



Full wwPDB EM Validation Report ⓘ

Mar 16, 2026 – 01:22 PM UTC

PDB ID : 7PO4 / pdb_00007po4
EMDB ID : EMD-13562
Title : Assembly intermediate of human mitochondrial ribosome large subunit (largely unfolded rRNA with MALSU1, L0R8F8 and ACP)
Authors : Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on : 2021-09-08
Resolution : 2.56 Å(reported)
Based on initial model : 6ZM6

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

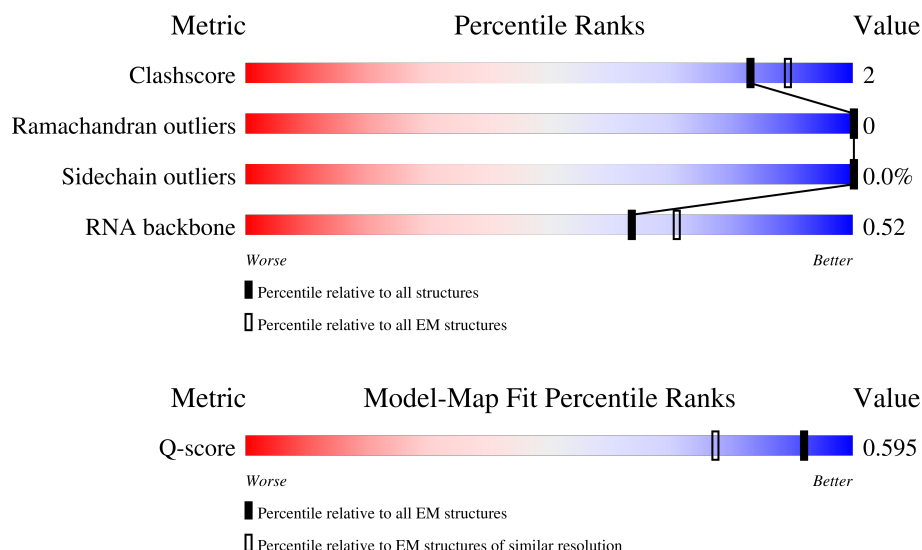
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 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.



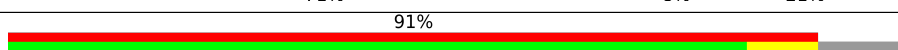
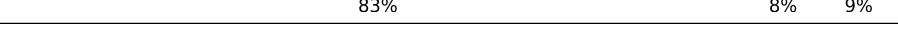
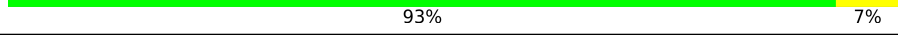
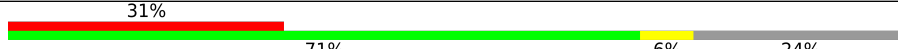
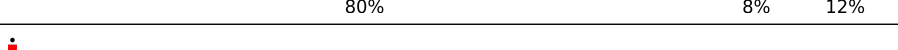
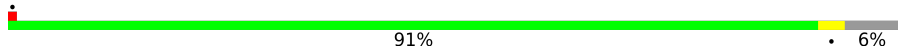
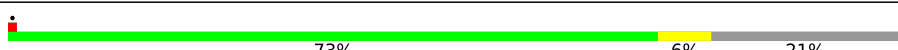
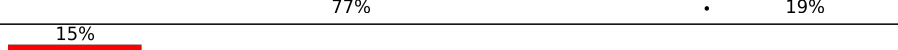
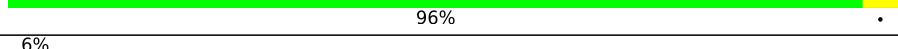
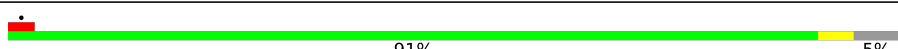
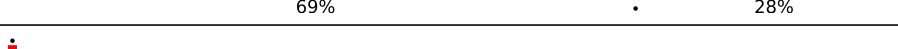
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7558 (2.06 - 3.06)

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

Mol	Chain	Length	Quality of chain
1	A	1561	
2	B	72	
3	D	305	

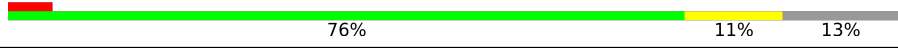
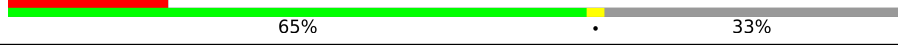
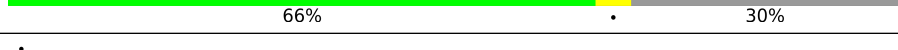
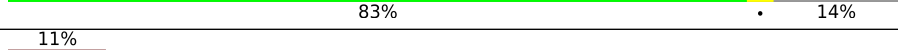
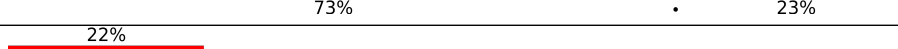
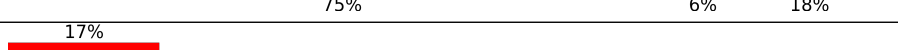
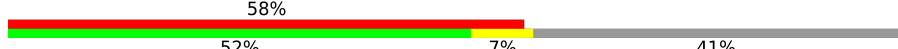
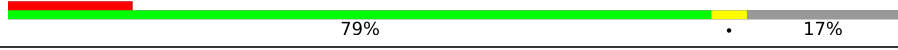
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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	177	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	152	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	

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Mol	Chain	Length	Quality of chain
29	5	423	
30	6	380	
31	7	338	
32	8	206	
33	9	137	
34	a	142	
35	b	214	
36	c	332	
37	d	306	
38	e	279	
39	f	212	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	k	111	
45	l	138	
46	m	128	
47	o	102	
48	p	206	
49	q	222	
50	r	196	
51	s	439	
52	t	198	
52	u	198	

