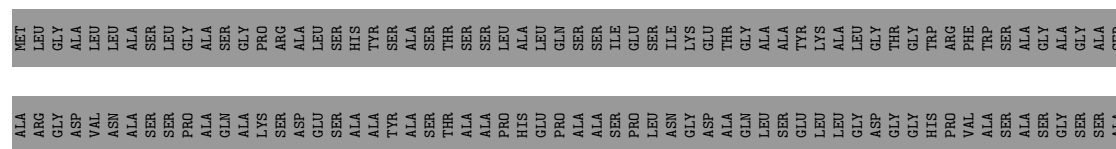








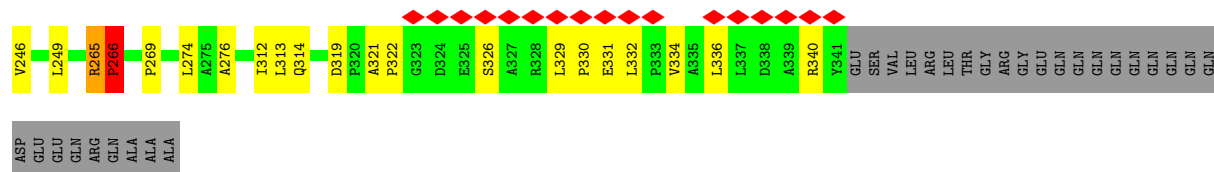
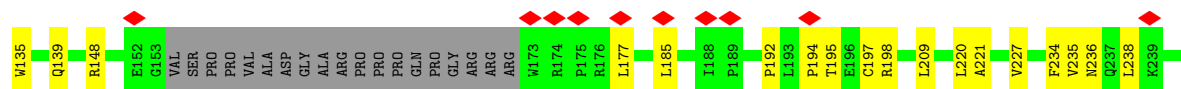
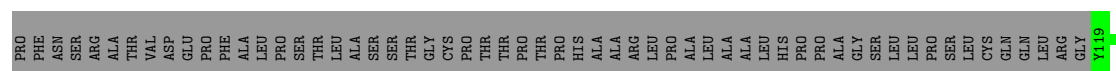
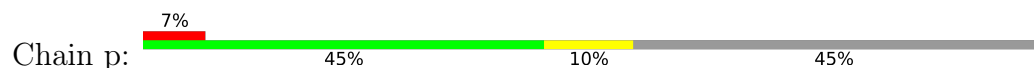
• Molecule 11: Mitochondrial ribosomal protein L19



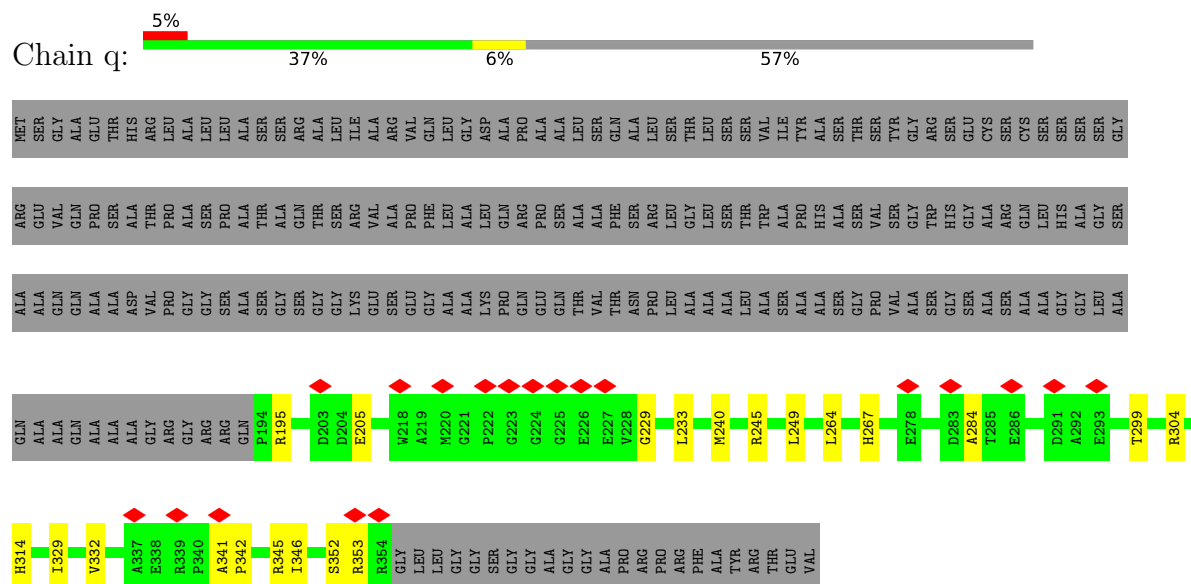
• Molecule 12: 50S ribosomal protein L20



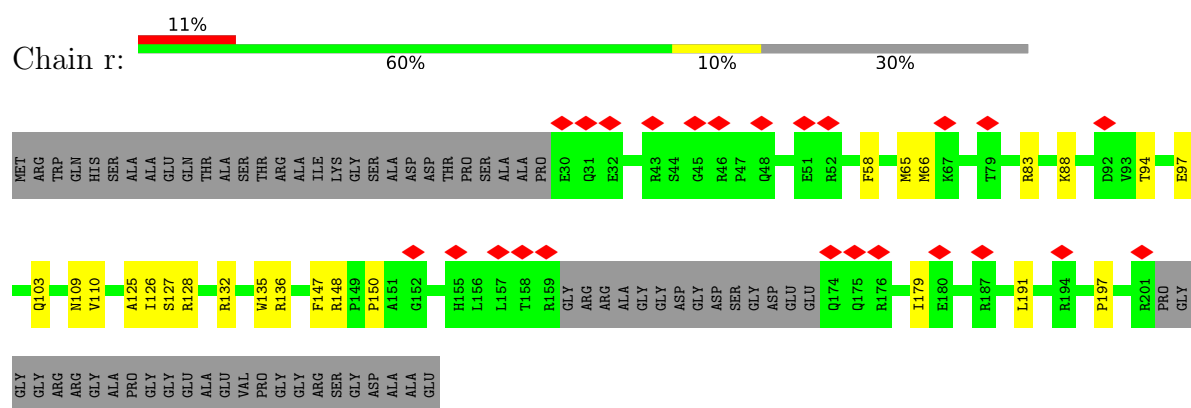
• Molecule 13: bL21m



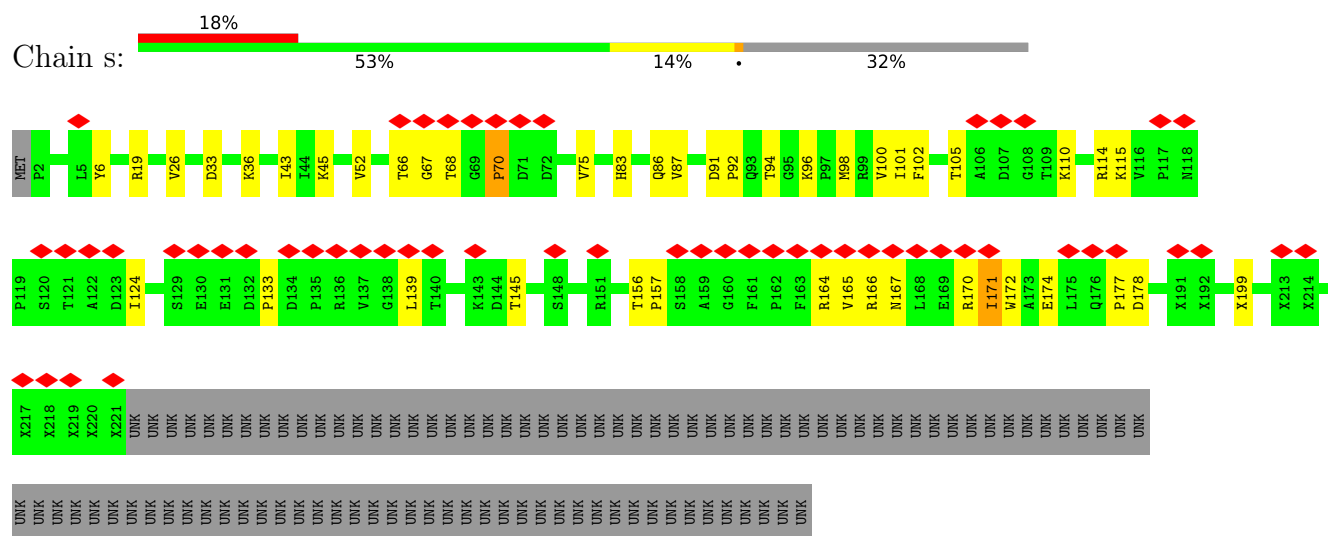
- Molecule 14: uL22m



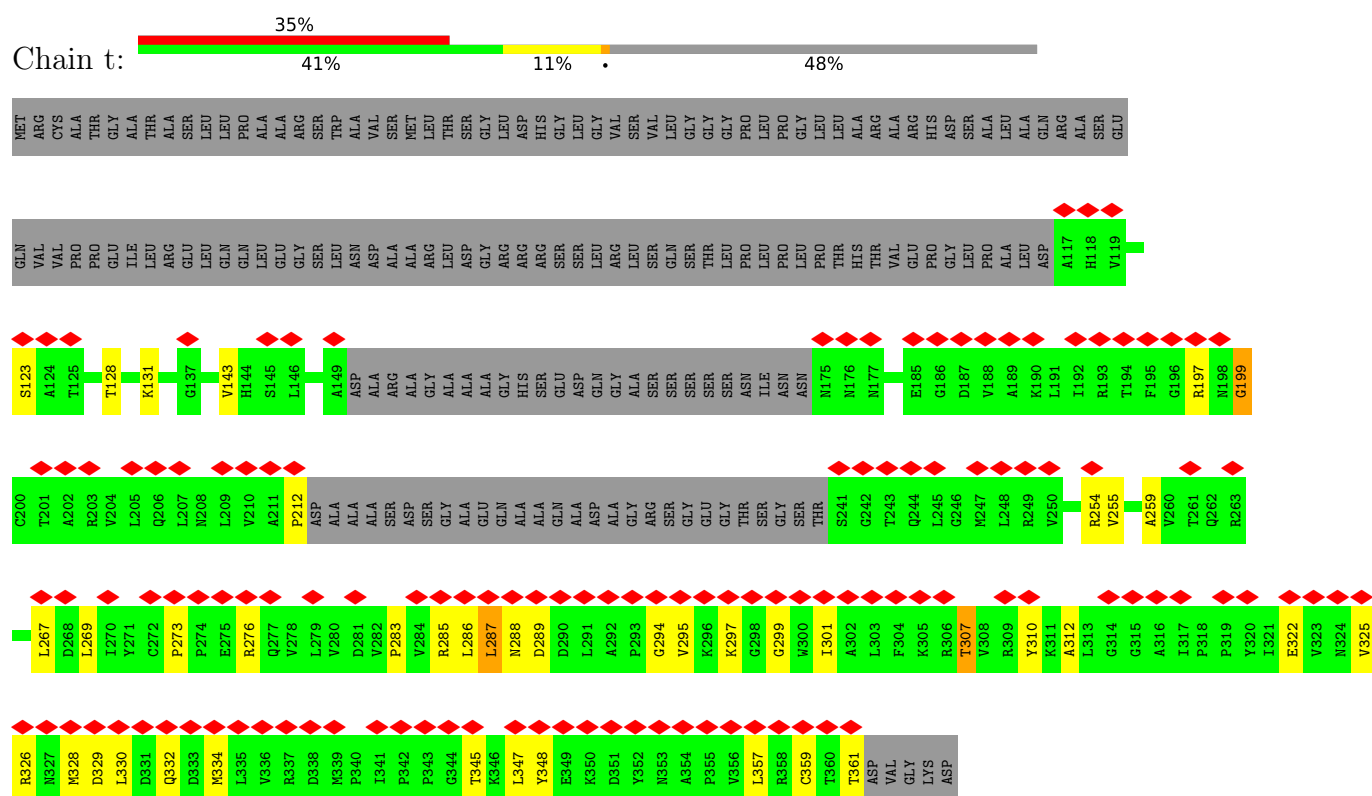
- Molecule 15: Mitochondrial ribosomal protein L23



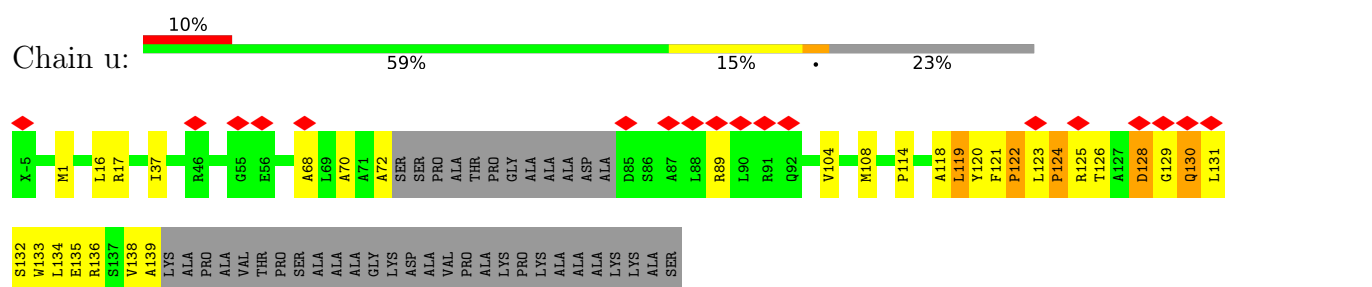
- Molecule 16: KOW domain-containing protein,uL24m



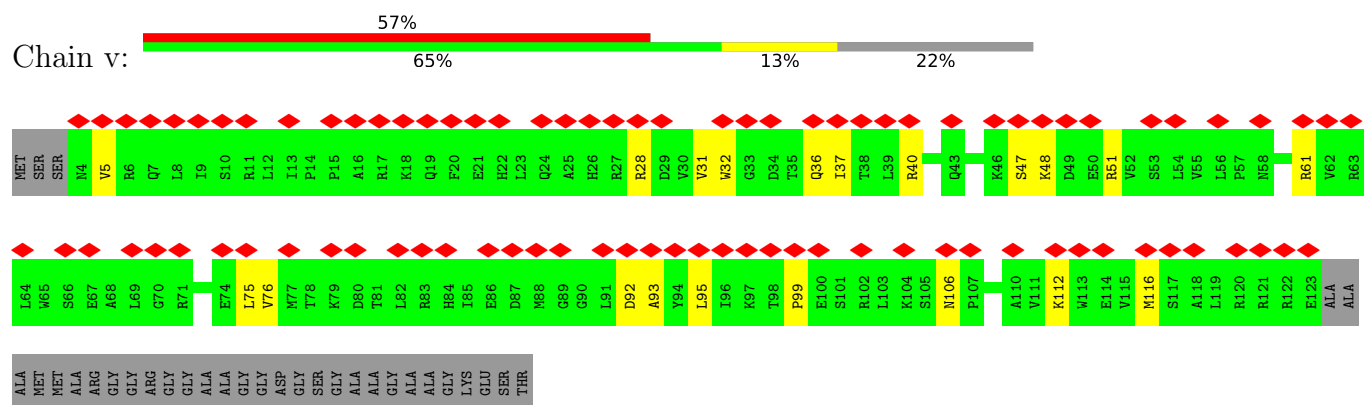
- Molecule 17: Ribosomal_TL5_C domain-containing protein



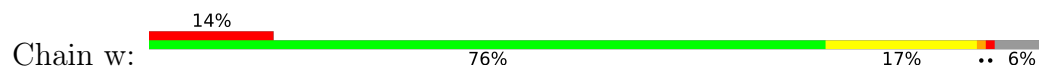
- Molecule 18: bL27m

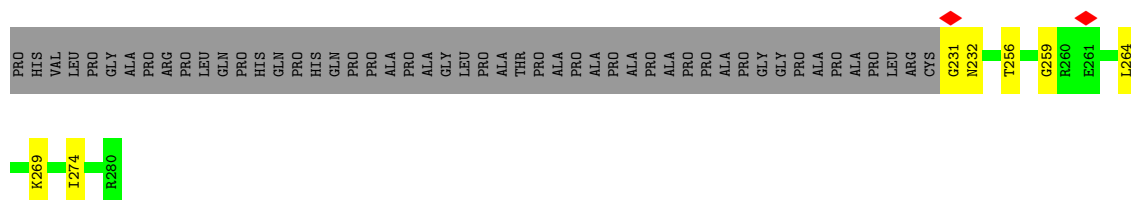


- Molecule 19: bL28m

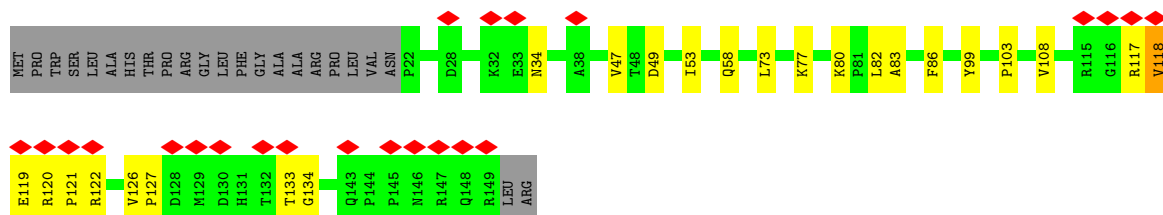


- Molecule 20: uL29m

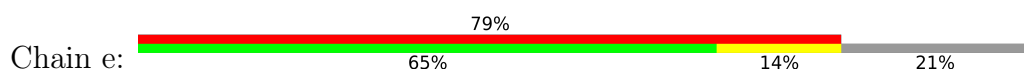




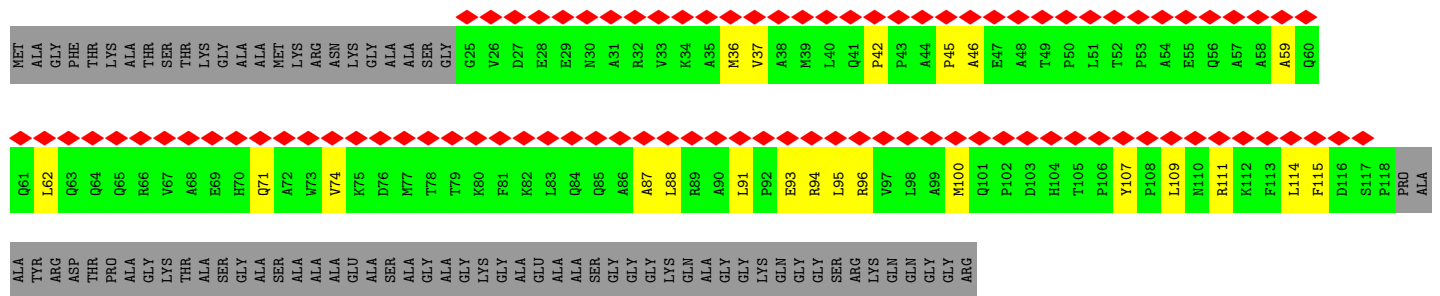
• Molecule 25: bL35m



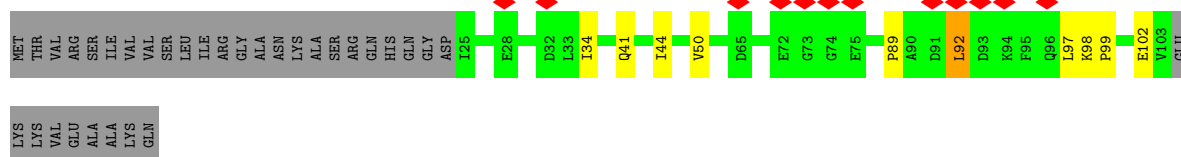
• Molecule 26: Plastid ribosomal protein L6



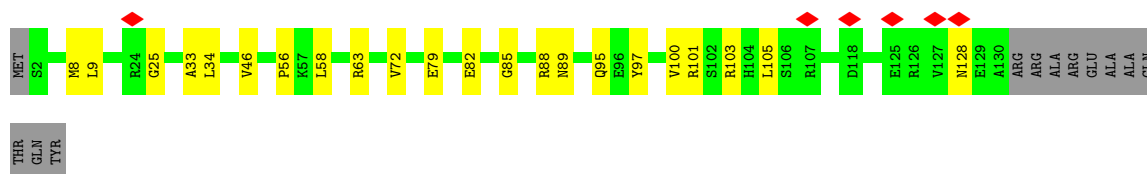
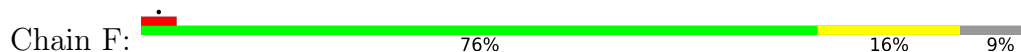
• Molecule 27: mL40



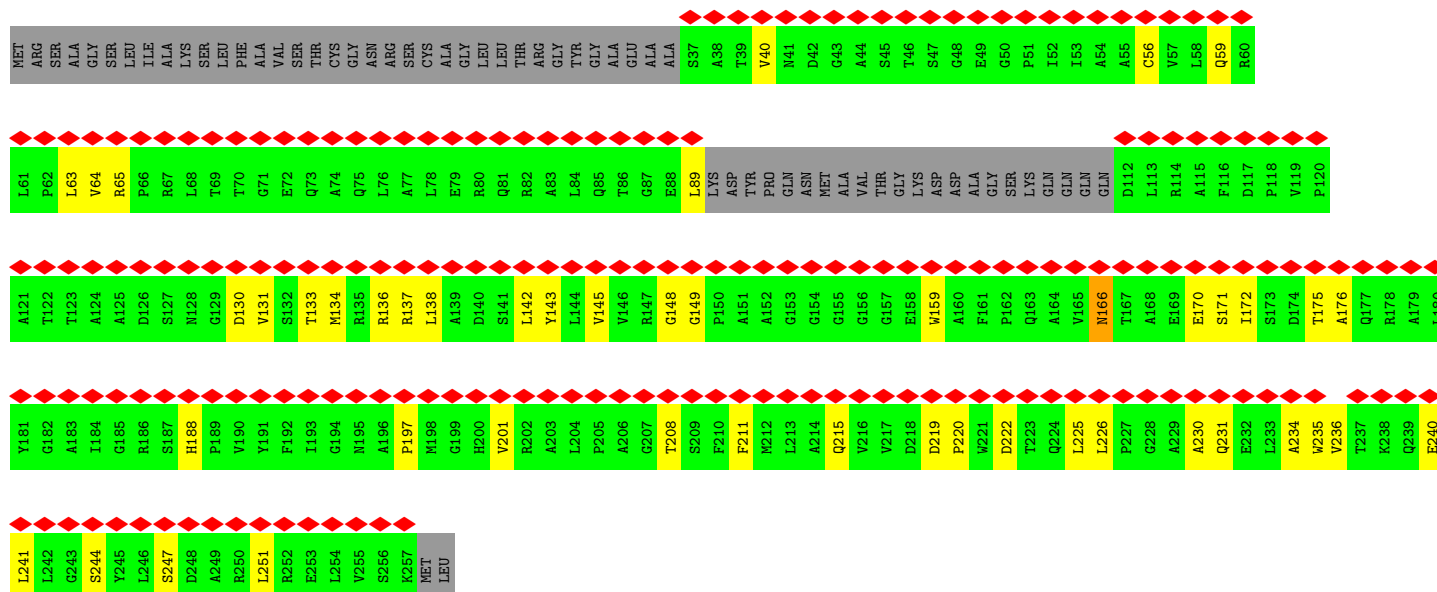
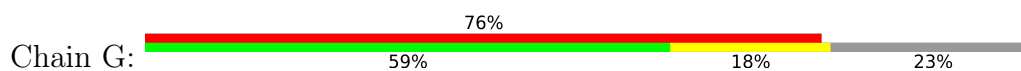
• Molecule 28: mL41



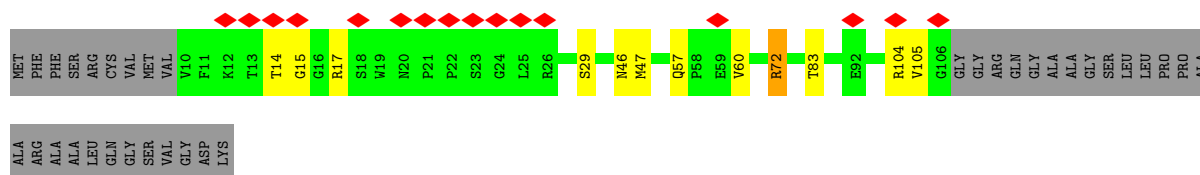
- Molecule 29: mL43



- Molecule 30: Mitochondrial ribosomal protein L17

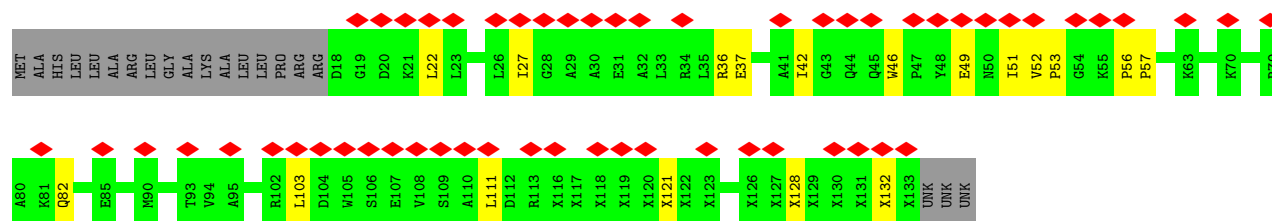


- Molecule 31: mL63/57/60



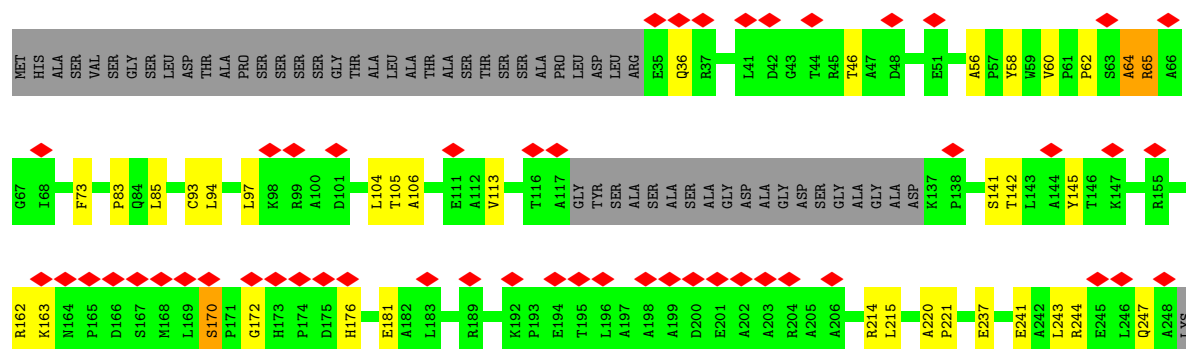
- Molecule 32: mL59/64

Chain J: 



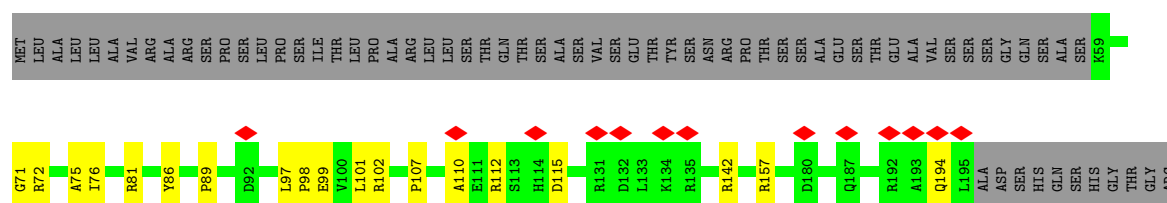
- Molecule 33: mL80

Chain K: 

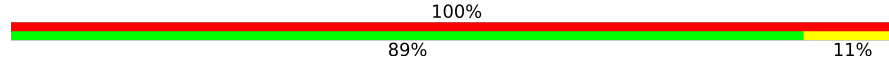


- Molecule 34: mL87

Chain L: 

