Full wwPDB EM Validation Report

Aug 27, 2026 – 11:18 am BST

PDB ID	:	9HCH / pdb_00009hch
EMDB ID	:	EMD-52049
Title	:	Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, GTPBP7 and the MALSU1-L0R8F8-mt-ACP complex, State C1 (SAMC knock-out)
Authors	:	Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenberg, A.
Deposited on	:	2024-11-10
Resolution	:	2.85 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 (i) 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 (1)) were used in the production of this report:

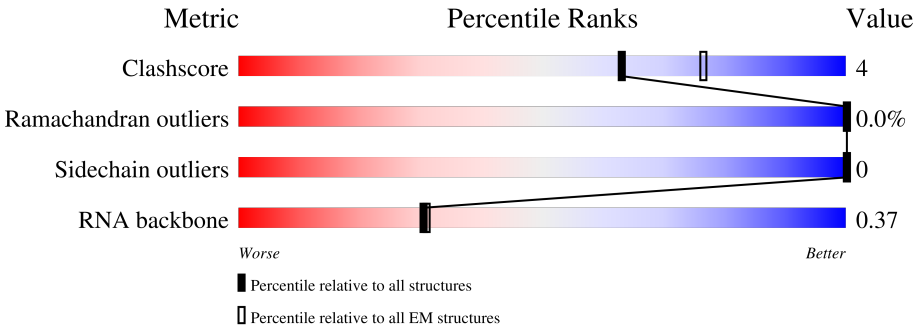
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

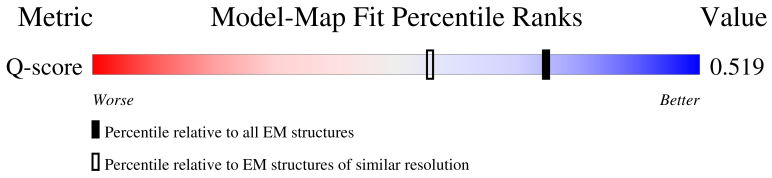
1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 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.





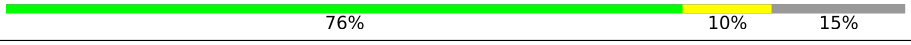
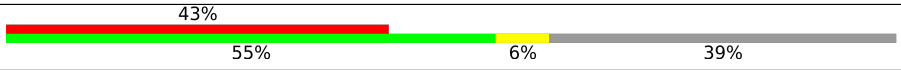
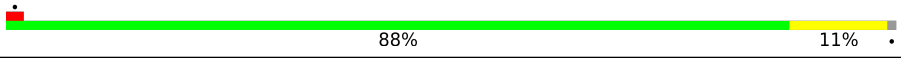
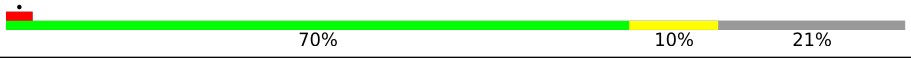
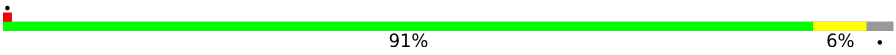
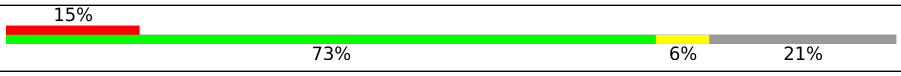
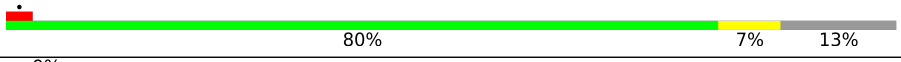
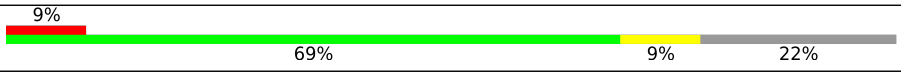
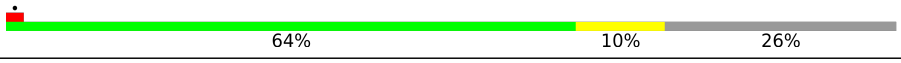
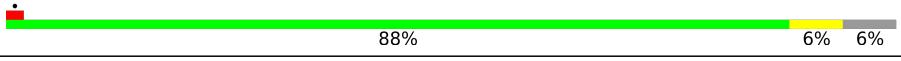
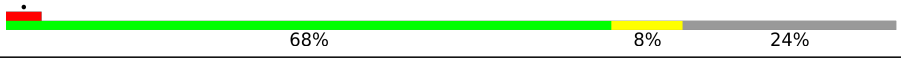
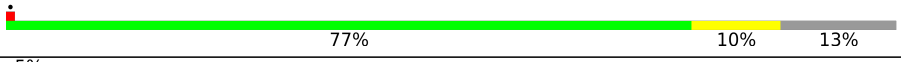
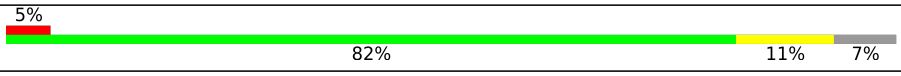
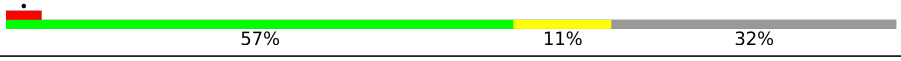
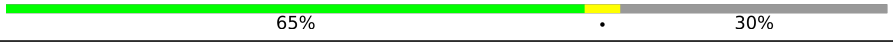
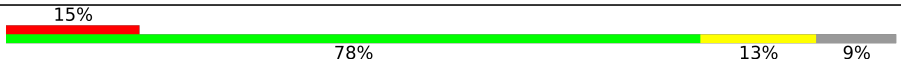
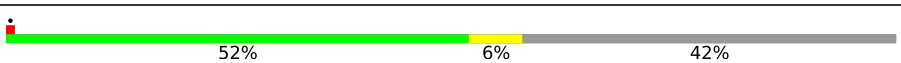
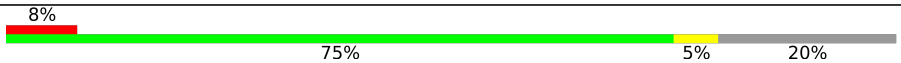
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11965 (2.35 - 3.35)

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 <=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	1584	5% 54% 28% 9% 9%
2	B	68	44% 37% 32% 22% 9%
3	D	246	84% 8% 8%

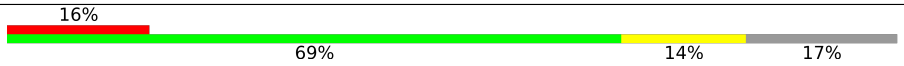
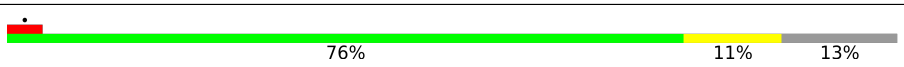
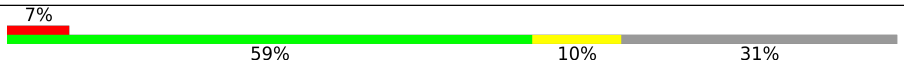
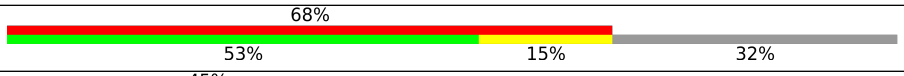
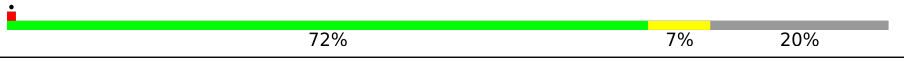
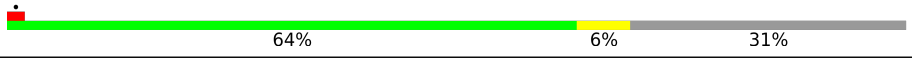
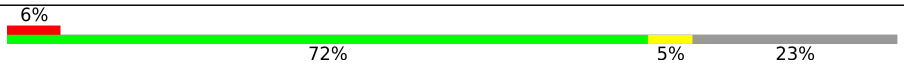
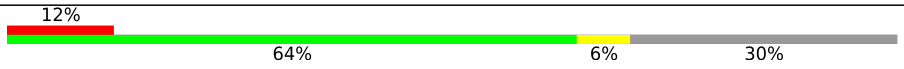
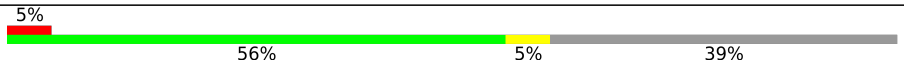
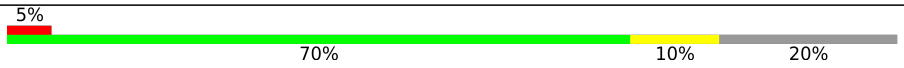
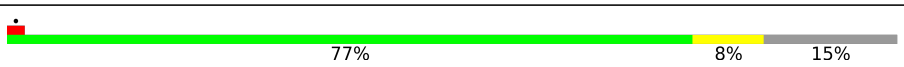
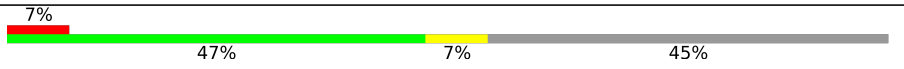
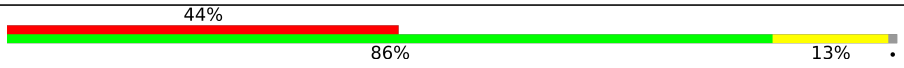
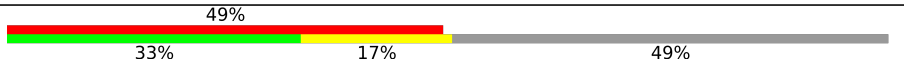
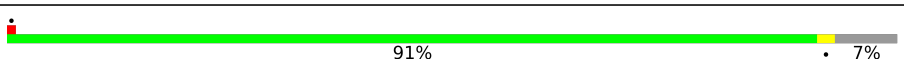
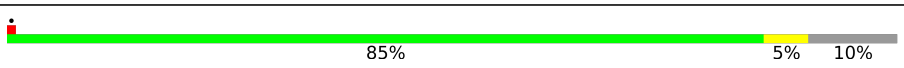
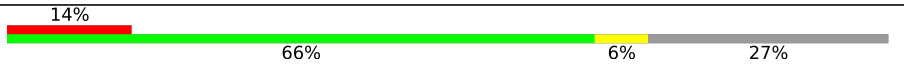
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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	294	
6	H	265	
7	I	262	
8	J	192	
9	K	178	
10	L	145	
11	M	295	
12	N	251	
13	O	176	
14	P	180	
15	Q	292	
16	R	149	
17	S	209	
18	T	206	
19	U	146	
20	V	216	
21	W	148	
22	X	294	
23	Y	252	
24	Z	160	
25	x	356	
26	0	187	
27	1	65	
28	2	92	

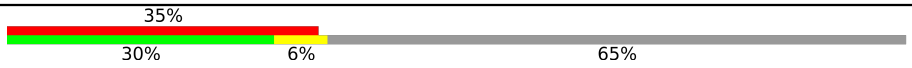
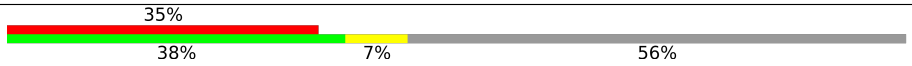
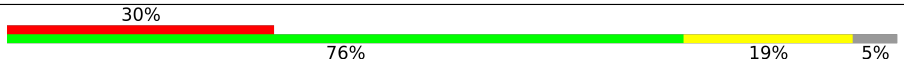
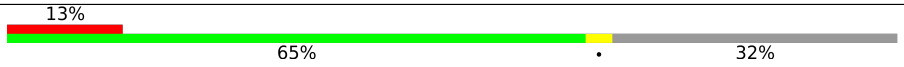
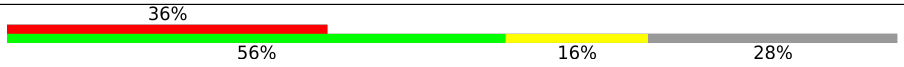
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Mol	Chain	Length	Quality of chain
29	3	188	
30	4	101	
31	6	380	
32	7	336	
33	b	159	
34	c	303	
35	d	306	
36	e	283	
37	f	211	
38	g	166	
39	h	159	
40	i	128	
41	j	121	
42	o	102	
43	p	206	
44	q	222	
45	r	196	
46	s	442	
47	u	228	
48	v	70	
49	w	156	
50	5	423	
51	8	206	
52	9	135	
53	a	142	

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Mol	Chain	Length	Quality of chain
54	m	127	
55	l	135	
56	z	326	
57	y	346	
58	k	118	

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 198705 atoms, of which 91907 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA (1584-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	1441	46100	13756	15471	5518	9914	1441	0	0

- Molecule 2 is a RNA chain called tRNA-Phe (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	62	1993	595	667	244	425	62	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	227	3598	1105	1830	349	305	9	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	308	4901	1577	2442	432	442	8	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	250	4030	1286	2025	364	349	6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	H	95	1593	492	814	150	137	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	161	Total	C	H	N	O	S	0	0
			2700	851	1393	235	214	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	175	Total	C	H	N	O	S	0	0
			2720	846	1394	234	243	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	177	Total	C	H	N	O	S	0	0
			2893	927	1444	262	253	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1837	560	944	174	155	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	287	Total	C	H	N	O	S	0	0
			4692	1475	2377	428	406	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	198	Total	C	H	N	O	S	0	0
			3264	1051	1639	289	275	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	153	Total	C	H	N	O	S	0	0
			2541	795	1282	240	219	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	141	Total	C	H	N	O	S	0	0
			2302	725	1148	221	203	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	217	Total	C	H	N	O	S	0	0
			3612	1150	1822	309	322	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	140	Total	C	H	N	O	S	0	0
			2385	738	1224	233	187	3		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	159	Total	C	H	N	O	S	0	0
			2673	840	1372	233	226	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	166	Total	C	H	N	O	S	0	0
			2771	871	1402	256	234	8		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	127	Total	C	H	N	O	S	0	0
			2109	675	1057	196	178	3		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	201	Total	C	H	N	O	S	0	0
			3295	1043	1643	305	298	6		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	100	Total	C	H	N	O	S	0	0
			1602	515	808	141	135	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m,Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	242	Total	C	H	N	O	S	0	0
			4072	1304	2051	358	355	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	176	Total	C	H	N	O	S	0	0
			3076	973	1553	290	255	5		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	121	Total	C	H	N	O	S	0	0
			2026	632	1039	182	170	3		

- Molecule 25 is a protein called 5-cytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	x	325	Total	C	H	N	O	S	1	0
			5110	1626	2546	448	473	17		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	0	108	Total	C	H	N	O	S	0	0
			1789	546	908	174	155	6		

- Molecule 27 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	52	Total	C	H	N	O	0	0
			900	278	472	80	70		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	46	Total	C	H	N	O	S	0	0
			787	235	407	86	58	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	95	Total	C	H	N	O	S	0	0
			1695	528	872	164	127	4		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	37	Total	C	H	N	O	S	0	0
			676	206	354	68	45	3		

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	6	315	Total	C	H	N	O	S	0	0
			5248	1726	2559	487	470	6		

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	7	292	Total	C	H	N	O	S	0	0
			4757	1517	2378	409	438	15		

- Molecule 33 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	b	148	Total	C	H	N	O	S	0	0
			2376	731	1195	234	214	2		

- Molecule 34 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	c	281	Total	C	H	N	O	S	0	0
			4535	1450	2273	392	412	8		

- Molecule 35 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	d	211	Total	C	H	N	O	S	0	0
			3471	1119	1728	309	304	11		

- Molecule 36 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	e	193	Total	C	H	N	O	S	0	0
			3174	1013	1598	278	279	6		

- Molecule 37 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	f	104	Total	C	H	N	O	S	0	0
			1674	533	836	141	160	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	g	132	Total	C	H	N	O	S	0	0
			2184	709	1094	187	192	2		

- Molecule 39 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	h	110	Total	C	H	N	O	S	0	0
			1739	552	867	156	160	4		

- Molecule 40 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	i	97	Total	C	H	N	O	S	0	0
			1685	540	854	161	128	2		

- Molecule 41 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	j	93	Total	C	H	N	O	S	0	0
			1512	467	768	145	130	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	78	Total	C	H	N	O	S	0	0
			1263	402	623	118	116	4		

- Molecule 43 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	144	Total	C	H	N	O	S	0	0
			2374	735	1198	218	219	4		

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	135	Total	C	H	N	O	S	0	0
			2253	703	1123	223	199	5		

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	157	Total	C	H	N	O	S	0	0
			2604	812	1329	242	210	11		

- Molecule 46 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	s	377	Total	C	H	N	O	S	0	0
			6103	1938	3058	555	540	12		

- Molecule 47 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	125	Total	C	H	N	O	S	0	0
			2041	659	1012	170	191	9		

- Molecule 48 is a protein called Predicted gene, 55359.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	69	Total	C	H	N	O	S	0	0
			1189	374	603	112	99	1		

- Molecule 49 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	79	Total	C	H	N	O	S	0	0
			1277	410	640	95	127	5		

- Molecule 50 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	5	394	Total	C	H	N	O	S	0	0
			6468	2081	3243	564	571	9		

- Molecule 51 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	8	70	Total	C	H	N	O	S	0	0
			1163	368	574	102	117	2		

- Molecule 52 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	9	122	Total	C	H	N	O	S	0	0
			1973	635	990	167	179	2		

- Molecule 53 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	a	103	Total	C	H	N	O	S	0	0
			1703	542	843	156	159	3		

- Molecule 54 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	m	45	Total	C	H	N	O	S	0	0
			769	233	395	77	61	3		

- Molecule 55 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	l	60	Total	C	H	N	O	S	0	0
			1007	315	505	94	91	2		

- Molecule 56 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	z	311	Total	C	H	N	O	S	0	0
			5001	1562	2546	444	433	16		

- Molecule 57 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	237	Total	C	H	N	O	S	0	0
			3938	1238	1995	345	351	9		

- Molecule 58 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	k	85	Total	C	H	N	O	S	0	0
			1331	413	667	121	125	5		

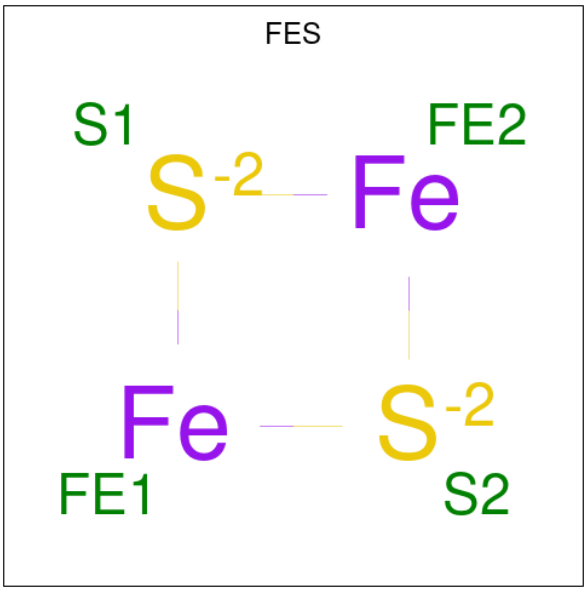
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	96	Total	Mg	0
			96	96	
59	E	1	Total	Mg	0
			1	1	
59	M	1	Total	Mg	0
			1	1	
59	O	1	Total	Mg	0
			1	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

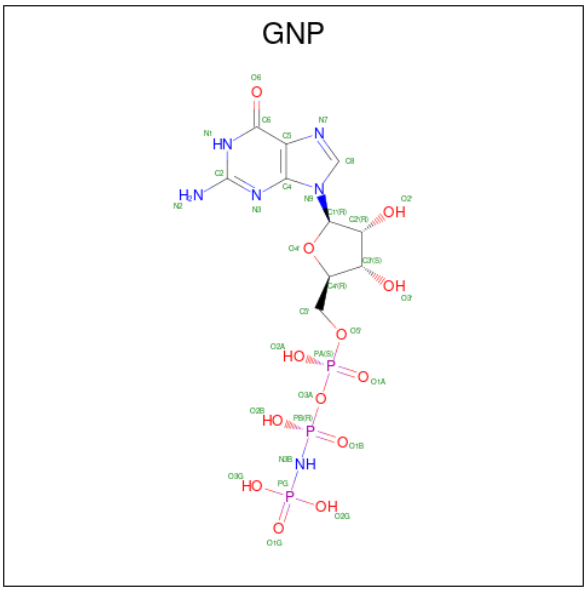
Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 62 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
62	z	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	AltConf
63	A	1	Total O 1 1	0

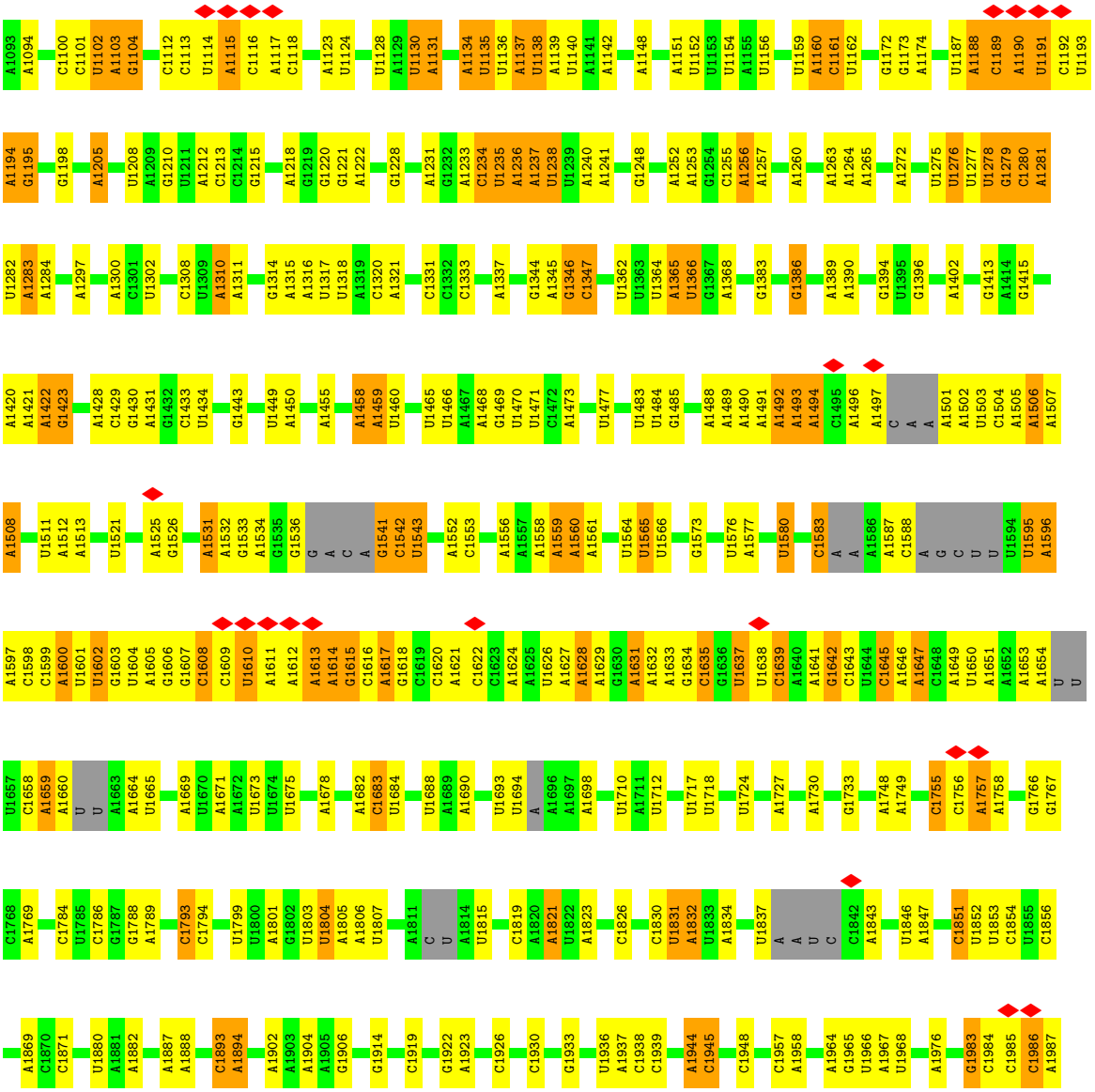
3 Residue-property plots (i)

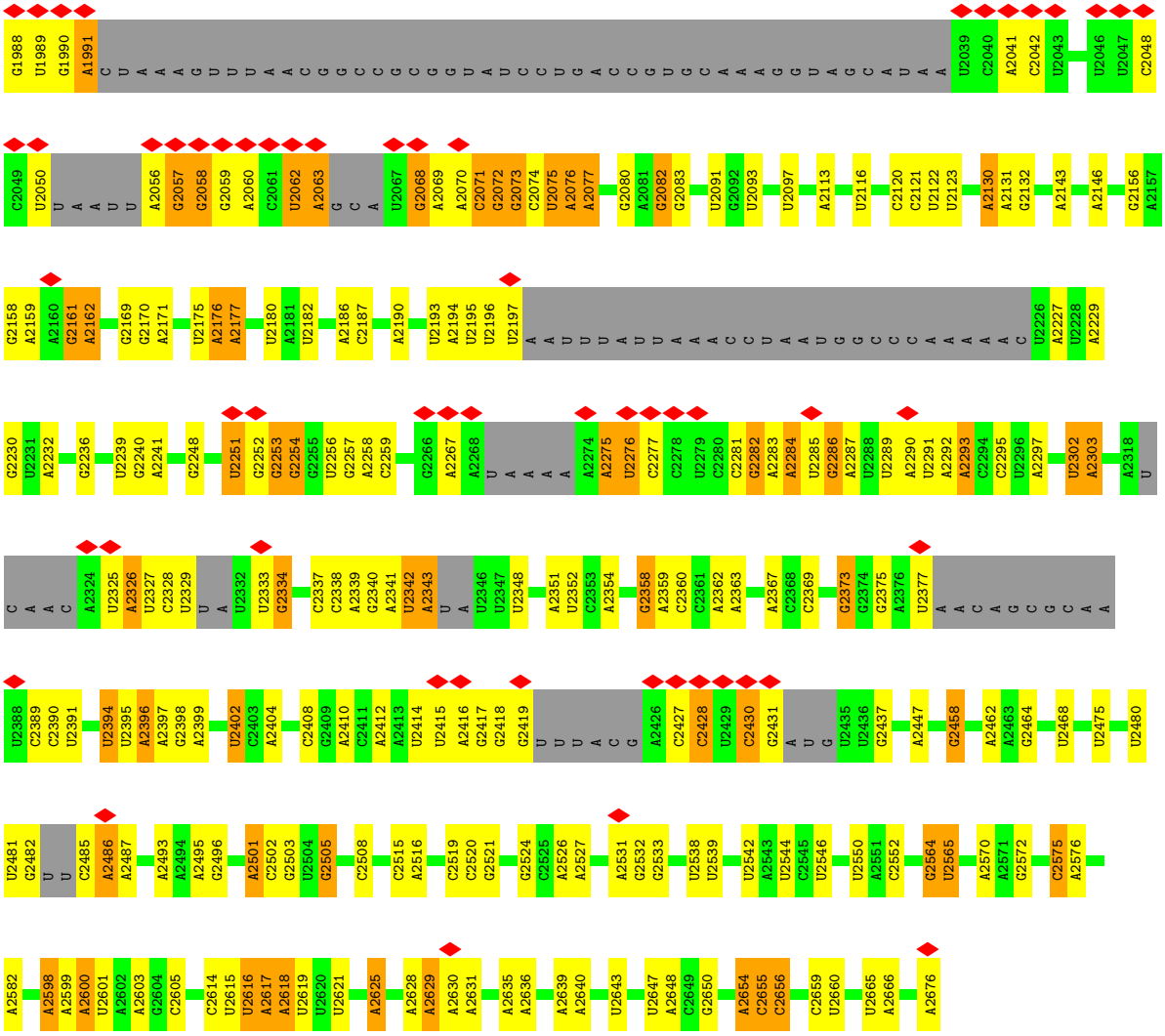
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S rRNA (1584-MER)

Chain A:

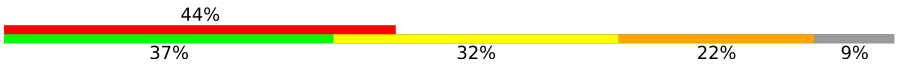


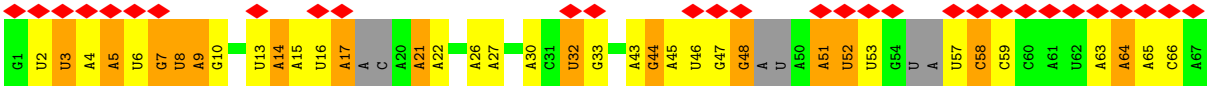




• Molecule 2: tRNA-Phe (68-MER)

Chain B:

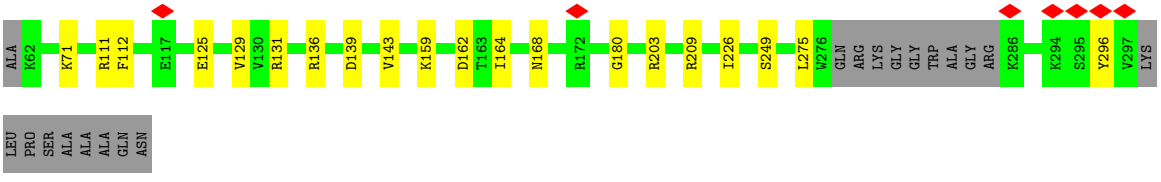




• Molecule 3: Large ribosomal subunit protein uL2m

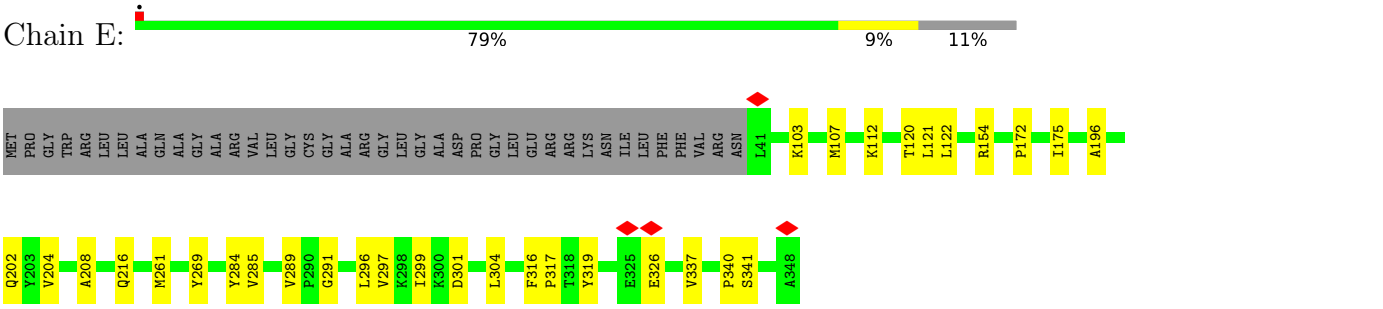
Chain D:





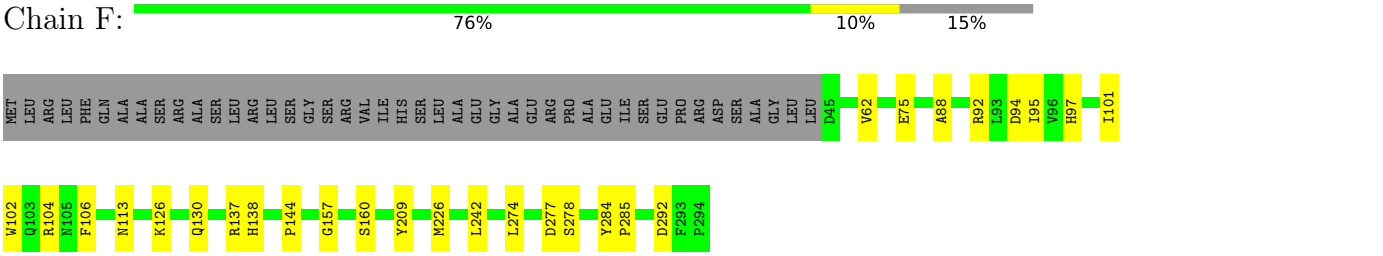
• Molecule 4: Large ribosomal subunit protein uL3m

Chain E:



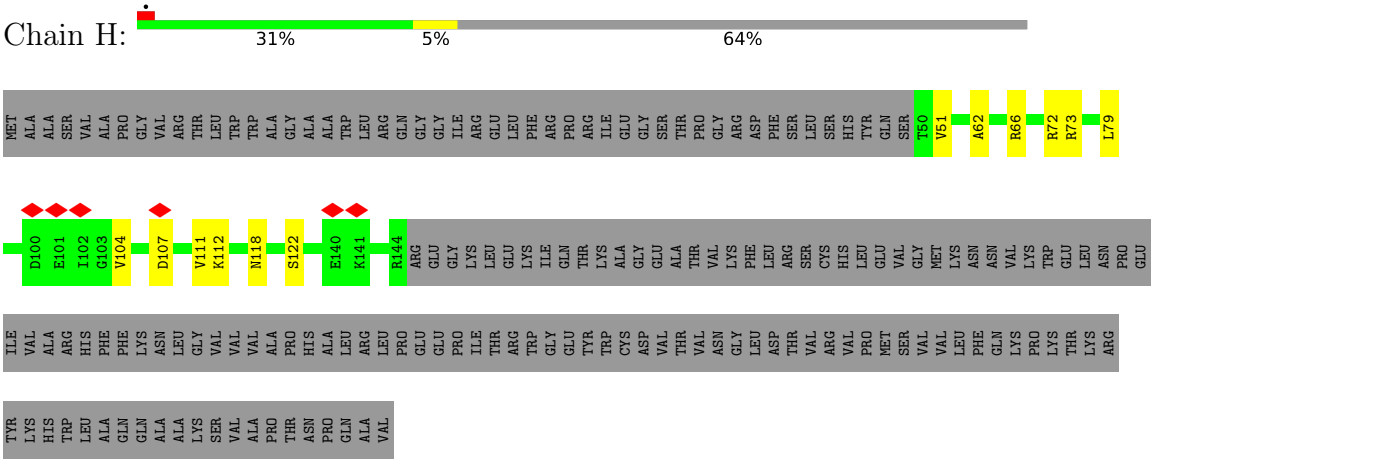
• Molecule 5: Large ribosomal subunit protein uL4m

Chain F:



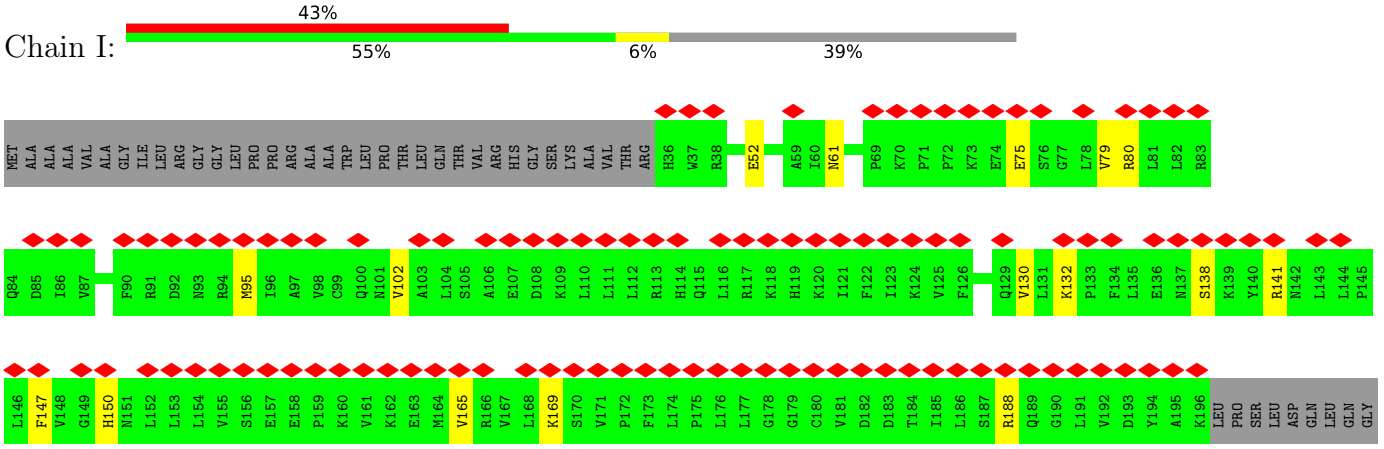
• Molecule 6: Large ribosomal subunit protein bL9m

Chain H:



• Molecule 7: Large ribosomal subunit protein uL10m

Chain I:

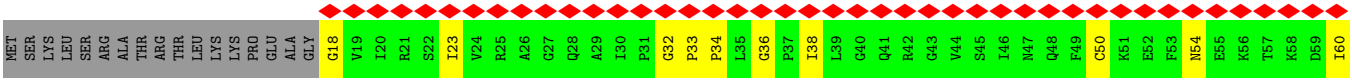


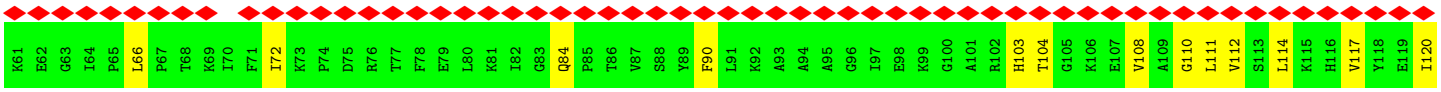


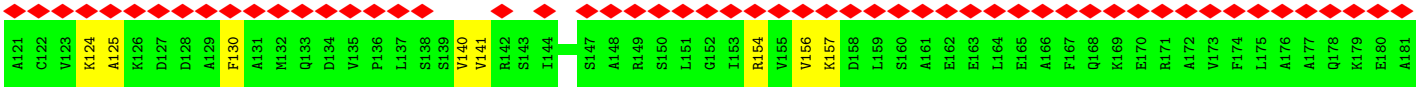
• Molecule 8: Large ribosomal subunit protein uL11m

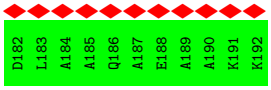
Chain J:











• Molecule 9: Large ribosomal subunit protein uL13m

Chain K:

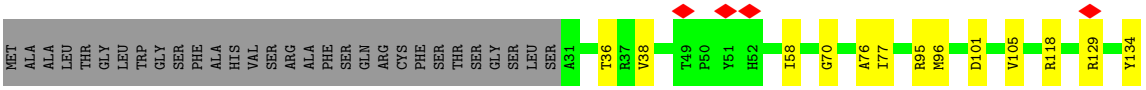




• Molecule 10: Large ribosomal subunit protein uL14m

Chain L:

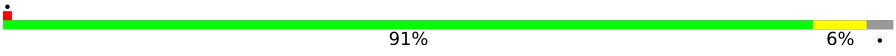






• Molecule 11: Large ribosomal subunit protein uL15m

Chain M:

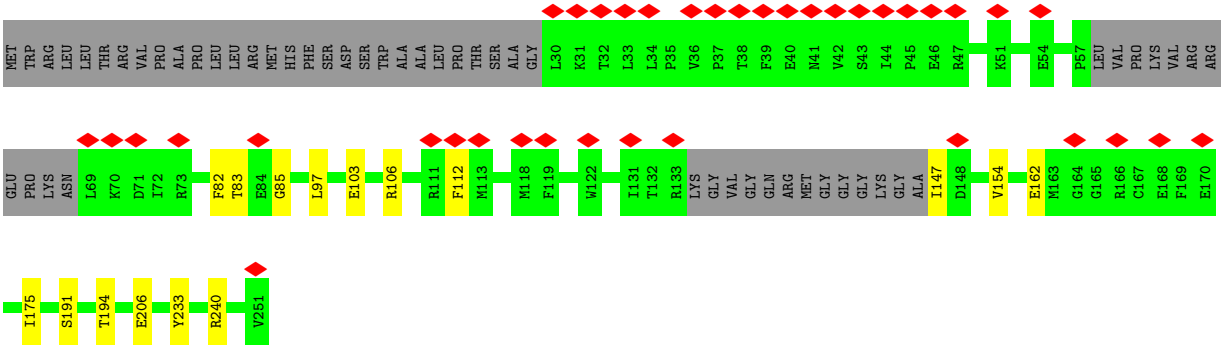




• Molecule 12: Large ribosomal subunit protein uL16m

Chain N:

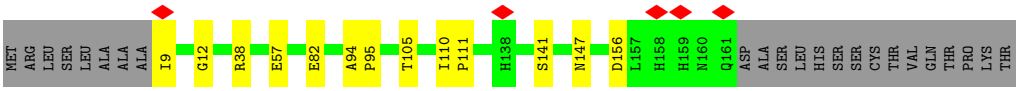




• Molecule 13: Large ribosomal subunit protein bL17m

Chain O:

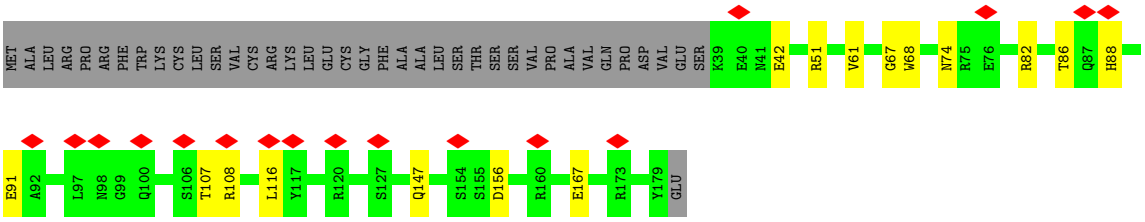




• Molecule 14: Large ribosomal subunit protein uL18m

Chain P:

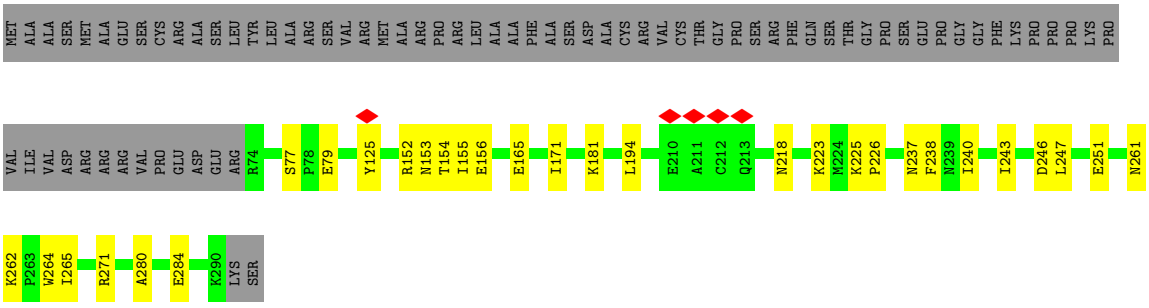




• Molecule 15: Large ribosomal subunit protein bL19m

Chain Q:





• Molecule 16: Large ribosomal subunit protein bL20m

Chain R:

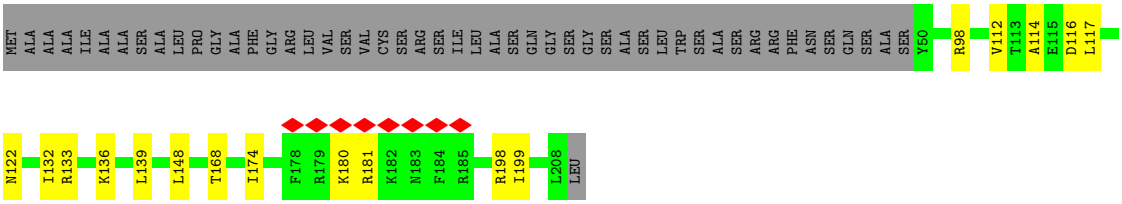




• Molecule 17: Large ribosomal subunit protein bL21m

Chain S:

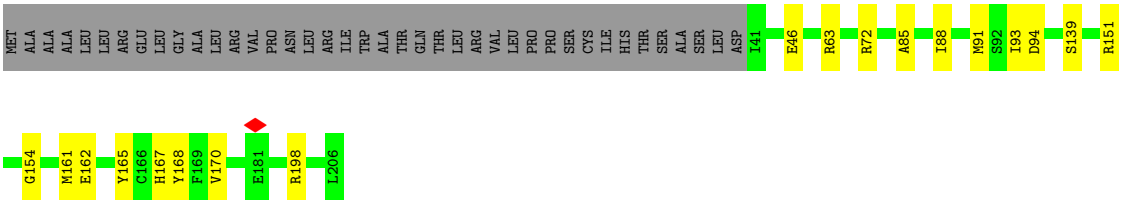




• Molecule 18: Large ribosomal subunit protein uL22m

Chain T:

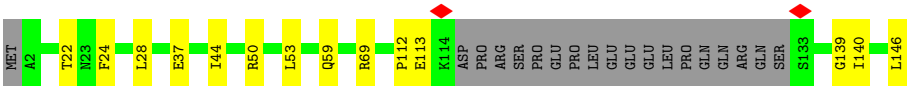




• Molecule 19: Large ribosomal subunit protein uL23m

Chain U:

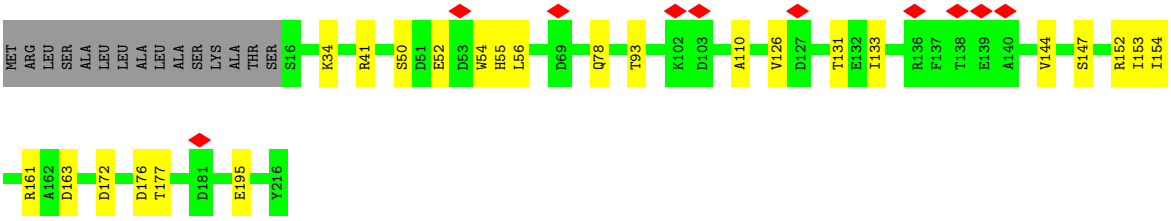




• Molecule 20: Large ribosomal subunit protein uL24m

Chain V:

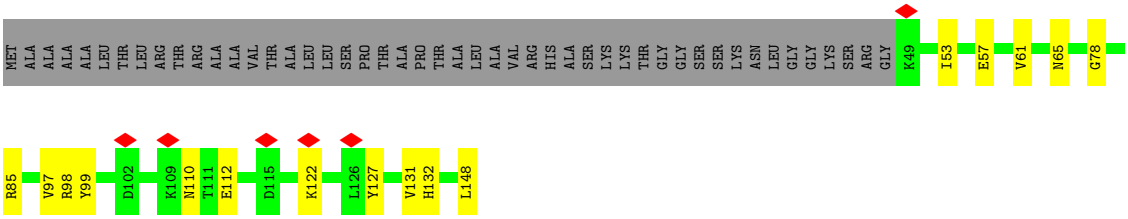




• Molecule 21: Large ribosomal subunit protein bL27m

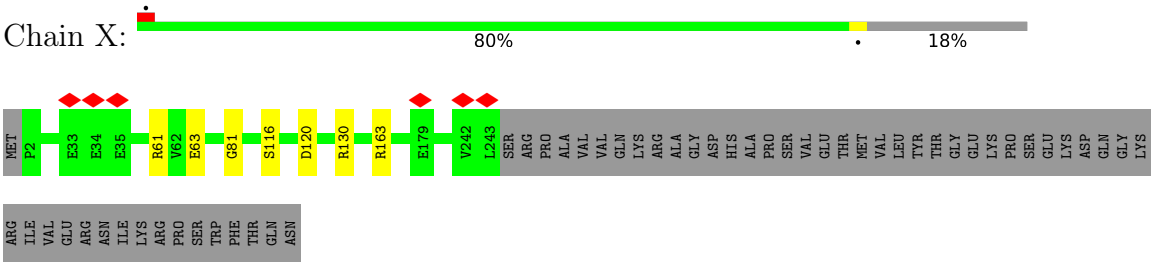
Chain W:





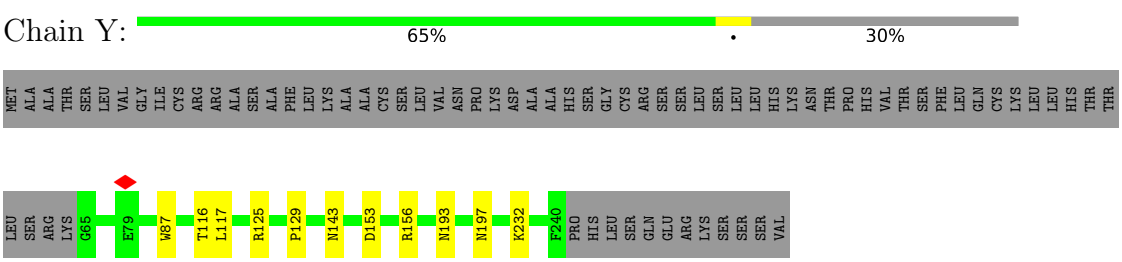
• Molecule 22: Large ribosomal subunit protein bL28m,Large ribosomal subunit protein bL32m

Chain X:



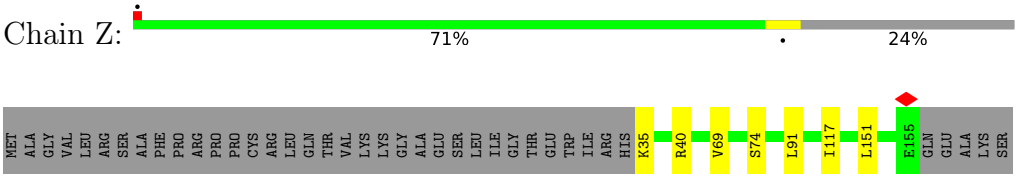
• Molecule 23: Large ribosomal subunit protein uL29m

Chain Y:



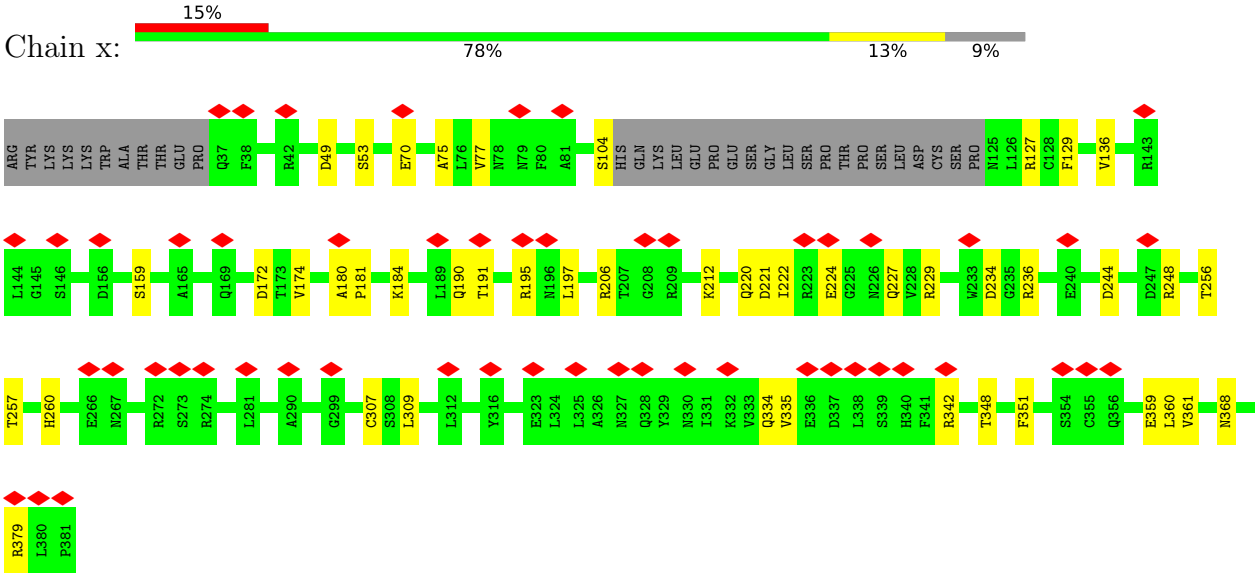
• Molecule 24: Large ribosomal subunit protein uL30m

Chain Z:



• Molecule 25: 5-cytosine rRNA methyltransferase NSUN4

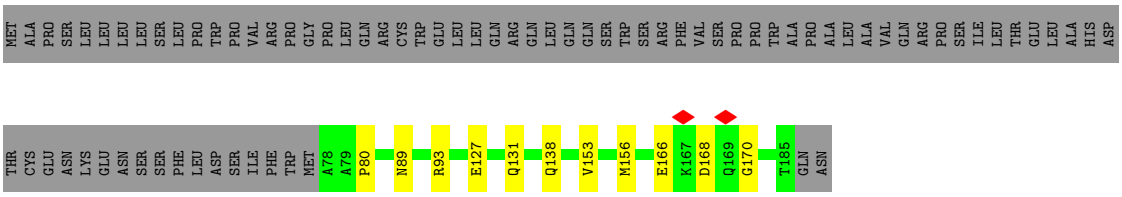
Chain x:



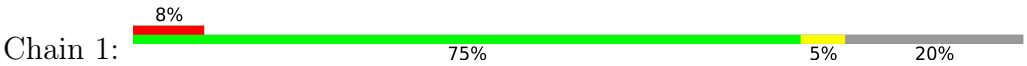
• Molecule 26: Large ribosomal subunit protein bL32m

Chain 0:

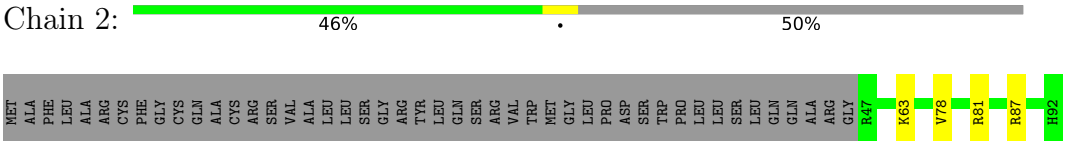




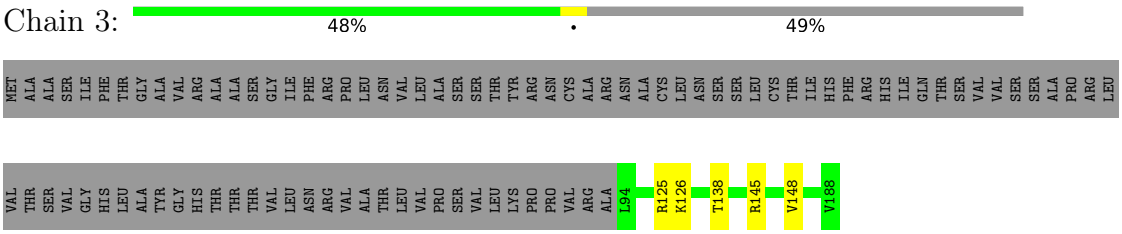
• Molecule 27: Large ribosomal subunit protein bL33m



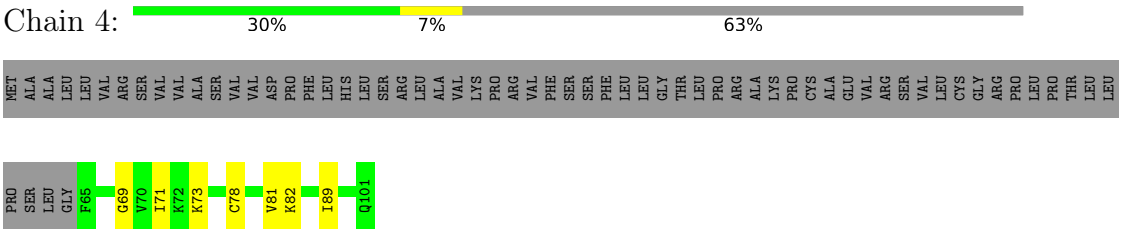
• Molecule 28: Large ribosomal subunit protein bL34m



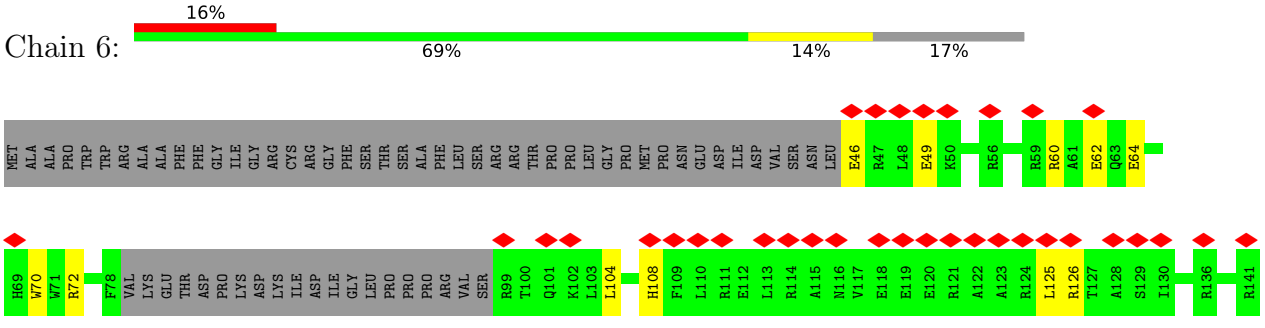
• Molecule 29: Large ribosomal subunit protein bL35m