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Mol	Chain	Length	Quality of chain
52	v	198	15%14%85%
52	w	198	16%13%84%
52	x	198	16%16%84%
52	y	198	16%16%84%
53	za	234	50%47%
54	zb	70	9%94%
55	zc	156	48%52%44%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 186318 atoms, of which 85917 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16SrRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1145	Total	C	H	N	O	P	0	0
			36467	10915	12165	4406	7836	1145		

- Molecule 2 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total	C	H	N	O	P	0	0
			2293	685	769	269	498	72		

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	214	Total	C	H	N	O	S	0	0
			3360	1023	1703	335	291	8		

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	284	Total	C	H	N	O	S	0	0
			4526	1457	2269	384	405	11		

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	249	Total	C	H	N	O	S	0	0
			4053	1293	2042	366	346	6		

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	97	Total	C	H	N	O		0	0
			1649	508	847	155	139			

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	206	Total	C	H	N	O	S	0	0
			3397	1065	1740	297	284	11		

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	175	Total	C	H	N	O	S	0	0
			2738	847	1408	237	244	2		

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	177	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	269	Total	C	H	N	O	S	0	0
			4357	1383	2208	379	382	5		

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	191	Total	C	H	N	O	S	0	0
			3114	995	1560	279	271	9		

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	154	Total	C	H	N	O	S	0	0
			2554	792	1295	241	219	7		

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	144	Total	C	H	N	O	S	0	0
			2339	733	1166	224	211	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	220	Total	C	H	N	O	S	0	0
			3707	1174	1873	326	325	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	140	Total	C	H	N	O	S	0	0
			2369	732	1215	231	187	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	161	Total	C	H	N	O	S	0	0
			2659	835	1366	227	227	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	166	Total	C	H	N	O	S	0	0
			2780	875	1411	254	233	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	152	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	205	Total	C	H	N	O	S	0	0
			3364	1068	1688	298	302	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	102	Total	C	H	N	O	S	0	0
			1647	523	835	152	134	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	244	Total	C	H	N	O	S	0	0
			4104	1322	2060	352	365	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	110	Total	C	H	N	O	S	0	0
			1799	554	901	176	162	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	55	Total	C	H	N	O	S	0	0
			954	290	499	87	76	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	2	46	Total	C	H	N	O	S	0	0
			784	233	407	83	60	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	95	Total	C	H	N	O	S	0	0
			1716	539	884	162	128	3		

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	5	394	Total	C	H	N	O	S	0	0
			6417	2073	3207	560	566	11		

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	6	354	Total	C	H	N	O	S	0	0
			5790	1881	2842	525	533	9		

- Molecule 31 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	7	294	Total	C	H	N	O	S	0	0
			4788	1529	2398	405	438	18		

- Molecule 32 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	8	138	Total	C	H	N	O	S	0	0
			2363	746	1193	205	217	2		

- Molecule 33 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

- Molecule 34 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	a	100	Total	C	H	N	O	S	0	0
			1652	529	812	152	154	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
35	b	150	Total	C	H	N	O	S	0	0
			2392	744	1196	231	218	3		

- Molecule 36 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	c	286	Total	C	H	N	O	S	0	0
			4621	1470	2322	397	423	9		

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	d	236	Total	C	H	N	O	S	0	0
			3851	1233	1918	335	351	14		

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	e	228	Total	C	H	N	O	S	0	0
			3699	1174	1851	326	342	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	f	153	Total	C	H	N	O	S	0	0
			2449	778	1229	201	237	4		

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	h	110	Total	C	H	N	O	S	0	0
			1777	568	882	156	168	3		

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	i	93	Total	C	H	N	O	S	0	0
			1612	509	820	157	122	4		

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

- Molecule 44 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	k	101	Total	C	H	N	O	S	0	0
			1558	479	784	148	142	5		

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	l	82	Total	C	H	N	O	S	0	0
			1363	437	675	120	128	3		

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	m	64	Total	C	H	N	O	S	0	0
			1096	330	560	111	93	2		

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	o	82	Total	C	H	N	O	S	0	0
			1395	438	697	141	116	3		

- Molecule 48 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	p	147	Total	C	H	N	O	S	0	0
			2431	748	1226	228	225	4		

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	q	161	Total	C	H	N	O	S	0	0
			2678	841	1328	260	244	5		

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	r	162	Total	C	H	N	O	S	0	0
			2659	839	1337	252	223	8		

- Molecule 51 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	s	386	Total	C	H	N	O	S	0	0
			6296	2023	3141	559	559	14		

- Molecule 52 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	t	46	Total	C	H	N	O		0	0
			732	228	378	56	70			
52	u	32	Total	C	H	N	O		0	0
			541	168	284	40	49			
52	v	29	Total	C	H	N	O		0	0
			486	152	253	36	45			
52	w	31	Total	C	H	N	O		0	0
			520	159	275	39	47			
52	x	31	Total	C	H	N	O		0	0
			520	159	275	39	47			
52	y	31	Total	C	H	N	O		0	0
			520	159	275	39	47			

- Molecule 53 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	za	123	Total	C	H	N	O	S	0	0
			2019	648	1007	169	185	10		

- Molecule 54 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	zb	69	Total	C	H	N	O		0	0
			1194	372	605	116	101			

- Molecule 55 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	zc	87	Total	C	H	N	O	S	0	0
			1397	452	692	103	144	6		

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

Mol	Chain	Residues	Atoms		AltConf
56	A	33	Total	Mg	0
			33	33	
56	B	1	Total	Mg	0
			1	1	
56	g	1	Total	Mg	0
			1	1	