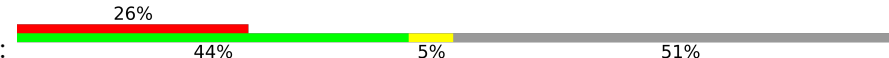


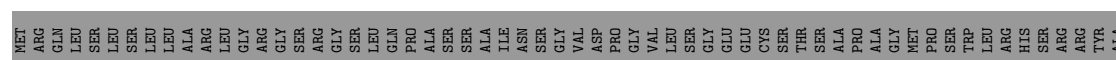
- Molecule 35: bL36m

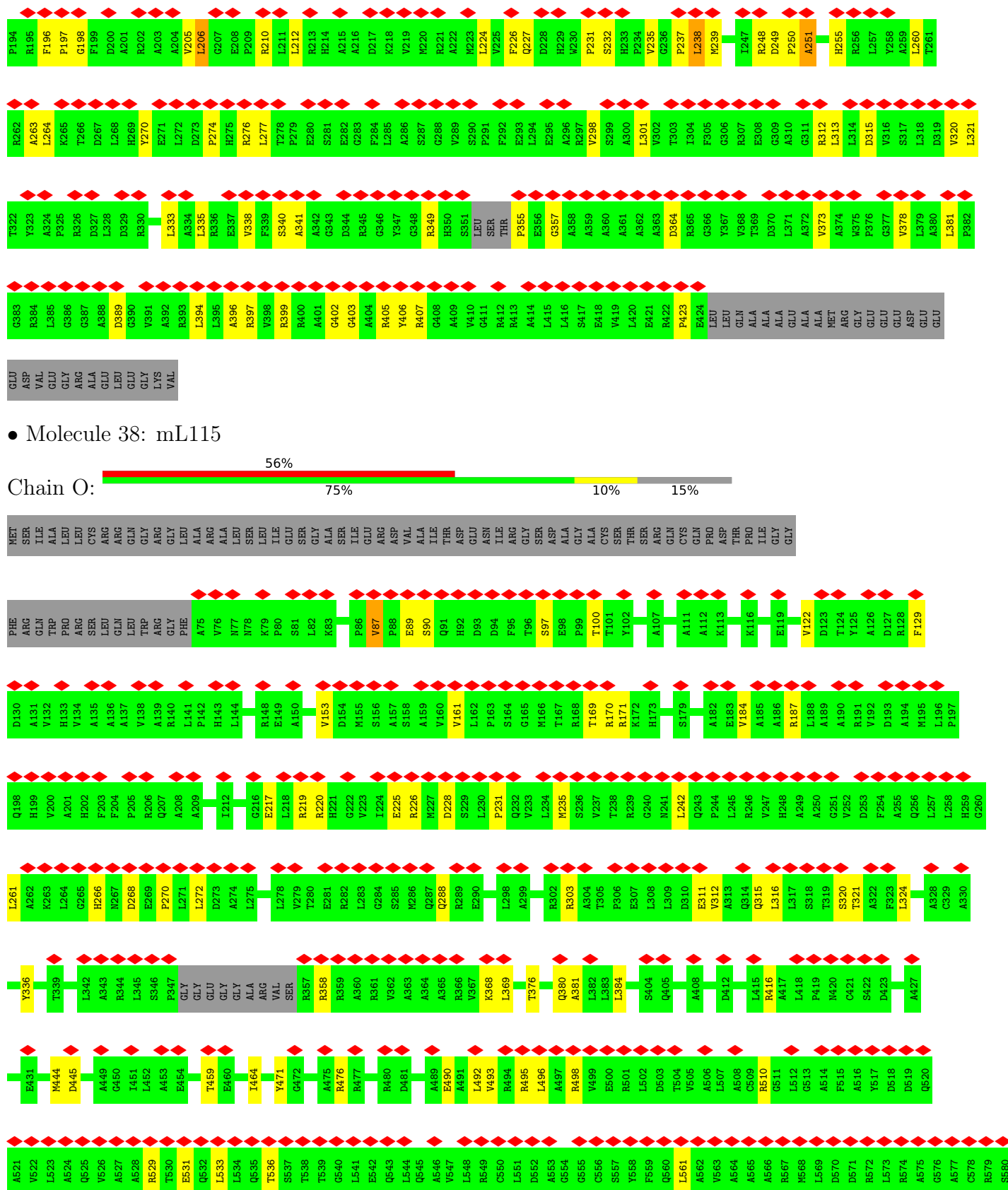
Chain C: 



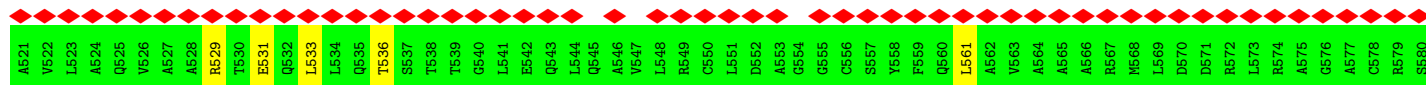
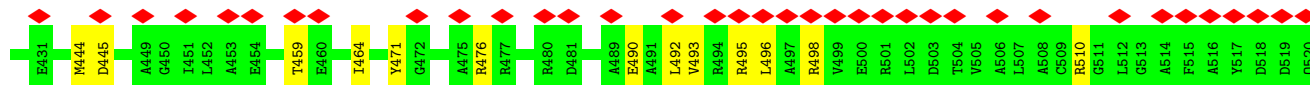
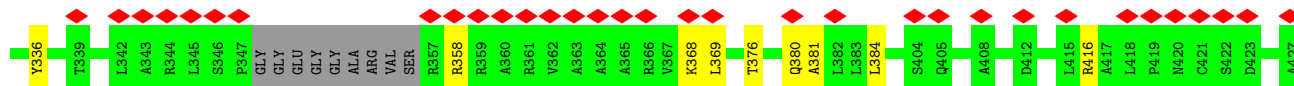
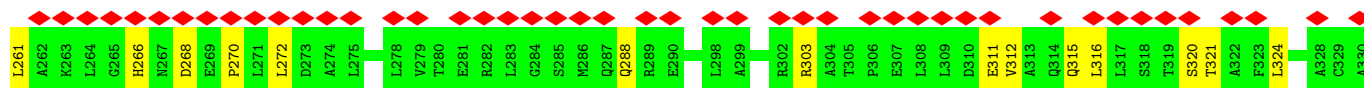
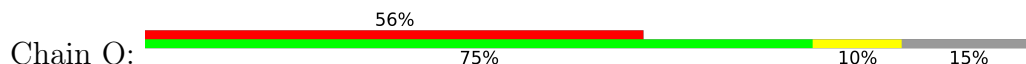
- Molecule 36: mL113

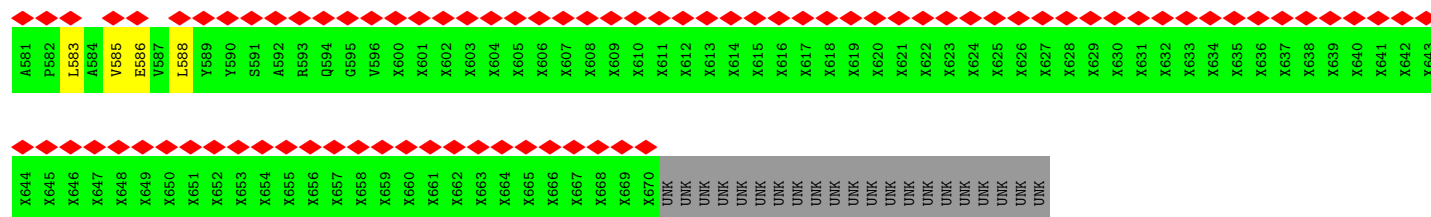
Chain M: 



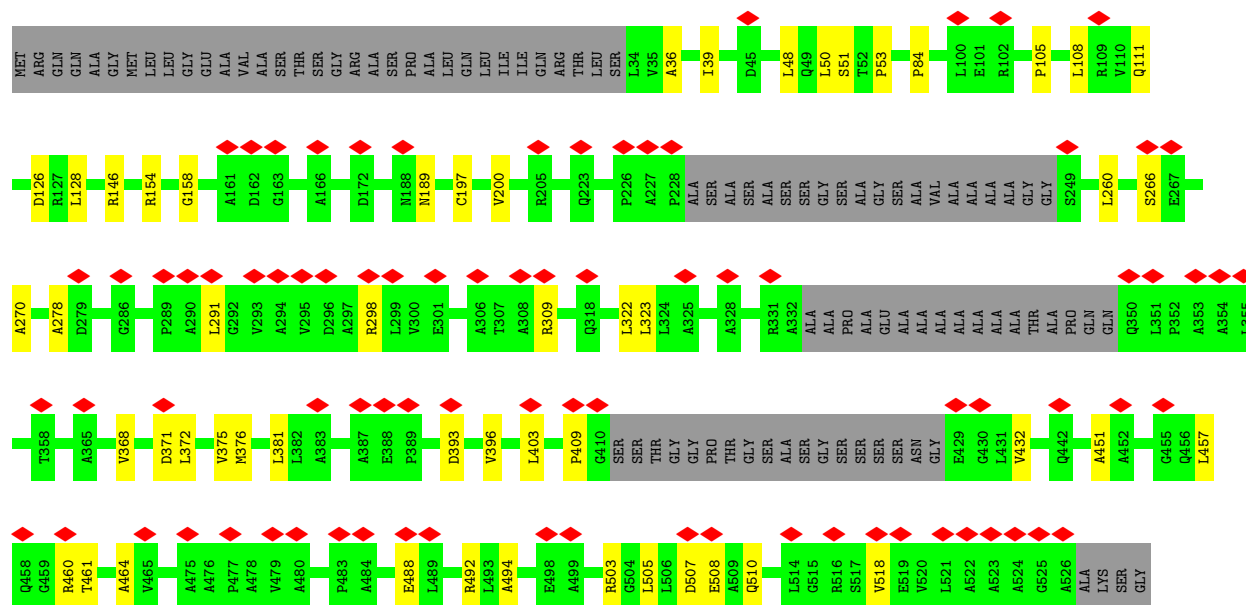


• Molecule 38: mL115

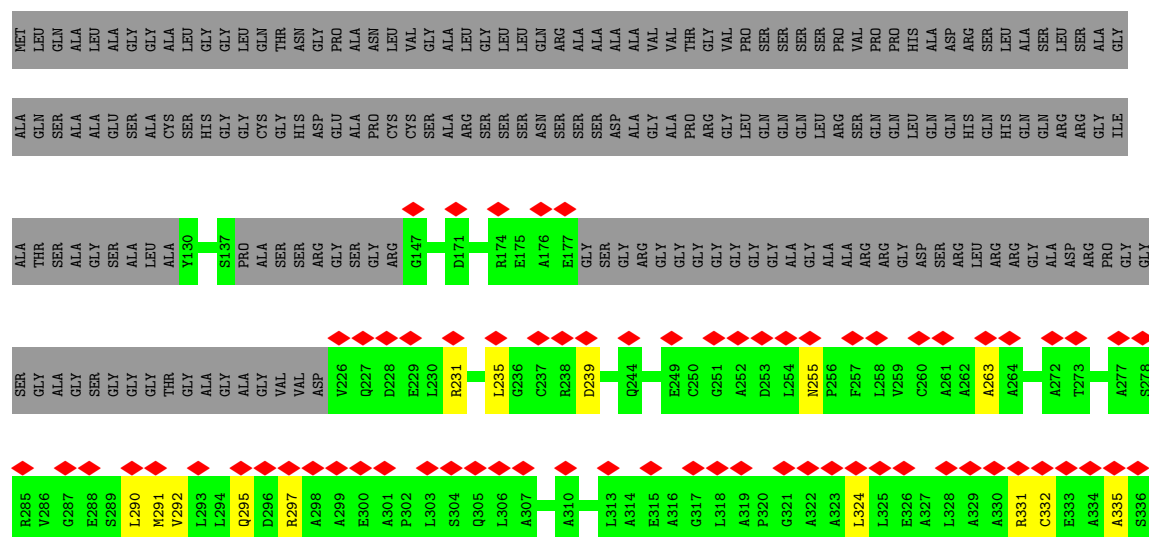


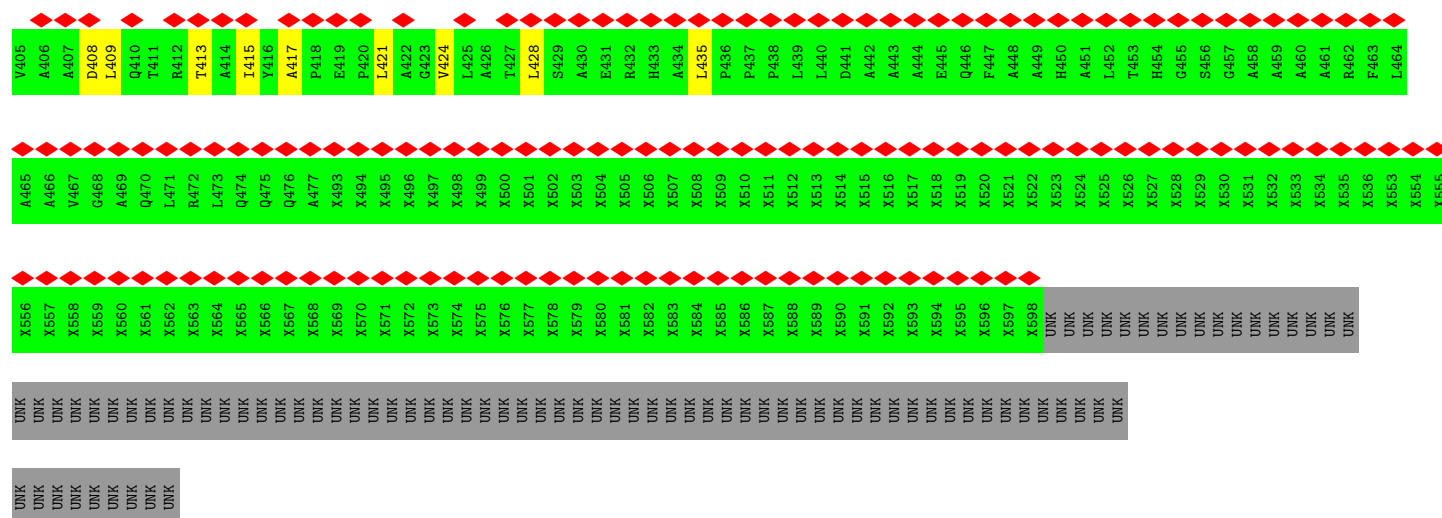


• Molecule 39: mL116

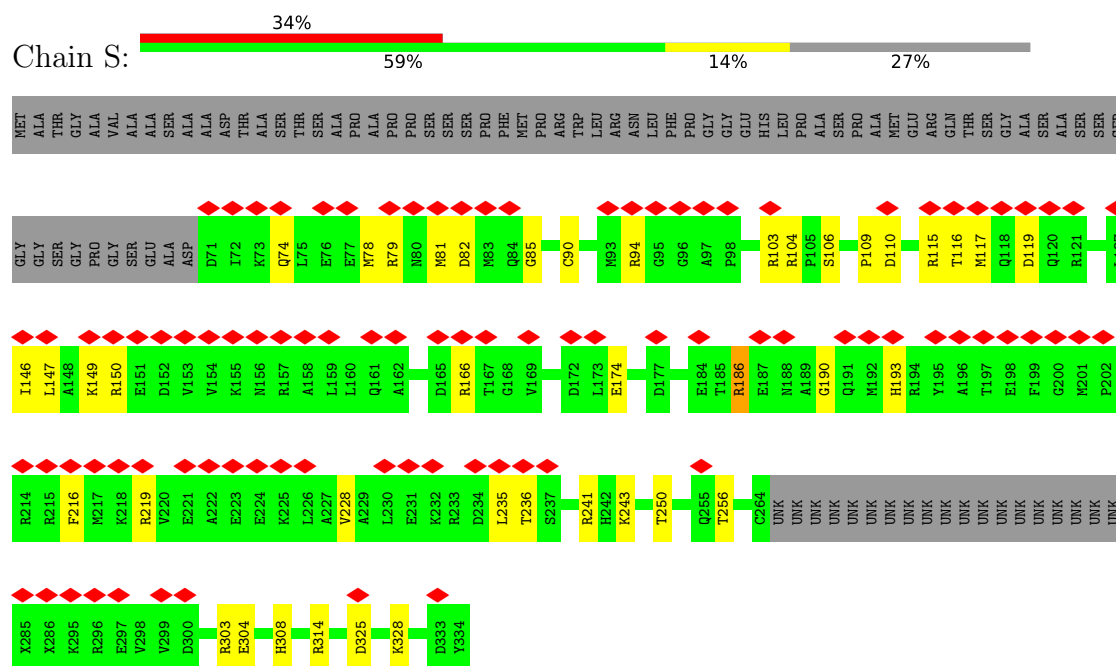


• Molecule 40: mL117

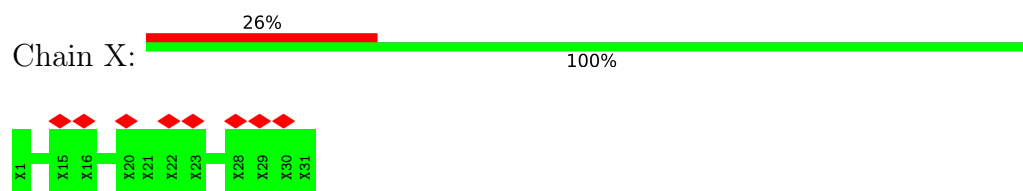




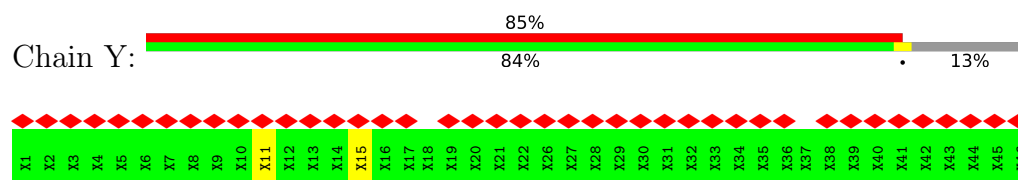
• Molecule 42: mL119

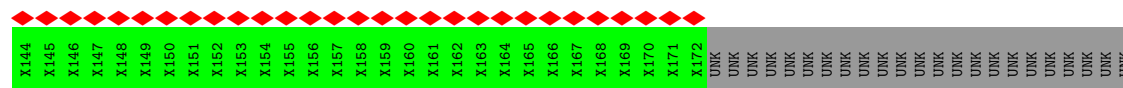
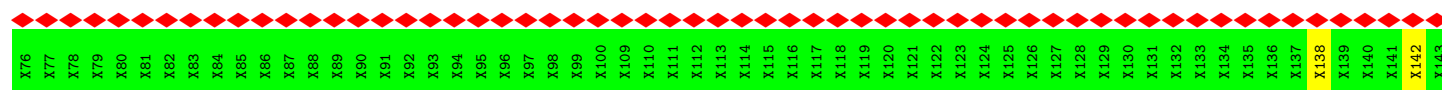


• Molecule 43: Unk1

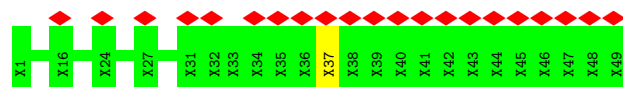


• Molecule 44: PPR*

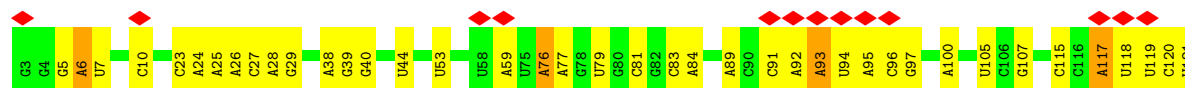




• Molecule 45: Unk2



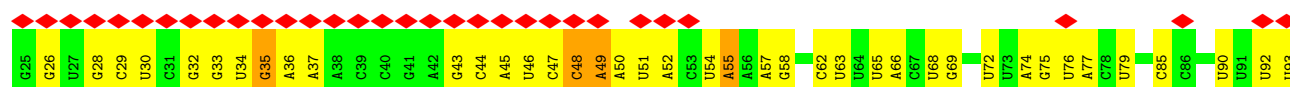
• Molecule 46: L1 rRNA



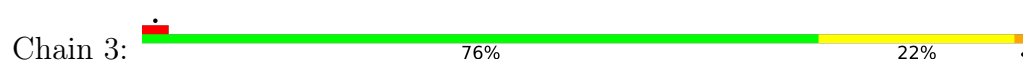
• Molecule 47: L2a rRNA

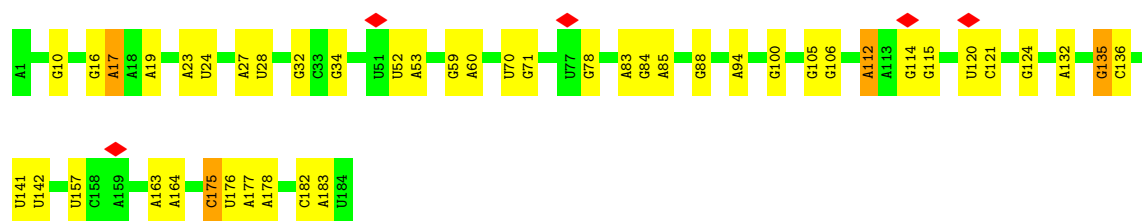


• Molecule 48: L3a rRNA (5S)

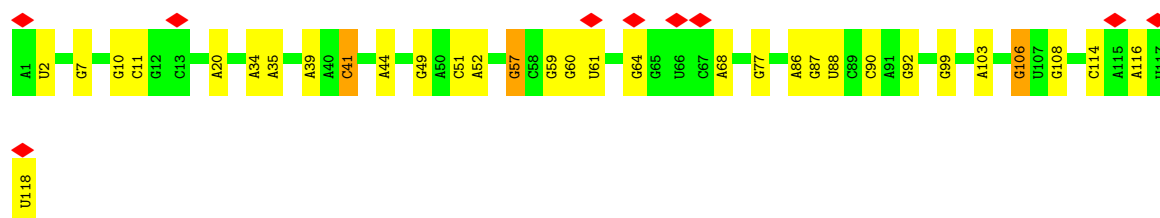
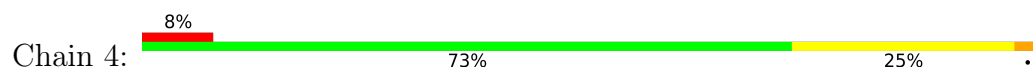


• Molecule 49: L3b rRNA

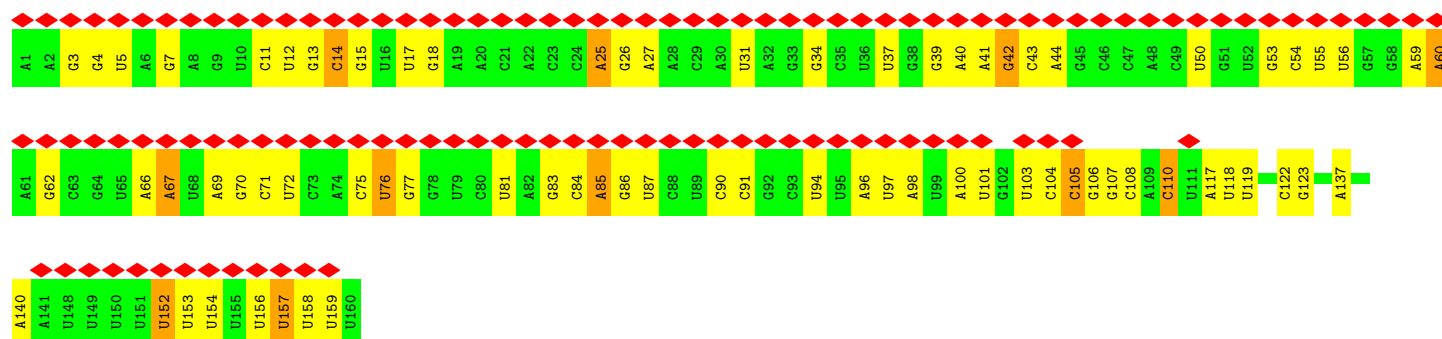
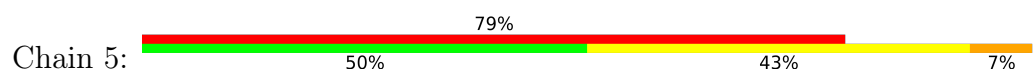




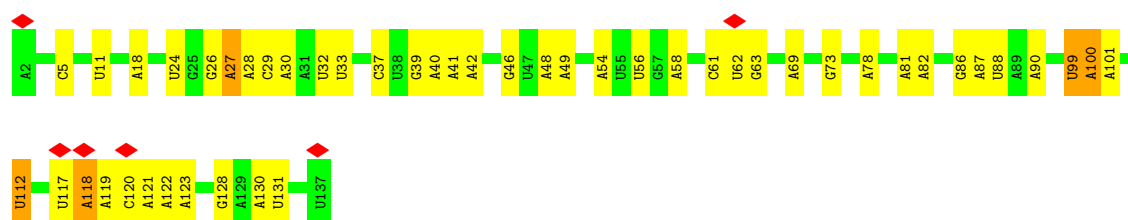
• Molecule 50: L4 rRNA



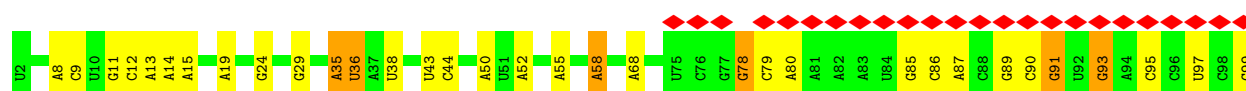
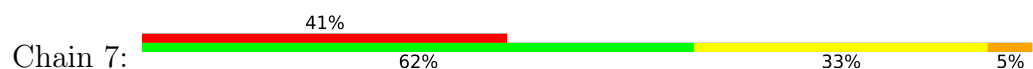
• Molecule 51: L5 rRNA