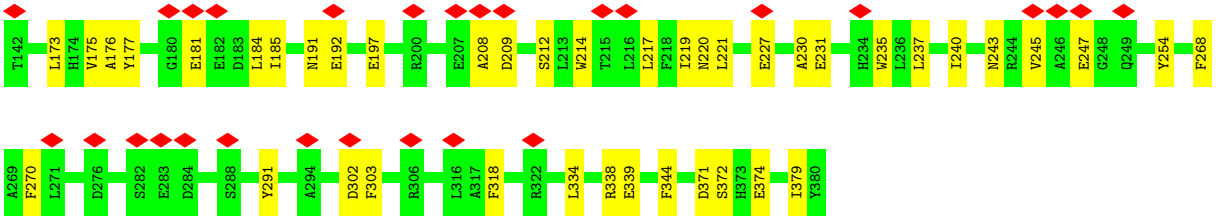


• Molecule 30: Large ribosomal subunit protein bL36m



• Molecule 31: Large ribosomal subunit protein mL38

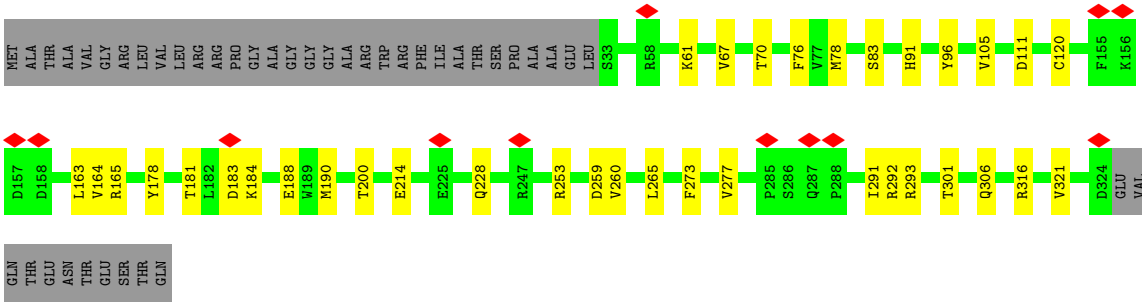




• Molecule 32: Large ribosomal subunit protein mL39

Chain 7:





• Molecule 33: Large ribosomal subunit protein mL43

Chain b:

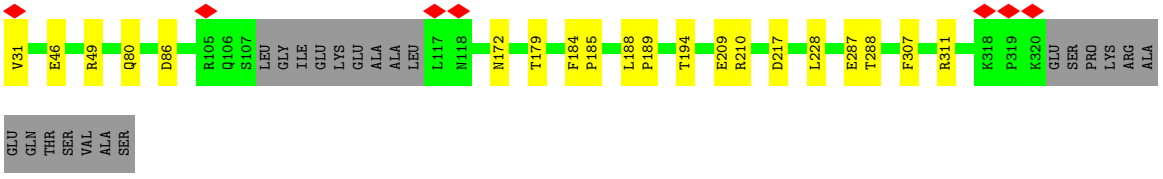




• Molecule 34: Large ribosomal subunit protein mL44

Chain c:

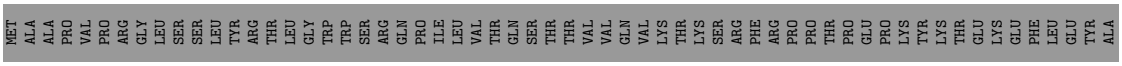


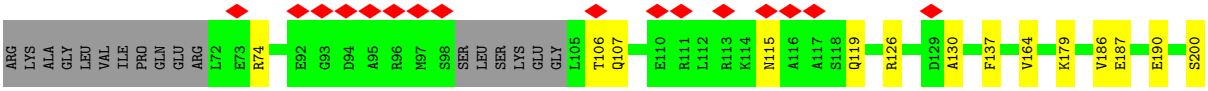


• Molecule 35: Large ribosomal subunit protein mL45

Chain d:



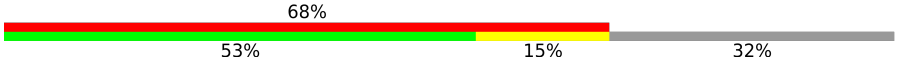


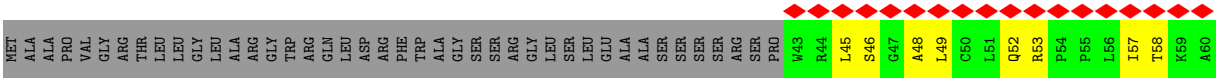


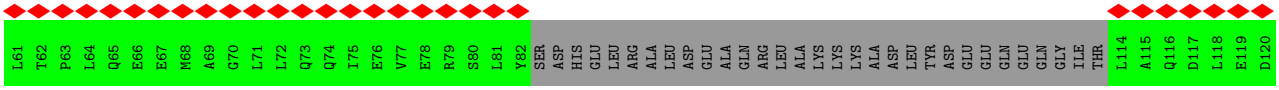


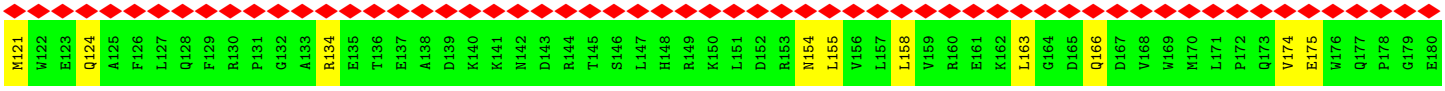
• Molecule 36: Large ribosomal subunit protein mL46

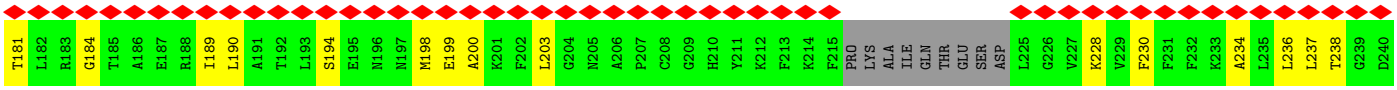
Chain e:

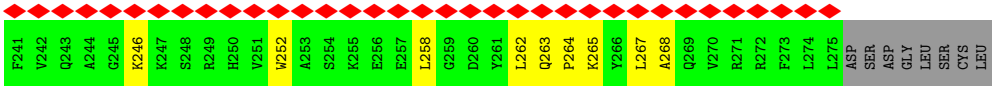










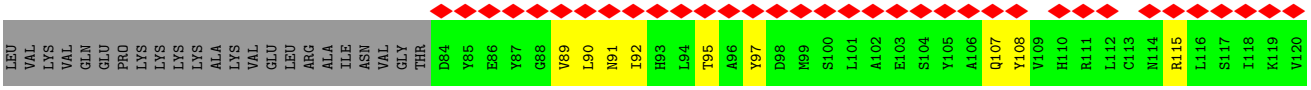


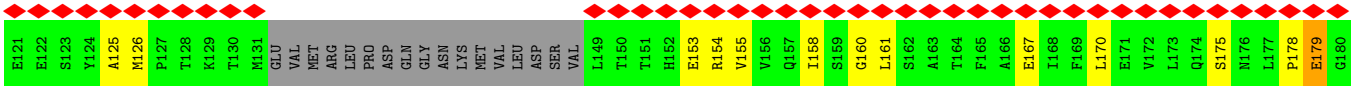
• Molecule 37: Large ribosomal subunit protein mL48

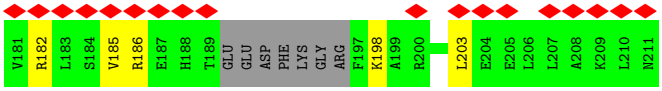
Chain f:







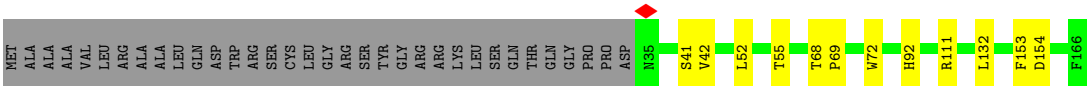




• Molecule 38: Large ribosomal subunit protein mL49

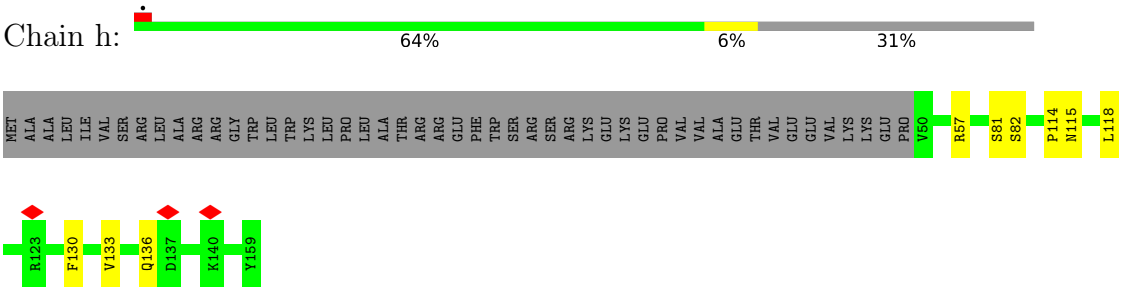
Chain g:





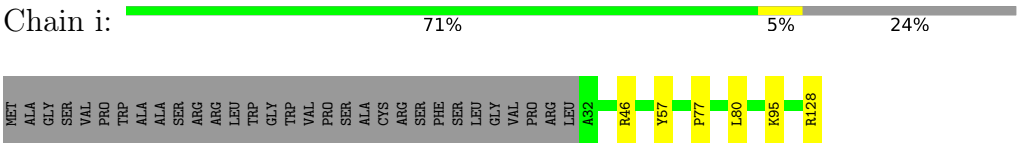
• Molecule 39: Large ribosomal subunit protein mL50

Chain h:



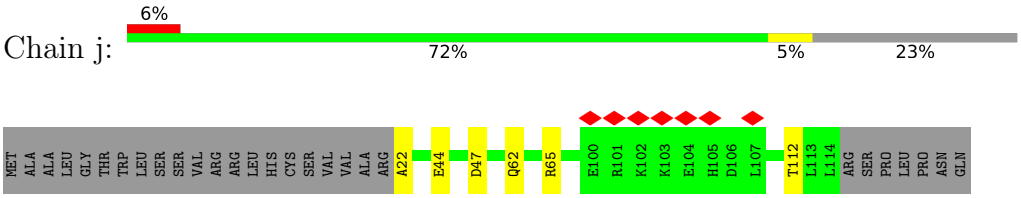
• Molecule 40: Large ribosomal subunit protein mL51

Chain i:



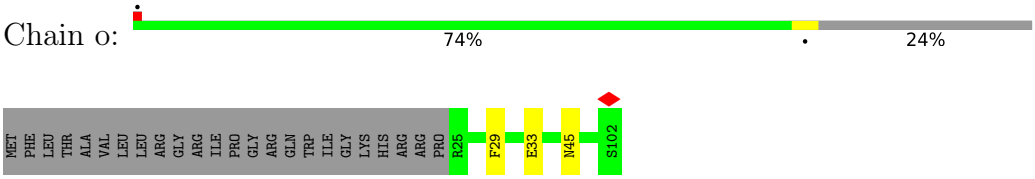
• Molecule 41: Large ribosomal subunit protein mL52

Chain j:



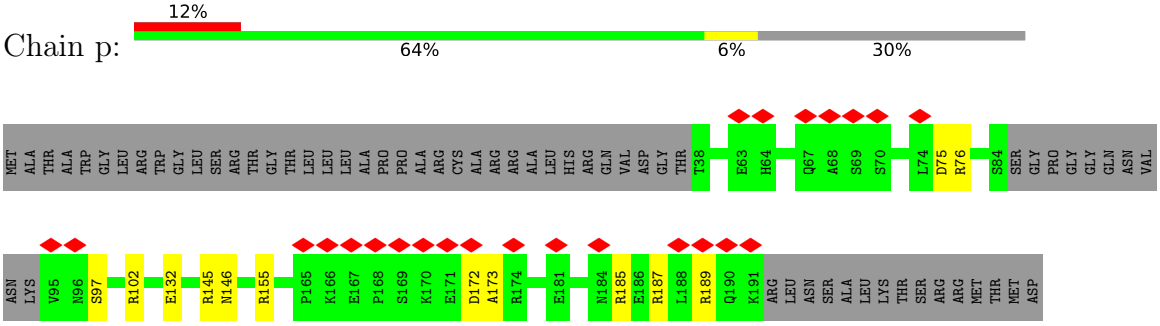
• Molecule 42: Large ribosomal subunit protein mL63

Chain o:



• Molecule 43: Large ribosomal subunit protein mL62

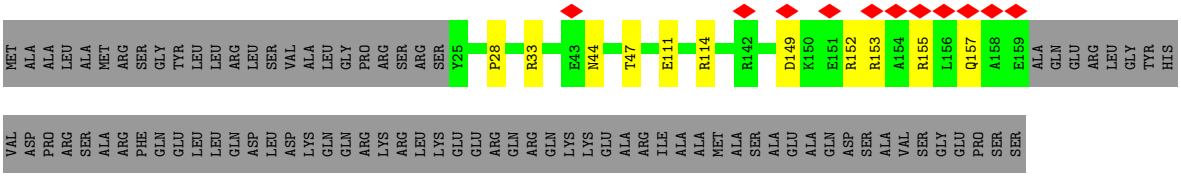
Chain p:



• Molecule 44: Large ribosomal subunit protein mL64

Chain q:

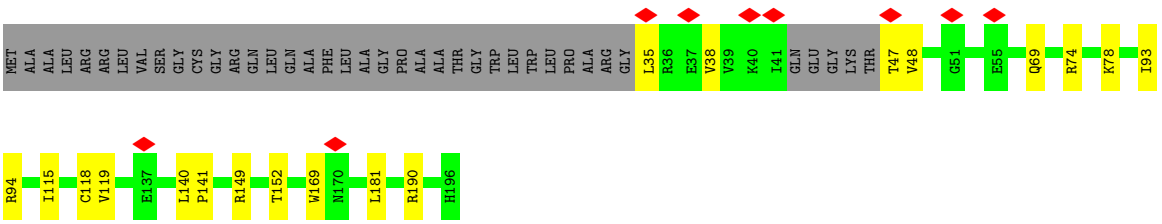




• Molecule 45: Large ribosomal subunit protein mL66

Chain r:

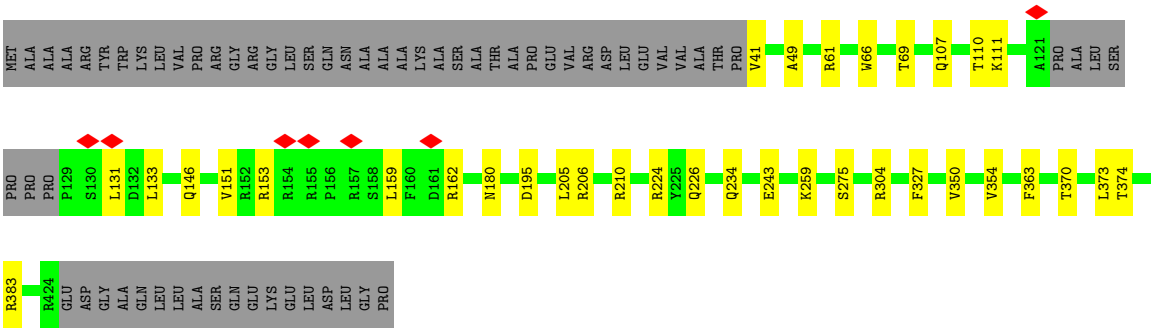




• Molecule 46: Large ribosomal subunit protein mL65

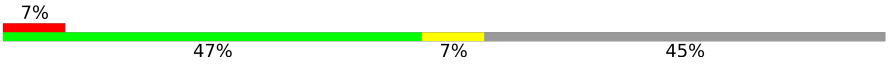
Chain s:

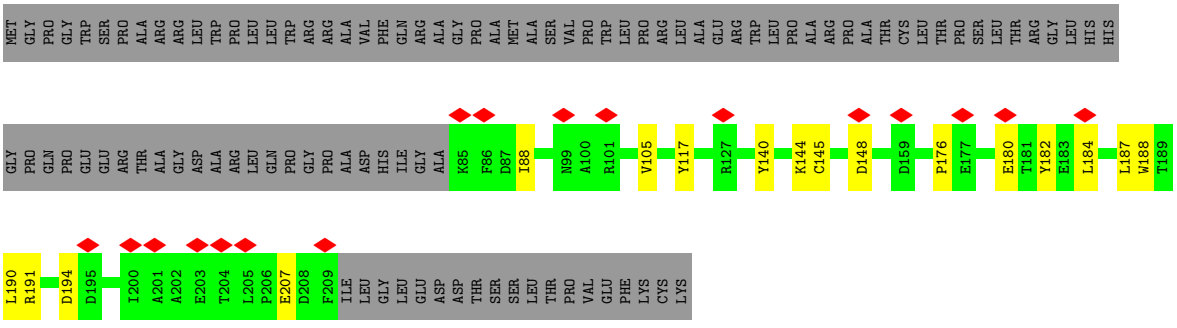




• Molecule 47: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:

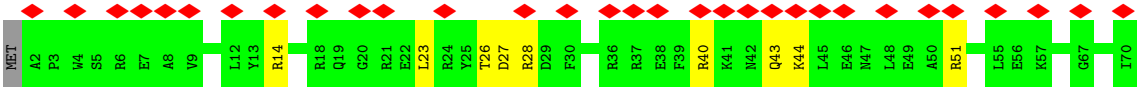




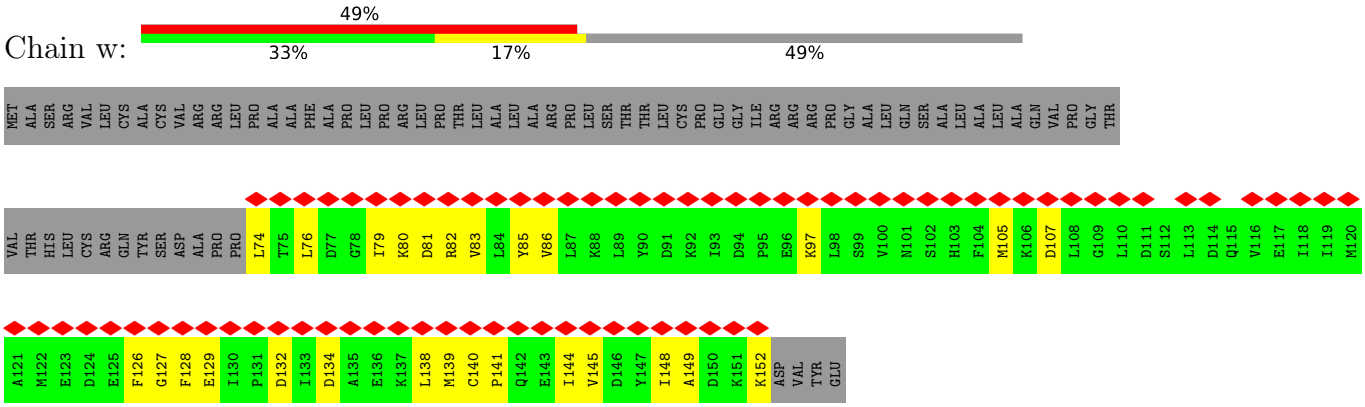
• Molecule 48: Predicted gene, 55359

Chain v:

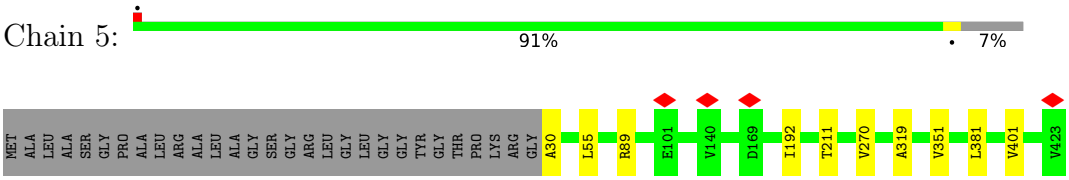




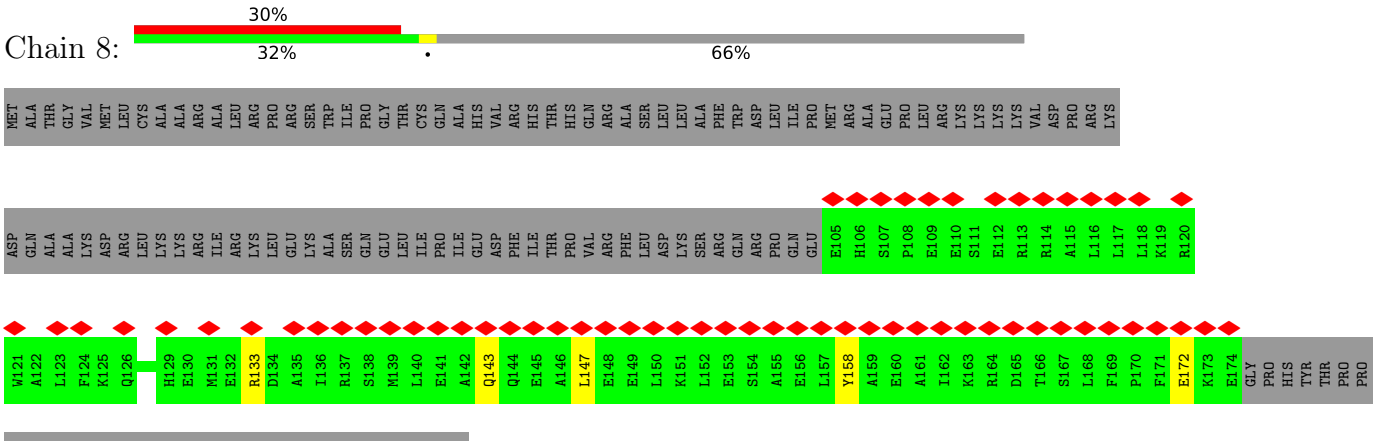
• Molecule 49: Acyl carrier protein, mitochondrial



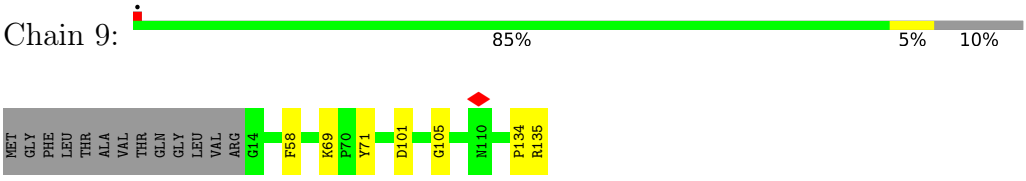
• Molecule 50: Large ribosomal subunit protein mL37



• Molecule 51: Large ribosomal subunit protein mL40

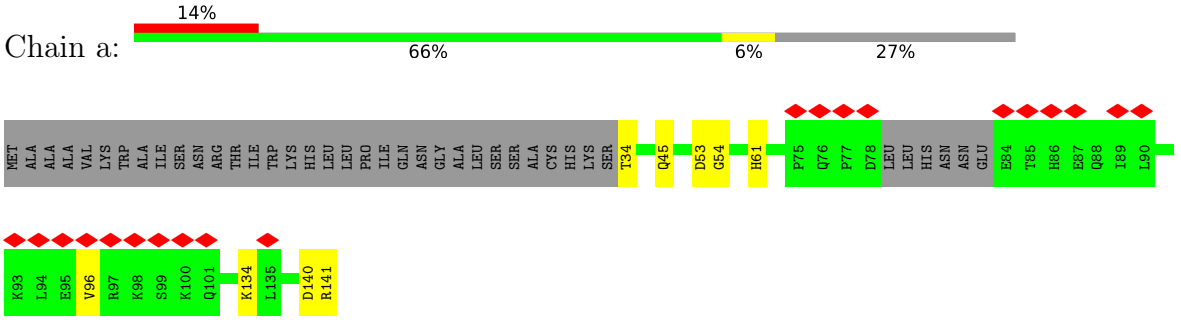


• Molecule 52: Large ribosomal subunit protein mL41



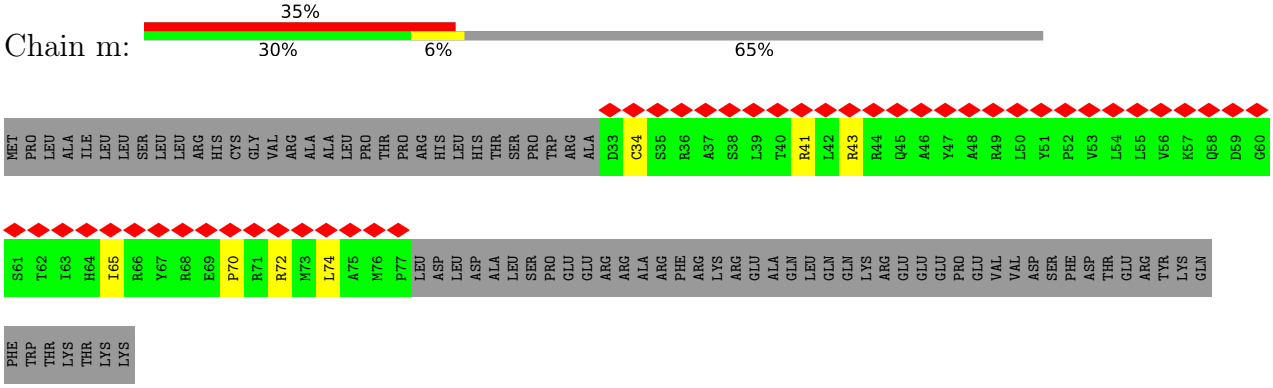
• Molecule 53: Large ribosomal subunit protein mL42

Chain a:



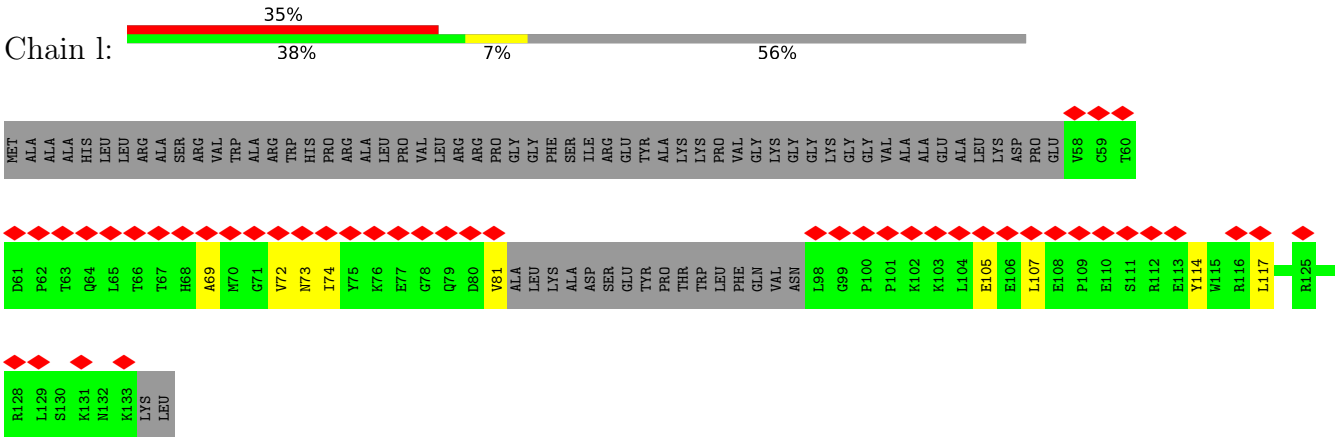
• Molecule 54: Large ribosomal subunit protein mL55

Chain m:



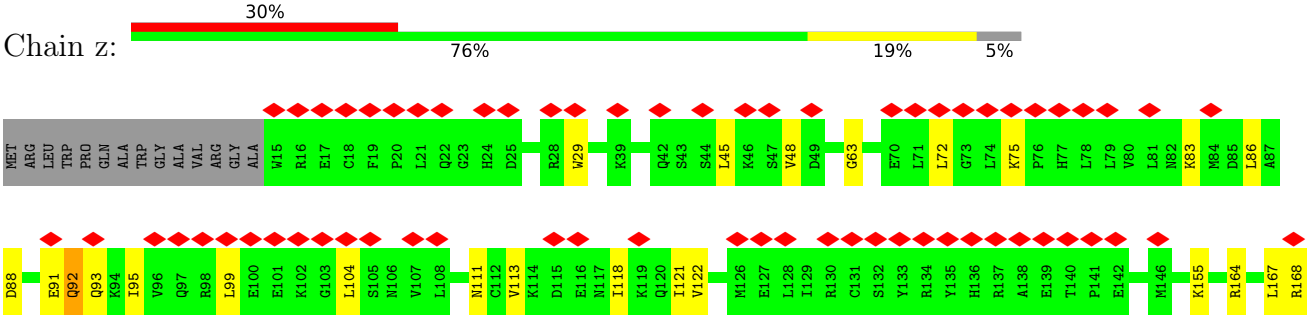
• Molecule 55: Large ribosomal subunit protein mL54

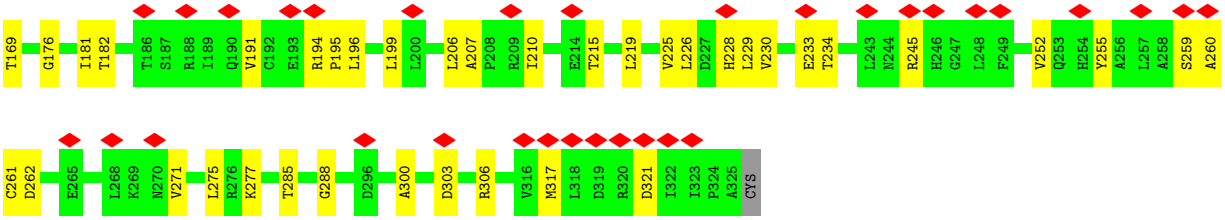
Chain l:



• Molecule 56: Mitochondrial ribosome-associated GTPase 1

Chain z:

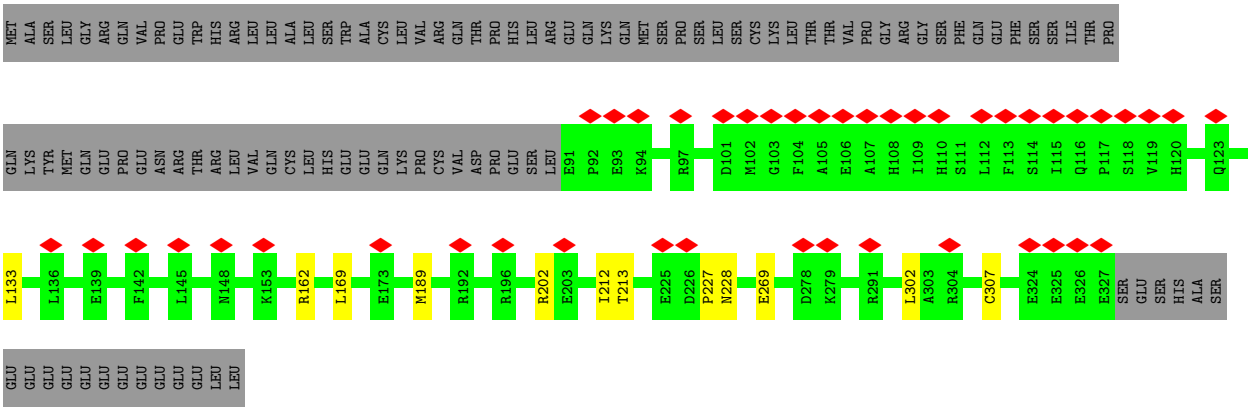




• Molecule 57: Transcription termination factor 4, mitochondrial

Chain y:

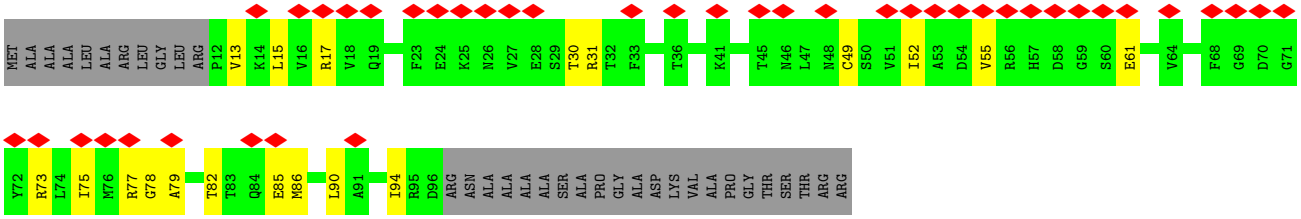




• Molecule 58: Large ribosomal subunit protein mL53

Chain k:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	457.2925, 457.2925, 457.2925	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.846838, 0.846838, 0.846838	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.16	0/34254	0.29	0/53277
2	B	0.14	0/1483	0.29	0/2299
3	D	0.12	0/1802	0.28	0/2424
4	E	0.13	0/2535	0.28	0/3443
5	F	0.14	0/2061	0.29	0/2805
6	H	0.10	0/793	0.25	0/1066
7	I	0.09	0/1339	0.25	0/1813
8	J	0.09	0/1346	0.29	0/1809
9	K	0.12	0/1491	0.25	0/2022
10	L	0.12	0/908	0.28	0/1224
11	M	0.12	0/2369	0.26	0/3197
12	N	0.08	0/1670	0.22	0/2252
13	O	0.13	0/1285	0.30	0/1732
14	P	0.08	0/1181	0.23	0/1600
15	Q	0.12	0/1832	0.27	0/2471
16	R	0.14	0/1182	0.26	0/1585
17	S	0.13	0/1328	0.29	0/1798
18	T	0.15	0/1402	0.29	0/1885
19	U	0.13	0/1080	0.27	0/1464
20	V	0.12	0/1695	0.26	0/2295
21	W	0.11	0/816	0.27	0/1105
22	X	0.11	0/2075	0.24	0/2806
23	Y	0.12	0/1561	0.22	0/2093
24	Z	0.11	0/1013	0.27	0/1368
25	x	0.09	0/2620	0.24	0/3549
26	0	0.13	0/896	0.28	0/1200
27	1	0.08	0/434	0.24	0/578
28	2	0.14	0/387	0.27	0/514
29	3	0.14	0/843	0.28	0/1122
30	4	0.10	0/328	0.26	0/430
31	6	0.10	0/2783	0.26	0/3781
32	7	0.10	0/2436	0.23	0/3300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	b	0.13	0/1203	0.30	0/1625
34	c	0.11	0/2313	0.24	0/3128
35	d	0.10	0/1792	0.26	0/2429
36	e	0.09	0/1608	0.26	0/2165
37	f	0.09	0/851	0.27	0/1149
38	g	0.13	0/1126	0.28	0/1533
39	h	0.10	0/894	0.24	0/1216
40	i	0.15	0/855	0.28	0/1147
41	j	0.10	0/759	0.26	0/1019
42	o	0.10	0/655	0.23	0/880
43	p	0.09	0/1195	0.24	0/1603
44	q	0.10	0/1161	0.23	0/1571
45	r	0.12	0/1309	0.28	0/1767
46	s	0.12	0/3118	0.26	0/4232
47	u	0.08	0/1053	0.22	0/1425
48	v	0.08	0/596	0.22	0/795
49	w	0.13	0/646	0.32	0/869
50	5	0.11	0/3317	0.25	0/4519
51	8	0.07	0/598	0.21	0/799
52	9	0.12	0/1009	0.25	0/1358
53	a	0.13	0/884	0.28	0/1197
54	m	0.10	0/380	0.26	0/510
55	l	0.07	0/512	0.22	0/689
56	z	0.10	0/2500	0.27	0/3380
57	y	0.07	0/1980	0.20	0/2667
58	k	0.08	0/674	0.24	0/910
All	All	0.13	0/112216	0.27	0/158889

