Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 11:25 AM EDT

PDB ID	:	9PR4 / pdb_00009pr4
EMDB ID	:	EMD-71797
Title	:	In Situ Structure of the Human Mitochondrial Large Subunit 39S in Complex with TACO1
Authors	:	Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on	:	2025-07-23
Resolution	:	2.77 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

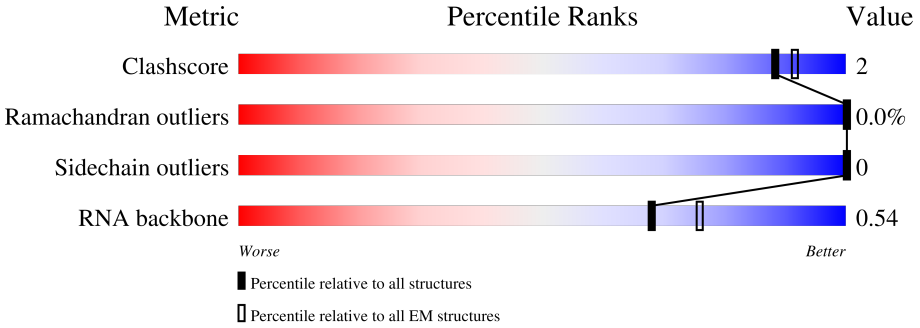
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

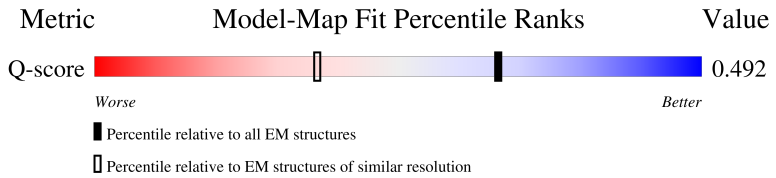
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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

Mol	Chain	Length	Quality of chain
1	0	188	58% 41%
2	1	65	5% 78% 8% 14%
3	2	92	50% 50%

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Mol	Chain	Length	Quality of chain
4	3	188	48% 49%
5	4	103	34% 63%
6	5	423	90% 7%
7	6	380	91% 7%
8	7	338	81% 6% 13%
9	8	206	22% 63% 5% 33%
10	9	137	89% 9%
11	C	297	49% 38% 18% 44%
12	D	305	77% 22%
13	E	348	85% 12%
14	F	311	78% 19%
15	G	198	36% 22% 14% 64%
15	t	198	13% 23% 77%
15	u	198	12% 14% 84%
15	v	198	16% 15% 84%
15	w	198	16% 15% 84%
15	x	198	16% 14% 84%
15	y	198	16% 13% 84%
16	H	267	33% 72% 24%
17	I	261	17% 75% 6% 19%
18	J	192	15% 85% 6% 9%
19	K	178	98%
20	L	145	77% 21%
21	M	296	96%
22	N	251	84% 12%

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Mol	Chain	Length	Quality of chain
23	O	175	83% 5% 12%
24	P	180	78% 20%
25	Q	292	73% 25%
26	R	149	93% 6%
27	S	205	77% 21%
28	T	206	80% 19%
29	U	153	13% 95% 5%
30	V	216	91% 5%
31	W	148	76% 22%
32	X	256	93% 5%
33	Y	250	72% 28%
34	Z	161	74% 24%
35	b	215	68% 30%
36	d	306	15% 72% 13% 15%
37	e	279	36% 76% 9% 15%
38	g	166	79% 19%
39	h	158	68% 30%
40	i	128	75% 24%
41	j	123	5% 76% 24%
42	k	112	88% 9%
43	l	138	5% 58% 41%
44	m	128	20% 45% 5% 49%
45	n	43	49% 74% 26%
46	o	102	90% 8%
47	q	222	23% 70% 9% 20%

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Mol	Chain	Length	Quality of chain
48	r	196	81% 17%
49	z	325	75% 67% 11% 22%
50	A	1558	75% 23%
51	c	332	85% 14%
52	f	212	21% 66% 8% 26%
53	p	206	8% 70% 29%
54	s	439	85% 12%
55	OX	435	6% 9% 90%
56	a	142	13% 70% 27%
57	B	72	12% 56% 35% 10%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 111602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	110	898	554	176	162	6	0	0

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	56	464	296	89	77	2	0	0

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	233	83	60	1	0	0

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	95	832	539	162	128	3	0	0

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	342	217	72	49	4	0	0

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	394	3210	2073	560	566	11	0	0

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	354	2948	1881	525	533	9	0	0

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	294	2390	1529	405	438	18	0	0

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	139	1179	752	207	218	2	0	0

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	124	997	644	170	181	2	0	0

- Molecule 11 is a protein called Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	166	1286	796	226	258	6	0	0

- Molecule 12 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	238	1859	1157	376	317	9	0	0

- Molecule 13 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	305	2406	1545	418	432	11	0	0

- Molecule 14 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	252	2031	1305	370	350	6	0	0

- Molecule 15 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	G	72	558	358	97	103	0	0
			Total	C	N	O		
15	t	46	354	228	56	70	0	0
			Total	C	N	O		
15	u	32	257	168	40	49	0	0
			Total	C	N	O		
15	v	32	257	168	40	49	0	0
			Total	C	N	O		
15	w	31	245	159	39	47	0	0
			Total	C	N	O		
15	x	31	245	159	39	47	0	0
			Total	C	N	O		
15	y	31	245	159	39	47	0	0

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	202	1661	1067	304	286	4	0	0

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	212	1695	1088	304	292	11	0	0

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	175	1330	847	237	244	2	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	178	1455	936	259	253	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP H2QWN0
K	132	TYR	ASP	conflict	UNP H2QWN0

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	115	890	559	171	155	5	0	0

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	291	2327	1483	430	408	6	0	0

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	222	1786	1143	326	307	10	0	0

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	154	1259	792	241	219	7	0	0

- Molecule 24 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	144	1173	733	224	211	5	0	0

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	220	1834	1174	326	325	9	0	0

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	140	1154	732	231	187	4	0	0

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	161	1293	835	227	227	4	0	0

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	166	1369	875	254	233	7	0	0

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	152	1248	786	234	225	3	0	0

- Molecule 30 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	205	1676	1068	298	302	8	0	0

- Molecule 31 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	116	904	577	171	153	3	0	0

- Molecule 32 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	244	2044	1322	352	365	5	0	0

- Molecule 33 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	181	1556	995	298	259	4	0	0

- Molecule 34 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	122	996	636	186	171	3	0	0

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	150	1193	742	231	217	3	0	0

- Molecule 36 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	259	2124	1357	369	384	14	0	0

- Molecule 37 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	238	1931	1222	339	364	6	0	0

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	g	134	1113	719	193	199	2	0	0

- Molecule 39 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	h	110	895	568	156	168	3	0	0

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	i	97	828	532	165	127	4	0	0

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	j	94	745	463	144	136	2	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	k	102	774	479	148	142	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q96EL3

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	l	82	688	437	120	128	3	0	0

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	m	65	541	333	112	94	2	0	0

- Molecule 45 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	n	32	160	96	32	32	0	0

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	94	798	501	165	129	3	0	0

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	177	1495	929	292	269	5	0	0

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	r	162	1322	839	252	223	8	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	z	252	2027	1304	336	381	6	0	0

- Molecule 50 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	A	1558	33070	14843	5963	10706	1558	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 2756414513
A	?	-	C	deletion	GB 2756414513
A	?	-	U	deletion	GB 2756414513

- Molecule 51 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	c	286	2299	1470	397	423	9	0	0

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	f	157	1252	799	207	242	4	0	0

- Molecule 53 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	p	147	1205	748	228	225	4	0	0

- Molecule 54 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	s	385	3148	2018	558	558	14	0	0

- Molecule 55 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	OX	42	359	221	75	62	1	0	0

- Molecule 56 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	a	103	865	543	155	162	5	0	0

- Molecule 57 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	B	72	1524	685	269	498	72	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	0	1	1	1	0
			Total	Zn	
58	4	1	1	1	0

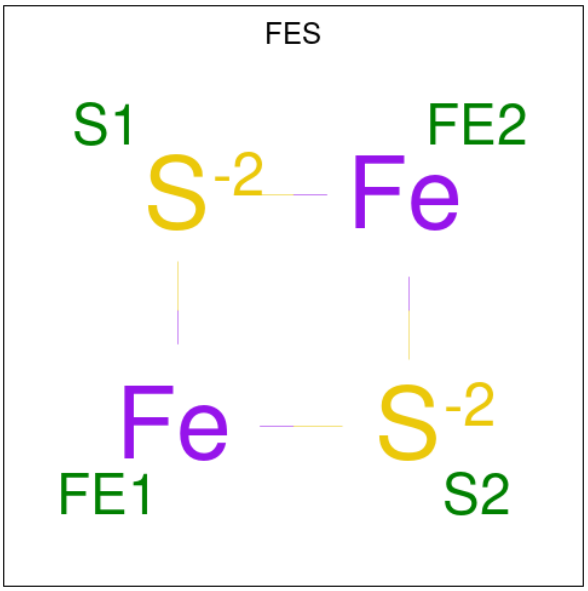
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
59	3	1	1	1	0
			Total	K	
59	6	1	1	1	0
			Total	K	
59	D	1	1	1	0
			Total	K	
59	M	1	1	1	0
			Total	K	
59	N	1	1	1	0
			Total	K	
59	W	1	1	1	0
			Total	K	
59	o	1	1	1	0
			Total	K	
59	A	29	29	29	0

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

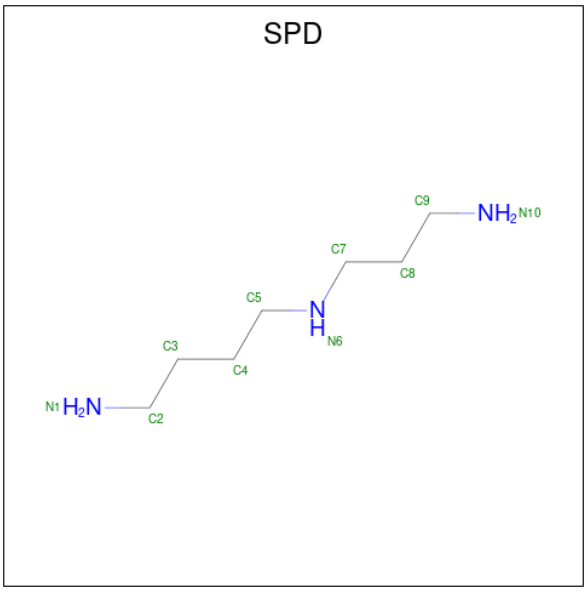
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	D	2	2	2	0
			Total	Mg	
60	E	1	1	1	0
			Total	Mg	
60	g	1	1	1	0
			Total	Mg	
60	A	137	137	137	0

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



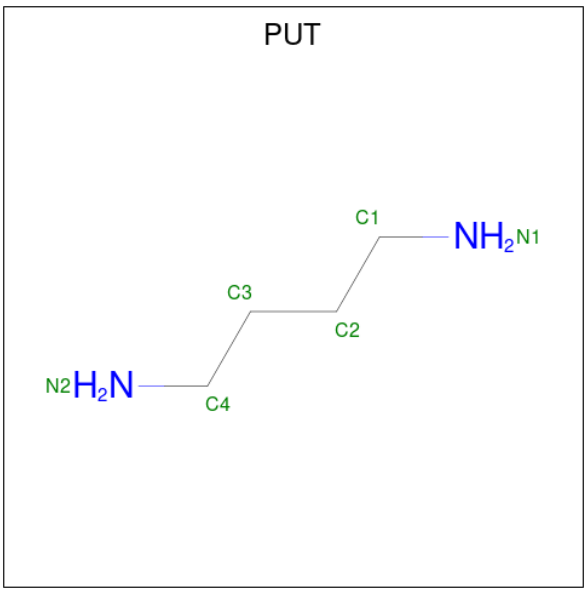
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
61	r	1	4	2	2	0

- Molecule 62 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



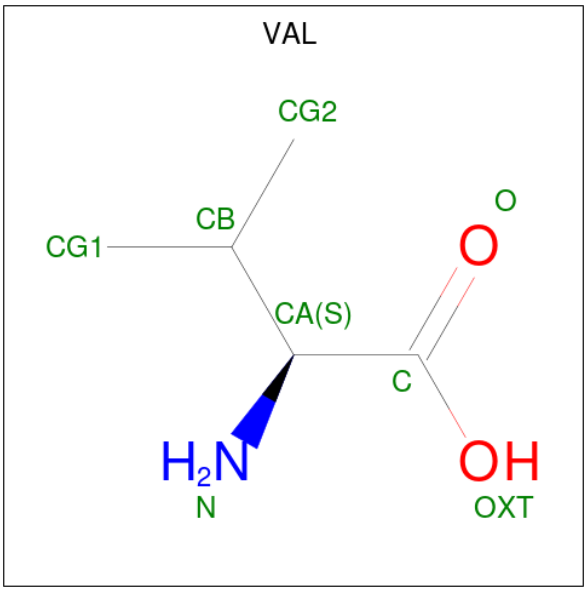
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
62	A	1	10	7	3	0
62	A	1	Total	C	N	0
			10	7	3	

- Molecule 63 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	A	1	6	4	2	0

- Molecule 64 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



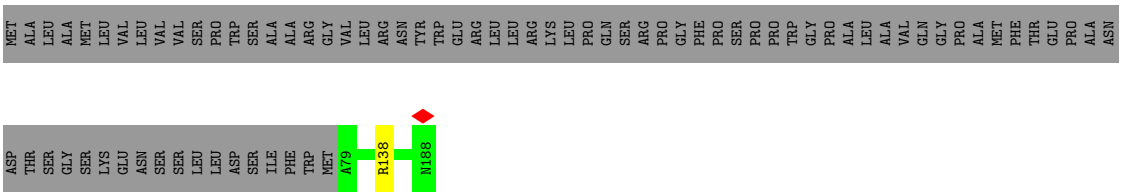
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
64	B	1	7	5	1	1	0

3 Residue-property plots (i)

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

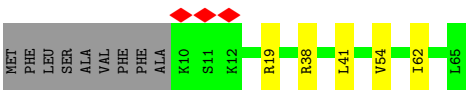
- Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:



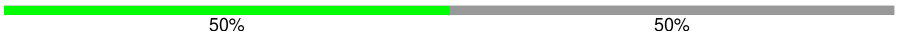
- Molecule 2: 39S ribosomal protein L33, mitochondrial

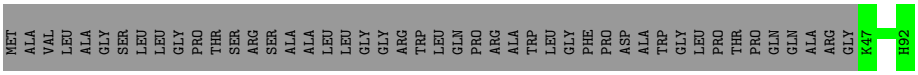
Chain 1:



- Molecule 3: 39S ribosomal protein L34, mitochondrial

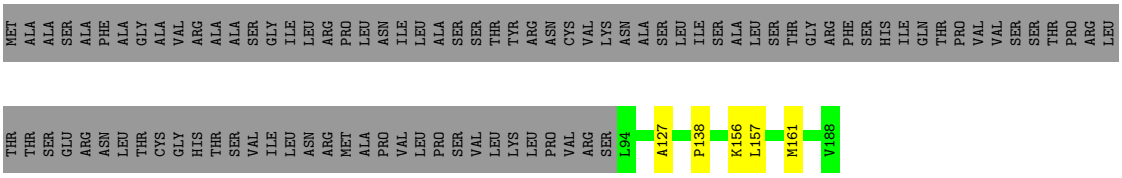
Chain 2:





- Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3:



- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:

MET ALA ASN LEU PHE ILE ARG LYS MET VAL ASN PRO LEU LEU TYR LEU SER ARG HIS THR VAL LYS PRO ARG ALA LEU SER THR PHE LEU PHE GLY SER ILE ARG GLY ALA ALA PRO VAL ALA VAL GLU PRO GLY ALA ALA VAL ARG SER LEU LEU SER PRO GLY LEU LEU PRO HIS LEU

LEU PRO ALA LEU GLY F66 K69 L72 M103

• Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:

MET ALA LEU ALA SER GLY PRO ALA ARG ARG ALA LEU ALA GLY SER GLY GLN LEU GLY LEU GLY GLY PHE GLY ALA PRO ARG ARG GLY A30 L98 L113 I129 Q165 T166 T167 T175 R201 R215 T232 D272 A311 F354 L364 L373 R395

L417 A423

• Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:

MET ALA ALA PRO TRP TRP ARG ALA ALA LEU CYS GLU CYS ARG ARG TRP ARG GLY PHE SER THR SER ALA VAL LEU GLY R27 K81 T82 D83 P84 K85 E86 R106 L161 E181 V187 Y206 W214 L225 H234 P257 D276 T300 F319 Y380

• Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:

MET GLU ALA LEU ALA MET GLY SER ARG ALA LEU ARG LEU TRP LEU VAL ALA PRO GLY GLY GLY ILE LYS TRP ARG PHE ILE ALA THR SER SER ALA SER Q34 R61 L107 P112 W113 D114 K117 L128 N139 M150 G151 C152 V153 I154 L166 V174 Y181

F260 P267 F276 L286 R296 L302 P303 V304 L317 D327 GLN SER LYS ALA THR GLU GLU CYS THR SER THR

• Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:

MET THR ALA SER VAL LEU ARG SER ILE SER LEU ALA LEU ARG PRO THR SER GLY LEU LEU GLY THR TRP GLN THR GLN LEU ARG GLU THR HIS GLN ARG ALA SER LEU LEU SER PHE TRP GLU LEU ILE PRO MET ARG SER GLU PRO LEU ARG LYS LYS LYS LYS VAL ASP PRO LYS LYS

ASP GLN GLU ALA K65 E66 R67 L68 K69 R70 K71 I72 R73 K74 L75 E76 K77 A78 T79 Q80 F88 P91 L92 L95 D96 K97 A98 R99 Q103 V104 E105 L106 L117 K125 I136 R137 A138 E141 E145 E148 E149 L152 E153 L157 R164 K173

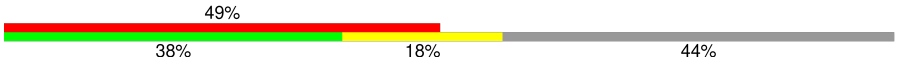
I182 P187 R191 Y192 N193 D194 V198 Y199 T200 Q201 V202 E203 PHE LYS ARG

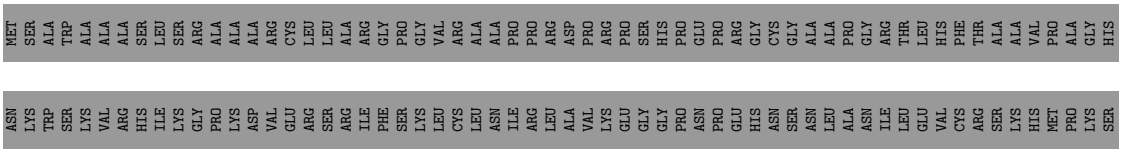
• Molecule 10: 39S ribosomal protein L41, mitochondrial

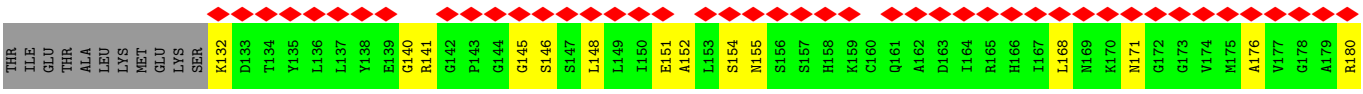
Chain 9:

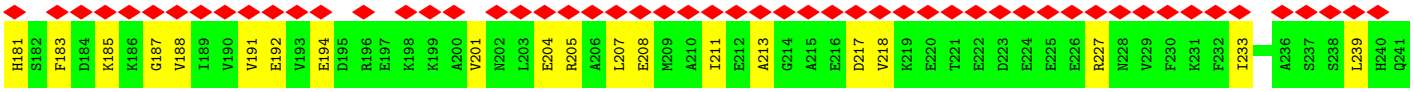
• Molecule 11: Translational activator of cytochrome c oxidase 1

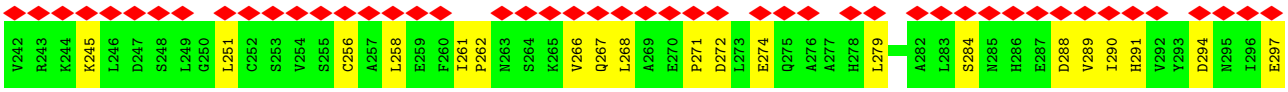
Chain C:





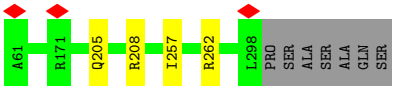






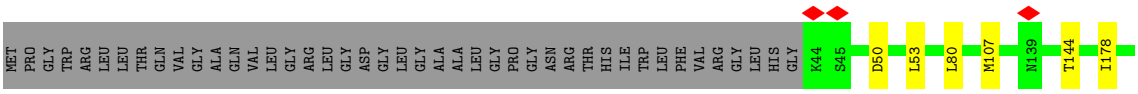
• Molecule 12: 39S ribosomal protein L2, mitochondrial