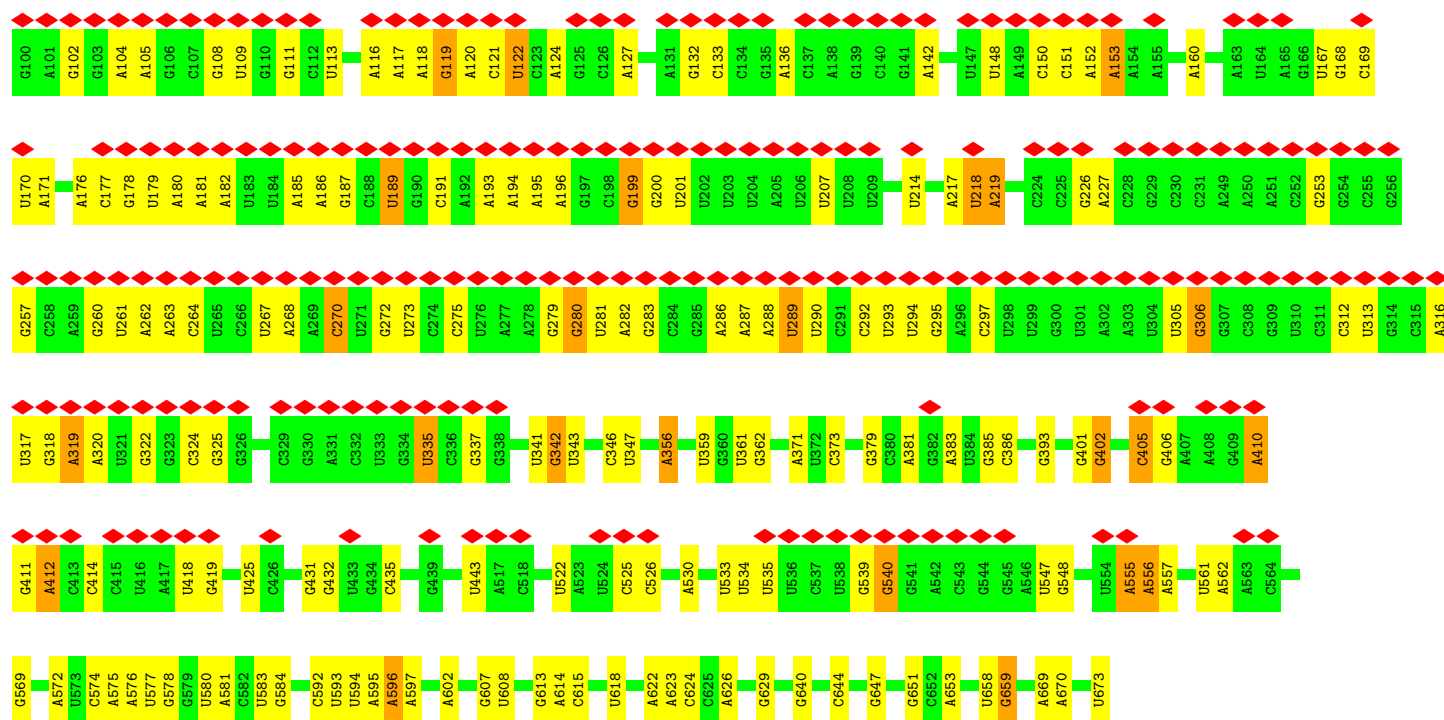


• Molecule 52: L6 rRNA

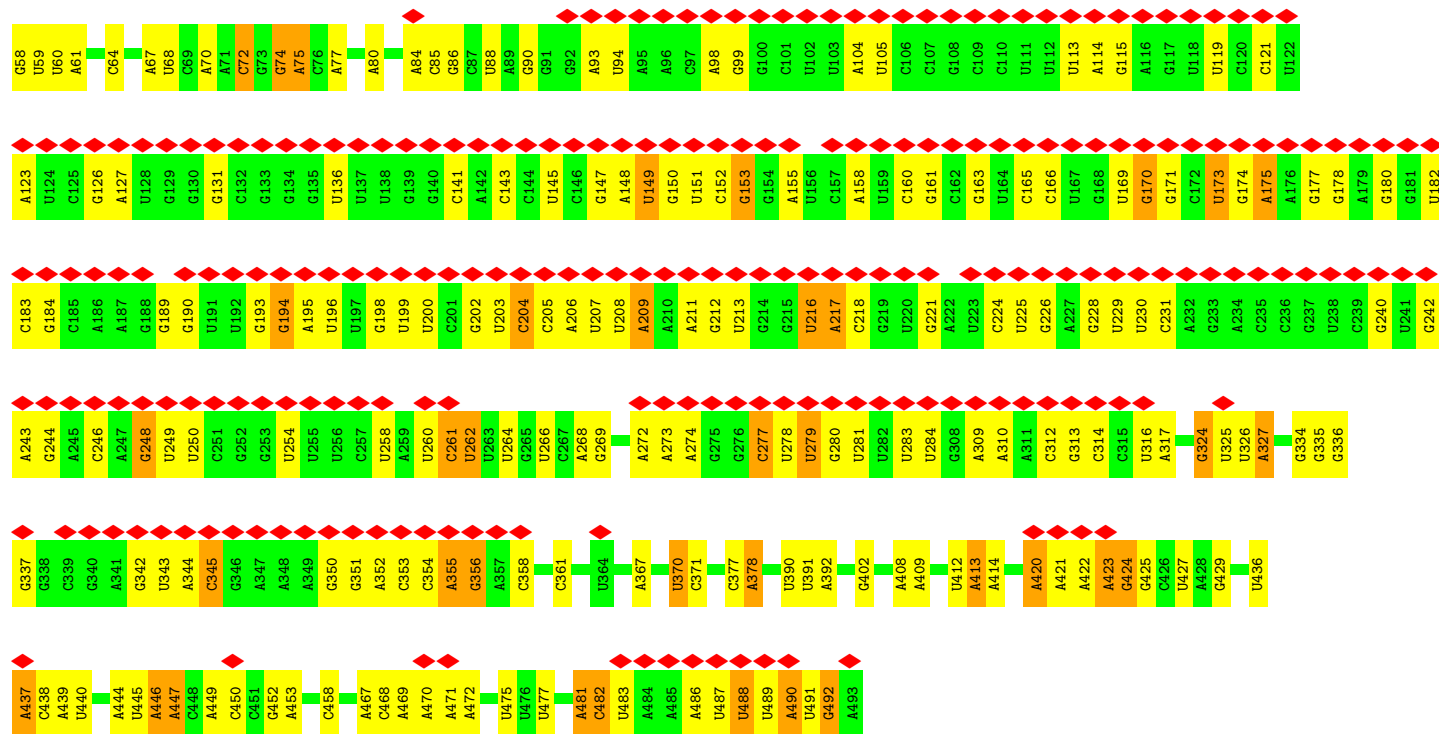


• Molecule 53: L7 rRNA





• Molecule 54: L8 rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	a	0.94	0/2039	1.17	4/2766 (0.1%)
2	b	0.90	0/2397	1.12	6/3264 (0.2%)
3	c	0.90	0/2492	1.18	9/3374 (0.3%)
4	d	0.96	0/1410	1.20	7/1918 (0.4%)
5	f	0.94	0/471	1.20	0/633
6	i	0.25	0/1266	0.55	2/1711 (0.1%)
7	j	0.95	0/959	1.22	2/1284 (0.2%)
8	k	0.87	0/1655	1.15	6/2237 (0.3%)
9	l	0.91	0/1098	1.10	1/1474 (0.1%)
10	m	0.89	1/1488 (0.1%)	1.18	9/2009 (0.4%)
11	n	0.91	1/1440 (0.1%)	1.36	8/1954 (0.4%)
12	o	0.30	0/905	0.55	0/1211
13	p	0.90	1/1640 (0.1%)	1.30	7/2231 (0.3%)
14	q	0.29	0/1300	0.57	0/1754
15	r	0.30	0/1370	0.61	0/1854
16	s	0.90	0/1442	1.18	4/1958 (0.2%)
17	t	0.95	0/1517	1.25	7/2057 (0.3%)
18	u	0.91	0/994	1.27	7/1342 (0.5%)
19	v	0.25	0/1017	0.59	0/1372
20	w	0.87	0/992	1.12	4/1339 (0.3%)
21	x	0.37	1/1434 (0.1%)	0.52	0/1933
22	y	0.95	0/555	1.32	5/748 (0.7%)
23	z	0.29	0/449	0.84	2/600 (0.3%)
24	A	0.28	0/433	0.53	0/575
25	B	0.89	0/1094	1.17	2/1481 (0.1%)
26	e	0.97	0/1254	1.17	2/1692 (0.1%)
27	D	0.24	0/757	0.61	0/1030
28	E	0.85	0/650	1.10	2/877 (0.2%)
29	F	0.30	0/1058	0.58	0/1428
30	G	0.88	0/1509	1.03	1/2054 (0.0%)
31	I	0.29	0/795	0.68	3/1069 (0.3%)
32	J	0.92	0/769	1.16	1/1039 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.89	0/1615	1.09	1/2192 (0.0%)
34	L	0.27	0/1205	0.51	0/1630
36	M	0.86	0/3027	0.99	2/4123 (0.0%)
37	N	0.93	1/2163 (0.0%)	1.15	7/2937 (0.2%)
38	O	0.26	0/3974	0.66	0/5407
39	P	0.28	0/3195	0.65	2/4362 (0.0%)
40	Q	3.89	6/1969 (0.3%)	0.70	3/2668 (0.1%)
41	R	0.25	0/2184	0.62	0/2967
42	S	0.29	0/1947	0.72	3/2603 (0.1%)
46	1	0.29	0/3844	0.48	1/5979 (0.0%)
47	2	0.29	0/2034	0.41	1/3164 (0.0%)
48	0	0.23	0/1779	0.50	0/2768
49	3	0.28	0/4401	0.41	0/6859
50	4	0.31	0/2846	0.42	0/4437
51	5	0.22	0/3522	0.45	0/5477
52	6	0.32	0/3266	0.48	0/5088
53	7	0.22	0/13815	0.41	0/21523
54	8	0.22	0/9830	0.47	0/15312
All	All	0.77	11/105265 (0.0%)	0.77	121/151764 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	k	0	1
13	p	0	1
19	v	0	1
23	z	0	1
29	F	0	1
33	K	0	2
38	O	0	2
40	Q	0	2
42	S	0	1
All	All	0	12

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Q	556	ARG	CZ-NH2	150.95	3.29	1.33
40	Q	608	HIS	CG-ND1	40.82	1.83	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Q	608	HIS	CD2-NE2	39.74	1.81	1.37
40	Q	608	HIS	ND1-CE1	35.10	1.67	1.32
40	Q	608	HIS	CE1-NE2	34.80	1.67	1.32
40	Q	608	HIS	CG-CD2	33.96	1.73	1.35
37	N	355	PRO	N-CD	-8.55	1.35	1.47
21	x	149	VAL	C-N	8.42	1.45	1.33
10	m	76	THR	C-O	-7.95	1.14	1.24
11	n	165	THR	N-CA	5.48	1.50	1.46
13	p	340	ARG	C-O	-5.09	1.17	1.24

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	m	76	THR	CA-C-O	-10.66	109.25	120.55
7	j	107	PRO	CB-CA-C	-9.46	95.96	111.56
22	y	110	PRO	N-CA-C	9.04	121.73	110.70
11	n	157	LYS	N-CA-CB	8.79	125.35	110.49
13	p	265	ARG	CB-CA-C	8.45	123.32	109.46
18	u	124	PRO	N-CA-C	-8.42	97.82	111.21
40	Q	625	PRO	N-CA-CB	8.11	110.50	103.36
11	n	186	ARG	N-CA-C	-8.05	93.65	110.80
8	k	142	GLY	N-CA-C	7.87	122.02	112.49
33	K	64	ALA	CA-C-O	-7.85	112.62	120.70
10	m	75	ARG	N-CA-C	7.77	119.53	111.14
18	u	70	ALA	N-CA-C	-7.63	104.58	114.04
40	Q	556	ARG	NE-CZ-NH1	-7.54	113.96	121.50
3	c	342	ARG	N-CA-CB	-7.50	99.10	110.12
11	n	163	THR	N-CA-C	7.48	119.08	111.07
13	p	266	PRO	CA-N-CD	-7.40	101.65	112.00
8	k	310	PRO	N-CA-C	-7.23	101.88	110.70
37	N	423	PRO	N-CA-CB	7.22	110.20	103.41
4	d	189	MET	N-CA-C	-7.17	104.90	112.93
31	I	105	VAL	N-CA-C	-7.14	105.76	112.83
42	S	235	LEU	CA-C-N	6.99	138.59	125.66
42	S	235	LEU	C-N-CA	6.99	138.59	125.66
10	m	76	THR	CA-CB-OG1	-6.96	99.16	109.60
17	t	299	GLY	N-CA-C	6.87	122.63	110.95
13	p	265	ARG	N-CA-C	-6.81	100.38	109.84
30	G	172	ILE	N-CA-C	6.81	116.93	110.53
37	N	172	LYS	N-CA-C	-6.71	104.11	112.90
20	w	13	CYS	N-CA-C	-6.71	105.65	114.31
11	n	241	VAL	N-CA-C	-6.64	95.52	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	244	VAL	N-CA-C	-6.61	101.69	108.96
20	w	5	VAL	N-CA-C	-6.61	105.20	112.80
16	s	170	ARG	CA-C-O	-6.57	113.60	120.70
10	m	76	THR	CB-CA-C	6.57	121.70	110.79
37	N	403	GLY	CA-C-O	-6.57	113.90	121.00
25	B	133	THR	CA-C-O	-6.50	112.12	119.98
2	b	104	ILE	N-CA-C	-6.46	106.44	112.83
16	s	66	THR	N-CA-C	-6.40	100.95	110.23
17	t	287	LEU	N-CA-C	6.30	117.81	111.07
3	c	341	GLY	N-CA-C	6.25	119.12	111.93
18	u	133	TRP	N-CA-C	-6.19	106.09	113.21
8	k	152	GLN	N-CA-C	-6.19	105.89	113.50
1	a	202	ILE	N-CA-C	-6.17	106.98	112.90
39	P	189	ASN	CA-C-N	6.15	133.28	121.54
39	P	189	ASN	C-N-CA	6.15	133.28	121.54
23	z	19	ALA	CA-C-N	6.13	133.24	121.54
23	z	19	ALA	C-N-CA	6.13	133.24	121.54
28	E	41	GLN	CB-CA-C	6.11	120.05	111.86
13	p	340	ARG	CA-C-O	-6.10	111.79	120.51
28	E	92	LEU	N-CA-C	-6.06	105.72	112.57
13	p	326	SER	N-CA-C	-6.02	105.76	114.12
17	t	297	LYS	N-CA-C	-6.00	104.66	111.14
11	n	180	ARG	N-CA-C	-5.96	99.43	108.67
7	j	107	PRO	CA-C-O	-5.96	109.75	120.60
2	b	94	PRO	N-CA-C	5.93	124.68	112.47
1	a	234	ARG	CB-CG-CD	-5.90	97.72	111.30
36	M	453	PHE	N-CA-C	-5.88	106.65	113.88
10	m	75	ARG	CA-C-O	-5.86	114.67	120.70
2	b	286	ASN	CA-C-O	-5.85	114.53	121.32
22	y	79	TYR	CA-C-O	-5.83	114.12	120.36
1	a	93	ALA	N-CA-C	-5.79	106.35	113.41
13	p	265	ARG	CA-C-O	-5.73	114.21	120.69
6	i	75	HIS	CA-C-N	5.72	132.47	121.54
6	i	75	HIS	C-N-CA	5.72	132.47	121.54
17	t	123	SER	N-CA-C	5.70	117.17	111.07
40	Q	556	ARG	N-CA-C	5.68	119.96	112.35
36	M	478	LEU	N-CA-C	-5.63	106.39	113.20
31	I	72	ARG	CA-CB-CG	5.62	125.34	114.10
3	c	92	ALA	N-CA-C	-5.60	105.80	113.30
3	c	348	LEU	CA-C-O	-5.57	115.06	121.47
26	e	37	PRO	N-CA-C	-5.54	101.17	111.03
3	c	338	GLY	CA-C-O	-5.53	116.95	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	n	157	LYS	CB-CA-C	-5.53	99.42	110.42
10	m	164	VAL	N-CA-C	-5.49	107.44	113.43
18	u	68	ALA	N-CA-C	-5.49	103.45	110.53
3	c	336	ASP	CA-CB-CG	5.47	118.07	112.60
37	N	355	PRO	CA-N-CD	5.46	119.64	112.00
22	y	104	VAL	CA-C-N	-5.44	112.85	122.26
22	y	104	VAL	C-N-CA	-5.44	112.85	122.26
31	I	60	VAL	CA-CB-CG1	5.43	119.63	110.40
17	t	285	ARG	CB-CA-C	5.40	118.15	109.07
1	a	246	GLN	CA-C-O	-5.40	115.11	121.16
26	e	36	VAL	N-CA-C	5.40	120.55	108.88
10	m	78	ARG	N-CA-C	-5.39	105.49	111.36
3	c	253	PRO	N-CA-C	-5.38	102.69	111.68
3	c	356	VAL	N-CA-C	-5.37	107.58	113.43
37	N	251	ALA	N-CA-C	-5.36	106.87	113.41
25	B	134	GLY	N-CA-C	5.36	119.88	112.37
18	u	122	PRO	N-CA-C	-5.31	103.73	111.33
8	k	183	GLU	N-CA-CB	5.29	119.39	114.10
18	u	128	ASP	N-CA-C	-5.29	105.52	111.28
2	b	387	PRO	N-CD-CG	-5.28	95.28	103.20
20	w	11	LEU	N-CA-C	-5.28	105.53	111.28
10	m	79	GLU	CB-CA-C	5.26	119.83	109.72
37	N	156	LEU	N-CA-C	5.26	115.64	109.60
10	m	76	THR	N-CA-C	5.25	117.00	111.28
16	s	133	PRO	N-CA-CB	-5.24	97.75	103.25
8	k	284	ARG	CA-C-O	-5.22	115.89	122.63
13	p	331	GLU	CA-C-O	-5.22	115.45	122.44
4	d	188	GLY	N-CA-C	-5.22	107.43	115.73
4	d	107	PRO	N-CA-C	5.19	117.03	110.70
42	S	149	LYS	CA-CB-CG	-5.18	103.74	114.10
11	n	156	PRO	CB-CA-C	-5.17	104.09	112.62
16	s	167	ASN	CA-C-O	-5.16	115.40	120.82
17	t	307	THR	CB-CA-C	5.14	120.01	112.09
18	u	120	TYR	N-CA-C	-5.14	106.78	113.16
46	l	177	C	P-O3'-C3'	5.13	127.89	120.20
3	c	348	LEU	N-CA-C	-5.10	102.93	110.48
17	t	199	GLY	N-CA-C	-5.09	101.10	113.18
47	2	81	U	P-O3'-C3'	5.09	127.84	120.20
4	d	111	VAL	CB-CA-C	5.09	115.07	110.13
37	N	173	GLY	N-CA-C	-5.09	101.12	113.18
4	d	193	VAL	N-CA-C	-5.08	108.02	112.90
4	d	97	PRO	N-CA-C	5.07	120.20	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	n	157	LYS	CA-CB-CG	5.07	124.24	114.10
20	w	67	ALA	N-CA-C	-5.07	107.22	113.41
4	d	136	PRO	N-CA-C	-5.05	106.63	113.40
2	b	286	ASN	CB-CA-C	-5.04	102.79	111.45
2	b	128	LEU	N-CA-C	5.02	117.79	109.46
22	y	105	GLU	CB-CA-C	5.02	118.38	109.65
8	k	184	VAL	N-CA-C	-5.00	106.21	113.07
32	J	56	PRO	N-CA-C	-5.00	105.23	110.58

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	F	97	TYR	Peptide
33	K	170	SER	Mainchain
33	K	64	ALA	Mainchain
38	O	87	VAL	Peptide
38	O	90	SER	Peptide
40	Q	556	ARG	Sidechain
40	Q	741	UNK	Peptide
42	S	186	ARG	Sidechain
8	k	290	LEU	Mainchain
13	p	265	ARG	Mainchain
19	v	99	PRO	Peptide
23	z	19	ALA	Peptide

5.2 Too-close contacts [i](#)

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	a	1993	0	2022	37	0
2	b	2325	0	2347	50	0
3	c	2497	0	2500	31	0
4	d	1382	0	1437	31	0
5	f	464	0	482	11	0
6	i	1234	0	1264	13	0
7	j	941	0	989	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	k	1620	0	1647	23	0
9	l	1079	0	1163	23	0
10	m	1459	0	1511	18	0
11	n	1406	0	1454	42	0
12	o	890	0	944	6	0
13	p	1606	0	1671	28	0
14	q	1270	0	1276	16	0
15	r	1335	0	1354	17	0
16	s	1565	0	1469	26	0
17	t	1489	0	1551	26	0
18	u	1007	0	1027	36	0
19	v	997	0	1035	13	0
20	w	974	0	1001	25	0
21	x	1397	0	1414	14	0
22	y	542	0	536	11	0
23	z	439	0	475	8	0
24	A	427	0	450	5	0
25	B	1058	0	1043	23	0
26	e	1238	0	1323	20	0
27	D	740	0	747	18	0
28	E	636	0	655	12	0
29	F	1036	0	1044	14	0
30	G	1482	0	1466	33	0
31	I	780	0	817	11	0
32	J	842	0	784	12	0
33	K	1571	0	1559	24	0
34	L	1167	0	1131	13	0
35	C	180	0	39	2	0
36	M	3152	0	3059	29	0
37	N	2116	0	2091	46	0
38	O	4260	0	4067	42	0
39	P	3151	0	3314	38	0
40	Q	3073	0	2217	42	0
41	R	2594	0	2291	38	0
42	S	1967	0	1931	29	0
43	X	155	0	35	0	0
44	Y	745	0	164	2	0
45	Z	245	0	51	1	0
46	1	3440	0	1740	21	0
47	2	1821	0	916	14	0
48	0	1592	0	805	12	0
49	3	3933	0	1980	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	4	2538	0	1277	13	0
51	5	3156	0	1598	16	0
52	6	2913	0	1467	20	0
53	7	12344	0	6227	73	0
54	8	8792	0	4436	72	0
55	y	1	0	0	0	0
56	0	1	0	0	0	0
56	1	6	0	0	0	0
56	2	7	0	0	0	0
56	3	12	0	0	0	0
56	4	8	0	0	0	0
56	5	3	0	0	0	0
56	6	6	0	0	0	0
56	7	18	0	0	0	0
56	8	7	0	0	0	0
56	Q	1	0	0	0	0
57	S	4	0	0	0	0
All	All	103129	0	81293	1015	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 6.

