



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 06:47 pm BST

PDB ID : 9HCF / pdb_00009hcf
EMDB ID : EMD-52047
Title : Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, GTPBP7, GTPBP10 and the MALSU-L0R8F8-mtACP complex with uL16m, State B2 (SAMC knock-out)
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.
Deposited on : 2024-11-08
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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

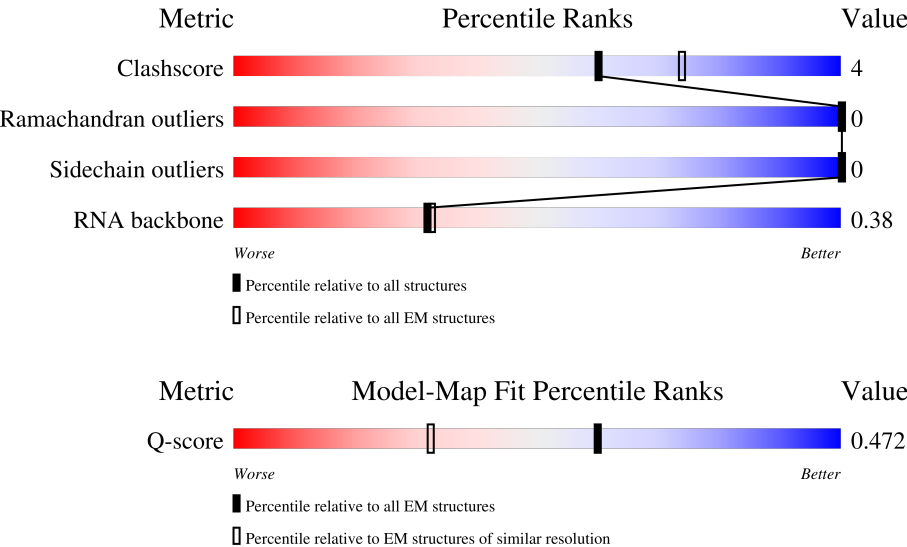
1 Overall quality at a glance i

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1584	10% 55% 26% 8% 10%
2	B	68	43% 44% 31% 16% 9%
3	D	246	5% 82% 10% 8%

Continued on next page...

Continued from previous page...

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	381	
26	1	65	
27	2	92	
28	3	188	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	4	101	
30	6	380	
31	7	336	
32	b	159	
33	f	211	
34	h	159	
35	i	128	
36	j	121	
37	o	102	
38	q	222	
39	r	196	
40	s	442	
41	u	228	
42	v	70	
43	5	423	
44	8	206	
45	9	135	
46	a	142	
47	m	127	
48	z	326	
49	l	135	
50	y	346	
51	w	156	
52	c	308	
53	g	166	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	k	118	63% 67% 5% 28%
55	0	187	53% 5% 42%
56	d	306	26% 67% 10% 22%
57	e	283	67% 55% 13% 32%
58	p	206	19% 64% 6% 30%
59	t	366	60% 69% 19% 12%

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 202333 atoms, of which 93796 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 (1432-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1428	Total	C	H	N	O	P	0	0
			45695	13636	15333	5478	9820	1428		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1842	U	C	conflict	GB 10336604
A	2197	A	U	conflict	GB 10336604
A	2431	A	G	conflict	GB 10336604

- Molecule 2 is a RNA chain called RNA (63-MER).

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	308	Total	C	H	N	O	S	0	0
			4900	1577	2441	432	442	8		

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

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

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

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

- 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	97	Total	C	H	N	O	S	0	0
			1543	487	796	126	131	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	184	Total	C	H	N	O	S	0	0
			3037	978	1521	273	255	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	155	Total	C	H	N	O	S	0	0
			2582	813	1323	222	222	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	120	Total	C	H	N	O	S	0	0
			2004	626	1026	180	169	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 bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	52	Total	C	H	N	O		0	0
			900	278	472	80	70			

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	2	46	Total	C	H	N	O	S	0	0
			787	235	407	86	58	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	95	Total	C	H	N	O	S	0	0
			1695	528	872	164	127	4		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	37	Total	C	H	N	O	S	0	0
			676	206	354	68	45	3		

- Molecule 30 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	6	315	Total	C	H	N	O	S	0	0
			5248	1726	2559	487	470	6		

- Molecule 31 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	7	292	Total	C	H	N	O	S	0	0
			4757	1517	2378	409	438	15		

- Molecule 32 is a protein called Large ribosomal subunit protein mL43.

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

- Molecule 33 is a protein called Large ribosomal subunit protein mL48.

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

- Molecule 34 is a protein called Large ribosomal subunit protein mL50.

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

- Molecule 35 is a protein called Large ribosomal subunit protein mL51.

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

- Molecule 36 is a protein called Large ribosomal subunit protein mL52.

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

- Molecule 37 is a protein called Large ribosomal subunit protein mL63.

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

- Molecule 38 is a protein called Large ribosomal subunit protein mL64.

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

- Molecule 39 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	r	157	Total	C	H	N	O	S	0	0
			2606	812	1331	242	210	11		

- Molecule 40 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	s	377	Total	C	H	N	O	S	0	0
			6104	1938	3059	555	540	12		

- Molecule 41 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 42 is a protein called Predicted gene, 55359.

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

- Molecule 43 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	5	394	Total	C	H	N	O	S	0	0
			6468	2081	3243	564	571	9		

- Molecule 44 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	8	67	Total	C	H	N	O	S	0	0
			1121	354	557	97	111	2		

- Molecule 45 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	9	122	Total	C	H	N	O	S	0	0
			1973	635	990	167	179	2		

- Molecule 46 is a protein called Large ribosomal subunit protein mL42.

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

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

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

- Molecule 48 is a protein called Mitochondrial ribosome-associated GTPase 1.

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

- Molecule 49 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	l	65	Total	C	H	N	O	S	0	0
			1108	355	549	101	102	1		

- Molecule 50 is a protein called Transcription termination factor 4, mitochondrial.

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

- Molecule 51 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 52 is a protein called Large ribosomal subunit protein mL44.

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

- Molecule 53 is a protein called Large ribosomal subunit protein mL49.

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

- Molecule 54 is a protein called Large ribosomal subunit protein mL53.

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

- Molecule 55 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	0	108	Total	C	H	N	O	S	0	0
			1789	546	908	174	155	6		

- Molecule 56 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	d	238	Total	C	H	N	O	S	0	0
			3901	1262	1940	348	341	10		

- Molecule 57 is a protein called Large ribosomal subunit protein mL46.

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

- Molecule 58 is a protein called Large ribosomal subunit protein mL62.

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

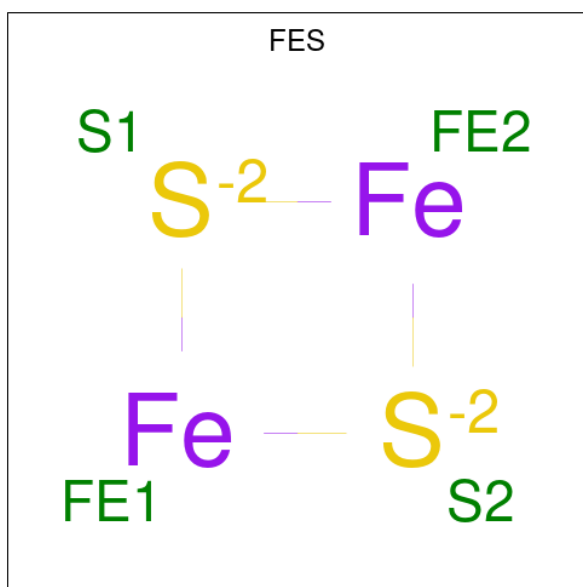
- Molecule 59 is a protein called GTP-binding protein 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	t	321	Total	C	H	N	O	S	0	0
			5015	1569	2551	431	455	9		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	96	Total	Mg	0
			96	96	
60	M	1	Total	Mg	0
			1	1	
60	O	1	Total	Mg	0
			1	1	
60	R	1	Total	Mg	0
			1	1	

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

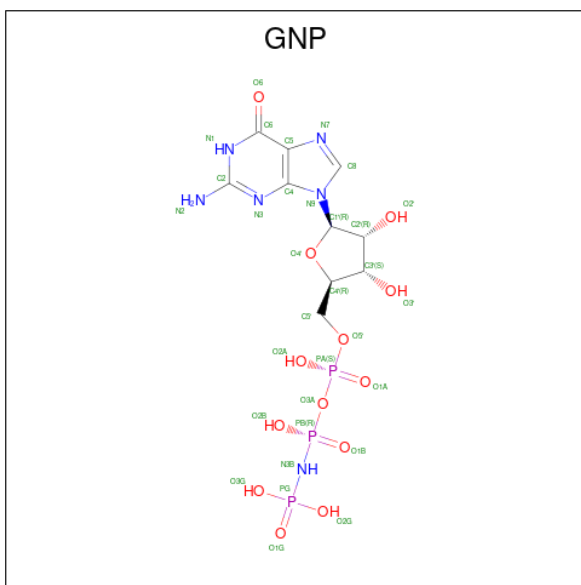


Mol	Chain	Residues	Atoms			AltConf
61	I	1	Total	Fe	S	0
			4	2	2	

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	4	1	Total	Zn	0
			1	1	
62	0	1	Total	Zn	0
			1	1	

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

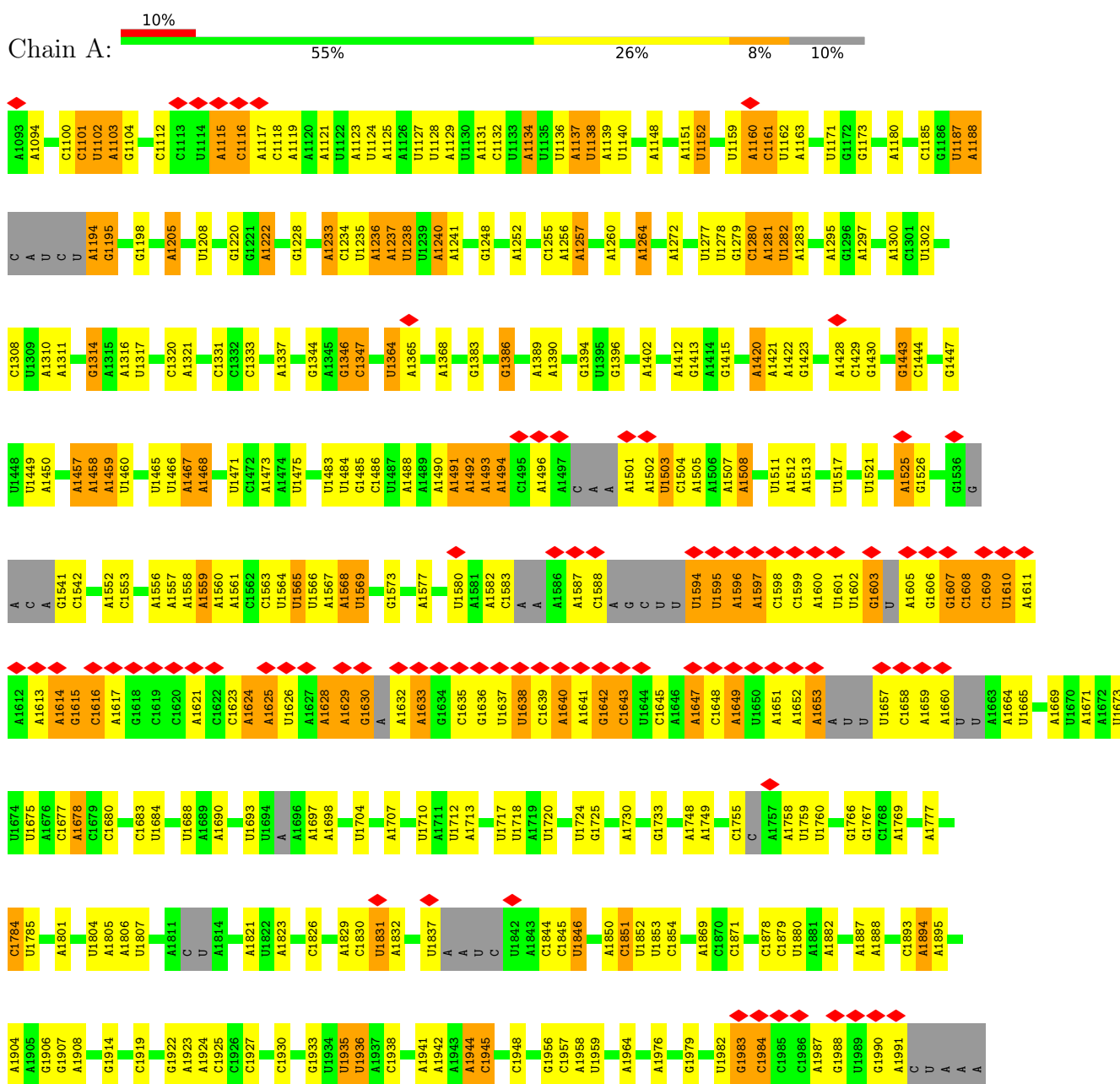


Mol	Chain	Residues	Atoms						AltConf
63	z	1	Total 45	C 10	H 13	N 6	O 13	P 3	0
63	t	1	Total 45	C 10	H 13	N 6	O 13	P 3	0

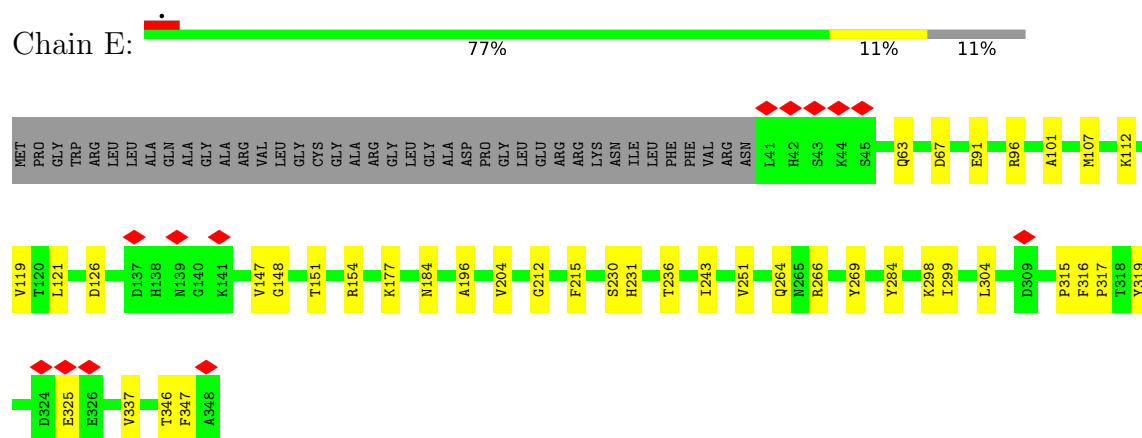
3 Residue-property plots [i](#)

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.

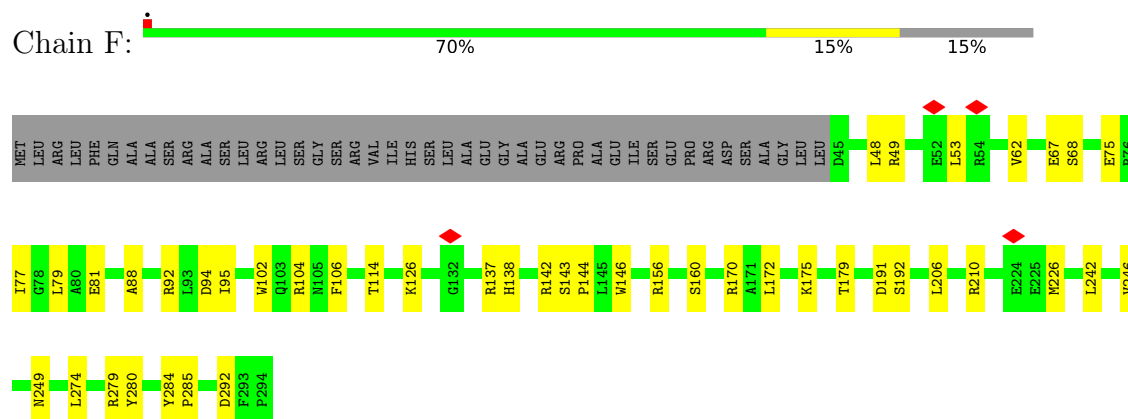
• Molecule 1: 16S rRNA (1432-MER)



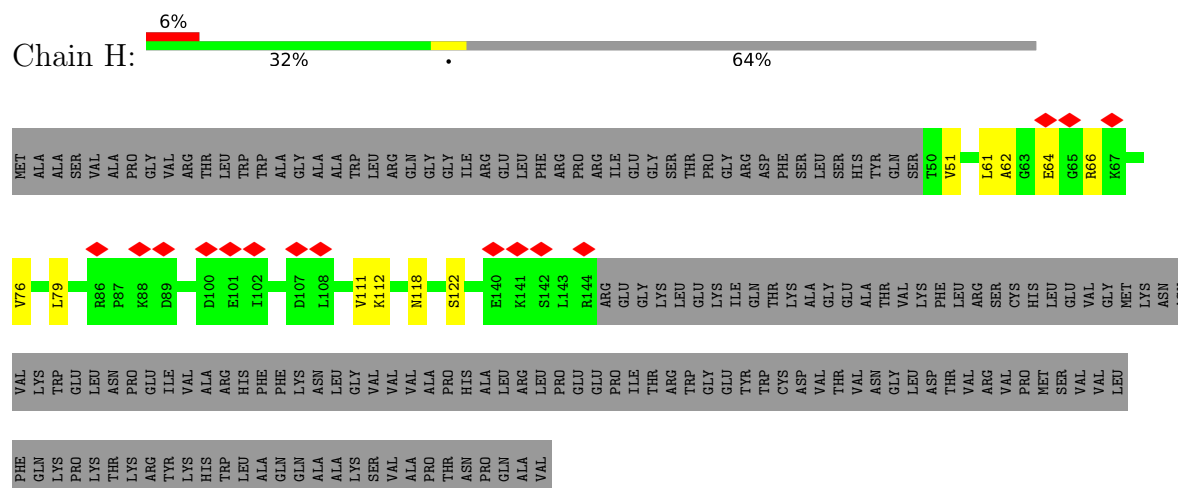
- Chain E:



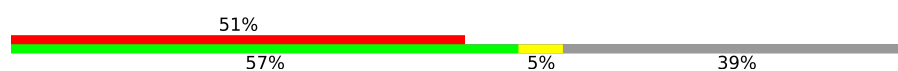
- Chain F:

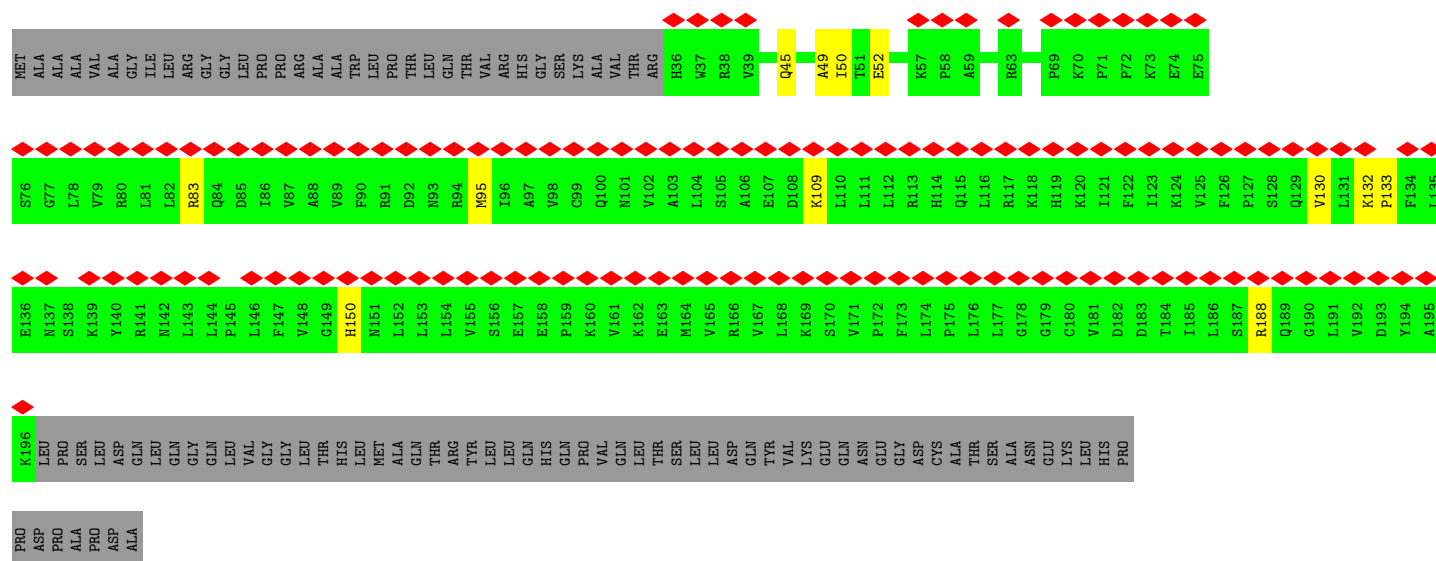


- Chain H:

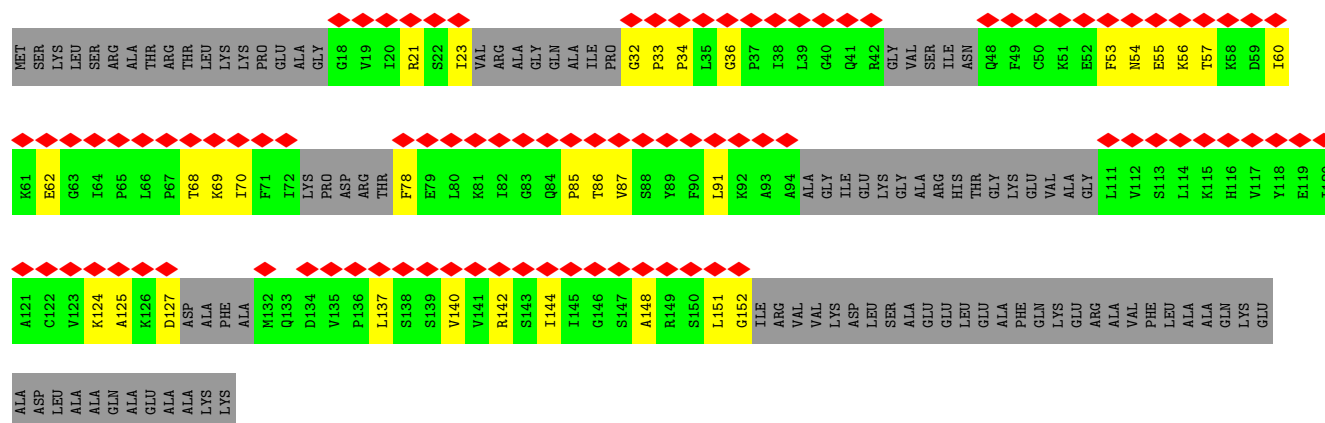
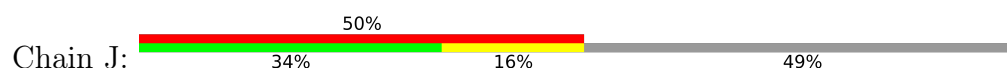


- Chain I:





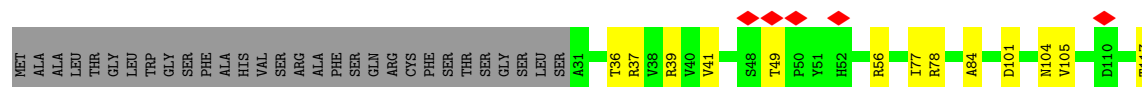
• Molecule 8: Large ribosomal subunit protein uL11m

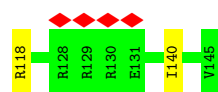


• Molecule 9: Large ribosomal subunit protein uL13m



• Molecule 10: Large ribosomal subunit protein uL14m

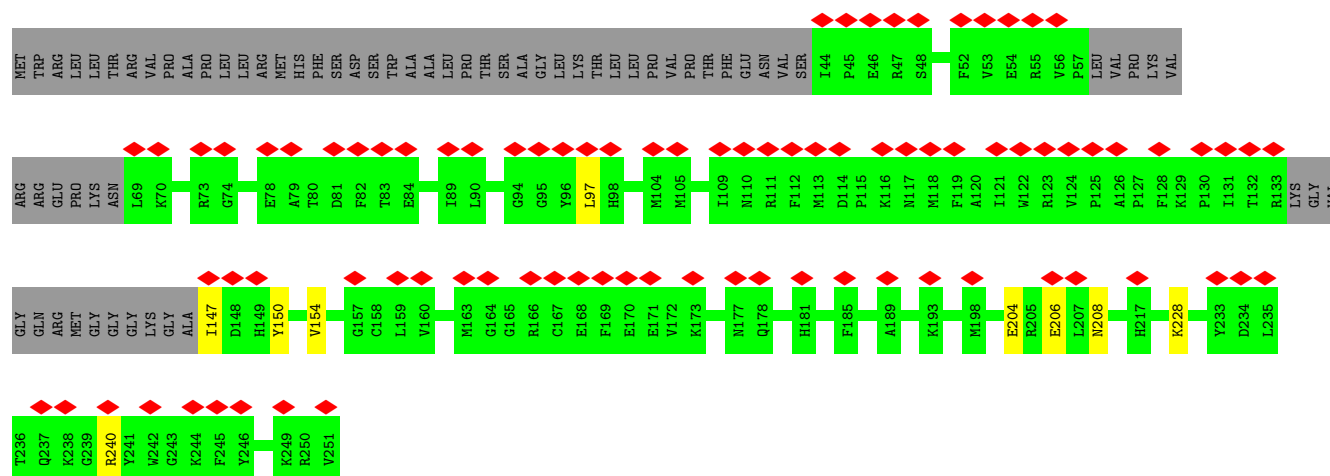




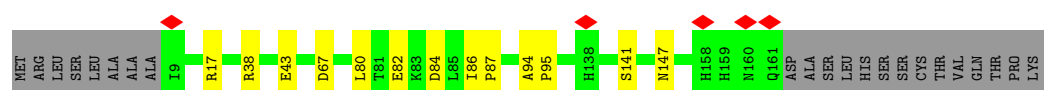
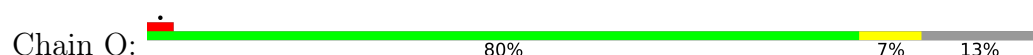
- Molecule 11: Large ribosomal subunit protein uL15m