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	30629	15471	15492	210	0
2	B	1326	667	670	23	0
3	D	1768	1830	1830	15	0
4	E	2459	2442	2441	19	0
5	F	2005	2025	2024	19	0
6	H	779	814	814	7	0
7	I	1307	1393	1393	11	0
8	J	1326	1394	1394	18	0
9	K	1449	1444	1444	13	0
10	L	893	944	944	12	0
11	M	2315	2377	2377	14	0
12	N	1625	1639	1639	10	0
13	O	1259	1282	1282	8	0
14	P	1154	1148	1148	15	0
15	Q	1790	1822	1822	19	0
16	R	1161	1224	1224	6	0
17	S	1301	1372	1372	16	0
18	T	1369	1402	1402	13	0
19	U	1052	1057	1057	12	0
20	V	1652	1643	1643	20	0
21	W	794	808	808	15	0
22	X	2021	2051	2051	4	0
23	Y	1523	1553	1553	10	0
24	Z	987	1039	1039	7	0
25	x	2564	2546	2546	30	0
26	0	881	908	908	7	0
27	1	428	472	472	2	0
28	2	380	407	407	3	0
29	3	823	872	872	3	0
30	4	322	354	354	6	0
31	6	2689	2559	2559	42	0
32	7	2379	2378	2378	23	0
33	b	1181	1195	1195	18	0
34	c	2262	2273	2273	15	0
35	d	1743	1728	1728	21	0
36	e	1576	1598	1598	27	0
37	f	838	836	836	24	0
38	g	1090	1094	1094	12	0
39	h	872	867	867	7	0
40	i	831	854	854	7	0
41	j	744	768	768	6	0
42	o	640	623	623	2	0
43	p	1176	1198	1198	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	1130	1123	1123	7	0
45	r	1275	1329	1329	15	0
46	s	3045	3058	3057	25	0
47	u	1029	1012	1012	12	0
48	v	586	603	603	5	0
49	w	637	640	640	24	0
50	5	3225	3243	3243	8	0
51	8	589	574	574	4	0
52	9	983	990	990	5	0
53	a	860	843	843	6	0
54	m	374	395	395	8	0
55	l	502	505	505	7	0
56	z	2455	2546	2546	48	0
57	y	1943	1995	1995	7	0
58	k	664	667	667	13	0
59	A	96	0	0	0	0
59	E	1	0	0	0	0
59	M	1	0	0	0	0
59	O	1	0	0	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
61	r	4	0	0	0	0
62	z	32	13	13	3	0
63	A	1	0	0	0	0
All	All	106798	91907	91928	820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (820) 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)
1:A:1965:G:OP1	3:D:136:ARG:NH2	2.09	0.85
1:A:2080:G:O2'	1:A:2082:G:OP2	1.95	0.84
3:D:139:ASP:OD1	3:D:249:SER:OG	1.95	0.83
47:u:140:TYR:OH	47:u:148:ASP:OD2	1.96	0.83
4:E:107:MET:HE3	4:E:121:LEU:HD11	1.62	0.82
1:A:2275:A:O2'	1:A:2276:U:OP1	1.97	0.82
14:P:82:ARG:NH2	31:6:62:GLU:OE1	2.13	0.81
46:s:66:TRP:O	46:s:69:THR:OG1	2.00	0.80
1:A:2076:A:O2'	1:A:2077:A:OP2	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2286:G:O2'	25:x:212:LYS:NZ	2.15	0.79
17:S:139:LEU:HD13	17:S:148:LEU:HD23	1.62	0.78
1:A:2326:A:OP1	21:W:85:ARG:NH2	2.16	0.78
1:A:1531:A:HO2'	24:Z:35:LYS:N	1.82	0.77
1:A:1308:C:OP2	38:g:111:ARG:NH2	2.19	0.76
1:A:2505:G:O2'	1:A:2508:C:OP2	2.04	0.75
12:N:206:GLU:OE2	12:N:240:ARG:NH2	2.19	0.75
32:7:190:MET:SD	32:7:292:ARG:NH2	2.59	0.75
31:6:374:GLU:OE2	43:p:145:ARG:NH2	2.19	0.75
20:V:177:THR:HG23	52:9:71:TYR:O	1.87	0.74
49:w:80:LYS:HG2	49:w:145:VAL:HG11	1.69	0.74
1:A:2254:G:O6	1:A:2428:C:N4	2.20	0.74
56:z:72:LEU:HD12	56:z:72:LEU:O	1.88	0.74
15:Q:155:ILE:HG22	15:Q:156:GLU:OE1	1.88	0.74
3:D:296:TYR:OH	57:y:269:GLU:OE2	2.05	0.73
1:A:1620:C:O2'	8:J:104:THR:OG1	1.99	0.73
56:z:63:GLY:HA3	56:z:219:LEU:HD11	1.71	0.73
19:U:139:GLY:O	35:d:179:LYS:NZ	2.22	0.73
20:V:177:THR:HG22	52:9:69:LYS:H	1.54	0.72
1:A:2072:G:O2'	1:A:2073:G:OP1	2.07	0.72
17:S:116:ASP:OD1	17:S:117:LEU:N	2.22	0.72
1:A:1598:C:N4	1:A:1645:C:OP1	2.23	0.72
31:6:247:GLU:OE1	31:6:247:GLU:N	2.23	0.72
21:W:127:TYR:OH	31:6:64:GLU:OE2	2.09	0.71
16:R:10:LEU:HD13	16:R:13:ARG:HD3	1.73	0.70
18:T:198:ARG:NH2	34:c:287:GLU:OE1	2.24	0.70
1:A:1265:A:OP1	33:b:4:ARG:NH2	2.25	0.70
2:B:65:A:OP1	36:e:265:LYS:NZ	2.19	0.70
12:N:85:GLY:N	12:N:162:GLU:OE2	2.25	0.70
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.25	0.69
45:r:48:VAL:HG22	58:k:75:ILE:HB	1.74	0.69
46:s:206:ARG:HD2	46:s:373:LEU:HD12	1.74	0.69
32:7:183:ASP:OD1	32:7:184:LYS:N	2.25	0.69
55:l:107:LEU:HD11	55:l:117:LEU:HD12	1.74	0.69
48:v:23:LEU:O	48:v:28:ARG:NE	2.24	0.69
35:d:226:ASP:OD1	35:d:232:MET:HE2	1.91	0.69
56:z:45:LEU:O	56:z:75:LYS:NZ	2.25	0.69
56:z:226:LEU:O	56:z:229:LEU:HD23	1.93	0.69
7:I:61:ASN:OD1	45:r:78:LYS:NZ	2.27	0.68
45:r:93:ILE:HD11	45:r:119:VAL:HG21	1.76	0.68
34:c:46:GLU:OE1	34:c:49:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:263:GLN:N	36:e:263:GLN:OE1	2.27	0.67
2:B:22:A:OP2	2:B:45:A:N6	2.27	0.67
7:I:75:GLU:O	7:I:80:ARG:NH2	2.28	0.67
14:P:68:TRP:N	21:W:78:GLY:O	2.27	0.67
1:A:1620:C:O2'	8:J:103:HIS:O	2.12	0.67
1:A:1102:U:O2'	1:A:1103:A:OP2	2.09	0.67
47:u:88:ILE:HD11	47:u:105:VAL:HG11	1.77	0.66
32:7:228:GLN:OE1	32:7:228:GLN:N	2.27	0.66
57:y:162:ARG:NH2	57:y:189:MET:O	2.27	0.66
31:6:46:GLU:N	31:6:46:GLU:OE1	2.29	0.66
32:7:61:LYS:NZ	35:d:278:LYS:O	2.29	0.65
1:A:1984:C:H5	1:A:2068:G:H21	1.44	0.65
9:K:26:GLN:NE2	9:K:147:GLN:OE1	2.30	0.65
12:N:82:PHE:O	12:N:83:THR:OG1	2.11	0.65
1:A:1846:U:O2'	50:5:270:VAL:O	2.15	0.65
20:V:54:TRP:NE1	20:V:56:LEU:O	2.30	0.65
1:A:1205:A:N6	1:A:1208:U:OP2	2.29	0.65
3:D:125:GLU:HB3	3:D:143:VAL:HG22	1.78	0.65
5:F:126:LYS:NZ	5:F:130:GLN:OE1	2.28	0.65
6:H:104:VAL:N	6:H:107:ASP:OD2	2.29	0.64
4:E:121:LEU:HD22	4:E:284:TYR:CE1	2.32	0.64
5:F:209:TYR:O	39:h:57:ARG:NH1	2.30	0.64
49:w:76:LEU:HD22	49:w:149:ALA:HB1	1.78	0.64
48:v:43:GLN:O	48:v:51:ARG:NH2	2.30	0.64
6:H:62:ALA:O	6:H:66:ARG:NH1	2.30	0.64
8:J:84:GLN:NE2	8:J:124:LYS:O	2.31	0.64
1:A:1804:U:O2	19:U:69:ARG:NH1	2.31	0.64
1:A:2342:U:O2'	1:A:2343:A:OP1	2.14	0.64
5:F:126:LYS:NZ	5:F:138:HIS:O	2.31	0.63
20:V:177:THR:HG21	23:Y:87:TRP:CZ2	2.34	0.63
44:q:44:ASN:O	44:q:47:THR:HG22	1.98	0.63
1:A:1493:A:O2'	21:W:57:GLU:OE1	2.12	0.63
35:d:244:GLU:N	35:d:244:GLU:OE1	2.31	0.63
7:I:52:GLU:N	7:I:52:GLU:OE1	2.32	0.63
7:I:138:SER:O	7:I:141:ARG:NH1	2.31	0.63
23:Y:87:TRP:O	23:Y:143:ASN:ND2	2.32	0.63
47:u:188:TRP:O	47:u:191:ARG:NH1	2.31	0.63
36:e:264:PRO:O	36:e:268:ALA:N	2.29	0.63
35:d:106:THR:OG1	35:d:107:GLN:N	2.31	0.62
37:f:160:GLY:O	37:f:161:LEU:HD22	2.00	0.62
25:x:221:ASP:OD1	25:x:222:ILE:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1983:G:O2'	1:A:2068:G:N2	2.27	0.62
1:A:2057:G:O2'	1:A:2058:G:OP1	2.18	0.62
31:6:70:TRP:O	31:6:72:ARG:NH2	2.33	0.62
56:z:245:ARG:NH2	56:z:321:ASP:OD2	2.32	0.62
58:k:17:ARG:HG2	58:k:52:ILE:HD11	1.82	0.62
1:A:1237:A:O2'	1:A:1238:U:OP1	2.14	0.62
1:A:1786:C:OP1	18:T:165:TYR:OH	2.18	0.62
14:P:86:THR:OG1	14:P:88:HIS:O	2.18	0.61
23:Y:117:LEU:HD21	23:Y:129:PRO:HD2	1.82	0.61
20:V:93:THR:HG21	20:V:110:ALA:HB1	1.82	0.61
46:s:159:LEU:HD23	46:s:159:LEU:O	2.00	0.61
1:A:1893:C:O2'	1:A:1894:A:OP2	2.17	0.61
41:j:112:THR:HG22	41:j:112:THR:O	1.99	0.61
1:A:1280:C:N3	1:A:1281:A:N6	2.47	0.60
1:A:2617:A:O2'	1:A:2618:A:OP2	2.19	0.60
43:p:172:ASP:OD1	43:p:173:ALA:N	2.34	0.60
1:A:2625:A:O3'	45:r:94:ARG:NH1	2.34	0.60
21:W:148:LEU:O	31:6:339:GLU:N	2.34	0.60
56:z:63:GLY:CA	56:z:219:LEU:HD11	2.31	0.60
20:V:78:GLN:OE1	35:d:74:ARG:NH1	2.34	0.60
1:A:2402:U:O4	1:A:2458:G:N2	2.33	0.60
14:P:51:ARG:NH2	31:6:221:LEU:O	2.35	0.60
34:c:209:GLU:OE1	34:c:209:GLU:N	2.34	0.60
32:7:163:LEU:HD22	32:7:178:TYR:HE2	1.65	0.60
50:5:401:VAL:O	50:5:401:VAL:HG13	2.01	0.60
1:A:1628:A:O2'	1:A:1647:A:N3	2.34	0.60
35:d:126:ARG:O	35:d:130:ALA:N	2.35	0.60
20:V:93:THR:CG2	20:V:110:ALA:HB1	2.32	0.59
8:J:125:ALA:HB2	8:J:140:VAL:HG21	1.83	0.59
58:k:13:VAL:HG23	58:k:49:CYS:HB3	1.82	0.59
35:d:115:ASN:O	35:d:119:GLN:N	2.35	0.59
15:Q:237:ASN:OD1	15:Q:238:PHE:N	2.36	0.59
7:I:132:LYS:NZ	7:I:147:PHE:O	2.32	0.59
20:V:161:ARG:NH2	20:V:163:ASP:OD2	2.36	0.59
25:x:221:ASP:OD2	44:q:155:ARG:NH1	2.35	0.59
53:a:34:THR:HG22	53:a:34:THR:O	2.02	0.59
49:w:126:PHE:CE2	49:w:148:ILE:HD13	2.38	0.59
22:X:61:ARG:NH2	22:X:63:GLU:OE2	2.35	0.59
2:B:9:A:OP1	2:B:45:A:O2'	2.19	0.59
31:6:219:ILE:HG21	31:6:231:GLU:HG3	1.85	0.59
25:x:180:ALA:HB3	25:x:181:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:196:LEU:HD23	56:z:196:LEU:O	2.02	0.59
37:f:178:PRO:O	37:f:179:GLU:HB3	2.03	0.58
56:z:191:VAL:HG21	56:z:199:LEU:HG	1.86	0.58
18:T:88:ILE:HA	18:T:91:MET:HE2	1.84	0.58
36:e:158:LEU:HD21	36:e:262:LEU:HD11	1.84	0.58
47:u:207:GLU:N	47:u:207:GLU:OE1	2.36	0.58
10:L:70:GLY:O	10:L:134:TYR:OH	2.13	0.58
32:7:76:PHE:HB3	32:7:78:MET:HE3	1.86	0.58
55:l:69:ALA:N	55:l:81:VAL:O	2.33	0.58
14:P:74:ASN:O	14:P:147:GLN:NE2	2.35	0.58
39:h:136:GLN:N	39:h:136:GLN:OE1	2.34	0.57
2:B:57:U:H2'	2:B:58:C:O4'	2.05	0.57
1:A:1215:G:N2	1:A:1218:A:OP2	2.36	0.57
25:x:309:LEU:CD1	25:x:360:LEU:HD21	2.34	0.57
1:A:1263:A:OP1	53:a:134:LYS:NZ	2.37	0.57
34:c:80:GLN:O	34:c:210:ARG:NH2	2.38	0.57
56:z:91:GLU:O	56:z:93:GLN:N	2.38	0.57
37:f:97:TYR:CZ	54:m:65:ILE:HG22	2.40	0.57
1:A:1115:A:H4'	1:A:1115:A:OP2	2.05	0.56
19:U:59:GLN:NE2	52:9:58:PHE:O	2.38	0.56
1:A:2334:G:N2	1:A:2358:G:O4'	2.38	0.56
5:F:75:GLU:OE2	39:h:57:ARG:NH2	2.37	0.56
29:3:125:ARG:NH1	29:3:145:ARG:O	2.39	0.56
33:b:89:VAL:HG12	33:b:89:VAL:O	2.05	0.56
48:v:14:ARG:NH1	49:w:132:ASP:OD2	2.39	0.56
21:W:112:GLU:OE1	21:W:112:GLU:N	2.33	0.56
40:i:77:PRO:HD2	40:i:80:LEU:HD11	1.87	0.56
44:q:111:GLU:OE1	44:q:114:ARG:NH2	2.37	0.56
6:H:118:ASN:O	6:H:122:SER:OG	2.24	0.56
39:h:115:ASN:HA	39:h:118:LEU:HD13	1.87	0.56
1:A:1564:U:O2'	1:A:1577:A:N3	2.38	0.56
56:z:194:ARG:HB2	56:z:195:PRO:HD3	1.88	0.56
12:N:97:LEU:HD12	12:N:154:VAL:HG21	1.88	0.56
56:z:167:LEU:HG	56:z:169:THR:HG23	1.88	0.56
36:e:46:SER:OG	36:e:228:LYS:O	2.22	0.55
1:A:1854:C:OP2	46:s:304:ARG:NH1	2.40	0.55
14:P:61:VAL:HG12	14:P:61:VAL:O	2.07	0.55
1:A:1383:G:O2'	1:A:1386:G:O2'	2.20	0.55
5:F:277:ASP:O	5:F:278:SER:OG	2.17	0.55
32:7:293:ARG:NH1	32:7:321:VAL:O	2.39	0.55
41:j:62:GLN:OE1	41:j:65:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:G:OP2	23:Y:232:LYS:NZ	2.39	0.55
31:6:181:GLU:N	31:6:181:GLU:OE1	2.39	0.55
49:w:80:LYS:CG	49:w:145:VAL:HG11	2.37	0.55
11:M:283:LYS:NZ	38:g:41:SER:OG	2.40	0.55
1:A:1237:A:HO2'	1:A:1238:U:P	2.31	0.54
49:w:138:LEU:HD12	49:w:139:MET:N	2.22	0.54
1:A:2524:G:N2	1:A:2527:A:OP2	2.31	0.54
25:x:190:GLN:O	25:x:191:THR:OG1	2.24	0.54
56:z:259:SER:O	56:z:260:ALA:HB3	2.06	0.54
5:F:113:ASN:OD1	5:F:157:GLY:N	2.35	0.54
17:S:136:LYS:NZ	41:j:47:ASP:OD1	2.25	0.54
20:V:177:THR:HG21	23:Y:87:TRP:HZ2	1.72	0.54
30:4:71:ILE:CG2	30:4:89:ILE:HD12	2.38	0.54
25:x:75:ALA:O	25:x:129:PHE:N	2.37	0.54
8:J:18:GLY:N	8:J:72:ILE:O	2.39	0.54
55:l:107:LEU:HD13	55:l:114:TYR:HA	1.90	0.54
1:A:1234:C:H3'	1:A:1235:U:C5'	2.38	0.54
31:6:212:SER:O	31:6:214:TRP:NE1	2.41	0.54
32:7:163:LEU:HD22	32:7:178:TYR:CE2	2.42	0.54
1:A:1389:A:OP2	18:T:154:GLY:O	2.26	0.54
1:A:2057:G:O2'	1:A:2058:G:P	2.66	0.54
33:b:131:HIS:CE1	33:b:134:THR:HG23	2.43	0.54
56:z:275:LEU:O	56:z:277:LYS:NZ	2.33	0.54
1:A:1583:C:OP2	45:r:190:ARG:NH2	2.41	0.53
13:O:57:GLU:OE2	13:O:105:THR:OG1	2.25	0.53
1:A:1154:U:OP1	6:H:73:ARG:NH1	2.40	0.53
17:S:112:VAL:HG13	17:S:199:ILE:HG13	1.89	0.53
37:f:92:ILE:CD1	37:f:158:ILE:HD12	2.38	0.53
1:A:1646:A:H2'	1:A:1647:A:H5"	1.90	0.53
1:A:1815:U:O3'	50:5:89:ARG:NH1	2.41	0.53
8:J:117:VAL:HG12	8:J:141:VAL:HG23	1.90	0.53
4:E:269:TYR:HB3	4:E:304:LEU:HD11	1.91	0.53
7:I:150:HIS:O	58:k:31:ARG:NH2	2.42	0.53
26:0:127:GLU:OE2	26:0:131:GLN:NE2	2.41	0.53
32:7:200:THR:HG22	32:7:277:VAL:H	1.73	0.53
56:z:271:VAL:HG13	56:z:300:ALA:HB1	1.89	0.53
36:e:45:LEU:HD23	36:e:228:LYS:HE2	1.91	0.53
54:m:70:PRO:O	54:m:72:ARG:NH1	2.42	0.53
49:w:81:ASP:O	49:w:85:TYR:N	2.41	0.52
1:A:1188:A:O2'	1:A:1189:C:OP2	2.23	0.52
2:B:48:G:N2	2:B:59:C:O2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:172:ASP:O	25:x:195:ARG:N	2.42	0.52
31:6:104:LEU:O	31:6:108:HIS:ND1	2.42	0.52
1:A:1755:C:OP1	26:0:138:GLN:NE2	2.42	0.52
21:W:99:TYR:CD2	21:W:131:VAL:HG22	2.44	0.52
1:A:1595:U:O2'	1:A:1596:A:O5'	2.24	0.52
15:Q:153:ASN:OD1	15:Q:154:THR:N	2.42	0.52
25:x:220:GLN:O	25:x:224:GLU:N	2.36	0.52
5:F:92:ARG:HG2	5:F:95:ILE:HD12	1.90	0.52
1:A:1283:A:O4'	1:A:2130:A:N6	2.42	0.52
33:b:33:LEU:HD11	33:b:47:VAL:HG21	1.91	0.52
37:f:97:TYR:CE2	54:m:65:ILE:HG22	2.45	0.52
1:A:1431:A:OP2	1:A:2171:A:O2'	2.28	0.52
1:A:1789:A:N1	18:T:151:ARG:HD3	2.25	0.52
4:E:216:GLN:HG3	4:E:261:MET:HE2	1.92	0.52
10:L:129:ARG:NH2	15:Q:125:TYR:O	2.43	0.52
55:l:74:ILE:HG22	55:l:74:ILE:O	2.10	0.52
1:A:1390:A:OP2	1:A:1938:C:N4	2.42	0.52
14:P:167:GLU:O	43:p:187:ARG:NH1	2.42	0.52
38:g:68:THR:HG22	38:g:69:PRO:HD2	1.92	0.52
39:h:81:SER:O	39:h:82:SER:OG	2.14	0.52
17:S:139:LEU:HD13	17:S:148:LEU:CD2	2.36	0.51
1:A:1134:A:N7	23:Y:197:ASN:ND2	2.58	0.51
1:A:2395:U:O4	1:A:2396:A:N6	2.42	0.51
16:R:14:LEU:HD23	16:R:16:ASP:H	1.76	0.51
47:u:88:ILE:HD12	47:u:117:TYR:CD2	2.46	0.51
31:6:302:ASP:OD1	31:6:303:PHE:N	2.43	0.51
1:A:1188:A:H61	44:q:33:ARG:HA	1.75	0.51
10:L:96:MET:HE1	15:Q:171:ILE:HD11	1.92	0.51
15:Q:251:GLU:OE1	15:Q:251:GLU:N	2.38	0.51
31:6:176:ALA:HB3	31:6:184:LEU:HD12	1.92	0.51
34:c:31:VAL:HG13	34:c:31:VAL:O	2.10	0.51
45:r:93:ILE:HG22	45:r:94:ARG:O	2.10	0.51
53:a:96:VAL:O	53:a:96:VAL:HG13	2.09	0.51
29:3:126:LYS:HD3	29:3:148:VAL:HG21	1.92	0.51
45:r:47:THR:N	58:k:73:ARG:O	2.43	0.51
56:z:99:LEU:HG	56:z:104:LEU:HD12	1.92	0.51
46:s:131:LEU:HD11	46:s:133:LEU:HD23	1.92	0.51
1:A:1156:U:O3'	40:i:95:LYS:NZ	2.44	0.51
2:B:32:U:N3	54:m:43:ARG:O	2.44	0.51
1:A:2116:U:O2'	26:0:80:PRO:O	2.28	0.51
36:e:190:LEU:HD22	36:e:198:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1799:U:O2	23:Y:125:ARG:NH2	2.45	0.50
1:A:1990:G:H3'	1:A:1991:A:H4'	1.93	0.50
4:E:208:ALA:HB2	4:E:297:VAL:HG12	1.94	0.50
21:W:61:VAL:HG21	21:W:97:VAL:CG2	2.41	0.50
49:w:134:ASP:OD1	49:w:134:ASP:N	2.44	0.50
1:A:2614:C:O2	9:K:97:ARG:NH2	2.42	0.50
2:B:4:A:H2'	2:B:5:A:C8	2.47	0.50
36:e:58:THR:HG22	54:m:34:CYS:SG	2.51	0.50
1:A:1160:A:O2'	1:A:1161:C:P	2.70	0.50
56:z:261:CYS:SG	56:z:262:ASP:N	2.84	0.50
17:S:168:THR:HG22	33:b:107:GLN:HG2	1.92	0.50
21:W:61:VAL:HG13	21:W:65:ASN:HB2	1.92	0.50
46:s:354:VAL:HG12	46:s:363:PHE:CD2	2.47	0.50
1:A:1832:A:H4'	1:A:1832:A:OP1	2.12	0.50
3:D:203:ARG:O	50:5:30:ALA:N	2.45	0.50
33:b:12:THR:HG22	33:b:13:SER:N	2.27	0.50
57:y:169:LEU:O	57:y:213:THR:HG22	2.12	0.50
1:A:1137:A:O2'	1:A:1138:U:OP1	2.27	0.50
1:A:2656:C:H2'	1:A:2656:C:O2	2.12	0.50
23:Y:153:ASP:OD1	23:Y:156:ARG:NH2	2.41	0.50
46:s:354:VAL:HG12	46:s:363:PHE:HD2	1.76	0.50
8:J:33:PRO:N	8:J:34:PRO:HD2	2.27	0.50
26:0:166:GLU:OE1	26:0:166:GLU:N	2.37	0.50
36:e:262:LEU:HD23	36:e:267:LEU:HB3	1.94	0.50
12:N:147:ILE:O	12:N:147:ILE:HG23	2.11	0.49
15:Q:181:LYS:O	15:Q:218:ASN:N	2.40	0.49
25:x:136:VAL:HG12	25:x:136:VAL:O	2.13	0.49
37:f:126:MET:SD	37:f:155:VAL:HG23	2.52	0.49
53:a:53:ASP:OD1	53:a:54:GLY:N	2.45	0.49
14:P:42:GLU:OE2	31:6:338:ARG:NH1	2.45	0.49
58:k:86:MET:O	58:k:90:LEU:HD23	2.12	0.49
17:S:112:VAL:CG1	17:S:199:ILE:HG21	2.42	0.49
20:V:133:ILE:HG21	20:V:154:ILE:HD12	1.94	0.49
1:A:1458:A:H4'	1:A:1459:A:OP1	2.11	0.49
1:A:1688:U:O2'	17:S:122:ASN:ND2	2.46	0.49
4:E:202:GLN:NE2	4:E:301:ASP:OD1	2.45	0.49
49:w:105:MET:HG2	49:w:139:MET:CE	2.43	0.49
30:4:71:ILE:HG22	30:4:89:ILE:HD12	1.94	0.49
37:f:160:GLY:C	37:f:161:LEU:HD22	2.37	0.49
31:6:371:ASP:OD1	31:6:372:SER:N	2.44	0.49
46:s:205:LEU:CD2	46:s:224:ARG:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1469:G:O2'	11:M:55:GLU:OE1	2.31	0.49
10:L:58:ILE:HD11	10:L:76:ALA:HB2	1.95	0.49
18:T:85:ALA:O	18:T:139:SER:OG	2.30	0.49
3:D:226:ILE:HD11	57:y:133:LEU:HD22	1.95	0.49
20:V:50:SER:OG	20:V:52:GLU:OE1	2.31	0.49
36:e:48:ALA:N	36:e:230:PHE:O	2.46	0.49
45:r:115:ILE:O	45:r:119:VAL:HG23	2.12	0.49
1:A:1236:A:H2'	1:A:1237:A:O4'	2.12	0.49
1:A:1345:A:OP1	28:2:63:LYS:NZ	2.41	0.49
17:S:98:ARG:NH2	17:S:114:ALA:O	2.45	0.48
33:b:89:VAL:O	33:b:89:VAL:CG1	2.60	0.48
38:g:132:LEU:HD21	38:g:153:PHE:HZ	1.77	0.48
49:w:141:PRO:O	49:w:145:VAL:HG23	2.13	0.48
19:U:146:LEU:HD11	35:d:240:LYS:HB2	1.94	0.48
35:d:190:GLU:OE2	35:d:215:ARG:NH1	2.45	0.48
53:a:45:GLN:O	53:a:61:HIS:HA	2.14	0.48
49:w:79:ILE:HG22	49:w:145:VAL:HG22	1.95	0.48
56:z:191:VAL:HG21	56:z:199:LEU:CG	2.42	0.48
1:A:1134:A:H1'	1:A:1135:U:H5'	1.96	0.48
1:A:2600:A:O2'	13:O:12:GLY:O	2.29	0.48
38:g:132:LEU:HD21	38:g:153:PHE:CZ	2.49	0.48
2:B:43:A:H2'	2:B:44:G:O4'	2.14	0.48
25:x:244:ASP:OD1	25:x:379:ARG:NH1	2.46	0.48
56:z:181:ILE:HD11	62:z:401:GNP:O1A	2.14	0.48
1:A:2341:A:O2'	27:1:60:LYS:NZ	2.47	0.48
8:J:32:GLY:O	8:J:36:GLY:N	2.42	0.48
20:V:126:VAL:HB	20:V:152:ARG:NH1	2.29	0.48
25:x:348:THR:O	25:x:348:THR:HG22	2.14	0.48
1:A:1821:A:C2	3:D:129:VAL:HG11	2.49	0.48
5:F:97:HIS:CE1	5:F:101:ILE:HD12	2.49	0.48
8:J:90:PHE:CE2	8:J:120:ILE:HG21	2.49	0.48
11:M:190:ILE:HD11	38:g:52:LEU:HD22	1.96	0.48
17:S:180:LYS:O	17:S:181:ARG:HG2	2.13	0.48
1:A:1235:U:H1'	1:A:1236:A:OP2	2.14	0.48
33:b:6:THR:HG22	33:b:7:SER:N	2.28	0.48
46:s:226:GLN:NE2	46:s:275:SER:OG	2.46	0.48
55:l:69:ALA:HB1	55:l:72:VAL:HG13	1.95	0.48
9:K:174:ASP:O	45:r:35:LEU:N	2.47	0.47
35:d:213:THR:HG22	35:d:247:VAL:HG22	1.95	0.47
1:A:2071:C:O2'	56:z:168:ARG:O	2.32	0.47
34:c:307:PHE:O	34:c:307:PHE:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:90:LEU:HD23	37:f:185:VAL:CG1	2.44	0.47
26:0:153:VAL:HG21	26:0:170:GLY:O	2.14	0.47
31:6:60:ARG:O	31:6:60:ARG:NH1	2.47	0.47
51:8:172:GLU:OE1	51:8:172:GLU:N	2.46	0.47
1:A:1317:U:OP1	11:M:132:LYS:NZ	2.42	0.47
1:A:1607:G:N1	1:A:1608:C:O2	2.47	0.47
1:A:2283:A:H2'	1:A:2284:A:O4'	2.14	0.47
21:W:98:ARG:N	21:W:132:HIS:O	2.41	0.47
31:6:175:VAL:HG11	31:6:270:PHE:CE2	2.48	0.47
45:r:69:GLN:O	45:r:74:ARG:NH2	2.46	0.47
57:y:202:ARG:HG2	57:y:212:ILE:HD11	1.97	0.47
10:L:142:GLN:HG3	47:u:187:LEU:HD21	1.96	0.47
13:O:38:ARG:NE	13:O:82:GLU:OE1	2.44	0.47
16:R:149:HIS:O	24:Z:151:LEU:N	2.46	0.47
32:7:67:VAL:O	32:7:67:VAL:HG22	2.14	0.47
1:A:1210:G:O2'	1:A:1221:G:O6	2.25	0.47
1:A:1458:A:H1'	1:A:1459:A:C8	2.49	0.47
25:x:257:THR:HG23	25:x:257:THR:O	2.15	0.47
25:x:342:ARG:NE	25:x:359:GLU:OE1	2.40	0.47
38:g:154:ASP:OD1	38:g:154:ASP:N	2.48	0.47
46:s:151:VAL:HG12	46:s:153:ARG:HG3	1.96	0.47
1:A:1278:U:H2'	1:A:1279:G:H5"	1.96	0.47
1:A:1712:U:OP2	40:i:46:ARG:NH1	2.41	0.47
19:U:112:PRO:O	19:U:113:GLU:HB2	2.14	0.47
20:V:55:HIS:HB2	20:V:133:ILE:HD11	1.97	0.47
25:x:180:ALA:CB	25:x:181:PRO:CD	2.93	0.47
25:x:334:GLN:NE2	25:x:335:VAL:O	2.48	0.47
31:6:173:LEU:HD21	31:6:175:VAL:HG23	1.97	0.47
46:s:41:VAL:HG22	46:s:41:VAL:O	2.15	0.47
1:A:1142:A:OP2	6:H:72:ARG:NH1	2.47	0.47
5:F:62:VAL:HG21	5:F:88:ALA:HB2	1.96	0.47
5:F:226:MET:SD	5:F:242:LEU:HD21	2.54	0.47
8:J:114:LEU:HG	8:J:157:LYS:O	2.15	0.47
31:6:191:ASN:OD1	31:6:192:GLU:N	2.48	0.47
32:7:259:ASP:OD1	32:7:260:VAL:N	2.47	0.47
33:b:21:ARG:NE	34:c:217:ASP:OD2	2.40	0.47
1:A:1190:A:H4'	1:A:1191:U:H2'	1.96	0.47
1:A:2070:A:H3'	1:A:2071:C:H5"	1.97	0.47
1:A:2122:U:O2'	1:A:2546:U:H5'	2.15	0.47
31:6:208:ALA:O	31:6:209:ASP:CB	2.62	0.47
1:A:1507:A:H3'	1:A:1508:A:H5"	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1613:A:H4'	1:A:1614:A:OP1	2.15	0.47
1:A:2253:G:N2	1:A:2430:C:O4'	2.48	0.47
1:A:1501:A:OP1	24:Z:40:ARG:NH1	2.47	0.46
7:I:95:MET:SD	7:I:95:MET:N	2.84	0.46
20:V:144:VAL:HG21	20:V:153:ILE:HD12	1.96	0.46
21:W:110:ASN:OD1	21:W:110:ASN:O	2.33	0.46
24:Z:69:VAL:HG23	24:Z:91:LEU:HD21	1.97	0.46
33:b:45:GLU:HB2	33:b:94:VAL:HG22	1.96	0.46
46:s:107:GLN:O	46:s:111:LYS:N	2.48	0.46
47:u:182:TYR:HB3	47:u:184:LEU:HD12	1.97	0.46
1:A:1819:C:OP2	3:D:71:LYS:NZ	2.47	0.46
1:A:2161:G:O2'	1:A:2162:A:H5'	2.15	0.46
2:B:14:A:N1	2:B:21:A:O2'	2.45	0.46
5:F:284:TYR:HB2	5:F:285:PRO:HD2	1.97	0.46
56:z:86:LEU:HD23	56:z:86:LEU:H	1.80	0.46
1:A:1542:C:H2'	1:A:1543:U:H5'	1.98	0.46
1:A:1710:U:O2'	5:F:104:ARG:NH2	2.48	0.46
1:A:1757:A:O2'	46:s:210:ARG:NH1	2.48	0.46
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.98	0.46
20:V:195:GLU:OE1	20:V:195:GLU:N	2.46	0.46
25:x:70:GLU:O	25:x:368:ASN:ND2	2.48	0.46
36:e:154:ASN:C	36:e:155:LEU:HD12	2.40	0.46
56:z:215:THR:O	56:z:219:LEU:HD13	2.15	0.46
2:B:4:A:H2	2:B:63:A:H61	1.63	0.46
7:I:102:VAL:HG22	7:I:102:VAL:O	2.16	0.46
10:L:38:VAL:HG21	10:L:105:VAL:HG13	1.97	0.46
36:e:53:ARG:HH11	36:e:155:LEU:HD13	1.80	0.46
47:u:144:LYS:O	47:u:145:CYS:SG	2.72	0.46
56:z:91:GLU:O	56:z:92:GLN:C	2.59	0.46
1:A:2598:A:N1	15:Q:261:ASN:O	2.49	0.46
46:s:205:LEU:HB2	46:s:374:THR:HG22	1.97	0.46
1:A:1172:G:OP2	1:A:1174:A:N6	2.49	0.46
1:A:2501:A:H5'	1:A:2503:G:O3'	2.16	0.46
7:I:188:ARG:NH2	58:k:55:VAL:O	2.48	0.46
35:d:164:VAL:HG12	35:d:261:MET:HB3	1.96	0.46
36:e:203:LEU:HD13	37:f:170:LEU:HD21	1.98	0.46
37:f:167:GLU:OE1	51:8:143:GLN:NE2	2.48	0.46
56:z:29:TRP:HE1	56:z:225:VAL:HG13	1.80	0.46
1:A:2629:A:N3	1:A:2629:A:H2'	2.31	0.46
38:g:72:TRP:NE1	38:g:92:HIS:O	2.42	0.46
40:i:80:LEU:HD12	40:i:80:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:118:ILE:O	56:z:121:ILE:HG22	2.15	0.46
41:j:112:THR:O	41:j:112:THR:CG2	2.63	0.46
49:w:128:PHE:O	49:w:129:GLU:HB2	2.15	0.46
1:A:1966:U:H2'	3:D:209:ARG:HG3	1.98	0.45
1:A:1986:C:H4'	1:A:1986:C:OP1	2.16	0.45
11:M:155:VAL:O	11:M:175:THR:HA	2.16	0.45
1:A:1831:U:H4'	1:A:1831:U:OP1	2.16	0.45
22:X:116:SER:O	22:X:120:ASP:N	2.49	0.45
49:w:81:ASP:OD1	49:w:82:ARG:N	2.50	0.45
56:z:83:LYS:HB3	56:z:86:LEU:HD21	1.98	0.45
1:A:2075:U:OP2	1:A:2076:A:O2'	2.34	0.45
12:N:103:GLU:OE1	12:N:106:ARG:NH2	2.48	0.45
31:6:177:TYR:N	31:6:185:ILE:O	2.44	0.45
31:6:217:LEU:HD21	31:6:219:ILE:HD12	1.98	0.45
1:A:1188:A:H1'	1:A:1189:C:C5'	2.46	0.45
2:B:27:A:OP1	37:f:115:ARG:NE	2.49	0.45
10:L:118:ARG:NH2	47:u:194:ASP:OD2	2.48	0.45
30:4:81:VAL:HG12	30:4:82:LYS:N	2.31	0.45
37:f:126:MET:HE2	37:f:153:GLU:CB	2.47	0.45
56:z:121:ILE:HG23	56:z:122:VAL:N	2.31	0.45
5:F:102:TRP:O	5:F:106:PHE:HD1	1.99	0.45
10:L:77:ILE:HG23	10:L:77:ILE:O	2.16	0.45
15:Q:265:ILE:HG12	15:Q:271:ARG:NH1	2.32	0.45
17:S:181:ARG:O	17:S:181:ARG:CG	2.64	0.45
25:x:256:THR:O	25:x:256:THR:HG22	2.16	0.45
36:e:199:GLU:OE1	36:e:238:THR:OG1	2.34	0.45
1:A:1188:A:H1'	1:A:1189:C:OP2	2.17	0.45
1:A:2293:A:OP1	29:3:138:THR:OG1	2.31	0.45
4:E:154:ARG:O	32:7:306:GLN:NE2	2.49	0.45
12:N:112:PHE:CD1	12:N:175:ILE:HG21	2.52	0.45
36:e:174:VAL:HG12	36:e:175:GLU:N	2.32	0.45
1:A:1102:U:O2'	1:A:1103:A:P	2.75	0.45
1:A:1228:G:O6	20:V:41:ARG:NH1	2.43	0.45
2:B:64:A:H2'	2:B:65:A:C8	2.52	0.45
12:N:112:PHE:CE1	12:N:175:ILE:HG21	2.50	0.45
35:d:186:VAL:HG12	35:d:187:GLU:N	2.32	0.45
55:l:105:GLU:OE1	55:l:105:GLU:N	2.44	0.45
15:Q:240:ILE:HG21	15:Q:243:ILE:HD12	1.98	0.45
31:6:185:ILE:HG12	43:p:189:ARG:HG3	1.99	0.45
36:e:194:SER:O	36:e:246:LYS:NZ	2.39	0.45
45:r:149:ARG:HD3	45:r:152:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:181:ARG:O	17:S:181:ARG:HG3	2.17	0.45
32:7:70:THR:HG23	32:7:96:TYR:OH	2.16	0.45
2:B:8:U:O3'	2:B:45:A:H1'	2.17	0.45
3:D:111:ARG:NH2	3:D:180:GLY:O	2.41	0.45
31:6:214:TRP:N	31:6:240:ILE:O	2.47	0.45
37:f:95:THR:HG23	37:f:182:ARG:HB3	1.98	0.45
56:z:303:ASP:OD1	56:z:306:ARG:NH1	2.50	0.45
1:A:1256:A:O2'	1:A:2121:C:H5	2.00	0.44
14:P:116:LEU:C	14:P:116:LEU:HD12	2.43	0.44
35:d:200:SER:OG	35:d:208:MET:SD	2.74	0.44
49:w:138:LEU:HD12	49:w:140:CYS:H	1.82	0.44
56:z:271:VAL:CG1	56:z:300:ALA:HB1	2.47	0.44
1:A:1237:A:O2'	1:A:1238:U:P	2.74	0.44
1:A:1560:A:N6	1:A:1561:A:H62	2.15	0.44
3:D:159:LYS:N	3:D:162:ASP:OD2	2.45	0.44
34:c:228:LEU:HB2	34:c:307:PHE:CD2	2.52	0.44
39:h:114:PRO:O	39:h:118:LEU:HD12	2.17	0.44
1:A:1612:A:H2'	1:A:1613:A:O4'	2.16	0.44
1:A:2062:U:H3'	1:A:2063:A:H5"	1.99	0.44
3:D:143:VAL:HG21	3:D:164:ILE:HD11	1.98	0.44
12:N:191:SER:N	12:N:194:THR:OG1	2.51	0.44
36:e:52:GLN:O	36:e:236:LEU:N	2.45	0.44
38:g:68:THR:CG2	38:g:69:PRO:HD2	2.47	0.44
45:r:140:LEU:HD12	45:r:141:PRO:O	2.17	0.44
1:A:1488:A:H2'	1:A:1489:A:O4'	2.18	0.44
39:h:130:PHE:O	39:h:133:VAL:HG22	2.18	0.44
51:8:147:LEU:HD23	51:8:158:TYR:HE1	1.83	0.44
58:k:90:LEU:O	58:k:94:ILE:HG12	2.18	0.44
1:A:1635:C:N4	1:A:1642:G:H22	2.14	0.44
1:A:2177:A:N3	1:A:2362:A:O2'	2.40	0.44
1:A:2617:A:O2'	1:A:2618:A:C8	2.70	0.44
25:x:257:THR:HA	25:x:307:CYS:SG	2.57	0.44
32:7:78:MET:HB3	32:7:83:SER:OG	2.18	0.44
46:s:49:ALA:O	46:s:61:ARG:NH1	2.43	0.44
49:w:74:LEU:HD13	49:w:152:LYS:HB3	1.99	0.44
57:y:227:PRO:O	57:y:228:ASN:HB2	2.18	0.44
1:A:1137:A:HO2'	1:A:1138:U:P	2.40	0.44
1:A:2617:A:N6	1:A:2643:U:O4'	2.50	0.44
25:x:234:ASP:OD1	25:x:236:ARG:N	2.50	0.44
26:0:156:MET:HE1	26:0:168:ASP:OD1	2.18	0.44
46:s:110:THR:HG23	46:s:327:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:w:74:LEU:HD12	49:w:79:ILE:HD11	1.99	0.44
1:A:1894:A:OP1	13:O:9:ILE:N	2.50	0.44
2:B:63:A:H2'	2:B:64:A:C1'	2.48	0.44
10:L:96:MET:HE2	15:Q:165:GLU:H	1.82	0.44
11:M:61:ARG:O	40:i:128:ARG:NH2	2.46	0.44
19:U:28:LEU:O	23:Y:116:THR:HG23	2.18	0.44
19:U:146:LEU:HD23	35:d:222:LEU:HB3	1.99	0.44
31:6:220:ASN:O	31:6:231:GLU:HB2	2.18	0.44
1:A:2373:G:OP1	5:F:137:ARG:NH1	2.41	0.44
4:E:121:LEU:HD22	4:E:284:TYR:CD1	2.53	0.44
5:F:160:SER:HB3	40:i:80:LEU:HD13	1.99	0.44
18:T:168:TYR:CE2	18:T:170:VAL:HG13	2.53	0.44
31:6:235:TRP:HB3	31:6:254:TYR:HA	2.00	0.44
1:A:2073:G:P	56:z:164:ARG:HE	2.41	0.44
1:A:2113:A:OP1	18:T:162:GLU:N	2.49	0.44
1:A:2281:C:H2'	1:A:2282:G:O4'	2.18	0.44
2:B:3:U:H3'	2:B:4:A:H8	1.83	0.44
8:J:23:ILE:O	8:J:23:ILE:HG23	2.17	0.44
16:R:14:LEU:HD22	16:R:17:ARG:HB2	1.99	0.44
37:f:125:ALA:HB2	37:f:154:ARG:NE	2.32	0.44
1:A:2575:C:H4'	1:A:2575:C:OP1	2.18	0.43
4:E:154:ARG:HG2	4:E:172:PRO:HG3	1.99	0.43
8:J:110:GLY:O	8:J:111:LEU:HD12	2.18	0.43
32:7:111:ASP:OD1	32:7:265:LEU:N	2.43	0.43
33:b:47:VAL:O	33:b:51:VAL:HG12	2.17	0.43
35:d:235:GLN:HB2	35:d:240:LYS:HZ1	1.83	0.43
37:f:92:ILE:HD13	37:f:158:ILE:HD12	2.00	0.43
1:A:1493:A:O2'	21:W:99:TYR:HB2	2.17	0.43
9:K:101:VAL:O	9:K:101:VAL:HG12	2.18	0.43
11:M:190:ILE:HD11	38:g:52:LEU:CD2	2.48	0.43
14:P:107:THR:HG22	14:P:107:THR:O	2.17	0.43
19:U:37:GLU:OE2	46:s:259:LYS:NZ	2.37	0.43
25:x:159:SER:O	25:x:184:LYS:NZ	2.40	0.43
37:f:198:LYS:HB2	37:f:203:LEU:HD11	2.00	0.43
46:s:146:GLN:O	46:s:151:VAL:HG23	2.18	0.43
54:m:65:ILE:HD11	54:m:74:LEU:HD12	2.01	0.43
1:A:1610:U:H1'	1:A:1617:A:H61	1.82	0.43
4:E:120:THR:HG21	4:E:289:VAL:HG23	2.01	0.43
8:J:50:CYS:O	8:J:54:ASN:N	2.44	0.43
9:K:67:PHE:HD2	9:K:72:TRP:CE2	2.36	0.43
15:Q:246:ASP:OD1	15:Q:247:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:257:THR:OG1	25:x:260:HIS:HB3	2.18	0.43
37:f:92:ILE:HD11	37:f:158:ILE:HD12	2.00	0.43
1:A:1556:A:H2'	1:A:1559:A:H61	1.82	0.43
1:A:2389:C:H2'	1:A:2390:C:O4'	2.18	0.43
14:P:156:ASP:OD1	14:P:156:ASP:N	2.51	0.43
15:Q:194:LEU:HD23	15:Q:223:LYS:O	2.19	0.43
34:c:184:PHE:HA	34:c:185:PRO:C	2.43	0.43
36:e:121:MET:O	36:e:124:GLN:NE2	2.49	0.43
38:g:42:VAL:HG12	38:g:42:VAL:O	2.18	0.43
48:v:40:ARG:O	48:v:44:LYS:HG2	2.18	0.43
56:z:48:VAL:O	56:z:75:LYS:NZ	2.41	0.43
1:A:2654:A:C3'	1:A:2655:C:H5'	2.48	0.43
11:M:237:MET:O	43:p:155:ARG:NH2	2.51	0.43
25:x:104:SER:O	25:x:104:SER:OG	2.37	0.43
31:6:197:GLU:OE2	43:p:185:ARG:NH2	2.52	0.43
36:e:181:THR:HG23	36:e:184:GLY:H	1.83	0.43
49:w:97:LYS:NZ	49:w:107:ASP:OD2	2.27	0.43
56:z:176:GLY:N	56:z:181:ILE:HD13	2.33	0.43
56:z:255:TYR:CD1	56:z:271:VAL:HG23	2.52	0.43
1:A:1188:A:H1'	1:A:1189:C:P	2.59	0.43
17:S:198:ARG:NH2	33:b:13:SER:OG	2.52	0.43
18:T:93:ILE:HG23	18:T:94:ASP:N	2.33	0.43
23:Y:193:ASN:O	23:Y:197:ASN:ND2	2.51	0.43
45:r:118:CYS:SG	45:r:181:LEU:HD11	2.58	0.43
1:A:1561:A:N3	1:A:1561:A:H2'	2.34	0.43
1:A:1580:U:C2	45:r:169:TRP:CD1	3.07	0.43
4:E:103:LYS:NZ	4:E:291:GLY:O	2.49	0.43
13:O:141:SER:O	13:O:147:ASN:ND2	2.52	0.43
26:0:89:ASN:O	26:0:93:ARG:HG2	2.18	0.43
30:4:71:ILE:HG22	30:4:89:ILE:CD1	2.48	0.43
33:b:15:LEU:HD11	34:c:172:ASN:HB2	2.00	0.43
34:c:86:ASP:N	34:c:86:ASP:OD1	2.50	0.43
47:u:187:LEU:C	47:u:187:LEU:HD23	2.44	0.43
56:z:210:ILE:O	56:z:210:ILE:HG22	2.19	0.43
1:A:1489:A:O2'	1:A:1506:A:N1	2.51	0.43
1:A:1615:G:H2'	1:A:1616:C:O4'	2.19	0.43
13:O:94:ALA:HB3	13:O:95:PRO:HD3	2.00	0.43
36:e:155:LEU:HD23	36:e:252:TRP:HB3	2.00	0.43
40:i:57:TYR:OH	44:q:28:PRO:O	2.29	0.43
49:w:105:MET:HG2	49:w:139:MET:HE1	2.01	0.43
56:z:225:VAL:HG11	56:z:230:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:A:OP1	1:A:2063:A:O4'	2.37	0.43
4:E:326:GLU:O	4:E:326:GLU:HG2	2.18	0.43
9:K:17:MET:HE3	9:K:142:VAL:HG11	2.00	0.43
9:K:136:ASP:OD1	9:K:137:ILE:N	2.52	0.43
31:6:177:TYR:O	31:6:185:ILE:N	2.44	0.43
1:A:2337:C:H2'	1:A:2338:C:O4'	2.19	0.43
7:I:165:VAL:O	7:I:169:LYS:N	2.41	0.43
36:e:190:LEU:HD13	36:e:200:ALA:HB3	2.01	0.43
1:A:1194:A:HO2'	1:A:1195:G:P	2.42	0.42
1:A:1231:A:OP2	20:V:34:LYS:NZ	2.51	0.42
1:A:1365:A:H4'	1:A:1366:U:O4'	2.19	0.42
1:A:1621:A:H61	1:A:1631:A:C2'	2.32	0.42
3:D:112:PHE:CZ	3:D:168:ASN:HB2	2.54	0.42
4:E:340:PRO:O	4:E:341:SER:OG	2.32	0.42
7:I:79:VAL:HG22	7:I:130:VAL:HG11	2.01	0.42
50:5:351:VAL:HG22	50:5:381:LEU:HD23	2.01	0.42
1:A:1492:A:H1'	1:A:1493:A:O4'	2.19	0.42
1:A:1492:A:H4'	1:A:1493:A:OP1	2.18	0.42
1:A:1542:C:C2'	1:A:1543:U:H5'	2.49	0.42
1:A:2302:U:O2'	1:A:2303:A:P	2.77	0.42
5:F:292:ASP:OD1	38:g:55:THR:HG22	2.19	0.42
8:J:34:PRO:O	8:J:38:ILE:HD12	2.19	0.42
11:M:103:LEU:CD2	11:M:108:ARG:HE	2.32	0.42
25:x:77:VAL:HG22	25:x:127:ARG:HG3	2.01	0.42
25:x:197:LEU:N	25:x:227:GLN:O	2.52	0.42
32:7:188:GLU:OE1	32:7:188:GLU:N	2.52	0.42
34:c:287:GLU:HG3	34:c:288:THR:HG23	2.01	0.42
36:e:237:LEU:O	36:e:238:THR:HG23	2.19	0.42
1:A:1137:A:O2'	1:A:1138:U:P	2.77	0.42
1:A:1683:C:O2	1:A:1683:C:C2'	2.67	0.42
31:6:125:LEU:O	31:6:126:ARG:HG2	2.19	0.42
31:6:227:GLU:OE1	31:6:230:ALA:N	2.44	0.42
33:b:17:ASN:O	33:b:21:ARG:O	2.37	0.42
43:p:75:ASP:OD1	43:p:76:ARG:N	2.53	0.42
49:w:83:VAL:HA	49:w:86:VAL:HG22	2.01	0.42
56:z:181:ILE:N	62:z:401:GNP:O3G	2.52	0.42
56:z:226:LEU:O	56:z:228:HIS:N	2.52	0.42
1:A:1533:G:OP1	12:N:233:TYR:OH	2.27	0.42
28:2:78:VAL:HG22	28:2:81:ARG:HH22	1.85	0.42
30:4:73:LYS:NZ	30:4:78:CYS:O	2.53	0.42
32:7:164:VAL:HG13	32:7:165:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:49:LEU:HB3	36:e:189:ILE:HG21	2.01	0.42
46:s:110:THR:O	46:s:110:THR:HG22	2.18	0.42
46:s:370:THR:CG2	46:s:383:ARG:HB2	2.50	0.42
1:A:1346:G:H4'	1:A:1347:C:OP2	2.20	0.42
1:A:2485:C:H2'	1:A:2486:A:C8	2.54	0.42
4:E:122:LEU:HD12	4:E:285:VAL:HG21	2.01	0.42
19:U:140:ILE:HD11	35:d:232:MET:SD	2.60	0.42
32:7:78:MET:HE1	32:7:91:HIS:CD2	2.54	0.42
46:s:243:GLU:HA	46:s:350:VAL:HG21	2.01	0.42
1:A:1310:A:C5	31:6:379:ILE:HG21	2.54	0.42
1:A:1420:A:N1	3:D:275:LEU:HD12	2.34	0.42
1:A:1455:A:O2'	1:A:1477:U:H5"	2.19	0.42
1:A:2302:U:HO2'	1:A:2303:A:P	2.42	0.42
2:B:7:G:H5"	2:B:8:U:OP1	2.19	0.42
9:K:60:ILE:HG21	9:K:133:ILE:HD11	2.02	0.42
13:O:156:ASP:OD2	32:7:316:ARG:NH2	2.53	0.42
15:Q:280:ALA:O	15:Q:284:GLU:OE1	2.38	0.42
53:a:140:ASP:O	53:a:141:ARG:O	2.38	0.42
2:B:9:A:H4'	2:B:10:G:OP1	2.19	0.42
2:B:15:A:O2'	2:B:17:A:N6	2.48	0.42
8:J:60:ILE:HG21	8:J:66:LEU:HD11	2.01	0.42
15:Q:225:LYS:HB2	15:Q:226:PRO:CD	2.50	0.42
18:T:72:ARG:O	18:T:167:HIS:CD2	2.72	0.42
24:Z:117:ILE:O	42:o:45:ASN:ND2	2.50	0.42
25:x:49:ASP:O	25:x:53:SER:OG	2.37	0.42
34:c:188:LEU:N	34:c:189:PRO:HD2	2.34	0.42
35:d:186:VAL:HG12	35:d:187:GLU:H	1.84	0.42
36:e:258:LEU:HD12	36:e:262:LEU:HD13	2.01	0.42
56:z:111:ASN:OD1	56:z:113:VAL:HG22	2.20	0.42
1:A:1189:C:H4'	1:A:1190:A:OP1	2.20	0.42
1:A:1494:A:O2'	21:W:53:ILE:HD11	2.20	0.42
5:F:94:ASP:OD1	5:F:94:ASP:N	2.52	0.42
9:K:154:ARG:NH1	9:K:156:ASP:OD1	2.53	0.42
18:T:46:GLU:OE1	18:T:46:GLU:N	2.42	0.42
25:x:351:PHE:CE1	25:x:361:VAL:HG22	2.55	0.42
27:1:15:THR:O	27:1:65:LEU:N	2.48	0.42
31:6:217:LEU:HD21	31:6:219:ILE:CD1	2.49	0.42
32:7:105:VAL:HG13	32:7:120:CYS:SG	2.60	0.42
33:b:148:LEU:O	33:b:149:ARG:CB	2.67	0.42
37:f:175:SER:O	54:m:34:CYS:HA	2.20	0.42
58:k:78:GLY:O	58:k:79:ALA:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1610:U:H1'	1:A:1617:A:N6	2.35	0.42
1:A:2062:U:C3'	1:A:2063:A:H5"	2.50	0.42
2:B:51:A:C6	2:B:52:U:O4	2.73	0.42
5:F:274:LEU:O	5:F:277:ASP:OD1	2.37	0.42
9:K:90:VAL:HG22	9:K:94:GLN:HB2	2.02	0.42
25:x:174:VAL:HA	25:x:248:ARG:O	2.19	0.42
1:A:1607:G:N3	1:A:1607:G:H2'	2.35	0.42
8:J:112:VAL:O	8:J:156:VAL:O	2.38	0.42
31:6:208:ALA:N	31:6:243:ASN:OD1	2.43	0.42
33:b:40:SER:OG	33:b:44:ARG:NH1	2.53	0.42
36:e:57:ILE:HG21	36:e:134:ARG:HA	2.02	0.42
56:z:233:GLU:HG2	56:z:234:THR:N	2.34	0.42
1:A:1610:U:C6	1:A:1610:U:OP2	2.73	0.41
9:K:171:THR:O	9:K:171:THR:HG23	2.19	0.41
19:U:44:ILE:HG21	19:U:53:LEU:HD12	2.02	0.41
22:X:163:ARG:HE	50:5:55:LEU:HD11	1.85	0.41
25:x:180:ALA:HB1	25:x:206:ARG:HB3	2.01	0.41
43:p:102:ARG:NE	43:p:132:GLU:OE2	2.50	0.41
49:w:79:ILE:HG21	49:w:148:ILE:HB	2.02	0.41
56:z:155:LYS:NZ	62:z:401:GNP:O2G	2.52	0.41
58:k:61:GLU:OE2	58:k:77:ARG:NH1	2.53	0.41
1:A:1130:U:O2'	1:A:1131:A:O5'	2.36	0.41
1:A:1220:G:N7	28:2:87:ARG:NH2	2.59	0.41
1:A:1724:U:O2	16:R:12:ASN:ND2	2.53	0.41
1:A:1906:G:O2'	10:L:36:THR:HG22	2.20	0.41
14:P:91:GLU:OE2	14:P:108:ARG:NH2	2.45	0.41
1:A:1576:U:OP2	41:j:22:ALA:N	2.54	0.41
1:A:1600:A:N6	1:A:1645:C:OP2	2.53	0.41
1:A:2251:U:H4'	1:A:2251:U:OP1	2.20	0.41
1:A:2302:U:C2'	1:A:2303:A:O5'	2.68	0.41
2:B:30:A:OP1	54:m:41:ARG:NE	2.53	0.41
8:J:108:VAL:HG21	8:J:154:ARG:HB2	2.02	0.41
11:M:167:GLU:OE2	11:M:219:ARG:NH2	2.52	0.41
14:P:61:VAL:HG11	31:6:344:PHE:CE2	2.55	0.41
37:f:95:THR:HG23	37:f:95:THR:O	2.21	0.41
42:o:29:PHE:CZ	42:o:33:GLU:OE2	2.73	0.41
43:p:97:SER:O	43:p:146:ASN:ND2	2.53	0.41
44:q:153:ARG:O	44:q:157:GLN:N	2.46	0.41
1:A:1275:U:H5"	11:M:46:ARG:NH2	2.35	0.41
1:A:1541:G:H2'	1:A:1542:C:O4'	2.20	0.41
1:A:1659:A:OP2	1:A:1659:A:N3	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1831:U:OP1	1:A:1831:U:C4'	2.68	0.41
1:A:2075:U:H3'	1:A:2076:A:H2'	2.02	0.41
1:A:2616:U:C6	1:A:2616:U:OP2	2.73	0.41
4:E:112:LYS:NZ	4:E:337:VAL:O	2.53	0.41
15:Q:77:SER:OG	15:Q:79:GLU:OE1	2.37	0.41
17:S:132:ILE:HG22	17:S:133:ARG:N	2.35	0.41
11:M:115:ILE:HG13	11:M:151:ILE:HD11	2.02	0.41
14:P:67:GLY:HA3	21:W:78:GLY:O	2.20	0.41
20:V:172:ASP:HB2	20:V:176:ASP:HB2	2.02	0.41
37:f:107:GLN:HG3	37:f:108:TYR:N	2.35	0.41
50:5:211:THR:HG21	50:5:319:ALA:O	2.21	0.41
1:A:1856:C:OP2	19:U:50:ARG:NE	2.52	0.41
1:A:2073:G:O5'	56:z:164:ARG:NE	2.54	0.41
1:A:2074:C:H2'	1:A:2075:U:O5'	2.20	0.41
1:A:2564:G:H1'	1:A:2565:U:OP2	2.21	0.41
11:M:232:ARG:HH21	11:M:243:LEU:HD21	1.86	0.41
18:T:63:ARG:O	35:d:230:ARG:HD3	2.21	0.41
20:V:133:ILE:HG22	20:V:147:SER:HA	2.03	0.41
35:d:267:PRO:HG2	35:d:270:ALA:HB2	2.03	0.41
36:e:52:GLN:N	36:e:234:ALA:O	2.52	0.41
49:w:80:LYS:HA	49:w:145:VAL:HG21	2.02	0.41
1:A:1275:U:H2'	1:A:1276:U:O4'	2.21	0.41
1:A:1637:U:H2'	1:A:1639:C:OP2	2.20	0.41
2:B:9:A:OP2	2:B:9:A:H3'	2.21	0.41
2:B:13:U:O2'	2:B:14:A:P	2.79	0.41
6:H:111:VAL:HG12	6:H:112:LYS:N	2.35	0.41
14:P:91:GLU:OE2	14:P:108:ARG:NE	2.47	0.41
56:z:181:ILE:HG13	56:z:182:THR:N	2.35	0.41
56:z:225:VAL:HG11	56:z:230:VAL:CG2	2.50	0.41
56:z:259:SER:O	56:z:260:ALA:CB	2.68	0.41
1:A:1712:U:H4'	11:M:23:LEU:HD12	2.03	0.41
1:A:2394:U:OP1	30:4:69:GLY:N	2.52	0.41
22:X:81:GLY:O	22:X:130:ARG:NE	2.49	0.41
37:f:89:VAL:HG23	37:f:89:VAL:O	2.21	0.41
47:u:190:LEU:N	47:u:190:LEU:HD12	2.36	0.41
49:w:127:GLY:C	49:w:128:PHE:CD1	2.99	0.41
49:w:138:LEU:HD22	49:w:144:ILE:HD13	2.01	0.41
56:z:252:VAL:HG11	56:z:260:ALA:HB2	2.03	0.41
58:k:30:THR:HG23	58:k:31:ARG:N	2.35	0.41
1:A:1422:A:C5'	1:A:1423:G:OP1	2.69	0.41
1:A:1821:A:O2'	3:D:131:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1851:C:O2	46:s:162:ARG:NH1	2.47	0.41
4:E:204:VAL:HG21	4:E:299:ILE:CG1	2.51	0.41
9:K:67:PHE:HB3	9:K:71:LYS:HB2	2.02	0.41
13:O:110:ILE:CG2	13:O:111:PRO:HD2	2.51	0.41
15:Q:262:LYS:HA	15:Q:264:TRP:CZ3	2.55	0.41
17:S:98:ARG:HG3	34:c:311:ARG:O	2.20	0.41
18:T:151:ARG:HE	18:T:161:MET:HE2	1.86	0.41
19:U:22:THR:HG22	19:U:24:PHE:H	1.85	0.41
21:W:122:LYS:N	31:6:49:GLU:O	2.42	0.41
24:Z:151:LEU:HD21	41:j:44:GLU:OE1	2.20	0.41
31:6:268:PHE:O	31:6:318:PHE:HA	2.21	0.41
46:s:180:ASN:OD1	50:5:192:ILE:HD12	2.21	0.41
52:9:101:ASP:O	52:9:105:GLY:N	2.54	0.41
52:9:134:PRO:O	52:9:135:ARG:C	2.64	0.41
55:l:72:VAL:HG23	55:l:73:ASN:N	2.35	0.41
57:y:302:LEU:O	57:y:307:CYS:N	2.54	0.41
58:k:15:LEU:HD21	58:k:17:ARG:HE	1.86	0.41
1:A:1433:C:H2'	1:A:1434:U:C6	2.56	0.41
1:A:1506:A:H2'	1:A:1507:A:O4'	2.21	0.41
1:A:1639:C:OP2	1:A:1639:C:C6	2.73	0.41
1:A:1944:A:O2'	1:A:1945:C:OP1	2.36	0.41
1:A:2072:G:O2'	1:A:2073:G:P	2.78	0.41
1:A:2175:U:O2'	1:A:2176:A:H2'	2.21	0.41
1:A:2617:A:O2'	1:A:2618:A:P	2.79	0.41
2:B:26:A:O2'	51:8:133:ARG:NH2	2.53	0.41
31:6:237:LEU:HD13	31:6:240:ILE:HD11	2.02	0.41
32:7:181:THR:HG22	32:7:291:ILE:HG12	2.03	0.41
32:7:273:PHE:HB2	32:7:301:THR:HG22	2.02	0.41
37:f:91:ASN:N	37:f:186:ARG:O	2.52	0.41
49:w:139:MET:HE3	49:w:139:MET:HA	2.03	0.41
56:z:206:LEU:O	56:z:207:ALA:HB2	2.21	0.41
1:A:1103:A:H2'	1:A:1104:G:O4'	2.21	0.40
1:A:1333:C:H5"	5:F:144:PRO:HD2	2.03	0.40
1:A:1793:C:H2'	1:A:1794:C:O4'	2.21	0.40
1:A:2076:A:HO2'	1:A:2077:A:P	2.32	0.40
20:V:131:THR:O	20:V:131:THR:HG23	2.21	0.40
31:6:212:SER:O	31:6:214:TRP:CD1	2.73	0.40
33:b:134:THR:O	33:b:135:ASN:HB2	2.22	0.40
56:z:88:ASP:O	56:z:317:MET:HE3	2.20	0.40
1:A:1113:C:H2'	1:A:1114:U:O4'	2.21	0.40
1:A:1565:U:H5'	24:Z:74:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:U:O3'	8:J:130:PHE:HB2	2.21	0.40
1:A:1985:C:H3'	1:A:1986:C:H5"	2.02	0.40
1:A:2630:A:N3	1:A:2630:A:H3'	2.36	0.40
4:E:175:ILE:HG22	4:E:296:LEU:HD23	2.04	0.40
9:K:177:ARG:NH2	45:r:38:VAL:HG23	2.37	0.40
10:L:95:ARG:O	10:L:96:MET:HB2	2.21	0.40
16:R:84:PRO:O	16:R:88:VAL:HG22	2.22	0.40
31:6:240:ILE:HD12	31:6:245:VAL:HA	2.04	0.40
32:7:214:GLU:OE1	32:7:253:ARG:NE	2.50	0.40
48:v:26:THR:HG22	48:v:27:ASP:N	2.36	0.40
56:z:285:THR:HG22	56:z:288:GLY:O	2.21	0.40
1:A:2599:A:C8	15:Q:271:ARG:HG2	2.55	0.40
25:x:229:ARG:NH1	37:f:198:LYS:O	2.54	0.40
31:6:291:TYR:CE1	31:6:334:LEU:HD12	2.56	0.40
34:c:179:THR:HG23	34:c:194:THR:HG21	2.04	0.40
46:s:195:ASP:HB2	46:s:234:GLN:HG2	2.04	0.40
47:u:176:PRO:O	47:u:180:GLU:OE1	2.40	0.40
56:z:95:ILE:HD11	56:z:317:MET:SD	2.61	0.40
1:A:1212:A:H2'	1:A:1213:C:O4'	2.22	0.40
1:A:1422:A:H5'	1:A:1423:G:OP1	2.22	0.40
1:A:2267:A:N1	1:A:2276:U:O4	2.55	0.40
4:E:196:ALA:HB3	4:E:319:TYR:CD2	2.57	0.40
17:S:174:ILE:HD12	33:b:2:THR:HB	2.04	0.40
31:6:334:LEU:H	31:6:334:LEU:HD23	1.86	0.40
36:e:163:LEU:N	36:e:166:GLN:O	2.47	0.40
44:q:149:ASP:HA	44:q:152:ARG:HG3	2.04	0.40
58:k:82:THR:HG23	58:k:85:GLU:H	1.87	0.40
1:A:1985:C:H3'	1:A:1986:C:C5'	2.52	0.40
6:H:51:VAL:HG13	6:H:79:LEU:CD1	2.51	0.40
35:d:137:PHE:CE2	35:d:212:VAL:HG11	2.57	0.40
37:f:178:PRO:O	37:f:179:GLU:CB	2.68	0.40
46:s:370:THR:HG22	46:s:383:ARG:HB2	2.04	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	
3	D	223/246 (91%)	221 (99%)	2 (1%)	0	100	100
4	E	306/348 (88%)	293 (96%)	13 (4%)	0	100	100
5	F	248/294 (84%)	245 (99%)	3 (1%)	0	100	100
6	H	93/265 (35%)	93 (100%)	0	0	100	100
7	I	159/262 (61%)	156 (98%)	3 (2%)	0	100	100
8	J	173/192 (90%)	167 (96%)	6 (4%)	0	100	100
9	K	175/178 (98%)	175 (100%)	0	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	285/295 (97%)	281 (99%)	4 (1%)	0	100	100
12	N	192/251 (76%)	190 (99%)	2 (1%)	0	100	100
13	O	151/176 (86%)	149 (99%)	2 (1%)	0	100	100
14	P	139/180 (77%)	137 (99%)	2 (1%)	0	100	100
15	Q	215/292 (74%)	212 (99%)	3 (1%)	0	100	100
16	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
17	S	157/209 (75%)	151 (96%)	6 (4%)	0	100	100
18	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
19	U	123/146 (84%)	122 (99%)	1 (1%)	0	100	100
20	V	199/216 (92%)	196 (98%)	3 (2%)	0	100	100
21	W	98/148 (66%)	97 (99%)	1 (1%)	0	100	100
22	X	240/294 (82%)	236 (98%)	4 (2%)	0	100	100
23	Y	174/252 (69%)	174 (100%)	0	0	100	100
24	Z	119/160 (74%)	118 (99%)	1 (1%)	0	100	100
25	x	322/356 (90%)	310 (96%)	12 (4%)	0	100	100
26	0	106/187 (57%)	106 (100%)	0	0	100	100
27	1	50/65 (77%)	50 (100%)	0	0	100	100
28	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
29	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
30	4	35/101 (35%)	35 (100%)	0	0	100	100
31	6	311/380 (82%)	295 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	7	290/336 (86%)	280 (97%)	10 (3%)	0	100	100
33	b	146/159 (92%)	142 (97%)	4 (3%)	0	100	100
34	c	277/303 (91%)	273 (99%)	4 (1%)	0	100	100
35	d	205/306 (67%)	199 (97%)	6 (3%)	0	100	100
36	e	187/283 (66%)	178 (95%)	9 (5%)	0	100	100
37	f	98/211 (46%)	96 (98%)	1 (1%)	1 (1%)	12	25
38	g	130/166 (78%)	128 (98%)	2 (2%)	0	100	100
39	h	108/159 (68%)	105 (97%)	3 (3%)	0	100	100
40	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
41	j	91/121 (75%)	88 (97%)	3 (3%)	0	100	100
42	o	76/102 (74%)	76 (100%)	0	0	100	100
43	p	140/206 (68%)	135 (96%)	5 (4%)	0	100	100
44	q	133/222 (60%)	133 (100%)	0	0	100	100
45	r	153/196 (78%)	146 (95%)	7 (5%)	0	100	100
46	s	373/442 (84%)	365 (98%)	8 (2%)	0	100	100
47	u	123/228 (54%)	120 (98%)	3 (2%)	0	100	100
48	v	67/70 (96%)	67 (100%)	0	0	100	100
49	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
50	5	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
51	8	68/206 (33%)	67 (98%)	1 (2%)	0	100	100
52	9	120/135 (89%)	118 (98%)	2 (2%)	0	100	100
53	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
54	m	43/127 (34%)	41 (95%)	2 (5%)	0	100	100
55	l	56/135 (42%)	56 (100%)	0	0	100	100
56	z	309/326 (95%)	293 (95%)	15 (5%)	1 (0%)	36	54
57	y	235/346 (68%)	232 (99%)	3 (1%)	0	100	100
58	k	83/118 (70%)	78 (94%)	5 (6%)	0	100	100
All	All	9019/12025 (75%)	8818 (98%)	199 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	z	92	GLN