All (1015) 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)
40:Q:608:HIS:CE1	40:Q:608:HIS:ND1	1.67	1.59
40:Q:608:HIS:CD2	40:Q:608:HIS:NE2	1.81	1.48
40:Q:608:HIS:ND1	40:Q:608:HIS:CG	1.83	1.46
40:Q:556:ARG:NH2	40:Q:608:HIS:CE1	2.12	1.18
40:Q:556:ARG:NH2	40:Q:608:HIS:CG	2.15	1.14
1:a:74:LEU:CD2	1:a:277:LEU:HD22	1.75	1.13
40:Q:556:ARG:NH2	40:Q:608:HIS:CD2	2.17	1.13
40:Q:556:ARG:CZ	40:Q:608:HIS:CE1	2.32	1.11
20:w:11:LEU:CD1	20:w:14:VAL:HG13	1.81	1.11
1:a:74:LEU:HD21	1:a:277:LEU:HD22	1.33	1.09
20:w:11:LEU:HD13	20:w:14:VAL:HG13	1.10	1.08
40:Q:556:ARG:CZ	40:Q:608:HIS:CD2	2.37	1.07
52:6:26:G:N1	52:6:49:A:C2	2.21	1.07
40:Q:556:ARG:NH2	40:Q:608:HIS:ND1	2.04	1.05
52:6:26:G:N1	52:6:49:A:H2	1.54	1.05
40:Q:556:ARG:CZ	40:Q:608:HIS:CG	2.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:w:11:LEU:HD13	20:w:14:VAL:CG1	1.86	1.04
20:w:11:LEU:CD1	20:w:14:VAL:CG1	2.37	1.02
40:Q:556:ARG:NH2	40:Q:608:HIS:NE2	2.06	1.02
18:u:121:PHE:CZ	25:B:47:VAL:HG21	1.94	1.02
18:u:121:PHE:HZ	25:B:47:VAL:HG21	1.20	1.01
40:Q:556:ARG:CZ	40:Q:608:HIS:ND1	2.26	0.97
54:8:153:G:H1	54:8:225:U:H3	1.06	0.96
40:Q:556:ARG:CZ	40:Q:608:HIS:NE2	2.30	0.95
7:j:118:ARG:HG2	11:n:305:GLN:HG3	1.50	0.94
13:p:197:CYS:SG	13:p:238:LEU:HD23	2.07	0.93
3:c:337:SER:HA	3:c:386:ARG:HH22	1.36	0.90
53:7:189:U:H3	53:7:199:G:H1	0.95	0.90
11:n:142:LEU:HD11	41:R:300:LEU:HB2	1.53	0.89
54:8:171:G:H1	54:8:182:U:H3	1.21	0.88
53:7:257:G:H1	53:7:273:U:H3	0.92	0.88
18:u:124:PRO:HD3	39:P:51:SER:HB2	1.55	0.87
20:w:11:LEU:HD12	20:w:14:VAL:HG11	1.55	0.86
5:f:133:ARG:NE	53:7:443:U:O3'	2.09	0.85
2:b:295:LYS:HA	54:8:264:U:H5''	1.59	0.82
50:4:114:C:H42	51:5:117:A:H2	1.26	0.81
27:D:37:VAL:HG11	32:J:111:LEU:HD23	1.63	0.80
18:u:119:LEU:HB3	18:u:121:PHE:HD2	1.43	0.80
17:t:294:GLY:HA3	17:t:329:ASP:HA	1.62	0.80
37:N:205:VAL:HG21	37:N:212:LEU:HD11	1.62	0.79
54:8:114:A:H62	54:8:126:G:H21	1.28	0.79
52:6:26:G:H1	52:6:49:A:H2	0.80	0.79
37:N:205:VAL:CG2	37:N:212:LEU:HD11	2.14	0.77
32:J:52:VAL:HG23	32:J:53:PRO:HD3	1.66	0.76
20:w:11:LEU:HD12	20:w:14:VAL:CG1	2.10	0.75
4:d:127:LYS:HD3	4:d:131:ASP:HA	1.70	0.74
54:8:173:U:H3	54:8:180:G:H1	1.33	0.73
4:d:41:LEU:HD11	4:d:164:PRO:HD2	1.69	0.73
30:G:142:LEU:HD23	30:G:235:TRP:HB3	1.71	0.73
37:N:394:LEU:HD22	53:7:185:A:H5''	1.70	0.73
13:p:266:PRO:HG2	21:x:84:PRO:HA	1.72	0.72
1:a:116:ARG:HH12	49:3:32:G:H21	1.39	0.71
37:N:338:VAL:HG21	37:N:389:ASP:HB3	1.72	0.71
18:u:121:PHE:CE1	25:B:99:TYR:HA	2.25	0.71
10:m:89:LEU:HD22	10:m:159:LEU:HD11	1.71	0.71
50:4:114:C:N3	51:5:117:A:N1	2.39	0.71
2:b:95:LYS:HG2	2:b:97:ARG:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:8:114:A:H62	54:8:126:G:N2	1.88	0.70
18:u:119:LEU:HB3	18:u:121:PHE:CD2	2.26	0.70
7:j:107:PRO:O	7:j:108:ARG:HG2	1.92	0.69
2:b:262:ARG:HH22	54:8:266:U:H5'	1.58	0.69
2:b:164:VAL:HB	11:n:192:MET:HE1	1.75	0.68
29:F:95:GLN:NE2	52:6:40:A:N7	2.43	0.67
52:6:26:G:O6	52:6:49:A:N1	2.28	0.67
16:s:43:ILE:HG12	16:s:52:VAL:HG22	1.77	0.67
33:K:94:LEU:HD22	36:M:66:ILE:HD13	1.77	0.66
16:s:75:VAL:HG13	42:S:174:GLU:HG3	1.77	0.66
4:d:75:LEU:HD12	4:d:83:ALA:HB1	1.78	0.66
16:s:91:ASP:HB3	16:s:98:MET:HG2	1.78	0.66
25:B:117:ARG:HB3	53:7:673:U:H5''	1.77	0.66
27:D:87:ALA:HB1	30:G:197:PRO:HG2	1.78	0.66
39:P:510:GLN:HE21	47:2:86:U:H3	1.44	0.66
42:S:90:CYS:O	42:S:94:ARG:HB3	1.95	0.66
37:N:175:LEU:HD12	37:N:176:PRO:HD2	1.76	0.66
11:n:255:VAL:HA	11:n:261:GLY:HA2	1.77	0.66
48:0:48:C:H2'	48:0:49:A:H2'	1.78	0.66
38:O:235:MET:HE1	38:O:261:LEU:HD21	1.79	0.65
32:J:42:ILE:HG21	38:O:416:ARG:HD2	1.78	0.65
37:N:263:ALA:HB1	37:N:298:VAL:HG21	1.77	0.65
40:Q:624:GLY:HA2	40:Q:628:PHE:HD2	1.61	0.65
17:t:212:PRO:HD2	45:Z:37:UNK:HA	1.79	0.65
4:d:16:THR:HG23	4:d:175:GLU:HB2	1.78	0.65
2:b:377:ASP:HA	11:n:158:LEU:HD22	1.79	0.65
7:j:95:LYS:HA	7:j:115:LEU:HG	1.79	0.65
14:q:299:THR:HB	14:q:332:VAL:HB	1.79	0.64
9:l:146:PHE:HB3	50:4:57:G:H5'	1.80	0.64
4:d:187:GLY:HA2	4:d:191:LEU:HB3	1.79	0.64
15:r:135:TRP:CD1	28:E:44:ILE:HG13	2.31	0.64
25:B:118:VAL:HG22	53:7:673:U:H5'	1.80	0.64
18:u:124:PRO:HD3	39:P:51:SER:CB	2.27	0.64
38:O:226:ARG:HD2	38:O:228:ASP:H	1.62	0.64
53:7:261:U:H3	53:7:270:C:H42	1.46	0.64
18:u:134:LEU:HD11	25:B:77:LYS:HG2	1.80	0.63
13:p:148:ARG:HG3	39:P:368:VAL:HG11	1.81	0.63
52:6:26:G:C6	52:6:49:A:N1	2.66	0.63
9:l:135:CYS:HB3	9:l:179:ALA:HB1	1.81	0.63
11:n:160:GLN:HG3	11:n:198:GLU:HG3	1.79	0.63
36:M:372:ARG:HH22	36:M:374:ILE:HD13	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:t:287:LEU:HD12	17:t:322:GLU:HG2	1.81	0.63
8:k:247:CYS:HB3	8:k:252:ARG:HH21	1.63	0.62
40:Q:335:ALA:HA	40:Q:338:ARG:HD3	1.80	0.62
47:2:43:A:H62	52:6:58:A:H2	1.45	0.62
2:b:346:LEU:HD11	54:8:420:A:H5''	1.81	0.62
5:f:133:ARG:HE	53:7:443:U:H4'	1.62	0.62
21:x:165:LEU:HD13	21:x:209:ARG:HE	1.64	0.62
27:D:96:ARG:HB3	27:D:100:MET:HE2	1.80	0.62
34:L:102:ARG:NH2	34:L:115:ASP:OD2	2.33	0.62
8:k:178:GLN:OE1	18:u:125:ARG:NH2	2.33	0.62
4:d:18:ILE:HG22	4:d:76:ASP:HB2	1.80	0.62
53:7:187:G:H1	53:7:201:U:H3	1.47	0.62
5:f:104:PRO:HD2	5:f:128:ARG:HH22	1.64	0.61
11:n:214:ALA:HB2	11:n:241:VAL:HG23	1.80	0.61
1:a:167:LEU:HD11	1:a:179:TYR:HB3	1.82	0.61
2:b:378:VAL:HG13	11:n:158:LEU:HD11	1.81	0.61
4:d:22:ILE:HD11	4:d:166:ARG:HB3	1.82	0.61
34:L:71:GLY:HA2	34:L:89:PRO:HG3	1.82	0.61
2:b:258:GLY:HA2	2:b:300:PRO:HB3	1.81	0.61
30:G:133:THR:H	30:G:136:ARG:HH12	1.46	0.61
51:5:152:U:H5'	51:5:153:U:H5'	1.82	0.61
31:I:17:ARG:HE	50:4:87:G:H22	1.48	0.61
7:j:41:VAL:HG22	7:j:55:MET:HG2	1.81	0.61
7:j:98:SER:HB3	7:j:117:LYS:HB2	1.83	0.61
42:S:303:ARG:HH22	53:7:361:U:H5''	1.66	0.61
2:b:101:PRO:HG2	2:b:105:ALA:HB2	1.83	0.60
8:k:289:PRO:HD2	8:k:309:ILE:HG21	1.81	0.60
52:6:26:G:C2	52:6:49:A:H2	2.17	0.60
3:c:337:SER:HB2	3:c:341:GLY:HA3	1.84	0.60
12:o:83:ARG:NH2	51:5:122:C:OP1	2.34	0.60
42:S:143:SER:HA	42:S:146:ILE:HG12	1.83	0.60
44:Y:138:UNK:O	44:Y:142:UNK:N	2.34	0.60
10:m:133:LEU:HD11	10:m:154:ARG:HG3	1.84	0.60
18:u:114:PRO:HB3	25:B:53:ILE:HG21	1.83	0.60
21:x:10:VAL:HG13	21:x:67:THR:HG23	1.84	0.60
36:M:240:LEU:HA	36:M:243:VAL:HG12	1.84	0.60
9:l:155:ILE:HG22	17:t:259:ALA:H	1.67	0.60
12:o:49:ARG:NH1	51:5:123:G:OP2	2.34	0.60
17:t:273:PRO:HD2	17:t:276:ARG:HE	1.66	0.60
42:S:147:LEU:HA	42:S:150:ARG:HG2	1.83	0.60
48:0:34:U:H2'	48:0:35:G:H2'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:172:PRO:HG2	1:a:175:GLN:HB2	1.84	0.60
16:s:166:ARG:HG3	16:s:177:PRO:HB2	1.84	0.60
37:N:394:LEU:HA	37:N:397:ARG:HB3	1.81	0.60
18:u:122:PRO:HA	39:P:53:PRO:HD3	1.82	0.60
54:8:261:C:O2'	54:8:262:U:O2	2.16	0.59
11:n:224:VAL:HG12	11:n:227:ALA:H	1.66	0.59
38:O:219:ARG:HG3	38:O:225:GLU:HA	1.84	0.59
16:s:164:ARG:NH1	16:s:178:ASP:OD1	2.34	0.59
30:G:149:GLY:HA2	30:G:231:GLN:HB2	1.84	0.59
40:Q:608:HIS:CE1	40:Q:608:HIS:CD2	2.90	0.59
4:d:59:PRO:HG3	4:d:69:THR:HG22	1.85	0.59
20:w:111:GLU:HB2	20:w:116:LEU:HB3	1.85	0.59
54:8:160:C:H2'	54:8:161:G:H8	1.68	0.59
2:b:286:ASN:HB2	2:b:290:PRO:HG2	1.84	0.59
23:z:20:LYS:HG3	32:J:82:GLN:HG3	1.83	0.59
39:P:371:ASP:OD1	39:P:372:LEU:N	2.34	0.59
7:j:106:LYS:N	7:j:107:PRO:HD3	2.18	0.59
12:o:78:ASN:O	13:p:266:PRO:HD3	2.03	0.59
39:P:461:THR:HA	39:P:464:ALA:HB3	1.84	0.59
8:k:175:VAL:HG21	25:B:126:VAL:HG11	1.84	0.59
38:O:268:ASP:HB3	38:O:270:PRO:HD2	1.85	0.59
19:v:106:ASN:OD1	38:O:100:THR:OG1	2.20	0.58
19:v:28:ARG:NH1	38:O:97:SER:OG	2.37	0.58
6:i:148:PRO:O	29:F:128:ASN:ND2	2.36	0.58
38:O:498:ARG:HH22	46:1:93:A:H5'	1.68	0.58
7:j:17:LYS:HG3	7:j:46:ARG:HG2	1.85	0.58
13:p:220:LEU:HD21	13:p:249:LEU:HD22	1.86	0.58
23:z:29:LYS:NZ	23:z:55:GLU:OE1	2.34	0.58
38:O:493:VAL:HA	38:O:496:LEU:HD23	1.85	0.58
48:O:68:U:O2'	50:4:20:A:N3	2.36	0.58
25:B:118:VAL:HG23	25:B:119:GLU:H	1.69	0.58
16:s:68:THR:HB	16:s:70:PRO:HD2	1.84	0.58
54:8:277:C:O2'	54:8:313:G:N2	2.37	0.58
33:K:142:THR:HG23	33:K:145:TYR:H	1.68	0.58
40:Q:608:HIS:CE1	40:Q:608:HIS:CG	2.92	0.58
1:a:79:PRO:HA	1:a:85:ARG:HA	1.86	0.57
18:u:126:THR:HG22	39:P:48:LEU:HD21	1.86	0.57
42:S:236:THR:HA	42:S:241:ARG:HH21	1.69	0.57
53:7:286:A:N7	53:7:292:C:N4	2.51	0.57
6:i:115:SER:HB2	6:i:128:MET:HE2	1.86	0.57
53:7:414:C:O2'	53:7:540:G:N2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:108:PRO:HA	4:d:130:LEU:HG	1.86	0.57
18:u:119:LEU:CB	18:u:121:PHE:HD2	2.13	0.57
20:w:71:MET:HE3	28:E:44:ILE:HD12	1.87	0.57
18:u:134:LEU:HD11	25:B:77:LYS:CG	2.35	0.57
33:K:65:ARG:HB2	33:K:73:PHE:CZ	2.40	0.57
38:O:459:THR:O	38:O:495:ARG:NH2	2.37	0.57
39:P:403:LEU:O	39:P:492:ARG:NH1	2.38	0.57
37:N:186:PHE:HE1	37:N:205:VAL:HG11	1.70	0.57
38:O:496:LEU:HB3	38:O:529:ARG:HG2	1.87	0.57
41:R:374:ARG:HD3	54:8:492:G:H1'	1.87	0.57
10:m:144:TRP:HB2	41:R:415:ILE:HG21	1.85	0.56
19:v:112:LYS:HG2	19:v:116:MET:HE2	1.85	0.56
26:e:91:GLY:HA2	26:e:94:ARG:HE	1.69	0.56
36:M:91:VAL:O	36:M:95:SER:HB3	2.05	0.56
19:v:95:LEU:HD22	19:v:112:LYS:HB2	1.87	0.56
38:O:217:GLU:OE1	38:O:220:ARG:NH2	2.35	0.56
39:P:323:LEU:HB2	39:P:381:LEU:HD11	1.87	0.56
41:R:267:ASP:OD1	41:R:267:ASP:N	2.38	0.56
53:7:148:U:OP2	53:7:153:A:N6	2.37	0.56
1:a:237:SER:HB2	1:a:276:HIS:HA	1.86	0.56
36:M:497:LEU:O	36:M:501:SER:HB2	2.05	0.56
17:t:310:TYR:HB2	17:t:347:LEU:HA	1.86	0.56
38:O:312:VAL:HG22	38:O:369:LEU:HD22	1.87	0.56
3:c:317:LYS:HA	3:c:358:MET:HE1	1.87	0.56
13:p:329:LEU:HG	13:p:330:PRO:HD2	1.88	0.56
41:R:186:LEU:O	41:R:262:ARG:NH1	2.38	0.56
13:p:235:VAL:HG23	13:p:238:LEU:CD1	2.36	0.56
26:e:114:MET:HE1	26:e:132:VAL:HG12	1.87	0.56
37:N:335:LEU:HG	37:N:381:LEU:CD2	2.36	0.56
53:7:405:C:H2'	54:8:149:U:H3	1.70	0.56
54:8:279:U:O2'	54:8:280:G:N7	2.38	0.56
2:b:95:LYS:HE3	2:b:97:ARG:HG3	1.86	0.56
31:I:72:ARG:NH2	49:3:175:C:N3	2.52	0.56
37:N:312:ARG:HE	37:N:373:VAL:HG21	1.71	0.56
8:k:224:ILE:HB	8:k:276:LEU:HD11	1.88	0.56
13:p:195:THR:HG21	13:p:198:ARG:HE	1.69	0.56
13:p:197:CYS:SG	13:p:238:LEU:CD2	2.91	0.56
48:O:26:G:N2	48:O:46:U:O2	2.39	0.56
18:u:128:ASP:O	18:u:130:GLN:OE1	2.24	0.56
30:G:148:GLY:H	30:G:159:TRP:HA	1.70	0.56
53:7:257:G:O6	53:7:273:U:O4	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:168:GLY:HA2	9:l:240:GLU:HA	1.88	0.55
39:P:432:VAL:HG23	39:P:451:ALA:HB2	1.86	0.55
14:q:233:LEU:HD23	14:q:329:ILE:HD12	1.87	0.55
2:b:287:ARG:HG3	2:b:288:GLN:H	1.71	0.55
17:t:143:VAL:HG12	17:t:269:LEU:HB2	1.87	0.55
50:4:51:C:H2'	50:4:52:A:H8	1.72	0.55
1:a:152:VAL:HG22	1:a:168:VAL:HG22	1.89	0.55
2:b:137:SER:O	2:b:352:ARG:NH2	2.40	0.55
27:D:94:ARG:HG3	30:G:40:VAL:H	1.71	0.55
18:u:1:MET:HG3	18:u:16:LEU:HB3	1.89	0.55
39:P:393:ASP:HA	39:P:396:VAL:HG22	1.89	0.55
41:R:273:LEU:O	41:R:277:HIS:ND1	2.38	0.55
41:R:392:PRO:HB2	41:R:395:ARG:HB3	1.89	0.55
54:8:355:A:H4'	54:8:356:G:H5'	1.88	0.55
4:d:96:LEU:HD22	4:d:192:PRO:HD3	1.89	0.55
38:O:315:GLN:HE21	38:O:369:LEU:HD21	1.71	0.54
4:d:96:LEU:HD22	4:d:192:PRO:CD	2.38	0.54
30:G:222:ASP:HB3	30:G:225:LEU:HD13	1.88	0.54
53:7:555:A:N6	53:7:562:A:OP2	2.41	0.54
10:m:146:ARG:NH2	10:m:152:PRO:O	2.40	0.54
16:s:139:LEU:HD13	28:E:102:GLU:HB3	1.88	0.54
25:B:120:ARG:HG3	25:B:122:ARG:HD3	1.89	0.54
42:S:78:MET:HA	42:S:81:MET:HB3	1.89	0.54
54:8:226:G:OP2	54:8:226:G:N2	2.38	0.54
18:u:118:ALA:HB2	39:P:50:LEU:HD23	1.89	0.54
25:B:34:ASN:OD1	49:3:10:G:O2'	2.25	0.54
32:J:46:TRP:HZ2	32:J:53:PRO:HG2	1.73	0.54
36:M:339:LEU:HD21	36:M:430:HIS:HA	1.88	0.54
37:N:238:LEU:HD11	37:N:274:PRO:HB2	1.90	0.54
42:S:304:GLU:O	42:S:308:HIS:ND1	2.37	0.54
26:e:34:ILE:HG22	26:e:101:VAL:HB	1.89	0.54
37:N:175:LEU:HD13	37:N:212:LEU:HB2	1.90	0.54
8:k:152:GLN:HG3	49:3:135:G:H5''	1.88	0.54
39:P:503:ARG:HB3	39:P:505:LEU:HD13	1.89	0.54
39:P:457:LEU:O	39:P:503:ARG:NH1	2.41	0.54
40:Q:292:VAL:HA	40:Q:295:GLN:HG2	1.90	0.54
40:Q:681:ASP:HA	40:Q:685:LEU:HD13	1.89	0.54
42:S:250:THR:HG21	42:S:282:UNK:HA	1.90	0.54
7:j:106:LYS:H	7:j:107:PRO:HD3	1.72	0.54
9:l:233:ARG:HB2	9:l:236:GLN:HG2	1.90	0.54
30:G:130:ASP:O	30:G:136:ARG:NE	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:248:ARG:HD3	37:N:250:PRO:HD2	1.91	0.53
39:P:376:MET:SD	47:2:86:U:O2'	2.67	0.53
48:0:35:G:O2'	48:0:37:A:N7	2.40	0.53
29:F:34:LEU:HD11	29:F:46:VAL:HG11	1.90	0.53
30:G:201:VAL:H	30:G:208:THR:HG23	1.73	0.53
33:K:214:ARG:NH1	33:K:220:ALA:O	2.40	0.53
3:c:334:LEU:HD12	3:c:352:LEU:HD11	1.90	0.53
14:q:353:ARG:NH1	54:8:482:C:O2	2.41	0.53
16:s:33:ASP:HB2	16:s:36:LYS:HD2	1.89	0.53
36:M:432:THR:HG21	36:M:473:ALA:HB1	1.90	0.53
48:0:26:G:N1	48:0:46:U:N3	2.56	0.53
51:5:39:G:N2	51:5:67:A:OP1	2.41	0.53
53:7:160:A:H61	53:7:226:G:HO2'	1.51	0.53
3:c:337:SER:HA	3:c:386:ARG:NH2	2.17	0.53
19:v:61:ARG:HG2	19:v:76:VAL:HG22	1.90	0.53
9:l:152:ASN:ND2	50:4:10:G:H5''	2.24	0.53
11:n:160:GLN:HB3	11:n:197:ARG:HB3	1.90	0.53
27:D:93:GLU:HA	27:D:96:ARG:HD3	1.91	0.53
33:K:60:VAL:O	33:K:65:ARG:NH2	2.41	0.53
53:7:280:G:N2	53:7:319:A:OP2	2.42	0.53
7:j:97:ARG:HE	7:j:99:MET:HG2	1.74	0.53
2:b:257:GLN:HG2	2:b:261:ARG:HD2	1.91	0.53
17:t:255:VAL:HG12	17:t:267:LEU:HD13	1.90	0.53
34:L:102:ARG:HH11	34:L:110:ALA:HB1	1.74	0.53
16:s:101:ILE:HG21	16:s:115:LYS:HD3	1.90	0.52
21:x:18:ARG:NH1	21:x:63:VAL:O	2.42	0.52
30:G:63:LEU:HB2	30:G:138:LEU:HD22	1.91	0.52
31:I:83:THR:HG22	39:P:108:LEU:HD13	1.90	0.52
13:p:235:VAL:CG2	13:p:238:LEU:CD1	2.87	0.52
1:a:74:LEU:HD23	1:a:277:LEU:HD22	1.84	0.52
2:b:241:ALA:HB1	2:b:384:PRO:HD3	1.90	0.52
9:l:185:VAL:HG11	9:l:260:PHE:HD2	1.74	0.52
36:M:103:VAL:HG23	36:M:145:LEU:HD22	1.91	0.52
2:b:139:ARG:NH1	2:b:343:ASP:OD1	2.42	0.52
14:q:304:ARG:O	46:1:125:G:O2'	2.28	0.52
14:q:352:SER:O	54:8:482:C:N4	2.42	0.52
16:s:102:PHE:HB3	16:s:110:LYS:HD3	1.92	0.52
39:P:270:ALA:O	39:P:309:ARG:NH2	2.42	0.52
54:8:166:C:O2'	54:8:209:A:N3	2.41	0.52
7:j:103:GLU:HG3	7:j:105:ASN:HD22	1.75	0.52
14:q:249:LEU:HD11	22:y:68:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:514:ARG:HD2	37:N:227:GLN:HG3	1.91	0.52
3:c:126:LEU:HD22	3:c:246:LEU:HA	1.91	0.52
20:w:45:VAL:HG12	28:E:99:PRO:HG3	1.91	0.52
26:e:55:ASN:HB2	26:e:104:VAL:HA	1.92	0.52
3:c:315:GLU:OE1	3:c:318:ARG:NH2	2.43	0.52
24:A:256:THR:HG23	24:A:259:GLY:H	1.74	0.52
39:P:84:PRO:HB3	39:P:128:LEU:HD23	1.92	0.52
6:i:56:THR:O	47:2:14:U:O2'	2.27	0.52
19:v:32:TRP:HH2	19:v:37:ILE:HG23	1.75	0.52
11:n:292:LEU:HD23	11:n:295:ARG:HD3	1.91	0.52
20:w:11:LEU:CB	20:w:14:VAL:HG22	2.39	0.52
38:O:510:ARG:NH1	46:1:180:U:OP2	2.43	0.52
39:P:409:PRO:HD3	39:P:492:ARG:HG2	1.92	0.52
53:7:412:A:N6	54:8:149:U:OP1	2.43	0.52
4:d:17:ALA:HA	4:d:76:ASP:HB3	1.92	0.52
11:n:220:VAL:HA	11:n:276:VAL:HG12	1.92	0.52
20:w:63:PRO:HG3	20:w:72:ARG:HG3	1.92	0.52
30:G:170:GLU:OE1	30:G:175:THR:OG1	2.28	0.52
39:P:372:LEU:HA	39:P:375:VAL:HG22	1.92	0.52
54:8:114:A:N6	54:8:126:G:H21	2.03	0.52
4:d:54:ALA:HA	4:d:73:VAL:HG22	1.92	0.51
20:w:68:HIS:O	20:w:72:ARG:HG2	2.10	0.51
51:5:105:C:N4	51:5:108:C:OP2	2.44	0.51
20:w:113:VAL:HG23	20:w:115:LYS:H	1.75	0.51
30:G:56:CYS:HB2	30:G:176:ALA:HB1	1.91	0.51
7:j:107:PRO:HD2	7:j:109:TRP:HD1	1.75	0.51
13:p:236:ASN:O	13:p:238:LEU:HD12	2.10	0.51
21:x:168:ARG:NH2	52:6:46:G:N7	2.50	0.51
23:z:9:VAL:HG23	23:z:31:PRO:HD2	1.93	0.51
38:O:228:ASP:HA	38:O:231:PRO:HG3	1.92	0.51
54:8:177:G:N2	54:8:351:G:O2'	2.43	0.51
3:c:413:ILE:HG12	39:P:158:GLY:HA2	1.92	0.51
15:r:136:ARG:HB2	28:E:50:VAL:HG13	1.92	0.51
20:w:11:LEU:HB2	20:w:14:VAL:HG22	1.92	0.51
34:L:76:ILE:HD13	53:7:8:A:H4'	1.92	0.51
36:M:515:GLN:OE1	36:M:519:ARG:NE	2.39	0.51
17:t:329:ASP:H	17:t:332:GLN:HB3	1.76	0.51
53:7:342:G:N2	53:7:346:C:O2'	2.44	0.51
54:8:177:G:H22	54:8:351:G:H1'	1.75	0.51
26:e:188:ARG:HD3	26:e:189:TYR:H	1.76	0.51
14:q:240:MET:SD	46:1:53:U:O2'	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:P:266:SER:OG	39:P:298:ARG:NH1	2.43	0.51
53:7:160:A:N6	53:7:226:G:O2'	2.36	0.51
2:b:105:ALA:HA	2:b:108:VAL:HG12	1.93	0.51
2:b:317:LYS:HE3	2:b:381:VAL:HG11	1.93	0.51
9:l:185:VAL:HG12	9:l:259:LYS:HB2	1.93	0.51
22:y:106:GLN:HG3	22:y:108:PRO:HD3	1.93	0.51
30:G:133:THR:O	30:G:136:ARG:NH1	2.43	0.51
36:M:304:ARG:NH2	36:M:397:VAL:O	2.44	0.51
37:N:394:LEU:HD21	53:7:186:A:P	2.51	0.51
8:k:172:LYS:HE3	54:8:74:G:H1	1.77	0.51
10:m:77:ASP:HA	10:m:80:LEU:HD12	1.93	0.51
3:c:357:VAL:HG23	3:c:358:MET:HG3	1.93	0.50
7:j:76:GLN:HB3	11:n:263:VAL:HG13	1.93	0.50
13:p:209:LEU:HD21	13:p:332:LEU:HD21	1.93	0.50
19:v:40:ARG:NH1	53:7:522:U:OP2	2.43	0.50
30:G:219:ASP:N	30:G:219:ASP:OD1	2.44	0.50
37:N:174:LEU:HB3	37:N:210:ARG:HG2	1.92	0.50
11:n:253:TYR:HD1	11:n:263:VAL:HB	1.77	0.50
53:7:93:G:N1	53:7:136:A:OP1	2.44	0.50
53:7:167:U:O2'	53:7:171:A:N3	2.41	0.50
54:8:84:A:N6	54:8:246:C:OP1	2.44	0.50
27:D:115:PHE:H	30:G:64:VAL:HA	1.75	0.50
30:G:133:THR:HG22	30:G:134:MET:H	1.76	0.50
39:P:460:ARG:NH1	47:2:85:U:OP2	2.36	0.50
48:0:65:U:H2'	48:0:66:A:H8	1.76	0.50
1:a:74:LEU:HD22	1:a:277:LEU:HD13	1.93	0.50
30:G:145:VAL:HB	30:G:234:ALA:HB3	1.93	0.50
38:O:585:VAL:HG23	38:O:588:LEU:HD12	1.94	0.50
41:R:172:LEU:HD12	41:R:201:VAL:HG13	1.92	0.50
51:5:14:C:H3'	51:5:15:G:H8	1.75	0.50
33:K:83:PRO:HB3	54:8:390:U:H2'	1.93	0.50
40:Q:291:MET:HB2	40:Q:324:LEU:HD22	1.94	0.50
40:Q:570:SER:O	40:Q:623:ARG:NH2	2.44	0.50
41:R:354:ALA:HB2	41:R:390:LEU:HD22	1.92	0.50
9:l:145:VAL:HG11	9:l:207:VAL:HG13	1.94	0.50
38:O:531:GLU:HB3	38:O:561:LEU:HB3	1.94	0.50
13:p:234:PHE:O	29:F:103:ARG:HB3	2.12	0.50
30:G:236:VAL:HB	30:G:240:GLU:HG2	1.92	0.50
37:N:396:ALA:O	37:N:399:ARG:NH1	2.44	0.50
37:N:402:GLY:H	37:N:405:ARG:HH21	1.60	0.50
38:O:288:GLN:NE2	38:O:320:SER:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:8:327:A:H62	54:8:427:U:H3	1.60	0.50
1:a:242:VAL:HG22	1:a:252:VAL:HG22	1.93	0.50
7:j:10:ILE:HD13	7:j:84:LEU:HG	1.94	0.50
11:n:267:PRO:HD2	11:n:270:MET:SD	2.52	0.50
25:B:58:GLN:HG2	25:B:80:LYS:HG2	1.94	0.50
36:M:511:ARG:HD2	37:N:231:PRO:HG3	1.93	0.50
37:N:340:SER:O	37:N:407:ARG:NH2	2.44	0.50
39:P:260:LEU:HD12	39:P:291:LEU:HD11	1.94	0.50
42:S:119:ASP:OD1	42:S:119:ASP:N	2.45	0.50
51:5:55:U:O2	51:5:76:U:O2'	2.30	0.50
6:i:45:LEU:HD11	6:i:131:LEU:HB2	1.94	0.49
13:p:334:VAL:HG23	13:p:336:LEU:HG	1.94	0.49
42:S:106:SER:H	42:S:117:MET:HE1	1.77	0.49
54:8:170:G:N2	54:8:183:C:O2	2.38	0.49
13:p:235:VAL:HG21	13:p:238:LEU:HD11	1.94	0.49
30:G:188:HIS:HD2	30:G:220:PRO:HD2	1.76	0.49
34:L:72:ARG:NH1	34:L:86:TYR:O	2.43	0.49
39:P:278:ALA:HA	39:P:322:LEU:HD13	1.94	0.49
40:Q:556:ARG:NE	40:Q:608:HIS:ND1	2.58	0.49
40:Q:556:ARG:NE	40:Q:608:HIS:CG	2.80	0.49
46:1:25:A:H2	46:1:44:U:H5'	1.78	0.49
46:1:76:A:H5''	46:1:77:A:H5'	1.94	0.49
1:a:211:ARG:HG3	1:a:264:LEU:HB3	1.94	0.49
19:v:31:VAL:HG21	19:v:75:LEU:HD13	1.93	0.49
25:B:83:ALA:HB3	25:B:86:PHE:HD2	1.78	0.49
40:Q:680:MET:O	40:Q:684:SER:OG	2.30	0.49
49:3:163:A:H2'	49:3:164:A:H8	1.77	0.49
53:7:556:A:H2	53:7:561:U:H3	1.60	0.49
34:L:142:ARG:NH2	53:7:29:G:O3'	2.45	0.49
2:b:111:LYS:HZ1	6:i:142:GLN:H	1.59	0.49
3:c:417:VAL:HG21	39:P:154:ARG:HD2	1.95	0.49
9:l:169:ILE:HG13	9:l:253:LEU:HD12	1.95	0.49
10:m:139:LEU:HD13	41:R:417:ALA:HA	1.95	0.49
16:s:91:ASP:OD2	16:s:114:ARG:NH2	2.44	0.49
25:B:126:VAL:N	25:B:127:PRO:HD3	2.28	0.49
1:a:74:LEU:CD2	1:a:277:LEU:CD2	2.69	0.49
12:o:52:TRP:O	12:o:56:ILE:HG13	2.13	0.49
37:N:264:LEU:HB3	37:N:270:TYR:HB3	1.95	0.49
37:N:349:ARG:HB3	37:N:357:GLY:HA2	1.93	0.49
50:4:51:C:H2'	50:4:52:A:C8	2.48	0.49
8:k:226:TYR:HB3	25:B:108:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:120:ARG:HH12	54:8:58:G:H4'	1.77	0.49
25:B:49:ASP:OD1	25:B:53:ILE:N	2.45	0.49
41:R:164:ARG:HH22	54:8:482:C:H41	1.61	0.49
17:t:334:MET:HB3	17:t:357:LEU:HB2	1.95	0.49
26:e:128:LEU:HD12	26:e:140:LEU:HD11	1.94	0.49
1:a:86:HIS:O	1:a:282:ASN:ND2	2.46	0.48
18:u:104:VAL:HG12	18:u:108:MET:HE2	1.94	0.48
36:M:391:ASP:OD1	36:M:393:ARG:NH2	2.46	0.48
37:N:180:SER:HA	37:N:183:ARG:HG2	1.94	0.48
38:O:381:ALA:HA	38:O:384:LEU:HD22	1.94	0.48
40:Q:556:ARG:NH1	40:Q:608:HIS:NE2	2.61	0.48
41:R:382:GLY:HA2	41:R:385:ARG:HG2	1.95	0.48
2:b:262:ARG:NH1	2:b:299:LEU:O	2.46	0.48
40:Q:539:UNK:HA	40:Q:548:SER:HA	1.95	0.48
54:8:246:C:O2'	54:8:248:G:OP1	2.31	0.48
5:f:111:LEU:HA	5:f:142:ALA:HA	1.95	0.48
17:t:312:ALA:HA	17:t:345:THR:HG23	1.96	0.48
49:3:182:C:H2'	49:3:183:A:H8	1.78	0.48
53:7:189:U:O4	53:7:199:G:O6	2.30	0.48
1:a:195:MET:H	1:a:206:ASN:ND2	2.11	0.48
16:s:67:GLY:O	16:s:68:THR:HG23	2.14	0.48
34:L:99:GLU:HB2	34:L:112:ARG:HA	1.96	0.48
19:v:5:VAL:HG11	38:O:87:VAL:HA	1.95	0.48
36:M:143:ASP:OD1	36:M:173:HIS:NE2	2.42	0.48
40:Q:614:ARG:NH2	40:Q:660:SER:O	2.42	0.48
2:b:256:PHE:HA	2:b:302:CYS:HA	1.95	0.48
13:p:269:PRO:HD2	21:x:87:PRO:HG2	1.95	0.48
34:L:97:LEU:HD12	34:L:98:PRO:HD2	1.96	0.48
38:O:464:ILE:HG21	38:O:492:LEU:HB2	1.96	0.48
41:R:163:ASN:OD1	41:R:190:ASN:ND2	2.45	0.48
42:S:115:ARG:HG3	42:S:116:THR:HG23	1.96	0.48
46:1:176:U:O2'	46:1:178:G:N2	2.46	0.48
54:8:171:G:O6	54:8:182:U:O4	2.31	0.48
4:d:104:GLY:HA3	4:d:195:SER:HA	1.96	0.48
8:k:180:PRO:HG2	25:B:103:PRO:HB3	1.95	0.48
15:r:197:PRO:O	52:6:118:A:N6	2.47	0.48
42:S:79:ARG:HD2	42:S:193:HIS:HB3	1.95	0.48
7:j:98:SER:HB3	7:j:117:LYS:HD3	1.95	0.48
22:y:54:LEU:HD13	22:y:58:ARG:HD2	1.95	0.48
27:D:88:LEU:HA	27:D:91:LEU:HD21	1.96	0.48
2:b:164:VAL:HB	11:n:192:MET:CE	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:134:LEU:CD1	18:u:136:ARG:NH2	2.77	0.48
20:w:95:ASN:OD1	20:w:98:ARG:NH1	2.46	0.48
40:Q:263:ALA:HB2	40:Q:290:LEU:HD21	1.96	0.48
8:k:188:HIS:CE1	8:k:229:LEU:HD23	2.49	0.48
9:l:193:ILE:HG23	9:l:197:ALA:HB3	1.96	0.48
17:t:288:ASN:H	17:t:325:VAL:HG12	1.77	0.48
22:y:58:ARG:HD3	54:8:261:C:H5''	1.96	0.48
36:M:96:ALA:O	36:M:148:ARG:NH1	2.47	0.48
51:5:85:A:N1	51:5:86:G:O6	2.47	0.48
10:m:92:ARG:NH2	10:m:157:SER:O	2.46	0.47
14:q:267:HIS:NE2	53:7:359:U:OP1	2.47	0.47
16:s:45:LYS:H	42:S:104:ARG:HH12	1.60	0.47
18:u:125:ARG:HG2	18:u:135:GLU:HB2	1.95	0.47
37:N:226:PHE:HB2	37:N:249:ASP:HB2	1.96	0.47
39:P:197:CYS:HA	39:P:200:VAL:HG12	1.96	0.47
3:c:313:TYR:HE2	46:1:105:U:H4'	1.79	0.47
16:s:105:THR:HG21	16:s:124:ILE:HD11	1.96	0.47
23:z:15:LEU:HB3	23:z:53:PHE:HB3	1.97	0.47
30:G:130:ASP:OD1	30:G:130:ASP:N	2.43	0.47
21:x:173:GLU:OE1	21:x:176:ARG:NH2	2.47	0.47
37:N:198:GLY:HA3	37:N:237:PRO:HD3	1.96	0.47
4:d:147:GLY:HA2	4:d:150:LEU:HD12	1.97	0.47
11:n:245:GLY:N	54:8:469:A:OP2	2.48	0.47
27:D:91:LEU:HD13	27:D:95:LEU:HB3	1.95	0.47
30:G:166:ASN:C	30:G:166:ASN:HD22	2.23	0.47
33:K:241:GLU:OE1	33:K:244:ARG:NH2	2.47	0.47
2:b:139:ARG:NH2	2:b:238:HIS:O	2.47	0.47
2:b:197:CYS:HA	41:R:152:TYR:N	2.29	0.47
53:7:534:U:OP1	54:8:75:A:N6	2.46	0.47
23:z:19:ALA:HB2	23:z:51:VAL:HG11	1.95	0.47
37:N:175:LEU:CD1	37:N:212:LEU:HB2	2.45	0.47
40:Q:570:SER:HB3	40:Q:573:ASP:HB2	1.97	0.47
42:S:79:ARG:HG2	42:S:190:GLY:HA2	1.96	0.47
47:2:46:C:H2'	47:2:47:A:C8	2.49	0.47
13:p:227:VAL:HG21	13:p:312:ILE:HG13	1.96	0.47
15:r:66:MET:SD	15:r:88:LYS:HG3	2.54	0.47
16:s:83:HIS:HB3	16:s:86:GLN:HG3	1.97	0.47
18:u:126:THR:HB	18:u:130:GLN:HG3	1.97	0.47
36:M:230:GLN:HG3	36:M:233:ARG:HH11	1.78	0.47
41:R:369:LYS:O	41:R:372:THR:OG1	2.33	0.47
50:4:39:A:O2'	50:4:41:C:OP1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:7:119:G:H2'	53:7:120:A:H8	1.80	0.47
54:8:221:G:O2'	54:8:224:C:OP2	2.33	0.47
54:8:324:G:H21	54:8:429:G:H21	1.63	0.47
54:8:481:A:H5'	54:8:482:C:H5''	1.95	0.47
3:c:165:THR:O	46:1:139:A:H1'	2.14	0.47
15:r:179:ILE:HB	33:K:237:GLU:HG3	1.96	0.47
17:t:310:TYR:HB2	17:t:348:TYR:H	1.80	0.47
20:w:26:TRP:CH2	28:E:97:LEU:HD23	2.50	0.47
31:l:14:THR:OG1	31:l:15:GLY:N	2.47	0.47
42:S:103:ARG:HE	42:S:104:ARG:H	1.61	0.47
42:S:208:GLN:HG3	42:S:211:ARG:HD3	1.97	0.47
42:S:325:ASP:OD1	42:S:328:LYS:NZ	2.48	0.47
47:2:46:C:H2'	47:2:47:A:H8	1.79	0.47
52:6:99:U:H4'	52:6:100:A:H5''	1.97	0.47
1:a:151:VAL:HG22	1:a:193:VAL:HG22	1.97	0.47
3:c:130:PRO:HG2	40:Q:611:SER:HB2	1.97	0.47
4:d:152:TYR:O	4:d:156:GLU:N	2.46	0.47
38:O:311:GLU:OE1	38:O:336:TYR:OH	2.27	0.47
11:n:156:PRO:HB3	11:n:170:THR:HG23	1.97	0.47
15:r:94:THR:HB	15:r:97:GLU:HG3	1.97	0.47
17:t:254:ARG:NH1	48:0:85:C:O2	2.45	0.47