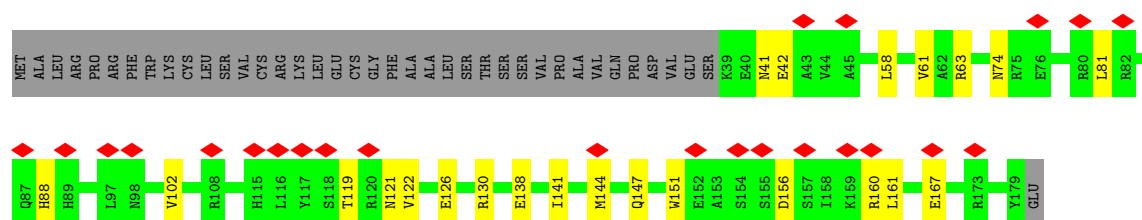
- Molecule 12: Large ribosomal subunit protein uL16m



- Molecule 13: Large ribosomal subunit protein bL17m

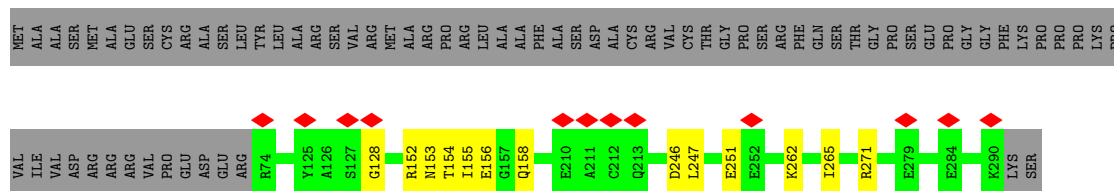


- Molecule 14: Large ribosomal subunit protein uL18m



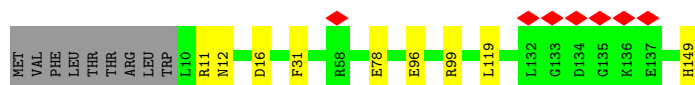
- Molecule 15: Large ribosomal subunit protein bL19m

Chain Q:  70% 26%



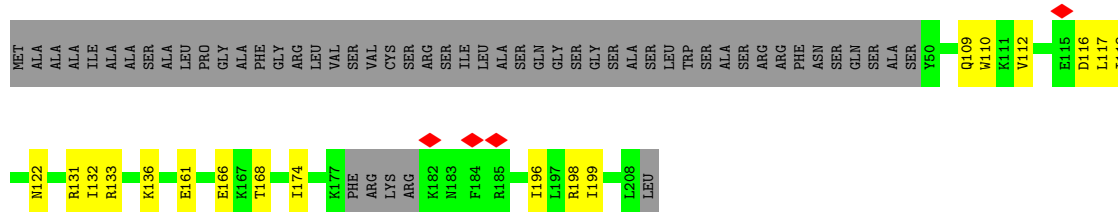
- Molecule 16: Large ribosomal subunit protein bL20m

Chain R:  88% 6% 6%



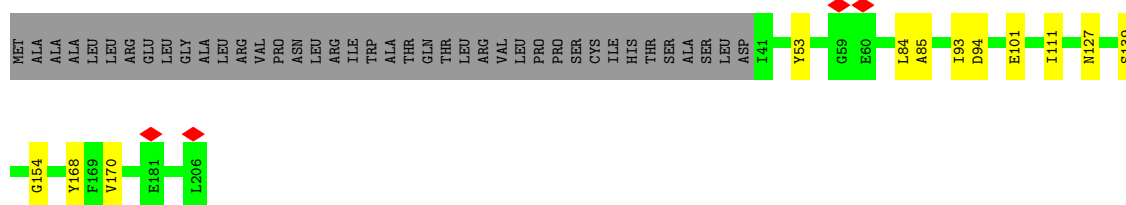
- Molecule 17: Large ribosomal subunit protein bL21m

Chain S:  66% 9% 26%



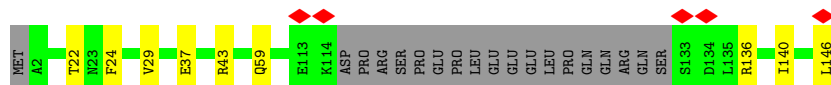
- Molecule 18: Large ribosomal subunit protein uL22m

Chain T:  75% 6% 19%



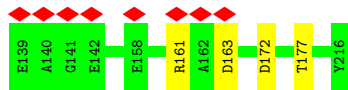
- Molecule 19: Large ribosomal subunit protein uL23m

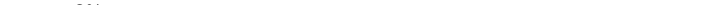
Chain U:  81% 6% 13%

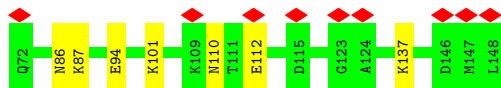


- Molecule 20: Large ribosomal subunit protein uL24m

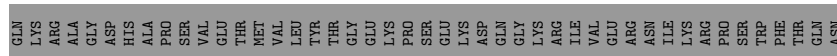
Chain V:  84% 9% 7%

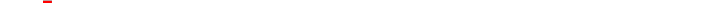


- Chain W:  8% 60% 7% 25%



- Chain X:



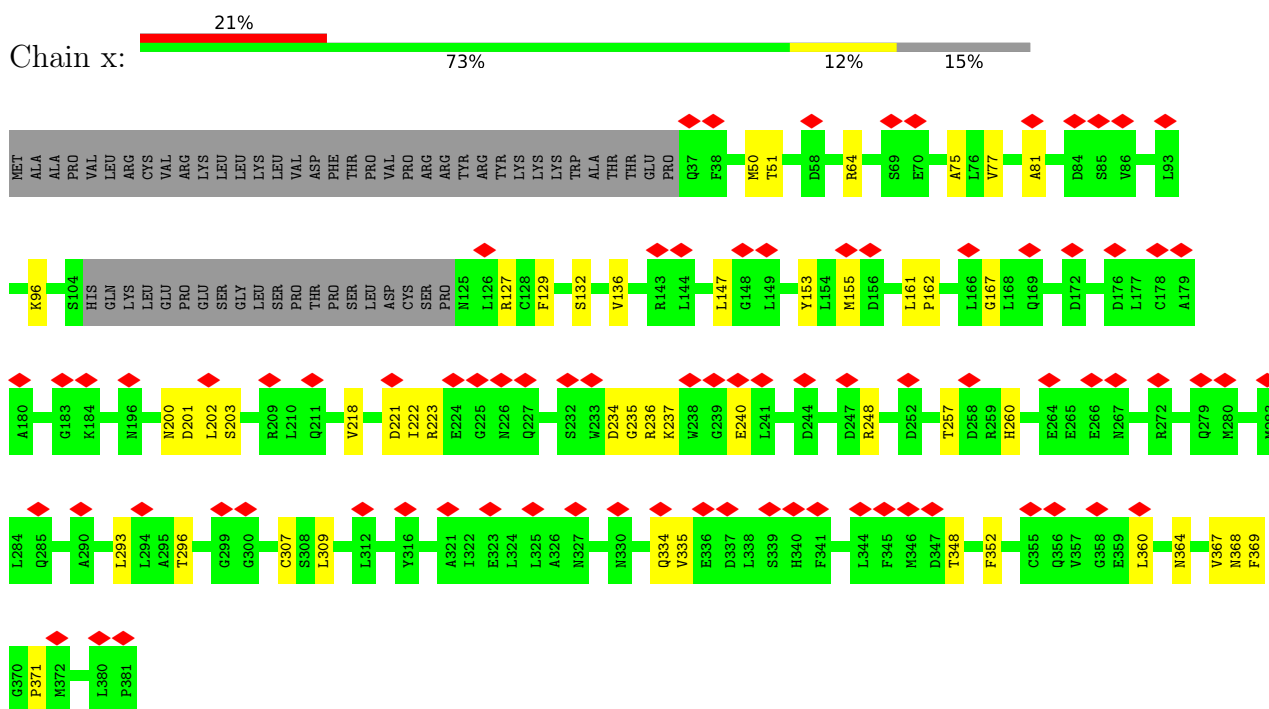
- Chain Y:  65% 5% 30%



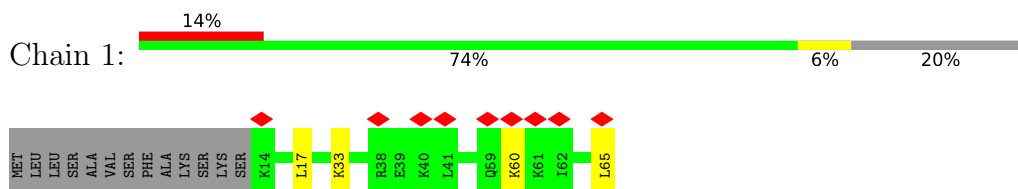
- Chain Z: 



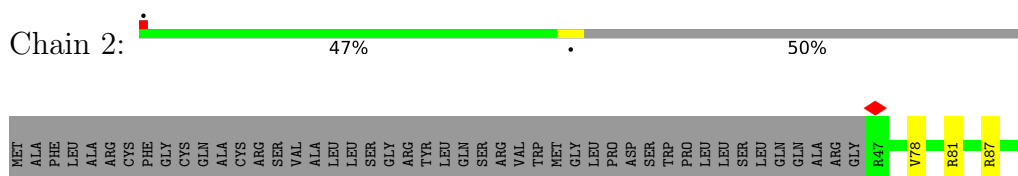
- 



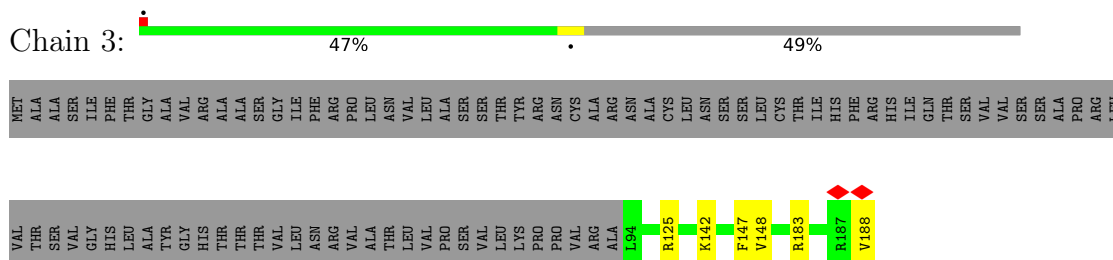
- Molecule 26: Large ribosomal subunit protein bL33m



- Molecule 27: Large ribosomal subunit protein bL34m



- Molecule 28: Large ribosomal subunit protein bL35m



- Molecule 29: Large ribosomal subunit protein bL36m



MET ALA ALA ALA LEU VAL ARG SER VAL VAL ALA ALA SER VAL VAL ASP PRO PHE LEU HIS LEU SER LEU ARG LEU VAL VAL LYS PRO ARG VAL PHE SER SER PHE LEU LEU GLY THR LEU PRO ARG ALA LYS PRO CYS ALA GLU VAL ARG SER VAL VAL CYS GLY ARG PRO PRO THR LEU

PRO SER LEU GLY F65 F66 F67 K73 K76 D77 C78 V81 K82 R83 T93 H97 K98 Q99 R100 Q101

• Molecule 30: Large ribosomal subunit protein mL38

Chain 6: 17% 67% 16% 17%

MET ALA ALA PRO TRP ARG ALA ALA PHE PHE GLY ILE GLY ARG CYS ARG GLY PHE SER THR ALA LEU SER ARG THR PRO PRO LEU GLY MET PRO ASN GLU ASP ILE ASP VAL SER ASN LEU E46 R47 L48 E49 K50 Y51 R52 E55 R56 Y57 R60 A61 E54 W70 W71 W72 F78 VAL LYS THR ASP PRO LYS LYS ILE ASP ILE GLY PRO PRO PRO ARG VAL SER L104 H108 F109 L110 R111 E112 L113 R114 A115 E118 E119 E120 R121 A122 R123 R124 L125 R126 T127 A128 S129 I130 A137 E138 W139 E140 R141 G144 P145 R159 D160 A165 P169 W170 L173 H174 V175 A176 G180 E181 E182 D183 L184 Y188 H189 E192 A198 S199 R200 E203 Y206 E207 A208 D209 K210 D211 T215 L216 L217 F218 L219 N220 L221 D222 G223 H224 L225 L226 E227 V233 L236 S242 N243 R244 V245 A246 E247 T251 Y254 R267 F270 L271 L272 F273 K274 Q275 D276 K277 V280 E283 D284 Q292 L293 R296 R299 D302 F303 Y304 Q308 G315 L316 A317 L334 L335 R338 F344 Y345 R346 K355 E360 T380

• Molecule 31: Large ribosomal subunit protein mL39

Chain 7: 11% 78% 9% 13%

MET ALA THR ALA VAL GLY ARG LEU VAL LEU ARG ARG PRO GLY ALA GLY GLY ALA ARG TRP ARG PHE ILE ALA THR SER PRO ALA ALA GLU LEU S33 E39 M40 R41 R47 Q42 T56 P57 R58 E63 V67 V77 W95 V105 D106 D111 C120 D131 A144 L147 I151 F155 K156 D157 D158 V164 R165 L182 D183 K184 E188 P191 E214 D217 E225 L226 F227 Q228 D235 F236 L237 E238 A241 S242 Q243 N244 P245 E246 R247 R253 D256 D259 V260 S261 E262 F273 V280 L283 N284 F285 S286 Q287 P288 R289 R292 R293 T301 Q306 V321 T322 E323 D324 VAL ARG GLN THR GLU ASN THR GLU THR THR GLN

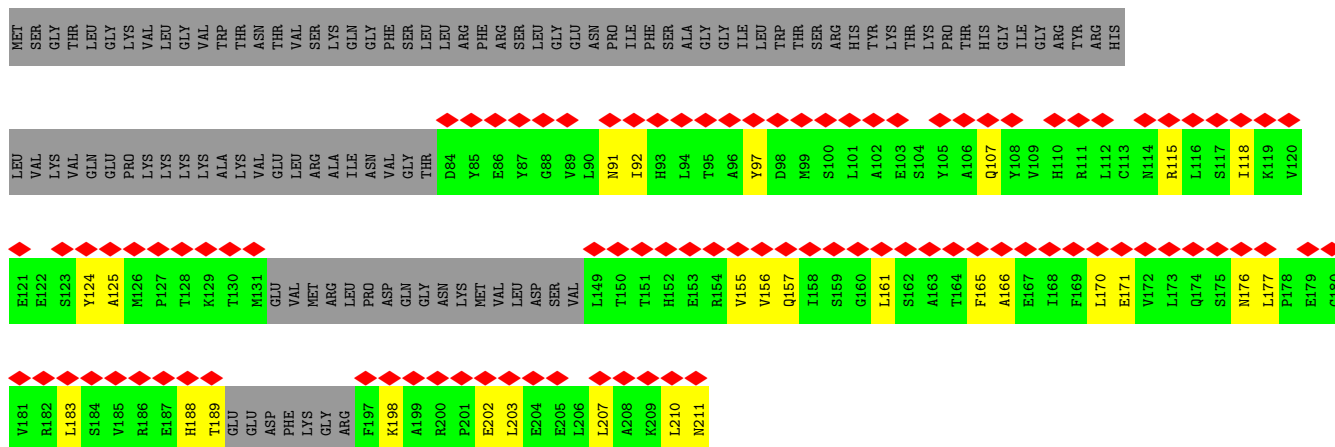
• Molecule 32: Large ribosomal subunit protein mL43

Chain b: 81% 12% 7%

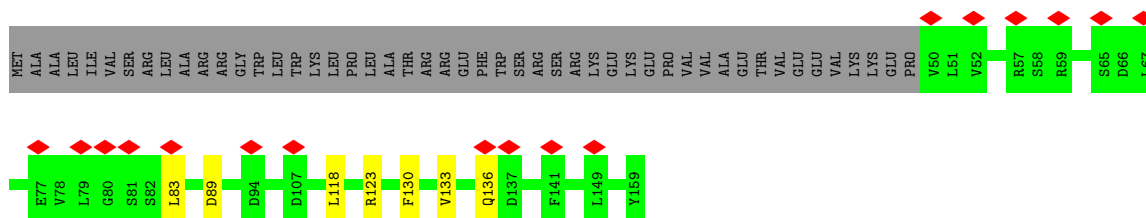
MET T2 T6 S7 T12 S13 R21 D36 E45 F46 V47 V51 V65 N66 P67 V69 V94 Q107 H131 T134 N135 K136 R137 R149 ASP SER ALA PRO ALA SER MET GLN ALA GLN

• Molecule 33: Large ribosomal subunit protein mL48

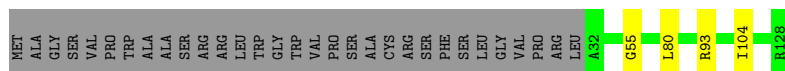
Chain f: 46% 36% 13% 51%



• Molecule 34: Large ribosomal subunit protein mL50



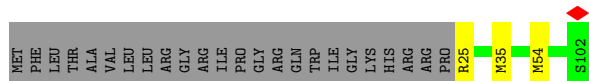
• Molecule 35: Large ribosomal subunit protein mL51



• Molecule 36: Large ribosomal subunit protein mL52

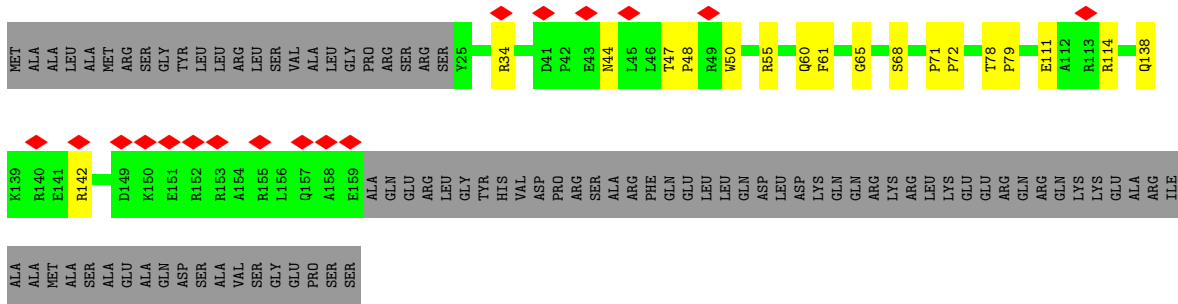


• Molecule 37: Large ribosomal subunit protein mL63

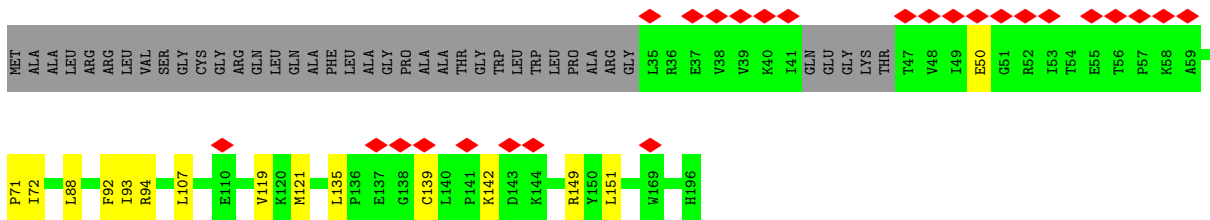


• Molecule 38: Large ribosomal subunit protein mL64

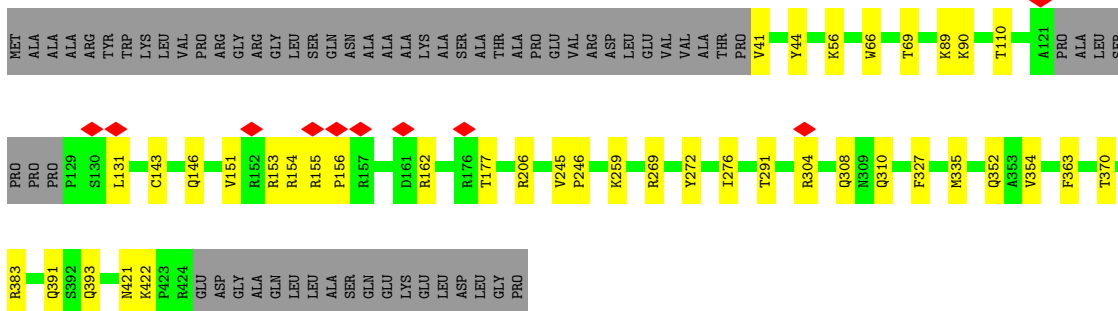
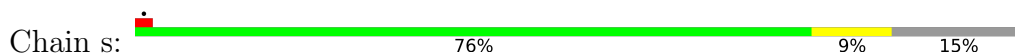




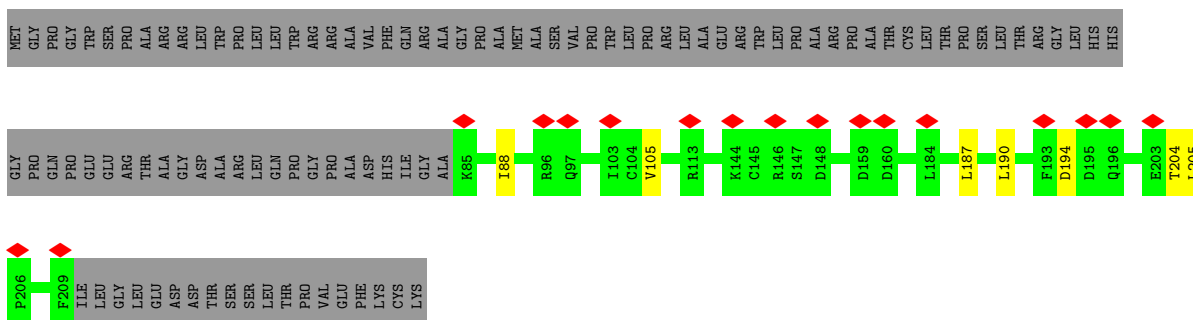
- Molecule 39: Large ribosomal subunit protein mL66



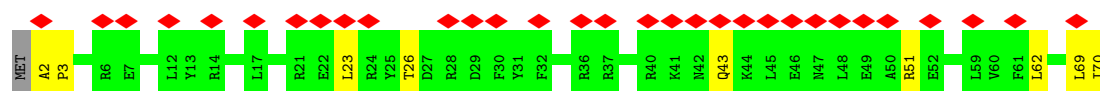
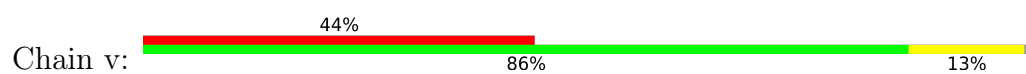
- Molecule 40: Large ribosomal subunit protein mL65



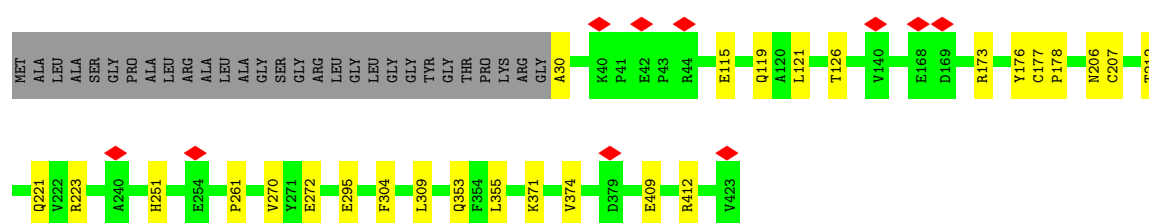
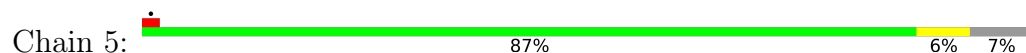
- Molecule 41: Mitochondrial assembly of ribosomal large subunit protein 1



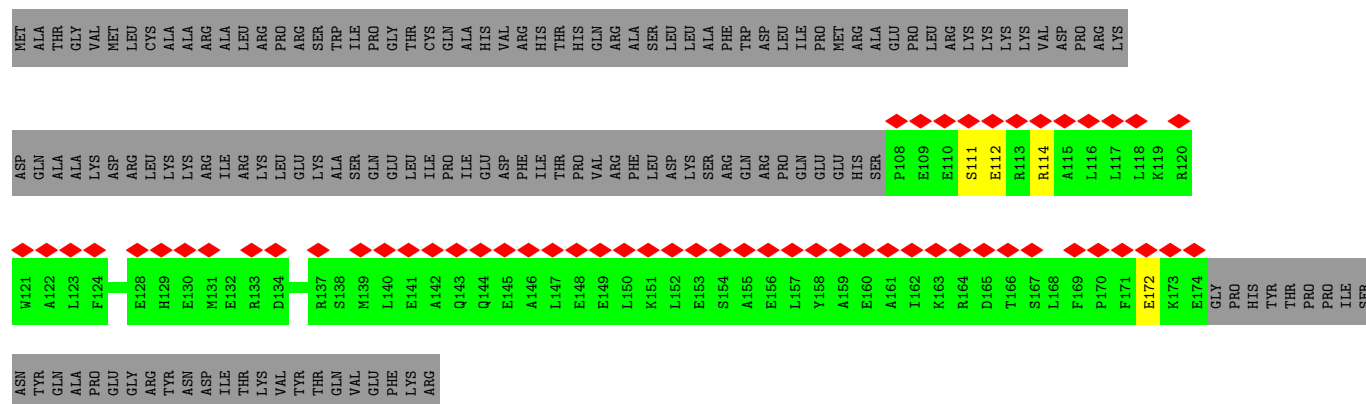
- Molecule 42: Predicted gene, 55359



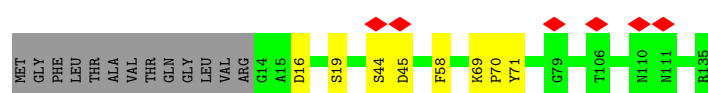
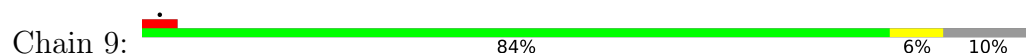
- Molecule 43: Large ribosomal subunit protein mL37