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Mol	Chain	Res	Type
37	f	179	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	186/197 (94%)	186 (100%)	0	100	100
4	E	270/298 (91%)	270 (100%)	0	100	100
5	F	216/250 (86%)	216 (100%)	0	100	100
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	149/230 (65%)	149 (100%)	0	100	100
8	J	138/152 (91%)	138 (100%)	0	100	100
9	K	157/158 (99%)	157 (100%)	0	100	100
10	L	99/122 (81%)	99 (100%)	0	100	100
11	M	248/252 (98%)	248 (100%)	0	100	100
12	N	175/216 (81%)	175 (100%)	0	100	100
13	O	133/152 (88%)	133 (100%)	0	100	100
14	P	123/157 (78%)	123 (100%)	0	100	100
15	Q	197/258 (76%)	197 (100%)	0	100	100
16	R	119/128 (93%)	119 (100%)	0	100	100
17	S	145/180 (81%)	145 (100%)	0	100	100
18	T	147/180 (82%)	147 (100%)	0	100	100
19	U	114/133 (86%)	114 (100%)	0	100	100
20	V	179/190 (94%)	179 (100%)	0	100	100
21	W	84/116 (72%)	84 (100%)	0	100	100
22	X	219/265 (83%)	219 (100%)	0	100	100
23	Y	162/228 (71%)	162 (100%)	0	100	100
24	Z	114/146 (78%)	114 (100%)	0	100	100
25	x	283/311 (91%)	283 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	0	97/170 (57%)	97 (100%)	0	100	100
27	1	49/60 (82%)	49 (100%)	0	100	100
28	2	40/77 (52%)	40 (100%)	0	100	100
29	3	88/165 (53%)	88 (100%)	0	100	100
30	4	35/90 (39%)	35 (100%)	0	100	100
31	6	280/335 (84%)	280 (100%)	0	100	100
32	7	269/301 (89%)	269 (100%)	0	100	100
33	b	130/138 (94%)	130 (100%)	0	100	100
34	c	245/262 (94%)	245 (100%)	0	100	100
35	d	189/272 (70%)	189 (100%)	0	100	100
36	e	166/238 (70%)	166 (100%)	0	100	100
37	f	93/185 (50%)	93 (100%)	0	100	100
38	g	122/148 (82%)	122 (100%)	0	100	100
39	h	100/143 (70%)	100 (100%)	0	100	100
40	i	87/111 (78%)	87 (100%)	0	100	100
41	j	75/99 (76%)	75 (100%)	0	100	100
42	o	65/85 (76%)	65 (100%)	0	100	100
43	p	129/177 (73%)	129 (100%)	0	100	100
44	q	117/187 (63%)	117 (100%)	0	100	100
45	r	142/168 (84%)	142 (100%)	0	100	100
46	s	329/378 (87%)	329 (100%)	0	100	100
47	u	115/197 (58%)	115 (100%)	0	100	100
48	v	60/61 (98%)	60 (100%)	0	100	100
49	w	73/135 (54%)	73 (100%)	0	100	100
50	5	356/372 (96%)	356 (100%)	0	100	100
51	8	62/182 (34%)	62 (100%)	0	100	100
52	9	104/114 (91%)	104 (100%)	0	100	100
53	a	97/129 (75%)	97 (100%)	0	100	100
54	m	40/114 (35%)	40 (100%)	0	100	100
55	l	56/112 (50%)	56 (100%)	0	100	100
56	z	270/280 (96%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	y	220/322 (68%)	220 (100%)	0	100	100
58	k	76/95 (80%)	76 (100%)	0	100	100
All	All	8119/10449 (78%)	8119 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	234	GLN
4	E	281	ASN
4	E	294	ASN
5	F	97	HIS
8	J	48	GLN
9	K	74	GLN
10	L	104	ASN
11	M	31	ASN
11	M	113	GLN
11	M	218	ASN
13	O	100	GLN
14	P	88	HIS
15	Q	88	ASN
15	Q	172	GLN
18	T	127	ASN
24	Z	67	HIS
25	x	328	GLN
25	x	340	HIS
26	0	117	GLN
31	6	174	HIS
31	6	239	ASN
31	6	275	GLN
32	7	252	HIS
32	7	302	HIS
33	b	16	HIS
34	c	139	GLN
34	c	168	HIS
35	d	119	GLN
36	e	73	GLN
37	f	174	GLN
37	f	176	ASN
40	i	59	ASN