Chain D:



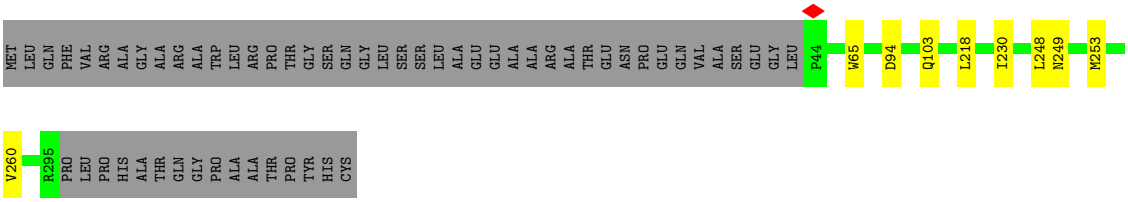
• Molecule 13: 39S ribosomal protein L3, mitochondrial

Chain E:



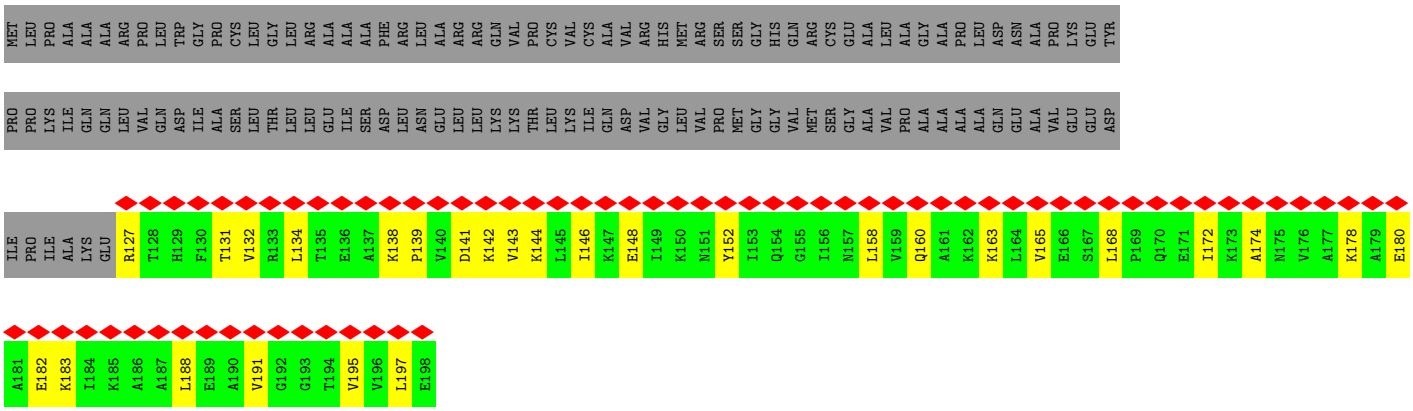
• Molecule 14: 39S ribosomal protein L4, mitochondrial

Chain F:



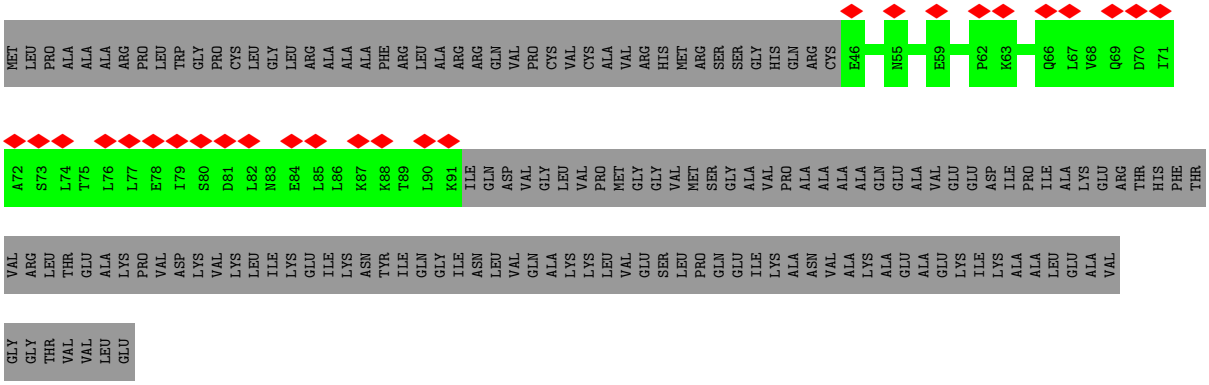
• Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain G:



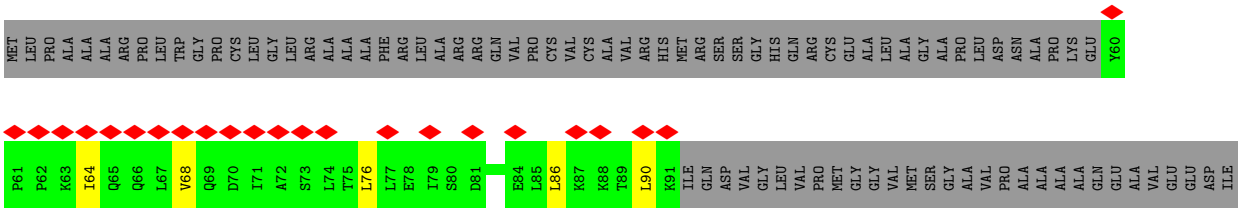
• Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain t:



• Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain u:



PRO ILE ALA LYS GLU ARG THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS ASN TYR ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL ALA LYS ALA GLU ALA

GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain v: 16% 15% 84%

MET LEU PRO ALA ALA ALA ARG PRO LEU TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA ALA PHE ARG LEU ALA ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS GLN ARG CYS GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU Y60

P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

ILE PRO ILE ALA LYS GLU ARG THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS ASN TYR ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL ALA LYS ALA GLU

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain w: 16% 15% 84%

MET LEU PRO ALA ALA ALA ARG PRO LEU TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA ALA PHE ARG LEU ALA ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS GLN ARG CYS GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR

P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

ILE PRO ILE ALA LYS GLU ARG THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS ASN TYR ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL ALA LYS ALA GLU

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain x: 16% 14% 84%

MET LEU PRO ALA ALA ALA ARG PRO LEU TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA ALA PHE ARG LEU ALA ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS GLN ARG CYS GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR

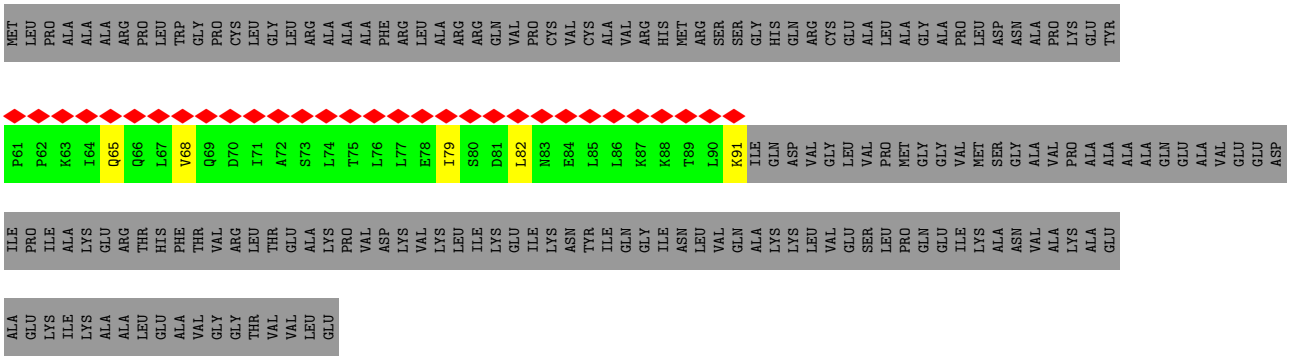
P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

ILE PRO ILE ALA LYS GLU ARG THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS ASN TYR ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL ALA LYS ALA GLU

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

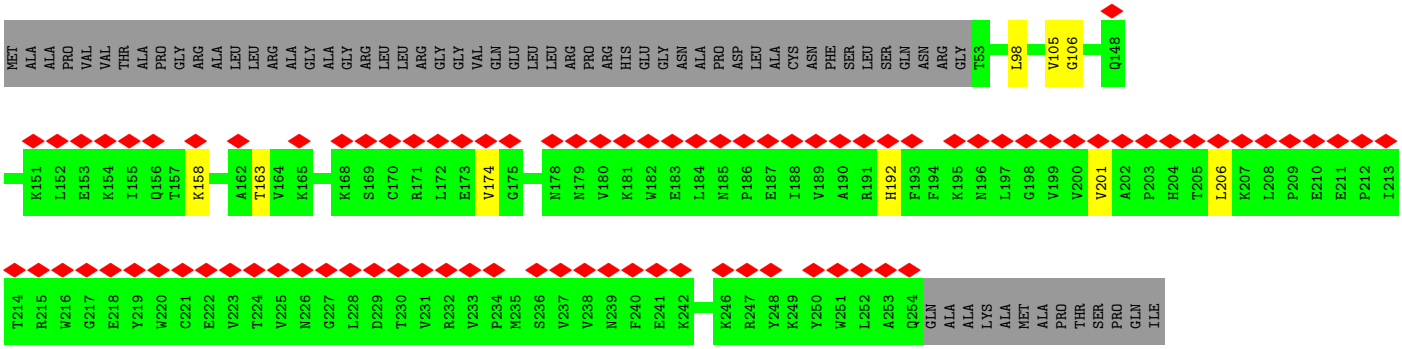
- Molecule 15: 39S ribosomal protein L12, mitochondrial

Chain y:



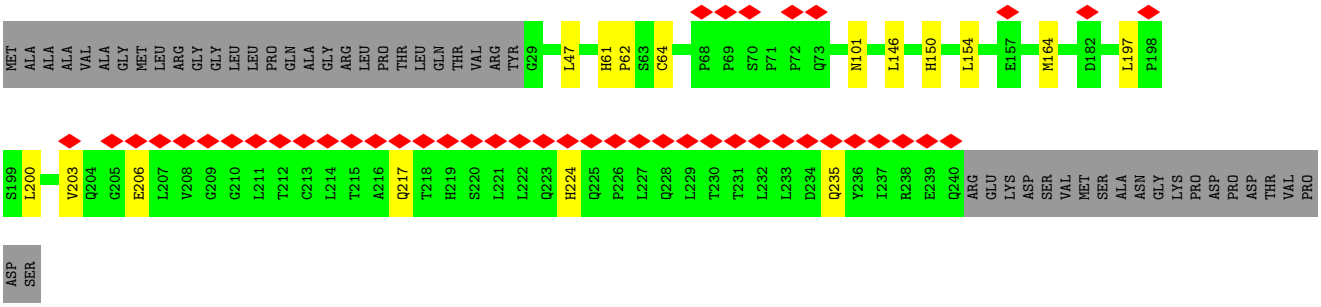
- Molecule 16: 39S ribosomal protein L9, mitochondrial

Chain H:



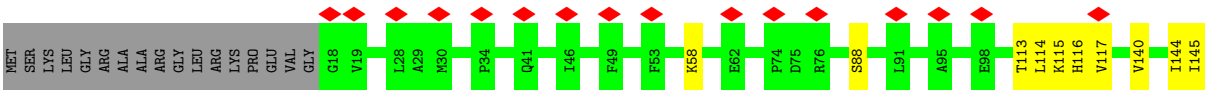
- Molecule 17: 39S ribosomal protein L10, mitochondrial

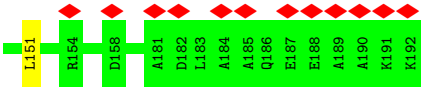
Chain I:



- Molecule 18: 39S ribosomal protein L11, mitochondrial

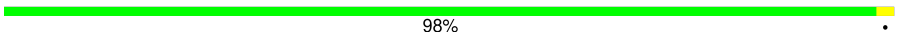
Chain J:





• Molecule 19: Large ribosomal subunit protein uL13m

Chain K:

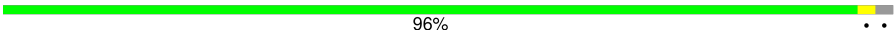


• Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L:

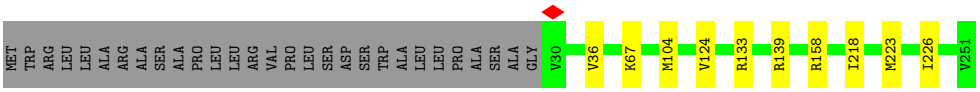
• Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:



• Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:

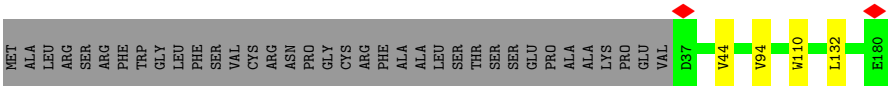


• Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:

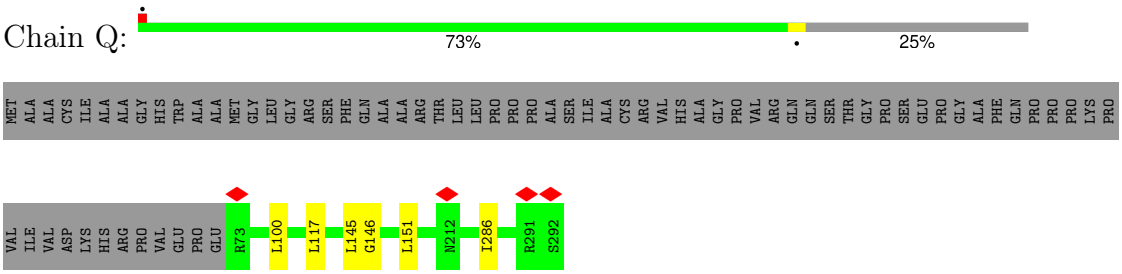
• Molecule 24: 39S ribosomal protein L18, mitochondrial

Chain P:



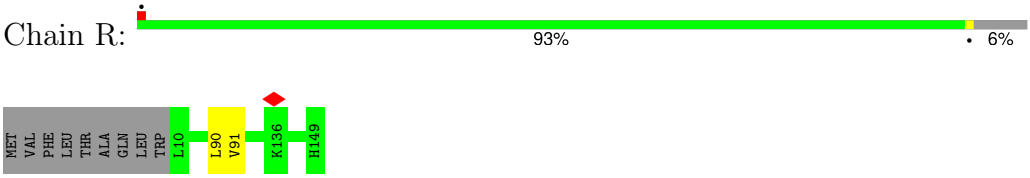
• Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q:



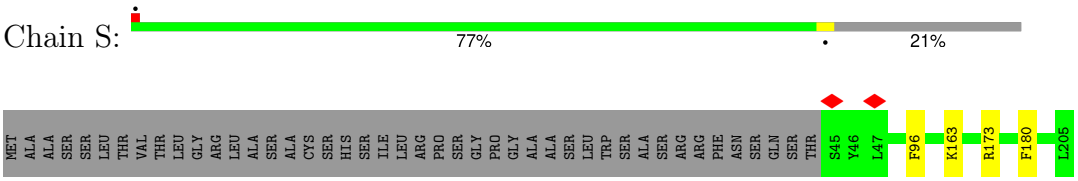
- Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R:



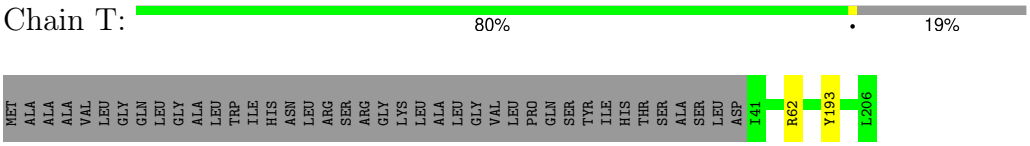
- Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S:



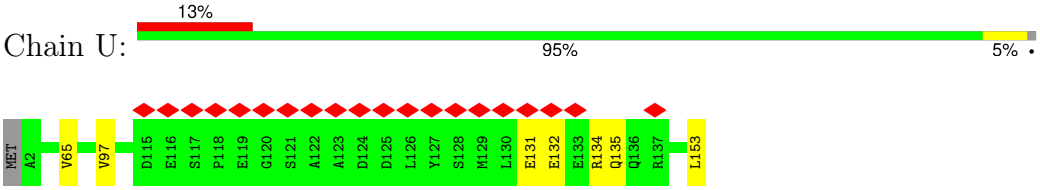
- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T:



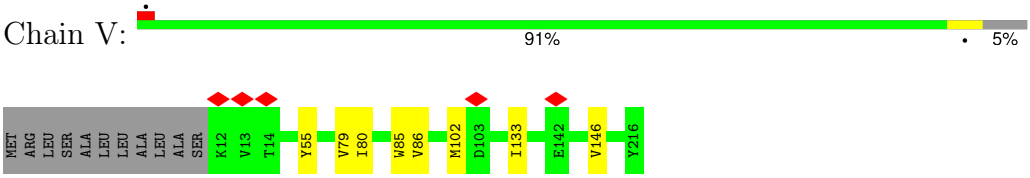
- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U:



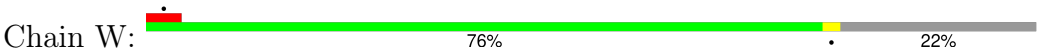
- Molecule 30: 39S ribosomal protein L24, mitochondrial

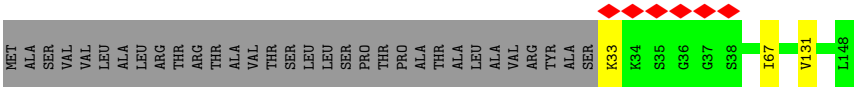
Chain V:



- Molecule 31: 39S ribosomal protein L27, mitochondrial

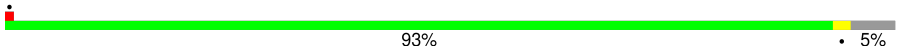
Chain W:

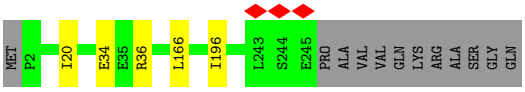




• Molecule 32: 39S ribosomal protein L28, mitochondrial

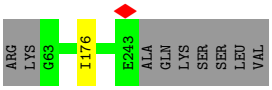
Chain X:





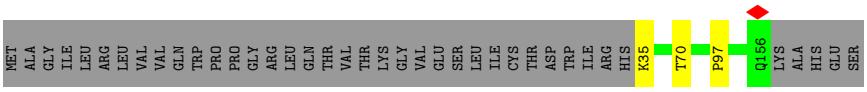
• Molecule 33: 39S ribosomal protein L47, mitochondrial

Chain Y:



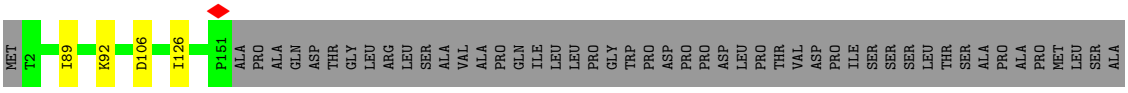
• Molecule 34: 39S ribosomal protein L30, mitochondrial

Chain Z:



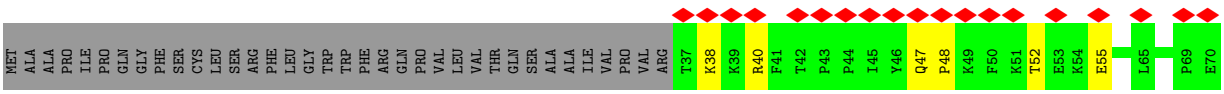
• Molecule 35: 39S ribosomal protein L43, mitochondrial

Chain b:



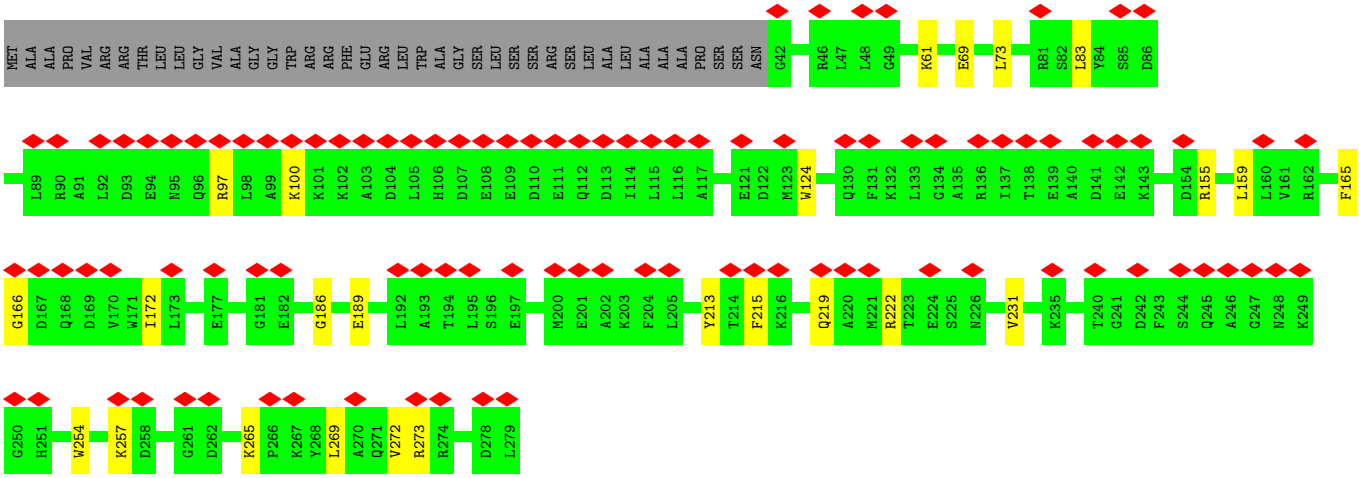
• Molecule 36: 39S ribosomal protein L45, mitochondrial