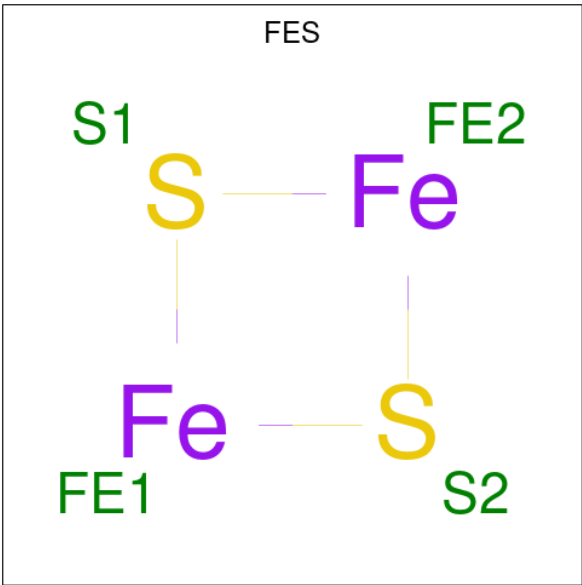
- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	7	Total	K	0
			7	7	
57	6	1	Total	K	0
			1	1	

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

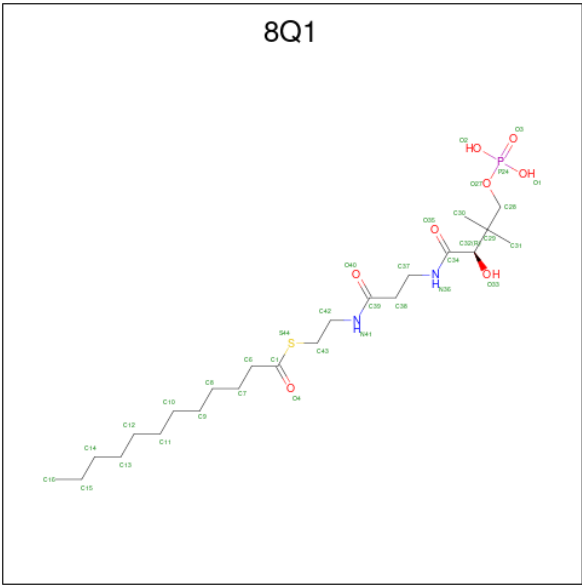
Mol	Chain	Residues	Atoms		AltConf
58	0	1	Total	Zn	0
			1	1	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 60 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
60	zc	1	Total	C	H	N	O	P	S	0
			77	23	43	2	7	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	1157	Total 1157	O 1157	0
61	B	26	Total 26	O 26	0
61	D	14	Total 14	O 14	0
61	E	77	Total 77	O 77	0
61	F	81	Total 81	O 81	0
61	H	7	Total 7	O 7	0
61	K	29	Total 29	O 29	0
61	L	38	Total 38	O 38	0
61	M	53	Total 53	O 53	0
61	N	1	Total 1	O 1	0
61	O	33	Total 33	O 33	0
61	P	52	Total 52	O 52	0
61	Q	79	Total 79	O 79	0
61	R	56	Total 56	O 56	0
61	S	35	Total 35	O 35	0
61	T	43	Total 43	O 43	0
61	U	44	Total 44	O 44	0
61	V	29	Total 29	O 29	0
61	W	16	Total 16	O 16	0
61	X	16	Total 16	O 16	0
61	Y	46	Total 46	O 46	0
61	Z	23	Total 23	O 23	0

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Mol	Chain	Residues	Atoms		AltConf
61	0	26	Total 26	O 26	0
61	2	32	Total 32	O 32	0
61	3	36	Total 36	O 36	0
61	5	32	Total 32	O 32	0
61	6	49	Total 49	O 49	0
61	7	11	Total 11	O 11	0
61	8	5	Total 5	O 5	0
61	9	29	Total 29	O 29	0
61	a	18	Total 18	O 18	0
61	b	54	Total 54	O 54	0
61	c	42	Total 42	O 42	0
61	d	7	Total 7	O 7	0
61	e	1	Total 1	O 1	0
61	f	6	Total 6	O 6	0
61	g	28	Total 28	O 28	0
61	h	7	Total 7	O 7	0
61	i	43	Total 43	O 43	0
61	j	27	Total 27	O 27	0
61	m	1	Total 1	O 1	0
61	o	16	Total 16	O 16	0
61	p	12	Total 12	O 12	0