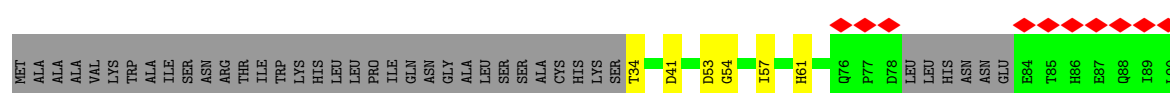
- Molecule 44: Large ribosomal subunit protein mL40

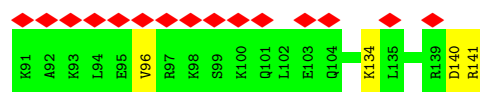


- Molecule 45: Large ribosomal subunit protein mL41

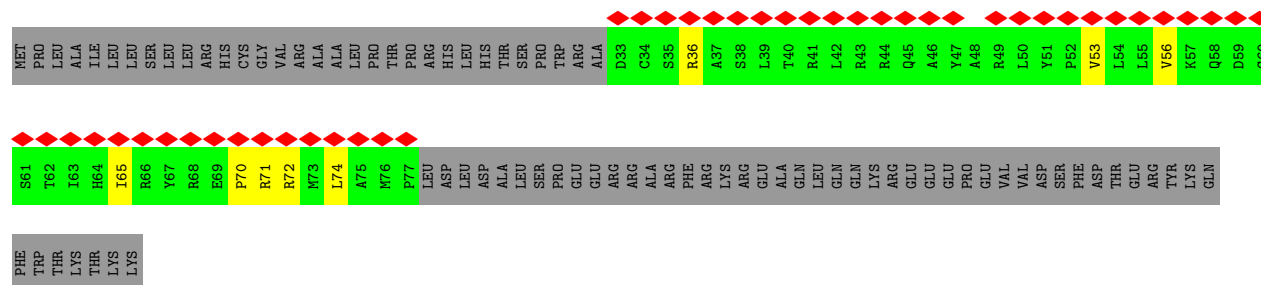


- Molecule 46: Large ribosomal subunit protein mL42

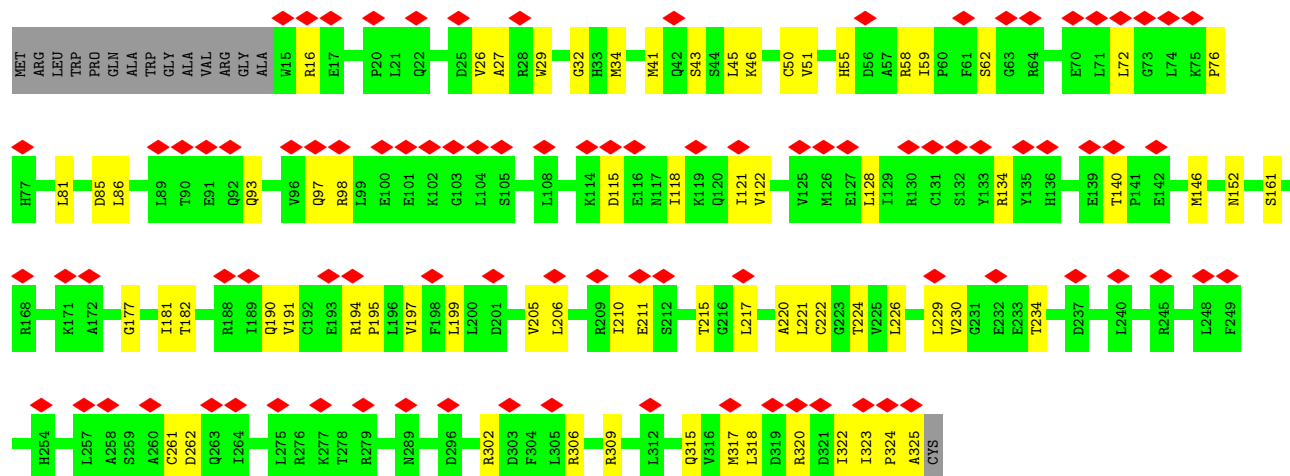
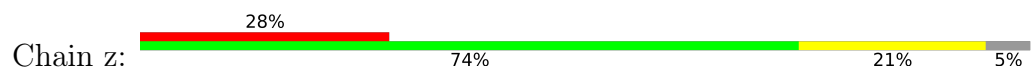




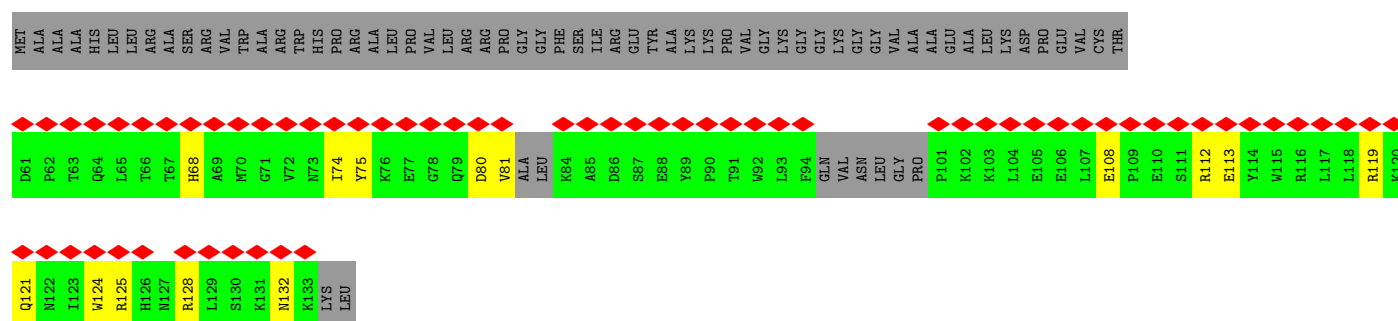
- Molecule 47: Large ribosomal subunit protein mL55



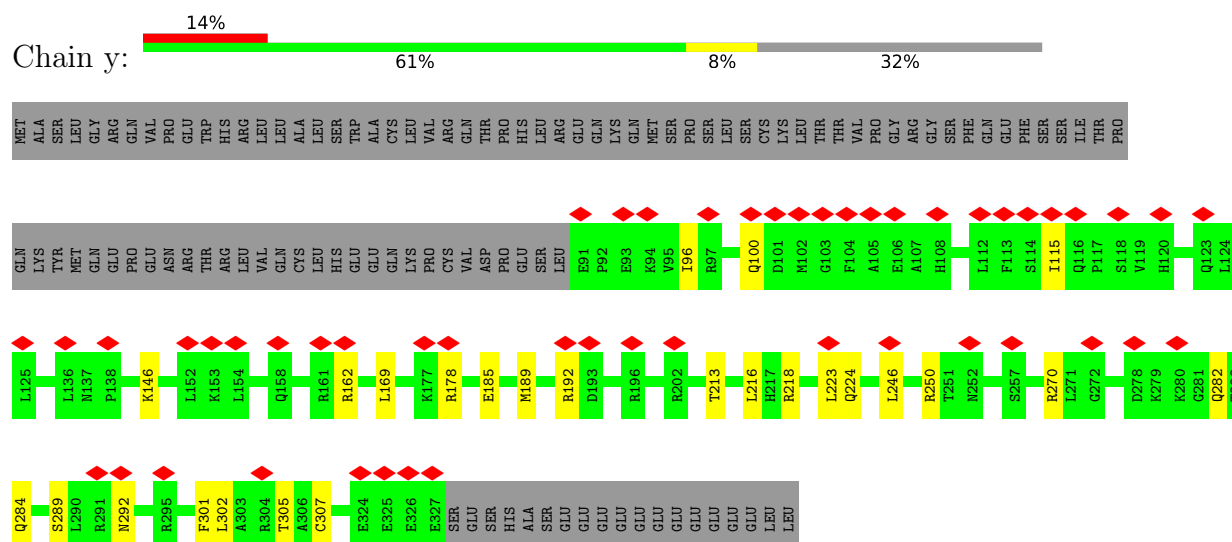
- Molecule 48: Mitochondrial ribosome-associated GTPase 1



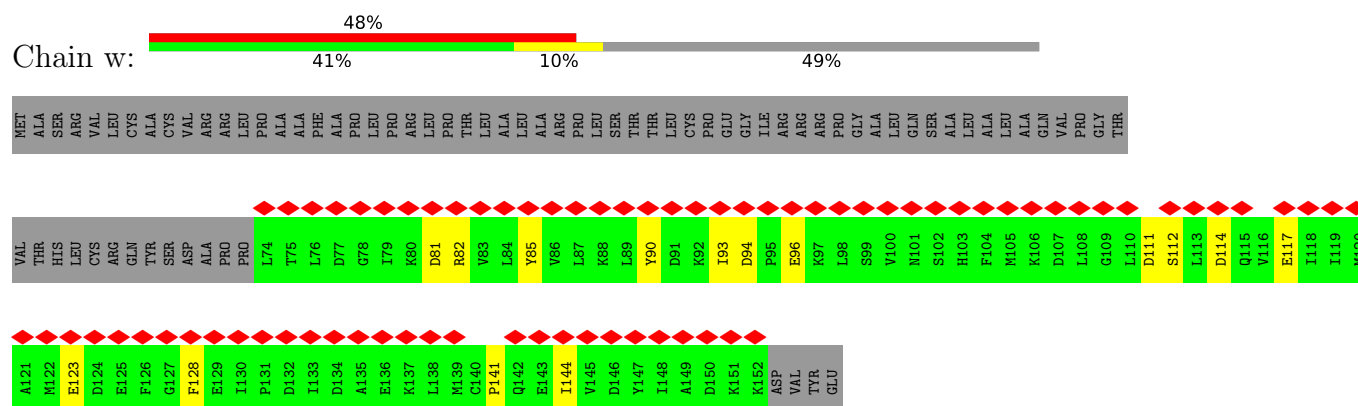
- Molecule 49: Large ribosomal subunit protein mL54



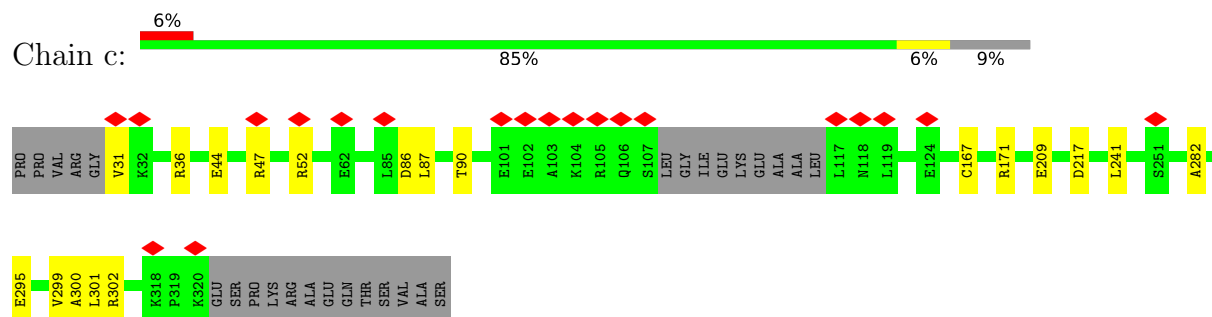
- Molecule 50: Transcription termination factor 4, mitochondrial



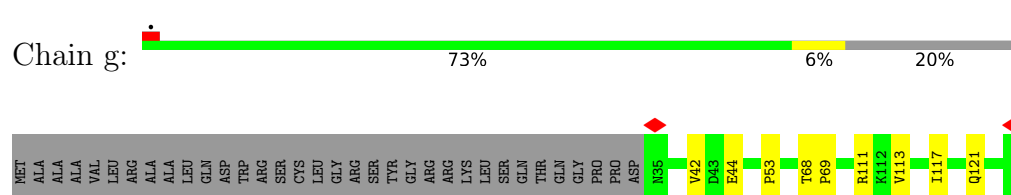
- Molecule 51: Acyl carrier protein, mitochondrial



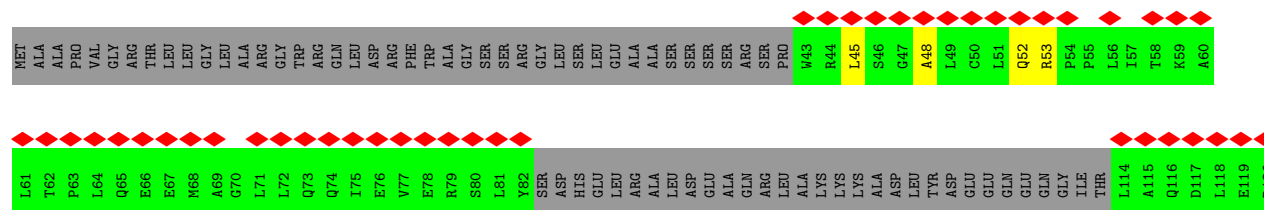
- Molecule 52: Large ribosomal subunit protein mL44

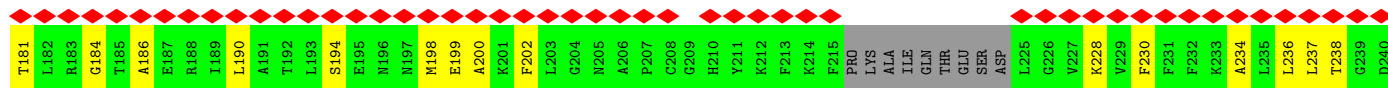


- Molecule 53: Large ribosomal subunit protein mL49

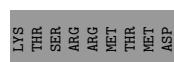
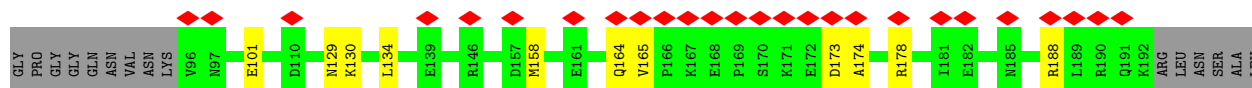
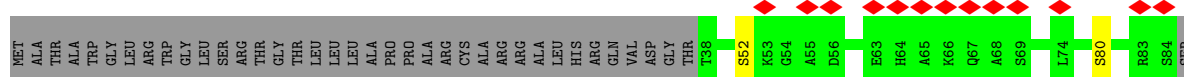


- Molecule 54: Large ribosomal subunit protein mL53

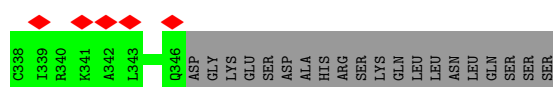
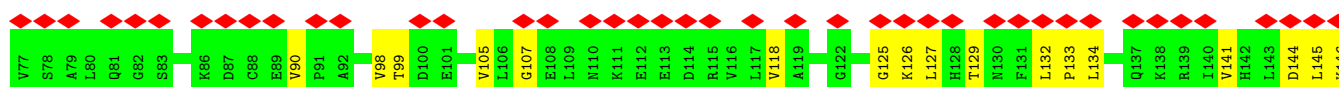
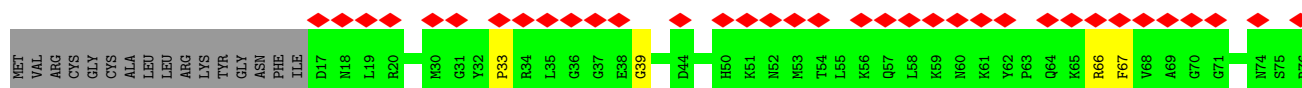




• Molecule 58: Large ribosomal subunit protein mL62



• Molecule 59: GTP-binding protein 10



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.060	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	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

5.1 Standard geometry

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

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	0/33973	0.29	0/52824
2	B	0.10	0/1483	0.24	0/2299
3	D	0.12	0/1802	0.29	0/2424
4	E	0.14	0/2535	0.31	0/3443
5	F	0.15	0/2061	0.31	0/2805
6	H	0.10	0/793	0.24	0/1066
7	I	0.10	0/1339	0.25	0/1813
8	J	0.11	0/756	0.31	0/1010
9	K	0.13	0/1491	0.26	0/2022
10	L	0.13	0/908	0.30	0/1224
11	M	0.13	0/2369	0.28	0/3197
12	N	0.08	0/1558	0.21	0/2097
13	O	0.12	0/1285	0.27	0/1732
14	P	0.08	0/1181	0.24	0/1600
15	Q	0.12	0/1832	0.28	0/2471
16	R	0.14	0/1182	0.27	0/1585
17	S	0.14	0/1284	0.29	0/1740
18	T	0.14	0/1402	0.28	0/1885
19	U	0.13	0/1080	0.27	0/1464
20	V	0.11	0/1695	0.26	0/2295
21	W	0.10	0/816	0.25	0/1105
22	X	0.12	0/2075	0.25	0/2806
23	Y	0.12	0/1561	0.23	0/2093
24	Z	0.11	0/1004	0.27	0/1357
25	x	0.08	0/2620	0.24	0/3549
26	1	0.09	0/434	0.24	0/578
27	2	0.16	0/387	0.29	0/514
28	3	0.15	0/843	0.28	0/1122
29	4	0.10	0/328	0.27	0/430
30	6	0.10	0/2783	0.26	0/3781
31	7	0.10	0/2436	0.24	0/3300
32	b	0.13	0/1203	0.31	0/1625

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.08	0/851	0.25	0/1149
34	h	0.09	0/894	0.22	0/1216
35	i	0.15	0/855	0.30	0/1147
36	j	0.12	0/759	0.27	0/1019
37	o	0.11	0/655	0.25	0/880
38	q	0.10	0/1161	0.26	0/1571
39	r	0.12	0/1309	0.31	0/1767
40	s	0.13	0/3118	0.30	0/4232
41	u	0.09	0/1053	0.24	0/1425
42	v	0.08	0/596	0.23	0/795
43	5	0.11	0/3317	0.27	0/4519
44	8	0.08	0/572	0.21	0/763
45	9	0.12	0/1009	0.27	0/1358
46	a	0.12	0/884	0.27	0/1197
47	m	0.08	0/380	0.21	0/510
48	z	0.11	0/2500	0.29	0/3380
49	l	0.10	0/572	0.28	0/768
50	y	0.08	0/1980	0.21	0/2667
51	w	0.10	0/646	0.26	0/869
52	c	0.11	0/2313	0.25	0/3128
53	g	0.12	0/1126	0.27	0/1533
54	k	0.09	0/674	0.25	0/910
55	0	0.13	0/896	0.28	0/1200
56	d	0.11	0/2017	0.29	0/2735
57	e	0.08	0/1608	0.24	0/2165
58	p	0.08	0/1195	0.23	0/1603
59	t	0.10	0/2504	0.27	0/3369
All	All	0.13	0/113943	0.27	0/161131