4:d:94:VAL:HG11	4:d:153:PRO:HG2	1.97	0.46
7:j:10:ILE:O	7:j:46:ARG:NH2	2.48	0.46
8:k:164:ASP:OD1	8:k:164:ASP:N	2.48	0.46
11:n:176:ARG:HH11	11:n:187:ARG:HH12	1.63	0.46
18:u:132:SER:C	18:u:134:LEU:H	2.22	0.46
38:O:272:LEU:HD12	38:O:303:ARG:HH12	1.80	0.46
15:r:65:MET:HE3	20:w:5:VAL:CG1	2.45	0.46
34:L:75:ALA:O	53:7:8:A:O2'	2.31	0.46
42:S:110:ASP:OD1	42:S:110:ASP:N	2.48	0.46
1:a:279:ARG:HG3	53:7:218:U:C2	2.51	0.46
4:d:17:ALA:HB3	4:d:173:VAL:HB	1.97	0.46
8:k:293:PRO:HD3	32:J:57:PRO:HB2	1.96	0.46
9:l:179:ALA:HA	9:l:182:ILE:HD12	1.96	0.46
18:u:129:GLY:O	18:u:130:GLN:HB2	2.15	0.46
26:e:148:VAL:HB	26:e:156:LEU:HD11	1.96	0.46
38:O:444:MET:O	38:O:471:TYR:OH	2.33	0.46
41:R:244:VAL:HA	41:R:247:ARG:HG2	1.97	0.46
54:8:408:A:O2'	54:8:472:A:OP1	2.32	0.46
11:n:140:ARG:HH21	11:n:143:ARG:HD2	1.80	0.46
17:t:288:ASN:HD22	17:t:326:ARG:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:t:301:ILE:HD13	17:t:325:VAL:HG21	1.97	0.46
53:7:539:G:O2'	54:8:141:C:OP1	2.30	0.46
10:m:42:LEU:HD23	10:m:115:ALA:HB2	1.98	0.46
13:p:276:ALA:HB2	13:p:313:LEU:HD21	1.96	0.46
26:e:110:LYS:HE2	26:e:110:LYS:HB2	1.80	0.46
29:F:100:VAL:HG21	29:F:105:LEU:HD13	1.97	0.46
36:M:511:ARG:HG3	37:N:231:PRO:HB3	1.96	0.46
53:7:58:A:N7	53:7:356:A:H1'	2.31	0.46
53:7:659:G:H21	54:8:74:G:H8	1.63	0.46
1:a:97:VAL:HG23	1:a:155:LEU:H	1.80	0.46
4:d:105:VAL:HB	4:d:193:VAL:HA	1.98	0.46
11:n:251:LYS:HG2	11:n:263:VAL:HG22	1.98	0.46
17:t:330:LEU:HD21	17:t:361:THR:HB	1.98	0.46
28:E:89:PRO:HD2	28:E:92:LEU:HD21	1.97	0.46
34:L:157:ARG:NH2	53:7:44:C:O2	2.43	0.46
41:R:374:ARG:NH1	54:8:492:G:O2'	2.49	0.46
32:J:49:GLU:HG2	32:J:51:ILE:H	1.81	0.46
36:M:518:ALA:CB	37:N:224:LEU:HD21	2.46	0.46
38:O:184:VAL:HG22	38:O:187:ARG:HH22	1.80	0.46
2:b:175:LEU:HD21	2:b:227:LEU:HD13	1.98	0.46
8:k:183:GLU:O	8:k:188:HIS:NE2	2.48	0.46
9:l:203:LEU:HD22	9:l:238:ILE:HB	1.97	0.46
9:l:243:ARG:HH22	17:t:289:ASP:CG	2.23	0.46
33:K:243:LEU:O	33:K:247:GLN:HB2	2.16	0.46
53:7:189:U:O2	53:7:199:G:N2	2.39	0.46
2:b:96:PRO:HG2	6:i:17:ILE:CG2	2.46	0.46
15:r:65:MET:CE	20:w:5:VAL:CG1	2.94	0.46
18:u:134:LEU:HD12	18:u:136:ARG:NH2	2.31	0.46
31:I:104:ARG:HH22	39:P:507:ASP:HB2	1.80	0.46
35:C:17:UNK:O	35:C:24:UNK:N	2.48	0.46
53:7:425:U:H1'	54:8:242:G:H21	1.81	0.46
54:8:335:G:H2'	54:8:336:G:H8	1.80	0.46
1:a:301:ILE:HG22	1:a:310:HIS:HB3	1.98	0.46
2:b:197:CYS:HG	41:R:152:TYR:N	2.14	0.46
10:m:169:ARG:HD3	34:L:194:GLN:NE2	2.31	0.46
11:n:161:ARG:NH2	11:n:193:HIS:HB3	2.31	0.46
17:t:295:VAL:HG12	17:t:301:ILE:HG23	1.98	0.46
34:L:81:ARG:NH1	34:L:101:LEU:O	2.49	0.46
36:M:486:LEU:HD23	36:M:490:LEU:HD22	1.98	0.46
46:1:83:C:H2'	46:1:84:A:H8	1.81	0.46
1:a:238:THR:HG21	53:7:217:A:H5''	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:108:VAL:HG23	6:i:14:LEU:HD22	1.97	0.45
13:p:235:VAL:CG2	13:p:238:LEU:HD11	2.46	0.45
13:p:321:ALA:HB3	13:p:322:PRO:HD3	1.98	0.45
26:e:53:GLY:HA3	26:e:104:VAL:HB	1.97	0.45
31:I:17:ARG:NH1	53:7:379:G:OP1	2.47	0.45
4:d:174:MET:SD	4:d:174:MET:N	2.89	0.45
20:w:5:VAL:HG12	20:w:5:VAL:O	2.15	0.45
31:I:29:SER:OG	50:4:106:G:OP2	2.32	0.45
53:7:580:U:H2'	53:7:581:A:H8	1.81	0.45
1:a:175:GLN:HE21	37:N:333:LEU:HD13	1.81	0.45
16:s:94:THR:OG1	16:s:96:LYS:NZ	2.48	0.45
17:t:310:TYR:HA	17:t:348:TYR:HB2	1.97	0.45
21:x:53:ARG:NH2	31:I:57:GLN:OE1	2.34	0.45
37:N:313:LEU:HD21	37:N:320:VAL:HG21	1.98	0.45
5:f:133:ARG:HE	53:7:443:U:C3'	2.28	0.45
16:s:172:TRP:HE1	16:s:199:UNK:HA	1.80	0.45
18:u:130:GLN:HB3	39:P:48:LEU:HD11	1.97	0.45
30:G:171:SER:O	30:G:175:THR:OG1	2.35	0.45
38:O:533:LEU:O	38:O:536:THR:OG1	2.34	0.45
2:b:225:ASP:OD1	2:b:225:ASP:N	2.44	0.45
4:d:194:LEU:HD12	27:D:107:TYR:O	2.16	0.45
22:y:54:LEU:HB3	22:y:59:ARG:HG3	1.97	0.45
33:K:62:PRO:HA	33:K:65:ARG:HG2	1.99	0.45
33:K:105:THR:OG1	33:K:106:ALA:N	2.48	0.45
54:8:335:G:H2'	54:8:336:G:C8	2.52	0.45
1:a:95:LEU:HD22	1:a:98:TYR:HB2	1.99	0.45
4:d:194:LEU:HB2	27:D:109:LEU:HD23	1.97	0.45
5:f:127:VAL:H	5:f:132:MET:HE2	1.80	0.45
9:l:149:GLU:HG2	9:l:151:ILE:HG22	1.99	0.45
13:p:227:VAL:CG2	13:p:312:ILE:HG13	2.47	0.45
15:r:125:ALA:HB3	15:r:135:TRP:HZ3	1.81	0.45
24:A:231:GLY:N	53:7:150:C:OP1	2.50	0.45
37:N:301:LEU:HD13	37:N:321:LEU:HD23	1.99	0.45
41:R:187:ASP:OD1	41:R:188:HIS:N	2.48	0.45
4:d:150:LEU:HD23	4:d:165:LEU:HD23	1.98	0.45
18:u:138:VAL:O	18:u:139:ALA:C	2.60	0.45
33:K:46:THR:HG1	33:K:141:SER:HG	1.62	0.45
53:7:283:G:H1	53:7:318:G:H21	1.64	0.45
53:7:306:G:H21	53:7:335:U:H4'	1.81	0.45
54:8:216:U:H5'	54:8:217:A:H5''	1.98	0.45
1:a:119:THR:HG22	1:a:121:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:152:ASN:HB3	9:l:233:ARG:HH21	1.82	0.45
30:G:131:VAL:HB	30:G:235:TRP:H	1.82	0.45
34:L:107:PRO:HD2	34:L:110:ALA:HB2	1.98	0.45
37:N:276:ARG:NH2	37:N:315:ASP:O	2.49	0.45
40:Q:570:SER:OG	40:Q:571:CYS:N	2.49	0.45
51:5:157:U:O2'	51:5:158:U:O4'	2.34	0.45
2:b:294:TRP:O	54:8:264:U:H4'	2.17	0.45
3:c:93:LEU:HD21	29:F:25:GLY:HA2	1.99	0.45
23:z:29:LYS:NZ	23:z:36:TRP:O	2.49	0.45
33:K:163:LYS:HG3	53:7:116:A:OP2	2.17	0.45
41:R:177:GLU:O	41:R:181:ARG:HB3	2.17	0.45
3:c:196:ARG:HA	3:c:203:GLY:HA2	1.99	0.45
20:w:38:ASP:OD2	28:E:97:LEU:HD22	2.17	0.45
26:e:126:LYS:HD2	26:e:126:LYS:HA	1.78	0.45
33:K:215:LEU:HD21	33:K:221:PRO:HG3	1.98	0.45
38:O:170:ARG:HG3	38:O:171:ARG:H	1.81	0.45
41:R:178:MET:O	41:R:182:GLU:HB3	2.17	0.45
4:d:105:VAL:HG22	4:d:112:PRO:HD3	2.00	0.44
10:m:26:LYS:HE2	10:m:73:ILE:HA	1.99	0.44
33:K:163:LYS:HA	33:K:176:HIS:HE1	1.82	0.44
38:O:153:VAL:HA	38:O:169:THR:HG22	1.97	0.44
51:5:3:G:O6	51:5:94:U:O2	2.36	0.44
14:q:229:GLY:HA3	14:q:284:ALA:HB2	1.99	0.44
15:r:127:SER:OG	15:r:128:ARG:N	2.49	0.44
21:x:63:VAL:O	31:I:46:ASN:ND2	2.43	0.44
26:e:183:LYS:HG3	26:e:185:LYS:HB2	1.99	0.44
29:F:56:PRO:HB2	29:F:72:VAL:HG23	1.97	0.44
33:K:172:GLY:HA3	53:7:113:U:O2	2.16	0.44
36:M:247:LEU:HB2	36:M:300:TRP:HH2	1.82	0.44
40:Q:332:CYS:HA	40:Q:335:ALA:HB3	1.99	0.44
41:R:177:GLU:HA	41:R:180:VAL:HG12	1.98	0.44
3:c:158:ARG:NH2	52:6:24:U:O2	2.49	0.44
4:d:41:LEU:HB3	27:D:36:MET:SD	2.56	0.44
10:m:33:LEU:HD23	10:m:87:VAL:HG21	1.99	0.44
22:y:104:VAL:O	42:S:243:LYS:HE2	2.17	0.44
26:e:42:VAL:HG22	26:e:51:VAL:HG22	2.00	0.44
26:e:188:ARG:HD2	26:e:192:GLU:HB2	1.98	0.44
38:O:266:HIS:ND1	38:O:268:ASP:OD1	2.32	0.44
49:3:17:A:N3	54:8:88:U:O2'	2.46	0.44
3:c:99:THR:O	3:c:108:ARG:NH1	2.51	0.44
3:c:104:PRO:HB2	3:c:146:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:s:19:ARG:NH1	16:s:100:VAL:O	2.41	0.44
36:M:497:LEU:O	36:M:501:SER:CB	2.65	0.44
37:N:274:PRO:HA	37:N:277:LEU:HD13	2.00	0.44
46:l:150:U:H2'	46:l:151:A:C8	2.52	0.44
8:k:161:MET:HE2	8:k:161:MET:HB3	1.84	0.44
14:q:264:LEU:HB3	22:y:71:LYS:HD2	1.99	0.44
25:B:121:PRO:HB2	54:8:59:U:H4'	1.98	0.44
13:p:192:PRO:O	13:p:194:PRO:HD3	2.18	0.44
19:v:92:ASP:OD1	19:v:93:ALA:N	2.51	0.44
29:F:85:GLY:O	29:F:89:ASN:ND2	2.50	0.44
40:Q:681:ASP:N	40:Q:681:ASP:OD1	2.49	0.44
41:R:409:LEU:O	41:R:413:THR:OG1	2.36	0.44
53:7:104:A:H3'	53:7:105:A:H8	1.81	0.44
2:b:195:GLN:HE22	41:R:265:TRP:HB3	1.81	0.44
5:f:137:TYR:HB2	5:f:142:ALA:HB3	2.00	0.44
14:q:245:ARG:HG2	22:y:68:LEU:HG	1.99	0.44
18:u:17:ARG:HH21	53:7:623:A:H1'	1.83	0.44
37:N:171:LYS:HE2	37:N:175:LEU:HG	1.98	0.44
51:5:85:A:C6	51:5:86:G:O6	2.71	0.44
53:7:410:A:N6	54:8:90:G:OP1	2.49	0.44
1:a:185:PRO:HG2	1:a:188:VAL:HG13	1.99	0.44
10:m:21:ARG:NH2	54:8:378:A:OP2	2.51	0.44
17:t:128:THR:HA	17:t:131:LYS:HG2	2.00	0.44
42:S:81:MET:O	42:S:186:ARG:NH1	2.51	0.44
53:7:122:U:O2'	53:7:124:A:N7	2.37	0.44
4:d:115:ARG:NH1	4:d:118:LYS:O	2.51	0.44
18:u:124:PRO:O	18:u:125:ARG:C	2.59	0.44
1:a:334:ARG:HB2	53:7:167:U:OP1	2.18	0.43
6:i:68:ALA:HB3	6:i:135:PRO:HA	1.99	0.43
9:l:148:ARG:HB3	9:l:176:ARG:HD3	1.99	0.43
9:l:189:LEU:HD13	9:l:241:MET:HE1	2.00	0.43
11:n:204:ARG:NE	11:n:269:TYR:OH	2.51	0.43
16:s:145:THR:CG2	28:E:98:LYS:H	2.30	0.43
18:u:122:PRO:O	18:u:123:LEU:C	2.57	0.43
39:P:494:ALA:HB2	39:P:518:VAL:HG21	2.00	0.43
42:S:228:VAL:HG22	42:S:256:THR:HG23	1.99	0.43
54:8:183:C:H2'	54:8:184:G:H8	1.83	0.43
3:c:193:GLY:H	49:3:16:G:H5''	1.82	0.43
8:k:291:PRO:HG2	8:k:308:GLN:HG3	2.00	0.43
17:t:301:ILE:HG22	17:t:359:CYS:HA	2.00	0.43
21:x:202:ARG:HH22	46:l:115:C:H6	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:7:580:U:H2'	53:7:581:A:C8	2.53	0.43
1:a:74:LEU:HD21	1:a:277:LEU:CD2	2.24	0.43
1:a:249:HIS:HB3	1:a:261:LEU:HG	2.00	0.43
2:b:167:VAL:HG11	2:b:235:GLY:HA2	2.00	0.43
18:u:126:THR:HG22	39:P:48:LEU:CD2	2.48	0.43
49:3:70:U:H2'	49:3:71:G:C8	2.53	0.43
14:q:345:ARG:HG3	22:y:73:GLU:HG2	1.99	0.43
20:w:115:LYS:NZ	20:w:119:GLU:OE1	2.49	0.43
33:K:162:ARG:NH2	33:K:181:GLU:OE1	2.51	0.43
37:N:180:SER:HA	37:N:183:ARG:CG	2.49	0.43
39:P:105:PRO:O	39:P:111:GLN:NE2	2.51	0.43
40:Q:608:HIS:ND1	40:Q:608:HIS:CD2	2.80	0.43
42:S:140:LYS:HD2	42:S:166:ARG:HD3	2.01	0.43
54:8:370:U:H2'	54:8:371:C:H6	1.83	0.43
2:b:200:PRO:HD3	41:R:155:TRP:CD1	2.54	0.43
2:b:287:ARG:H	53:7:402:G:H4'	1.83	0.43
5:f:120:ARG:HG3	5:f:121:ARG:H	1.84	0.43
8:k:121:ARG:NH1	8:k:122:ASP:O	2.51	0.43
29:F:8:MET:HA	29:F:63:ARG:HB2	1.99	0.43
1:a:256:SER:OG	53:7:168:G:N7	2.50	0.43
3:c:310:ILE:HG21	3:c:316:LEU:HB2	2.01	0.43
8:k:186:TYR:HE1	25:B:108:VAL:HG13	1.83	0.43
8:k:286:LEU:HD11	32:J:37:GLU:OE1	2.19	0.43
9:l:202:ARG:HB2	9:l:238:ILE:HA	2.01	0.43
36:M:402:THR:HG23	36:M:405:SER:H	1.83	0.43
40:Q:581:LEU:HD22	40:Q:609:PHE:HE1	1.84	0.43
53:7:547:U:O2'	54:8:72:C:OP2	2.36	0.43
53:7:596:A:H2'	53:7:597:A:C8	2.54	0.43
4:d:59:PRO:HD3	4:d:68:ALA:HA	2.00	0.43
5:f:110:VAL:HG12	5:f:124:VAL:HG22	2.01	0.43
6:i:97:PRO:HD2	6:i:100:ASP:HB2	2.01	0.43
11:n:267:PRO:HB2	11:n:270:MET:HB3	2.01	0.43
16:s:92:PRO:HD2	16:s:114:ARG:HH12	1.83	0.43
18:u:72:ALA:HA	18:u:89:ARG:HB3	2.00	0.43
26:e:180:GLU:HB2	26:e:183:LYS:HG2	1.99	0.43
33:K:36:GLN:HG2	33:K:85:LEU:HD21	2.01	0.43
52:6:41:A:H2'	52:6:42:A:C8	2.54	0.43
53:7:669:A:H2'	53:7:670:A:C8	2.54	0.43
11:n:138:PRO:HB2	11:n:143:ARG:HH22	1.84	0.43
11:n:243:LYS:O	11:n:244:LYS:NZ	2.49	0.43
16:s:26:VAL:HB	16:s:87:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:F:9:LEU:HD22	29:F:88:ARG:HA	2.01	0.43
46:1:160:G:H2'	46:1:161:G:H8	1.83	0.43
49:3:83:A:H2'	49:3:84:G:H8	1.83	0.43
53:7:289:U:O5'	54:8:249:U:O2'	2.36	0.43
53:7:583:U:H2'	53:7:584:G:H8	1.84	0.43
3:c:336:ASP:O	3:c:363:PRO:HD3	2.18	0.43
12:o:61:ARG:HH22	50:4:114:C:H5'	1.83	0.43
15:r:58:PHE:HA	20:w:43:TRP:CD1	2.54	0.43
15:r:83:ARG:NH1	15:r:147:PHE:O	2.47	0.43
27:D:42:PRO:HB2	27:D:45:PRO:HG3	2.01	0.43
33:K:93:CYS:HA	33:K:113:VAL:HG21	2.00	0.43
37:N:397:ARG:HA	37:N:406:TYR:CE2	2.54	0.43
38:O:161:VAL:HG21	46:1:151:A:H4'	2.00	0.43
41:R:421:LEU:HA	41:R:424:VAL:HG12	2.00	0.43
48:0:26:G:N1	48:0:46:U:C2	2.83	0.43
3:c:363:PRO:HB3	3:c:387:ILE:HG13	2.01	0.43
9:l:158:ASN:HD21	50:4:11:C:H5''	1.83	0.43
11:n:176:ARG:NH1	11:n:187:ARG:HH12	2.17	0.43
19:v:51:ARG:NH1	53:7:432:G:OP1	2.51	0.43
36:M:359:THR:OG1	36:M:360:ILE:N	2.51	0.43
6:i:77:LYS:NZ	51:5:110:C:OP2	2.37	0.42
18:u:134:LEU:HD12	18:u:136:ARG:HH21	1.84	0.42
30:G:59:GLN:HA	30:G:143:TYR:HD1	1.84	0.42
40:Q:331:ARG:O	40:Q:335:ALA:CB	2.67	0.42
7:j:117:LYS:HG2	11:n:258:ASP:OD2	2.19	0.42
11:n:140:ARG:HE	11:n:143:ARG:HG3	1.84	0.42
21:x:161:LYS:HE2	21:x:161:LYS:HB2	1.74	0.42
33:K:97:LEU:HD21	33:K:104:LEU:HB3	2.01	0.42
36:M:514:ARG:HA	36:M:517:MET:HE2	2.00	0.42
42:S:205:LYS:HB3	42:S:208:GLN:HB2	2.00	0.42
54:8:194:G:H2'	54:8:195:A:H8	1.85	0.42
2:b:194:ARG:NH2	54:8:453:A:H5'	2.34	0.42
2:b:330:GLN:H	2:b:330:GLN:HG3	1.75	0.42
13:p:135:TRP:O	13:p:139:GLN:HG2	2.19	0.42
18:u:125:ARG:HG2	18:u:135:GLU:CB	2.49	0.42
53:7:35:A:H1'	53:7:36:U:H2'	2.00	0.42
4:d:99:GLN:NE2	4:d:112:PRO:O	2.52	0.42
12:o:63:HIS:HB2	12:o:101:VAL:HG11	2.00	0.42
14:q:346:ILE:HD13	22:y:74:VAL:HG13	2.01	0.42
17:t:197:ARG:C	17:t:199:GLY:H	2.26	0.42
25:B:82:LEU:HD23	25:B:82:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:P:36:ALA:HB3	39:P:39:ILE:HD12	2.01	0.42
47:2:47:A:H2'	47:2:48:A:C8	2.53	0.42
47:2:79:G:H4'	47:2:80:A:H5'	2.01	0.42
49:3:182:C:H2'	49:3:183:A:C8	2.55	0.42
2:b:200:PRO:HG2	54:8:437:A:C8	2.55	0.42
13:p:220:LEU:HD23	13:p:220:LEU:HA	1.89	0.42
20:w:69:GLN:HG2	20:w:74:ILE:HB	1.99	0.42
30:G:226:LEU:HB2	30:G:230:ALA:HB2	2.01	0.42
37:N:341:ALA:N	37:N:364:ASP:OD1	2.46	0.42
41:R:247:ARG:HE	41:R:247:ARG:HB2	1.67	0.42
46:1:117:A:O2'	46:1:118:U:O4'	2.32	0.42
47:2:35:G:OP1	52:6:62:U:O2'	2.36	0.42
2:b:128:LEU:HD23	2:b:360:PRO:HB3	2.01	0.42
2:b:195:GLN:NE2	41:R:265:TRP:HB3	2.34	0.42
3:c:85:LEU:HG	29:F:33:ALA:HB2	2.01	0.42
11:n:152:TYR:OH	41:R:408:ASP:HA	2.20	0.42
11:n:161:ARG:CZ	11:n:193:HIS:HB3	2.50	0.42
13:p:319:ASP:OD1	13:p:319:ASP:N	2.53	0.42
32:J:22:LEU:HD21	32:J:27:ILE:HD12	2.01	0.42
36:M:425:GLN:O	36:M:455:ARG:NH1	2.48	0.42
38:O:122:VAL:HA	38:O:129:PHE:HZ	1.85	0.42
46:1:5:G:H2'	46:1:6:A:C8	2.54	0.42
3:c:195:ILE:HG13	3:c:196:ARG:HG2	2.01	0.42
15:r:103:GLN:HE21	15:r:110:VAL:HB	1.83	0.42
17:t:325:VAL:HG23	17:t:328:MET:SD	2.60	0.42
39:P:146:ARG:HE	39:P:146:ARG:HB2	1.71	0.42
54:8:412:U:H2'	54:8:413:A:C8	2.55	0.42
3:c:97:PRO:HD3	8:k:119:ASN:HB3	2.02	0.42
11:n:197:ARG:HD2	11:n:197:ARG:HA	1.88	0.42
21:x:165:LEU:HD12	52:6:37:C:H3'	2.00	0.42
23:z:37:LYS:NZ	23:z:55:GLU:O	2.38	0.42
38:O:316:LEU:HD11	38:O:368:LYS:HD2	2.02	0.42
41:R:428:LEU:HD22	41:R:435:LEU:HD11	2.01	0.42
1:a:75:ILE:N	1:a:89:SER:O	2.45	0.42
2:b:139:ARG:HH21	2:b:238:HIS:CE1	2.38	0.42
8:k:287:PRO:HG2	32:J:36:ARG:HH21	1.85	0.42
9:l:156:MET:HG3	48:0:65:U:H1'	2.02	0.42
13:p:274:LEU:HD12	13:p:314:GLN:HE21	1.85	0.42
36:M:247:LEU:HD21	36:M:313:PHE:HZ	1.85	0.42
37:N:206:LEU:HD13	37:N:206:LEU:HA	1.88	0.42
54:8:446:A:H4'	54:8:447:A:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:m:16:ARG:HG2	10:m:20:HIS:CE1	2.55	0.42
10:m:44:LYS:O	10:m:48:LEU:HB2	2.19	0.42
16:s:174:GLU:C	16:s:177:PRO:HD2	2.45	0.42
24:A:264:LEU:HD23	24:A:264:LEU:HA	1.90	0.42
35:C:18:UNK:HA	35:C:23:UNK:HA	2.01	0.42
40:Q:550:LEU:HD12	40:Q:550:LEU:HA	1.92	0.42
41:R:192:THR:HG22	41:R:274:ALA:HB2	2.01	0.42
46:1:23:C:O2	46:1:28:A:O2'	2.38	0.42
52:6:73:G:O2'	53:7:362:G:O6	2.35	0.42
53:7:78:G:O2'	53:7:80:A:N6	2.44	0.42
2:b:151:GLN:HG2	54:8:370:U:O2'	2.20	0.41
2:b:243:GLN:NE2	2:b:343:ASP:OD2	2.53	0.41
3:c:192:GLN:OE1	3:c:200:TRP:NE1	2.50	0.41
11:n:209:LEU:HD22	11:n:276:VAL:HG22	2.01	0.41
13:p:185:LEU:H	13:p:185:LEU:HD23	1.84	0.41
16:s:6:TYR:CZ	42:S:109:PRO:HD2	2.55	0.41
27:D:71:GLN:HA	27:D:74:VAL:HG12	2.02	0.41
27:D:96:ARG:O	27:D:100:MET:N	2.49	0.41
27:D:114:LEU:HB3	30:G:65:ARG:HB2	2.01	0.41
1:a:112:LYS:HB2	49:3:34:G:H5''	2.02	0.41
6:i:28:ASP:OD1	6:i:67:ASN:ND2	2.42	0.41
10:m:174:ILE:HG12	33:K:58:TYR:CD1	2.55	0.41
14:q:195:ARG:NH2	14:q:205:GLU:OE1	2.40	0.41
33:K:65:ARG:HD3	33:K:73:PHE:CD2	2.56	0.41
37:N:184:THR:O	37:N:188:HIS:ND1	2.52	0.41
37:N:260:LEU:HD12	37:N:260:LEU:HA	1.91	0.41
47:2:15:A:H2'	47:2:16:G:C8	2.56	0.41
54:8:173:U:C2	54:8:175:A:H5''	2.55	0.41
3:c:247:ILE:HD12	3:c:247:ILE:HA	1.86	0.41
9:l:162:LEU:HD23	9:l:240:GLU:HB2	2.01	0.41
26:e:94:ARG:HA	26:e:97:VAL:HG12	2.01	0.41
32:J:128:UNK:O	32:J:132:UNK:N	2.53	0.41
37:N:235:VAL:O	37:N:239:MET:N	2.52	0.41
38:O:358:ARG:HH12	46:1:181:A:H5'	1.85	0.41
41:R:186:LEU:HD23	41:R:186:LEU:HA	1.93	0.41
42:S:216:PHE:HA	42:S:219:ARG:HB3	2.02	0.41
49:3:84:G:H2'	49:3:85:A:C8	2.55	0.41
5:f:133:ARG:HE	53:7:443:U:C4'	2.29	0.41
7:j:113:LYS:HA	7:j:119:LEU:HD21	2.03	0.41
8:k:118:GLY:HA3	52:6:26:G:H21	1.85	0.41
16:s:171:ILE:H	16:s:171:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:46:ALA:HB3	30:G:89:LEU:HD12	2.02	0.41
27:D:59:ALA:HA	27:D:62:LEU:HD12	2.03	0.41
32:J:103:LEU:HD22	32:J:121:UNK:HA	2.02	0.41
33:K:56:ALA:HB2	33:K:73:PHE:HA	2.01	0.41
38:O:242:LEU:HD23	38:O:242:LEU:HA	1.88	0.41
38:O:324:LEU:O	38:O:380:GLN:NE2	2.46	0.41
40:Q:627:GLN:OE1	40:Q:627:GLN:N	2.51	0.41
54:8:336:G:H2'	54:8:337:G:H8	1.84	0.41
1:a:183:LEU:HD23	1:a:183:LEU:HA	1.92	0.41
7:j:43:LYS:HD3	7:j:43:LYS:HA	1.80	0.41
7:j:98:SER:CB	7:j:117:LYS:HD3	2.50	0.41
11:n:217:VAL:HA	11:n:237:VAL:HA	2.03	0.41
15:r:109:ASN:HB3	15:r:148:ARG:HB3	2.03	0.41
24:A:274:ILE:HG12	28:E:34:ILE:HG12	2.01	0.41
30:G:236:VAL:HG23	30:G:241:LEU:HD23	2.01	0.41
37:N:251:ALA:O	37:N:255:HIS:HB2	2.20	0.41
53:7:282:A:H3'	53:7:283:G:H8	1.84	0.41
54:8:195:A:H61	54:8:204:C:H42	1.68	0.41
10:m:74:VAL:HB	10:m:80:LEU:CD2	2.51	0.41
11:n:168:GLN:OE1	11:n:180:ARG:NH1	2.53	0.41
18:u:123:LEU:O	18:u:124:PRO:C	2.63	0.41
19:v:36:GLN:HG3	38:O:89:GLU:HG3	2.03	0.41
26:e:185:LYS:HE3	54:8:345:C:H5'	2.01	0.41
31:I:47:MET:HE1	48:0:79:U:H4'	2.03	0.41
47:2:34:G:H2'	47:2:35:G:C8	2.56	0.41
1:a:298:VAL:HG21	49:3:112:A:N7	2.36	0.41
2:b:260:MET:HE3	2:b:279:ARG:HA	2.02	0.41
3:c:181:PRO:HB2	3:c:182:TRP:H	1.77	0.41
8:k:195:ALA:O	8:k:199:GLN:HG3	2.20	0.41
11:n:305:GLN:H	11:n:305:GLN:HG2	1.74	0.41
20:w:14:VAL:CG2	20:w:15:PRO:HD3	2.51	0.41
30:G:159:TRP:H	30:G:247:SER:HB2	1.86	0.41
30:G:244:SER:O	30:G:244:SER:OG	2.37	0.41
40:Q:231:ARG:O	40:Q:235:LEU:HB2	2.21	0.41
54:8:60:U:H2'	54:8:61:A:C8	2.56	0.41
3:c:193:GLY:HA3	49:3:17:A:OP1	2.20	0.41
4:d:39:LEU:HA	4:d:42:TYR:HB2	2.02	0.41
10:m:171:GLU:HA	10:m:174:ILE:HD11	2.02	0.41
17:t:286:LEU:HD21	17:t:301:ILE:HD11	2.03	0.41
19:v:47:SER:OG	19:v:48:LYS:N	2.50	0.41
22:y:84:SER:HB3	22:y:90:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:126:LYS:HG3	26:e:142:ILE:HD11	2.01	0.41
29:F:79:GLU:HA	29:F:82:GLU:HG2	2.02	0.41
30:G:137:ARG:HB2	30:G:142:LEU:HD11	2.02	0.41
38:O:490:GLU:HA	38:O:493:VAL:HG12	2.02	0.41
41:R:191:LEU:HD13	41:R:259:VAL:HA	2.02	0.41
41:R:300:LEU:HD23	41:R:300:LEU:HA	1.95	0.41
41:R:387:TRP:HH2	41:R:398:GLY:HA2	1.85	0.41
44:Y:11:UNK:O	44:Y:15:UNK:N	2.53	0.41
50:4:90:C:O2'	50:4:103:A:N3	2.49	0.41
52:6:26:G:H3'	52:6:27:A:H5'	2.03	0.41
2:b:166:TRP:CZ2	11:n:175:THR:HG22	2.56	0.41
2:b:248:THR:HB	2:b:340:PHE:HB2	2.03	0.41
3:c:338:GLY:HA2	3:c:349:ARG:NH2	2.36	0.41
7:j:109:TRP:HE3	7:j:112:LEU:HD23	1.86	0.41
10:m:94:ARG:HA	10:m:132:ALA:HB1	2.02	0.41
13:p:246:VAL:HG21	13:p:334:VAL:HG11	2.03	0.41
16:s:156:THR:HA	16:s:157:PRO:HD3	1.93	0.41
21:x:136:ARG:HD2	21:x:136:ARG:HA	1.90	0.41
21:x:213:ARG:NH2	52:6:39:G:N7	2.69	0.41
29:F:58:LEU:HD22	29:F:72:VAL:HG11	2.02	0.41
36:M:119:ARG:NH1	36:M:120:LYS:HE3	2.36	0.41
37:N:205:VAL:HG13	37:N:206:LEU:HD22	2.02	0.41
38:O:583:LEU:HA	38:O:586:GLU:HB2	2.03	0.41
42:S:82:ASP:HB3	42:S:85:GLY:H	1.85	0.41
46:1:29:G:O2'	46:1:40:G:O6	2.36	0.41
47:2:14:U:H2'	47:2:15:A:C8	2.56	0.41
2:b:319:ASP:HA	2:b:381:VAL:HG12	2.02	0.41
4:d:44:LEU:HD21	4:d:161:LEU:HD21	2.03	0.41
5:f:157:ASP:O	5:f:160:ARG:NH1	2.54	0.41
11:n:180:ARG:H	11:n:180:ARG:HG2	1.66	0.41
14:q:314:HIS:O	53:7:19:A:N6	2.54	0.41
16:s:145:THR:HG21	28:E:98:LYS:H	1.86	0.41
24:A:269:LYS:NZ	46:1:39:G:OP2	2.54	0.41
36:M:414:ALA:HB2	36:M:458:LEU:HD11	2.03	0.41
36:M:514:ARG:HD2	37:N:227:GLN:CG	2.51	0.41
40:Q:255:ASN:HB3	40:Q:297:ARG:HD2	2.03	0.41
41:R:356:ALA:HA	41:R:359:LEU:HD12	2.03	0.41
51:5:42:G:H21	51:5:60:A:H2	1.69	0.41
54:8:240:G:N2	54:8:243:A:OP2	2.42	0.41
1:a:116:ARG:HH12	49:3:32:G:N2	2.13	0.40
1:a:301:ILE:CG2	1:a:310:HIS:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:96:PRO:HG2	6:i:17:ILE:HG23	2.02	0.40
2:b:262:ARG:NH2	54:8:266:U:H5'	2.32	0.40
7:j:8:LEU:HD13	7:j:82:ALA:HB3	2.02	0.40
7:j:96:VAL:HG23	7:j:115:LEU:HB3	2.03	0.40
11:n:156:PRO:O	11:n:157:LYS:HG2	2.21	0.40
20:w:45:VAL:HG23	28:E:92:LEU:HD12	2.02	0.40
27:D:111:ARG:NH2	30:G:215:GLN:HE21	2.19	0.40
37:N:335:LEU:HD21	37:N:378:VAL:HG22	2.02	0.40
38:O:261:LEU:HD23	38:O:261:LEU:HA	1.86	0.40
42:S:314:ARG:NH1	52:6:112:U:OP2	2.44	0.40
51:5:25:A:N7	51:5:27:A:N6	2.69	0.40
1:a:156:GLU:O	1:a:164:TRP:HB2	2.21	0.40
2:b:173:VAL:HG13	2:b:211:VAL:HG21	2.02	0.40
8:k:178:GLN:NE2	18:u:135:GLU:OE2	2.54	0.40
17:t:283:PRO:HA	17:t:307:THR:HA	2.03	0.40
38:O:321:THR:OG1	38:O:376:THR:OG1	2.39	0.40
39:P:403:LEU:HD11	39:P:488:GLU:HG3	2.03	0.40
54:8:408:A:H2'	54:8:409:A:H8	1.85	0.40
1:a:74:LEU:HD13	1:a:90:ILE:HA	2.04	0.40
1:a:162:SER:HB3	53:7:219:A:H5''	2.03	0.40
3:c:123:ILE:HD13	3:c:381:ARG:HD3	2.03	0.40
9:l:169:ILE:N	9:l:239:PHE:O	2.45	0.40
11:n:142:LEU:HD11	41:R:300:LEU:H	1.86	0.40
14:q:341:ALA:HA	14:q:342:PRO:HD3	1.90	0.40
23:z:28:GLU:OE2	53:7:574:C:N4	2.52	0.40
26:e:180:GLU:HG3	26:e:183:LYS:HD3	2.02	0.40
29:F:101:ARG:NE	47:2:8:A:OP1	2.46	0.40
37:N:196:PHE:HA	37:N:197:PRO:HD3	1.94	0.40
40:Q:239:ASP:OD1	40:Q:239:ASP:N	2.53	0.40
48:0:54:U:H2'	48:0:55:A:C8	2.56	0.40
53:7:91:G:H21	53:7:105:A:H62	1.69	0.40
54:8:423:A:H5''	54:8:424:G:C8	2.57	0.40
4:d:127:LYS:HE3	4:d:127:LYS:HB2	1.88	0.40
7:j:19:ALA:HB1	7:j:40:VAL:HB	2.03	0.40
7:j:99:MET:O	11:n:259:SER:HA	2.21	0.40
15:r:126:ILE:HD12	15:r:132:ARG:H	1.86	0.40
25:B:73:LEU:O	25:B:77:LYS:HG3	2.21	0.40
26:e:35:THR:HB	26:e:36:VAL:H	1.75	0.40
26:e:51:VAL:HB	26:e:100:LEU:HD21	2.03	0.40
30:G:211:PHE:HZ	30:G:251:LEU:HD11	1.87	0.40
38:O:445:ASP:OD2	38:O:476:ARG:NH2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:P:126:ASP:OD1	39:P:154:ARG:NH2	2.54	0.40
40:Q:681:ASP:O	40:Q:685:LEU:HB2	2.21	0.40
42:S:74:GLN:O	42:S:78:MET:HB2	2.20	0.40
54:8:153:G:O6	54:8:225:U:O4	2.40	0.40
54:8:488:U:O2'	54:8:490:A:OP1	2.37	0.40
2:b:318:VAL:HG22	2:b:325:VAL:HG12	2.04	0.40
6:i:8:ILE:HA	6:i:11:LEU:HG	2.04	0.40
7:j:98:SER:HB2	11:n:258:ASP:HB2	2.04	0.40
15:r:179:ILE:HB	33:K:237:GLU:CG	2.50	0.40
15:r:191:LEU:HD23	15:r:191:LEU:HA	1.98	0.40
18:u:16:LEU:HG	18:u:37:ILE:HB	2.03	0.40
31:I:104:ARG:NH2	39:P:508:GLU:OE1	2.54	0.40
41:R:245:ARG:HH12	41:R:282:ARG:HH11	1.68	0.40
46:1:160:G:H2'	46:1:161:G:C8	2.57	0.40
53:7:401:G:N2	53:7:402:G:O6	2.48	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	a	259/383 (68%)	251 (97%)	8 (3%)	0	100	100
2	b	302/417 (72%)	284 (94%)	16 (5%)	2 (1%)	18	53
3	c	301/427 (70%)	288 (96%)	11 (4%)	2 (1%)	18	53
4	d	182/216 (84%)	168 (92%)	14 (8%)	0	100	100
5	f	58/304 (19%)	54 (93%)	4 (7%)	0	100	100
6	i	150/277 (54%)	139 (93%)	11 (7%)	0	100	100
7	j	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	16	50
8	k	208/337 (62%)	198 (95%)	8 (4%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	l	134/270 (50%)	127 (95%)	6 (4%)	1 (1%)	18	53
10	m	175/183 (96%)	169 (97%)	5 (3%)	1 (1%)	21	56
11	n	171/312 (55%)	163 (95%)	6 (4%)	2 (1%)	10	40
12	o	108/115 (94%)	107 (99%)	1 (1%)	0	100	100
13	p	200/370 (54%)	187 (94%)	11 (6%)	2 (1%)	12	45
14	q	159/377 (42%)	150 (94%)	9 (6%)	0	100	100
15	r	154/226 (68%)	142 (92%)	11 (7%)	1 (1%)	21	56
16	s	177/309 (57%)	159 (90%)	16 (9%)	2 (1%)	11	43
17	t	186/366 (51%)	172 (92%)	14 (8%)	0	100	100
18	u	124/173 (72%)	121 (98%)	2 (2%)	1 (1%)	16	50
19	v	118/153 (77%)	107 (91%)	11 (9%)	0	100	100
20	w	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
21	x	163/214 (76%)	157 (96%)	6 (4%)	0	100	100
22	y	69/123 (56%)	63 (91%)	6 (9%)	0	100	100
23	z	51/59 (86%)	48 (94%)	3 (6%)	0	100	100
24	A	48/280 (17%)	46 (96%)	2 (4%)	0	100	100
25	B	126/151 (83%)	116 (92%)	9 (7%)	1 (1%)	16	50
26	e	162/207 (78%)	150 (93%)	12 (7%)	0	100	100
27	D	92/172 (54%)	80 (87%)	12 (13%)	0	100	100
28	E	77/112 (69%)	74 (96%)	3 (4%)	0	100	100
29	F	127/141 (90%)	116 (91%)	11 (9%)	0	100	100
30	G	195/259 (75%)	184 (94%)	11 (6%)	0	100	100
31	I	95/132 (72%)	93 (98%)	2 (2%)	0	100	100
32	J	94/134 (70%)	84 (89%)	10 (11%)	0	100	100
33	K	191/249 (77%)	184 (96%)	6 (3%)	1 (0%)	24	60
34	L	135/206 (66%)	126 (93%)	9 (7%)	0	100	100
36	M	385/876 (44%)	368 (96%)	17 (4%)	0	100	100
37	N	279/455 (61%)	262 (94%)	16 (6%)	1 (0%)	30	65
38	O	509/688 (74%)	459 (90%)	50 (10%)	0	100	100
39	P	430/530 (81%)	400 (93%)	30 (7%)	0	100	100
40	Q	260/820 (32%)	237 (91%)	23 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	R	280/653 (43%)	264 (94%)	16 (6%)	0	100	100
42	S	230/334 (69%)	210 (91%)	20 (9%)	0	100	100
All	All	7400/12257 (60%)	6926 (94%)	454 (6%)	20 (0%)	37	70