Chain d:



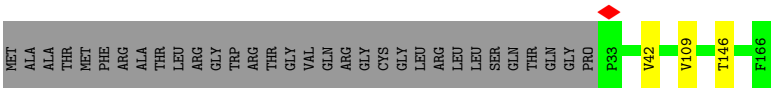
• Molecule 37: 39S ribosomal protein L46, mitochondrial

Chain e:



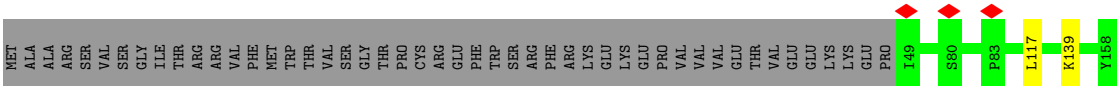
• Molecule 38: 39S ribosomal protein L49, mitochondrial

Chain g:



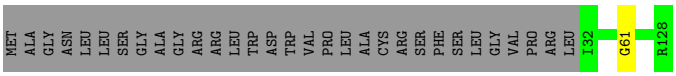
• Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h:



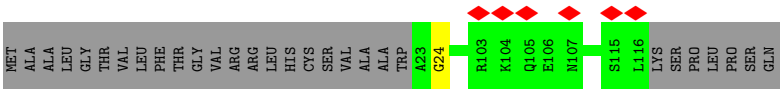
• Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i:



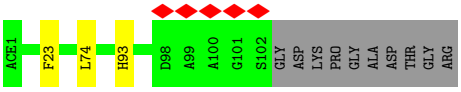
• Molecule 41: 39S ribosomal protein L52, mitochondrial

Chain j:



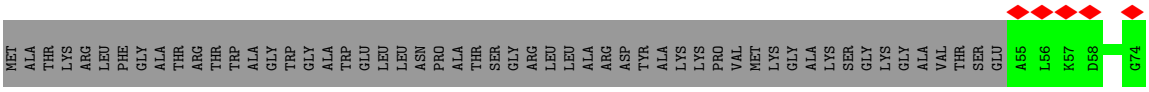
• Molecule 42: Large ribosomal subunit protein mL53

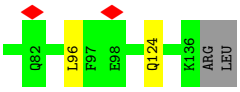
Chain k:



• Molecule 43: 39S ribosomal protein L54, mitochondrial

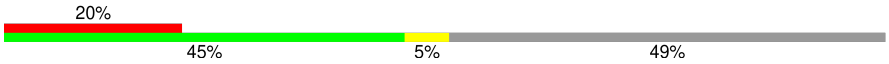
Chain l:

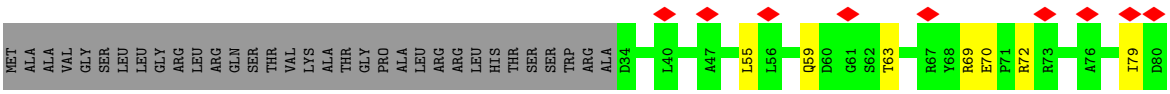


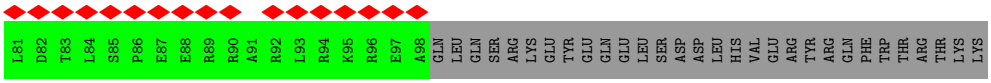


• Molecule 44: 39S ribosomal protein L55, mitochondrial

Chain m:

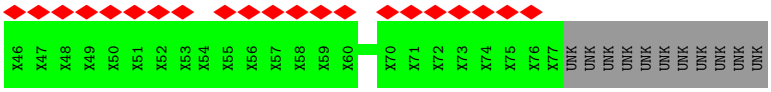






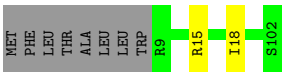
• Molecule 45: Nascent polypeptide

Chain n:



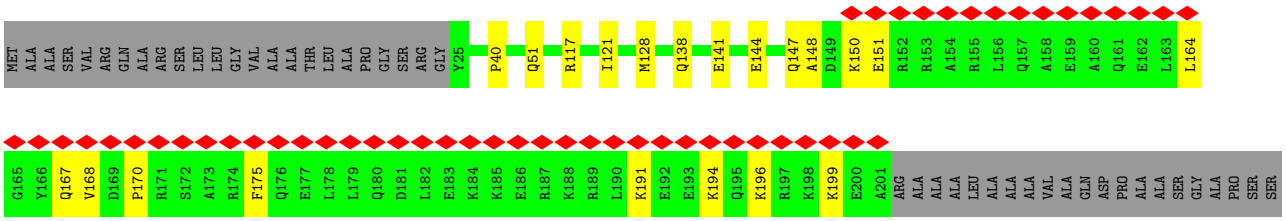
• Molecule 46: Ribosomal protein 63, mitochondrial

Chain o:



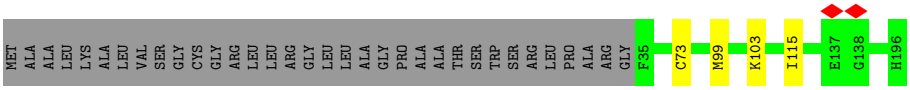
• Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



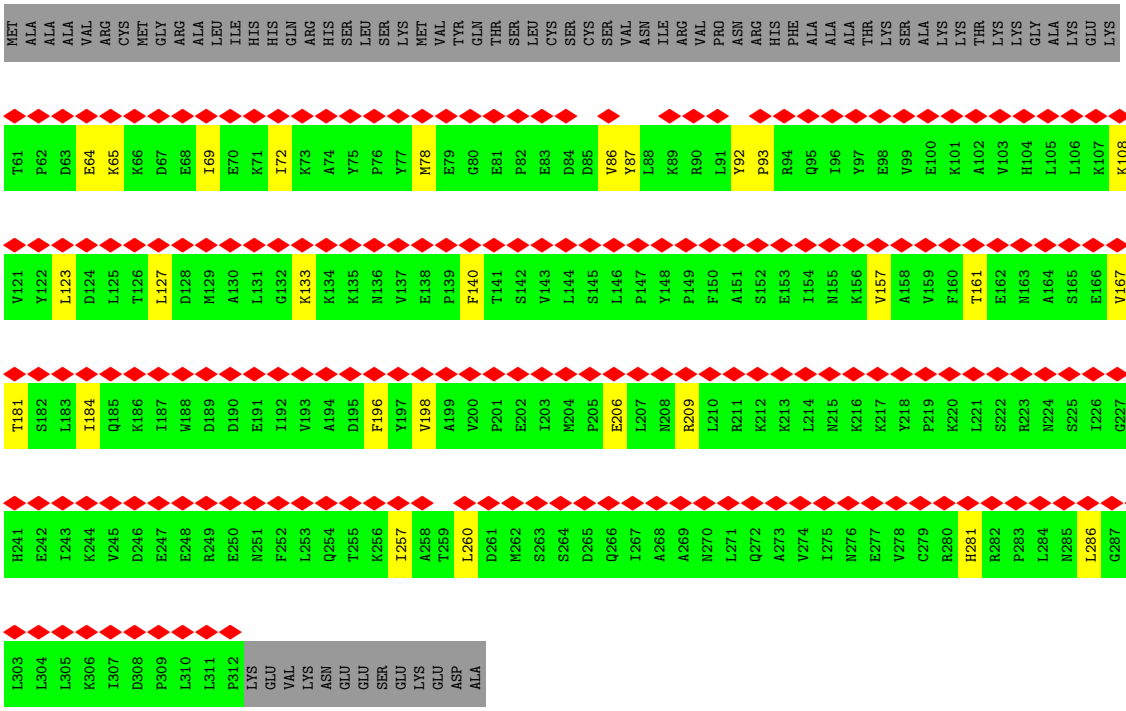
- Molecule 48: 39S ribosomal protein S18a, mitochondrial

Chain r:



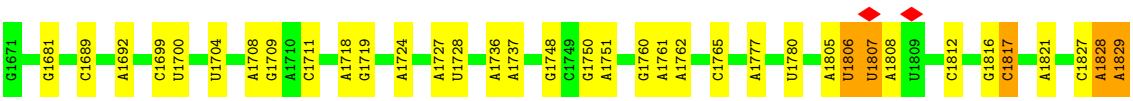
- Molecule 49: Large ribosomal subunit protein uL1m

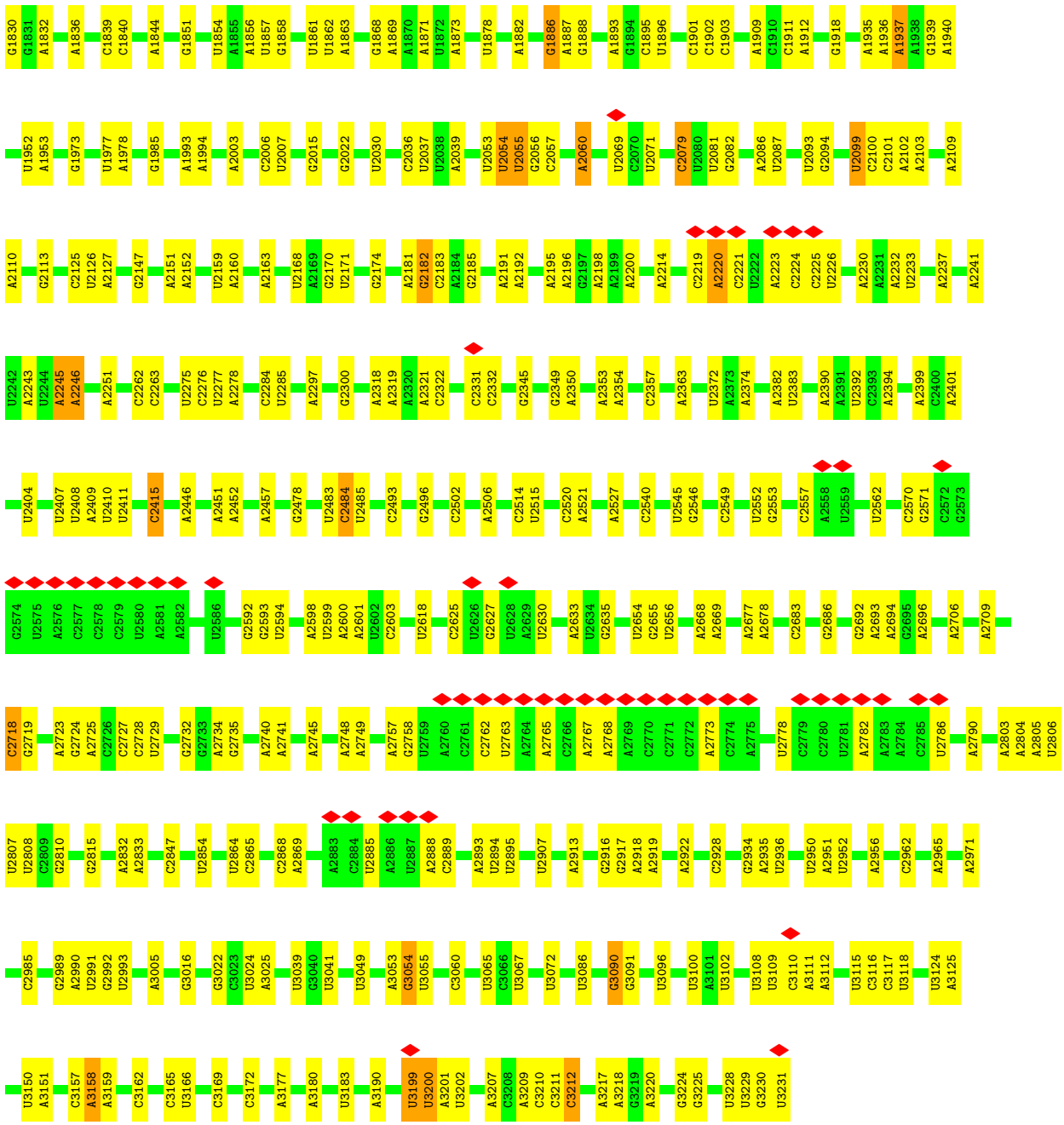
Chain z:



- Molecule 50: 16S mitochondrial rRNA

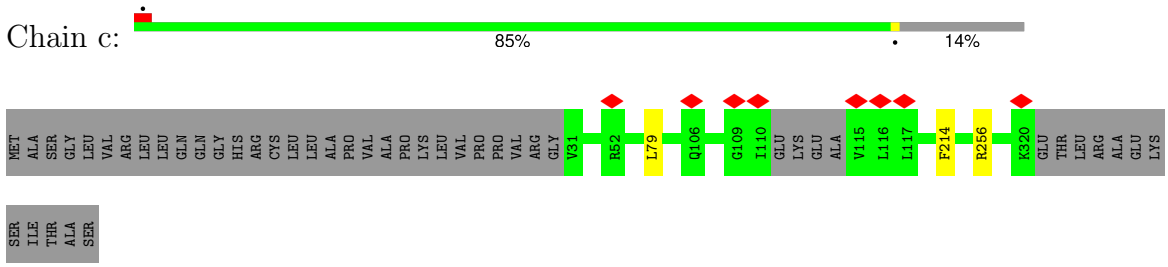
Chain A:





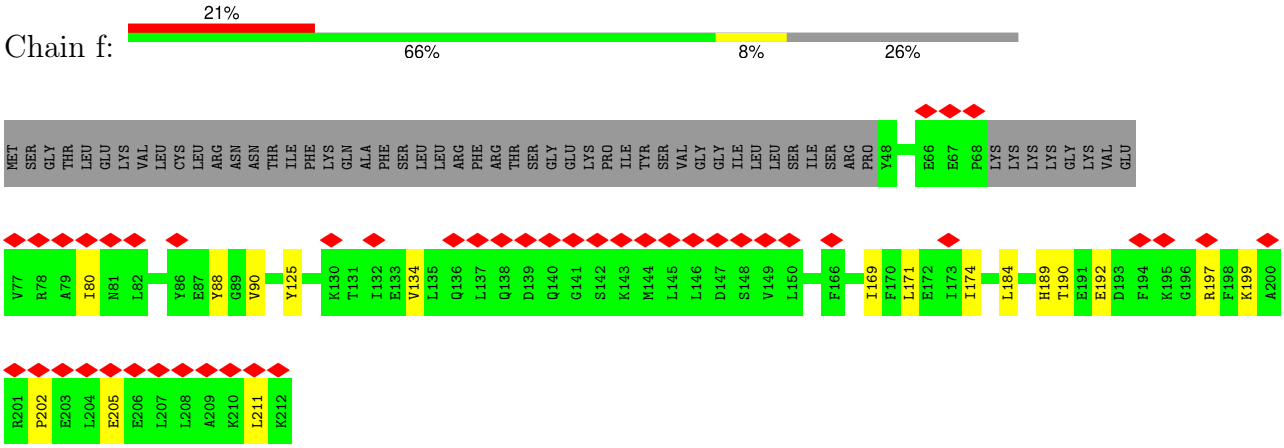
• Molecule 51: 39S ribosomal protein L44, mitochondrial

Chain c:



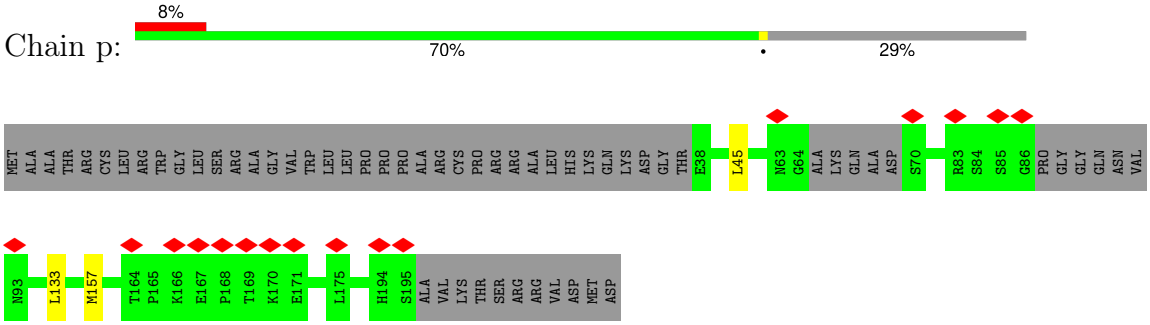
• Molecule 52: 39S ribosomal protein L48, mitochondrial

Chain f:



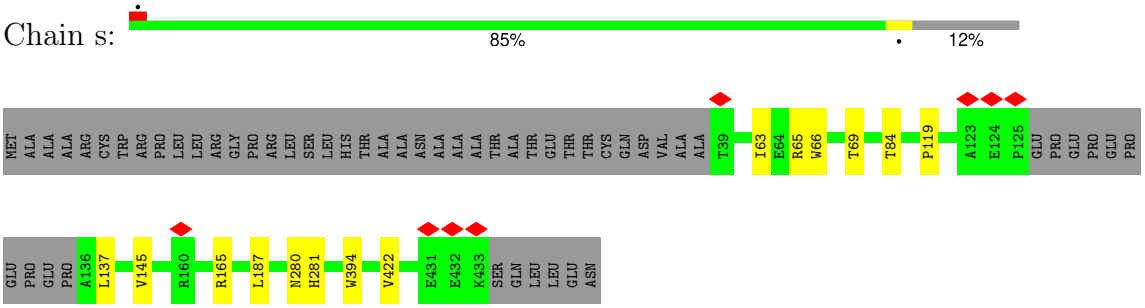
- Molecule 53: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



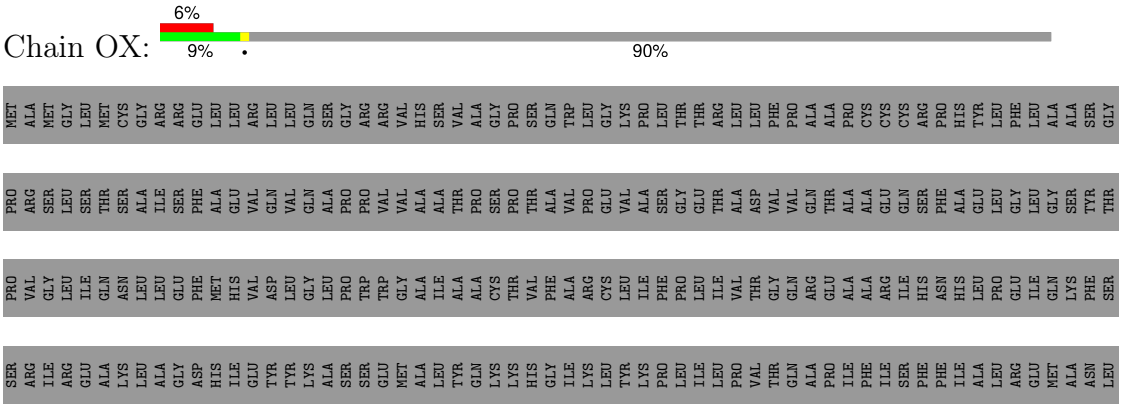
- Molecule 54: 39S ribosomal protein S30, mitochondrial

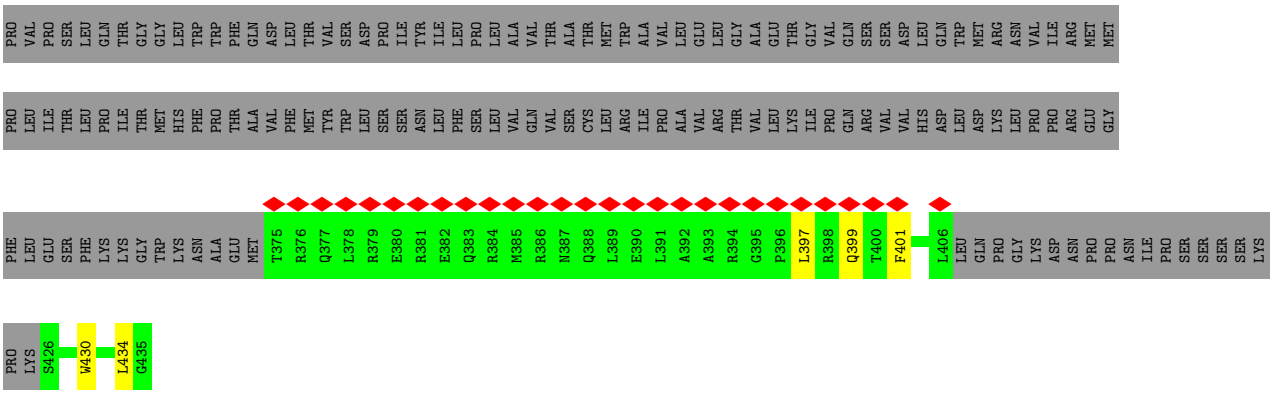
Chain s:



- Molecule 55: Mitochondrial inner membrane protein OXA1L

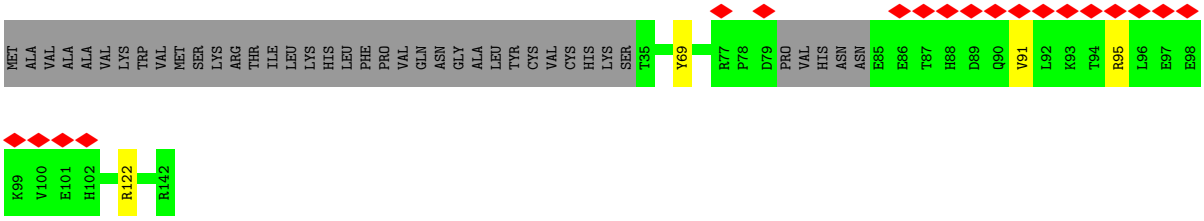
Chain OX:





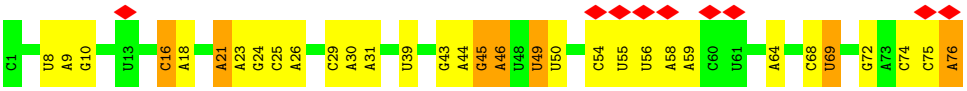
- Molecule 56: 39S ribosomal protein L42, mitochondrial

Chain a:



- Molecule 57: mitochondrial tRNAVal

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.795	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, FES, ZN, ACE, OMU, PSU, PUT, SPD, MG, 1MA, K, OMG

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	0	0.22	0/913	0.25	0/1224
2	1	0.21	0/469	0.28	0/621
3	2	0.26	0/383	0.28	0/507
4	3	0.26	0/853	0.27	0/1136
5	4	0.24	0/350	0.23	0/461
6	5	0.20	0/3305	0.28	0/4502
7	6	0.18	0/3043	0.28	0/4140
8	7	0.19	0/2447	0.29	0/3310
9	8	0.13	0/1204	0.29	0/1621
10	9	0.20	0/1025	0.26	0/1379
11	C	0.14	0/1302	0.31	0/1751
12	D	0.21	0/1896	0.28	0/2549
13	E	0.23	0/2475	0.30	0/3355
14	F	0.25	0/2090	0.30	0/2842
15	G	0.19	0/562	0.52	0/754
15	t	0.15	0/358	0.32	0/486
15	u	0.22	0/259	0.39	0/350
15	v	0.15	0/259	0.36	0/350
15	w	0.20	0/246	0.50	0/331
15	x	0.14	0/246	0.35	0/331
15	y	0.16	0/246	0.42	0/331
16	H	0.15	0/1698	0.29	0/2292
17	I	0.16	0/1731	0.31	0/2345
18	J	0.14	0/1348	0.29	0/1813
19	K	0.25	0/1497	0.27	0/2031
20	L	0.20	0/905	0.27	0/1218
21	M	0.24	0/2381	0.30	0/3212
22	N	0.21	0/1833	0.27	0/2468
23	O	0.23	0/1283	0.27	0/1727
24	P	0.20	0/1199	0.25	0/1623
25	Q	0.20	0/1875	0.26	0/2523
26	R	0.25	0/1175	0.26	0/1572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	S	0.25	0/1320	0.31	0/1789
28	T	0.23	0/1403	0.26	0/1886
29	U	0.24	0/1279	0.34	0/1730
30	V	0.19	0/1721	0.26	0/2333
31	W	0.24	0/926	0.26	0/1244
32	X	0.21	0/2099	0.25	0/2837
33	Y	0.23	0/1593	0.24	0/2136
34	Z	0.23	0/1021	0.27	0/1378
35	b	0.24	0/1218	0.28	0/1649
36	d	0.17	0/2181	0.32	0/2949
37	e	0.13	0/1970	0.31	0/2658
38	g	0.23	0/1151	0.28	0/1569
39	h	0.17	0/918	0.25	0/1249
40	i	0.26	0/850	0.27	0/1135
41	j	0.20	0/760	0.23	0/1023
42	k	0.14	0/783	0.23	0/1057
43	l	0.13	0/707	0.27	0/960
44	m	0.10	0/549	0.29	0/737
46	o	0.24	0/819	0.27	0/1097
47	q	0.17	0/1529	0.30	0/2055
48	r	0.22	0/1362	0.29	0/1846
49	z	0.14	0/2067	0.35	0/2793
50	A	0.26	0/36876	0.29	0/57402
51	c	0.20	0/2347	0.25	0/3171
52	f	0.16	0/1273	0.32	0/1716
53	p	0.17	0/1223	0.27	0/1641
54	s	0.23	0/3231	0.29	0/4389
55	OX	0.18	0/366	0.49	0/491
56	a	0.21	0/891	0.34	0/1208
57	B	0.17	0/1626	0.27	0/2523
All	All	0.22	0/116915	0.29	0/165806

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	1	0
2	1	464	0	511	3	0
3	2	377	0	406	0	0
4	3	832	0	883	4	0
5	4	342	0	361	2	0
6	5	3210	0	3206	9	0
7	6	2948	0	2841	6	0
8	7	2390	0	2397	11	0
9	8	1179	0	1205	13	0
10	9	997	0	987	1	0
11	C	1286	0	1270	33	0
12	D	1859	0	1920	2	0
13	E	2406	0	2415	5	0
14	F	2031	0	2065	6	0
15	G	558	0	612	20	0
15	t	354	0	377	0	0
15	u	257	0	283	4	0
15	v	257	0	283	1	0
15	w	245	0	275	3	0
15	x	245	0	275	2	0
15	y	245	0	275	4	0
16	H	1661	0	1734	6	0
17	I	1695	0	1785	12	0
18	J	1330	0	1407	8	0
19	K	1455	0	1452	2	0
20	L	890	0	941	2	0
21	M	2327	0	2395	6	0
22	N	1786	0	1817	9	0
23	O	1259	0	1294	5	0
24	P	1173	0	1165	3	0
25	Q	1834	0	1872	4	0
26	R	1154	0	1214	2	0
27	S	1293	0	1365	3	0
28	T	1369	0	1410	3	0
29	U	1248	0	1228	4	0
30	V	1676	0	1687	5	0
31	W	904	0	934	2	0
32	X	2044	0	2060	3	0
33	Y	1556	0	1597	1	0
34	Z	996	0	1044	2	0
35	b	1193	0	1191	3	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	2124	0	2125	28	0
37	e	1931	0	1916	17	0
38	g	1113	0	1097	2	0
39	h	895	0	881	2	0
40	i	828	0	857	1	0
41	j	745	0	746	1	0
42	k	774	0	784	2	0
43	l	688	0	673	2	0
44	m	541	0	564	5	0
45	n	160	0	40	0	0
46	o	798	0	804	2	0
47	q	1495	0	1492	15	0
48	r	1322	0	1348	3	0
49	z	2027	0	2076	21	0
50	A	33070	0	16793	104	0
51	c	2299	0	2320	2	0
52	f	1252	0	1269	16	0
53	p	1205	0	1223	2	0
54	s	3148	0	3131	8	0
55	OX	359	0	355	5	0
56	a	865	0	829	3	0
57	B	1524	0	779	16	0
58	0	1	0	0	0	0
58	4	1	0	0	0	0
59	3	1	0	0	0	0
59	6	1	0	0	0	0
59	A	29	0	0	0	0
59	D	1	0	0	0	0
59	M	1	0	0	0	0
59	N	1	0	0	0	0
59	W	1	0	0	0	0
59	o	1	0	0	0	0
60	A	137	0	0	0	0
60	D	2	0	0	0	0
60	E	1	0	0	0	0
60	g	1	0	0	0	0
61	r	4	0	0	0	0
62	A	20	0	38	0	0
63	A	6	0	12	0	0
64	B	7	0	8	2	0
All	All	111602	0	95515	397	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 2.