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 ⓘ

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	30362	15333	15360	222	0
2	B	1326	667	670	12	0
3	D	1768	1830	1830	19	0
4	E	2459	2441	2441	26	0
5	F	2005	2025	2024	31	0
6	H	779	814	814	8	0
7	I	1307	1393	1393	11	0
8	J	747	796	796	29	0
9	K	1449	1444	1444	9	0
10	L	893	944	944	14	0
11	M	2315	2377	2377	15	0
12	N	1516	1521	1521	7	0
13	O	1259	1282	1282	11	0
14	P	1154	1148	1148	19	0
15	Q	1790	1822	1822	9	0
16	R	1161	1224	1224	9	0
17	S	1259	1323	1323	14	0
18	T	1369	1402	1402	8	0
19	U	1052	1057	1057	8	0
20	V	1652	1643	1643	20	0
21	W	794	808	808	8	0
22	X	2021	2051	2051	12	0
23	Y	1523	1553	1553	10	0
24	Z	978	1026	1026	7	0
25	x	2564	2546	2546	33	0
26	1	428	472	472	3	0
27	2	380	407	407	3	0
28	3	823	872	872	5	0
29	4	322	354	354	5	0
30	6	2689	2559	2559	40	0
31	7	2379	2378	2378	22	0
32	b	1181	1195	1195	19	0
33	f	838	836	836	23	0
34	h	872	867	867	6	0
35	i	831	854	854	4	0
36	j	744	768	768	7	0
37	o	640	623	623	3	0
38	q	1130	1123	1123	10	0
39	r	1275	1331	1329	13	0
40	s	3045	3059	3057	29	0
41	u	1029	1012	1012	6	0
42	v	586	603	603	6	0
43	5	3225	3243	3243	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	8	564	557	557	3	0
45	9	983	990	990	6	0
46	a	860	843	843	8	0
47	m	374	395	395	5	0
48	z	2455	2546	2546	48	0
49	l	559	549	549	12	0
50	y	1943	1995	1995	17	0
51	w	637	640	640	8	0
52	c	2262	2273	2273	16	0
53	g	1090	1094	1094	8	0
54	k	664	667	667	5	0
55	0	881	908	908	9	0
56	d	1961	1940	1940	25	0
57	e	1576	1598	1598	26	0
58	p	1176	1198	1198	8	0
59	t	2464	2551	2551	46	0
60	A	96	0	0	0	0
60	M	1	0	0	0	0
60	O	1	0	0	0	0
60	R	1	0	0	0	0
61	I	4	0	0	0	0
62	0	1	0	0	0	0
62	4	1	0	0	0	0
63	t	32	13	13	2	0
63	z	32	13	13	1	0
All	All	108537	93796	93821	871	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 (871) 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)
15:Q:155:ILE:HG22	15:Q:156:GLU:OE1	1.74	0.88
1:A:1648:C:O2'	1:A:1649:A:O4'	1.92	0.86
1:A:2080:G:O2'	1:A:2082:G:OP2	1.94	0.86
1:A:1494:A:OP1	21:W:101:LYS:NZ	2.10	0.85
20:V:101:THR:OG1	20:V:103:ASP:OD1	1.96	0.83
1:A:1443:G:N2	1:A:1467:A:OP2	2.11	0.83
8:J:85:PRO:O	8:J:124:LYS:NZ	2.09	0.83
1:A:1616:C:O2	1:A:1635:C:N4	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:218:VAL:O	25:x:223:ARG:NH1	2.12	0.82
25:x:309:LEU:HD22	25:x:360:LEU:HD21	1.63	0.81
59:t:326:THR:OG1	63:t:501:GNP:N7	2.15	0.80
59:t:296:LEU:N	59:t:300:GLU:OE2	2.15	0.79
17:S:116:ASP:OD1	17:S:117:LEU:N	2.16	0.79
1:A:1630:G:O2'	1:A:1632:A:O4'	2.01	0.78
1:A:1628:A:N1	7:I:109:LYS:NZ	2.32	0.78
7:I:83:ARG:NH1	7:I:130:VAL:O	2.18	0.77
1:A:1458:A:O2'	1:A:1459:A:OP1	2.03	0.77
20:V:177:THR:HG23	45:9:71:TYR:O	1.86	0.76
1:A:2399:A:O2'	59:t:66:ARG:NH1	2.19	0.76
7:I:188:ARG:NH2	54:k:55:VAL:O	2.18	0.76
20:V:177:THR:HG22	45:9:69:LYS:H	1.47	0.76
52:c:167:CYS:SG	52:c:171:ARG:NH1	2.59	0.75
1:A:1205:A:N6	1:A:1208:U:OP2	2.19	0.75
1:A:1613:A:O2'	1:A:1617:A:OP1	2.04	0.75
5:F:279:ARG:NH1	5:F:280:TYR:O	2.20	0.75
30:6:206:TYR:CE2	30:6:208:ALA:HB2	2.22	0.75
1:A:1160:A:O2'	1:A:1161:C:OP2	2.05	0.74
29:4:73:LYS:NZ	29:4:78:CYS:O	2.21	0.73
23:Y:193:ASN:O	23:Y:197:ASN:ND2	2.21	0.73
1:A:1628:A:OP2	49:l:112:ARG:NH2	2.22	0.73
56:d:91:TYR:OH	56:d:120:ARG:NH1	2.22	0.72
1:A:1629:A:OP1	49:l:119:ARG:NH2	2.22	0.72
1:A:2295:C:OP2	28:3:142:LYS:NZ	2.21	0.72
41:u:88:ILE:HD11	41:u:105:VAL:HG11	1.71	0.71
1:A:2431:A:N3	1:A:2531:A:N6	2.39	0.71
5:F:249:ASN:ND2	35:i:55:GLY:O	2.24	0.70
1:A:1636:G:N1	1:A:1640:A:OP2	2.24	0.70
34:h:89:ASP:O	34:h:123:ARG:NH1	2.25	0.70
1:A:1784:C:OP1	56:d:65:LYS:NZ	2.21	0.70
2:B:35:A:OP1	33:f:107:GLN:NE2	2.25	0.69
19:U:136:ARG:NH2	31:7:63:GLU:OE2	2.26	0.69
30:6:217:LEU:HD13	30:6:236:LEU:HD13	1.75	0.69
1:A:1444:C:OP2	11:M:58:ARG:NH1	2.25	0.69
1:A:1704:U:OP2	11:M:35:ARG:NH2	2.25	0.69
8:J:91:LEU:HD12	8:J:151:LEU:HD11	1.75	0.69
59:t:152:GLY:O	59:t:231:LEU:N	2.25	0.68
1:A:1237:A:O2'	1:A:1238:U:OP1	2.12	0.68
1:A:1846:U:O2'	43:5:270:VAL:O	2.09	0.68
1:A:2627:U:O2'	1:A:2629:A:N6	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:54:ASN:OD1	8:J:55:GLU:N	2.27	0.67
1:A:1707:A:OP1	52:c:36:ARG:NH2	2.27	0.67
11:M:286:ASP:OD1	11:M:287:GLU:N	2.28	0.67
31:7:259:ASP:OD1	31:7:260:VAL:N	2.27	0.67
1:A:2176:A:N6	1:A:2525:C:OP1	2.28	0.67
2:B:27:A:OP1	33:f:115:ARG:NH2	2.27	0.67
3:D:86:ASP:OD1	3:D:88:THR:OG1	2.11	0.67
31:7:228:GLN:OE1	31:7:228:GLN:N	2.29	0.67
48:z:76:PRO:HB2	48:z:128:LEU:HD21	1.76	0.66
1:A:1161:C:OP1	6:H:66:ARG:NE	2.27	0.66
10:L:39:ARG:NH2	15:Q:158:GLN:OE1	2.27	0.66
34:h:136:GLN:N	34:h:136:GLN:OE1	2.29	0.66
26:1:17:LEU:HB2	26:1:65:LEU:HD23	1.77	0.66
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.28	0.66
19:U:37:GLU:OE2	40:s:259:LYS:NZ	2.24	0.66
1:A:1102:U:O2'	1:A:1103:A:OP2	2.12	0.65
10:L:49:THR:O	10:L:78:ARG:NH2	2.28	0.65
18:T:127:ASN:ND2	56:d:235:ASP:OD2	2.28	0.65
22:X:35:GLU:N	22:X:35:GLU:OE1	2.28	0.65
30:6:208:ALA:HB3	30:6:243:ASN:N	2.11	0.65
56:d:244:GLN:OE1	56:d:249:LYS:NZ	2.25	0.65
1:A:2524:G:N2	1:A:2527:A:OP2	2.28	0.65
30:6:51:TYR:O	30:6:56:ARG:NH2	2.29	0.65
36:j:87:ILE:HD11	37:o:54:MET:HG2	1.79	0.65
20:V:54:TRP:CZ2	20:V:79:VAL:HG11	2.32	0.65
1:A:1564:U:O2'	1:A:1577:A:N3	2.29	0.64
25:x:364:ASN:O	25:x:368:ASN:N	2.29	0.64
32:b:137:ARG:NH1	46:a:41:ASP:OD2	2.31	0.64
20:V:177:THR:HG21	23:Y:87:TRP:HZ2	1.63	0.64
39:r:93:ILE:HD11	39:r:119:VAL:HG21	1.80	0.64
48:z:206:LEU:HD21	48:z:224:THR:HG22	1.79	0.63
50:y:284:GLN:OE1	50:y:284:GLN:N	2.31	0.63
19:U:140:ILE:CD1	56:d:241:MET:HE3	2.29	0.63
6:H:62:ALA:O	6:H:66:ARG:NH1	2.30	0.63
1:A:1493:A:O2'	21:W:57:GLU:OE1	2.10	0.63
14:P:88:HIS:O	14:P:119:THR:OG1	2.16	0.63
2:B:64:A:O3'	57:e:265:LYS:NZ	2.32	0.63
21:W:112:GLU:OE1	21:W:112:GLU:N	2.29	0.63
48:z:222:CYS:SG	48:z:224:THR:OG1	2.56	0.63
55:0:111:GLU:N	55:0:111:GLU:OE1	2.32	0.63
59:t:245:THR:HG22	59:t:245:THR:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1935:U:O2'	1:A:1936:U:O5'	2.16	0.62
16:R:149:HIS:O	24:Z:151:LEU:N	2.32	0.62
59:t:39:GLY:N	59:t:125:GLY:O	2.32	0.62
30:6:46:GLU:N	30:6:46:GLU:OE1	2.33	0.62
1:A:1163:A:OP1	35:i:93:ARG:NH1	2.33	0.62
14:P:42:GLU:OE2	30:6:338:ARG:NH1	2.33	0.62
49:l:74:ILE:HG22	49:l:74:ILE:O	2.00	0.62
4:E:91:GLU:OE1	4:E:184:ASN:ND2	2.31	0.61
3:D:125:GLU:HB3	3:D:143:VAL:HG22	1.81	0.61
30:6:160:ASP:OD2	30:6:267:ARG:NH2	2.31	0.61
32:b:89:VAL:HG12	32:b:89:VAL:O	2.00	0.61
20:V:161:ARG:NH2	20:V:163:ASP:OD2	2.33	0.61
1:A:1894:A:O2'	4:E:215:PHE:O	2.18	0.61
49:l:68:HIS:NE2	49:l:80:ASP:OD2	2.33	0.61
43:5:119:GLN:NE2	43:5:261:PRO:O	2.34	0.61
48:z:115:ASP:HA	48:z:118:ILE:HD12	1.81	0.61
1:A:1237:A:HO2'	1:A:1238:U:P	2.24	0.61
4:E:121:LEU:HD22	4:E:284:TYR:CE1	2.35	0.61
20:V:177:THR:HG21	23:Y:87:TRP:CZ2	2.36	0.60
5:F:191:ASP:OD1	5:F:192:SER:N	2.34	0.60
19:U:140:ILE:HD11	56:d:241:MET:HE3	1.83	0.60
1:A:1488:A:OP1	24:Z:38:LYS:NZ	2.32	0.60
1:A:1603:G:N2	1:A:1624:A:O4'	2.34	0.60
42:v:43:GLN:O	42:v:51:ARG:NH2	2.33	0.60
39:r:71:PRO:HD2	39:r:107:LEU:HD23	1.83	0.60
57:e:155:LEU:HD23	57:e:252:TRP:HB3	1.83	0.60
57:e:194:SER:O	57:e:246:LYS:NZ	2.32	0.60
14:P:121:ASN:OD1	14:P:122:VAL:N	2.35	0.60
31:7:293:ARG:NH1	31:7:321:VAL:O	2.34	0.60
50:y:185:GLU:OE2	50:y:224:GLN:NE2	2.35	0.60
21:W:62:HIS:ND1	21:W:94:GLU:OE1	2.34	0.59
48:z:43:SER:O	48:z:46:LYS:NZ	2.32	0.59
17:S:131:ARG:NE	17:S:161:GLU:OE1	2.34	0.59
59:t:284:ASP:OD1	59:t:285:ALA:N	2.35	0.59
1:A:2625:A:O3'	39:r:94:ARG:NH1	2.36	0.59
48:z:194:ARG:HB2	48:z:195:PRO:HD3	1.84	0.59
15:Q:251:GLU:OE1	15:Q:251:GLU:N	2.35	0.59
1:A:1850:A:H61	40:s:155:ARG:NH2	2.00	0.59
30:6:216:LEU:O	30:6:236:LEU:HD12	2.03	0.59
33:f:161:LEU:HD11	33:f:166:ALA:HA	1.85	0.59
59:t:181:THR:O	59:t:182:THR:OG1	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1621:A:N6	1:A:1632:A:OP1	2.33	0.58
1:A:2267:A:OP2	1:A:2268:A:O2'	2.20	0.58
46:a:34:THR:HG22	46:a:34:THR:O	2.03	0.58
19:U:22:THR:HG22	19:U:24:PHE:H	1.68	0.58
43:5:409:GLU:OE1	43:5:412:ARG:NH2	2.37	0.58
50:y:162:ARG:NH2	50:y:189:MET:O	2.37	0.58
1:A:1308:C:OP2	53:g:111:ARG:NH2	2.36	0.58
1:A:2341:A:O2'	26:1:60:LYS:NZ	2.36	0.58
9:K:73:GLU:OE2	39:r:149:ARG:NH2	2.34	0.58
1:A:1851:C:O2	40:s:162:ARG:NH2	2.36	0.58
1:A:2634:U:OP2	29:4:83:ARG:NE	2.37	0.58
59:t:99:THR:HG22	59:t:105:VAL:HG22	1.85	0.58
1:A:1228:G:N7	20:V:41:ARG:NH2	2.51	0.58
17:S:136:LYS:NZ	36:j:42:LEU:O	2.35	0.58
30:6:170:TRP:NE1	36:j:112:THR:O	2.35	0.58
1:A:1467:A:H4'	1:A:1467:A:OP1	2.02	0.58
58:p:173:ASP:OD1	58:p:174:ALA:N	2.37	0.58
1:A:1595:U:H4'	1:A:1596:A:OP1	2.04	0.57
59:t:98:VAL:N	59:t:107:GLY:O	2.30	0.57
1:A:1984:C:O2	50:y:250:ARG:NH1	2.33	0.57
1:A:2182:U:O4	22:X:104:VAL:N	2.37	0.57
1:A:1101:C:O2'	1:A:1102:U:OP2	2.21	0.57
22:X:36:ARG:NH1	22:X:151:GLU:OE1	2.37	0.57
34:h:83:LEU:O	34:h:83:LEU:HD23	2.04	0.57
17:S:168:THR:HG22	32:b:107:GLN:HG2	1.86	0.57
31:7:214:GLU:OE1	31:7:253:ARG:NE	2.37	0.57
8:J:87:VAL:HG13	8:J:151:LEU:CD2	2.34	0.57
12:N:228:LYS:NZ	24:Z:77:ARG:O	2.32	0.57
14:P:126:GLU:OE1	14:P:160:ARG:NH2	2.37	0.57
59:t:246:PRO:O	59:t:248:ARG:NH2	2.36	0.57
17:S:112:VAL:CG2	17:S:199:ILE:HG13	2.35	0.57
25:x:367:VAL:HG12	25:x:369:PHE:H	1.69	0.57
1:A:1688:U:O2'	17:S:122:ASN:ND2	2.38	0.57
31:7:95:TRP:CG	55:0:108:ILE:HD11	2.40	0.57
56:d:253:GLU:N	56:d:253:GLU:OE1	2.34	0.57
1:A:1594:U:O2'	1:A:1595:U:OP2	2.19	0.57
1:A:2570:A:O2'	59:t:197:GLN:OE1	2.23	0.57
12:N:147:ILE:HG23	12:N:150:TYR:HE1	1.70	0.57
25:x:221:ASP:OD1	25:x:222:ILE:N	2.37	0.57
10:L:84:ALA:HB1	10:L:105:VAL:CG1	2.35	0.57
36:j:112:THR:O	36:j:112:THR:HG22	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:234:ASP:OD1	25:x:236:ARG:N	2.38	0.56
33:f:171:GLU:HG2	57:e:275:LEU:HD11	1.86	0.56
40:s:308:GLN:OE1	40:s:310:GLN:NE2	2.38	0.56
1:A:1607:G:O2'	8:J:152:GLY:N	2.38	0.56
1:A:1615:G:N2	1:A:1633:A:OP2	2.33	0.56
11:M:190:ILE:O	11:M:194:LEU:HD23	2.05	0.56
19:U:59:GLN:NE2	45:9:58:PHE:O	2.38	0.56
59:t:132:LEU:HB2	59:t:133:PRO:HD3	1.87	0.56
59:t:132:LEU:HB2	59:t:133:PRO:CD	2.35	0.56
40:s:370:THR:HG22	40:s:383:ARG:HB2	1.88	0.56
14:P:167:GLU:O	58:p:188:ARG:NH1	2.38	0.56
48:z:118:ILE:HD13	48:z:161:SER:HB3	1.87	0.56
1:A:1610:U:O2'	1:A:1613:A:N6	2.38	0.55
56:d:135:ARG:O	56:d:139:ALA:N	2.39	0.55
13:O:43:GLU:OE2	55:0:130:ARG:NE	2.39	0.55
49:l:128:ARG:O	49:l:132:ASN:ND2	2.39	0.55
51:w:111:ASP:OD1	51:w:112:SER:N	2.38	0.55
2:B:14:A:N1	2:B:21:A:O2'	2.40	0.55
8:J:68:THR:HG23	8:J:68:THR:O	2.06	0.55
20:V:50:SER:OG	20:V:52:GLU:OE1	2.25	0.55
27:2:78:VAL:HG22	27:2:81:ARG:HH21	1.71	0.55
1:A:2395:U:O4	1:A:2396:A:N6	2.40	0.55
1:A:1295:A:N1	1:A:1447:G:O2'	2.31	0.55
36:j:87:ILE:HG22	36:j:91:LYS:HE3	1.87	0.55
40:s:354:VAL:HG12	40:s:363:PHE:CD2	2.41	0.55
1:A:1594:U:O2	1:A:1653:A:O2'	2.14	0.55
1:A:2617:A:O2'	1:A:2618:A:OP2	2.20	0.55
4:E:101:ALA:HB3	4:E:299:ILE:HD11	1.89	0.55
1:A:1517:U:H5'	28:3:188:VAL:HG22	1.88	0.55
4:E:347:PHE:O	15:Q:128:GLY:N	2.40	0.55
5:F:226:MET:SD	5:F:242:LEU:HD21	2.47	0.55
14:P:130:ARG:NH2	30:6:130:ILE:O	2.38	0.55
8:J:62:GLU:N	8:J:62:GLU:OE1	2.40	0.54
29:4:67:THR:HG23	29:4:67:THR:O	2.06	0.54
1:A:1608:C:O2'	1:A:1609:C:O5'	2.24	0.54
4:E:346:THR:HG23	4:E:346:THR:O	2.08	0.54
52:c:209:GLU:OE1	52:c:209:GLU:N	2.36	0.54
59:t:203:LEU:HB2	59:t:204:PRO:HD2	1.90	0.54
12:N:147:ILE:HG22	12:N:147:ILE:O	2.07	0.54
48:z:181:ILE:HD11	63:z:401:GNP:O1A	2.08	0.54
57:e:262:LEU:HD23	57:e:267:LEU:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:t:221:LEU:HD12	59:t:224:LEU:HD12	1.89	0.54
59:t:288:LYS:O	59:t:292:LEU:N	2.37	0.54
1:A:2507:U:O2'	4:E:236:THR:HG21	2.07	0.54
48:z:62:SER:HB3	48:z:215:THR:HG23	1.88	0.54
59:t:211:HIS:ND1	59:t:212:MET:SD	2.80	0.54
1:A:2505:G:O2'	1:A:2508:C:OP2	2.24	0.54
7:I:150:HIS:O	54:k:31:ARG:NH2	2.41	0.54
25:x:334:GLN:NE2	25:x:335:VAL:O	2.41	0.54
38:q:60:GLN:O	38:q:68:SER:OG	2.26	0.54
40:s:131:LEU:HD12	40:s:131:LEU:O	2.07	0.54
41:u:204:THR:C	41:u:205:LEU:HD22	2.33	0.54
32:b:12:THR:HG22	32:b:13:SER:N	2.23	0.54
51:w:94:ASP:O	51:w:96:GLU:N	2.40	0.54
57:e:264:PRO:O	57:e:268:ALA:N	2.37	0.54
36:j:62:GLN:OE1	36:j:65:ARG:NH1	2.41	0.53
5:F:175:LYS:O	5:F:179:THR:HG23	2.09	0.53
6:H:64:GLU:OE1	22:X:61:ARG:NH2	2.42	0.53
8:J:57:THR:HA	8:J:60:ILE:HG22	1.89	0.53
30:6:104:LEU:O	30:6:108:HIS:ND1	2.41	0.53
30:6:270:PHE:N	30:6:317:ALA:O	2.39	0.53
57:e:158:LEU:HD21	57:e:262:LEU:HD11	1.90	0.53
1:A:1724:U:O2	16:R:12:ASN:ND2	2.41	0.53
13:O:80:LEU:HD12	13:O:86:ILE:HD13	1.90	0.53
1:A:2057:G:O2'	1:A:2058:G:P	2.67	0.53
30:6:304:TYR:O	30:6:308:GLN:N	2.40	0.53
33:f:91:ASN:OD1	33:f:157:GLN:NE2	2.41	0.53
58:p:164:GLN:NE2	58:p:165:VAL:O	2.41	0.53
1:A:2275:A:O2'	1:A:2276:U:O5'	2.23	0.53
46:a:96:VAL:O	46:a:96:VAL:HG13	2.08	0.53
1:A:2292:A:H3'	1:A:2293:A:C5'	2.39	0.53
47:m:70:PRO:O	47:m:72:ARG:NH1	2.40	0.53
4:E:63:GLN:NE2	4:E:67:ASP:OD1	2.42	0.53
3:D:194:ILE:HD11	3:D:227:ILE:HD12	1.90	0.53
52:c:295:GLU:O	52:c:299:VAL:HG23	2.09	0.53
56:d:275:VAL:HG13	56:d:275:VAL:O	2.09	0.53
3:D:248:VAL:O	3:D:249:SER:OG	2.26	0.53
22:X:81:GLY:N	22:X:131:THR:OG1	2.42	0.52
1:A:1649:A:HO2'	7:I:150:HIS:CD2	2.27	0.52
8:J:56:LYS:NZ	8:J:60:ILE:HD13	2.24	0.52
17:S:198:ARG:NH2	32:b:13:SER:OG	2.42	0.52
4:E:154:ARG:O	31:7:306:GLN:NE2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:117:THR:O	10:L:118:ARG:NH1	2.41	0.52
25:x:293:LEU:O	25:x:296:THR:HG22	2.08	0.52
25:x:309:LEU:HD21	25:x:371:PRO:HB2	1.90	0.52
1:A:1568:A:O2'	1:A:1569:U:P	2.67	0.52
52:c:299:VAL:HG12	52:c:299:VAL:O	2.09	0.52
9:K:26:GLN:NE2	9:K:147:GLN:OE1	2.42	0.52
49:l:124:TRP:O	49:l:128:ARG:N	2.40	0.52
57:e:150:LYS:HB2	57:e:155:LEU:HD11	1.92	0.52
1:A:1492:A:H1'	1:A:1493:A:O4'	2.09	0.52
1:A:2057:G:O2'	1:A:2058:G:OP1	2.27	0.52
1:A:2639:A:OP1	39:r:142:LYS:N	2.36	0.52
1:A:1759:U:P	40:s:56:LYS:HZ3	2.32	0.52
1:A:2325:U:O2'	1:A:2326:A:O2'	2.27	0.52
3:D:203:ARG:O	43:5:30:ALA:N	2.43	0.52
30:6:220:ASN:O	30:6:222:ASP:N	2.43	0.52
4:E:112:LYS:NZ	4:E:337:VAL:O	2.42	0.52
13:O:67:ASP:OD2	40:s:44:TYR:OH	2.27	0.52
30:6:139:TRP:O	30:6:144:GLY:N	2.43	0.52
1:A:1314:G:N7	5:F:170:ARG:NH2	2.57	0.51
11:M:43:ARG:HD3	11:M:44:ARG:HG3	1.92	0.51
14:P:61:VAL:HG12	14:P:61:VAL:O	2.09	0.51
30:6:233:VAL:O	30:6:296:ARG:NH1	2.43	0.51
1:A:1608:C:H1'	1:A:1609:C:OP1	2.10	0.51
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.92	0.51
25:x:136:VAL:HG12	25:x:136:VAL:O	2.10	0.51
48:z:234:THR:HG22	48:z:234:THR:O	2.11	0.51
25:x:200:ASN:OD1	25:x:201:ASP:N	2.43	0.51
26:1:33:LYS:HG2	26:1:65:LEU:HD21	1.91	0.51
1:A:1895:A:N6	1:A:2105:A:O2'	2.44	0.51
31:7:273:PHE:HB2	31:7:301:THR:HG22	1.92	0.51
59:t:144:ASP:OD2	59:t:146:LYS:HE3	2.11	0.51
1:A:2275:A:HO2'	1:A:2276:U:C5'	2.24	0.51
8:J:56:LYS:HZ1	8:J:60:ILE:HD13	1.75	0.51
52:c:44:GLU:OE1	52:c:47:ARG:NH2	2.43	0.51
5:F:114:THR:O	5:F:156:ARG:NH1	2.43	0.51
33:f:171:GLU:CG	57:e:275:LEU:HD11	2.41	0.51
41:u:88:ILE:HD11	41:u:105:VAL:CG1	2.38	0.51
48:z:134:ARG:NH2	48:z:140:THR:OG1	2.43	0.51
1:A:2666:A:OP2	4:E:212:GLY:N	2.40	0.51
23:Y:153:ASP:OD1	23:Y:156:ARG:NH2	2.35	0.51
48:z:190:GLN:OE1	50:y:282:GLN:NE2	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:A:OP2	1:A:1938:C:N4	2.42	0.51
23:Y:193:ASN:OD1	23:Y:195:ARG:N	2.43	0.51
51:w:81:ASP:O	51:w:85:TYR:N	2.36	0.51
56:d:199:GLU:OE2	56:d:224:ARG:NH2	2.42	0.51
56:d:222:THR:HG22	56:d:256:VAL:HG22	1.93	0.51
1:A:1507:A:H3'	1:A:1508:A:H5''	1.93	0.51
1:A:1556:A:N6	1:A:1559:A:O2'	2.44	0.51
1:A:1568:A:O2'	1:A:1569:U:OP2	2.29	0.51
3:D:113:ARG:O	3:D:148:ARG:NH2	2.38	0.51
3:D:248:VAL:O	3:D:248:VAL:HG12	2.10	0.51
4:E:96:ARG:NH1	4:E:315:PRO:O	2.44	0.50
7:I:45:GLN:NE2	37:o:25:ARG:O	2.44	0.50
14:P:41:ASN:ND2	30:6:335:LEU:O	2.44	0.50
56:d:126:ALA:O	56:d:207:ARG:NH1	2.44	0.50
38:q:61:PHE:O	38:q:65:GLY:N	2.42	0.50
48:z:34:MET:HE3	48:z:206:LEU:H	1.75	0.50
52:c:31:VAL:HG13	52:c:31:VAL:O	2.10	0.50
57:e:53:ARG:HB3	57:e:155:LEU:HB2	1.93	0.50
10:L:77:ILE:HG23	10:L:77:ILE:O	2.11	0.50
28:3:183:ARG:NH2	30:6:355:LYS:O	2.41	0.50
1:A:1831:U:H2'	1:A:1832:A:O4'	2.12	0.50
2:B:31:C:O2'	2:B:32:U:OP1	2.23	0.50
5:F:49:ARG:NH1	5:F:81:GLU:O	2.43	0.50
1:A:2102:U:OP2	13:O:17:ARG:NE	2.41	0.50
5:F:62:VAL:HG21	5:F:88:ALA:HB2	1.93	0.50
50:y:289:SER:OG	50:y:292:ASN:ND2	2.45	0.50
50:y:302:LEU:O	50:y:307:CYS:N	2.44	0.50
57:e:154:ASN:C	57:e:155:LEU:HD12	2.37	0.50
1:A:1759:U:OP1	40:s:56:LYS:NZ	2.40	0.50
2:B:47:G:H3'	2:B:48:G:H5''	1.93	0.50
2:B:48:G:H1	2:B:58:C:H42	1.59	0.50
1:A:1222:A:OP1	5:F:142:ARG:NH2	2.37	0.50
20:V:54:TRP:CH2	20:V:79:VAL:HG11	2.46	0.50
50:y:185:GLU:OE1	50:y:185:GLU:N	2.42	0.50
1:A:2615:U:O2'	9:K:97:ARG:NH2	2.44	0.50
33:f:177:LEU:HD13	33:f:183:LEU:HG	1.93	0.49
40:s:90:LYS:NZ	40:s:272:TYR:O	2.42	0.49
1:A:1364:U:H2'	1:A:1365:A:O4'	2.12	0.49
6:H:118:ASN:O	6:H:122:SER:OG	2.26	0.49
31:7:67:VAL:O	31:7:67:VAL:HG22	2.12	0.49
31:7:147:LEU:HD23	31:7:151:ILE:HD12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:293:ARG:NH2	31:7:323:GLU:OE2	2.45	0.49
31:7:105:VAL:HG13	31:7:120:CYS:SG	2.52	0.49
32:b:21:ARG:NE	52:c:217:ASP:OD2	2.45	0.49
32:b:89:VAL:O	32:b:89:VAL:CG1	2.59	0.49
38:q:111:GLU:OE1	38:q:114:ARG:NH2	2.39	0.49
53:g:68:THR:HG22	53:g:69:PRO:HD2	1.94	0.49
1:A:1725:G:C8	16:R:11:ARG:HB2	2.47	0.49
1:A:2275:A:O2'	1:A:2276:U:P	2.69	0.49
33:f:118:ILE:HD11	33:f:165:PHE:CZ	2.48	0.49
59:t:221:LEU:CD1	59:t:224:LEU:HD12	2.42	0.49
14:P:58:LEU:O	58:p:178:ARG:NH2	2.43	0.49
1:A:1567:A:H2'	1:A:1568:A:H5'	1.95	0.49
33:f:176:ASN:OD1	47:m:36:ARG:NH1	2.44	0.49
39:r:93:ILE:HG22	39:r:94:ARG:O	2.12	0.49
1:A:2153:G:O6	1:A:2543:A:H2	1.96	0.49
1:A:2158:G:H2'	1:A:2159:A:H5'	1.94	0.49
30:6:247:GLU:OE1	30:6:247:GLU:N	2.46	0.49
33:f:118:ILE:HD11	33:f:165:PHE:CE2	2.48	0.49
3:D:107:ILE:HD11	3:D:140:ILE:HG21	1.94	0.49
11:M:275:ASN:ND2	11:M:278:ASP:OD2	2.45	0.49
31:7:183:ASP:OD1	31:7:184:LYS:N	2.44	0.49
32:b:131:HIS:CE1	32:b:134:THR:HG23	2.48	0.49
40:s:245:VAL:HG22	40:s:246:PRO:HD2	1.94	0.49
48:z:261:CYS:SG	48:z:262:ASP:N	2.86	0.49
59:t:285:ALA:O	59:t:289:LEU:N	2.39	0.49
1:A:1720:U:O2'	11:M:26:LEU:O	2.31	0.49
39:r:121:MET:HE3	39:r:151:LEU:HA	1.95	0.49
4:E:325:GLU:OE1	4:E:325:GLU:N	2.37	0.48
21:W:54:LYS:NZ	21:W:69:THR:OG1	2.46	0.48
48:z:93:GLN:OE1	48:z:97:GLN:NE2	2.46	0.48
5:F:126:LYS:NZ	5:F:138:HIS:O	2.46	0.48
30:6:236:LEU:O	30:6:251:THR:OG1	2.29	0.48
5:F:284:TYR:HB2	5:F:285:PRO:HD2	1.95	0.48
33:f:170:LEU:HD12	33:f:171:GLU:N	2.29	0.48
1:A:1710:U:O2'	5:F:104:ARG:NH2	2.41	0.48
20:V:54:TRP:CH2	20:V:56:LEU:O	2.65	0.48
8:J:69:LYS:NZ	8:J:127:ASP:OD2	2.44	0.48
16:R:78:GLU:OE1	32:b:135:ASN:ND2	2.45	0.48
25:x:240:GLU:N	25:x:240:GLU:OE1	2.46	0.48
44:8:172:GLU:OE1	44:8:172:GLU:N	2.47	0.48
48:z:16:ARG:NH2	48:z:262:ASP:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:g:121:GLN:OE1	53:g:138:THR:OG1	2.29	0.48
1:A:1603:G:O2'	8:J:87:VAL:HG12	2.13	0.48
8:J:144:ILE:O	8:J:148:ALA:N	2.44	0.48
15:Q:246:ASP:OD1	15:Q:247:LEU:N	2.47	0.48
30:6:219:ILE:HG22	30:6:221:LEU:H	1.78	0.48
39:r:50:GLU:OE1	54:k:77:ARG:NH2	2.46	0.48
39:r:72:ILE:HG12	39:r:107:LEU:HD22	1.95	0.48
53:g:113:VAL:HG11	53:g:117:ILE:HD12	1.96	0.48
59:t:146:LYS:HB2	59:t:226:ARG:HG3	1.94	0.48
5:F:79:LEU:HD11	34:h:118:LEU:HD23	1.94	0.48
8:J:53:PHE:O	8:J:57:THR:N	2.44	0.48
48:z:98:ARG:NH1	48:z:325:ALA:O	2.43	0.48
1:A:1565:U:H5'	24:Z:74:SER:HB2	1.95	0.48
49:l:121:GLN:O	49:l:125:ARG:N	2.36	0.48
1:A:1346:G:H4'	1:A:1347:C:OP2	2.14	0.48
1:A:1908:A:OP1	10:L:56:ARG:NH2	2.47	0.48
1:A:1983:G:N1	1:A:2069:A:O4'	2.46	0.48
14:P:102:VAL:HG11	14:P:141:ILE:HD11	1.95	0.48
17:S:110:TRP:CE3	17:S:118:ILE:HD12	2.48	0.48
1:A:2469:U:HO2'	1:A:2617:A:H8	1.60	0.48
5:F:102:TRP:O	5:F:106:PHE:HD1	1.96	0.48
48:z:29:TRP:HE3	48:z:229:LEU:HD21	1.79	0.48
1:A:1420:A:C6	3:D:275:LEU:HD12	2.48	0.47
14:P:161:LEU:C	14:P:161:LEU:HD23	2.39	0.47
22:X:7:PRO:HD2	22:X:10:LEU:HD12	1.96	0.47
52:c:86:ASP:N	52:c:86:ASP:OD1	2.45	0.47
14:P:74:ASN:O	14:P:147:GLN:NE2	2.41	0.47
23:Y:117:LEU:HD21	23:Y:129:PRO:HD2	1.96	0.47
40:s:153:ARG:HG2	43:5:206:ASN:O	2.13	0.47
43:5:173:ARG:HA	43:5:176:TYR:CE1	2.49	0.47
1:A:1596:A:H3'	1:A:1597:A:C8	2.48	0.47
15:Q:153:ASN:OD1	15:Q:154:THR:N	2.46	0.47
45:9:16:ASP:OD2	45:9:19:SER:OG	2.19	0.47
56:d:231:LEU:HD21	56:d:233:ILE:HG13	1.96	0.47
1:A:2373:G:OP1	5:F:137:ARG:NH1	2.36	0.47
43:5:355:LEU:HD11	43:5:374:VAL:CG2	2.45	0.47
1:A:1680:C:OP1	16:R:99:ARG:NH2	2.44	0.47
40:s:391:GLN:O	40:s:393:GLN:NE2	2.47	0.47
59:t:281:ASP:OD1	59:t:281:ASP:N	2.48	0.47
1:A:1412:A:OP1	3:D:90:ARG:NH2	2.44	0.47
15:Q:265:ILE:HG12	15:Q:271:ARG:NH1	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:A:O2'	1:A:1138:U:OP1	2.30	0.47
1:A:1208:U:O4'	20:V:40:ARG:NH2	2.47	0.47
1:A:1383:G:O2'	1:A:1386:G:O2'	2.25	0.47
1:A:1560:A:N6	1:A:1561:A:H62	2.12	0.47
1:A:1630:G:C4	1:A:1632:A:H1'	2.50	0.47
1:A:1760:U:O2'	13:O:82:GLU:OE2	2.32	0.47
1:A:2589:C:C2'	1:A:2590:C:H5'	2.45	0.47
5:F:95:ILE:HD13	5:F:172:LEU:HD23	1.97	0.47
16:R:119:LEU:HD11	46:a:57:ILE:HD13	1.95	0.47
24:Z:136:SER:OG	24:Z:147:VAL:O	2.31	0.47
48:z:55:HIS:HB3	48:z:81:LEU:HD23	1.95	0.47
48:z:86:LEU:HD23	48:z:86:LEU:H	1.80	0.47
59:t:146:LYS:O	59:t:226:ARG:NH1	2.47	0.47
1:A:1180:A:O2'	6:H:61:LEU:O	2.29	0.47
1:A:2451:C:O2'	1:A:2556:U:OP1	2.28	0.47
43:5:309:LEU:HD23	43:5:353:GLN:OE1	2.15	0.47
1:A:1121:A:N3	1:A:1127:U:O2'	2.44	0.47
1:A:1925:C:O3'	48:z:306:ARG:NH2	2.47	0.47
5:F:143:SER:HG	5:F:146:TRP:CD1	2.33	0.47
8:J:60:ILE:HD12	49:l:75:TYR:CE1	2.50	0.47
22:X:51:LYS:HD3	22:X:62:VAL:HG11	1.97	0.47
30:6:209:ASP:OD1	30:6:210:LYS:N	2.48	0.47
59:t:126:LYS:HB2	59:t:129:THR:HG22	1.96	0.47
1:A:1608:C:O2'	1:A:1609:C:P	2.73	0.47
12:N:147:ILE:HG23	12:N:150:TYR:CE1	2.50	0.47
1:A:1194:A:H3'	23:Y:230:LYS:NZ	2.30	0.46
25:x:64:ARG:NH1	50:y:270:ARG:O	2.41	0.46
42:v:69:LEU:O	42:v:70:ILE:C	2.59	0.46
48:z:26:VAL:HG22	48:z:27:ALA:N	2.30	0.46
50:y:96:ILE:O	50:y:100:GLN:N	2.45	0.46
1:A:1907:G:OP1	10:L:37:ARG:N	2.46	0.46
1:A:2347:U:H2'	1:A:2348:U:O4'	2.15	0.46
8:J:70:ILE:HD11	8:J:78:PHE:CE2	2.50	0.46
12:N:97:LEU:HD12	12:N:154:VAL:HG21	1.97	0.46
43:5:223:ARG:NH2	43:5:272:GLU:O	2.48	0.46
59:t:172:THR:N	59:t:173:PRO:HD3	2.30	0.46
1:A:2175:U:O2'	1:A:2176:A:H2'	2.14	0.46
1:A:2480:U:O2'	48:z:29:TRP:O	2.33	0.46
4:E:126:ASP:OD2	4:E:151:THR:OG1	2.22	0.46
4:E:269:TYR:HB3	4:E:304:LEU:HD11	1.97	0.46
30:6:121:ARG:NH1	44:8:112:GLU:OE2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:G:O6	20:V:41:ARG:NH1	2.47	0.46
18:T:168:TYR:CE2	18:T:170:VAL:HG13	2.51	0.46
19:U:29:VAL:HG11	19:U:43:ARG:HG3	1.98	0.46
1:A:1134:A:OP2	23:Y:194:LYS:NZ	2.34	0.46
14:P:151:TRP:NE1	30:6:55:GLU:OE2	2.47	0.46
25:x:167:GLY:O	25:x:248:ARG:NH1	2.49	0.46
1:A:1389:A:OP2	18:T:154:GLY:O	2.33	0.46
1:A:1625:A:OP1	8:J:142:ARG:NH1	2.48	0.46
25:x:153:TYR:HD2	25:x:155:MET:HE2	1.81	0.46
32:b:6:THR:HG22	32:b:7:SER:N	2.31	0.46
33:f:161:LEU:HD12	33:f:165:PHE:HD2	1.79	0.46
43:5:212:THR:HG22	43:5:221:GLN:HG2	1.96	0.46
1:A:2325:U:O3'	1:A:2326:A:H4'	2.16	0.46
8:J:137:LEU:O	8:J:140:VAL:HG22	2.16	0.46
11:M:155:VAL:O	11:M:175:THR:HA	2.15	0.46
48:z:191:VAL:HG21	48:z:199:LEU:HG	1.98	0.46
59:t:118:VAL:CG1	59:t:141:VAL:HG21	2.46	0.46
11:M:37:ARG:HB3	11:M:44:ARG:HD3	1.98	0.46
40:s:146:GLN:O	40:s:151:VAL:HG23	2.16	0.46