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Mol	Chain	Res	Type
40	i	65	ASN
41	j	94	GLN
45	r	167	HIS
46	s	71	HIS
46	s	107	GLN
46	s	226	GLN
46	s	228	ASN
46	s	337	GLN
48	v	54	GLN
49	w	103	HIS
50	5	302	GLN
50	5	407	GLN
53	a	110	GLN
55	l	132	ASN
56	z	24	HIS
56	z	82	ASN
57	y	123	GLN
57	y	158	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1421/1584 (89%)	478 (33%)	33 (2%)
2	B	58/68 (85%)	23 (39%)	2 (3%)
All	All	1479/1652 (89%)	501 (33%)	35 (2%)

All (501) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	A
1	A	1100	C
1	A	1101	C
1	A	1102	U
1	A	1103	A
1	A	1104	G
1	A	1112	C
1	A	1115	A
1	A	1116	C
1	A	1117	A
1	A	1118	C
1	A	1123	A

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Mol	Chain	Res	Type
1	A	1124	U
1	A	1128	U
1	A	1131	A
1	A	1134	A
1	A	1135	U
1	A	1136	U
1	A	1137	A
1	A	1138	U
1	A	1139	A
1	A	1140	U
1	A	1148	A
1	A	1151	A
1	A	1152	U
1	A	1159	U
1	A	1160	A
1	A	1161	C
1	A	1162	U
1	A	1173	G
1	A	1187	U
1	A	1188	A
1	A	1189	C
1	A	1190	A
1	A	1191	U
1	A	1192	C
1	A	1193	U
1	A	1194	A
1	A	1195	G
1	A	1198	G
1	A	1205	A
1	A	1222	A
1	A	1233	A
1	A	1234	C
1	A	1235	U
1	A	1236	A
1	A	1237	A
1	A	1238	U
1	A	1240	A
1	A	1241	A
1	A	1248	G
1	A	1252	A
1	A	1253	A
1	A	1255	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	1256	A
1	A	1257	A
1	A	1260	A
1	A	1264	A
1	A	1272	A
1	A	1276	U
1	A	1277	U
1	A	1278	U
1	A	1279	G
1	A	1280	C
1	A	1281	A
1	A	1282	U
1	A	1283	A
1	A	1284	A
1	A	1297	A
1	A	1300	A
1	A	1302	U
1	A	1310	A
1	A	1311	A
1	A	1314	G
1	A	1315	A
1	A	1316	A
1	A	1318	U
1	A	1320	C
1	A	1321	A
1	A	1331	C
1	A	1337	A
1	A	1344	G
1	A	1346	G
1	A	1347	C
1	A	1362	U
1	A	1364	U
1	A	1365	A
1	A	1366	U
1	A	1368	A
1	A	1386	G
1	A	1394	G
1	A	1396	G
1	A	1402	A
1	A	1413	G
1	A	1415	G
1	A	1421	A

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Mol	Chain	Res	Type
1	A	1422	A
1	A	1423	G
1	A	1428	A
1	A	1429	C
1	A	1430	G
1	A	1443	G
1	A	1449	U
1	A	1450	A
1	A	1458	A
1	A	1459	A
1	A	1460	U
1	A	1465	U
1	A	1466	U
1	A	1468	A
1	A	1470	U
1	A	1471	U
1	A	1473	A
1	A	1483	U
1	A	1484	U
1	A	1485	G
1	A	1490	A
1	A	1491	A
1	A	1492	A
1	A	1493	A
1	A	1494	A
1	A	1496	A
1	A	1497	A
1	A	1502	A
1	A	1503	U
1	A	1504	C
1	A	1505	A
1	A	1506	A
1	A	1508	A
1	A	1511	U
1	A	1512	A
1	A	1513	A
1	A	1521	U
1	A	1525	A
1	A	1526	G
1	A	1531	A
1	A	1532	A
1	A	1534	A

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Mol	Chain	Res	Type
1	A	1536	G
1	A	1542	C
1	A	1543	U
1	A	1552	A
1	A	1553	C
1	A	1558	A
1	A	1559	A
1	A	1560	A
1	A	1565	U
1	A	1566	U
1	A	1573	G
1	A	1580	U
1	A	1583	C
1	A	1587	A
1	A	1588	C
1	A	1595	U
1	A	1596	A
1	A	1597	A
1	A	1599	C
1	A	1600	A
1	A	1601	U
1	A	1602	U
1	A	1603	G
1	A	1604	U
1	A	1605	A
1	A	1606	G
1	A	1608	C
1	A	1609	C
1	A	1610	U
1	A	1611	A
1	A	1613	A
1	A	1614	A
1	A	1615	G
1	A	1617	A
1	A	1618	G
1	A	1622	C
1	A	1624	A
1	A	1626	U
1	A	1627	A
1	A	1628	A
1	A	1629	A
1	A	1631	A

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Mol	Chain	Res	Type
1	A	1632	A
1	A	1633	A
1	A	1634	G
1	A	1635	C
1	A	1637	U
1	A	1638	U
1	A	1639	C
1	A	1641	A
1	A	1642	G
1	A	1643	C
1	A	1645	C
1	A	1647	A
1	A	1649	A
1	A	1650	U
1	A	1651	A
1	A	1653	A
1	A	1654	A
1	A	1658	C
1	A	1659	A
1	A	1660	A
1	A	1664	A
1	A	1665	U
1	A	1669	A
1	A	1671	A
1	A	1673	U
1	A	1675	U
1	A	1678	A
1	A	1682	A
1	A	1683	C
1	A	1684	U
1	A	1690	A
1	A	1693	U
1	A	1694	U
1	A	1698	A
1	A	1717	U
1	A	1718	U
1	A	1727	A
1	A	1730	A
1	A	1733	G
1	A	1748	A
1	A	1749	A
1	A	1755	C

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Mol	Chain	Res	Type
1	A	1756	C
1	A	1757	A
1	A	1758	A
1	A	1766	G
1	A	1767	G
1	A	1769	A
1	A	1784	C
1	A	1788	G
1	A	1793	C
1	A	1801	A
1	A	1804	U
1	A	1805	A
1	A	1806	A
1	A	1807	U
1	A	1821	A
1	A	1823	A
1	A	1826	C
1	A	1830	C
1	A	1831	U
1	A	1832	A
1	A	1834	A
1	A	1837	U
1	A	1843	A
1	A	1847	A
1	A	1851	C
1	A	1852	U
1	A	1853	U
1	A	1869	A
1	A	1871	C
1	A	1880	U
1	A	1882	A
1	A	1887	A
1	A	1888	A
1	A	1894	A
1	A	1902	A
1	A	1904	A
1	A	1914	G
1	A	1919	C
1	A	1922	G
1	A	1923	A
1	A	1926	C
1	A	1930	C

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Mol	Chain	Res	Type
1	A	1933	G
1	A	1936	U
1	A	1937	A
1	A	1939	C
1	A	1944	A
1	A	1945	C
1	A	1948	C
1	A	1957	C
1	A	1958	A
1	A	1964	A
1	A	1968	U
1	A	1976	A
1	A	1983	G
1	A	1986	C
1	A	1987	A
1	A	1988	G
1	A	1989	U
1	A	1991	A
1	A	2041	A
1	A	2042	C
1	A	2048	C
1	A	2050	U
1	A	2057	G
1	A	2058	G
1	A	2059	G
1	A	2060	A
1	A	2062	U
1	A	2063	A
1	A	2068	G
1	A	2069	A
1	A	2071	C
1	A	2073	G
1	A	2075	U
1	A	2076	A
1	A	2077	A
1	A	2082	G
1	A	2083	G
1	A	2091	U
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2123	U

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Mol	Chain	Res	Type
1	A	2130	A
1	A	2131	A
1	A	2132	G
1	A	2143	A
1	A	2146	A
1	A	2156	G
1	A	2158	G
1	A	2159	A
1	A	2161	G
1	A	2162	A
1	A	2169	G
1	A	2170	G
1	A	2176	A
1	A	2177	A
1	A	2180	U
1	A	2182	U
1	A	2186	A
1	A	2187	C
1	A	2190	A
1	A	2193	U
1	A	2194	A
1	A	2195	U
1	A	2196	U
1	A	2197	U
1	A	2227	A
1	A	2229	A
1	A	2230	G
1	A	2232	A
1	A	2236	G
1	A	2239	U
1	A	2240	G
1	A	2241	A
1	A	2248	G
1	A	2251	U
1	A	2252	G
1	A	2253	G
1	A	2254	G
1	A	2256	U
1	A	2257	G
1	A	2258	A
1	A	2259	C
1	A	2275	A

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Mol	Chain	Res	Type
1	A	2276	U
1	A	2277	C
1	A	2282	G
1	A	2284	A
1	A	2285	U
1	A	2286	G
1	A	2287	A
1	A	2289	U
1	A	2290	A
1	A	2291	U
1	A	2292	A
1	A	2293	A
1	A	2295	C
1	A	2297	A
1	A	2303	A
1	A	2325	U
1	A	2326	A
1	A	2327	U
1	A	2328	C
1	A	2329	U
1	A	2333	U
1	A	2334	G
1	A	2339	A
1	A	2340	G
1	A	2342	U
1	A	2343	A
1	A	2348	U
1	A	2351	A
1	A	2352	U
1	A	2354	A
1	A	2358	G
1	A	2359	A
1	A	2360	C
1	A	2363	A
1	A	2367	A
1	A	2369	C
1	A	2373	G
1	A	2375	G
1	A	2377	U
1	A	2391	U
1	A	2394	U
1	A	2396	A

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Mol	Chain	Res	Type
1	A	2397	A
1	A	2398	G
1	A	2399	A
1	A	2402	U
1	A	2404	A
1	A	2408	C
1	A	2410	A
1	A	2412	A
1	A	2414	U
1	A	2415	U
1	A	2416	A
1	A	2417	G
1	A	2418	G
1	A	2419	G
1	A	2427	C
1	A	2428	C
1	A	2430	C
1	A	2431	G
1	A	2437	G
1	A	2447	A
1	A	2458	G
1	A	2462	A
1	A	2464	G
1	A	2468	U
1	A	2475	U
1	A	2480	U
1	A	2481	U
1	A	2482	G
1	A	2486	A
1	A	2487	A
1	A	2493	A
1	A	2495	A
1	A	2496	G
1	A	2501	A
1	A	2502	C
1	A	2505	G
1	A	2515	C
1	A	2516	A
1	A	2519	C
1	A	2520	C
1	A	2521	G
1	A	2526	A

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Mol	Chain	Res	Type
1	A	2531	A
1	A	2532	G
1	A	2533	G
1	A	2538	U
1	A	2539	U
1	A	2542	U
1	A	2544	U
1	A	2550	U
1	A	2552	C
1	A	2564	G
1	A	2565	U
1	A	2570	A
1	A	2572	G
1	A	2575	C
1	A	2576	A
1	A	2582	A
1	A	2598	A
1	A	2600	A
1	A	2601	U
1	A	2603	A
1	A	2605	C
1	A	2615	U
1	A	2616	U
1	A	2617	A
1	A	2618	A
1	A	2619	U
1	A	2621	U
1	A	2625	A
1	A	2628	A
1	A	2629	A
1	A	2631	A
1	A	2635	A
1	A	2636	A
1	A	2639	A
1	A	2640	A
1	A	2647	U
1	A	2648	A
1	A	2650	G
1	A	2654	A
1	A	2655	C
1	A	2656	C
1	A	2659	C

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Mol	Chain	Res	Type
1	A	2660	U
1	A	2665	U
1	A	2666	A
1	A	2676	A
2	B	2	U
2	B	3	U
2	B	5	A
2	B	6	U
2	B	7	G
2	B	8	U
2	B	9	A
2	B	14	A
2	B	16	U
2	B	17	A
2	B	21	A
2	B	32	U
2	B	33	G
2	B	44	G
2	B	46	U
2	B	47	G
2	B	48	G
2	B	51	A
2	B	52	U
2	B	53	U
2	B	58	C
2	B	64	A
2	B	66	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	U
1	A	1134	A
1	A	1137	A
1	A	1188	A
1	A	1189	C
1	A	1190	A
1	A	1194	A
1	A	1235	U
1	A	1237	A
1	A	1281	A
1	A	1422	A

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Mol	Chain	Res	Type
1	A	1428	A
1	A	1458	A
1	A	1492	A
1	A	1541	G
1	A	1613	A
1	A	1638	U
1	A	1642	G
1	A	1683	C
1	A	1803	U
1	A	1893	C
1	A	1944	A
1	A	1967	A
1	A	2056	A
1	A	2057	G
1	A	2072	G
1	A	2076	A
1	A	2275	A
1	A	2302	U
1	A	2342	U
1	A	2414	U
1	A	2564	G
1	A	2659	C
2	B	8	U
2	B	52	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	2509	1	18,21,22	0.50	0	22,30,33	0.58	0

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
1	PSU	A	2509	1	-	0/7/25/26	0/2/2/2

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.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 103 ligands modelled in this entry, 101 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	FES	r	201	7,45	0,4,4	-	-	-		
62	GNP	z	401	-	33,34,34	1.13	5 (15%)	46,54,54	0.63	0

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
61	FES	r	201	7,45	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GNP	z	401	-	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	z	401	GNP	PB-O2B	-3.18	1.48	1.56
62	z	401	GNP	PG-O1G	3.02	1.50	1.46
62	z	401	GNP	C6-N1	-2.93	1.33	1.38
62	z	401	GNP	PG-O3G	-2.13	1.51	1.56
62	z	401	GNP	PG-O2G	-2.09	1.51	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	GNP	PB-N3B-PG-O1G
62	z	401	GNP	PG-N3B-PB-O1B

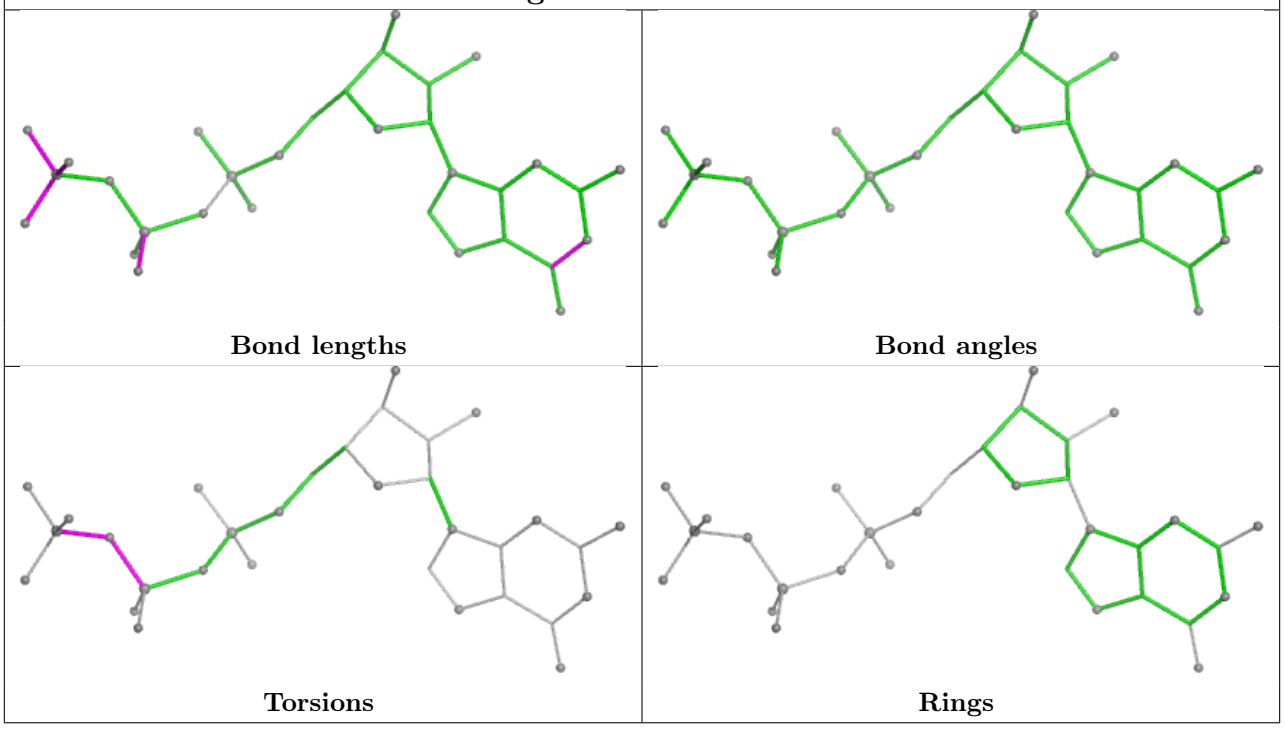
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	z	401	GNP	3	0

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

Ligand GNP z 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

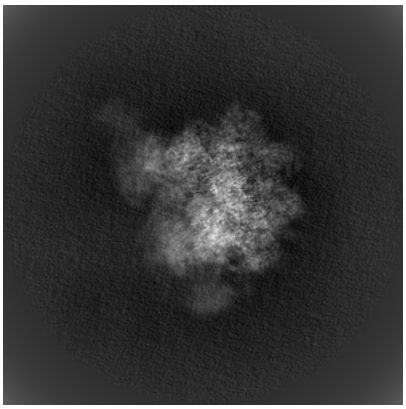
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52049. These allow visual inspection of the internal detail of the map and identification of artifacts.

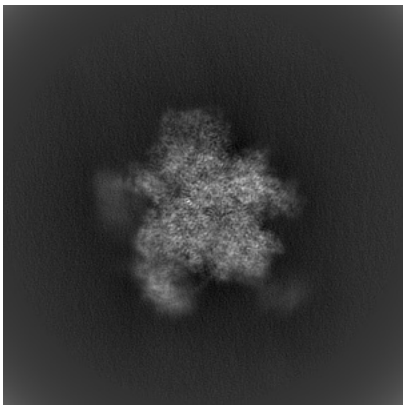
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

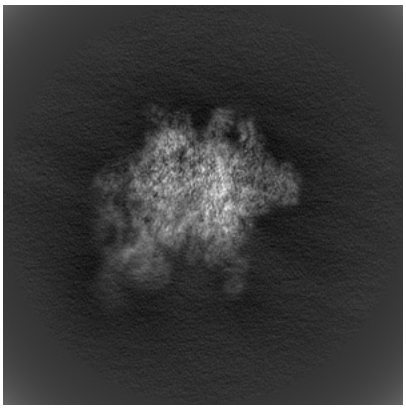
6.1.1 Primary map



X

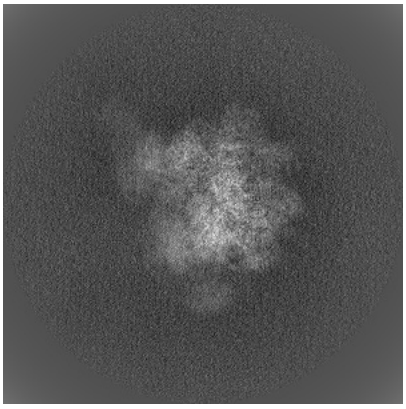


Y

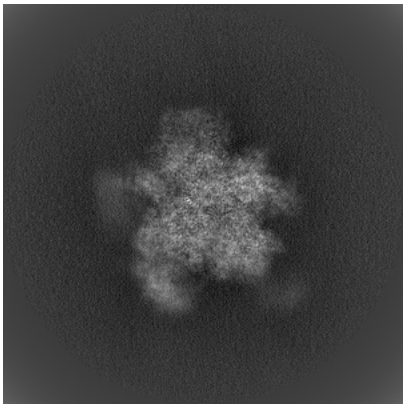


Z

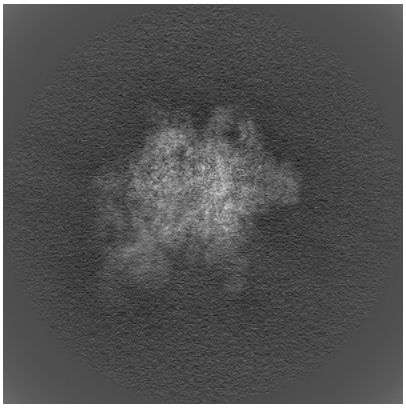
6.1.2 Raw map



X



Y

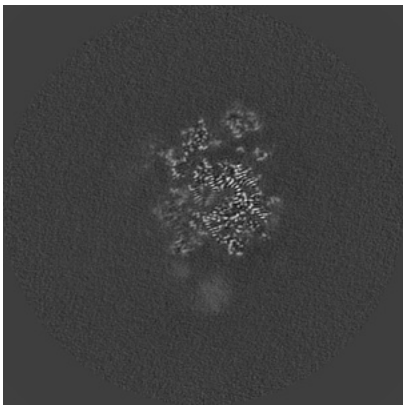


Z

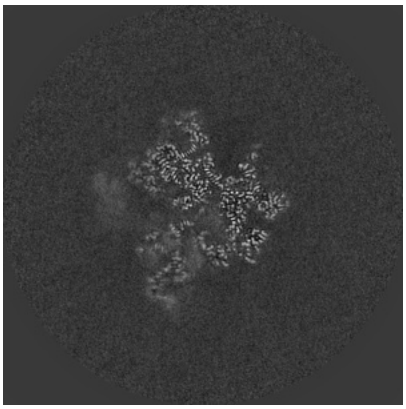
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

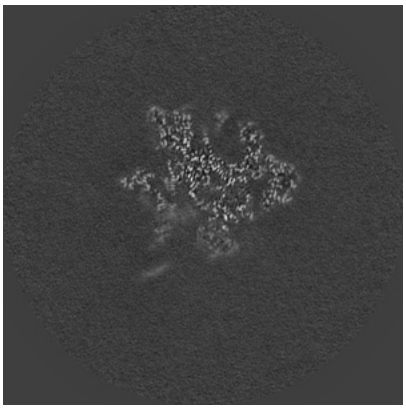
6.2.1 Primary map



X Index: 270

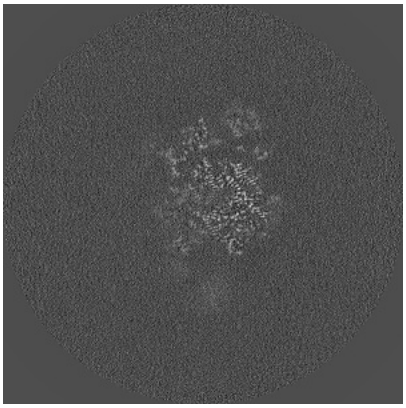


Y Index: 270

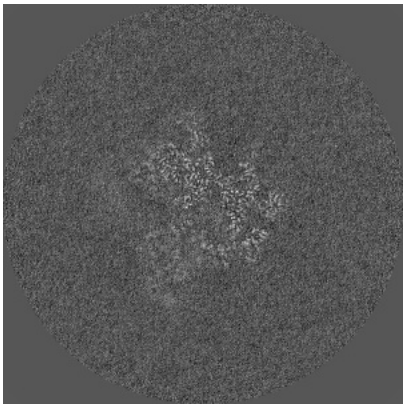


Z Index: 270

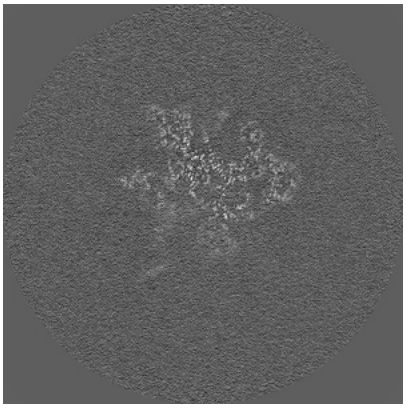
6.2.2 Raw map



X Index: 270



Y Index: 270

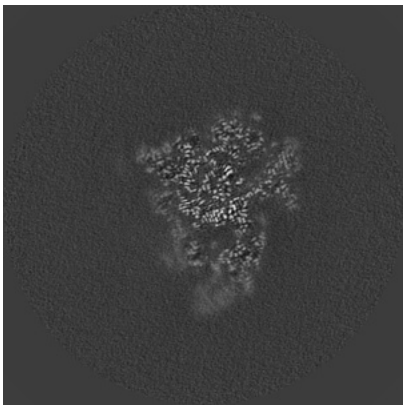


Z Index: 270

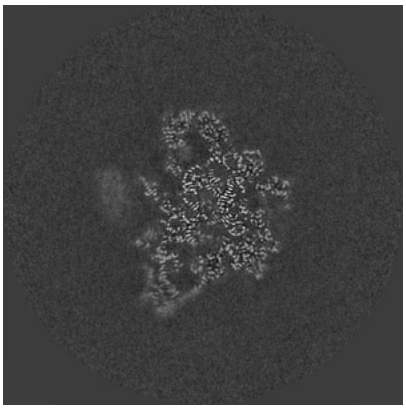
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

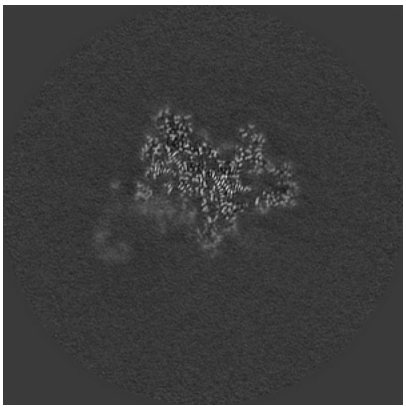
6.3.1 Primary map



X Index: 296

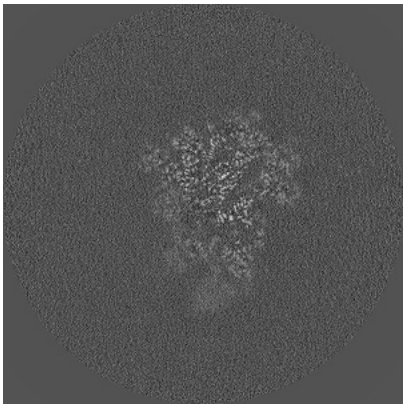


Y Index: 297

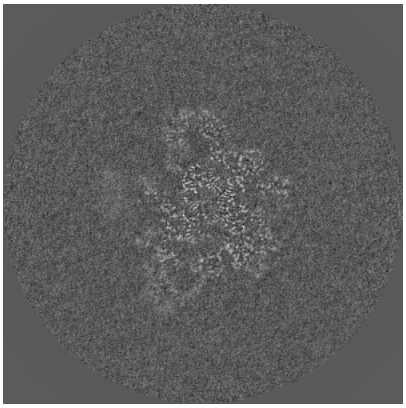


Z Index: 254

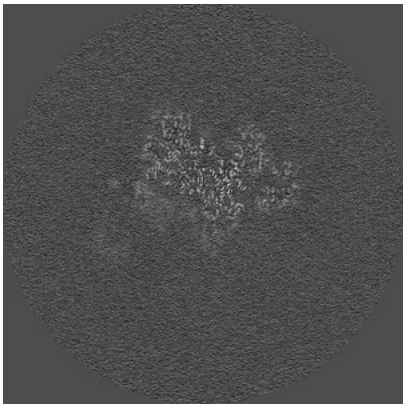
6.3.2 Raw map



X Index: 291



Y Index: 297

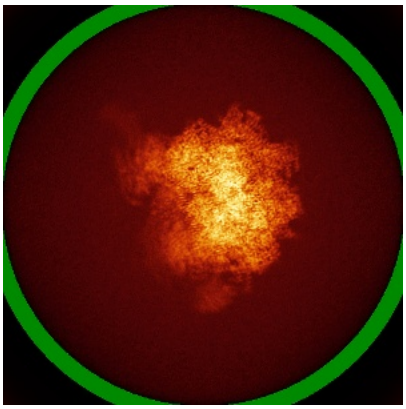


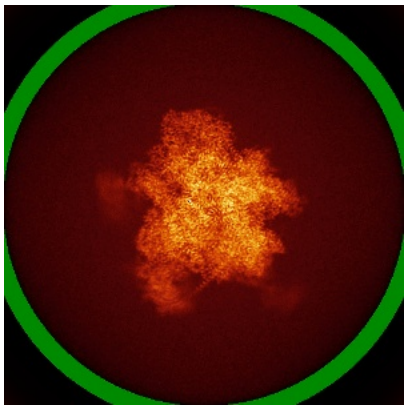
Z Index: 256

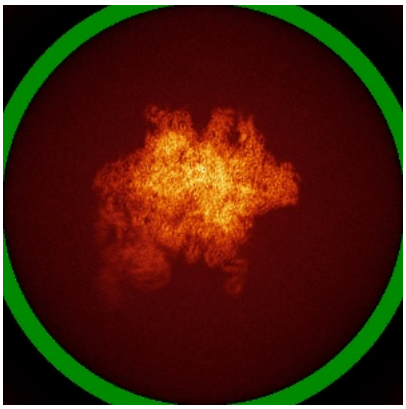
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