All (397) 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)
17:I:64:CYS:HB3	48:r:73:CYS:SG	2.20	0.80
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.66	0.76
28:T:62:ARG:HE	36:d:230:ARG:HD2	1.51	0.75
14:F:103:GLN:HE22	14:F:249:ASN:HD22	1.35	0.75
15:G:143:VAL:HA	15:G:146:ILE:HG12	1.71	0.73
11:C:211:ILE:HD12	15:G:143:VAL:HG12	1.74	0.70
15:G:134:LEU:HA	15:G:195:VAL:HA	1.73	0.69
11:C:268:LEU:HD23	11:C:272:ASP:HB3	1.74	0.69
15:x:64:ILE:HG21	15:y:82:LEU:HD21	1.76	0.67
30:V:79:VAL:HG12	30:V:86:VAL:HG12	1.75	0.67
15:G:165:VAL:HA	15:G:168:LEU:HG	1.76	0.66
32:X:20:ILE:HG22	55:OX:434:LEU:HD23	1.80	0.64
49:z:127:LEU:HD22	49:z:290:VAL:HG13	1.79	0.64
36:d:186:VAL:HG21	36:d:239:PRO:HB3	1.80	0.64
49:z:181:THR:HA	49:z:184:ILE:HD12	1.80	0.63
12:D:205:GLN:HA	12:D:208:ARG:HH21	1.63	0.62
11:C:192:GLU:HA	11:C:227:ARG:HH12	1.64	0.62
15:G:132:VAL:HG23	15:G:172:ILE:HB	1.82	0.60
36:d:52:THR:HG23	36:d:55:GLU:H	1.67	0.60
57:B:30:A:H2'	57:B:31:A:H8	1.67	0.60
36:d:208:VAL:HG22	36:d:253:THR:HG23	1.84	0.60
50:A:2545:U:H5"	50:A:2546:G:H5'	1.85	0.59
36:d:138:PRO:HG3	36:d:194:VAL:HG23	1.85	0.59
49:z:161:THR:HB	49:z:167:VAL:HG22	1.85	0.59
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.85	0.59
37:e:265:LYS:HZ3	57:B:76:A:H8	1.51	0.59
11:C:191:VAL:HG11	11:C:251:LEU:HD23	1.84	0.58
15:G:131:THR:HA	15:G:174:ALA:HA	1.85	0.58
50:A:1857:U:H2'	50:A:1858:G:C8	2.38	0.58
13:E:244:ALA:HB1	13:E:248:ILE:HD11	1.84	0.58
49:z:184:ILE:HD13	49:z:206:GLU:HB2	1.86	0.58
11:C:217:ASP:HB2	11:C:233:ILE:HB	1.86	0.58
11:C:267:GLN:HG3	11:C:297:GLU:HB3	1.85	0.58
32:X:34:GLU:OE2	32:X:36:ARG:HB2	2.04	0.58
49:z:108:LYS:O	49:z:112:LEU:HB2	2.04	0.58
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.86	0.57
4:3:138:PRO:HG2	50:A:2854:U:H4'	1.84	0.57
47:q:167:GLN:HB2	52:f:199:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:218:ILE:HG23	22:N:223:MET:HB2	1.87	0.57
34:Z:35:LYS:N	50:A:2103:A:HO2'	2.04	0.56
15:G:138:LYS:HB2	15:G:141:ASP:HB2	1.87	0.56
9:8:187:PRO:HG2	44:m:79:ILE:HD11	1.87	0.56
15:y:79:ILE:HA	15:y:82:LEU:HB2	1.87	0.56
50:A:2409:A:H2'	50:A:2410:U:C6	2.40	0.56
8:7:286:LEU:HD11	8:7:296:ARG:HB2	1.87	0.56
50:A:2099:U:H2'	50:A:2100:C:C6	2.40	0.56
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.87	0.55
18:J:140:VAL:O	18:J:144:ILE:HG12	2.06	0.55
50:A:2740:A:H2'	50:A:2741:A:C8	2.41	0.55
22:N:124:VAL:HG12	22:N:158:ARG:HE	1.70	0.55
49:z:115:THR:HG22	50:A:2778:U:H5"	1.87	0.55
8:7:107:LEU:HD13	8:7:128:LEU:HD11	1.88	0.55
11:C:239:LEU:HD11	11:C:256:CYS:HB2	1.89	0.55
11:C:207:LEU:HD22	15:G:158:LEU:HD13	1.88	0.55
54:s:63:ILE:HA	54:s:66:TRP:CD1	2.42	0.54
37:e:213:TYR:HB3	37:e:231:VAL:HB	1.89	0.54
54:s:145:VAL:HG21	54:s:187:LEU:HD11	1.89	0.53
54:s:137:LEU:HD21	54:s:422:VAL:HG11	1.90	0.53
22:N:124:VAL:HA	22:N:158:ARG:HH21	1.73	0.53
48:r:99:MET:HE1	48:r:115:ILE:HG22	1.89	0.53
47:q:168:VAL:HG12	47:q:175:PHE:HB2	1.91	0.53
37:e:257:LYS:HE2	37:e:273:ARG:HE	1.74	0.53
53:p:133:LEU:HD21	53:p:157:MET:HE1	1.90	0.53
11:C:152:ALA:HA	11:C:290:ILE:HG12	1.91	0.53
18:J:117:VAL:HG21	18:J:145:ILE:HG13	1.90	0.53
15:G:188:LEU:HA	15:G:191:VAL:HG12	1.91	0.53
30:V:102:MET:HE3	36:d:48:PRO:HG2	1.91	0.53
57:B:23:A:H2'	57:B:24:G:C8	2.44	0.53
11:C:168:LEU:HD23	11:C:279:LEU:HD11	1.90	0.53
15:G:134:LEU:HB2	15:G:195:VAL:HG22	1.91	0.53
19:K:60:MET:HE2	19:K:133:ILE:HD11	1.91	0.53
50:A:2055:U:H2'	50:A:2056:G:H8	1.74	0.53
37:e:172:ILE:HD13	57:B:76:A:C2	2.45	0.52
15:G:165:VAL:HG22	15:G:168:LEU:HD11	1.91	0.52
50:A:2093:U:H2'	50:A:2094:G:C8	2.45	0.52
50:A:2727:C:H2'	50:A:2728:C:C6	2.44	0.52
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.91	0.52
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.92	0.52
50:A:3158:A:H2'	50:A:3159:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:v:60:TYR:HB3	15:v:65:GLN:HE21	1.75	0.52
16:H:98:LEU:HD11	16:H:105:VAL:HG23	1.91	0.51
18:J:114:LEU:HB3	43:l:96:LEU:HD21	1.91	0.51
11:C:284:SER:HA	11:C:289:VAL:HG11	1.92	0.51
11:C:204:GLU:O	11:C:208:GLU:HG2	2.11	0.51
1:0:138:ARG:HB3	50:A:2321:A:C8	2.46	0.51
9:8:68:LEU:HD21	52:f:211:LEU:HB2	1.93	0.51
7:6:206:TYR:HH	7:6:214:TRP:CD1	2.29	0.51
15:G:132:VAL:HG12	15:G:197:LEU:HB3	1.92	0.51
15:G:132:VAL:HA	15:G:197:LEU:HA	1.93	0.51
55:OX:397:LEU:HD13	55:OX:399:GLN:HB3	1.94	0.50
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.27	0.50
16:H:201:VAL:HA	49:z:86:VAL:HG12	1.93	0.50
25:Q:100:LEU:HD21	25:Q:286:ILE:HG12	1.93	0.50
11:C:213:ALA:HA	11:C:245:LYS:HE3	1.94	0.50
18:J:88:SER:HA	18:J:151:LEU:HD11	1.93	0.50
2:1:54:VAL:HG13	47:q:128:MET:HE2	1.92	0.50
9:8:136:ILE:HD11	52:f:169:ILE:HG23	1.93	0.50
36:d:152:LEU:HD22	36:d:176:ILE:HD11	1.93	0.50
36:d:164:VAL:HG12	36:d:261:MET:HB3	1.94	0.50
50:A:2086:A:H2'	50:A:2087:U:C6	2.47	0.50
50:A:2718:C:H2'	50:A:2991:U:H4'	1.93	0.50
9:8:164:ARG:HG3	52:f:88:TYR:CE1	2.47	0.50
11:C:187:GLY:HA3	11:C:239:LEU:HB2	1.94	0.49
50:A:1839:C:H2'	50:A:1840:C:C6	2.48	0.49
37:e:166:GLY:HA3	64:B:101:VAL:HB	1.94	0.49
50:A:2392:U:H2'	50:A:2394:A:H62	1.76	0.49
9:8:201:GLN:HB2	52:f:199:LYS:HE2	1.93	0.49
29:U:153:LEU:HD21	36:d:220:GLN:HB2	1.95	0.49
15:x:86:LEU:HD23	15:x:90:LEU:HD12	1.94	0.49
50:A:1862:U:H2'	50:A:1863:A:H8	1.76	0.49
52:f:190:THR:HG23	52:f:192:GLU:HG3	1.94	0.49
20:L:32:ILE:HD11	20:L:103:ASN:HB3	1.94	0.49
50:A:2151:A:H2'	50:A:2152:A:C8	2.48	0.49
50:A:3158:A:H2'	50:A:3159:A:H8	1.77	0.49
51:c:79:LEU:HD13	51:c:214:PHE:HE2	1.77	0.49
25:Q:117:LEU:HD12	25:Q:151:LEU:HD21	1.94	0.49
15:G:144:LYS:HB3	15:G:191:VAL:HG22	1.93	0.49
50:A:2740:A:H2'	50:A:2741:A:H8	1.77	0.49
50:A:2894:U:H5"	50:A:2895:U:O4'	2.12	0.49
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:1952:U:H2'	50:A:1953:A:C8	2.47	0.48
16:H:163:THR:HG21	49:z:86:VAL:HG23	1.95	0.48
8:7:150:MET:O	8:7:154:ILE:HG12	2.13	0.48
15:G:148:GLU:O	15:G:152:TYR:HB3	2.14	0.48
50:A:2318:A:H2'	50:A:2319:A:C8	2.48	0.48
50:A:2006:C:H2'	50:A:2007:U:C6	2.49	0.48
30:V:55:TYR:HB2	30:V:133:ILE:HD11	1.94	0.47
50:A:2081:U:H2'	50:A:2082:G:C8	2.49	0.47
50:A:2734:A:H2'	50:A:2735:G:H8	1.78	0.47
50:A:2727:C:H2'	50:A:2728:C:H6	1.78	0.47
57:B:68:C:H2'	57:B:69:U:C6	2.49	0.47
15:y:65:GLN:HA	15:y:68:VAL:HG12	1.97	0.47
15:G:139:PRO:HA	15:G:142:LYS:HE2	1.96	0.47
36:d:108:ARG:HA	36:d:111:ARG:HD2	1.96	0.47
9:8:125:LYS:HD3	57:B:29:C:H5"	1.96	0.47
47:q:117:ARG:O	47:q:121:ILE:HG12	2.15	0.47
47:q:191:LYS:HA	47:q:194:LYS:HG2	1.95	0.47
55:OX:399:GLN:HE21	55:OX:401:PHE:HD1	1.62	0.47
47:q:196:LYS:HA	47:q:199:LYS:HD2	1.97	0.47
50:A:1806:U:H4'	50:A:1807:U:H5'	1.97	0.47
50:A:2410:U:H2'	50:A:2411:U:H6	1.78	0.47
50:A:3211:C:H4'	50:A:3212:C:H5	1.79	0.47
8:7:302:LEU:HD23	23:O:144:LEU:HD23	1.97	0.47
17:I:154:LEU:HD12	17:I:164:MET:HE3	1.96	0.47
50:A:2127:A:H4'	50:A:2251:A:C5	2.50	0.47
52:f:80:ILE:HG23	52:f:90:VAL:HG12	1.97	0.47
11:C:180:ARG:NH1	11:C:181:HIS:HB3	2.29	0.46
36:d:204:ASN:O	36:d:205:GLN:HG2	2.15	0.46
44:m:55:LEU:HD23	44:m:63:THR:HG21	1.96	0.46
47:q:40:PRO:HG2	47:q:51:GLN:HB3	1.96	0.46
37:e:159:LEU:HD12	37:e:254:TRP:CH2	2.51	0.46
47:q:138:GLN:O	47:q:141:GLU:HG3	2.15	0.46
49:z:119:GLN:HB2	49:z:260:LEU:HD12	1.95	0.46
52:f:202:PRO:HA	52:f:205:GLU:HG3	1.98	0.46
36:d:90:PRO:HB2	36:d:269:TRP:HZ2	1.81	0.46
50:A:2408:U:H2'	50:A:2409:A:H8	1.80	0.46
16:H:106:GLY:HA2	16:H:158:LYS:HB2	1.98	0.46
50:A:1828:A:H4'	50:A:1829:A:C8	2.50	0.46
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.98	0.46
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.98	0.46
47:q:147:GLN:O	47:q:150:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:z:157:VAL:HG22	49:z:196:PHE:HB3	1.96	0.46
7:6:161:LEU:HD23	7:6:300:THR:HG21	1.97	0.46
46:o:15:ARG:HB3	46:o:18:ILE:HG12	1.97	0.46
50:A:2514:C:H2'	50:A:2515:U:H6	1.81	0.46
57:B:29:C:H2'	57:B:30:A:H8	1.81	0.46
13:E:50:ASP:HA	13:E:53:LEU:HG	1.98	0.46
16:H:201:VAL:HG11	16:H:206:LEU:HG	1.98	0.46
50:A:1935:A:C2	50:A:1936:A:H1'	2.51	0.46
50:A:2483:U:H2'	50:A:2484:C:O4'	2.16	0.46
11:C:148:LEU:HD23	11:C:294:ASP:HB3	1.97	0.46
11:C:271:PRO:O	11:C:274:GLU:HG3	2.15	0.46
50:A:2805:A:H2'	50:A:2806:U:C6	2.51	0.46
9:8:117:LEU:HD11	37:e:69:GLU:HB3	1.98	0.46
22:N:36:VAL:HG11	43:l:124:GLN:HB3	1.98	0.46
27:S:163:LYS:HB2	35:b:106:ASP:HB3	1.98	0.46
50:A:2677:A:H2'	50:A:2678:A:C8	2.51	0.46
11:C:201:VAL:HG22	11:C:205:ARG:HH12	1.80	0.45
22:N:67:LYS:HE2	50:A:2110:A:H5'	1.98	0.45
42:k:74:LEU:HD13	42:k:93:HIS:CD2	2.51	0.45
50:A:3054:G:H2'	50:A:3055:U:C6	2.51	0.45
21:M:40:PRO:HG3	50:A:1868:G:H2'	1.99	0.45
36:d:38:LYS:HE2	36:d:40:ARG:HH12	1.81	0.45
11:C:205:ARG:HA	11:C:208:GLU:HG2	1.96	0.45
11:C:185:LYS:HD2	11:C:258:LEU:HB3	1.99	0.45
15:G:160:GLN:HA	15:G:163:LYS:HG2	1.98	0.45
49:z:133:LYS:HE3	49:z:286:LEU:HD13	1.99	0.45
11:C:207:LEU:HG	11:C:218:VAL:HG21	1.99	0.45
50:A:2803:A:H2'	50:A:2804:A:O4'	2.16	0.45
50:A:3224:G:H2'	50:A:3225:G:H8	1.82	0.45
11:C:154:SER:HB3	11:C:288:ASP:OD1	2.16	0.45
17:I:61:HIS:CD2	17:I:62:PRO:HD2	2.52	0.45
30:V:146:VAL:HG21	55:OX:401:PHE:CE1	2.52	0.45
54:s:84:THR:HB	54:s:280:ASN:HB2	1.98	0.45
8:7:166:LEU:HB3	8:7:181:TYR:HE2	1.82	0.45
23:O:44:ALA:HB3	23:O:49:VAL:HG23	1.98	0.45
49:z:64:GLU:HG2	49:z:65:LYS:N	2.31	0.45
50:A:2415:C:H3'	54:s:165:ARG:NH2	2.32	0.45
22:N:133:ARG:HD3	50:A:2109:A:H5'	1.98	0.45
49:z:69:ILE:HA	49:z:72:ILE:HG12	1.99	0.45
16:H:174:VAL:HG12	16:H:192:HIS:HB3	1.99	0.45
17:I:101:ASN:HB3	17:I:150:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:96:PHE:HB3	35:b:126:ILE:HD13	1.99	0.45
37:e:61:LYS:HE2	37:e:155:ARG:HD2	1.99	0.45
52:f:125:TYR:CD1	52:f:197:ARG:HD3	2.52	0.45
4:3:157:LEU:HG	4:3:161:MET:HE2	1.98	0.44
17:I:224:HIS:H	15:w:87:LYS:HZ1	1.65	0.44
36:d:90:PRO:HB3	36:d:245:TYR:CE2	2.52	0.44
36:d:205:GLN:HE21	36:d:207:ASN:HD21	1.65	0.44
50:A:2245:A:H4'	50:A:2246:A:OP1	2.17	0.44
50:A:2757:A:H2'	50:A:2758:G:O4'	2.16	0.44
50:A:3199:U:H5"	50:A:3200:U:H4'	1.98	0.44
6:5:129:ILE:HD11	6:5:373:LEU:HD22	1.99	0.44
21:M:281:LYS:HG2	38:g:42:VAL:HG22	1.99	0.44
33:Y:176:ILE:HG21	55:OX:430:TRP:CG	2.52	0.44
50:A:1862:U:H2'	50:A:1863:A:C8	2.52	0.44
50:A:1939:G:O2'	50:A:1973:G:H4'	2.18	0.44
57:B:43:G:H2'	57:B:44:A:C8	2.51	0.44
5:4:103:MET:HE1	50:A:2952:U:H5'	1.98	0.44
21:M:177:ALA:HB1	21:M:203:ARG:HH12	1.82	0.44
37:e:269:LEU:HA	37:e:272:VAL:HG12	1.99	0.44
50:A:1750:G:H2'	50:A:1751:A:C8	2.52	0.44
52:f:90:VAL:HG13	52:f:189:HIS:HB3	2.00	0.44
7:6:225:LEU:HB3	24:P:44:VAL:HG13	1.99	0.44
25:Q:146:GLY:O	50:A:3151:A:H4'	2.17	0.44
5:4:69:LYS:HB2	5:4:72:LEU:HD23	2.00	0.44
14:F:94:ASP:HB2	21:M:30:ASN:HB2	1.99	0.44
36:d:140:LYS:HE2	36:d:144:ILE:HD11	2.00	0.44
47:q:141:GLU:HA	47:q:144:GLU:HG3	1.99	0.44
57:B:49:U:H2'	57:B:50:U:C6	2.53	0.44
14:F:248:LEU:HG	14:F:253:MET:HE2	2.00	0.44
37:e:165:PHE:O	64:B:101:VAL:N	2.50	0.44
15:w:76:LEU:HD23	15:w:76:LEU:H	1.82	0.44
11:C:171:ASN:HB2	11:C:279:LEU:HD13	2.00	0.44
14:F:218:LEU:HD13	14:F:230:ILE:HD11	2.00	0.44
7:6:106:ARG:HG2	24:P:110:TRP:CE2	2.53	0.43
8:7:276:PHE:HB2	8:7:304:VAL:HG22	2.00	0.43
36:d:201:SER:O	36:d:208:VAL:HG12	2.18	0.43
13:E:80:LEU:HD12	13:E:323:GLY:HA3	1.99	0.43
29:U:131:GLU:O	29:U:134:ARG:HG3	2.18	0.43
50:A:2060:A:C8	50:A:2079:C:C4	3.06	0.43
26:R:91:VAL:HG11	41:j:24:GLY:HA3	2.00	0.43
36:d:115:THR:O	36:d:119:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:2408:U:H2'	50:A:2409:A:C8	2.54	0.43
52:f:171:LEU:HD13	52:f:174:ILE:HD11	2.00	0.43
9:8:187:PRO:HG3	44:m:59:GLN:HA	2.01	0.43
34:Z:70:THR:HG22	34:Z:97:PRO:HA	2.00	0.43
36:d:100:LEU:HD22	36:d:108:ARG:HH21	1.83	0.43
19:K:20:LEU:HD22	19:K:141:LEU:HD13	1.99	0.43
50:A:1761:A:H2'	50:A:1762:A:C8	2.53	0.43
11:C:141:ARG:NH2	11:C:145:GLY:HA2	2.33	0.43
12:D:257:ILE:O	12:D:262:ARG:HD2	2.19	0.43
15:u:64:ILE:O	15:u:68:VAL:HG23	2.18	0.43
50:A:1851:G:H2'	50:A:2693:A:N7	2.33	0.43
50:A:1895:C:H2'	50:A:1896:U:C6	2.53	0.43
8:7:112:PRO:HB2	8:7:267:PRO:HG2	2.01	0.43
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.54	0.43
23:O:10:SER:HB2	50:A:2457:A:H3'	2.00	0.43
50:A:2277:U:H2'	50:A:2278:A:H8	1.83	0.43
50:A:3117:C:H2'	50:A:3118:U:H6	1.84	0.43
36:d:85:PHE:HZ	36:d:209:TYR:HB2	1.83	0.43
37:e:124:TRP:CD2	44:m:72:ARG:HG2	2.54	0.43
40:i:61:GLY:HA3	50:A:1886:G:H1	1.84	0.43
50:A:2053:U:HO2'	50:A:2054:U:H6	1.64	0.43
54:s:119:PRO:HG3	54:s:394:TRP:CD2	2.54	0.43
57:B:25:C:H2'	57:B:26:A:H8	1.84	0.43
11:C:188:VAL:HG22	11:C:233:ILE:HD12	2.01	0.43
22:N:104:MET:HE3	22:N:104:MET:HB3	1.89	0.43
49:z:116:SER:HB2	50:A:2778:U:O2'	2.19	0.43
50:A:2275:U:H2'	50:A:2276:C:C6	2.54	0.43
50:A:2868:C:H2'	50:A:2869:A:O4'	2.19	0.43
6:5:215:ARG:HD2	6:5:364:LEU:O	2.19	0.42
11:C:132:LYS:O	11:C:155:ASN:HA	2.19	0.42
13:E:107:MET:HE3	25:Q:145:LEU:HD12	2.00	0.42
36:d:40:ARG:HD3	36:d:40:ARG:HA	1.83	0.42
50:A:2552:U:C2	50:A:2553:G:C8	3.07	0.42
50:A:2668:A:H2'	50:A:2669:A:C8	2.54	0.42
50:A:2748:A:H2'	50:A:2749:A:H8	1.84	0.42
50:A:3150:U:C2	50:A:3151:A:C8	3.07	0.42
50:A:1829:A:H2'	50:A:1830:G:H8	1.83	0.42
11:C:140:GLY:HA2	11:C:176:ALA:H	1.84	0.42
24:P:94:VAL:HG23	24:P:132:LEU:HD21	2.01	0.42
36:d:168:CYS:HB2	36:d:262:HIS:O	2.19	0.42
49:z:78:MET:HE1	49:z:93:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:2182:G:H2'	50:A:2183:C:C6	2.54	0.42
57:B:21:A:H61	57:B:46:A:H2'	1.84	0.42
18:J:113:THR:HG23	18:J:115:LYS:H	1.83	0.42
28:T:62:ARG:NE	36:d:230:ARG:HD2	2.28	0.42
56:a:91:VAL:HG12	56:a:95:ARG:HE	1.84	0.42
17:I:203:VAL:HA	17:I:206:GLU:HB2	2.01	0.42
22:N:139:ARG:HE	31:W:33:LYS:HD3	1.83	0.42
6:5:354:PHE:HB3	6:5:417:LEU:HD11	2.01	0.42
6:5:417:LEU:HD23	6:5:417:LEU:HA	1.88	0.42
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.54	0.42
13:E:144:THR:HB	13:E:178:ILE:HG23	2.02	0.42
23:O:50:ASP:HB2	23:O:107:MET:HE1	1.99	0.42
36:d:208:VAL:H	36:d:253:THR:HG23	1.85	0.42
36:d:221:THR:HG22	36:d:239:PRO:HA	2.01	0.42
49:z:140:PHE:H	49:z:281:HIS:CD2	2.38	0.42
50:A:2410:U:H2'	50:A:2411:U:C6	2.53	0.42
50:A:2950:U:H2'	50:A:2951:A:H8	1.84	0.42
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.54	0.42
36:d:197:VAL:HG22	36:d:212:ILE:HG23	2.01	0.42
37:e:186:GLY:HA2	37:e:189:GLU:CD	2.44	0.42
15:u:86:LEU:O	15:u:90:LEU:HB2	2.20	0.42
49:z:198:VAL:HB	49:z:230:ILE:HG23	2.00	0.42
50:A:2815:OMG:HM23	50:A:2815:OMG:H1'	1.77	0.42
57:B:74:C:H2'	57:B:75:C:O4'	2.19	0.42
30:V:80:ILE:HB	30:V:85:TRP:HB2	2.01	0.42
47:q:170:PRO:HA	47:q:175:PHE:CD2	2.54	0.42
50:A:1861:U:H2'	50:A:1862:U:C6	2.55	0.42
29:U:132:GLU:HA	29:U:135:GLN:HB3	2.02	0.42
36:d:207:ASN:HA	36:d:253:THR:OG1	2.20	0.42
50:A:2275:U:H2'	50:A:2276:C:H6	1.84	0.42
50:A:2728:C:H2'	50:A:2729:U:H6	1.84	0.42
50:A:3124:U:H2'	50:A:3125:A:H8	1.85	0.42
9:8:117:LEU:HD22	37:e:73:LEU:HD23	2.01	0.41
17:I:200:LEU:HD13	15:u:76:LEU:HB3	2.02	0.41
28:T:193:TYR:HD1	56:a:122:ARG:HE	1.66	0.41
50:A:2056:G:H2'	50:A:2057:C:H6	1.85	0.41
50:A:3024:U:H2'	50:A:3025:A:H8	1.85	0.41
50:A:3115:U:H2'	50:A:3116:C:C6	2.55	0.41
9:8:173:LYS:HB3	52:f:184:LEU:HB3	2.02	0.41
11:C:183:PHE:HA	11:C:262:PRO:HA	2.01	0.41
49:z:184:ILE:HG22	49:z:209:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:192:TYR:HE1	52:f:134:VAL:HG22	1.85	0.41
11:C:268:LEU:HB3	11:C:272:ASP:HB2	2.02	0.41
15:G:180:GLU:O	15:G:183:LYS:HG3	2.20	0.41
17:I:235:GLN:OE1	15:y:91:LYS:HA	2.20	0.41
32:X:166:LEU:HD13	32:X:196:ILE:HD11	2.02	0.41
38:g:109:VAL:HG13	38:g:146:THR:HG23	2.03	0.41
48:r:103:LYS:NZ	50:A:2220:A:H5"	2.36	0.41
50:A:3090:G:H2'	50:A:3091:G:H8	1.84	0.41
50:A:3165:C:H2'	50:A:3166:U:C6	2.55	0.41
54:s:65:ARG:O	54:s:69:THR:HG23	2.20	0.41
15:G:127:ARG:HD2	15:G:127:ARG:HA	1.91	0.41
47:q:167:GLN:HB2	52:f:199:LYS:HZ2	1.85	0.41
50:A:2382:A:H2'	50:A:2383:U:C6	2.55	0.41
11:C:146:SER:HA	11:C:266:VAL:HG11	2.02	0.41
20:L:46:LEU:HD12	20:L:78:LYS:HD3	2.02	0.41
49:z:123:LEU:HD23	49:z:257:ILE:HD11	2.02	0.41
57:B:29:C:C2	57:B:30:A:C8	3.08	0.41
4:3:127:ALA:HA	21:M:79:PRO:HD3	2.02	0.41
4:3:156:LYS:HB2	4:3:156:LYS:HE3	1.84	0.41
27:S:173:ARG:HB3	27:S:180:PHE:HE2	1.86	0.41
39:h:139:LYS:HA	39:h:139:LYS:HD2	1.91	0.41
50:A:1737:A:H61	50:A:1760:G:H1'	1.85	0.41
6:5:98:LEU:HD22	6:5:272:ASP:HB3	2.03	0.41
8:7:317:LEU:HD23	8:7:317:LEU:HA	1.90	0.41
50:A:1816:G:H2'	50:A:1817:C:O4'	2.20	0.41
14:F:65:TRP:CD1	39:h:117:LEU:HD11	2.56	0.41
17:I:217:GLN:HE22	15:w:76:LEU:HD12	1.85	0.41
31:W:67:ILE:HG21	31:W:131:VAL:HG21	2.03	0.41
35:b:89:ILE:HA	35:b:92:LYS:HD2	2.03	0.41
50:A:1977:U:H2'	50:A:1978:A:H8	1.86	0.41
11:C:192:GLU:HG2	11:C:194:GLU:H	1.86	0.41
17:I:197:LEU:HD22	15:u:76:LEU:HD12	2.02	0.41
18:J:151:LEU:HD23	50:A:2174:G:H4'	2.03	0.41
47:q:148:ALA:O	47:q:151:GLU:HG3	2.20	0.41
49:z:175:ALA:HA	49:z:234:LEU:HD23	2.03	0.41
50:A:1936:A:H4'	50:A:1937:A:C8	2.55	0.41
50:A:2807:U:H2'	50:A:2808:U:C6	2.55	0.41
57:B:9:1MA:N3	57:B:45:G:H2'	2.35	0.41
6:5:167:THR:HG21	54:s:281:HIS:CE1	2.56	0.41
18:J:113:THR:HG22	18:J:116:HIS:ND1	2.35	0.41
37:e:215:PHE:CZ	57:B:76:A:H2'	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:o:15:ARG:HG3	50:A:2692:G:OP1	2.21	0.41
49:z:87:TYR:CD2	49:z:92:TYR:HB2	2.56	0.41
50:A:1911:C:H2'	50:A:1912:A:C8	2.56	0.41
50:A:1952:U:H2'	50:A:1953:A:H8	1.86	0.41
50:A:2549:C:N4	50:A:2562:U:H2'	2.36	0.41
14:F:218:LEU:HD23	14:F:260:VAL:HB	2.02	0.40
21:M:226:PRO:HG3	53:p:45:LEU:HD23	2.03	0.40
37:e:97:ARG:HA	37:e:100:LYS:HG2	2.01	0.40
37:e:219:GLN:HA	37:e:222:ARG:HB2	2.03	0.40
50:A:1718:A:H2'	50:A:1719:G:O4'	2.21	0.40
50:A:3150:U:H2'	50:A:3151:A:H8	1.86	0.40
9:8:136:ILE:HD11	52:f:169:ILE:CG2	2.51	0.40
29:U:65:VAL:HG13	29:U:97:VAL:HG13	2.04	0.40
36:d:208:VAL:HG23	36:d:252:LEU:HB2	2.04	0.40
50:A:2101:C:H2'	50:A:2102:A:H8	1.86	0.40
11:C:233:ILE:HG21	11:C:261:ILE:HG13	2.03	0.40
44:m:69:ARG:HG3	44:m:70:GLU:HG2	2.03	0.40
50:A:2598:A:H3'	50:A:2625:C:H42	1.86	0.40
51:c:256:ARG:HD2	56:a:69:TYR:CE2	2.56	0.40
57:B:16:C:H2'	57:B:18:A:O4'	2.20	0.40
6:5:113:LEU:HD12	6:5:311:ALA:HB1	2.03	0.40
15:G:178:LYS:NZ	15:G:182:GLU:HB3	2.35	0.40
17:I:146:LEU:HD11	42:k:23:PHE:CE2	2.57	0.40
18:J:58:LYS:HA	18:J:58:LYS:HD2	1.83	0.40
50:A:3201:A:H2'	50:A:3202:U:O4'	2.22	0.40
9:8:99:ARG:HG2	37:e:83:LEU:HB3	2.04	0.40
11:C:151:GLU:OE2	11:C:291:HIS:HB3	2.21	0.40
26:R:90:LEU:HD23	26:R:90:LEU:HA	1.92	0.40
47:q:167:GLN:HB2	52:f:199:LYS:HZ1	1.84	0.40
50:A:2170:G:H2'	50:A:2171:U:C5	2.56	0.40
50:A:2748:A:H2'	50:A:2749:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	385 (98%)	7 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	137/206 (66%)	135 (98%)	2 (2%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
11	C	164/297 (55%)	159 (97%)	5 (3%)	0	100	100
12	D	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
13	E	303/348 (87%)	294 (97%)	9 (3%)	0	100	100
14	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
15	G	70/198 (35%)	65 (93%)	5 (7%)	0	100	100
15	t	44/198 (22%)	43 (98%)	1 (2%)	0	100	100
15	u	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
15	v	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
15	w	29/198 (15%)	26 (90%)	3 (10%)	0	100	100
15	x	29/198 (15%)	28 (97%)	1 (3%)	0	100	100
15	y	29/198 (15%)	26 (90%)	3 (10%)	0	100	100
16	H	200/267 (75%)	196 (98%)	4 (2%)	0	100	100
17	I	210/261 (80%)	208 (99%)	2 (1%)	0	100	100
18	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
19	K	176/178 (99%)	175 (99%)	1 (1%)	0	100	100
20	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
21	M	289/296 (98%)	284 (98%)	5 (2%)	0	100	100
22	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
23	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
24	P	142/180 (79%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Q	218/292 (75%)	217 (100%)	1 (0%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
27	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
28	T	164/206 (80%)	164 (100%)	0	0	100	100
29	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
30	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
31	W	114/148 (77%)	112 (98%)	2 (2%)	0	100	100
32	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
33	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
34	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
35	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
36	d	257/306 (84%)	243 (95%)	13 (5%)	1 (0%)	30	57
37	e	236/279 (85%)	226 (96%)	10 (4%)	0	100	100
38	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
39	h	108/158 (68%)	103 (95%)	5 (5%)	0	100	100
40	i	95/128 (74%)	95 (100%)	0	0	100	100
41	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
42	k	100/112 (89%)	100 (100%)	0	0	100	100
43	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
44	m	63/128 (49%)	62 (98%)	1 (2%)	0	100	100
46	o	92/102 (90%)	92 (100%)	0	0	100	100
47	q	175/222 (79%)	175 (100%)	0	0	100	100
48	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
49	z	250/325 (77%)	235 (94%)	15 (6%)	0	100	100
51	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
52	f	153/212 (72%)	148 (97%)	5 (3%)	0	100	100
53	p	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
54	s	381/439 (87%)	372 (98%)	9 (2%)	0	100	100
55	OX	38/435 (9%)	34 (90%)	4 (10%)	0	100	100
56	a	99/142 (70%)	98 (99%)	1 (1%)	0	100	100
All	All	9288/13112 (71%)	9097 (98%)	190 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	d	47	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	129/190 (68%)	129 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
11	C	141/245 (58%)	141 (100%)	0	100	100
12	D	192/245 (78%)	192 (100%)	0	100	100
13	E	260/290 (90%)	260 (100%)	0	100	100
14	F	219/262 (84%)	219 (100%)	0	100	100
15	G	60/158 (38%)	60 (100%)	0	100	100
15	t	40/158 (25%)	40 (100%)	0	100	100
15	u	31/158 (20%)	31 (100%)	0	100	100
15	v	31/158 (20%)	31 (100%)	0	100	100
15	w	30/158 (19%)	30 (100%)	0	100	100
15	x	30/158 (19%)	30 (100%)	0	100	100
15	y	30/158 (19%)	30 (100%)	0	100	100
16	H	182/228 (80%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	I	194/232 (84%)	194 (100%)	0	100	100
18	J	138/150 (92%)	138 (100%)	0	100	100
19	K	155/155 (100%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	246/249 (99%)	246 (100%)	0	100	100
22	N	189/211 (90%)	189 (100%)	0	100	100
23	O	134/150 (89%)	134 (100%)	0	100	100
24	P	126/155 (81%)	126 (100%)	0	100	100
25	Q	202/256 (79%)	202 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	146/180 (81%)	146 (100%)	0	100	100
28	T	146/176 (83%)	146 (100%)	0	100	100
29	U	134/135 (99%)	134 (100%)	0	100	100
30	V	183/191 (96%)	183 (100%)	0	100	100
31	W	94/119 (79%)	94 (100%)	0	100	100
32	X	220/229 (96%)	220 (100%)	0	100	100
33	Y	163/223 (73%)	163 (100%)	0	100	100
34	Z	113/147 (77%)	113 (100%)	0	100	100
35	b	132/186 (71%)	132 (100%)	0	100	100
36	d	237/274 (86%)	237 (100%)	0	100	100
37	e	207/236 (88%)	207 (100%)	0	100	100
38	g	124/148 (84%)	124 (100%)	0	100	100
39	h	104/148 (70%)	104 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	74/97 (76%)	74 (100%)	0	100	100
42	k	83/89 (93%)	83 (100%)	0	100	100
43	l	76/116 (66%)	76 (100%)	0	100	100
44	m	58/113 (51%)	58 (100%)	0	100	100
46	o	80/87 (92%)	80 (100%)	0	100	100
47	q	153/178 (86%)	153 (100%)	0	100	100
48	r	147/169 (87%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	z	226/287 (79%)	226 (100%)	0	100	100
51	c	251/288 (87%)	251 (100%)	0	100	100
52	f	139/188 (74%)	139 (100%)	0	100	100
53	p	135/181 (75%)	135 (100%)	0	100	100
54	s	339/381 (89%)	339 (100%)	0	100	100
55	OX	38/372 (10%)	38 (100%)	0	100	100
56	a	99/133 (74%)	99 (100%)	0	100	100
All	All	8319/11221 (74%)	8319 (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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	31	ASN
4	3	178	GLN
6	5	94	HIS
6	5	150	GLN
6	5	195	HIS
6	5	214	ASN
6	5	343	GLN
7	6	163	HIS
7	6	295	GLN
8	7	69	HIS
9	8	186	GLN
11	C	275	GLN
14	F	103	GLN
17	I	119	HIS
19	K	40	GLN
19	K	94	GLN
22	N	210	GLN
25	Q	107	HIS
25	Q	132	GLN
26	R	89	ASN
27	S	196	ASN
29	U	41	GLN
32	X	4	HIS
32	X	177	HIS
33	Y	88	GLN