1:A:1468:A:N1	1:A:2373:G:O2'	2.44	0.46
55:0:153:VAL:HG21	55:0:170:GLY:O	2.16	0.46
7:I:95:MET:SD	7:I:95:MET:N	2.83	0.46
11:M:145:ASP:OD1	11:M:145:ASP:N	2.48	0.46
27:2:78:VAL:HG22	27:2:81:ARG:NH2	2.30	0.46
51:w:123:GLU:O	51:w:128:PHE:N	2.39	0.46
59:t:232:PHE:O	59:t:276:ALA:N	2.47	0.46
1:A:1829:A:H2'	1:A:1830:C:H5'	1.98	0.45
1:A:1936:U:H5	1:A:1941:A:N7	2.14	0.45
25:x:96:LYS:NZ	25:x:132:SER:OG	2.49	0.45
31:7:164:VAL:HG13	31:7:165:ARG:N	2.31	0.45
59:t:246:PRO:HB2	59:t:248:ARG:HG2	1.98	0.45
1:A:1220:G:N7	27:2:87:ARG:NH2	2.59	0.45
1:A:1845:C:OP2	40:s:154:ARG:NH1	2.50	0.45
14:P:63:ARG:NH2	21:W:137:LYS:O	2.42	0.45
17:S:166:GLU:HG2	17:S:168:THR:HG23	1.99	0.45
25:x:360:LEU:C	25:x:360:LEU:HD23	2.42	0.45
58:p:129:ASN:OD1	58:p:130:LYS:N	2.47	0.45
1:A:1629:A:H2'	1:A:1629:A:N3	2.31	0.45
1:A:1630:G:N3	1:A:1632:A:O2'	2.44	0.45
48:z:230:VAL:HG12	48:z:230:VAL:O	2.15	0.45
1:A:1264:A:OP1	46:a:134:LYS:NZ	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:95:TRP:CB	55:0:108:ILE:HD11	2.45	0.45
33:f:161:LEU:HD12	33:f:165:PHE:CD2	2.51	0.45
52:c:282:ALA:CB	52:c:300:ALA:HB2	2.46	0.45
53:g:68:THR:CG2	53:g:69:PRO:HD2	2.47	0.45
55:0:117:GLN:HB2	55:0:120:VAL:HG22	1.98	0.45
58:p:134:LEU:HD21	58:p:158:MET:HE1	1.97	0.45
4:E:107:MET:HG2	4:E:121:LEU:HD21	1.96	0.45
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.99	0.45
14:P:61:VAL:HG11	30:6:344:PHE:CE2	2.50	0.45
32:b:45:GLU:HB2	32:b:94:VAL:HG22	1.99	0.45
1:A:2156:G:O3'	55:0:81:LYS:NZ	2.50	0.45
3:D:248:VAL:O	3:D:249:SER:CB	2.65	0.45
30:6:198:ALA:O	30:6:254:TYR:OH	2.28	0.45
42:v:23:LEU:HD13	42:v:26:THR:HG23	1.98	0.45
1:A:1137:A:O2'	1:A:1138:U:P	2.75	0.45
25:x:234:ASP:OD1	25:x:235:GLY:N	2.49	0.45
48:z:323:ILE:HB	48:z:324:PRO:HD3	1.99	0.45
1:A:1420:A:N1	3:D:275:LEU:HD12	2.31	0.45
1:A:2122:U:O2'	1:A:2546:U:H5'	2.16	0.45
3:D:111:ARG:NH2	3:D:166:ASN:OD1	2.50	0.45
33:f:124:TYR:CG	33:f:125:ALA:N	2.84	0.45
40:s:66:TRP:O	40:s:69:THR:OG1	2.29	0.45
47:m:56:VAL:N	47:m:74:LEU:O	2.47	0.45
48:z:317:MET:O	48:z:318:LEU:C	2.60	0.45
56:d:188:LYS:CE	56:d:241:MET:HE1	2.46	0.45
31:7:77:VAL:HG23	31:7:77:VAL:O	2.16	0.45
40:s:110:THR:HG23	40:s:327:PHE:CD1	2.52	0.45
59:t:235:ASP:OD1	59:t:237:SER:N	2.50	0.45
1:A:2158:G:C2'	1:A:2159:A:H5'	2.47	0.44
1:A:2302:U:O2'	1:A:2303:A:P	2.75	0.44
41:u:187:LEU:C	41:u:187:LEU:HD23	2.42	0.44
1:A:1567:A:C2'	1:A:1568:A:H5'	2.47	0.44
2:B:7:G:N2	2:B:60:C:N3	2.64	0.44
23:Y:87:TRP:O	23:Y:143:ASN:ND2	2.48	0.44
57:e:174:VAL:HG12	57:e:175:GLU:N	2.32	0.44
14:P:81:LEU:HB2	14:P:144:MET:SD	2.58	0.44
1:A:1281:A:H4'	1:A:1282:U:OP1	2.17	0.44
8:J:33:PRO:N	8:J:34:PRO:HD2	2.33	0.44
8:J:56:LYS:O	8:J:60:ILE:N	2.51	0.44
48:z:152:ASN:ND2	48:z:177:GLY:O	2.50	0.44
48:z:221:LEU:O	48:z:309:ARG:NE	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:226:LEU:HB2	48:z:229:LEU:HD13	1.99	0.44
1:A:1137:A:HO2'	1:A:1138:U:P	2.39	0.44
13:O:86:ILE:HB	13:O:87:PRO:HD3	1.99	0.44
25:x:352:PHE:HE1	25:x:360:LEU:HD22	1.81	0.44
48:z:320:ARG:O	48:z:322:ILE:HD12	2.17	0.44
1:A:1240:A:OP1	52:c:52:ARG:NH2	2.50	0.44
1:A:1615:G:O4'	1:A:1632:A:C8	2.71	0.44
1:A:2481:U:O2'	48:z:32:GLY:N	2.51	0.44
8:J:60:ILE:HD11	8:J:85:PRO:HB3	1.99	0.44
8:J:125:ALA:HB2	8:J:137:LEU:HD22	1.98	0.44
32:b:134:THR:O	32:b:135:ASN:HB2	2.18	0.44
48:z:220:ALA:O	48:z:309:ARG:NH2	2.42	0.44
51:w:90:TYR:O	51:w:93:ILE:HG12	2.18	0.44
1:A:1237:A:O2'	1:A:1238:U:P	2.75	0.44
1:A:1496:A:H1'	1:A:1501:A:H61	1.82	0.44
1:A:1603:G:OP1	8:J:21:ARG:NH1	2.50	0.44
4:E:147:VAL:HG12	4:E:148:GLY:N	2.32	0.44
8:J:70:ILE:HG23	8:J:70:ILE:O	2.18	0.44
10:L:118:ARG:NH2	41:u:194:ASP:OD2	2.44	0.44
25:x:257:THR:HG23	25:x:257:THR:O	2.17	0.44
29:4:81:VAL:HG12	29:4:82:LYS:N	2.33	0.44
31:7:95:TRP:HB3	55:0:108:ILE:HD11	2.00	0.44
34:h:130:PHE:O	34:h:133:VAL:HG22	2.18	0.44
59:t:167:ARG:NH2	59:t:327:VAL:O	2.49	0.44
1:A:1152:U:O2'	22:X:96:LYS:O	2.29	0.44
4:E:177:LYS:HB3	4:E:298:LYS:HD2	2.00	0.44
10:L:36:THR:O	10:L:56:ARG:HA	2.18	0.44
13:O:38:ARG:NH2	13:O:82:GLU:OE1	2.48	0.44
57:e:199:GLU:OE1	57:e:238:THR:OG1	2.36	0.44
1:A:2302:U:HO2'	1:A:2303:A:P	2.41	0.44
3:D:139:ASP:OD1	3:D:249:SER:OG	2.16	0.44
4:E:264:GLN:OE1	4:E:266:ARG:NH2	2.44	0.44
5:F:284:TYR:O	5:F:285:PRO:C	2.61	0.44
9:K:3:SER:O	52:c:302:ARG:NH1	2.51	0.44
13:O:38:ARG:NE	13:O:82:GLU:OE1	2.47	0.44
25:x:257:THR:HA	25:x:307:CYS:SG	2.57	0.44
32:b:6:THR:HG22	32:b:7:SER:H	1.82	0.44
33:f:188:HIS:O	33:f:189:THR:C	2.60	0.44
48:z:41:MET:HG2	48:z:146:MET:HE3	2.00	0.44
48:z:98:ARG:NH1	48:z:322:ILE:O	2.51	0.44
59:t:161:LYS:N	63:t:501:GNP:O1B	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:U:OP1	11:M:132:LYS:HE2	2.17	0.43
1:A:1541:G:H2'	1:A:1542:C:O4'	2.17	0.43
1:A:1906:G:H4'	10:L:36:THR:HG22	2.00	0.43
1:A:1956:G:N7	3:D:231:SER:OG	2.48	0.43
1:A:2657:C:H5'	1:A:2658:U:OP1	2.18	0.43
13:O:84:ASP:OD1	13:O:84:ASP:N	2.50	0.43
33:f:97:TYR:CE2	47:m:65:ILE:HG22	2.53	0.43
48:z:217:LEU:O	48:z:221:LEU:HD23	2.18	0.43
59:t:207:ILE:HG22	59:t:208:GLU:N	2.33	0.43
1:A:1493:A:OP2	30:6:72:ARG:HG2	2.18	0.43
10:L:41:VAL:HG21	10:L:104:ASN:HB3	2.00	0.43
43:5:295:GLU:OE2	43:5:304:PHE:HB2	2.18	0.43
47:m:53:VAL:HG12	47:m:71:ARG:O	2.18	0.43
51:w:141:PRO:HA	51:w:144:ILE:HG22	2.00	0.43
1:A:1944:A:HO2'	1:A:1945:C:P	2.41	0.43
1:A:2617:A:O2'	1:A:2618:A:C8	2.71	0.43
2:B:15:A:O2'	2:B:17:A:N6	2.43	0.43
31:7:235:ASP:OD1	31:7:236:PHE:N	2.51	0.43
59:t:244:VAL:O	59:t:245:THR:OG1	2.26	0.43
1:A:2302:U:C2'	1:A:2303:A:O5'	2.66	0.43
39:r:92:PHE:CE2	39:r:107:LEU:HD11	2.53	0.43
56:d:195:VAL:HG12	56:d:196:GLU:H	1.83	0.43
57:e:48:ALA:N	57:e:230:PHE:O	2.51	0.43
1:A:1637:U:H3'	1:A:1638:U:H5''	2.00	0.43
4:E:230:SER:O	4:E:231:HIS:HB2	2.19	0.43
8:J:32:GLY:O	8:J:36:GLY:N	2.46	0.43
30:6:173:LEU:HD21	30:6:175:VAL:HG23	2.01	0.43
1:A:2188:U:OP1	50:y:192:ARG:NE	2.51	0.43
11:M:226:ALA:HB2	58:p:52:SER:HB3	2.01	0.43
21:W:110:ASN:OD1	21:W:110:ASN:O	2.36	0.43
40:s:370:THR:HG22	40:s:383:ARG:CB	2.47	0.43
56:d:50:GLU:N	56:d:51:PRO:CD	2.81	0.43
1:A:1280:C:O4'	1:A:1560:A:C4	2.71	0.43
1:A:2292:A:H4'	1:A:2293:A:OP2	2.19	0.43
1:A:2334:G:N2	1:A:2358:G:O4'	2.52	0.43
1:A:2676:A:H4'	1:A:2676:A:OP2	2.18	0.43
7:I:49:ALA:O	7:I:52:GLU:OE1	2.36	0.43
39:r:135:LEU:HD12	39:r:135:LEU:O	2.19	0.43
59:t:33:PRO:HA	59:t:127:LEU:HD22	2.00	0.43
59:t:303:LEU:H	59:t:303:LEU:HD23	1.84	0.43
1:A:1187:U:O3'	1:A:1188:A:H4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:C:O2'	1:A:1609:C:H3'	2.18	0.43
7:I:132:LYS:HB2	7:I:133:PRO:HD3	2.01	0.43
25:x:75:ALA:O	25:x:129:PHE:N	2.51	0.43
40:s:276:ILE:HD13	40:s:335:MET:SD	2.59	0.43
43:5:121:LEU:HD22	43:5:126:THR:HG23	2.00	0.43
48:z:50:CYS:SG	48:z:51:VAL:N	2.91	0.43
48:z:59:ILE:CG2	48:z:62:SER:HB2	2.49	0.43
57:e:52:GLN:N	57:e:234:ALA:O	2.51	0.43
59:t:145:LEU:O	59:t:146:LYS:C	2.61	0.43
59:t:151:VAL:HG12	59:t:229:GLN:HB2	2.01	0.43
59:t:314:LYS:O	59:t:315:ALA:HB3	2.19	0.43
1:A:1102:U:H5'	20:V:42:ARG:HD3	2.01	0.43
1:A:1233:A:OP2	20:V:94:HIS:NE2	2.49	0.43
4:E:204:VAL:HG21	4:E:299:ILE:CG2	2.49	0.43
17:S:132:ILE:HG22	17:S:133:ARG:N	2.33	0.43
20:V:82:GLN:OE1	20:V:82:GLN:N	2.46	0.43
32:b:47:VAL:O	32:b:51:VAL:HG12	2.19	0.43
1:A:1187:U:O2	38:q:34:ARG:HD3	2.18	0.42
1:A:1595:U:H1'	1:A:1596:A:H5''	2.01	0.42
1:A:2562:C:OP2	1:A:2563:A:O2'	2.28	0.42
8:J:23:ILE:HG23	8:J:86:THR:HG21	2.01	0.42
10:L:41:VAL:O	10:L:41:VAL:HG12	2.18	0.42
14:P:156:ASP:OD1	14:P:156:ASP:N	2.52	0.42
25:x:161:LEU:HB2	25:x:162:PRO:HD3	2.01	0.42
28:3:148:VAL:CG1	30:6:360:GLU:HA	2.48	0.42
38:q:48:PRO:HB2	38:q:50:TRP:CD1	2.54	0.42
57:e:181:THR:HG23	57:e:184:GLY:H	1.83	0.42
59:t:245:THR:N	59:t:246:PRO:CD	2.82	0.42
1:A:1707:A:H5'	16:R:16:ASP:OD2	2.18	0.42
1:A:1854:C:OP2	40:s:304:ARG:NH1	2.52	0.42
1:A:1983:G:H3'	1:A:1984:C:H5''	2.00	0.42
6:H:51:VAL:HG13	6:H:79:LEU:CD1	2.49	0.42
9:K:90:VAL:HG22	9:K:94:GLN:HB2	2.01	0.42
12:N:204:GLU:OE2	12:N:208:ASN:ND2	2.52	0.42
30:6:208:ALA:O	30:6:209:ASP:HB3	2.18	0.42
31:7:41:ARG:NE	31:7:226:ILE:O	2.52	0.42
40:s:206:ARG:HD2	40:s:373:LEU:HD12	2.00	0.42
42:v:23:LEU:HD13	42:v:26:THR:CG2	2.49	0.42
46:a:53:ASP:OD1	46:a:54:GLY:N	2.52	0.42
1:A:1607:G:C5	1:A:1608:C:C4	3.07	0.42
13:O:94:ALA:HB3	13:O:95:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:y:216:LEU:HD22	50:y:223:LEU:HD21	2.00	0.42
53:g:44:GLU:OE1	53:g:44:GLU:N	2.52	0.42
1:A:1563:C:OP2	24:Z:77:ARG:NH1	2.51	0.42
2:B:59:C:N3	2:B:60:C:N4	2.67	0.42
5:F:67:GLU:HG2	5:F:75:GLU:O	2.20	0.42
21:W:86:ASN:O	21:W:87:LYS:HB2	2.20	0.42
30:6:145:PRO:HB3	30:6:169:PRO:O	2.19	0.42
33:f:198:LYS:HB2	33:f:203:LEU:HD11	2.00	0.42
59:t:225:GLU:O	59:t:271:LYS:NZ	2.53	0.42
59:t:300:GLU:N	59:t:300:GLU:OE1	2.52	0.42
1:A:1160:A:HO2'	1:A:1161:C:P	2.38	0.42
1:A:2174:U:O2'	1:A:2526:A:N3	2.49	0.42
4:E:119:VAL:HG21	4:E:284:TYR:HB3	2.00	0.42
5:F:94:ASP:N	5:F:94:ASP:OD1	2.52	0.42
33:f:124:TYR:O	33:f:155:VAL:HB	2.20	0.42
40:s:143:CYS:SG	40:s:177:THR:HG21	2.60	0.42
43:5:177:CYS:HB3	43:5:178:PRO:HD3	2.01	0.42
48:z:195:PRO:HB2	48:z:197:VAL:HG23	2.01	0.42
57:e:186:ALA:HB1	57:e:202:PHE:CE1	2.54	0.42
25:x:237:LYS:HZ1	33:f:207:LEU:HB3	1.84	0.42
30:6:334:LEU:H	30:6:334:LEU:HD23	1.85	0.42
56:d:120:ARG:HD3	56:d:120:ARG:N	2.34	0.42
57:e:155:LEU:HD23	57:e:252:TRP:CB	2.49	0.42
1:A:1185:C:OP2	38:q:55:ARG:NH2	2.52	0.42
1:A:1821:A:C2	3:D:129:VAL:HG11	2.55	0.42
5:F:246:VAL:O	5:F:246:VAL:HG22	2.19	0.42
18:T:85:ALA:O	18:T:139:SER:OG	2.38	0.42
30:6:271:LEU:HD22	30:6:273:PHE:CZ	2.55	0.42
56:d:259:ARG:NH2	56:d:266:GLY:O	2.52	0.42
1:A:1333:C:H5''	5:F:144:PRO:HD2	2.02	0.42
1:A:1502:A:H2'	1:A:1503:U:H5''	2.01	0.42
1:A:1624:A:O3'	8:J:142:ARG:NH1	2.53	0.42
2:B:8:U:O3'	2:B:45:A:O2'	2.32	0.42
25:x:50:MET:HG3	25:x:51:THR:HG23	2.01	0.42
39:r:135:LEU:HD13	39:r:139:CYS:O	2.20	0.42
40:s:151:VAL:HG13	43:5:207:CYS:SG	2.59	0.42
40:s:421:ASN:OD1	40:s:422:LYS:N	2.53	0.42
49:l:108:GLU:N	49:l:108:GLU:OE1	2.52	0.42
50:y:178:ARG:NH2	50:y:218:ARG:O	2.53	0.42
56:d:195:VAL:HG12	56:d:196:GLU:N	2.35	0.42
3:D:157:ASN:N	3:D:179:GLU:OE2	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:196:ALA:HB3	4:E:319:TYR:CD2	2.55	0.42
4:E:243:ILE:HG21	4:E:251:VAL:HG22	2.01	0.42
6:H:111:VAL:HG12	6:H:112:LYS:N	2.34	0.42
20:V:103:ASP:OD1	20:V:104:HIS:N	2.52	0.42
50:y:301:PHE:O	50:y:305:THR:OG1	2.35	0.42
57:e:53:ARG:HH11	57:e:155:LEU:HD13	1.84	0.42
57:e:237:LEU:O	57:e:238:THR:HG23	2.20	0.42
1:A:1712:U:H2'	1:A:1713:A:O4'	2.20	0.42
1:A:1878:C:H2'	1:A:1879:C:O4'	2.20	0.42
1:A:2086:C:O2'	48:z:302:ARG:NH2	2.53	0.42
25:x:81:ALA:HB2	25:x:147:LEU:HD23	2.01	0.42
28:3:125:ARG:HD3	28:3:147:PHE:CE1	2.55	0.42
32:b:65:VAL:HG12	32:b:67:PRO:HD3	2.01	0.42
45:9:44:SER:O	45:9:45:ASP:HB2	2.20	0.42
50:y:115:ILE:HD11	50:y:146:LYS:HD2	2.02	0.42
1:A:1941:A:H4'	1:A:1942:A:O5'	2.20	0.41
3:D:109:PHE:HB3	3:D:205:ALA:HB3	2.02	0.41
5:F:92:ARG:HE	5:F:95:ILE:CD1	2.32	0.41
7:I:52:GLU:OE1	7:I:52:GLU:N	2.43	0.41
14:P:61:VAL:HG13	30:6:346:ARG:HH22	1.84	0.41
46:a:140:ASP:O	46:a:141:ARG:HG2	2.20	0.41
51:w:114:ASP:O	51:w:117:GLU:HG2	2.20	0.41
59:t:277:ILE:HB	59:t:323:PRO:HA	2.02	0.41
1:A:1257:A:H5'	16:R:31:PHE:CD1	2.55	0.41
1:A:1630:G:O3'	49:l:124:TRP:NE1	2.49	0.41
1:A:1677:C:H4'	1:A:1678:A:O4'	2.20	0.41
1:A:2659:C:H4'	1:A:2660:U:OP1	2.20	0.41
4:E:121:LEU:HD22	4:E:284:TYR:CD1	2.55	0.41
6:H:76:VAL:HG11	22:X:91:TYR:CE2	2.54	0.41
11:M:141:GLU:OE1	11:M:141:GLU:N	2.42	0.41
13:O:141:SER:O	13:O:147:ASN:ND2	2.53	0.41
40:s:155:ARG:CG	40:s:156:PRO:HD2	2.50	0.41
48:z:121:ILE:HG23	48:z:122:VAL:N	2.34	0.41
53:g:42:VAL:HG12	53:g:42:VAL:O	2.20	0.41
56:d:190:VAL:HG22	56:d:191:ARG:N	2.35	0.41
1:A:1116:C:O2	1:A:1116:C:O2'	2.32	0.41
5:F:160:SER:HB3	35:i:80:LEU:HD13	2.02	0.41
22:X:124:THR:O	22:X:124:THR:HG23	2.20	0.41
22:X:176:LEU:O	22:X:177:HIS:C	2.63	0.41
30:6:176:ALA:HB1	30:6:184:LEU:HB3	2.02	0.41
1:A:1115:A:O2'	1:A:1116:C:P	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:G:H3'	1:A:2258:A:O4'	2.20	0.41
1:A:2616:U:O2'	1:A:2617:A:O5'	2.35	0.41
16:R:96:GLU:O	17:S:109:GLN:NE2	2.46	0.41
19:U:146:LEU:HD11	56:d:249:LYS:HB2	2.01	0.41
25:x:237:LYS:HE3	33:f:210:LEU:HD11	2.01	0.41
25:x:348:THR:O	25:x:348:THR:HG22	2.20	0.41
30:6:224:HIS:O	30:6:225:LEU:C	2.64	0.41
34:h:133:VAL:O	34:h:133:VAL:HG23	2.19	0.41
43:5:115:GLU:HB2	43:5:119:GLN:HB2	2.02	0.41
45:9:69:LYS:HB3	45:9:70:PRO:CD	2.50	0.41
49:l:80:ASP:O	49:l:81:VAL:C	2.62	0.41
51:w:81:ASP:OD1	51:w:82:ARG:N	2.54	0.41
1:A:1187:U:H1'	1:A:1188:A:OP1	2.21	0.41
5:F:53:LEU:HD23	5:F:274:LEU:HD13	2.03	0.41
25:x:77:VAL:HG22	25:x:127:ARG:HG3	2.00	0.41
31:7:188:GLU:OE1	31:7:188:GLU:N	2.52	0.41
57:e:52:GLN:O	57:e:236:LEU:N	2.49	0.41
11:M:259:LYS:NZ	11:M:264:ILE:O	2.51	0.41
17:S:136:LYS:NZ	36:j:47:ASP:OD1	2.43	0.41
25:x:237:LYS:NZ	33:f:211:ASN:OD1	2.53	0.41
40:s:41:VAL:O	40:s:41:VAL:HG22	2.20	0.41
40:s:89:LYS:HG2	40:s:269:ARG:HB3	2.02	0.41
44:8:111:SER:HA	44:8:114:ARG:HE	1.84	0.41
46:a:61:HIS:O	46:a:61:HIS:ND1	2.54	0.41
48:z:34:MET:HE3	48:z:205:VAL:HA	2.03	0.41
54:k:90:LEU:O	54:k:94:ILE:HG12	2.21	0.41
56:d:160:CYS:O	56:d:164:SER:N	2.48	0.41
57:e:190:LEU:HD13	57:e:200:ALA:HB3	2.01	0.41
1:A:1457:A:OP1	1:A:1457:A:H4'	2.21	0.41
3:D:107:ILE:HG22	3:D:108:ASP:N	2.36	0.41
5:F:77:ILE:O	5:F:77:ILE:CG2	2.69	0.41
11:M:190:ILE:HD13	53:g:53:PRO:HD3	2.03	0.41
31:7:280:VAL:HG23	31:7:280:VAL:O	2.21	0.41
33:f:92:ILE:O	33:f:156:VAL:N	2.54	0.41
40:s:291:THR:HA	40:s:352:GLN:O	2.21	0.41
1:A:1194:A:HO2'	1:A:1195:G:P	2.43	0.41
1:A:1423:G:H4'	1:A:1936:U:H4'	2.03	0.41
1:A:1459:A:O2'	1:A:1525:A:H3'	2.21	0.41
9:K:101:VAL:O	9:K:101:VAL:CG1	2.68	0.41
25:x:257:THR:OG1	25:x:260:HIS:HB3	2.20	0.41
38:q:71:PRO:O	38:q:72:PRO:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:p:80:SER:OG	58:p:101:GLU:OE1	2.36	0.41
1:A:1236:A:H4'	1:A:1236:A:OP1	2.20	0.41
1:A:1614:A:H2'	1:A:1640:A:OP1	2.20	0.41
1:A:2285:U:H2'	1:A:2286:G:O4'	2.21	0.41
1:A:2635:A:OP2	1:A:2635:A:H4'	2.21	0.41
5:F:68:SER:O	5:F:210:ARG:NH2	2.36	0.41
8:J:87:VAL:HG13	8:J:151:LEU:HD21	2.01	0.41
15:Q:262:LYS:HB2	15:Q:265:ILE:HD12	2.02	0.41
17:S:174:ILE:HD12	32:b:2:THR:OG1	2.21	0.41
18:T:84:LEU:HB3	18:T:111:ILE:HD12	2.03	0.41
29:4:97:HIS:O	29:4:99:GLN:OE1	2.39	0.41
32:b:21:ARG:NH2	52:c:217:ASP:OD2	2.54	0.41
42:v:2:ALA:HB3	42:v:3:PRO:HD3	2.03	0.41
43:5:251:HIS:O	43:5:371:LYS:NZ	2.50	0.41
48:z:45:LEU:HD11	48:z:72:LEU:HD13	2.02	0.41
50:y:169:LEU:O	50:y:213:THR:HG22	2.20	0.41
50:y:246:LEU:CD2	50:y:250:ARG:CZ	2.99	0.41
52:c:87:LEU:O	52:c:90:THR:OG1	2.30	0.41
56:d:188:LYS:HD3	56:d:241:MET:HE1	2.03	0.41
57:e:271:ARG:HA	57:e:274:LEU:HB2	2.02	0.41
1:A:1194:A:O2'	1:A:1195:G:P	2.79	0.41
1:A:1504:C:H2'	1:A:1505:A:O4'	2.21	0.41
1:A:1628:A:O2'	1:A:1647:A:C2	2.74	0.41
1:A:2324:A:N3	1:A:2324:A:H2'	2.36	0.41
10:L:140:ILE:O	10:L:140:ILE:HG22	2.20	0.41
18:T:93:ILE:HG23	18:T:94:ASP:N	2.36	0.41
20:V:172:ASP:OD1	20:V:172:ASP:N	2.54	0.41
25:x:223:ARG:O	25:x:223:ARG:HG3	2.20	0.41
32:b:12:THR:HG22	32:b:13:SER:H	1.86	0.41
33:f:202:GLU:OE1	33:f:202:GLU:N	2.47	0.41
38:q:138:GLN:O	38:q:142:ARG:HG2	2.20	0.41
41:u:190:LEU:N	41:u:190:LEU:HD12	2.35	0.41
43:5:221:GLN:OE1	43:5:223:ARG:NH2	2.51	0.41
57:e:190:LEU:HD22	57:e:198:MET:HE1	2.03	0.41
1:A:1102:U:O2'	1:A:1103:A:P	2.79	0.40
14:P:138:GLU:HG3	30:6:188:TYR:CB	2.51	0.40
18:T:53:TYR:N	56:d:236:ARG:O	2.48	0.40
22:X:168:ARG:HD3	22:X:173:ASP:HB3	2.02	0.40
30:6:242:SER:OG	30:6:243:ASN:N	2.54	0.40
38:q:44:ASN:O	38:q:47:THR:HG22	2.21	0.40
39:r:88:LEU:HD23	39:r:88:LEU:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:58:ARG:HB2	48:z:59:ILE:HD12	2.03	0.40
48:z:85:ASP:O	48:z:315:GLN:NE2	2.49	0.40
52:c:241:LEU:HA	52:c:301:LEU:HD21	2.02	0.40
1:A:2517:G:O5'	1:A:2517:G:H8	2.04	0.40
2:B:13:U:O2'	2:B:14:A:P	2.80	0.40
5:F:206:LEU:C	5:F:206:LEU:HD23	2.46	0.40
17:S:166:GLU:OE1	17:S:196:ILE:HD12	2.22	0.40
18:T:101:GLU:OE1	55:0:115:LEU:HD12	2.22	0.40
20:V:131:THR:O	20:V:131:THR:HG23	2.20	0.40
23:Y:212:ARG:HD3	35:i:104:ILE:HD11	2.04	0.40
48:z:59:ILE:O	48:z:59:ILE:HG22	2.21	0.40
52:c:31:VAL:O	52:c:31:VAL:CG1	2.69	0.40
59:t:134:LEU:HD23	59:t:134:LEU:HA	1.97	0.40
1:A:2056:A:H4'	1:A:2057:G:OP1	2.20	0.40
1:A:2182:U:H5'	1:A:2183:A:OP2	2.21	0.40
8:J:54:ASN:OD1	8:J:54:ASN:C	2.64	0.40
9:K:17:MET:HE2	32:b:136:LYS:HE3	2.02	0.40
24:Z:69:VAL:HG23	24:Z:91:LEU:HD21	2.03	0.40
25:x:202:LEU:HD12	25:x:203:SER:N	2.36	0.40
30:6:215:THR:O	30:6:272:LEU:HD12	2.21	0.40
42:v:62:LEU:HD23	42:v:62:LEU:C	2.46	0.40
48:z:181:ILE:HG13	48:z:182:THR:N	2.36	0.40
49:l:113:GLU:OE1	49:l:113:GLU:N	2.49	0.40
59:t:67:PHE:CD2	59:t:90:VAL:HG22	2.57	0.40
1:A:1614:A:O2'	1:A:1640:A:O5'	2.40	0.40
1:A:2617:A:O2'	1:A:2618:A:P	2.79	0.40
5:F:48:LEU:HA	5:F:79:LEU:O	2.22	0.40
7:I:50:ILE:HD12	37:o:35:MET:SD	2.61	0.40
20:V:28:SER:O	20:V:32:LYS:HG3	2.22	0.40
31:7:191:PRO:HD2	31:7:280:VAL:HG21	2.03	0.40
38:q:78:THR:O	38:q:79:PRO:C	2.64	0.40
48:z:210:ILE:HG22	48:z:211:GLU:N	2.36	0.40
54:k:30:THR:HG23	54:k:31:ARG:N	2.36	0.40
56:d:246:ASP:OD1	56:d:246:ASP:N	2.54	0.40
57:e:45:LEU:HD23	57:e:228:LYS:HE2	2.03	0.40
1:A:1491:A:H62	1:A:1492:A:N6	2.20	0.40
1:A:1642:G:H5'	1:A:1643:C:OP2	2.21	0.40
5:F:292:ASP:OD1	5:F:292:ASP:N	2.53	0.40
9:K:112:LEU:HD22	9:K:121:MET:SD	2.62	0.40
12:N:206:GLU:OE2	12:N:240:ARG:NH2	2.49	0.40
30:6:292:GLN:O	30:6:293:LEU:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:e:163:LEU:N	57:e:166:GLN:O	2.45	0.40
59:t:194:ASP:O	59:t:195:PHE:HB2	2.22	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%)	217 (97%)	6 (3%)	0	100	100
4	E	306/348 (88%)	292 (95%)	14 (5%)	0	100	100
5	F	248/294 (84%)	244 (98%)	4 (2%)	0	100	100
6	H	93/265 (35%)	92 (99%)	1 (1%)	0	100	100
7	I	159/262 (61%)	152 (96%)	7 (4%)	0	100	100
8	J	85/192 (44%)	76 (89%)	9 (11%)	0	100	100
9	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
10	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
11	M	285/295 (97%)	276 (97%)	9 (3%)	0	100	100
12	N	178/251 (71%)	175 (98%)	3 (2%)	0	100	100
13	O	151/176 (86%)	148 (98%)	3 (2%)	0	100	100
14	P	139/180 (77%)	139 (100%)	0	0	100	100
15	Q	215/292 (74%)	211 (98%)	4 (2%)	0	100	100
16	R	138/149 (93%)	138 (100%)	0	0	100	100
17	S	151/209 (72%)	147 (97%)	4 (3%)	0	100	100
18	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
19	U	123/146 (84%)	123 (100%)	0	0	100	100
20	V	199/216 (92%)	194 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	98/148 (66%)	95 (97%)	3 (3%)	0	100	100
22	X	240/294 (82%)	239 (100%)	1 (0%)	0	100	100
23	Y	174/252 (69%)	173 (99%)	1 (1%)	0	100	100
24	Z	118/160 (74%)	116 (98%)	2 (2%)	0	100	100
25	x	322/381 (84%)	309 (96%)	13 (4%)	0	100	100
26	1	50/65 (77%)	50 (100%)	0	0	100	100
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	93 (100%)	0	0	100	100
29	4	35/101 (35%)	35 (100%)	0	0	100	100
30	6	311/380 (82%)	287 (92%)	24 (8%)	0	100	100
31	7	290/336 (86%)	284 (98%)	6 (2%)	0	100	100
32	b	146/159 (92%)	141 (97%)	5 (3%)	0	100	100
33	f	98/211 (46%)	92 (94%)	6 (6%)	0	100	100
34	h	108/159 (68%)	104 (96%)	4 (4%)	0	100	100
35	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
36	j	91/121 (75%)	88 (97%)	3 (3%)	0	100	100
37	o	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
38	q	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
39	r	153/196 (78%)	148 (97%)	5 (3%)	0	100	100
40	s	373/442 (84%)	367 (98%)	6 (2%)	0	100	100
41	u	123/228 (54%)	119 (97%)	4 (3%)	0	100	100
42	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
43	5	392/423 (93%)	386 (98%)	6 (2%)	0	100	100
44	8	65/206 (32%)	64 (98%)	1 (2%)	0	100	100
45	9	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
46	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
47	m	43/127 (34%)	42 (98%)	1 (2%)	0	100	100
48	z	309/326 (95%)	290 (94%)	19 (6%)	0	100	100
49	l	59/135 (44%)	54 (92%)	5 (8%)	0	100	100
50	y	235/346 (68%)	230 (98%)	5 (2%)	0	100	100
51	w	77/156 (49%)	65 (84%)	12 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	c	277/308 (90%)	269 (97%)	8 (3%)	0	100	100
53	g	130/166 (78%)	127 (98%)	3 (2%)	0	100	100
54	k	83/118 (70%)	80 (96%)	3 (4%)	0	100	100
55	o	106/187 (57%)	106 (100%)	0	0	100	100
56	d	230/306 (75%)	216 (94%)	14 (6%)	0	100	100
57	e	187/283 (66%)	177 (95%)	10 (5%)	0	100	100
58	p	140/206 (68%)	135 (96%)	5 (4%)	0	100	100
59	t	317/366 (87%)	291 (92%)	26 (8%)	0	100	100
All	All	9252/12421 (74%)	8961 (97%)	291 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	84/152 (55%)	84 (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	161/216 (74%)	161 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	R	119/128 (93%)	119 (100%)	0	100	100
17	S	141/180 (78%)	141 (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	113/146 (77%)	113 (100%)	0	100	100
25	x	283/334 (85%)	283 (100%)	0	100	100
26	1	49/60 (82%)	49 (100%)	0	100	100
27	2	40/77 (52%)	40 (100%)	0	100	100
28	3	88/165 (53%)	88 (100%)	0	100	100
29	4	35/90 (39%)	35 (100%)	0	100	100
30	6	280/335 (84%)	280 (100%)	0	100	100
31	7	269/301 (89%)	269 (100%)	0	100	100
32	b	130/138 (94%)	130 (100%)	0	100	100
33	f	93/185 (50%)	93 (100%)	0	100	100
34	h	100/143 (70%)	100 (100%)	0	100	100
35	i	87/111 (78%)	87 (100%)	0	100	100
36	j	75/99 (76%)	75 (100%)	0	100	100
37	o	65/85 (76%)	65 (100%)	0	100	100
38	q	117/187 (63%)	117 (100%)	0	100	100
39	r	142/168 (84%)	142 (100%)	0	100	100
40	s	329/378 (87%)	329 (100%)	0	100	100
41	u	115/197 (58%)	115 (100%)	0	100	100
42	v	60/61 (98%)	60 (100%)	0	100	100
43	5	356/372 (96%)	356 (100%)	0	100	100
44	8	59/182 (32%)	59 (100%)	0	100	100
45	9	104/114 (91%)	104 (100%)	0	100	100
46	a	97/129 (75%)	97 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m	40/114 (35%)	40 (100%)	0	100	100
48	z	270/280 (96%)	270 (100%)	0	100	100
49	l	61/112 (54%)	61 (100%)	0	100	100
50	y	220/322 (68%)	220 (100%)	0	100	100
51	w	73/135 (54%)	73 (100%)	0	100	100
52	c	245/266 (92%)	245 (100%)	0	100	100
53	g	122/148 (82%)	122 (100%)	0	100	100
54	k	76/95 (80%)	76 (100%)	0	100	100
55	o	97/170 (57%)	97 (100%)	0	100	100
56	d	210/272 (77%)	210 (100%)	0	100	100
57	e	166/238 (70%)	166 (100%)	0	100	100
58	p	129/177 (73%)	129 (100%)	0	100	100
59	t	266/306 (87%)	266 (100%)	0	100	100
All	All	8335/10782 (77%)	8335 (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 (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	228	GLN
4	E	227	GLN
4	E	281	ASN
5	F	153	HIS
11	M	31	ASN
12	N	217	HIS
13	O	109	GLN
13	O	138	HIS
13	O	161	GLN
15	Q	261	ASN
16	R	27	HIS
17	S	122	ASN
19	U	77	ASN
22	X	12	GLN
22	X	77	GLN
24	Z	67	HIS
25	x	79	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	x	328	GLN
30	6	239	ASN
30	6	275	GLN
30	6	292	GLN
31	7	289	ASN
32	b	16	HIS
32	b	66	ASN
32	b	120	HIS
32	b	123	ASN
32	b	141	HIS
33	f	174	GLN
34	h	86	ASN
34	h	96	HIS
35	i	65	ASN
37	o	94	HIS
39	r	131	HIS
40	s	107	GLN
40	s	226	GLN
40	s	228	ASN
40	s	233	ASN
43	5	88	HIS
43	5	195	HIS
43	5	269	HIS
43	5	287	HIS
43	5	343	GLN
46	a	70	HIS
48	z	97	GLN
50	y	292	ASN
52	c	139	GLN
55	0	117	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1405/1584 (88%)	427 (30%)	29 (2%)
2	B	58/68 (85%)	24 (41%)	2 (3%)
All	All	1463/1652 (88%)	451 (30%)	31 (2%)