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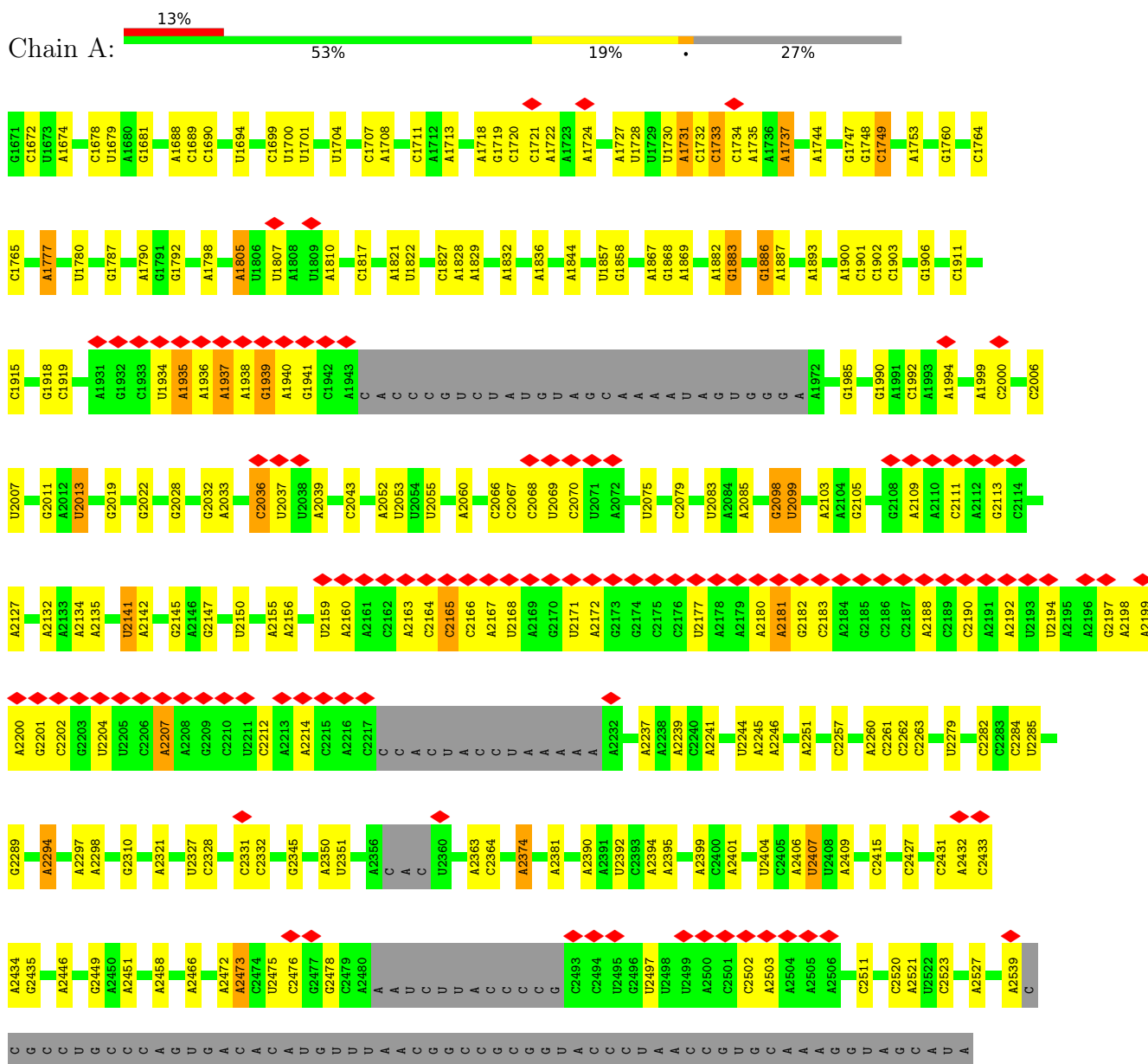
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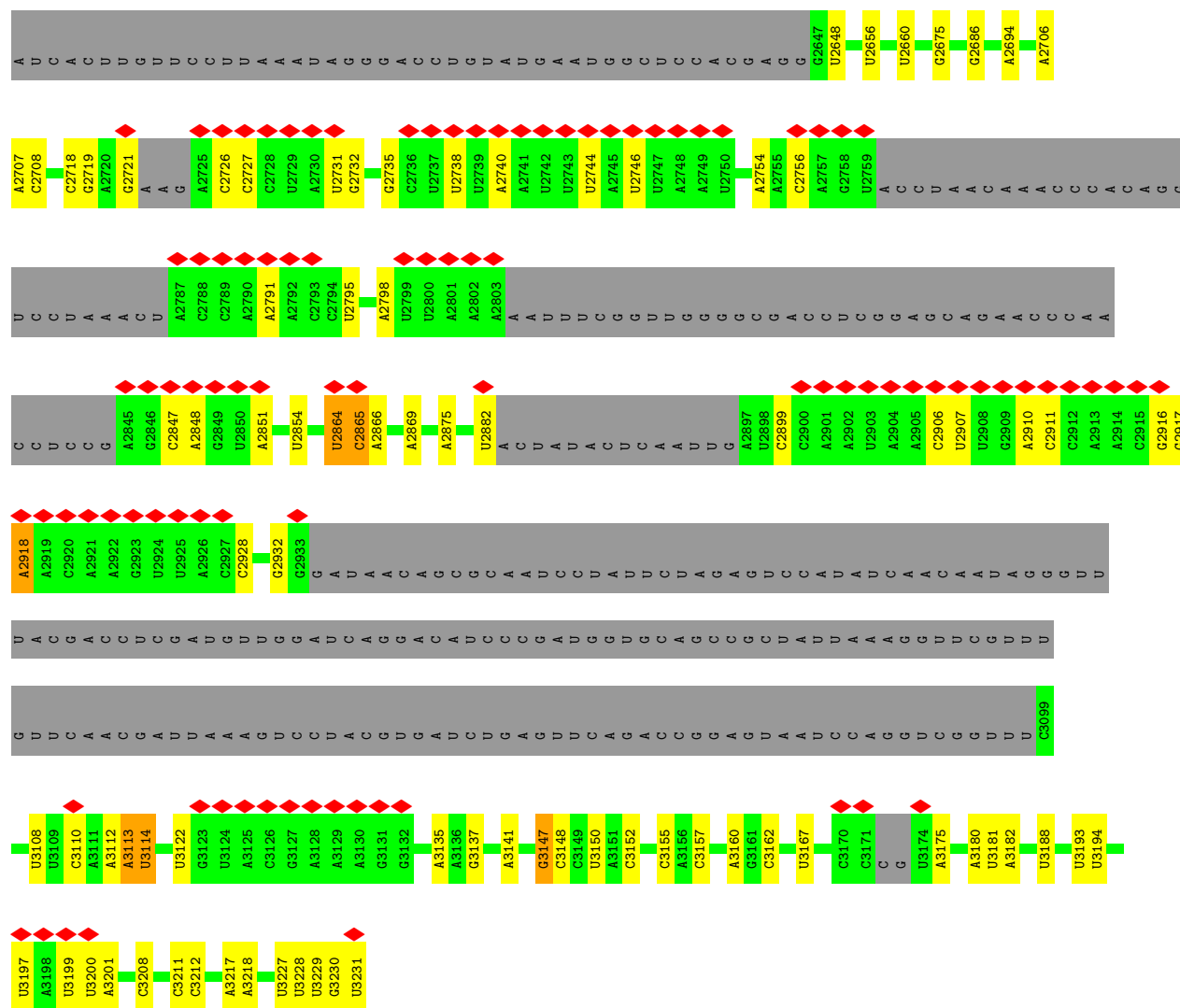
Mol	Chain	Residues	Atoms		AltConf
61	q	8	Total 8	O 8	0
61	r	7	Total 7	O 7	0
61	s	86	Total 86	O 86	0
61	za	5	Total 5	O 5	0