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	p	221	ALA
13	p	266	PRO
2	b	287	ARG
3	c	181	PRO
10	m	9	GLY
11	n	157	LYS
16	s	70	PRO
18	u	130	GLN
3	c	313	TYR
8	k	285	ARG
8	k	290	LEU
11	n	186	ARG
37	N	232	SER
33	K	170	SER
2	b	387	PRO
7	j	106	LYS
16	s	171	ILE
9	l	157	PRO
25	B	118	VAL
15	r	150	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	a	209/295 (71%)	209 (100%)	0	100	100
2	b	244/331 (74%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	254/313 (81%)	254 (100%)	0	100	100
4	d	144/164 (88%)	144 (100%)	0	100	100
5	f	47/209 (22%)	47 (100%)	0	100	100
6	i	133/214 (62%)	133 (100%)	0	100	100
7	j	99/99 (100%)	98 (99%)	1 (1%)	68	84
8	k	165/247 (67%)	165 (100%)	0	100	100
9	l	112/197 (57%)	112 (100%)	0	100	100
10	m	152/157 (97%)	150 (99%)	2 (1%)	61	81
11	n	153/245 (62%)	152 (99%)	1 (1%)	76	86
12	o	93/96 (97%)	93 (100%)	0	100	100
13	p	172/303 (57%)	171 (99%)	1 (1%)	78	88
14	q	128/269 (48%)	128 (100%)	0	100	100
15	r	143/184 (78%)	143 (100%)	0	100	100
16	s	156/157 (99%)	155 (99%)	1 (1%)	78	88
17	t	161/287 (56%)	161 (100%)	0	100	100
18	u	100/122 (82%)	98 (98%)	2 (2%)	48	76
19	v	109/122 (89%)	109 (100%)	0	100	100
20	w	106/112 (95%)	105 (99%)	1 (1%)	70	85
21	x	148/189 (78%)	148 (100%)	0	100	100
22	y	56/104 (54%)	55 (98%)	1 (2%)	51	77
23	z	49/54 (91%)	49 (100%)	0	100	100
24	A	45/219 (20%)	44 (98%)	1 (2%)	45	74
25	B	108/126 (86%)	108 (100%)	0	100	100
26	e	135/168 (80%)	135 (100%)	0	100	100
27	D	77/116 (66%)	77 (100%)	0	100	100
28	E	66/93 (71%)	66 (100%)	0	100	100
29	F	112/121 (93%)	112 (100%)	0	100	100
30	G	151/195 (77%)	150 (99%)	1 (1%)	76	86
31	I	82/105 (78%)	82 (100%)	0	100	100
32	J	75/87 (86%)	75 (100%)	0	100	100
33	K	158/193 (82%)	157 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	L	115/172 (67%)	115 (100%)	0	100	100
36	M	287/369 (78%)	287 (100%)	0	100	100
37	N	201/335 (60%)	198 (98%)	3 (2%)	57	80
38	O	403/466 (86%)	403 (100%)	0	100	100
39	P	301/353 (85%)	301 (100%)	0	100	100
40	Q	191/313 (61%)	191 (100%)	0	100	100
41	R	199/336 (59%)	199 (100%)	0	100	100
42	S	206/254 (81%)	206 (100%)	0	100	100
All	All	6045/8491 (71%)	6029 (100%)	16 (0%)	84	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	j	111	LYS
10	m	133	LEU
10	m	135	ARG
11	n	142	LEU
13	p	177	LEU
16	s	165	VAL
18	u	119	LEU
18	u	131	LEU
20	w	11	LEU
22	y	103	CYS
24	A	232	ASN
30	G	166	ASN
33	K	65	ARG
37	N	183	ARG
37	N	206	LEU
37	N	238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	143	GLN
1	a	175	GLN
1	a	206	ASN
1	a	220	HIS
1	a	275	ASN