All (451) 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	1119	A
1	A	1123	A
1	A	1124	U
1	A	1125	A
1	A	1128	U
1	A	1129	A
1	A	1131	A
1	A	1132	C
1	A	1134	A
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	1171	U
1	A	1173	G
1	A	1188	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1255	C
1	A	1256	A
1	A	1257	A
1	A	1260	A
1	A	1264	A
1	A	1272	A
1	A	1277	U
1	A	1278	U
1	A	1279	G
1	A	1280	C
1	A	1282	U
1	A	1283	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	1316	A
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	1364	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	1420	A
1	A	1421	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1422	A
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	1457	A
1	A	1459	A
1	A	1460	U
1	A	1465	U
1	A	1466	U
1	A	1467	A
1	A	1468	A
1	A	1471	U
1	A	1473	A
1	A	1475	U
1	A	1483	U
1	A	1484	U
1	A	1485	G
1	A	1486	C
1	A	1490	A
1	A	1491	A
1	A	1492	A
1	A	1493	A
1	A	1494	A
1	A	1503	U
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	1552	A
1	A	1553	C
1	A	1557	A
1	A	1558	A
1	A	1559	A
1	A	1565	U
1	A	1566	U
1	A	1568	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1569	U
1	A	1573	G
1	A	1580	U
1	A	1582	A
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	1598	C
1	A	1599	C
1	A	1600	A
1	A	1601	U
1	A	1602	U
1	A	1603	G
1	A	1606	G
1	A	1607	G
1	A	1609	C
1	A	1610	U
1	A	1611	A
1	A	1614	A
1	A	1615	G
1	A	1616	C
1	A	1623	C
1	A	1624	A
1	A	1625	A
1	A	1626	U
1	A	1628	A
1	A	1629	A
1	A	1630	G
1	A	1633	A
1	A	1638	U
1	A	1639	C
1	A	1640	A
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	1651	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1652	A
1	A	1653	A
1	A	1658	C
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	1683	C
1	A	1684	U
1	A	1690	A
1	A	1693	U
1	A	1697	A
1	A	1698	A
1	A	1717	U
1	A	1718	U
1	A	1730	A
1	A	1733	G
1	A	1748	A
1	A	1749	A
1	A	1755	C
1	A	1758	A
1	A	1766	G
1	A	1767	G
1	A	1769	A
1	A	1777	A
1	A	1784	C
1	A	1785	U
1	A	1801	A
1	A	1804	U
1	A	1805	A
1	A	1806	A
1	A	1807	U
1	A	1823	A
1	A	1826	C
1	A	1831	U
1	A	1837	U
1	A	1844	C
1	A	1846	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1893	C
1	A	1894	A
1	A	1904	A
1	A	1914	G
1	A	1919	C
1	A	1922	G
1	A	1923	A
1	A	1924	A
1	A	1927	C
1	A	1930	C
1	A	1933	G
1	A	1936	U
1	A	1944	A
1	A	1945	C
1	A	1948	C
1	A	1957	C
1	A	1958	A
1	A	1959	U
1	A	1964	A
1	A	1976	A
1	A	1979	G
1	A	1982	U
1	A	1983	G
1	A	1984	C
1	A	1987	A
1	A	1988	G
1	A	1990	G
1	A	1991	A
1	A	2040	C
1	A	2048	C
1	A	2050	U
1	A	2057	G
1	A	2058	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2059	G
1	A	2060	A
1	A	2063	A
1	A	2068	G
1	A	2069	A
1	A	2072	G
1	A	2077	A
1	A	2082	G
1	A	2091	U
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2123	U
1	A	2128	U
1	A	2131	A
1	A	2132	G
1	A	2143	A
1	A	2146	A
1	A	2155	C
1	A	2156	G
1	A	2158	G
1	A	2159	A
1	A	2160	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	2182	U
1	A	2183	A
1	A	2184	U
1	A	2186	A
1	A	2187	C
1	A	2190	A
1	A	2191	U
1	A	2193	U
1	A	2195	U
1	A	2197	A
1	A	2229	A
1	A	2230	G
1	A	2232	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2236	G
1	A	2248	G
1	A	2251	U
1	A	2252	G
1	A	2253	G
1	A	2255	G
1	A	2256	U
1	A	2257	G
1	A	2258	A
1	A	2259	C
1	A	2275	A
1	A	2276	U
1	A	2282	G
1	A	2284	A
1	A	2285	U
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	2303	A
1	A	2325	U
1	A	2326	A
1	A	2328	C
1	A	2329	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	2363	A
1	A	2367	A
1	A	2369	C
1	A	2375	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2391	U
1	A	2394	U
1	A	2397	A
1	A	2398	G
1	A	2399	A
1	A	2404	A
1	A	2410	A
1	A	2412	A
1	A	2414	U
1	A	2415	U
1	A	2416	A
1	A	2418	G
1	A	2427	C
1	A	2428	C
1	A	2429	U
1	A	2430	C
1	A	2431	A
1	A	2437	G
1	A	2447	A
1	A	2449	C
1	A	2458	G
1	A	2462	A
1	A	2464	G
1	A	2475	U
1	A	2481	U
1	A	2482	G
1	A	2486	A
1	A	2488	C
1	A	2495	A
1	A	2496	G
1	A	2498	C
1	A	2501	A
1	A	2502	C
1	A	2505	G
1	A	2509	U
1	A	2515	C
1	A	2516	A
1	A	2519	C
1	A	2520	C
1	A	2521	G
1	A	2523	A
1	A	2524	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2526	A
1	A	2531	A
1	A	2532	G
1	A	2533	G
1	A	2538	U
1	A	2539	U
1	A	2540	U
1	A	2542	U
1	A	2544	U
1	A	2550	U
1	A	2551	A
1	A	2552	C
1	A	2563	A
1	A	2564	G
1	A	2565	U
1	A	2570	A
1	A	2582	A
1	A	2590	C
1	A	2591	A
1	A	2595	U
1	A	2598	A
1	A	2599	A
1	A	2600	A
1	A	2601	U
1	A	2604	G
1	A	2605	C
1	A	2614	C
1	A	2615	U
1	A	2617	A
1	A	2618	A
1	A	2619	U
1	A	2621	U
1	A	2628	A
1	A	2629	A
1	A	2631	A
1	A	2635	A
1	A	2636	A
1	A	2640	A
1	A	2647	U
1	A	2648	A
1	A	2650	G
1	A	2656	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2657	C
1	A	2658	U
1	A	2659	C
1	A	2660	U
1	A	2665	U
1	A	2676	A
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	21	A
2	B	28	G
2	B	32	U
2	B	33	G
2	B	44	G
2	B	45	A
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	60	C
2	B	63	A
2	B	66	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1137	A
1	A	1187	U
1	A	1194	A
1	A	1234	C
1	A	1237	A
1	A	1281	A
1	A	1428	A
1	A	1458	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1467	A
1	A	1492	A
1	A	1594	U
1	A	1595	U
1	A	1596	A
1	A	1605	A
1	A	1608	C
1	A	1614	A
1	A	1657	U
1	A	1659	A
1	A	1935	U
1	A	1944	A
1	A	2056	A
1	A	2057	G
1	A	2076	A
1	A	2182	U
1	A	2275	A
1	A	2302	U
1	A	2414	U
1	A	2627	U
1	A	2659	C
2	B	31	C
2	B	52	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 101 are monoatomic - leaving 3 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	I	301	7,39	0,4,4	-	-	-		
63	GNP	z	401	-	33,34,34	1.15	5 (15%)	46,54,54	0.64	0
63	GNP	t	501	-	33,34,34	1.13	4 (12%)	46,54,54	0.70	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	FES	I	301	7,39	-	-	0/1/1/1
63	GNP	z	401	-	-	4/18/38/38	0/3/3/3
63	GNP	t	501	-	-	8/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	401	GNP	PB-O2B	-3.29	1.47	1.56
63	t	501	GNP	PG-O1G	3.19	1.51	1.46
63	t	501	GNP	PB-O2B	-3.17	1.48	1.56
63	z	401	GNP	PG-O1G	3.05	1.51	1.46
63	z	401	GNP	C6-N1	-2.89	1.33	1.38
63	t	501	GNP	C6-N1	-2.89	1.33	1.38
63	z	401	GNP	PG-O3G	-2.24	1.50	1.56
63	z	401	GNP	PG-O2G	-2.07	1.51	1.56
63	t	501	GNP	PG-O3G	-2.00	1.51	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	t	501	GNP	C4'-O4'-C1'	-2.08	104.88	109.47