3 Residue-property plots

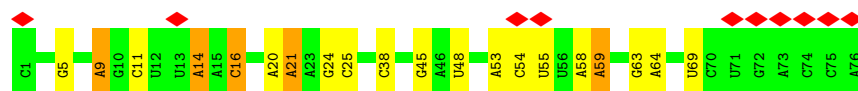
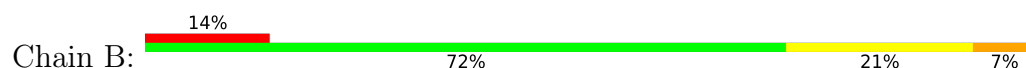
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16SrRNA

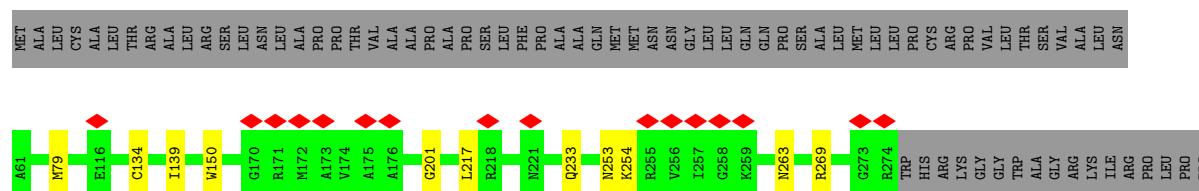




• Molecule 2: tRNAVal



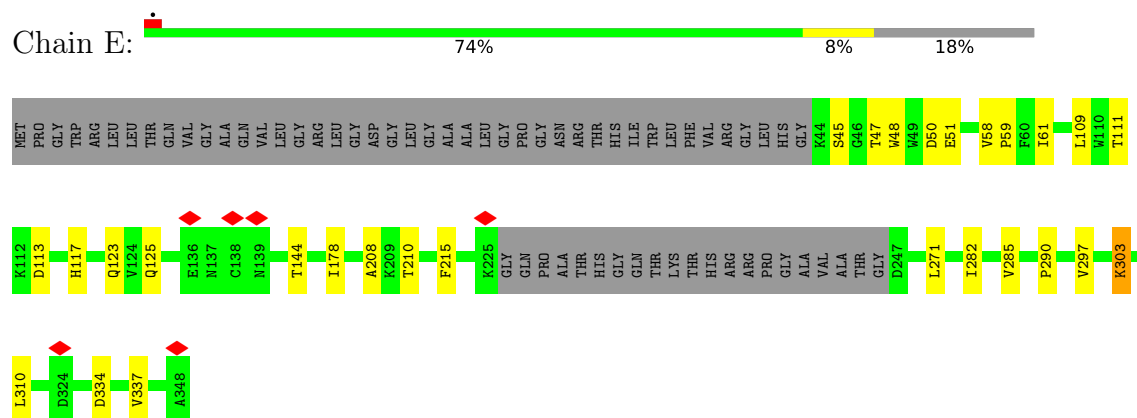
• Molecule 3: 39S ribosomal protein L2, mitochondrial



MET
LYS
SER
TYR
VAL
LEU
PRO
SER
ALA
ALA
GLN
SER

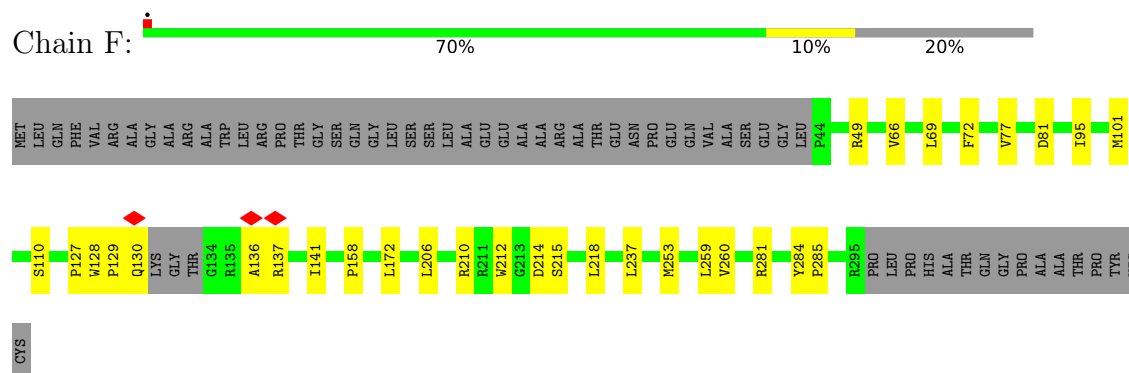
- Molecule 4: 39S ribosomal protein L3, mitochondrial

Chain E:



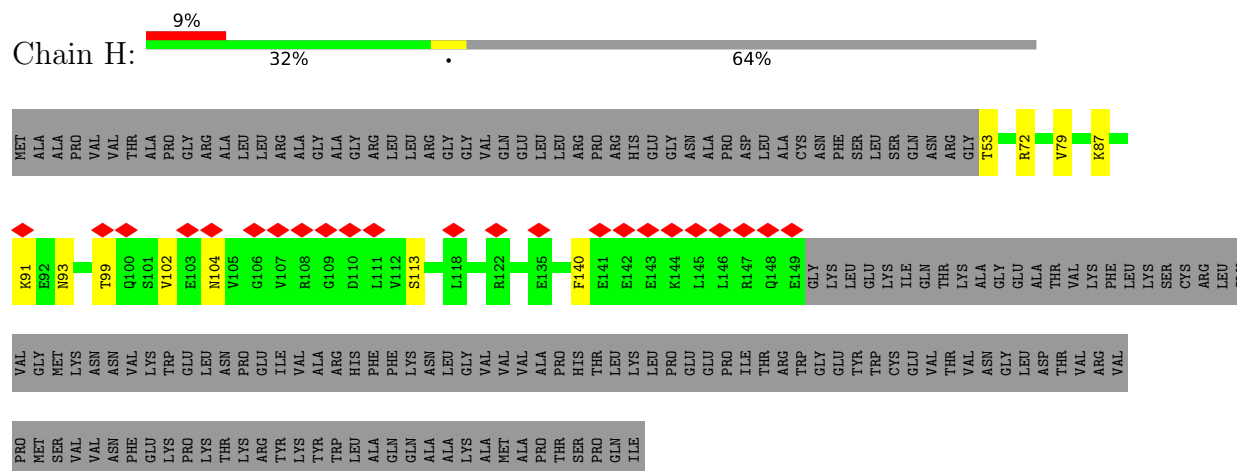
- Molecule 5: 39S ribosomal protein L4, mitochondrial

Chain F:



- Molecule 6: 39S ribosomal protein L9, mitochondrial

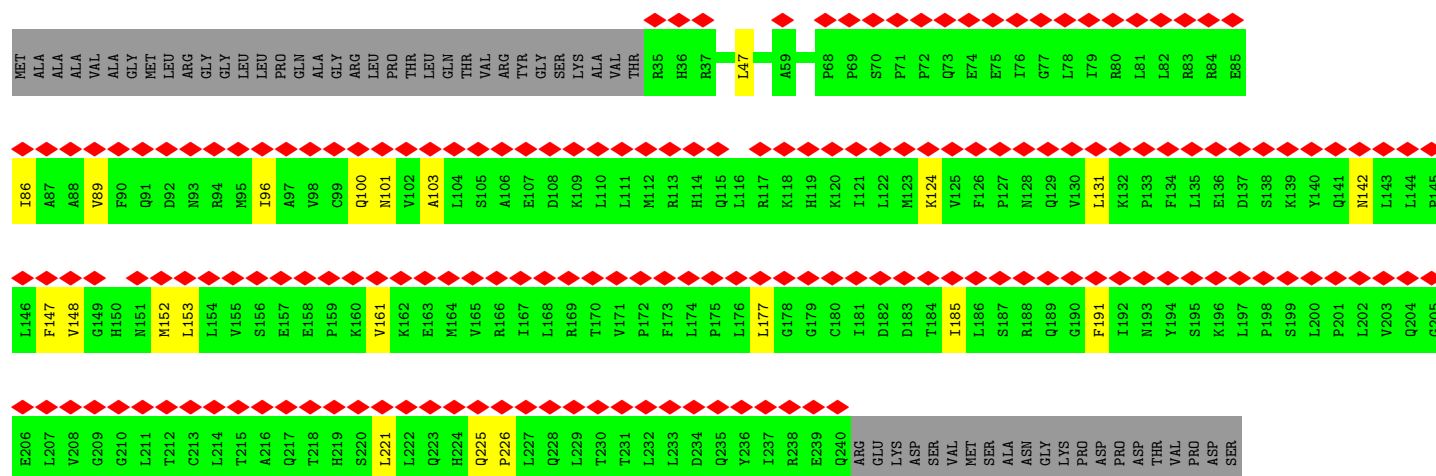
Chain H:



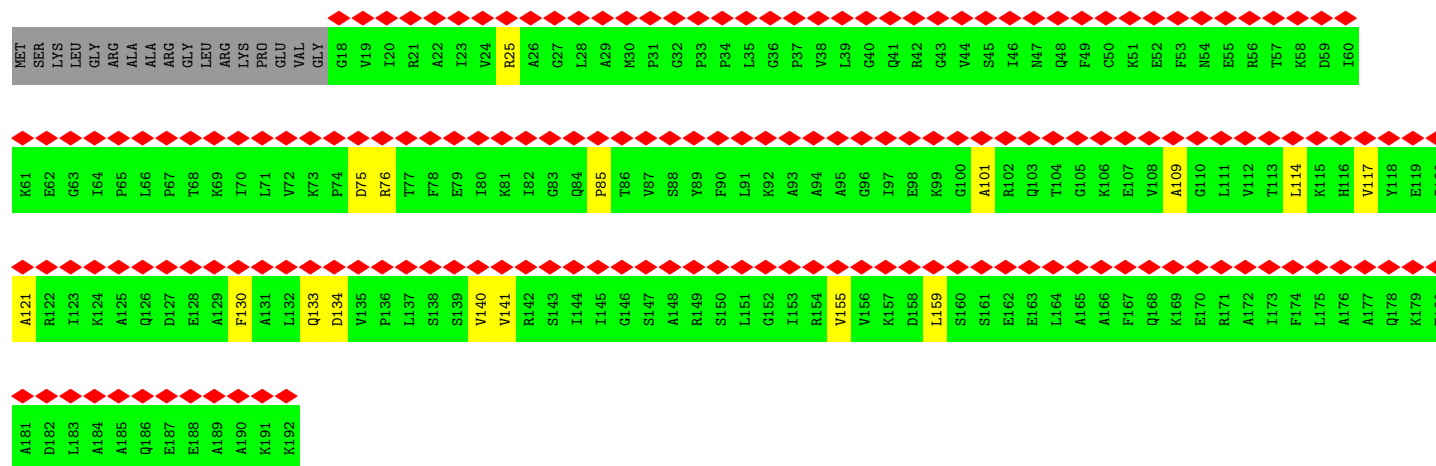
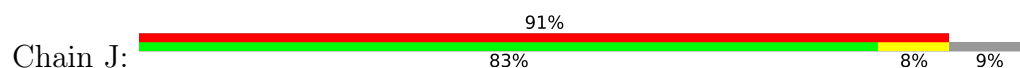
- Molecule 7: 39S ribosomal protein L10, mitochondrial