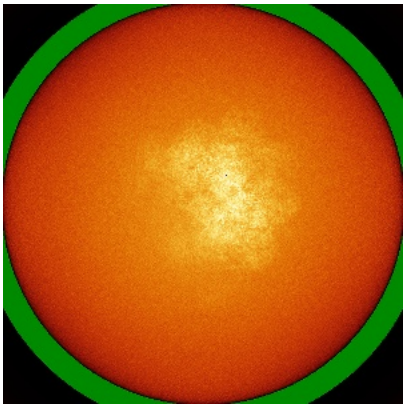
6.4.1 Primary map

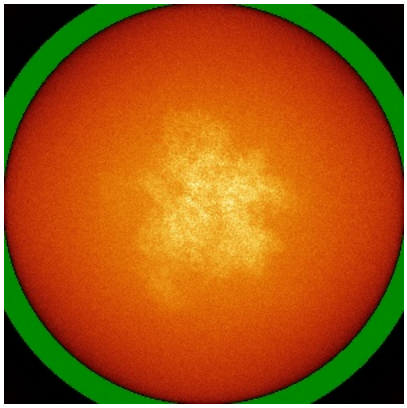

X

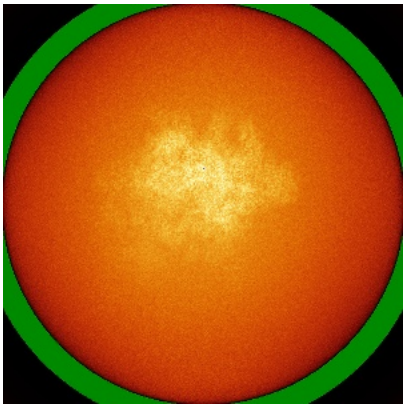

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

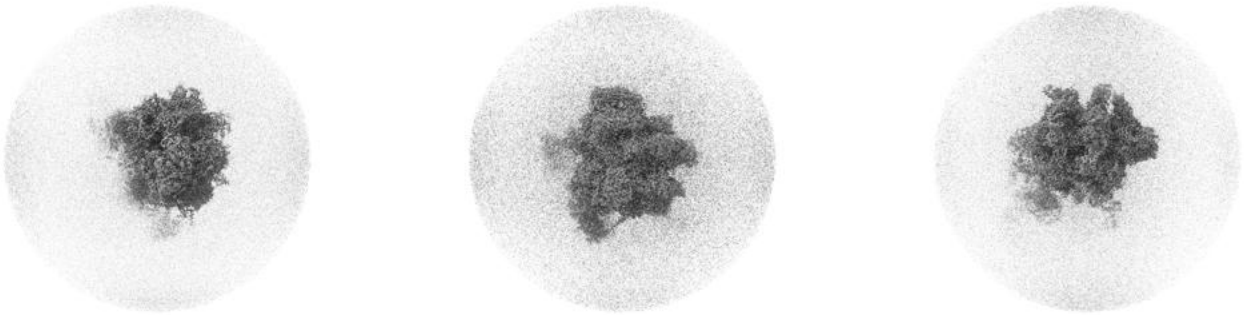
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

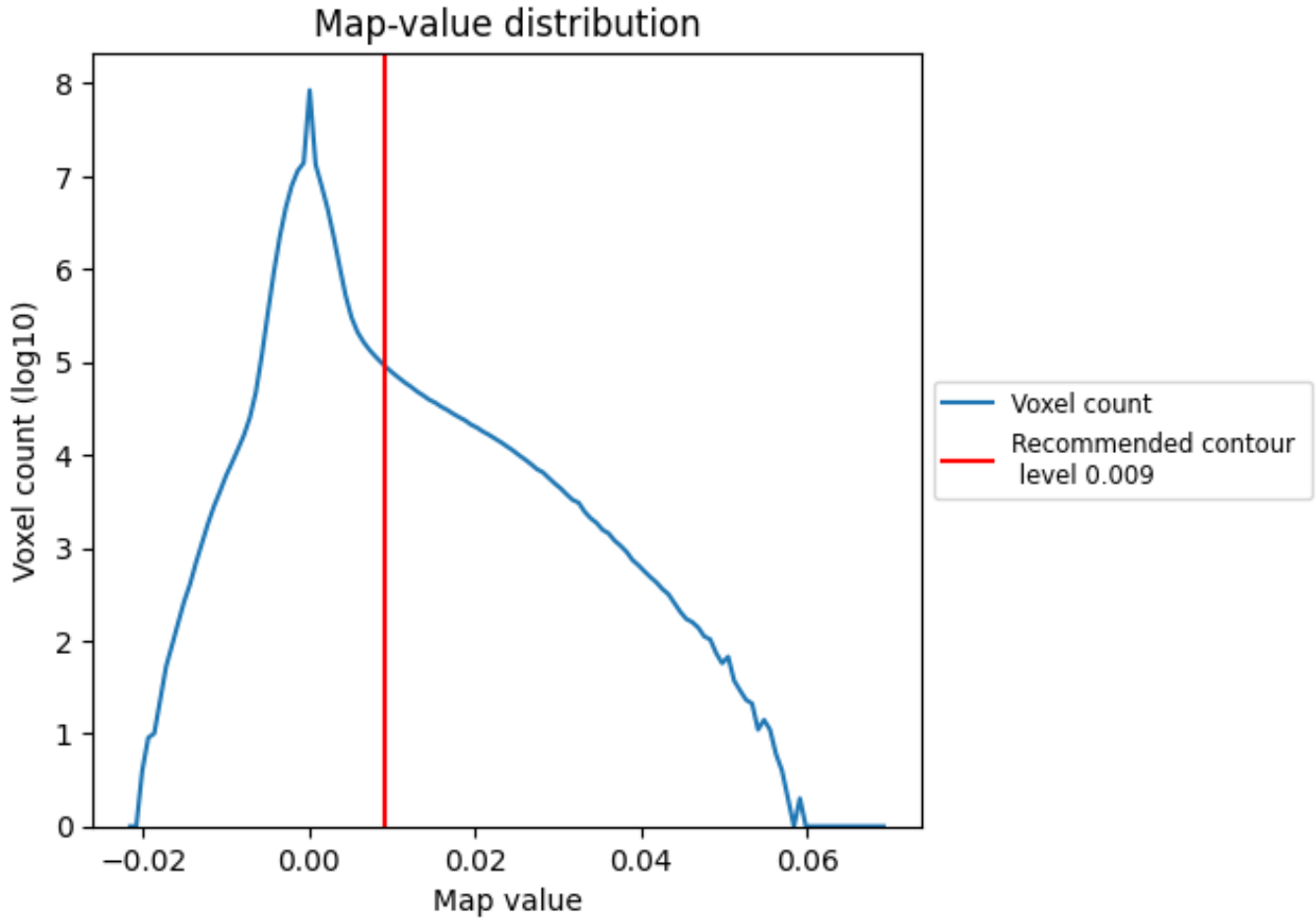
6.6 Mask visualisation (i)

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

7 Map analysis

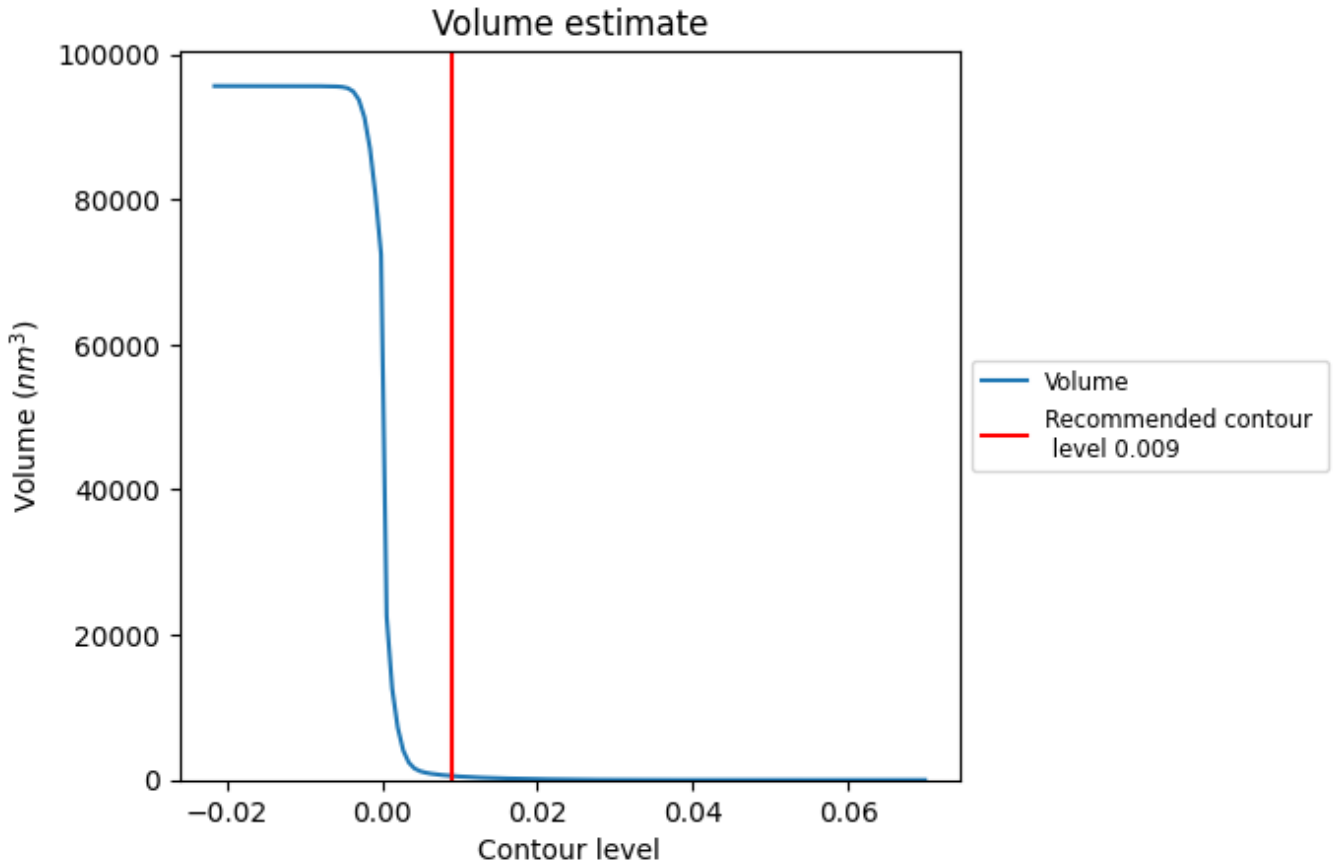
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

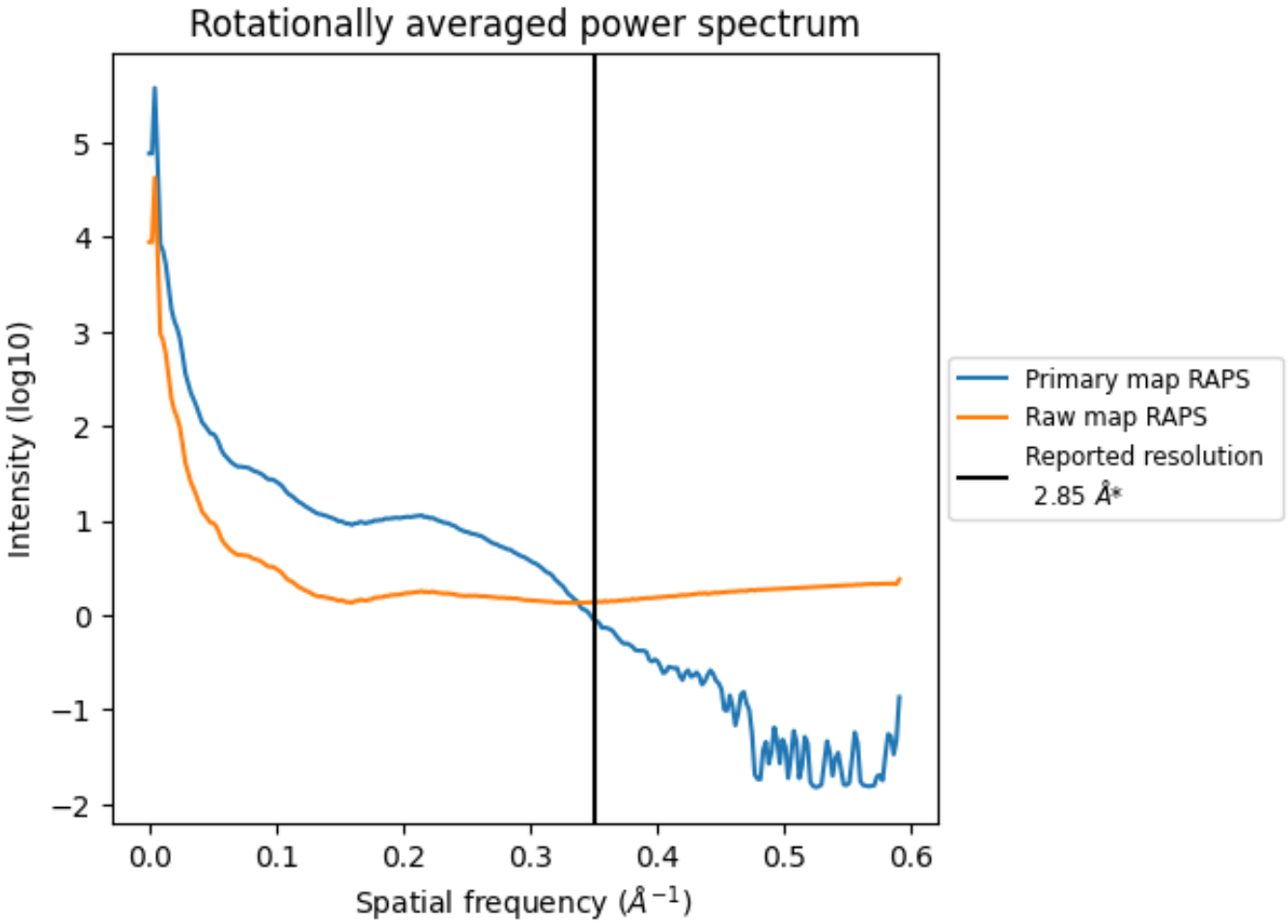
7.2 Volume estimate



The volume at the recommended contour level is 555 nm^3; this corresponds to an approximate mass of 502 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 (i)

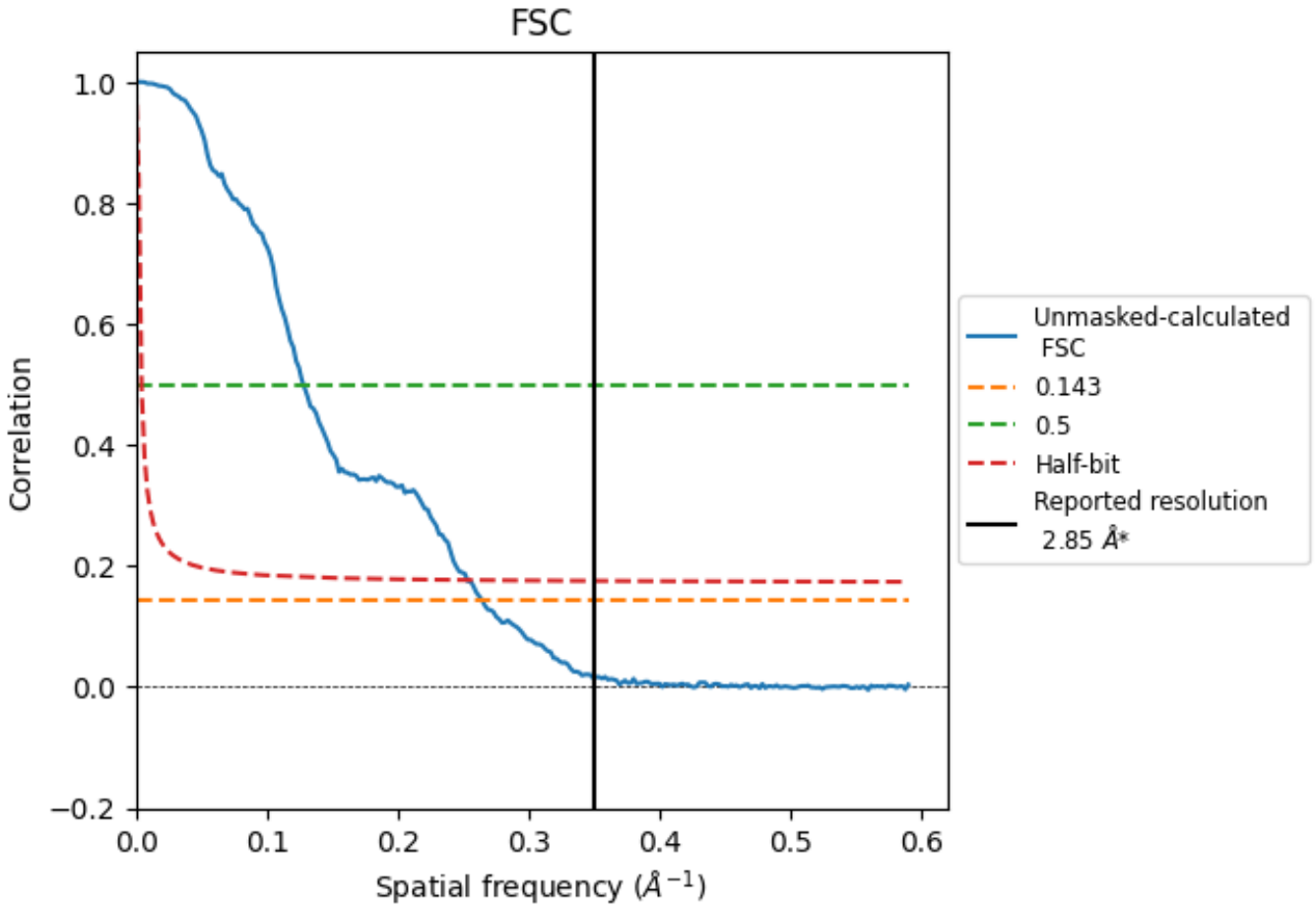


*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

8.2 Resolution estimates (i)

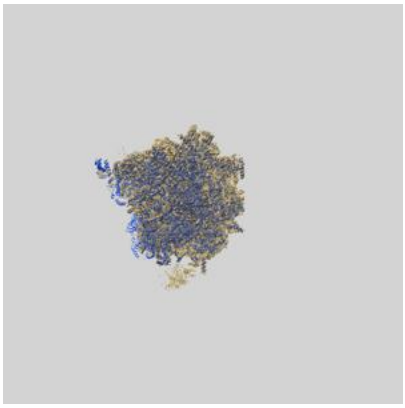
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.81	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.85 by more than 10 %

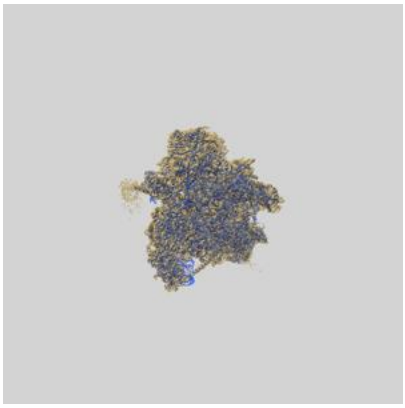
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52049 and PDB model 9HCH. Per-residue inclusion information can be found in section 3 on page 17.

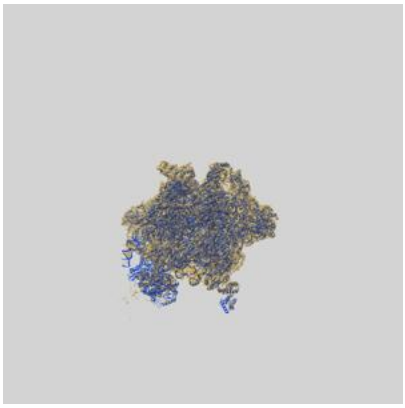
9.1 Map-model overlay



X



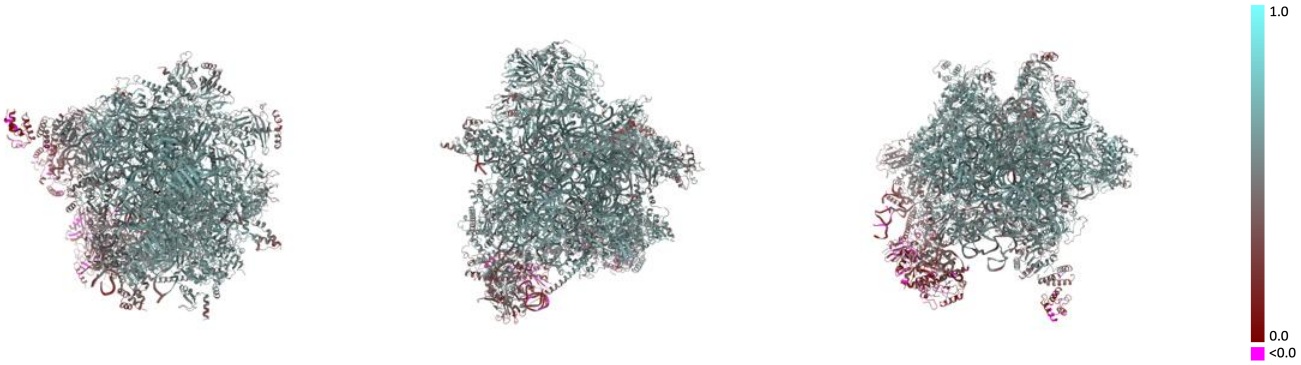
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

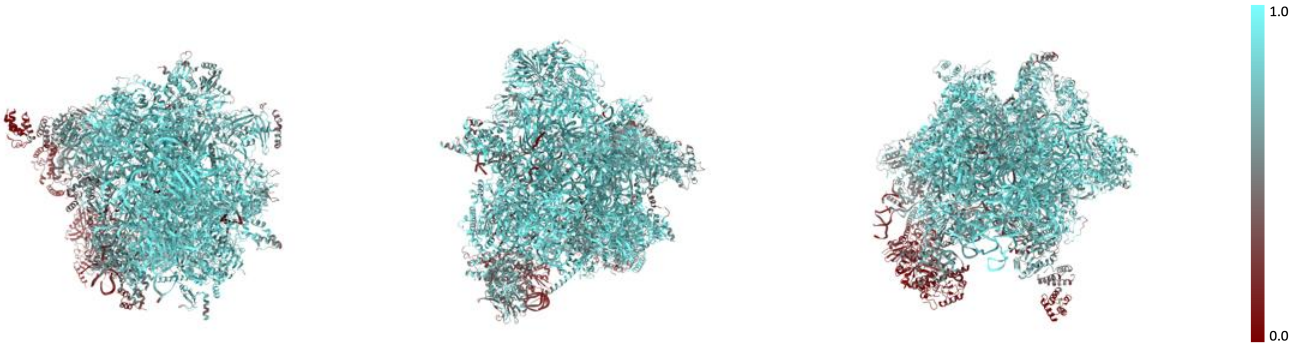
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

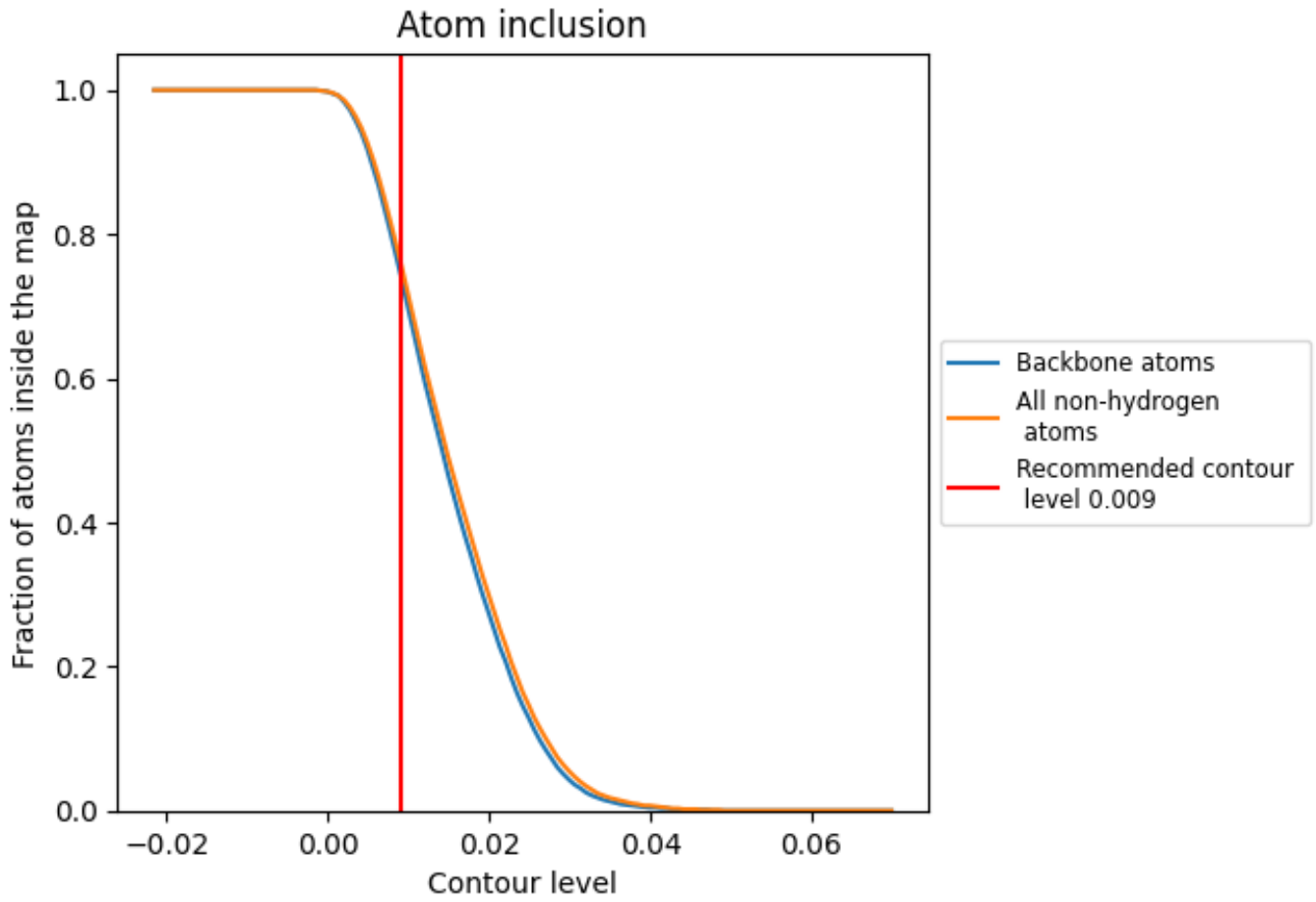
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.5190
0	0.8480	0.5720
1	0.7280	0.5280
2	0.9500	0.6500
3	0.9310	0.6290
4	0.7680	0.5470
5	0.8250	0.5710
6	0.6240	0.4100
7	0.7350	0.5160
8	0.1650	0.1920
9	0.8080	0.5570
A	0.8880	0.5650
B	0.3990	0.1710
D	0.8340	0.5800
E	0.8680	0.5890
F	0.8870	0.6040
H	0.7670	0.5440
I	0.3280	0.2630
J	0.0930	0.1730
K	0.8870	0.6040
L	0.7860	0.5640
M	0.8840	0.6020
N	0.5860	0.4880
O	0.8740	0.5960
P	0.6540	0.4370
Q	0.8200	0.5590
R	0.8940	0.6170
S	0.8090	0.5730
T	0.8800	0.6150
U	0.8960	0.6150
V	0.7770	0.5370
W	0.7180	0.5080
X	0.8360	0.5730
Y	0.8740	0.5950
Z	0.8310	0.5860



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.7110	0.5600
b	0.8930	0.6050
c	0.8120	0.5580
d	0.7010	0.4970
e	0.0230	0.1050
f	0.1160	0.1880
g	0.8660	0.5810
h	0.7570	0.5220
i	0.9280	0.6390
j	0.7820	0.5400
k	0.3880	0.3140
l	0.2130	0.2380
m	0.0400	0.1130
o	0.8510	0.5820
p	0.6510	0.4550
q	0.7360	0.4940
r	0.7980	0.5450
s	0.8620	0.5900
u	0.6290	0.4680
v	0.4270	0.3640
w	0.0730	0.1440
x	0.5980	0.4290
y	0.5950	0.4770
z	0.4950	0.4590