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Mol	Chain	Res	Type
1	a	282	ASN
1	a	304	ASN
2	b	195	GLN
2	b	288	GLN
3	c	184	GLN
4	d	98	ASN
6	i	46	GLN
7	j	70	GLN
7	j	105	ASN
8	k	123	ASN
8	k	308	GLN
9	l	139	GLN
9	l	158	ASN
11	n	150	GLN
11	n	160	GLN
12	o	24	ASN
13	p	136	GLN
13	p	139	GLN
13	p	236	ASN
14	q	281	HIS
15	r	60	ASN
15	r	181	GLN
16	s	152	GLN
17	t	288	ASN
17	t	324	ASN
17	t	327	ASN
17	t	353	ASN
19	v	24	GLN
19	v	26	HIS
20	w	68	HIS
20	w	94	GLN
21	x	49	ASN
23	z	33	ASN
24	A	232	ASN
24	A	238	GLN
25	B	60	ASN
25	B	112	HIS
26	e	55	ASN
26	e	89	GLN
26	e	93	ASN
28	E	96	GLN
29	F	41	ASN

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Mol	Chain	Res	Type
29	F	112	GLN
30	G	166	ASN
30	G	188	HIS
33	K	164	ASN
33	K	173	HIS
33	K	225	HIS
34	L	85	HIS
36	M	108	GLN
36	M	160	GLN
36	M	430	HIS
36	M	482	GLN
37	N	154	GLN
38	O	176	GLN
38	O	232	GLN
38	O	256	GLN
38	O	525	GLN
38	O	560	GLN
39	P	362	HIS
39	P	510	GLN
40	Q	135	ASN
40	Q	227	GLN
42	S	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	1	159/162 (98%)	43 (27%)	1 (0%)
47	2	85/86 (98%)	24 (28%)	2 (2%)
48	0	74/75 (98%)	31 (41%)	0
49	3	183/184 (99%)	32 (17%)	1 (0%)
50	4	117/118 (99%)	22 (18%)	0
51	5	146/149 (97%)	62 (42%)	1 (0%)
52	6	135/136 (99%)	35 (25%)	3 (2%)
53	7	574/578 (99%)	158 (27%)	5 (0%)
54	8	411/413 (99%)	153 (37%)	9 (2%)
All	All	1884/1901 (99%)	560 (29%)	22 (1%)

All (560) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	1	6	A

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Mol	Chain	Res	Type
46	1	7	U
46	1	10	C
46	1	24	A
46	1	26	A
46	1	27	C
46	1	38	A
46	1	59	A
46	1	76	A
46	1	79	U
46	1	81	C
46	1	89	A
46	1	91	C
46	1	92	A
46	1	93	A
46	1	94	U
46	1	95	A
46	1	96	C
46	1	97	G
46	1	100	A
46	1	107	G
46	1	117	A
46	1	119	U
46	1	120	C
46	1	121	U
46	1	125	G
46	1	136	U
46	1	137	G
46	1	140	C
46	1	143	A
46	1	156	U
46	1	158	U
46	1	159	U
46	1	163	A
46	1	167	G
46	1	168	A
46	1	170	U
46	1	172	C
46	1	176	U
46	1	177	C
46	1	178	G
46	1	179	U
46	1	181	A

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Mol	Chain	Res	Type
47	2	4	A
47	2	7	U
47	2	10	A
47	2	12	U
47	2	13	U
47	2	19	U
47	2	20	A
47	2	28	C
47	2	30	U
47	2	31	U
47	2	32	A
47	2	60	U
47	2	61	A
47	2	69	A
47	2	70	G
47	2	77	G
47	2	78	A
47	2	80	A
47	2	81	U
47	2	82	U
47	2	83	U
47	2	85	U
47	2	87	U
47	2	88	A
48	0	28	G
48	0	29	C
48	0	30	U
48	0	32	G
48	0	33	G
48	0	35	G
48	0	36	A
48	0	43	G
48	0	44	C
48	0	45	A
48	0	47	C
48	0	48	C
48	0	49	A
48	0	50	A
48	0	51	U
48	0	52	A
48	0	55	A
48	0	57	A

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Mol	Chain	Res	Type
48	0	58	G
48	0	62	C
48	0	63	U
48	0	69	G
48	0	72	U
48	0	74	A
48	0	75	G
48	0	76	U
48	0	77	A
48	0	90	U
48	0	92	U
48	0	93	U
48	0	99	A
49	3	17	A
49	3	19	A
49	3	23	A
49	3	24	U
49	3	27	A
49	3	28	U
49	3	52	U
49	3	53	A
49	3	59	G
49	3	60	A
49	3	78	G
49	3	88	G
49	3	94	A
49	3	100	G
49	3	105	G
49	3	106	G
49	3	112	A
49	3	114	G
49	3	115	G
49	3	120	U
49	3	121	C
49	3	124	G
49	3	132	A
49	3	135	G
49	3	136	C
49	3	141	U
49	3	142	U
49	3	157	U
49	3	175	C

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Mol	Chain	Res	Type
49	3	176	U
49	3	177	A
49	3	178	A
50	4	2	U
50	4	7	G
50	4	34	A
50	4	35	A
50	4	41	C
50	4	44	A
50	4	49	G
50	4	57	G
50	4	59	G
50	4	60	G
50	4	61	U
50	4	64	G
50	4	68	A
50	4	77	G
50	4	86	A
50	4	88	U
50	4	92	G
50	4	99	G
50	4	106	G
50	4	108	G
50	4	116	A
50	4	118	U
51	5	4	G
51	5	5	U
51	5	7	G
51	5	11	C
51	5	12	U
51	5	13	G
51	5	14	C
51	5	17	U
51	5	18	G
51	5	25	A
51	5	26	G
51	5	31	U
51	5	34	G
51	5	37	U
51	5	40	A
51	5	41	A
51	5	42	G

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Mol	Chain	Res	Type
51	5	43	C
51	5	44	A
51	5	50	U
51	5	53	G
51	5	54	C
51	5	56	U
51	5	59	A
51	5	60	A
51	5	62	G
51	5	66	A
51	5	67	A
51	5	69	A
51	5	70	G
51	5	71	C
51	5	72	U
51	5	75	C
51	5	76	U
51	5	77	G
51	5	81	U
51	5	83	G
51	5	84	C
51	5	85	A
51	5	87	U
51	5	90	C
51	5	91	C
51	5	96	A
51	5	97	U
51	5	98	A
51	5	100	A
51	5	101	U
51	5	103	U
51	5	104	C
51	5	105	C
51	5	106	G
51	5	107	G
51	5	110	C
51	5	118	U
51	5	119	U
51	5	137	A
51	5	140	A
51	5	152	U
51	5	154	U

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Mol	Chain	Res	Type
51	5	156	U
51	5	157	U
51	5	159	U
52	6	5	C
52	6	11	U
52	6	18	A
52	6	27	A
52	6	28	A
52	6	29	C
52	6	30	A
52	6	32	U
52	6	33	U
52	6	48	A
52	6	54	A
52	6	56	U
52	6	61	C
52	6	63	G
52	6	69	A
52	6	78	A
52	6	81	A
52	6	82	A
52	6	86	G
52	6	87	A
52	6	88	U
52	6	90	A
52	6	99	U
52	6	100	A
52	6	101	A
52	6	112	U
52	6	117	U
52	6	118	A
52	6	119	A
52	6	120	C
52	6	121	A
52	6	122	A
52	6	123	A
52	6	128	G
52	6	131	U
53	7	9	C
53	7	11	G
53	7	12	C
53	7	13	A

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Mol	Chain	Res	Type
53	7	14	A
53	7	15	A
53	7	24	G
53	7	35	A
53	7	36	U
53	7	38	U
53	7	43	U
53	7	50	A
53	7	52	A
53	7	55	A
53	7	58	A
53	7	68	A
53	7	78	G
53	7	79	C
53	7	85	G
53	7	86	C
53	7	87	A
53	7	89	G
53	7	90	C
53	7	91	G
53	7	93	G
53	7	95	C
53	7	97	U
53	7	99	G
53	7	102	G
53	7	109	U
53	7	111	G
53	7	117	A
53	7	118	A
53	7	119	G
53	7	121	C
53	7	122	U
53	7	127	A
53	7	132	G
53	7	133	C
53	7	142	A
53	7	151	C
53	7	152	A
53	7	153	A
53	7	169	C
53	7	170	U
53	7	176	A

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Mol	Chain	Res	Type
53	7	177	C
53	7	178	G
53	7	180	A
53	7	181	A
53	7	182	A
53	7	189	U
53	7	191	C
53	7	193	A
53	7	194	A
53	7	195	A
53	7	196	A
53	7	199	G
53	7	200	G
53	7	207	U
53	7	214	U
53	7	218	U
53	7	219	A
53	7	227	A
53	7	253	G
53	7	260	G
53	7	262	A
53	7	263	A
53	7	264	C
53	7	267	U
53	7	268	A
53	7	270	C
53	7	272	G
53	7	275	C
53	7	279	G
53	7	280	G
53	7	281	U
53	7	287	A
53	7	288	A
53	7	289	U
53	7	290	U
53	7	293	U
53	7	294	U
53	7	295	G
53	7	297	C
53	7	305	U
53	7	306	G
53	7	312	C

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Mol	Chain	Res	Type
53	7	313	U
53	7	316	A
53	7	317	U
53	7	319	A
53	7	320	A
53	7	322	G
53	7	324	C
53	7	325	G
53	7	335	U
53	7	337	G
53	7	341	U
53	7	342	G
53	7	343	U
53	7	347	U
53	7	356	A
53	7	371	A
53	7	373	C
53	7	381	A
53	7	383	A
53	7	385	G
53	7	386	C
53	7	393	G
53	7	402	G
53	7	405	C
53	7	406	G
53	7	410	A
53	7	411	G
53	7	412	A
53	7	418	U
53	7	419	G
53	7	431	G
53	7	435	C
53	7	525	C
53	7	526	C
53	7	530	A
53	7	533	U
53	7	535	U
53	7	540	G
53	7	548	G
53	7	555	A
53	7	556	A
53	7	557	A

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Mol	Chain	Res	Type
53	7	569	G
53	7	572	A
53	7	575	A
53	7	576	A
53	7	577	U
53	7	578	G
53	7	592	C
53	7	593	U
53	7	594	U
53	7	595	A
53	7	596	A
53	7	602	A
53	7	607	G
53	7	608	U
53	7	613	G
53	7	615	C
53	7	618	U
53	7	622	A
53	7	624	C
53	7	626	A
53	7	629	G
53	7	640	G
53	7	644	C
53	7	647	G
53	7	651	G
53	7	653	A
53	7	658	U
53	7	659	G
54	8	64	C
54	8	68	U
54	8	70	A
54	8	72	C
54	8	74	G
54	8	75	A
54	8	77	A
54	8	80	A
54	8	85	C
54	8	86	G
54	8	93	A
54	8	94	U
54	8	98	A
54	8	99	G

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Mol	Chain	Res	Type
54	8	104	A
54	8	105	U
54	8	113	U
54	8	115	G
54	8	119	U
54	8	121	C
54	8	123	A
54	8	127	A
54	8	131	G
54	8	136	U
54	8	143	C
54	8	145	U
54	8	147	G
54	8	148	A
54	8	149	U
54	8	150	G
54	8	151	U
54	8	152	C
54	8	153	G
54	8	155	A
54	8	158	A
54	8	163	G
54	8	165	C
54	8	169	U
54	8	170	G
54	8	173	U
54	8	174	G
54	8	175	A
54	8	178	G
54	8	189	G
54	8	190	G
54	8	193	G
54	8	194	G
54	8	196	U
54	8	198	G
54	8	199	U
54	8	200	U
54	8	202	G
54	8	203	U
54	8	204	C
54	8	205	C
54	8	206	A

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Mol	Chain	Res	Type
54	8	207	U
54	8	208	U
54	8	209	A
54	8	211	A
54	8	212	G
54	8	213	U
54	8	216	U
54	8	217	A
54	8	218	C
54	8	228	G
54	8	229	U
54	8	230	U
54	8	231	C
54	8	244	G
54	8	248	G
54	8	250	U
54	8	254	U
54	8	258	U
54	8	260	U
54	8	261	C
54	8	262	U
54	8	268	A
54	8	269	G
54	8	272	A
54	8	273	A
54	8	274	A
54	8	277	C
54	8	278	U
54	8	279	U
54	8	281	U
54	8	283	U
54	8	284	U
54	8	310	A
54	8	312	C
54	8	314	C
54	8	317	A
54	8	324	G
54	8	325	U
54	8	326	U
54	8	327	A
54	8	334	G
54	8	342	G

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Mol	Chain	Res	Type
54	8	343	U
54	8	344	A
54	8	345	C
54	8	350	G
54	8	352	A
54	8	353	C
54	8	354	C
54	8	355	A
54	8	356	G
54	8	358	C
54	8	361	C
54	8	367	A
54	8	370	U
54	8	377	C
54	8	378	A
54	8	391	U
54	8	392	A
54	8	402	G
54	8	413	A
54	8	414	A
54	8	420	A
54	8	421	A
54	8	422	A
54	8	423	A
54	8	424	G
54	8	425	G
54	8	436	U
54	8	437	A
54	8	438	C
54	8	439	A
54	8	440	U
54	8	444	A
54	8	445	U
54	8	446	A
54	8	447	A
54	8	449	A
54	8	450	C
54	8	452	G
54	8	458	C
54	8	467	A
54	8	468	C
54	8	470	A

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Mol	Chain	Res	Type
54	8	471	A
54	8	475	U
54	8	477	U
54	8	481	A
54	8	482	C
54	8	483	U
54	8	486	A
54	8	487	U
54	8	488	U
54	8	489	U
54	8	490	A
54	8	491	U
54	8	492	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	1	177	C
47	2	81	U
47	2	87	U
49	3	23	A
51	5	66	A
52	6	29	C
52	6	120	C
52	6	130	A
53	7	35	A
53	7	108	G
53	7	179	U
53	7	594	U
53	7	614	A
54	8	67	A
54	8	212	G
54	8	278	U
54	8	309	A
54	8	316	U
54	8	324	G
54	8	343	U
54	8	420	A
54	8	422	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	FES	S	401	42	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	FES	S	401	42	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	Q	6
53	7	3
44	Y	3
46	1	2
41	R	2
51	5	2
36	M	2
3	c	1
54	8	1
38	O	1
42	S	1
16	s	1
32	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	59:A	O3'	75:U	P	56.66
1	R	536:UNK	C	553:UNK	N	27.93
1	c	276:UNK	C	291:SER	N	25.05
1	5	111:U	O3'	117:A	P	21.41
1	R	477:ALA	C	493:UNK	N	21.21
1	7	231:C	O3'	249:A	P	20.90
1	M	550:UNK	C	572:UNK	N	19.54
1	8	284:U	O3'	308:G	P	19.48
1	Y	100:UNK	C	109:UNK	N	14.75
1	7	443:U	O3'	517:A	P	14.55
1	Q	367:UNK	C	386:UNK	N	13.78
1	Y	57:UNK	C	70:UNK	N	13.31
1	1	147:A	O3'	150:U	P	12.70
1	Y	22:UNK	C	26:UNK	N	10.61
1	O	596:VAL	C	600:UNK	N	9.67
1	Q	541:UNK	C	545:ALA	N	9.57
1	5	141:A	O3'	148:U	P	9.02
1	Q	411:UNK	C	444:UNK	N	8.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	286:UNK	C	295:LYS	N	8.47
1	s	180:ASP	C	191:UNK	N	7.42
1	7	586:U	O3'	591:A	P	7.42
1	Q	501:UNK	C	504:UNK	N	7.27
1	Q	693:CYS	C	705:UNK	N	7.13
1	J	113:ARG	C	116:UNK	N	7.12
1	M	523:PRO	C	530:UNK	N	5.32
1	Q	460:UNK	C	462:UNK	N	3.87

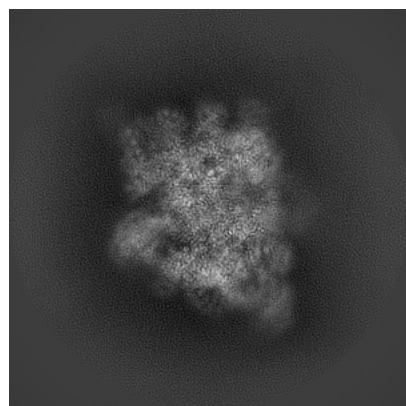
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13480. These allow visual inspection of the internal detail of the map and identification of artifacts.

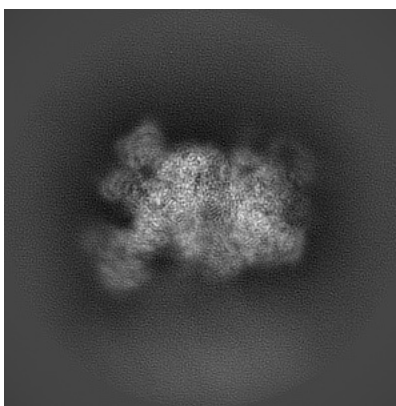
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

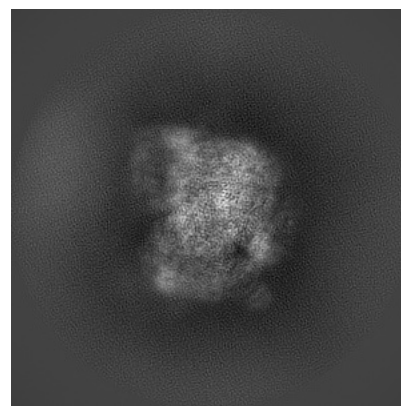
6.1.1 Primary map



X

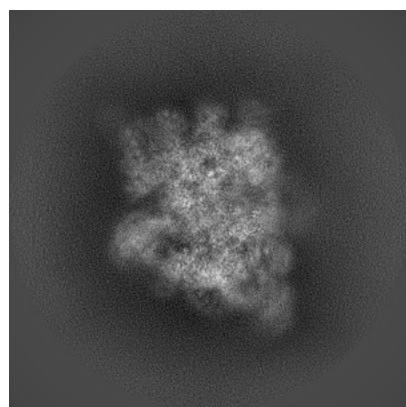


Y

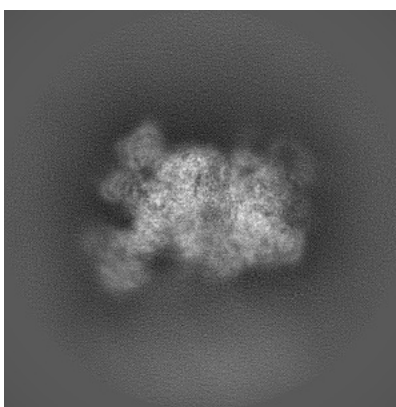


Z

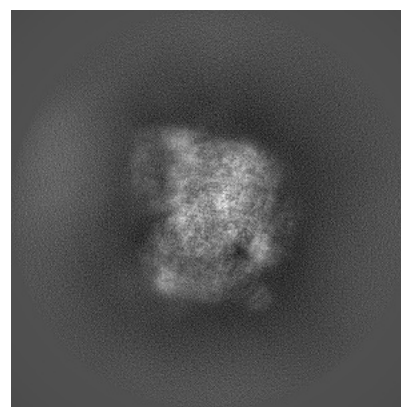
6.1.2 Raw map



X



Y

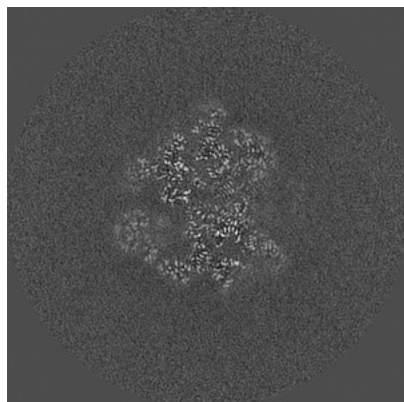


Z

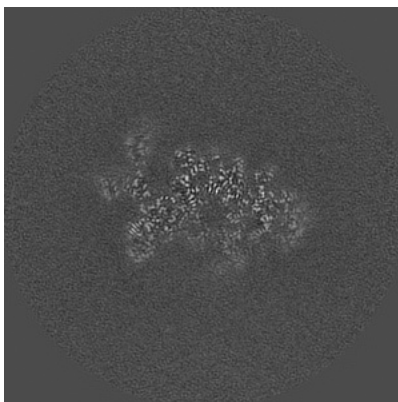
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

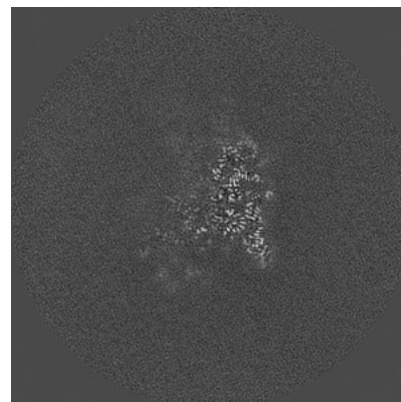
6.2.1 Primary map



X Index: 240

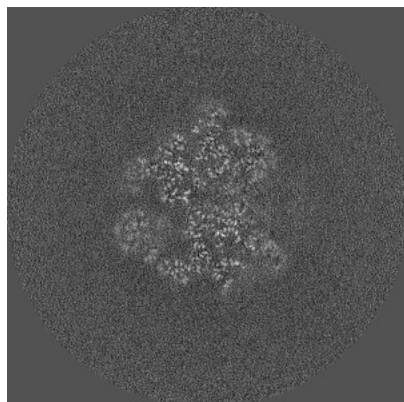


Y Index: 240

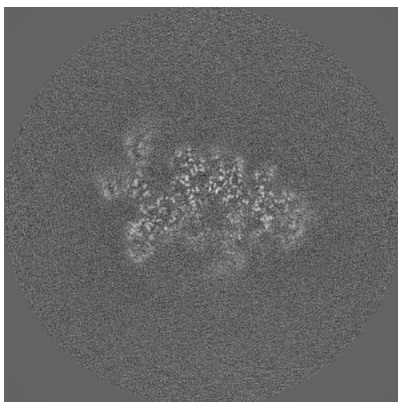


Z Index: 240

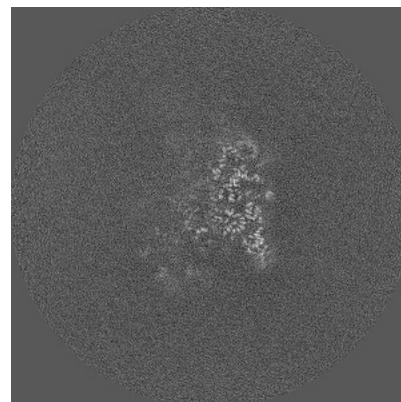
6.2.2 Raw map



X Index: 240



Y Index: 240

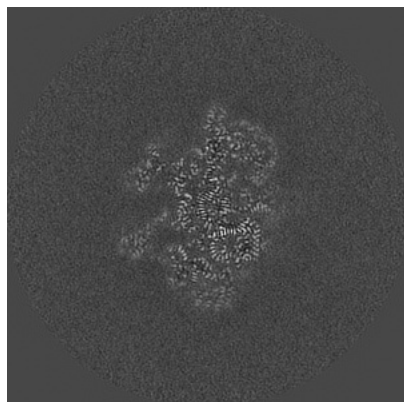


Z Index: 240

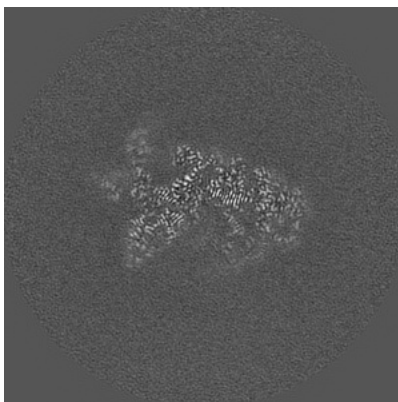
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

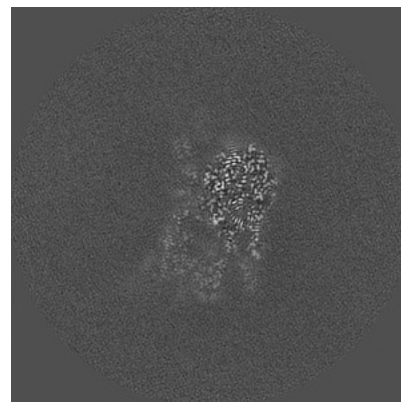
6.3.1 Primary map



X Index: 256

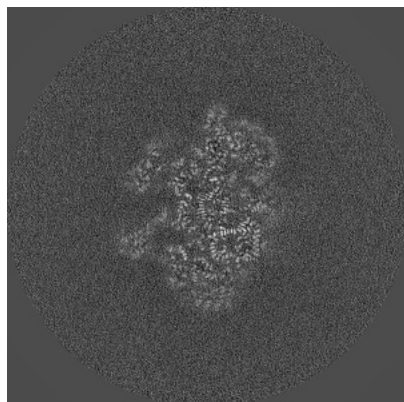


Y Index: 245

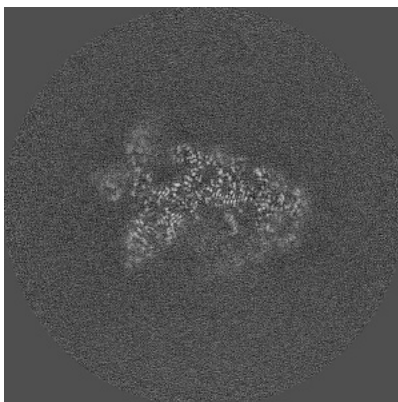


Z Index: 217

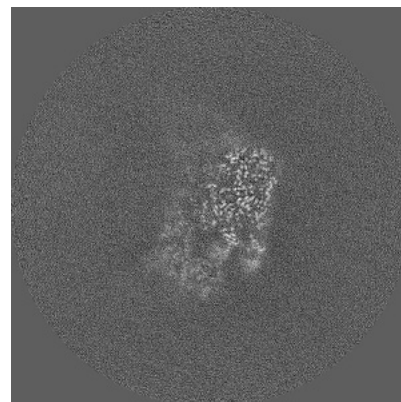
6.3.2 Raw map



X Index: 256



Y Index: 246

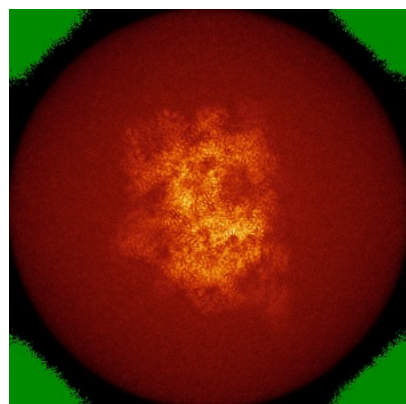


Z Index: 225

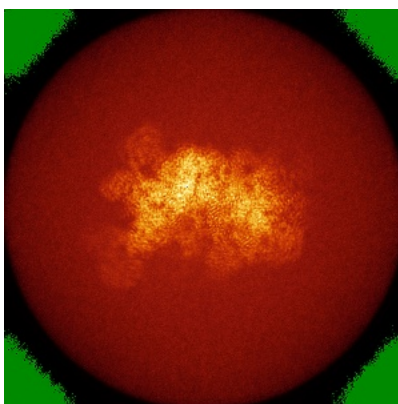
The images above show the largest variance slices of the map in three orthogonal directions.

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

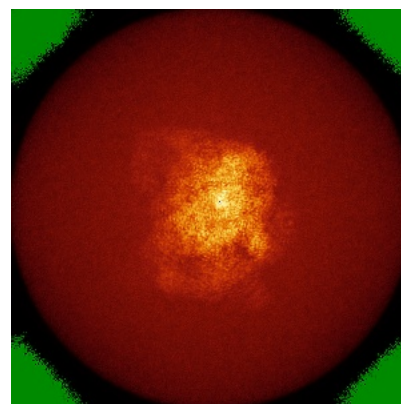
6.4.1 Primary map



X

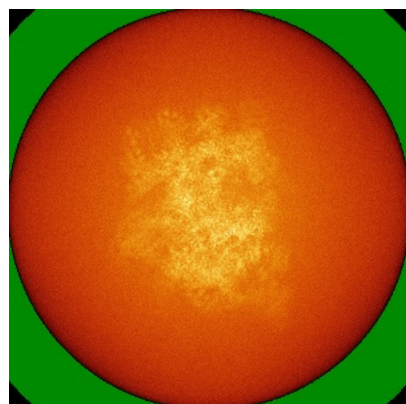


Y

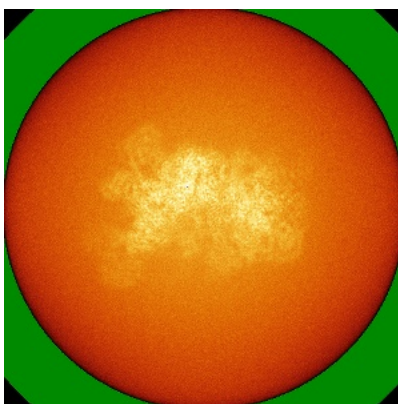


Z

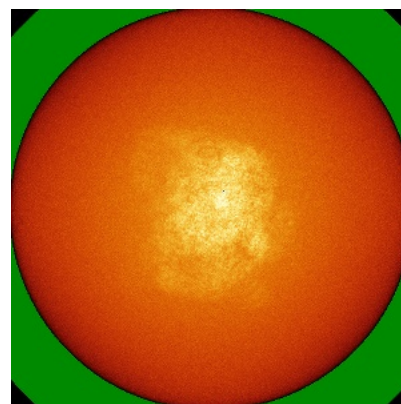
6.4.2 Raw map



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.