Chain I:





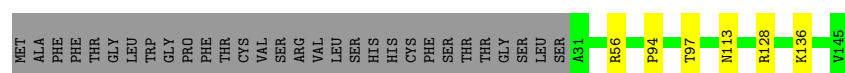
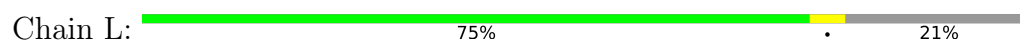
- Molecule 8: 39S ribosomal protein L11, mitochondrial



- Molecule 9: 39S ribosomal protein L13, mitochondrial

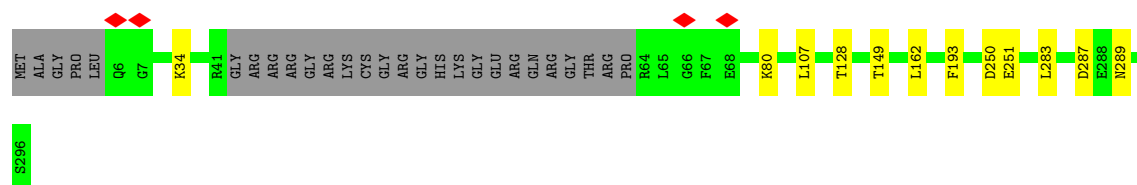


- Molecule 10: 39S ribosomal protein L14, mitochondrial

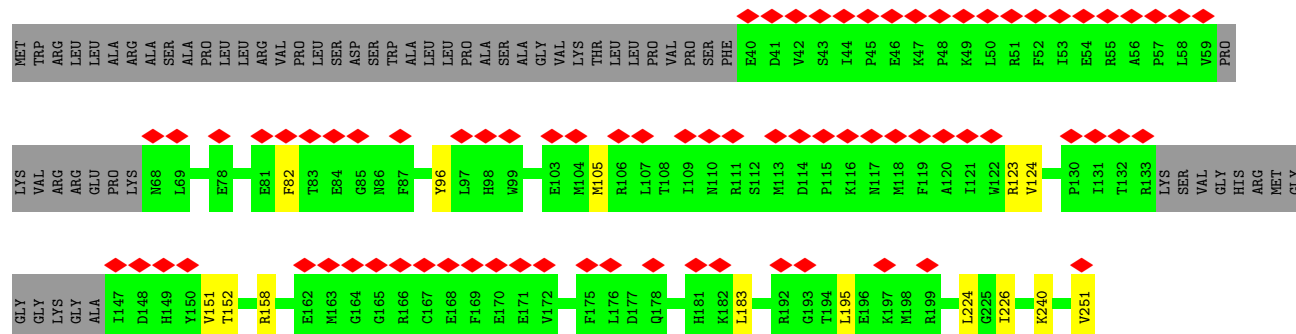


- Molecule 11: 39S ribosomal protein L15, mitochondrial

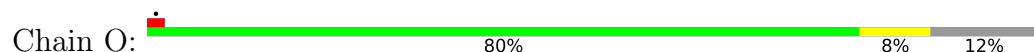




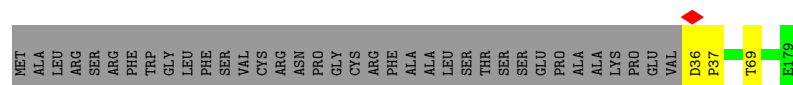
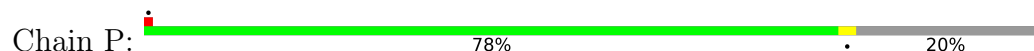
- Molecule 12: 39S ribosomal protein L16, mitochondrial



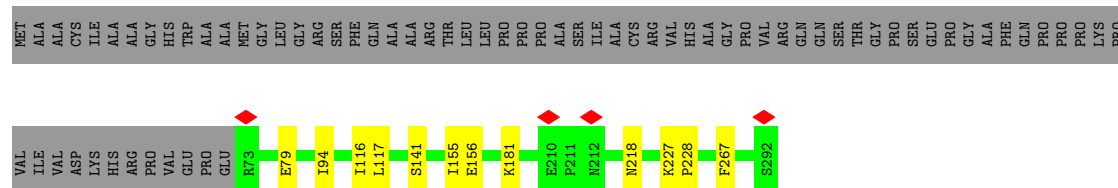
- Molecule 13: 39S ribosomal protein L17, mitochondrial



- Molecule 14: 39S ribosomal protein L18, mitochondrial

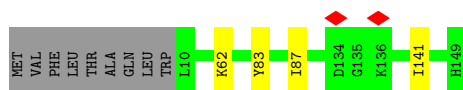


- Molecule 15: 39S ribosomal protein L19, mitochondrial

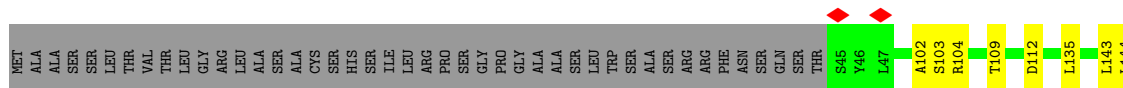


- Molecule 16: 39S ribosomal protein L20, mitochondrial

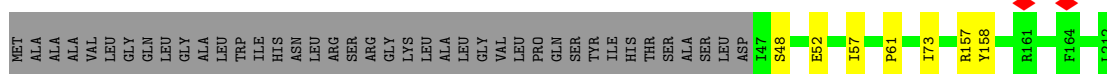
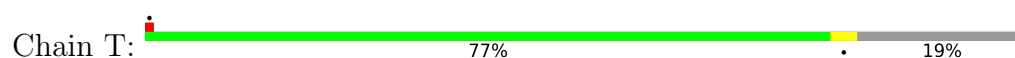