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Mol	Chain	Res	Type
35	b	90	HIS
36	d	47	GLN
36	d	205	GLN
37	e	67	GLN
37	e	106	HIS
37	e	150	ASN
37	e	248	ASN
37	e	251	HIS
42	k	19	GLN
43	l	100	ASN
47	q	60	GLN
48	r	79	HIS
15	t	65	GLN
15	w	83	ASN
49	z	110	GLN
49	z	251	ASN
51	c	73	GLN
51	c	168	HIS
52	f	189	HIS
53	p	117	GLN
54	s	107	GLN
54	s	164	HIS
54	s	281	HIS
54	s	420	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A	1556/1558 (99%)	247 (15%)	2 (0%)
57	B	70/72 (97%)	16 (22%)	0
All	All	1626/1630 (99%)	263 (16%)	2 (0%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A	1681	G
50	A	1689	C
50	A	1692	A
50	A	1699	C
50	A	1700	U
50	A	1704	U

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Mol	Chain	Res	Type
50	A	1708	A
50	A	1709	G
50	A	1711	C
50	A	1724	A
50	A	1727	A
50	A	1728	U
50	A	1736	A
50	A	1748	G
50	A	1765	C
50	A	1777	A
50	A	1780	U
50	A	1805	A
50	A	1806	U
50	A	1807	U
50	A	1808	A
50	A	1812	C
50	A	1817	C
50	A	1821	A
50	A	1827	C
50	A	1828	A
50	A	1829	A
50	A	1832	A
50	A	1836	A
50	A	1844	A
50	A	1854	U
50	A	1856	A
50	A	1869	A
50	A	1871	A
50	A	1873	A
50	A	1878	U
50	A	1882	A
50	A	1886	G
50	A	1887	A
50	A	1888	G
50	A	1893	A
50	A	1901	C
50	A	1902	C
50	A	1903	C
50	A	1909	A
50	A	1918	G
50	A	1937	A
50	A	1940	A

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Mol	Chain	Res	Type
50	A	1985	G
50	A	1993	A
50	A	1994	A
50	A	2003	A
50	A	2015	G
50	A	2022	G
50	A	2030	U
50	A	2036	C
50	A	2037	U
50	A	2039	A
50	A	2054	U
50	A	2055	U
50	A	2060	A
50	A	2069	U
50	A	2071	U
50	A	2079	C
50	A	2099	U
50	A	2113	G
50	A	2125	C
50	A	2126	U
50	A	2147	G
50	A	2159	U
50	A	2160	A
50	A	2163	A
50	A	2168	U
50	A	2181	A
50	A	2182	G
50	A	2185	G
50	A	2191	A
50	A	2192	A
50	A	2195	A
50	A	2196	A
50	A	2198	A
50	A	2200	A
50	A	2214	A
50	A	2219	C
50	A	2220	A
50	A	2221	C
50	A	2223	A
50	A	2224	C
50	A	2225	C
50	A	2226	U

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Mol	Chain	Res	Type
50	A	2230	A
50	A	2232	A
50	A	2233	U
50	A	2237	A
50	A	2241	A
50	A	2243	A
50	A	2245	A
50	A	2246	A
50	A	2262	C
50	A	2263	C
50	A	2284	C
50	A	2285	U
50	A	2297	A
50	A	2300	G
50	A	2322	C
50	A	2331	C
50	A	2332	C
50	A	2345	G
50	A	2349	G
50	A	2350	A
50	A	2353	A
50	A	2354	A
50	A	2357	C
50	A	2363	A
50	A	2372	U
50	A	2374	A
50	A	2390	A
50	A	2399	A
50	A	2401	A
50	A	2404	U
50	A	2407	U
50	A	2415	C
50	A	2446	A
50	A	2451	A
50	A	2452	A
50	A	2478	G
50	A	2485	U
50	A	2493	C
50	A	2496	G
50	A	2502	C
50	A	2506	A
50	A	2520	C

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Mol	Chain	Res	Type
50	A	2521	A
50	A	2527	A
50	A	2540	C
50	A	2557	C
50	A	2570	C
50	A	2571	G
50	A	2592	G
50	A	2593	G
50	A	2594	U
50	A	2599	U
50	A	2600	A
50	A	2601	A
50	A	2603	C
50	A	2618	U
50	A	2627	G
50	A	2630	U
50	A	2633	A
50	A	2635	G
50	A	2654	U
50	A	2655	G
50	A	2656	U
50	A	2683	C
50	A	2686	G
50	A	2694	A
50	A	2696	A
50	A	2706	A
50	A	2709	A
50	A	2718	C
50	A	2719	G
50	A	2723	A
50	A	2724	G
50	A	2725	A
50	A	2732	G
50	A	2745	A
50	A	2762	C
50	A	2763	U
50	A	2765	A
50	A	2767	A
50	A	2768	A
50	A	2773	A
50	A	2782	A
50	A	2786	U

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Mol	Chain	Res	Type
50	A	2790	A
50	A	2810	G
50	A	2832	A
50	A	2833	A
50	A	2847	C
50	A	2864	U
50	A	2865	C
50	A	2885	U
50	A	2888	A
50	A	2889	C
50	A	2893	A
50	A	2907	U
50	A	2913	A
50	A	2916	G
50	A	2917	G
50	A	2918	A
50	A	2919	A
50	A	2922	A
50	A	2928	C
50	A	2934	G
50	A	2935	A
50	A	2936	U
50	A	2956	A
50	A	2962	C
50	A	2965	A
50	A	2971	A
50	A	2985	C
50	A	2989	G
50	A	2990	A
50	A	2992	G
50	A	2993	U
50	A	3005	A
50	A	3016	G
50	A	3022	G
50	A	3041	U
50	A	3049	U
50	A	3053	A
50	A	3054	G
50	A	3060	C
50	A	3065	U
50	A	3072	U
50	A	3086	U

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Mol	Chain	Res	Type
50	A	3090	G
50	A	3096	U
50	A	3100	U
50	A	3102	U
50	A	3108	U
50	A	3109	U
50	A	3110	C
50	A	3111	A
50	A	3112	A
50	A	3157	C
50	A	3158	A
50	A	3162	C
50	A	3169	C
50	A	3172	C
50	A	3177	A
50	A	3180	A
50	A	3183	U
50	A	3190	A
50	A	3199	U
50	A	3200	U
50	A	3207	A
50	A	3209	A
50	A	3210	C
50	A	3212	C
50	A	3217	A
50	A	3218	A
50	A	3220	A
50	A	3228	U
50	A	3229	U
50	A	3230	G
50	A	3231	U
57	B	8	U
57	B	10	2MG
57	B	16	C
57	B	21	A
57	B	45	G
57	B	46	A
57	B	49	U
57	B	54	C
57	B	55	U
57	B	56	U
57	B	58	A

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Mol	Chain	Res	Type
57	B	59	A
57	B	64	A
57	B	69	U
57	B	72	G
57	B	76	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	A	2245	A
50	A	2484	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	2MG	B	10	57	23,26,27	0.36	0	33,38,41	0.42	0
57	PSU	B	39	57	18,21,22	1.03	1 (5%)	21,30,33	0.72	0
57	1MA	B	9	57	21,25,26	0.38	0	30,37,40	0.65	0
50	PSU	A	3067	50	18,21,22	1.12	2 (11%)	21,30,33	0.80	1 (4%)
50	1MA	A	2617	50	21,25,26	0.39	0	30,37,40	0.61	0
50	OMG	A	2815	59,50	23,26,27	0.35	0	32,38,41	0.41	0
50	OMG	A	3040	50	23,26,27	0.33	0	32,38,41	0.45	0
50	OMU	A	3039	59,50	19,22,23	0.31	0	25,31,34	0.74	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	2MG	B	10	57	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	B	39	57	-	0/7/25/26	0/2/2/2
57	1MA	B	9	57	-	0/7/25/26	0/3/3/3
50	PSU	A	3067	50	-	1/7/25/26	0/2/2/2
50	1MA	A	2617	50	-	0/7/25/26	0/3/3/3
50	OMG	A	2815	59,50	-	0/9/27/28	0/3/3/3
50	OMG	A	3040	50	-	0/9/27/28	0/3/3/3
50	OMU	A	3039	59,50	-	0/9/27/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	39	PSU	C6-C5	3.57	1.39	1.35
50	A	3067	PSU	C6-C5	3.53	1.39	1.35
50	A	3067	PSU	O4'-C1'	-2.58	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	A	3039	OMU	C2'-C1'-N1	-2.73	109.05	114.24
50	A	3067	PSU	O4'-C1'-C2'	2.39	108.46	105.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	A	3067	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	9	1MA	1	0
50	A	2815	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 179 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
64	VAL	B	101	57	4,6,7	0.78	0	6,7,9	1.02	1 (16%)
61	FES	r	201	48,17	0,4,4	-	-	-		
62	SPD	A	3303	-	9,9,9	0.15	0	8,8,8	0.28	0
62	SPD	A	3302	-	9,9,9	0.17	0	8,8,8	0.21	0
63	PUT	A	3304	-	5,5,5	0.13	0	4,4,4	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	VAL	B	101	57	-	0/5/6/8	-
61	FES	r	201	48,17	-	-	0/1/1/1
62	SPD	A	3303	-	-	1/7/7/7	-
62	SPD	A	3302	-	-	0/7/7/7	-
63	PUT	A	3304	-	-	0/3/3/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	B	101	VAL	O-C-CA	-2.33	118.78	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	A	3303	SPD	C2-C3-C4-C5

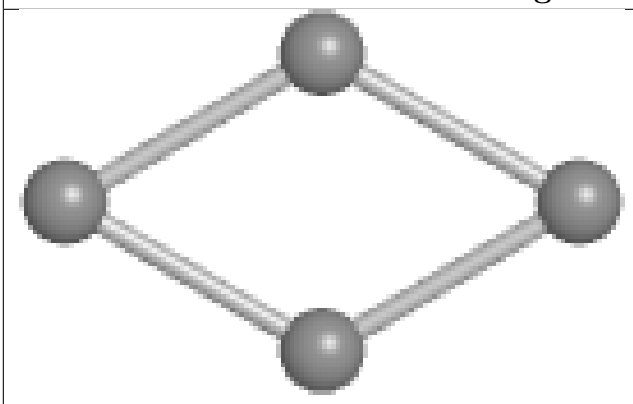
There are no ring outliers.

1 monomer is involved in 2 short contacts:

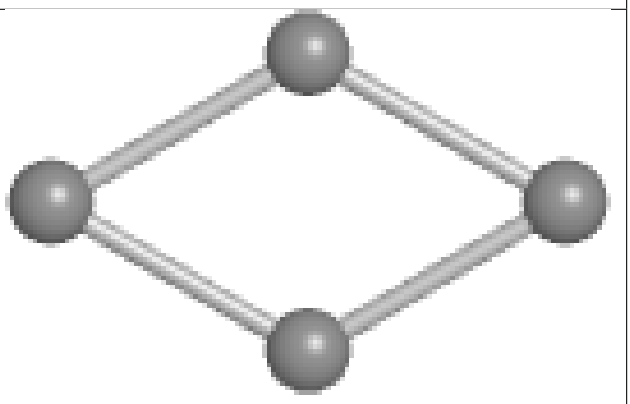
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	B	101	VAL	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

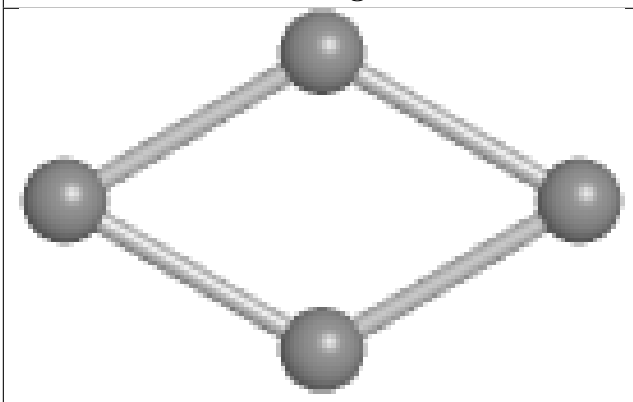
Ligand FES r 201



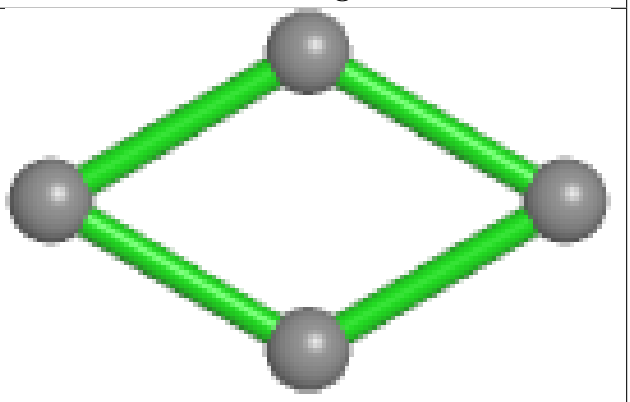
Bond lengths



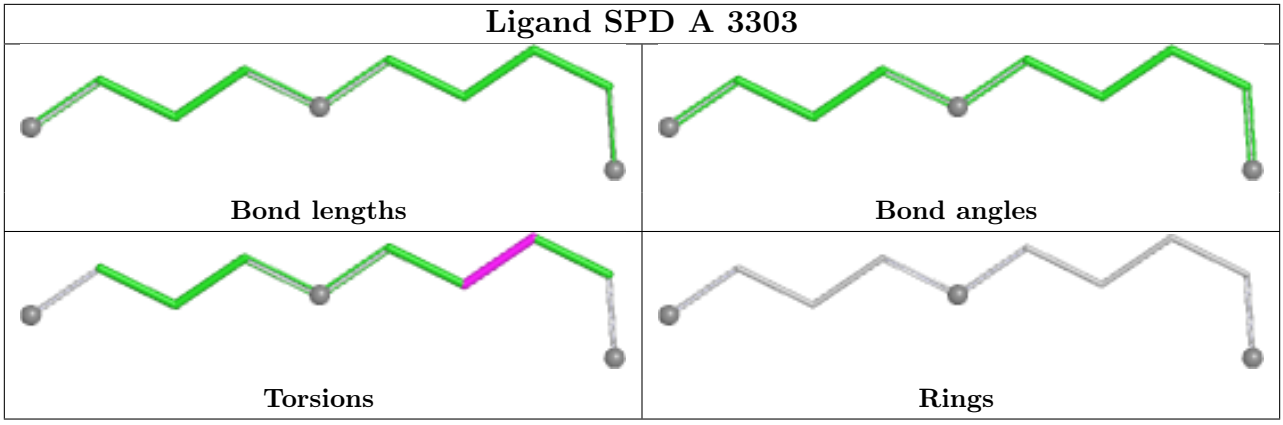
Bond angles

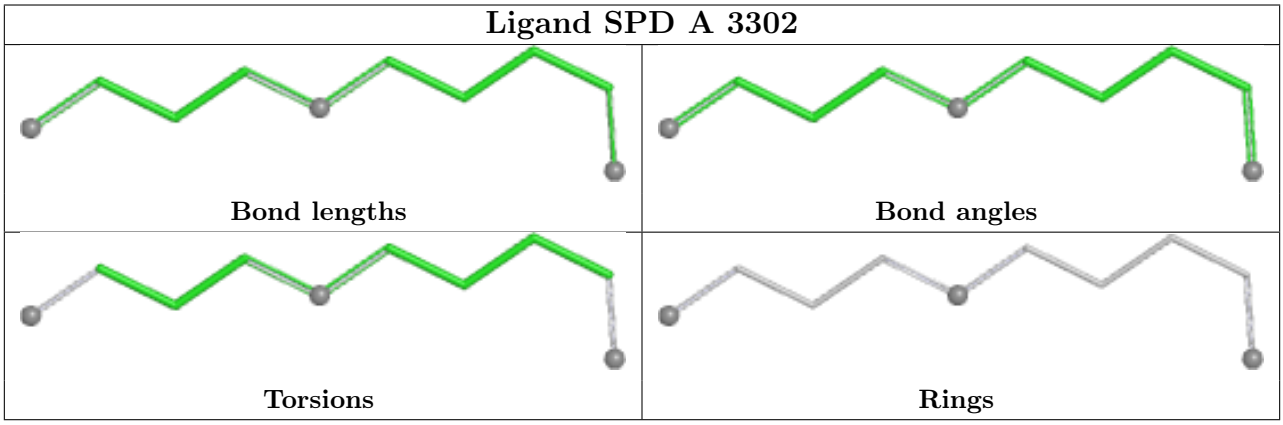


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
50	A	1
57	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	9.33
1	B	46:A	O3'	48:U	P	4.49

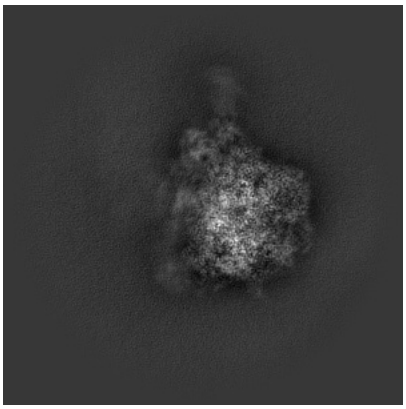
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-71797. These allow visual inspection of the internal detail of the map and identification of artifacts.