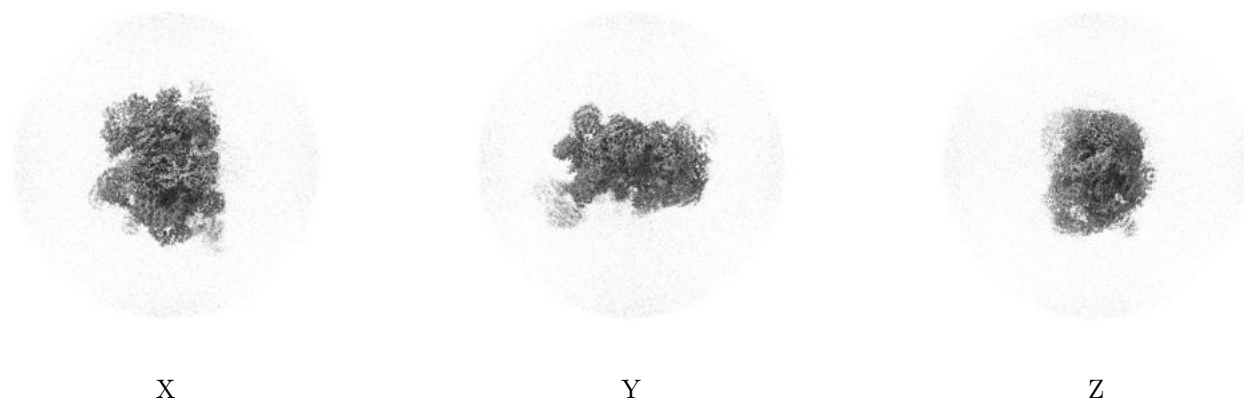
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

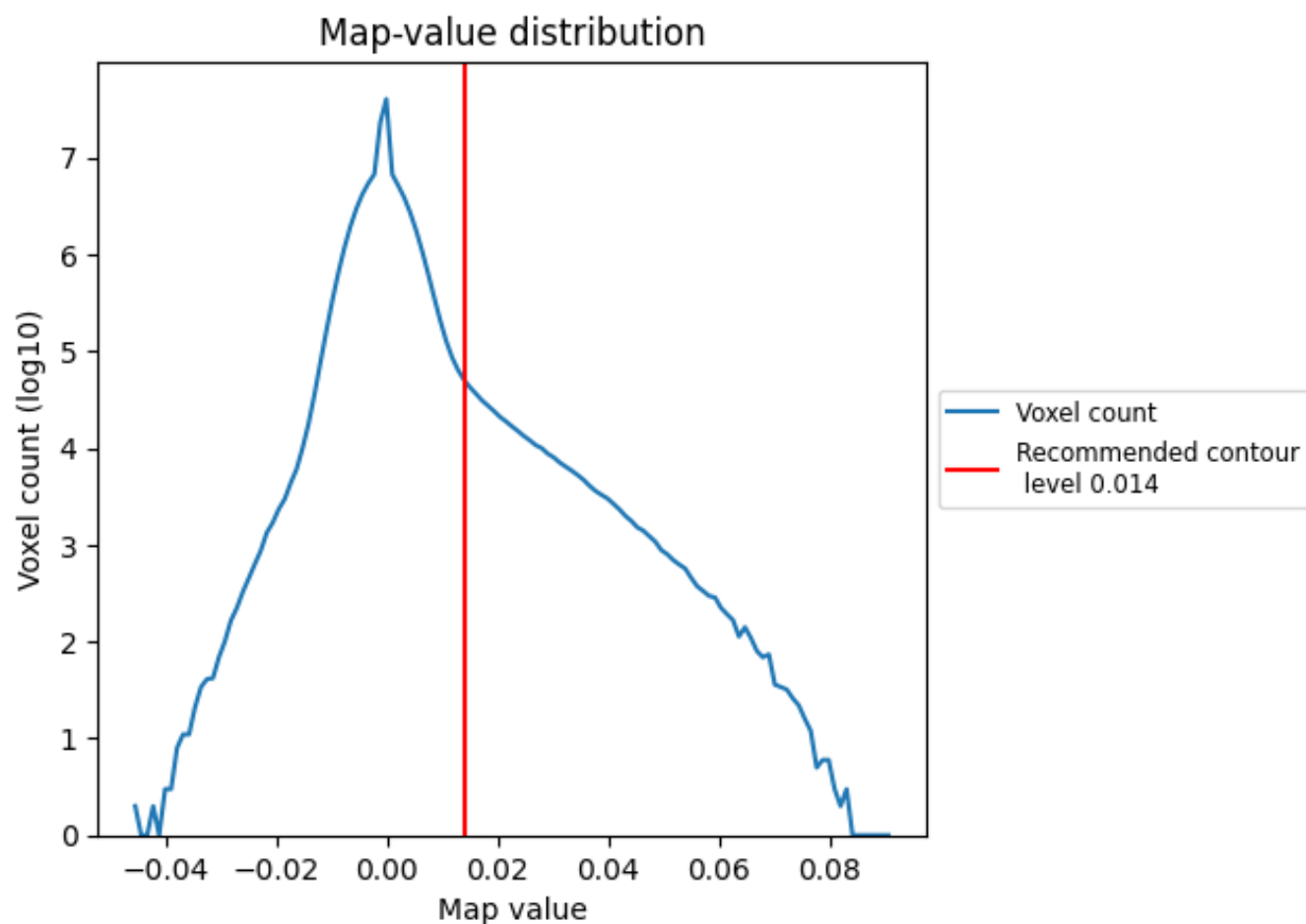
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

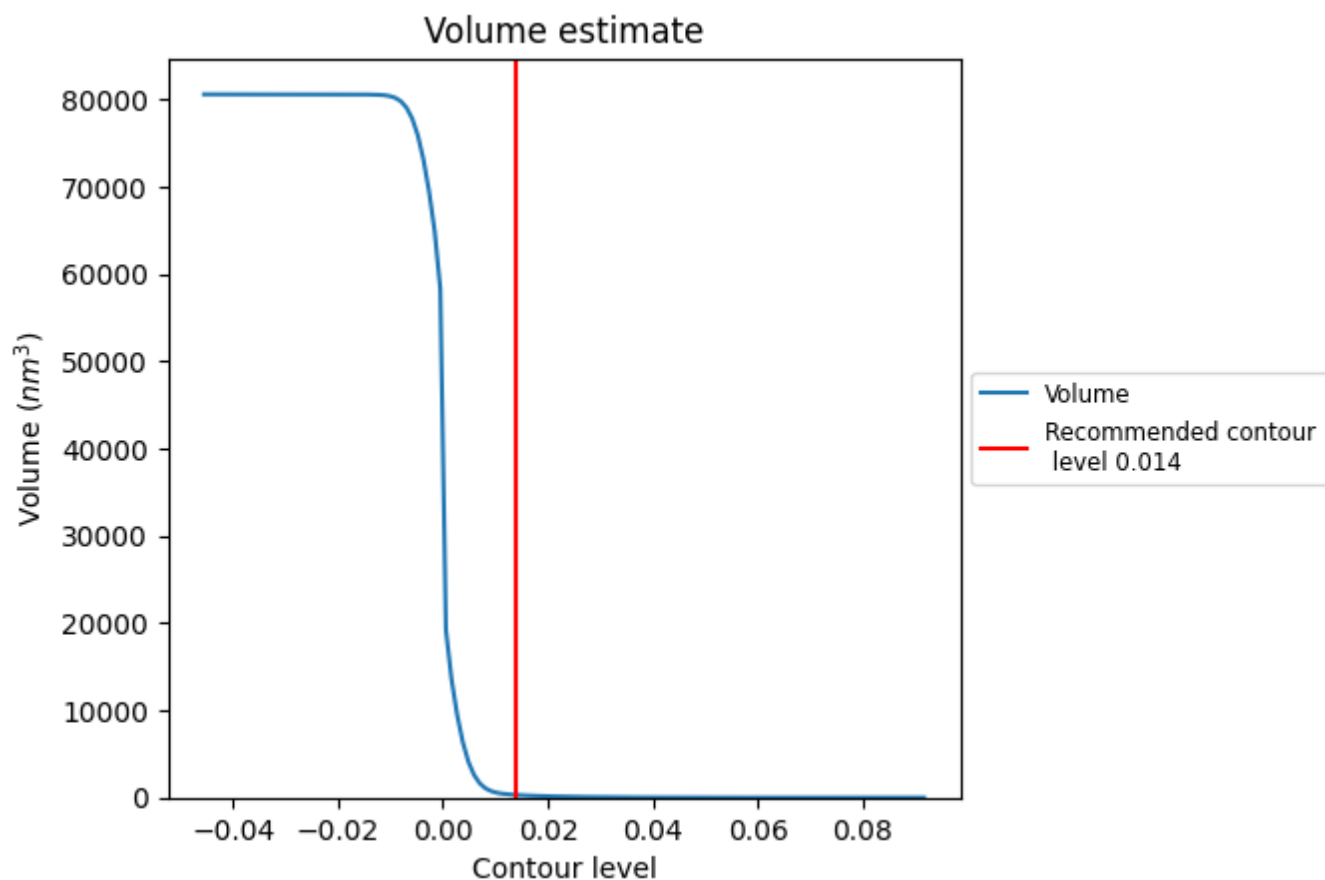
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

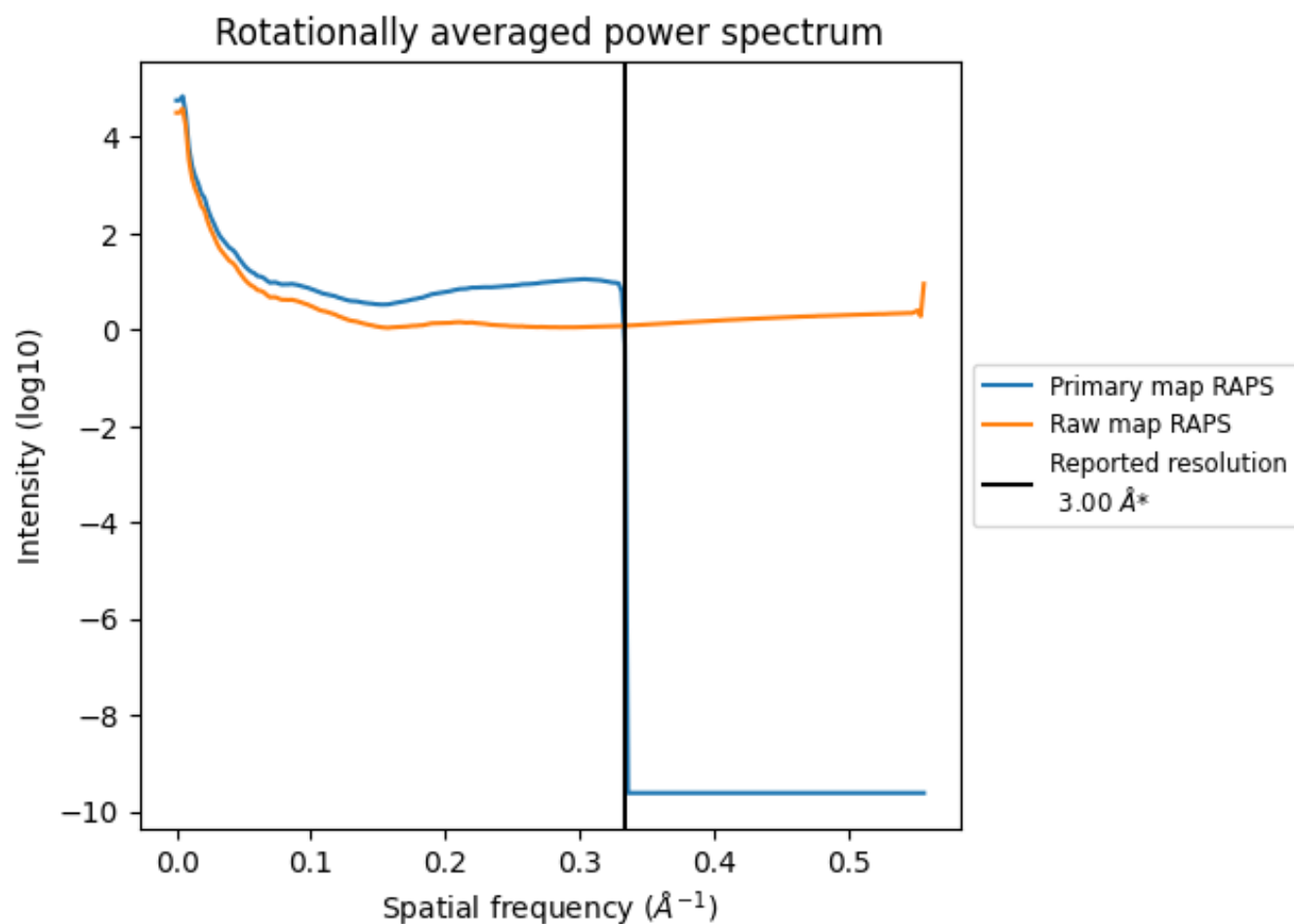
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 268 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

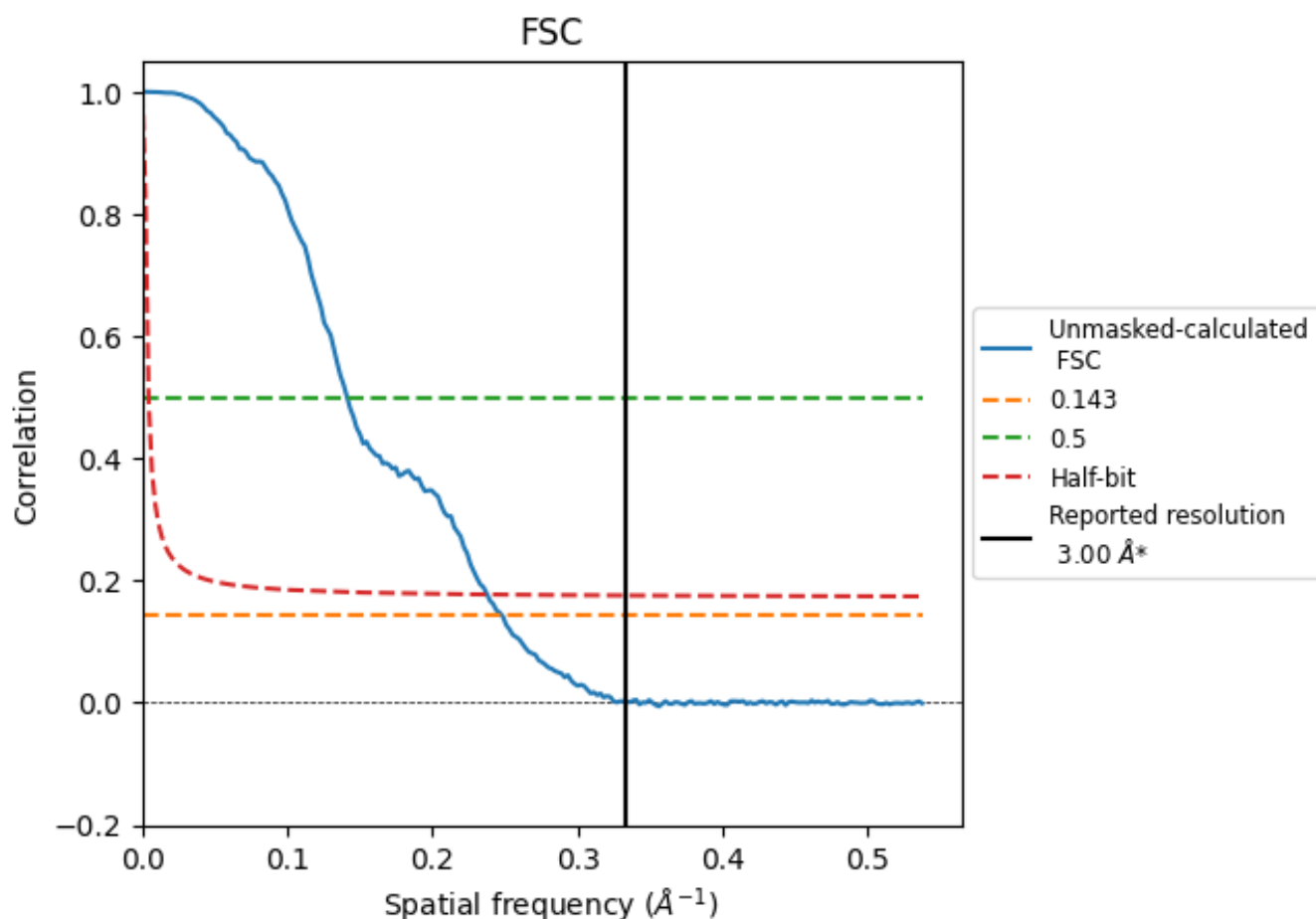


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

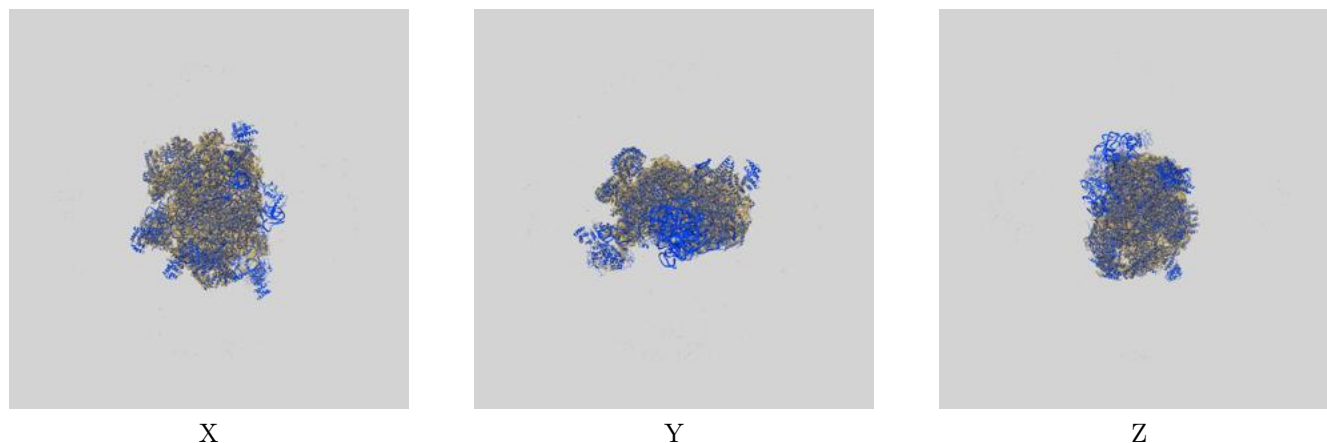
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.08	4.21

*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 4.03 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

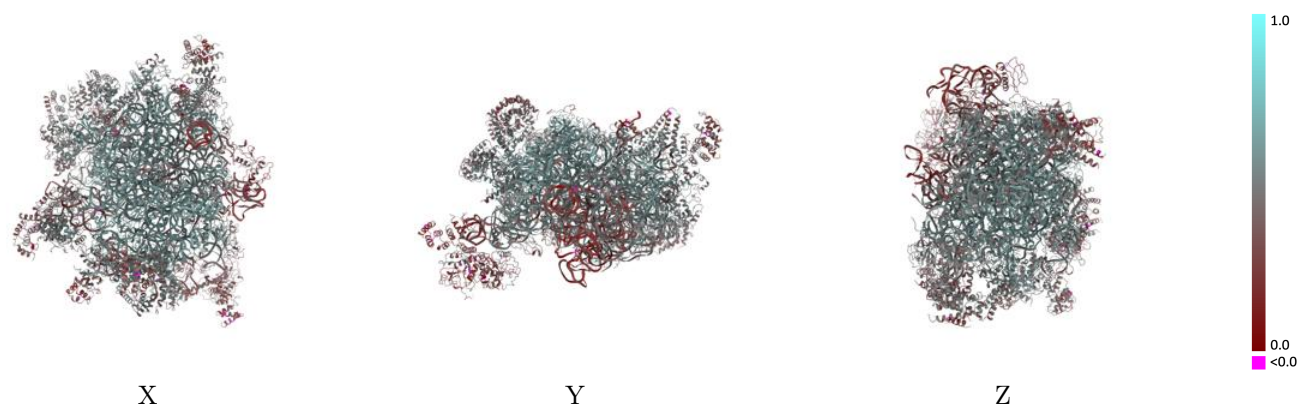
This section contains information regarding the fit between EMDB map EMD-13480 and PDB model 7PKT. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



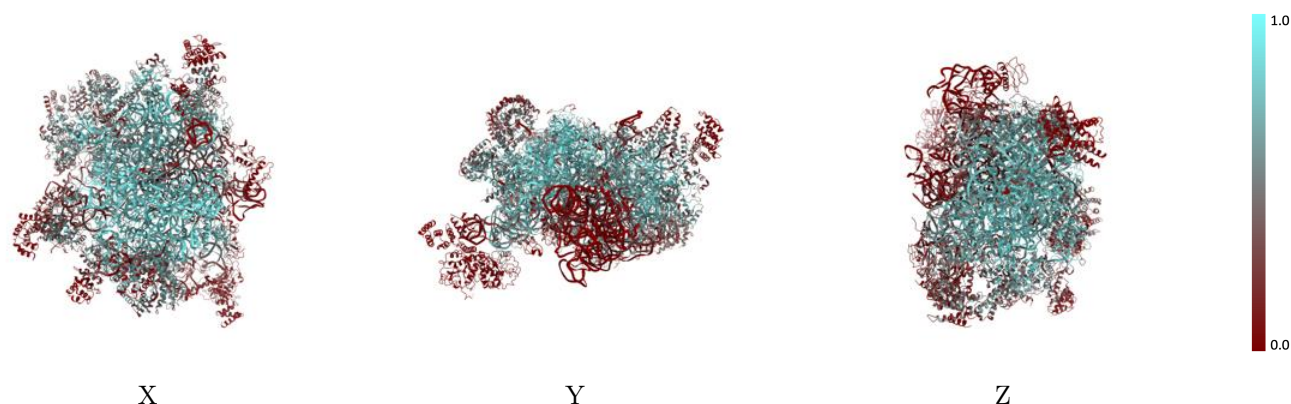
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



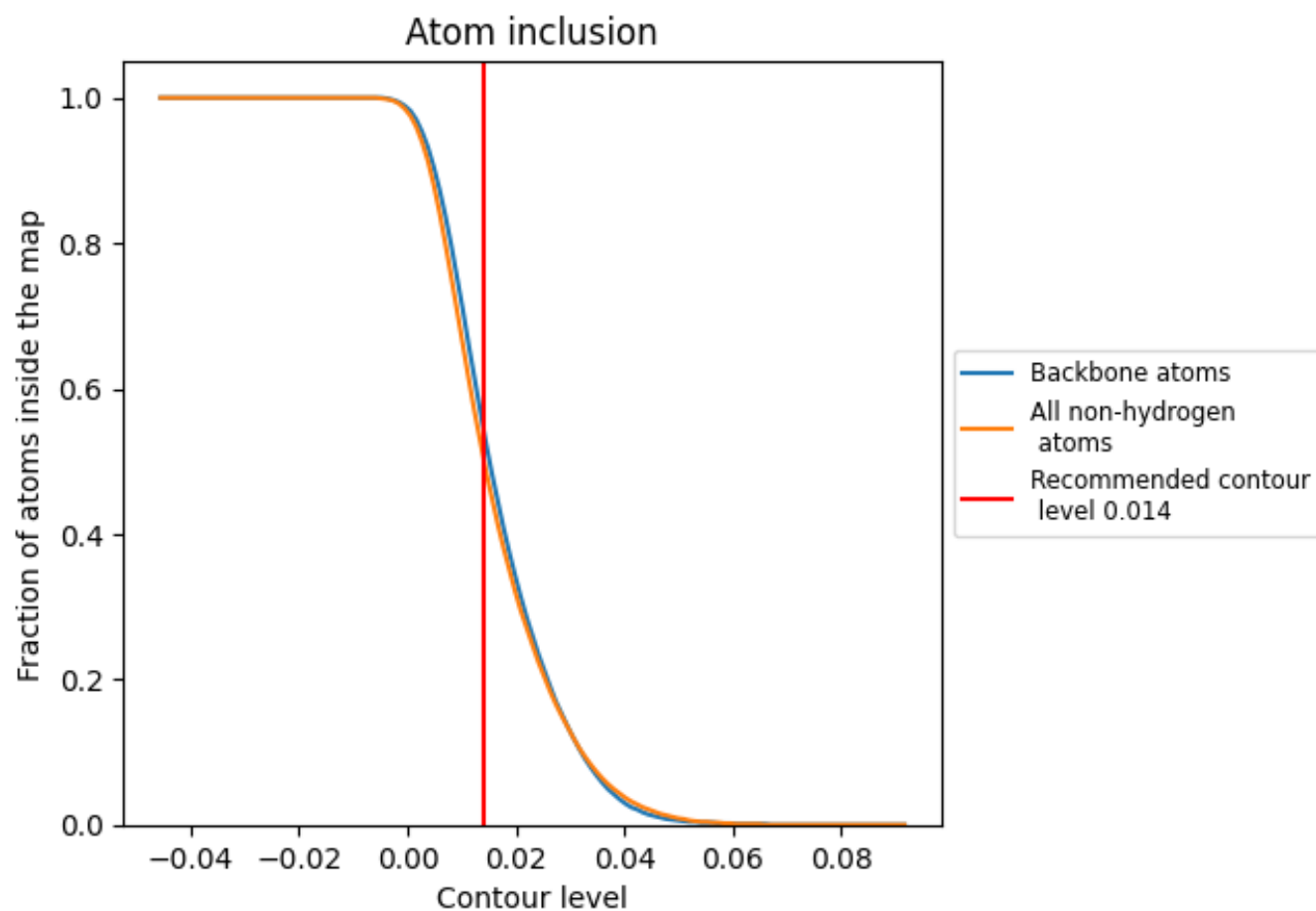
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 51% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5060	 0.4860
0	 0.3920	 0.4130
1	 0.6860	 0.5080
2	 0.8410	 0.5850
3	 0.8370	 0.5870
4	 0.8470	 0.5860
5	 0.2030	 0.3190
6	 0.8790	 0.5920
7	 0.5040	 0.4880
8	 0.3950	 0.4580
A	 0.8070	 0.6060
B	 0.6730	 0.5540
C	 0.0000	 0.3450
D	 0.0360	 0.3140
E	 0.6630	 0.5540
F	 0.8070	 0.5730
G	 0.0240	 0.3080
I	 0.6410	 0.5570
J	 0.4260	 0.4320
K	 0.5920	 0.5110
L	 0.7380	 0.5640
M	 0.4330	 0.4640
N	 0.3240	 0.4330
O	 0.3220	 0.4430
P	 0.6130	 0.5180
Q	 0.3650	 0.4270
R	 0.3000	 0.4340
S	 0.4790	 0.4690
X	 0.6520	 0.5040
Y	 0.0470	 0.2640
Z	 0.4900	 0.5040
a	 0.2330	 0.4870
b	 0.5380	 0.5210
c	 0.6640	 0.5470
d	 0.0570	 0.2890



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Chain	Atom inclusion	Q-score
e	 0.0010	 0.2910
f	 0.0860	 0.3620
i	 0.5540	 0.5510
j	 0.2890	 0.4600
k	 0.7240	 0.5670
l	 0.1280	 0.4360
m	 0.6520	 0.5370
n	 0.4750	 0.4570
o	 0.8120	 0.5880
p	 0.6820	 0.5270
q	 0.7290	 0.5750
r	 0.6880	 0.5620
s	 0.5890	 0.4980
t	 0.3190	 0.4350
u	 0.6690	 0.5380
v	 0.2800	 0.4740
w	 0.6580	 0.5290
x	 0.8010	 0.5880
y	 0.6960	 0.5550
z	 0.5840	 0.5070