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

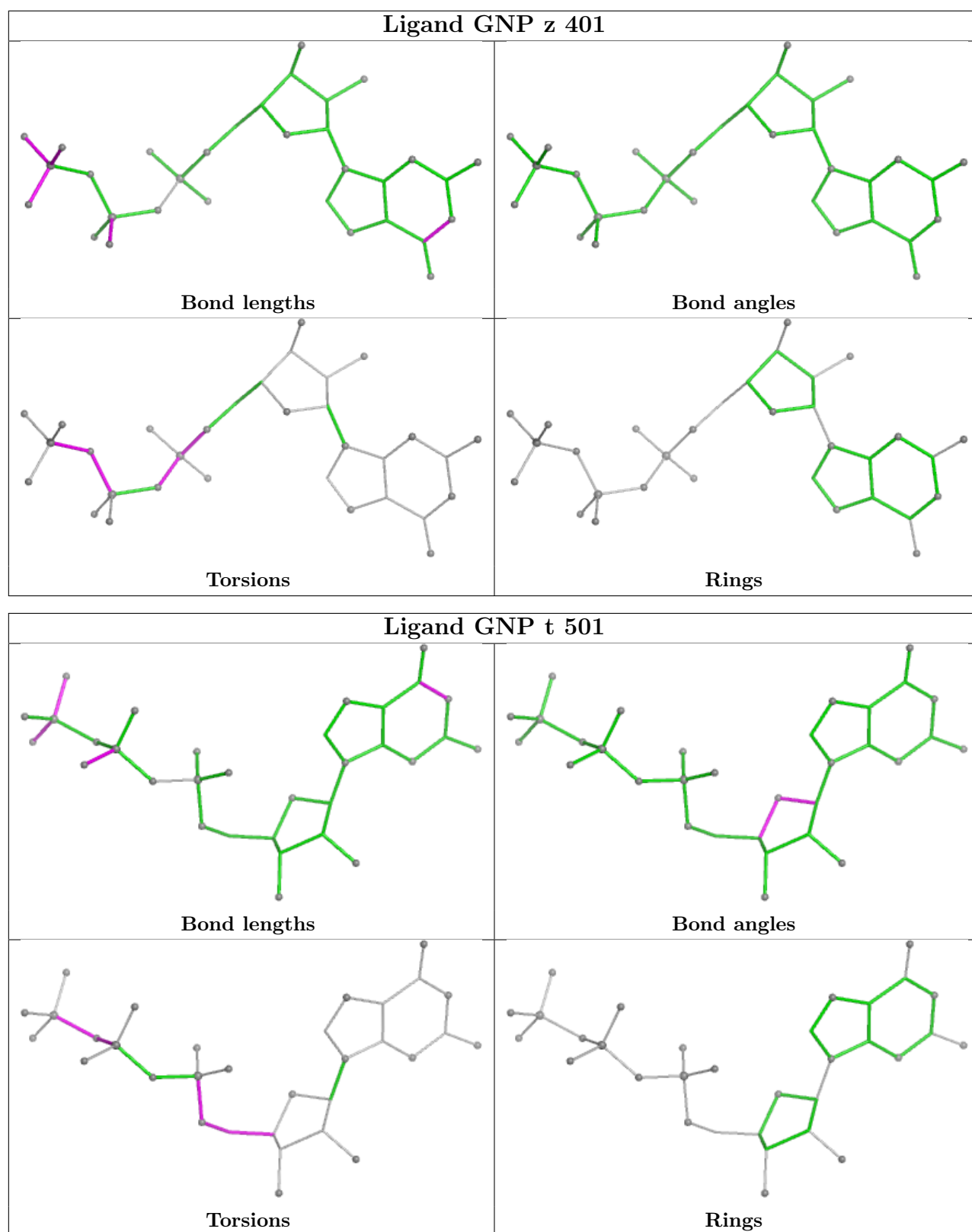
Mol	Chain	Res	Type	Atoms
63	z	401	GNP	PG-N3B-PB-O1B
63	z	401	GNP	C5'-O5'-PA-O1A
63	t	501	GNP	PB-N3B-PG-O1G
63	t	501	GNP	PG-N3B-PB-O1B
63	t	501	GNP	PG-N3B-PB-O3A
63	t	501	GNP	C5'-O5'-PA-O3A
63	t	501	GNP	C4'-C5'-O5'-PA
63	z	401	GNP	PB-O3A-PA-O1A
63	t	501	GNP	C5'-O5'-PA-O2A
63	t	501	GNP	C3'-C4'-C5'-O5'
63	t	501	GNP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	z	401	GNP	1	0
63	t	501	GNP	2	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

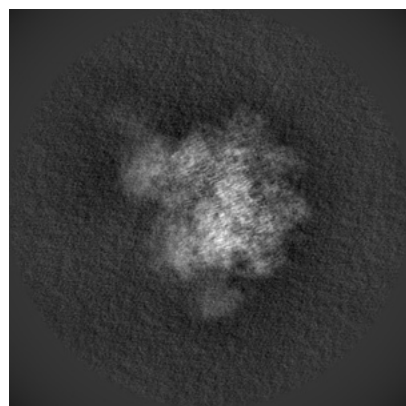
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52047. These allow visual inspection of the internal detail of the map and identification of artifacts.

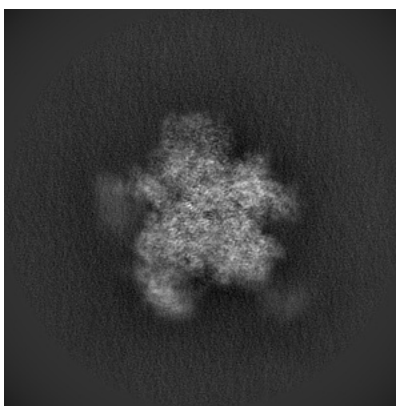
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

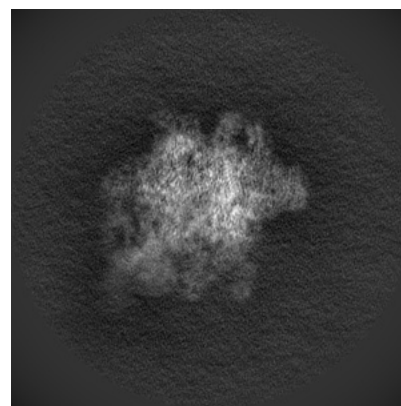
6.1.1 Primary map



X

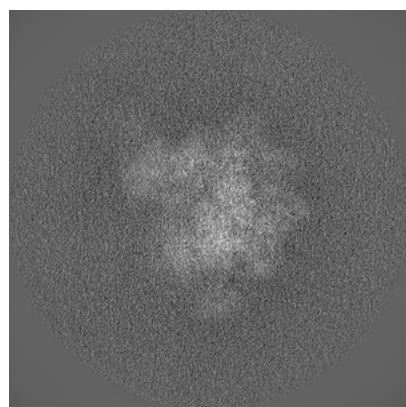


Y

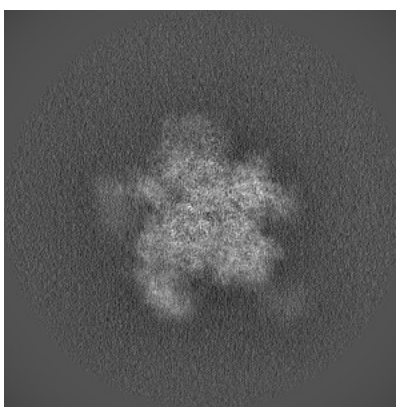


Z

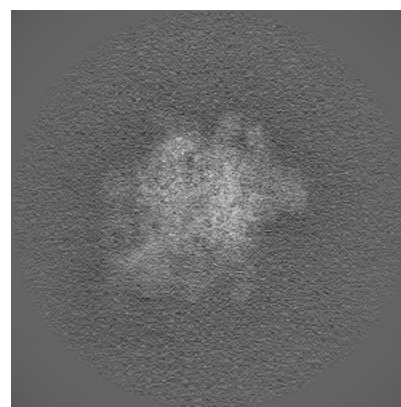
6.1.2 Raw map



X



Y

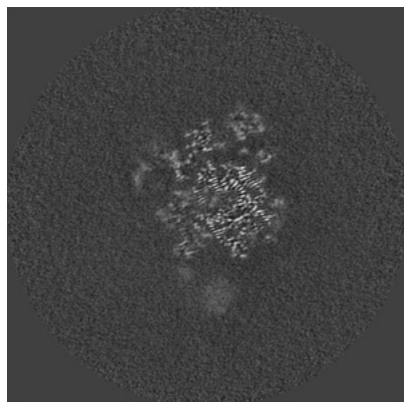


Z

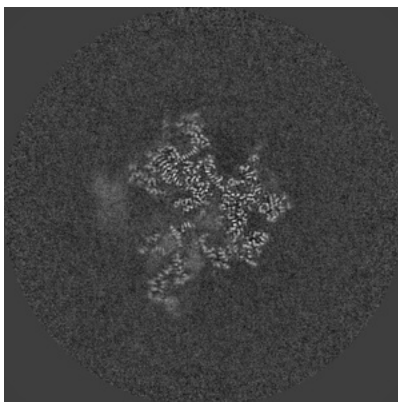
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

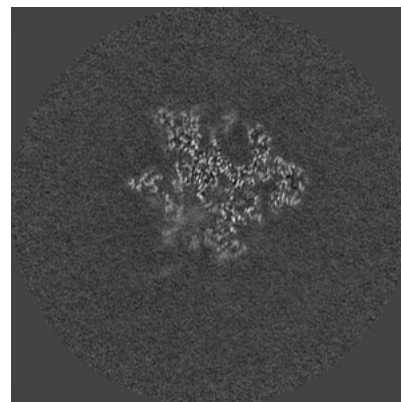
6.2.1 Primary map



X Index: 270

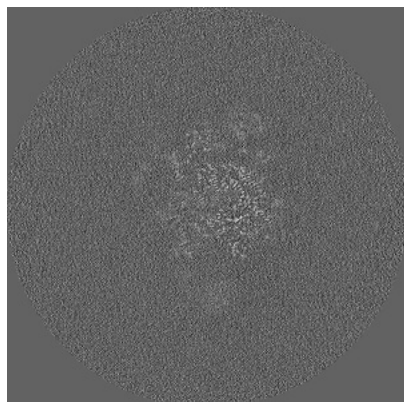


Y Index: 270

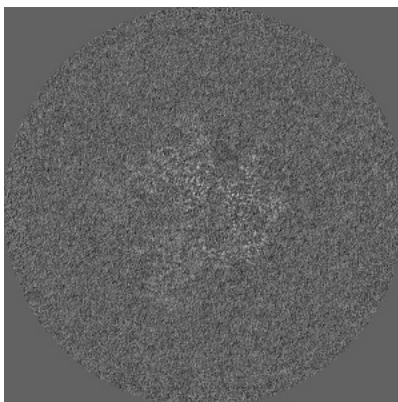


Z Index: 270

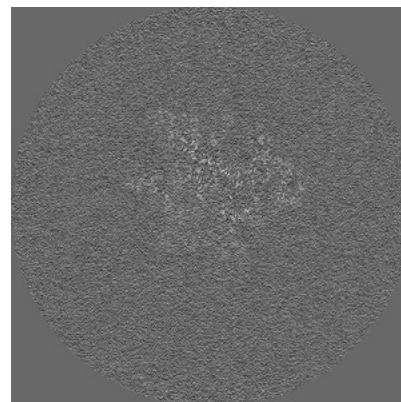
6.2.2 Raw map



X Index: 270



Y Index: 270

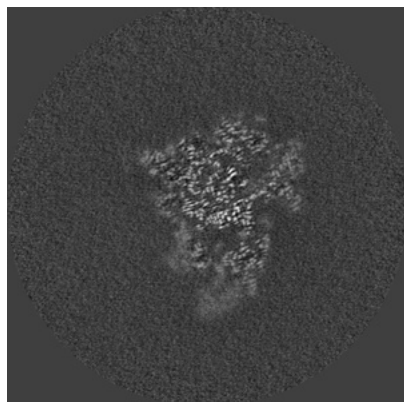


Z Index: 270

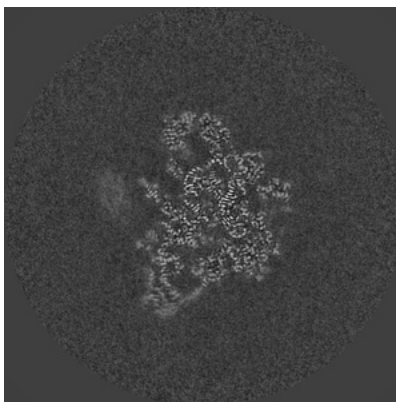
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

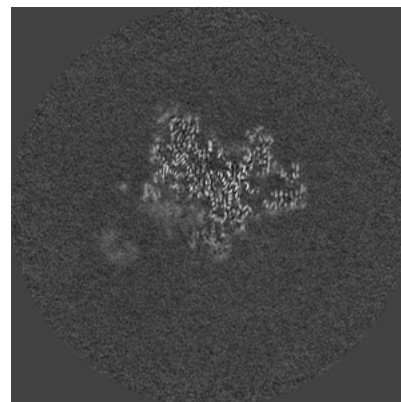
6.3.1 Primary map



X Index: 296

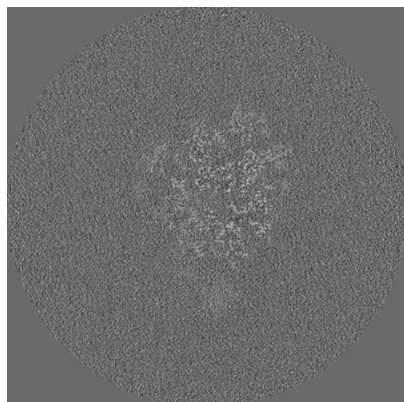


Y Index: 297

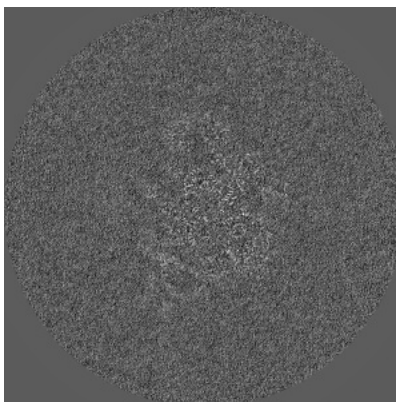


Z Index: 256

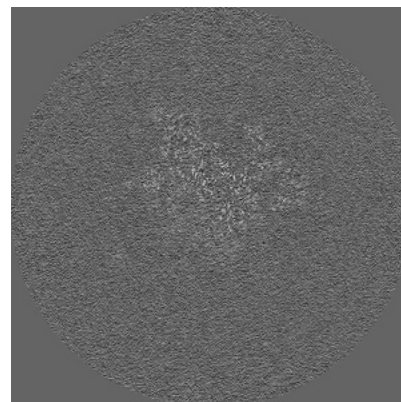
6.3.2 Raw map



X Index: 277



Y Index: 296

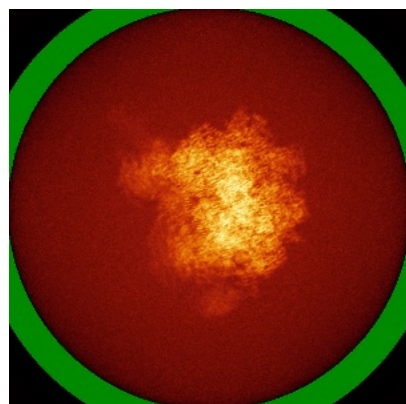


Z Index: 265

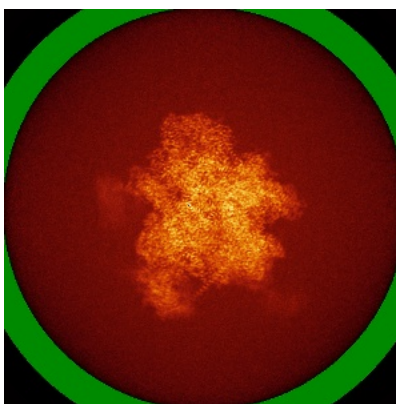
The images above show the largest variance slices of the map in three orthogonal directions.

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

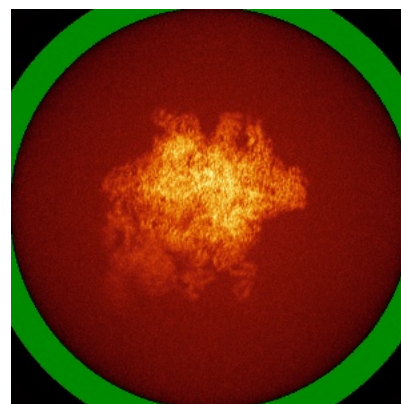
6.4.1 Primary map



X

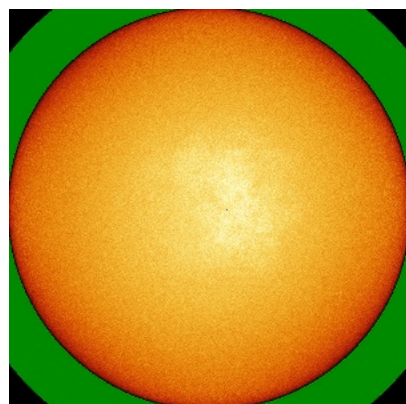


Y

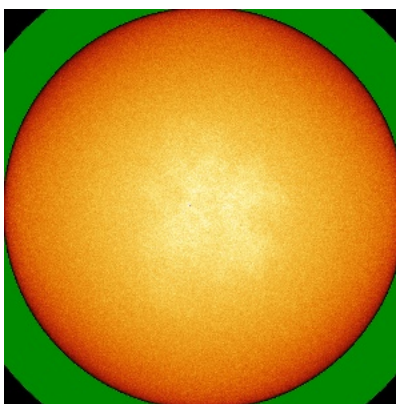


Z

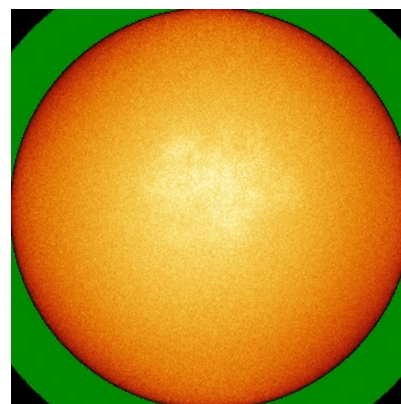
6.4.2 Raw map



X



Y

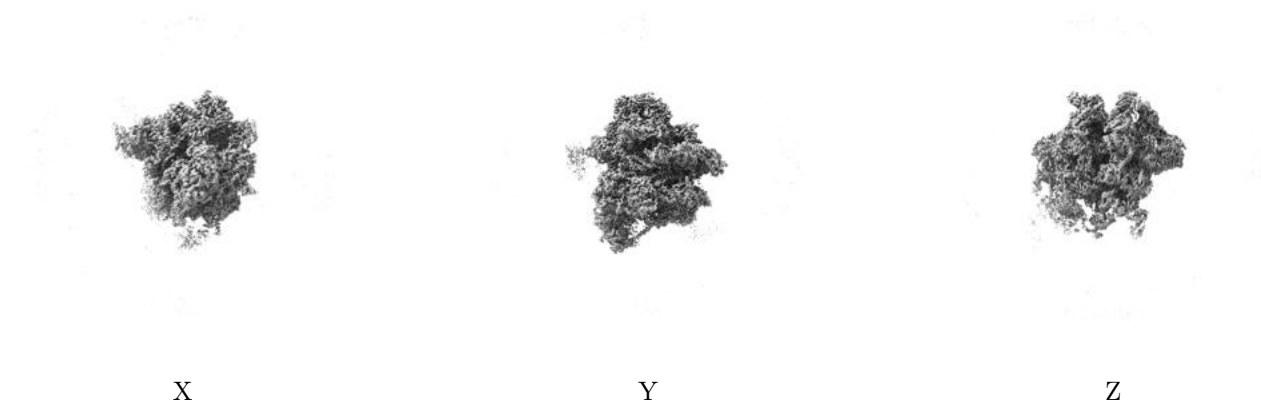


Z

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

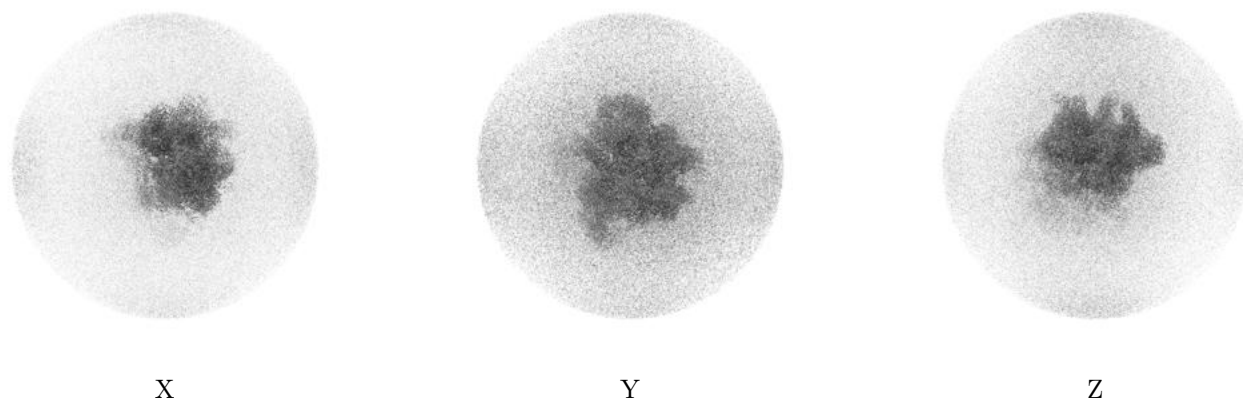
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