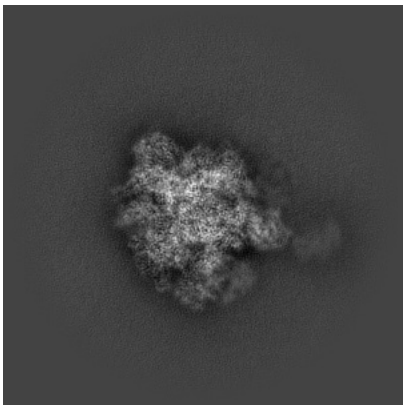
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

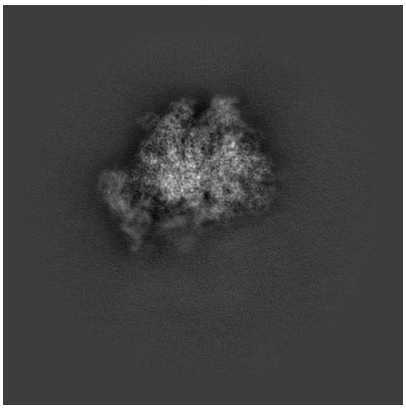
6.1.1 Primary map



X

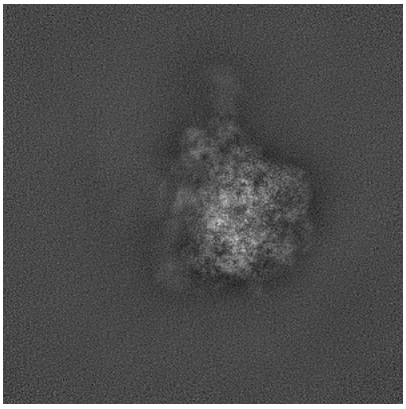


Y

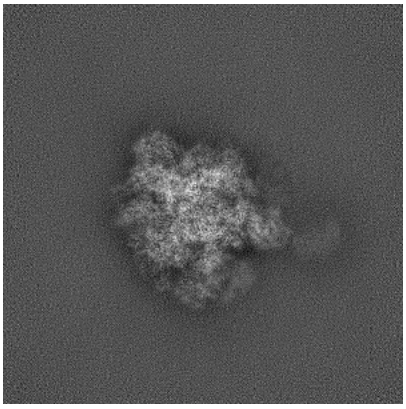


Z

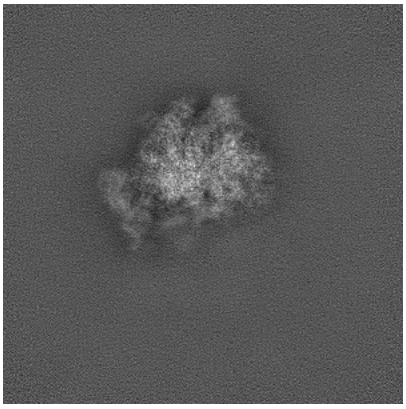
6.1.2 Raw map



X



Y

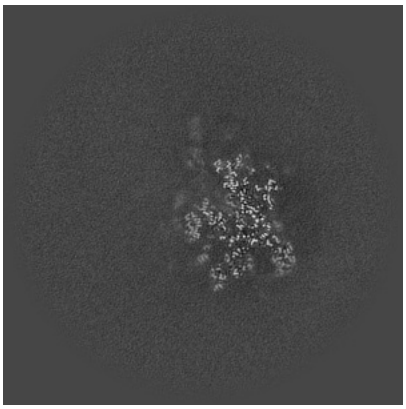


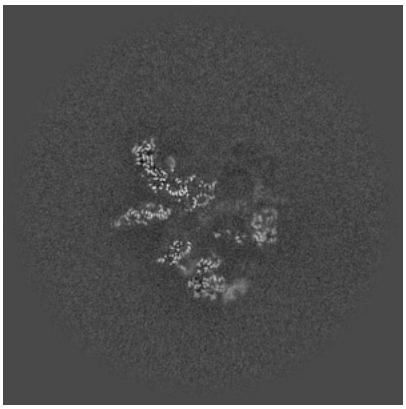
Z

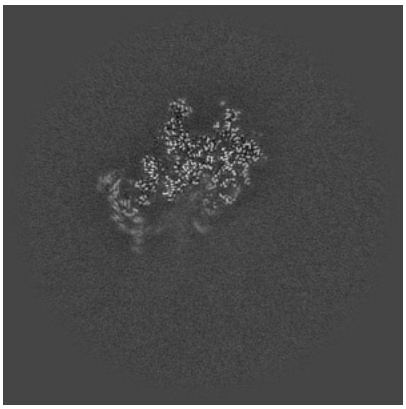
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

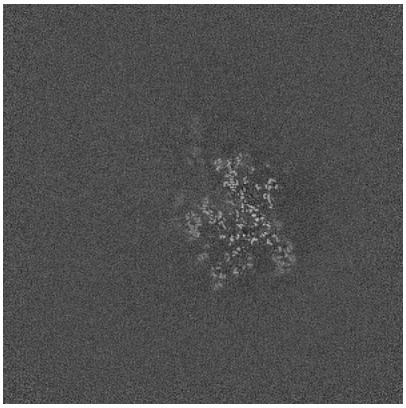
6.2.1 Primary map

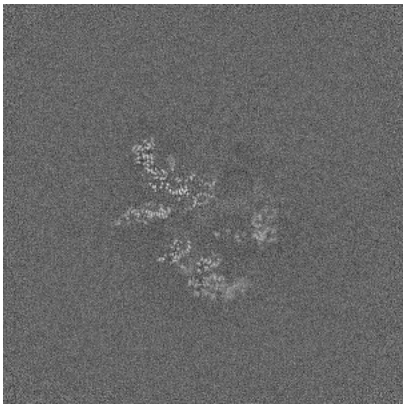

X Index: 240

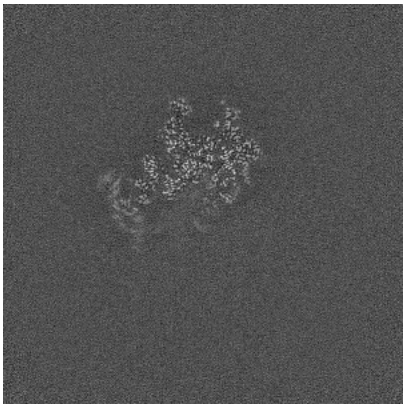

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

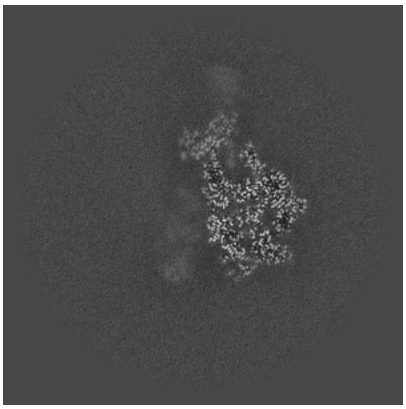

Y Index: 240


Z Index: 240

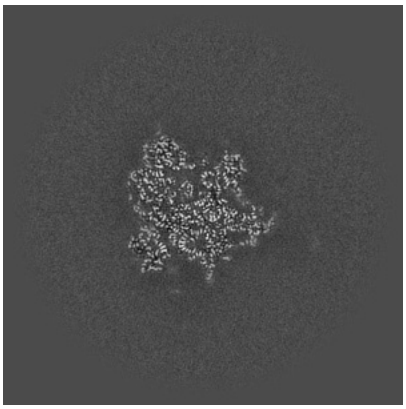
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

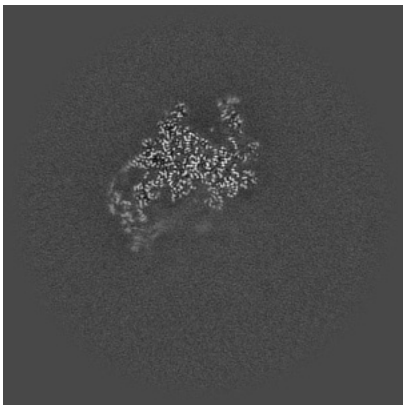
6.3.1 Primary map



X Index: 203

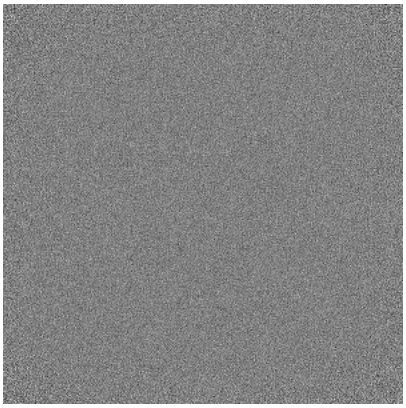


Y Index: 287

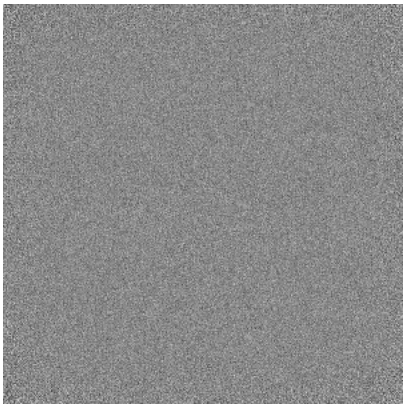


Z Index: 249

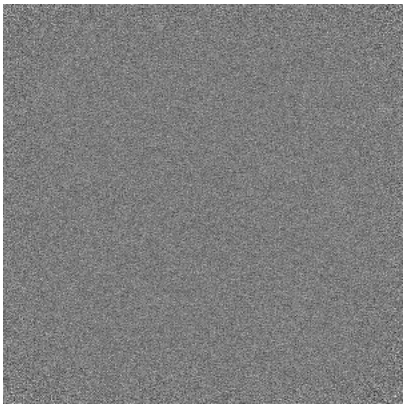
6.3.2 Raw map



X Index: 0



Y Index: 0

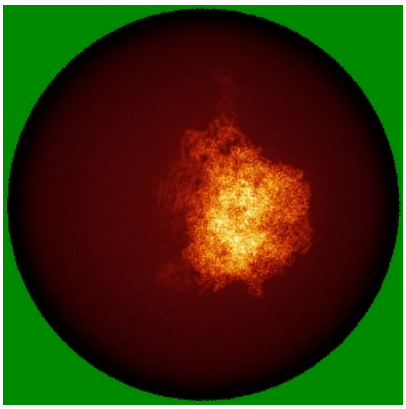


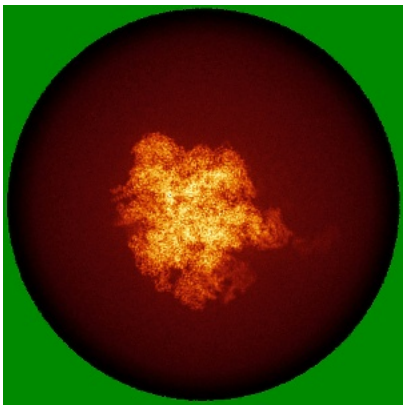
Z Index: 0

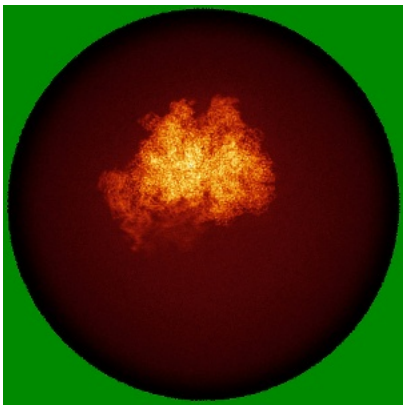
The images above show the largest variance slices of the map in three orthogonal directions.

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

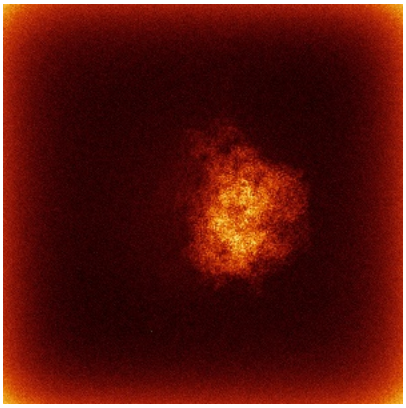
6.4.1 Primary map

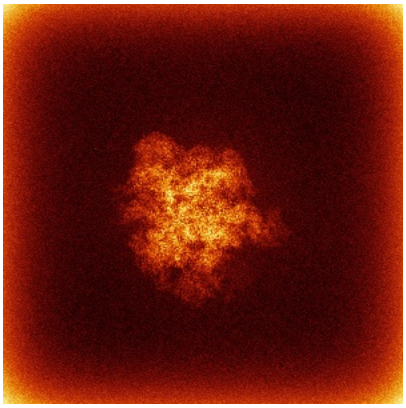

X

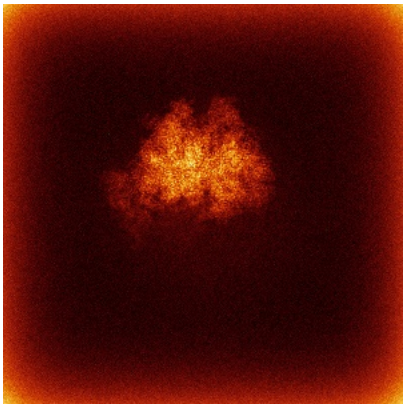

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

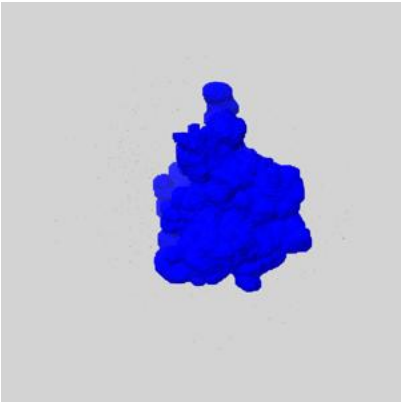
6.6 Mask visualisation (i)

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

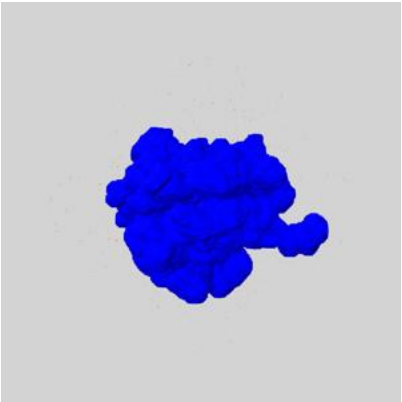
A mask typically either:

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

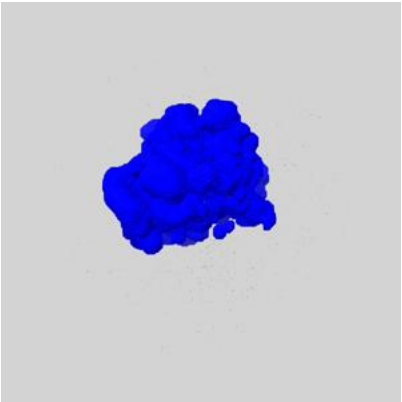
6.6.1 emd_71797_msk_1.map (i)



X



Y

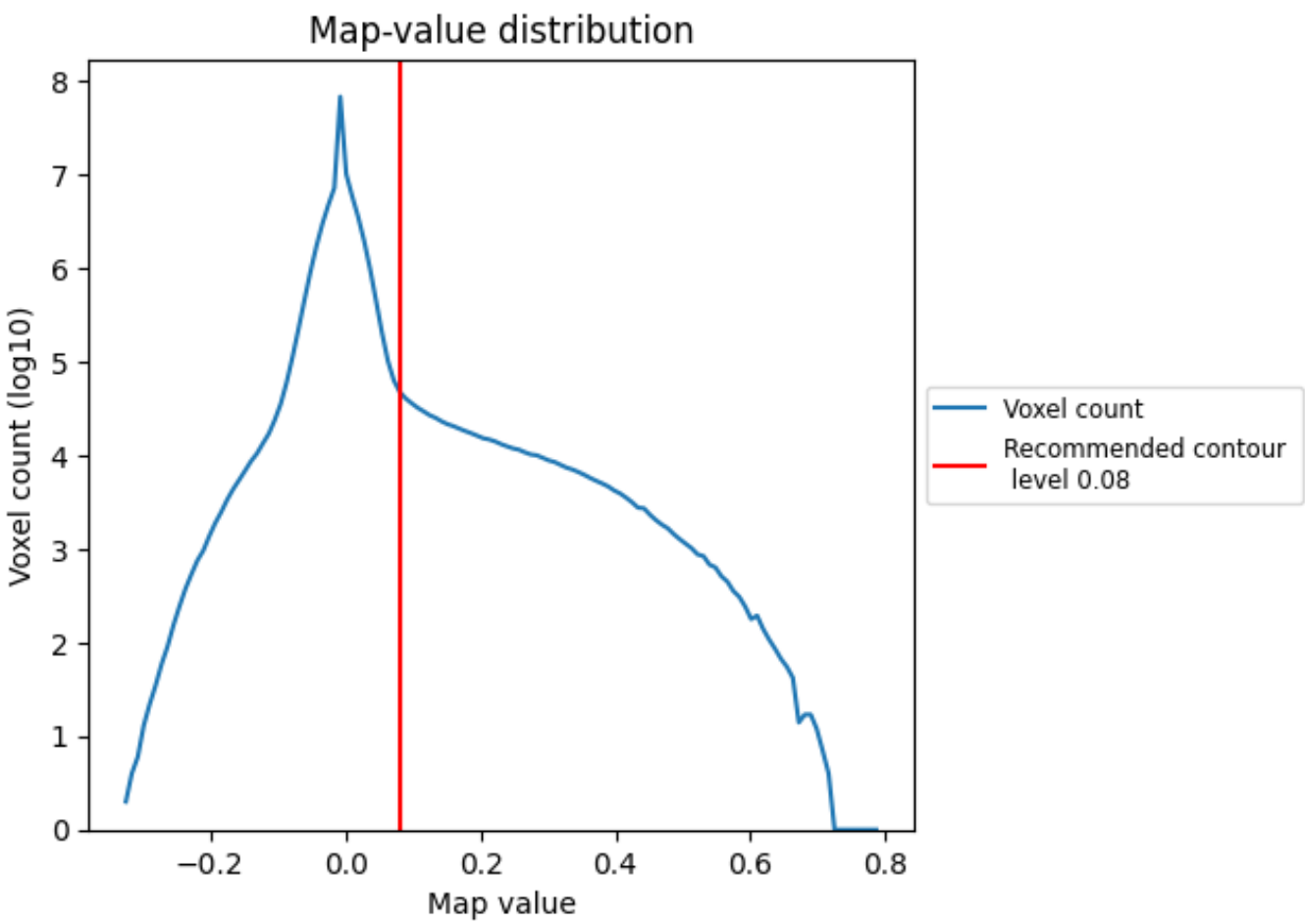


Z

7 Map analysis (i)

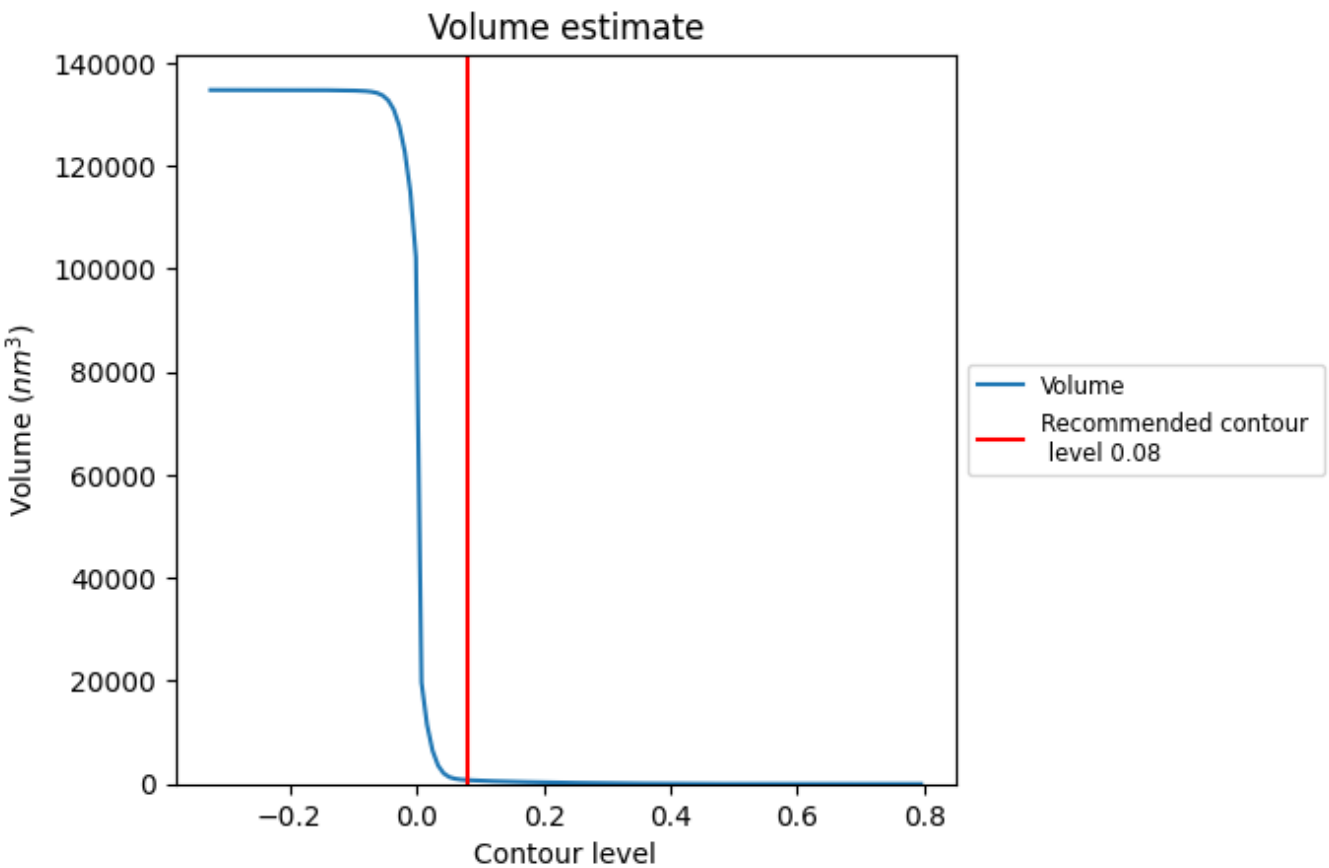
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

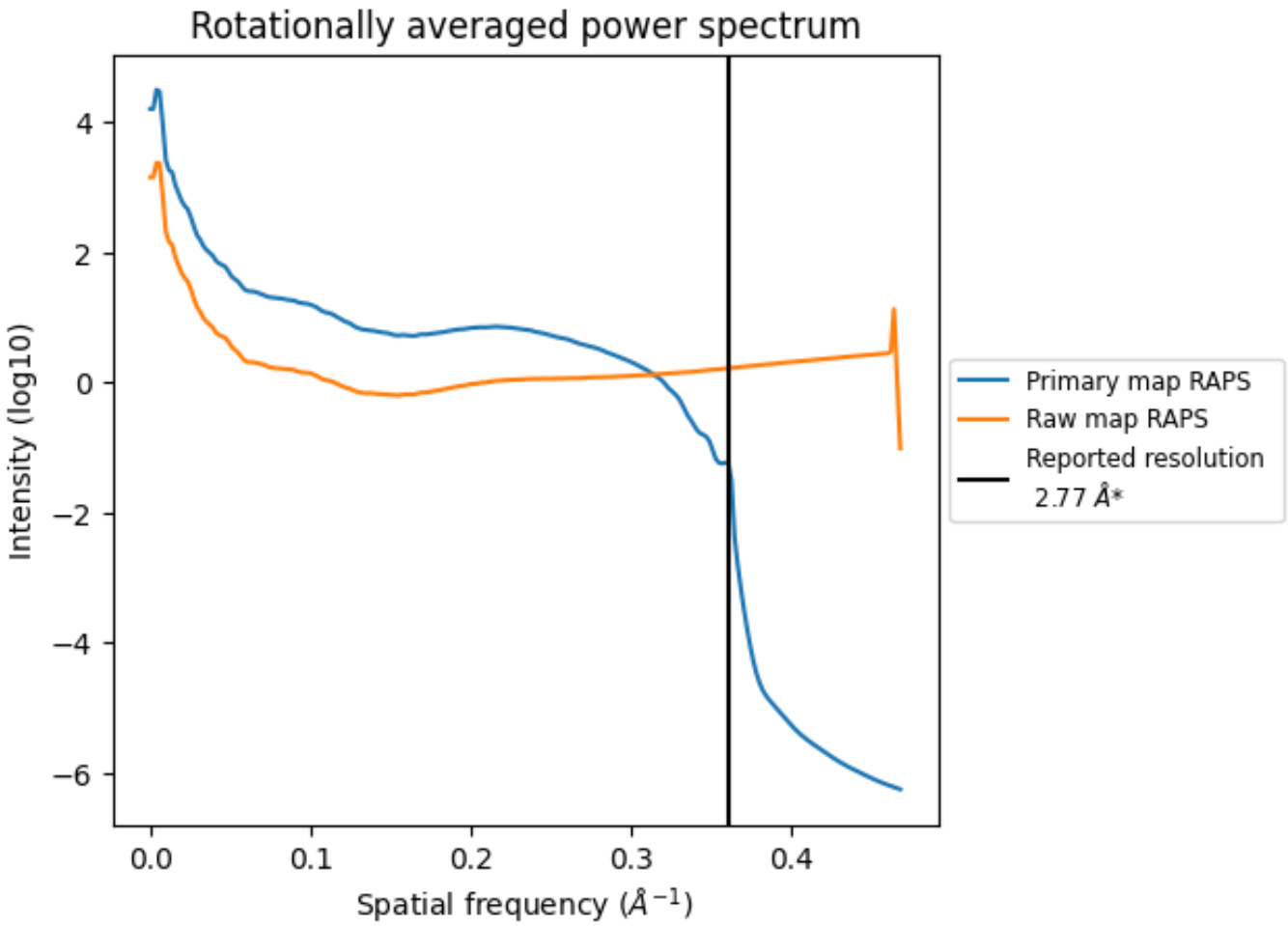
7.2 Volume estimate (i)



The volume at the recommended contour level is 762 nm^3; this corresponds to an approximate mass of 688 kDa.

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

7.3 Rotationally averaged power spectrum (i)

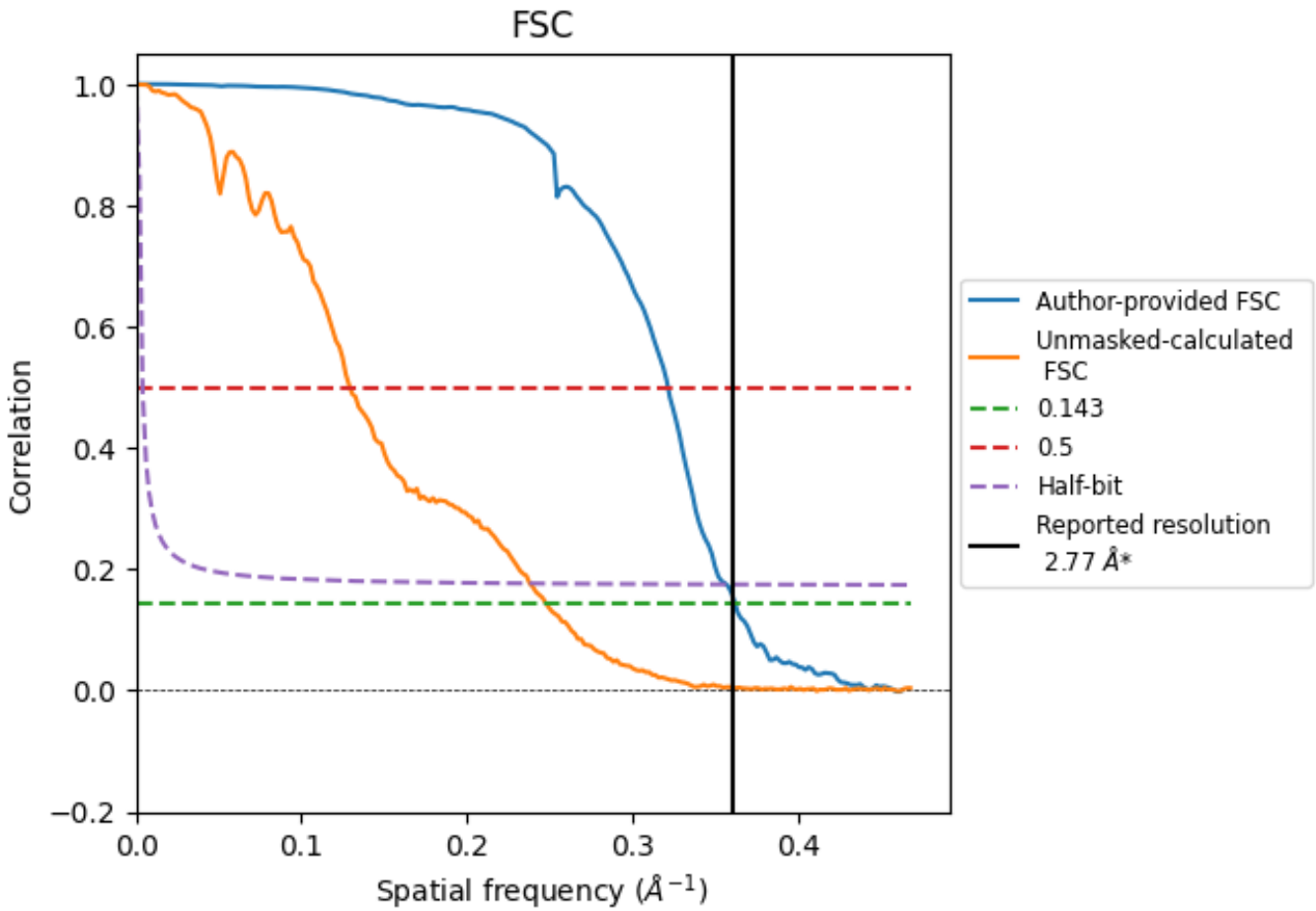


*Reported resolution corresponds to spatial frequency of 0.361 Å^{-1}

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 0.361 Å^{-1}

8.2 Resolution estimates (i)

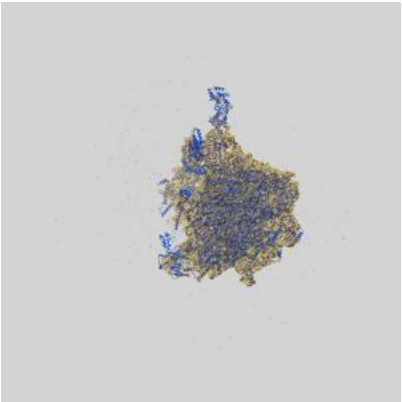
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.76	3.11	2.80
Unmasked-calculated*	4.03	7.73	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.77 by more than 10 %

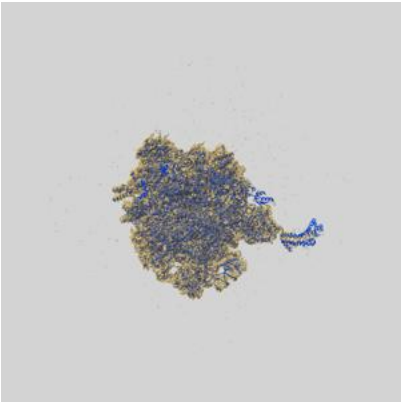
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-71797 and PDB model 9PR4. Per-residue inclusion information can be found in section 3 on page 18.

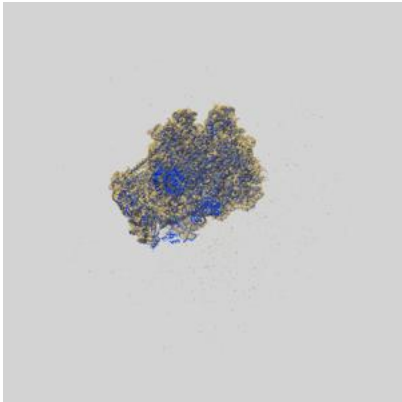
9.1 Map-model overlay (i)



X



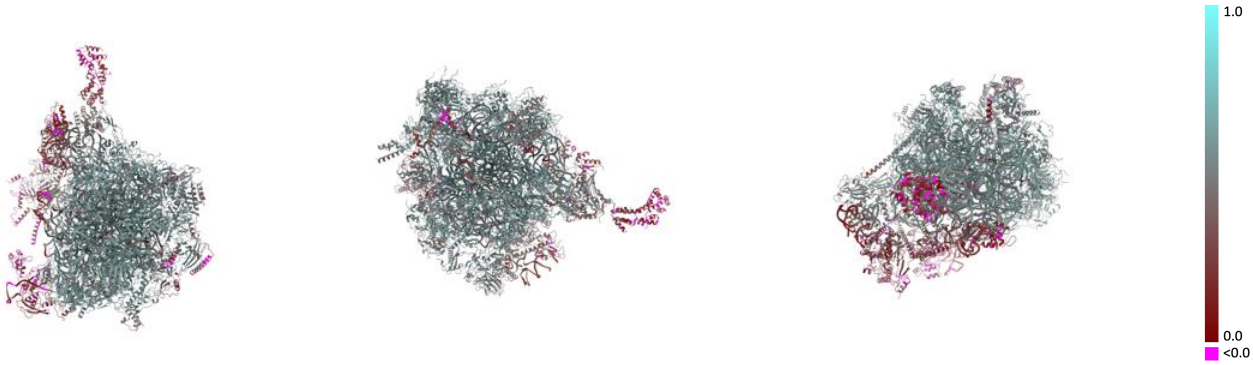
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

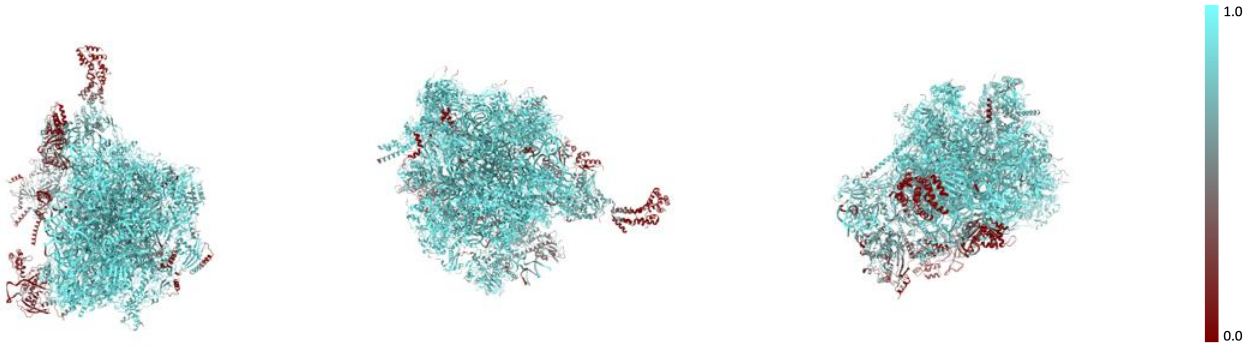
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

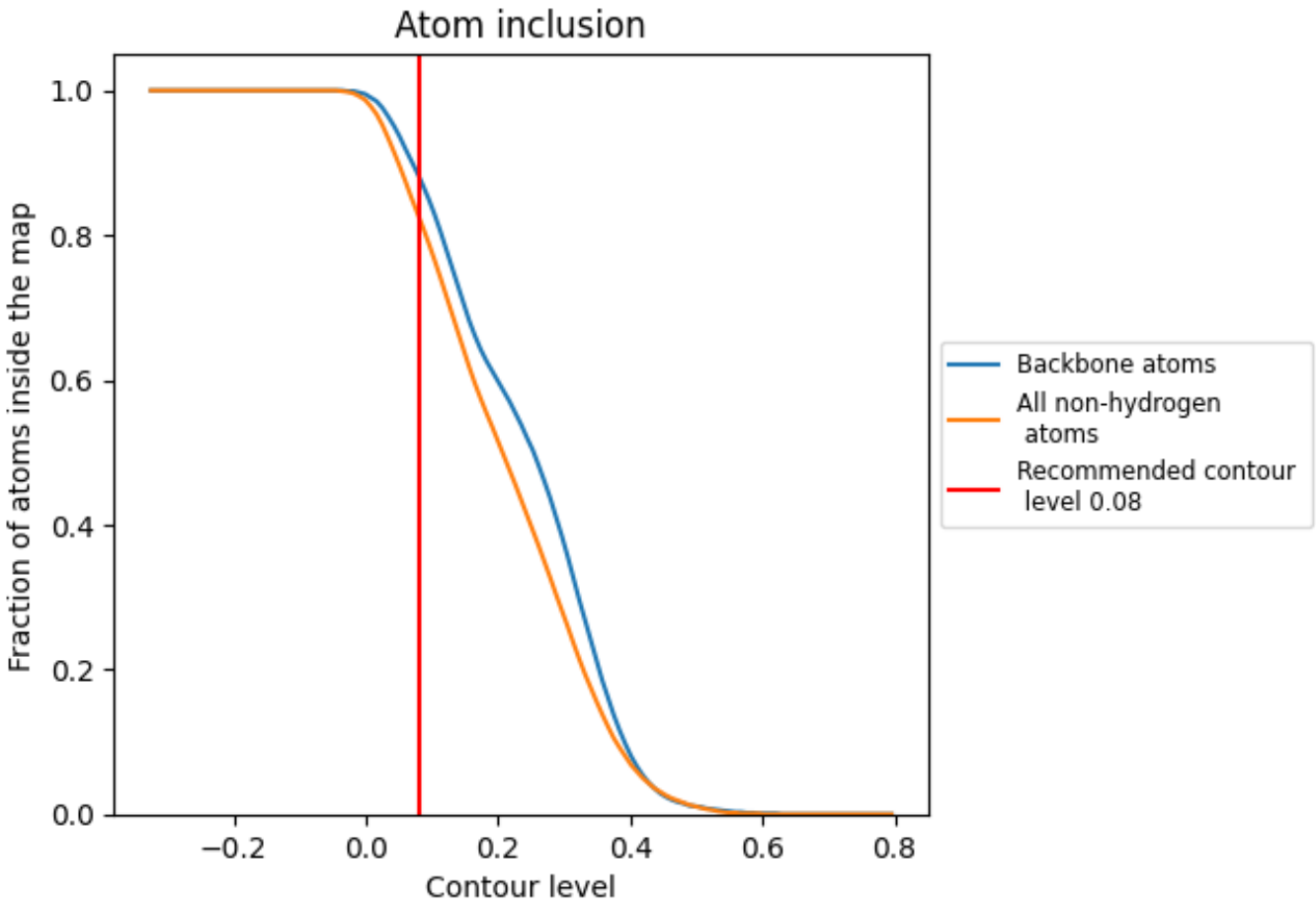
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4920
0	0.9060	0.5590
1	0.8270	0.5150
2	0.9610	0.5980
3	0.9610	0.5960
4	0.9140	0.5800
5	0.8950	0.5460
6	0.8430	0.4880
7	0.8480	0.5010
8	0.4920	0.2480
9	0.8940	0.5460
A	0.9380	0.5390
B	0.7830	0.3090
C	0.1750	0.2480
D	0.9090	0.5660
E	0.9200	0.5680
F	0.9460	0.5790
G	0.0270	0.1290
H	0.5080	0.3180
I	0.6250	0.3780
J	0.6230	0.3130
K	0.9460	0.5790
L	0.9060	0.5590
M	0.9380	0.5740
N	0.9070	0.5570
O	0.9290	0.5670
OX	0.3180	0.2900
P	0.8780	0.5300
Q	0.8910	0.5530
R	0.9330	0.5740
S	0.9230	0.5650
T	0.9350	0.5840
U	0.8160	0.4950
V	0.8510	0.5100
W	0.8980	0.5690

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Chain	Atom inclusion	Q-score
X	0.8980	0.5460
Y	0.9120	0.5620
Z	0.9280	0.5750
a	0.7720	0.4820
b	0.9420	0.5780
c	0.8950	0.5320
d	0.7130	0.4470
e	0.4500	0.1920
f	0.5340	0.2850
g	0.9210	0.5620
h	0.8600	0.5020
i	0.9510	0.5920
j	0.8500	0.5160
k	0.7850	0.4660
l	0.7270	0.3820
m	0.4590	0.2220
n	0.3750	0.3070
o	0.9500	0.5850
p	0.7770	0.4640
q	0.6100	0.3770
r	0.9070	0.5560
s	0.9060	0.5560
t	0.3340	0.2330
u	0.2620	0.1610
v	0.0310	0.0660
w	0.0330	0.0720
x	0.0200	0.0470
y	0.0120	0.0360
z	0.0690	0.0770