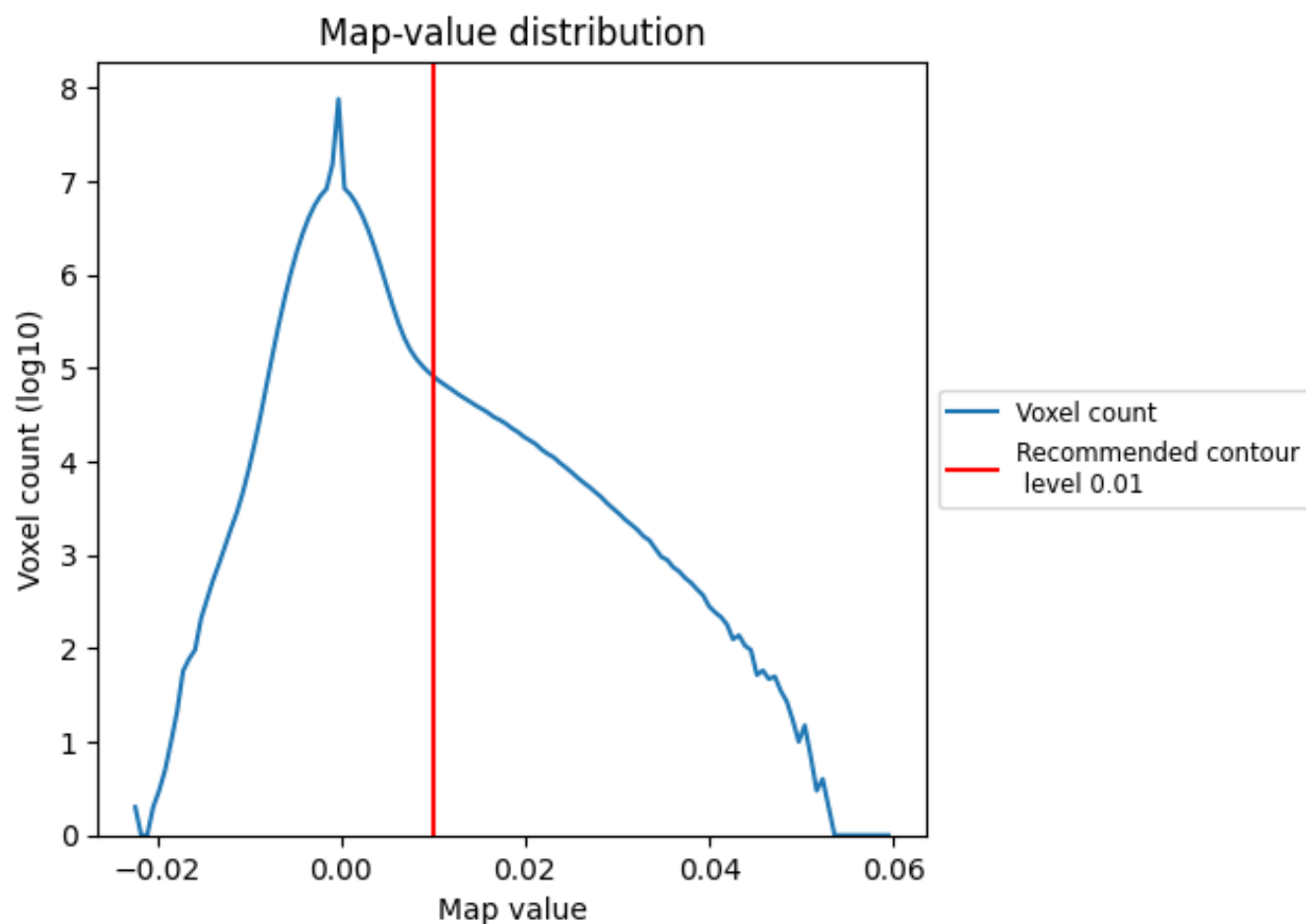
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

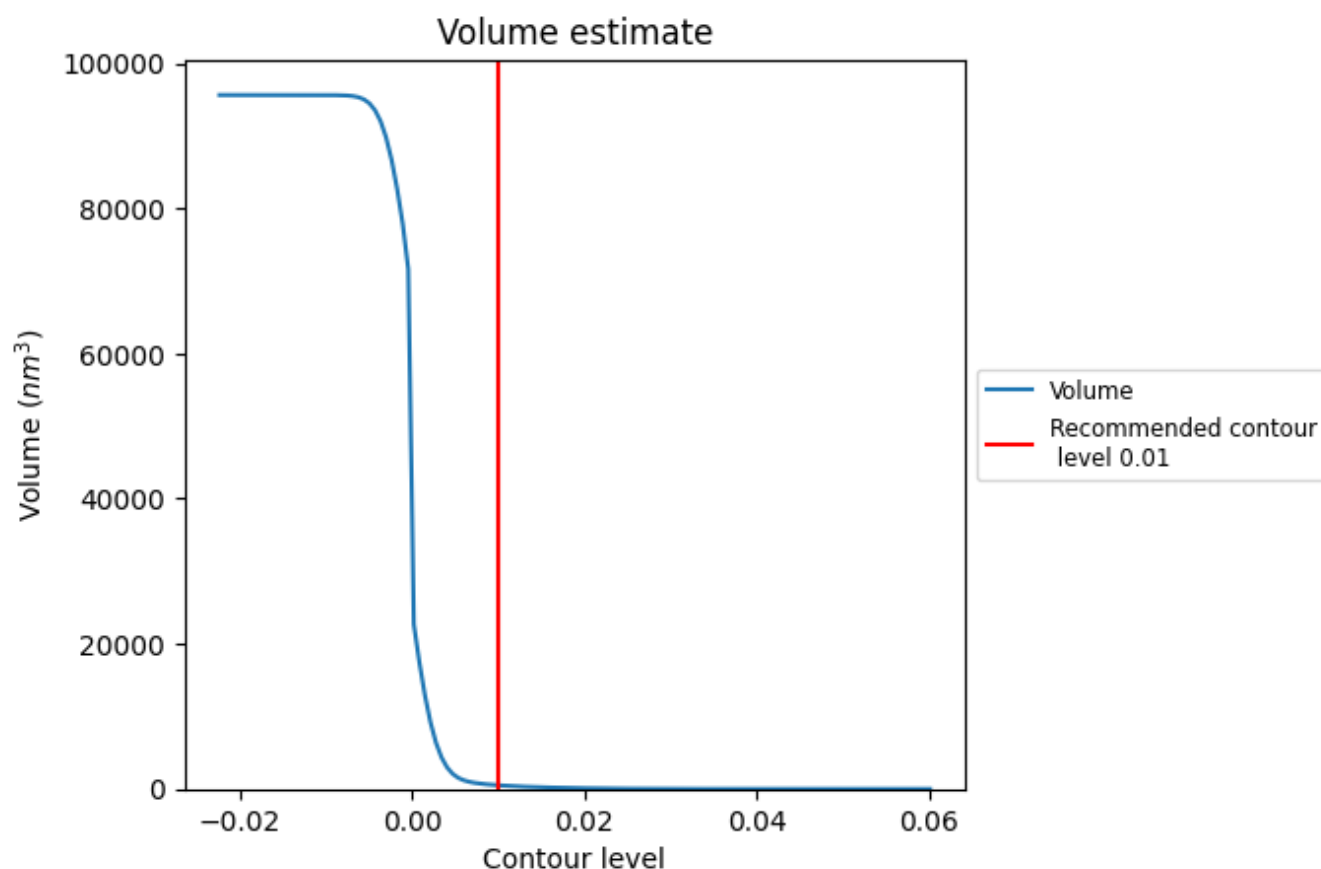
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

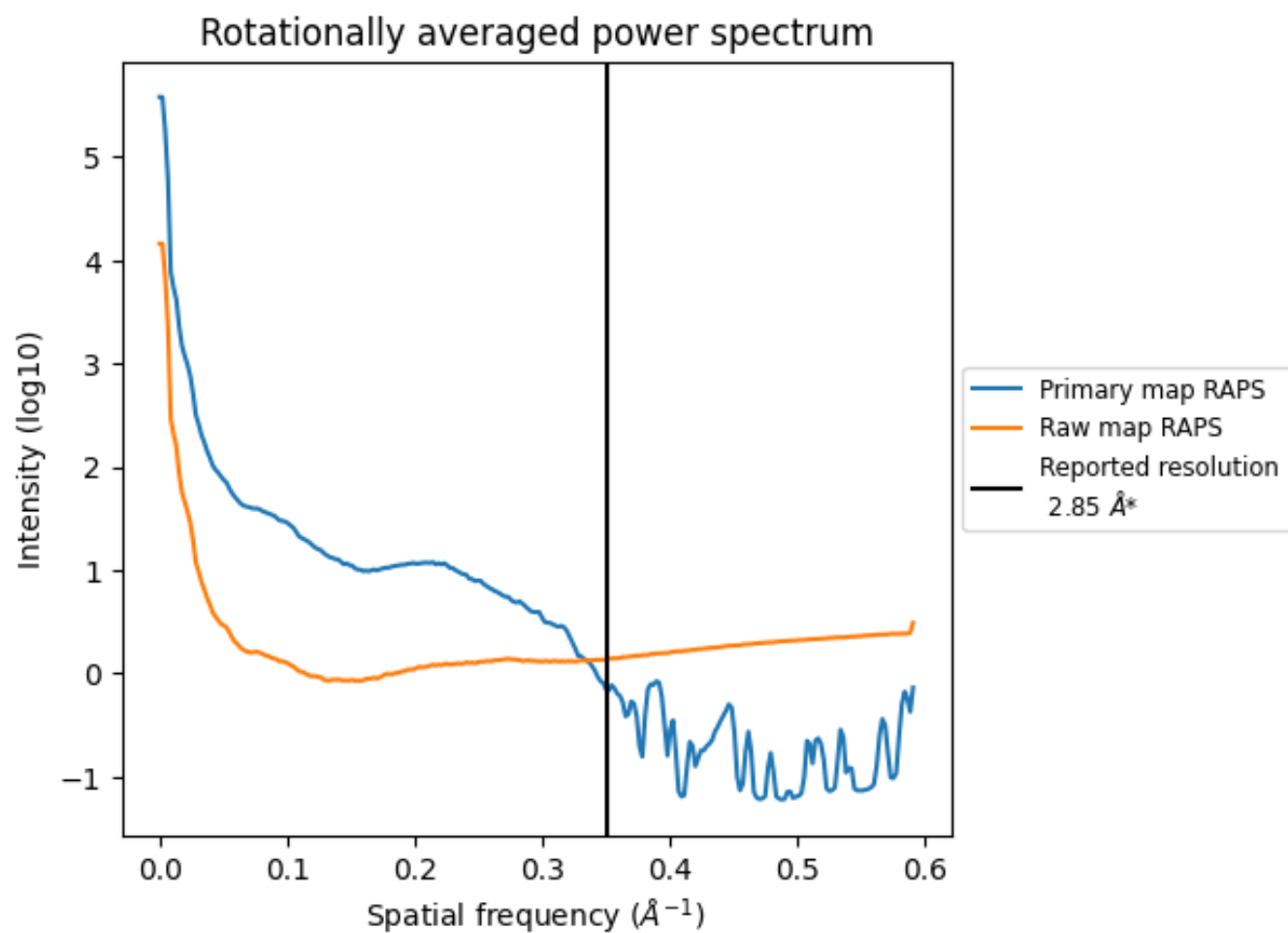
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

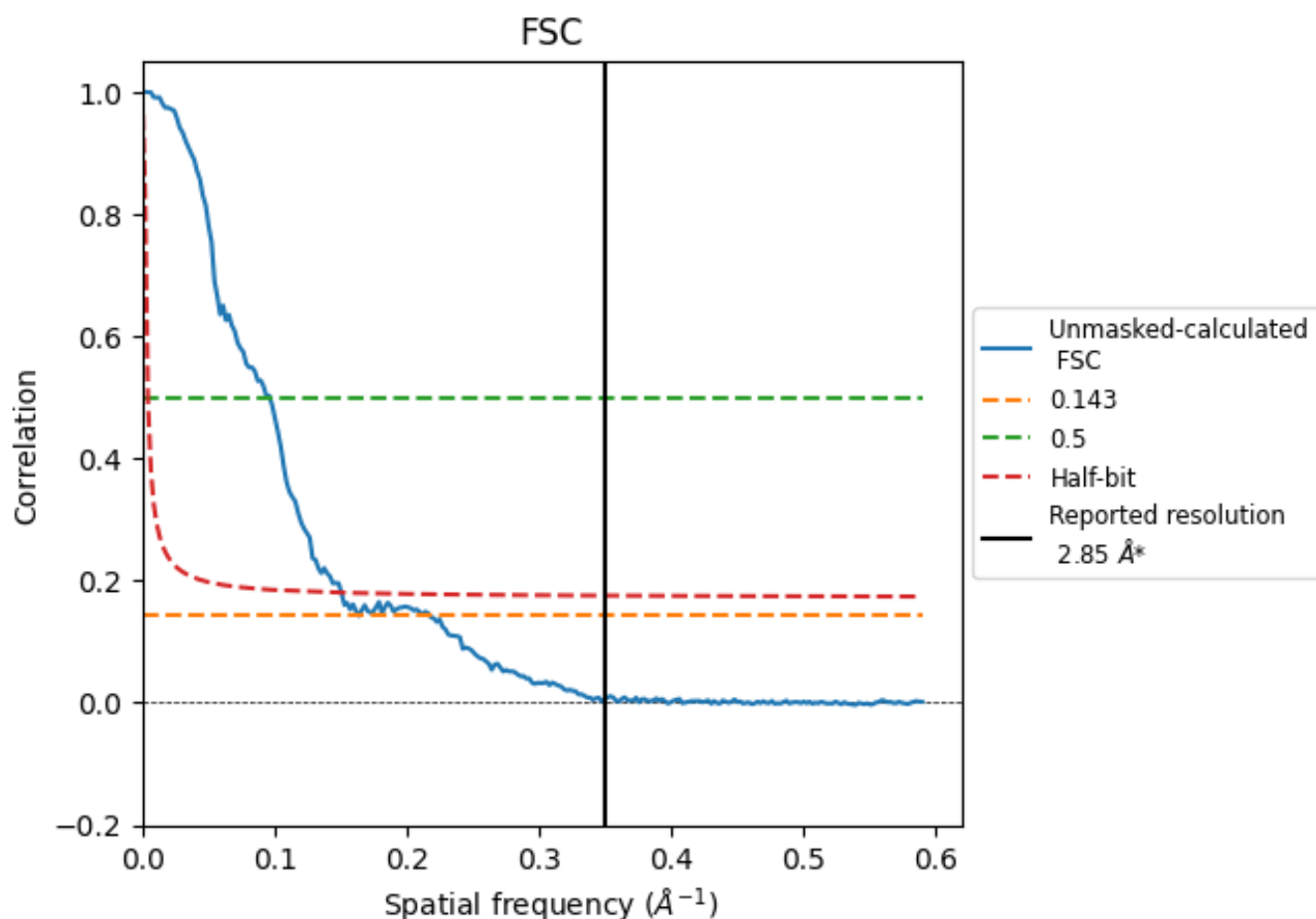


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

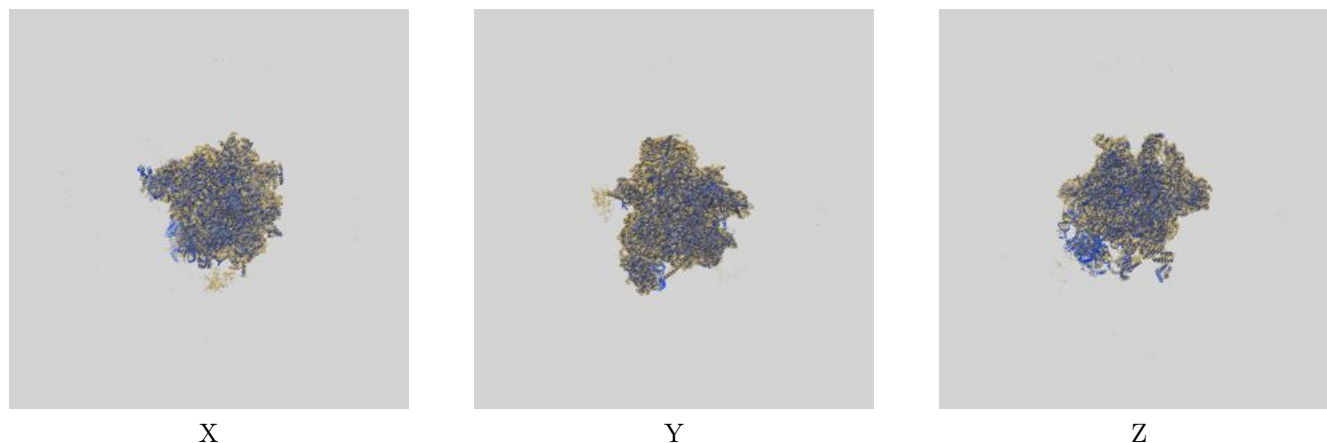
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.11	10.36	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.11 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

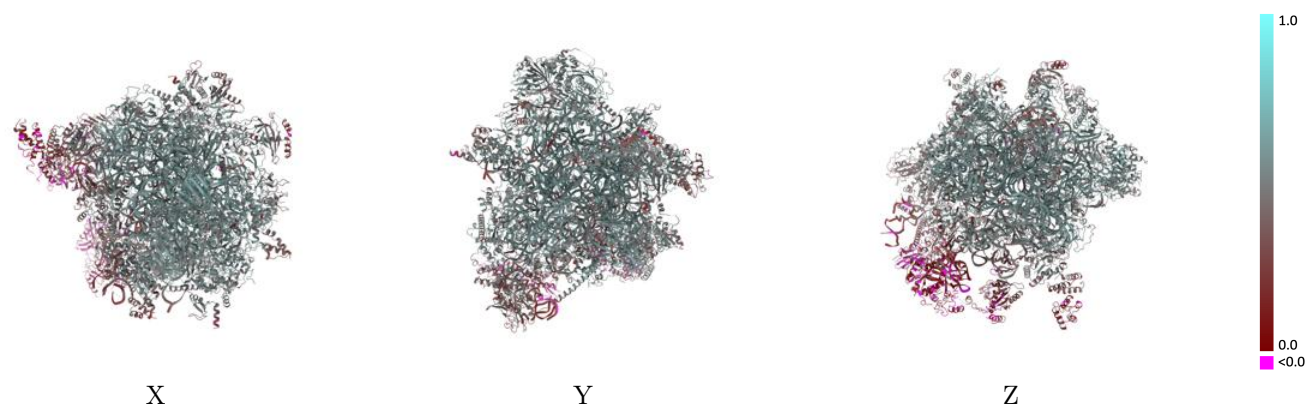
This section contains information regarding the fit between EMDB map EMD-52047 and PDB model 9HCF. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



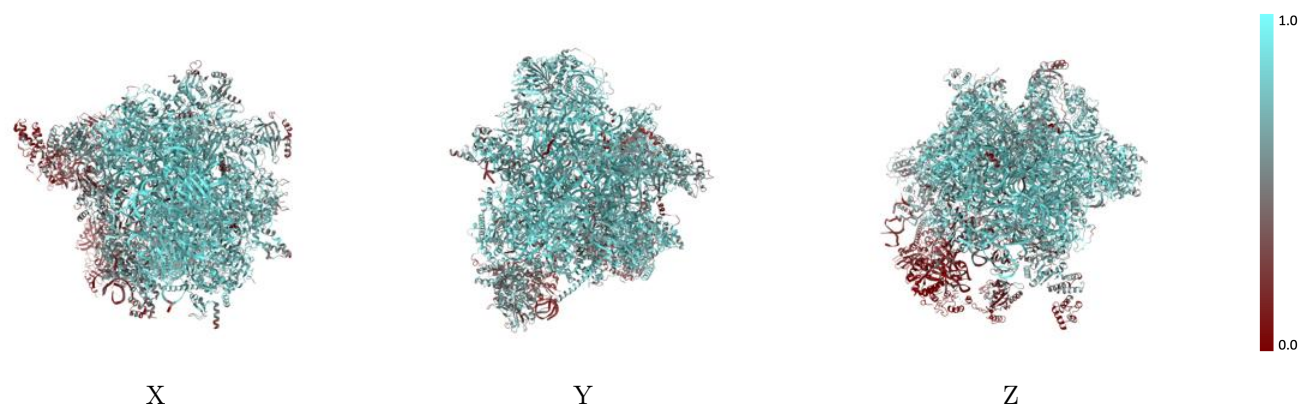
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



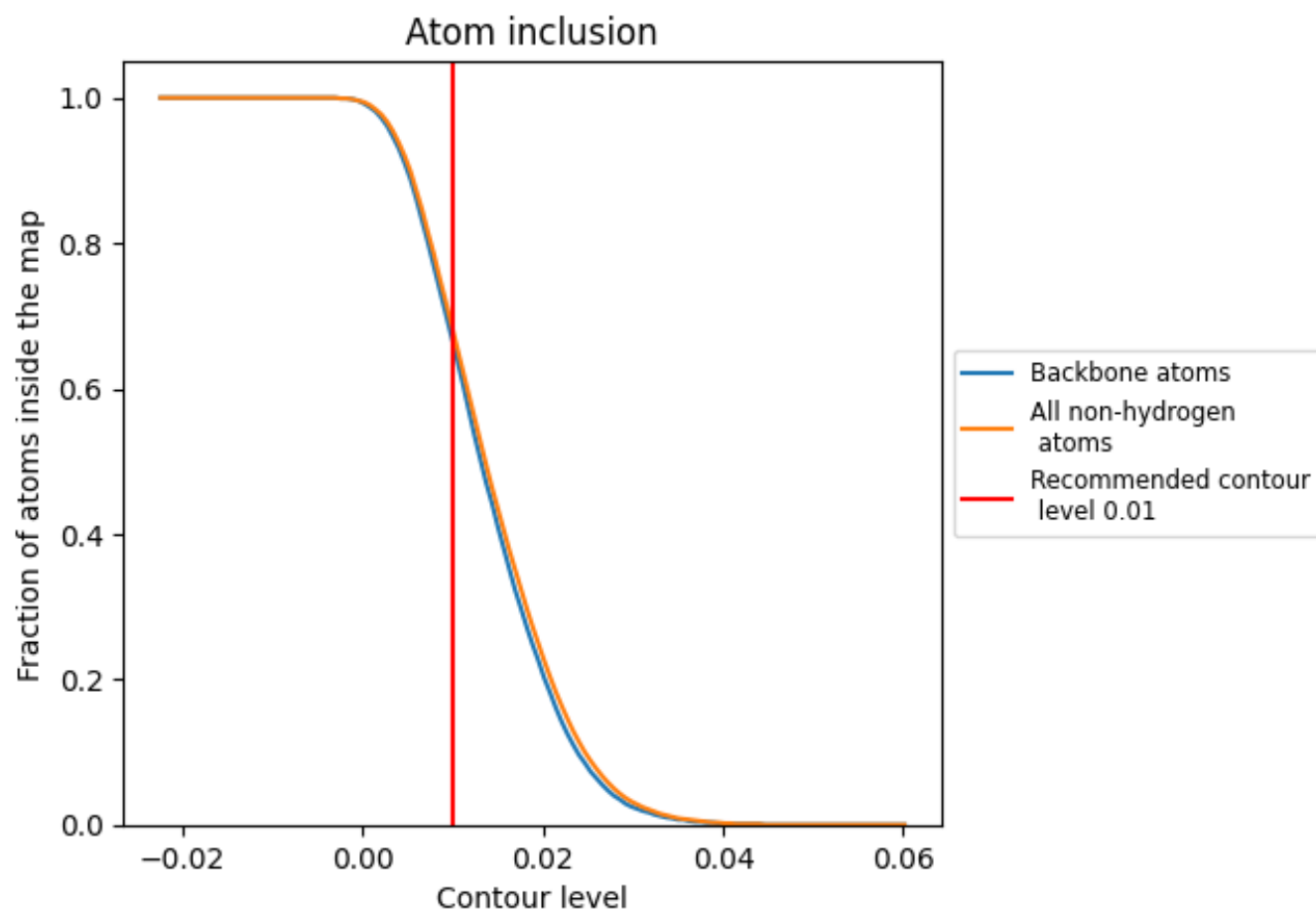
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 68% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.4720
0	 0.7380	 0.5220
1	 0.6400	 0.4980
2	 0.8890	 0.6070
3	 0.8500	 0.5900
4	 0.6490	 0.5120
5	 0.7460	 0.5240
6	 0.5920	 0.4000
7	 0.6300	 0.4520
8	 0.1780	 0.1740
9	 0.7020	 0.5080
A	 0.8150	 0.5180
B	 0.3930	 0.1940
D	 0.7610	 0.5480
E	 0.7910	 0.5470
F	 0.7960	 0.5590
H	 0.6480	 0.4910
I	 0.1680	 0.2080
J	 0.0520	 0.0830
K	 0.8000	 0.5580
L	 0.6970	 0.5260
M	 0.7960	 0.5540
N	 0.4100	 0.3650
O	 0.8010	 0.5500
P	 0.6080	 0.4340
Q	 0.7430	 0.5240
R	 0.8050	 0.5740
S	 0.7300	 0.5320
T	 0.8040	 0.5740
U	 0.8010	 0.5590
V	 0.6780	 0.4970
W	 0.6690	 0.4950
X	 0.7600	 0.5300
Y	 0.7820	 0.5390
Z	 0.7360	 0.5360



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.6350	 0.5130
b	 0.8040	 0.5530
c	 0.7060	 0.4990
d	 0.5140	 0.4190
e	 0.0410	 0.1020
f	 0.1390	 0.1870
g	 0.7790	 0.5300
h	 0.6470	 0.4610
i	 0.8480	 0.5930
j	 0.7010	 0.4930
k	 0.1860	 0.2070
l	 0.0660	 0.0770
m	 0.0820	 0.1440
o	 0.7430	 0.5220
p	 0.5700	 0.4170
q	 0.6730	 0.4390
r	 0.6890	 0.4900
s	 0.7740	 0.5420
t	 0.2770	 0.2280
u	 0.6070	 0.4460
v	 0.4610	 0.3100
w	 0.1360	 0.1530
x	 0.5420	 0.4270
y	 0.5580	 0.4490
z	 0.5210	 0.4480