- Molecule 17: 39S ribosomal protein L21, mitochondrial



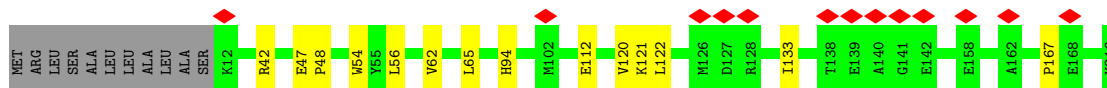
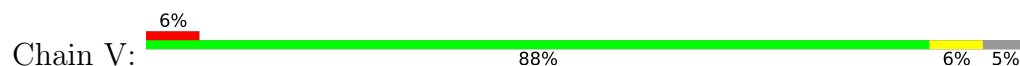
- Molecule 18: 39S ribosomal protein L22, mitochondrial



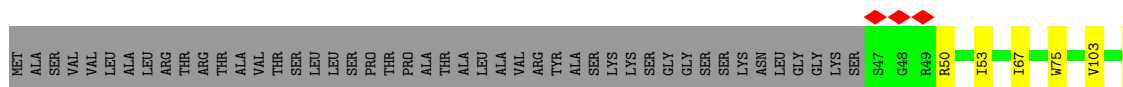
- Molecule 19: 39S ribosomal protein L23, mitochondrial



- Molecule 20: 39S ribosomal protein L24, mitochondrial

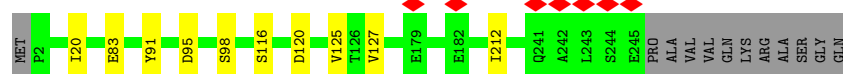


- Molecule 21: 39S ribosomal protein L27, mitochondrial



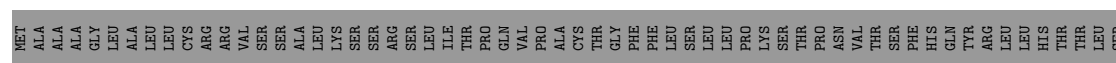
- Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X:  91% 5%



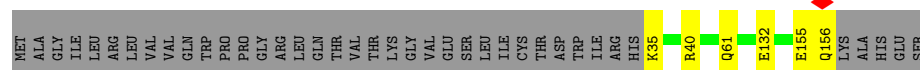
- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y:  69% 28%



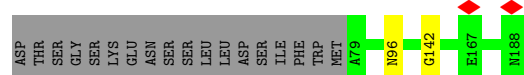
- Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z:  72% 24%



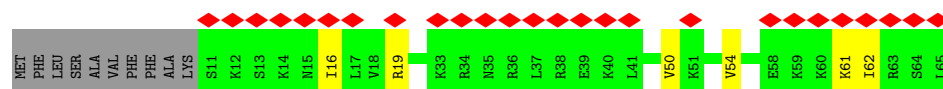
- Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0:  57% 41%



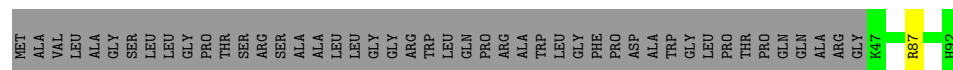
- Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1:  40% 75% 9% 15%



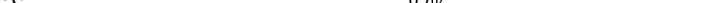
- Molecule 27: 39S ribosomal protein L34, mitochondrial

Chain 2:  49% 50%



- Molecule 28: 39S ribosomal protein L35, mitochondrial

MET	ALA	ALA	SER	GLY	ARG	PHE	GLY	ALA	VAL	ARG	ALA	SER	GLY	ILE	LEU	ASN	PRO	LEU	ASN	ILE	LEU	ALA	SER	SER	THR	TYR	ARG	ASN	CYS	VAL	LYS	ASN	ALA	SER	ILE	SER	ALA	LEU	SER	THR	GLY	ARG	PHE	SER	HIS	ILE	GLN	THR	PRO	VAL	VAL	SER	SER	THR	PRO	ARG
THR	SER	GLU	ARG	ASN	LEU	THR	CYS	GLY	HIS	THR	VAL	SER	ILE	LEU	ASN	ARG	MET	ALA	PRO	VAL	LEU	LYS	LEU	PRO	SER	VAL	LEU	LEU	PRO	VAL	ARG	SER	L94	K108	T162	K167	M170	L186	K187	V188																

Chain 5:  87% 6% 7%

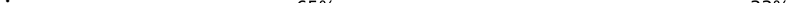
Sequence logo visualization of the 1000 Genomes Project. The top track shows the reference sequence (MET, ALA, LEU, ALA, SER, GLY, PRO, ALA, ARG, ALA, LEU, ALA, GLY, SER, GLY, GLN, LEU, LEU, GLY, PHE, GLY, ALA, PRO, ARG, ARG, GLY, A30, E56, Y105, R112, V140, D141, R144, A161, Q165, P178, R201, T212, E216, V222, I262, I270). The bottom track shows alternative alleles (V273, H289, T290, K296, L304, L355, N367, V376, Q384, R395, Y418, A423). Red diamonds indicate positions where the alternative allele is present in the population.

Chain 6: 

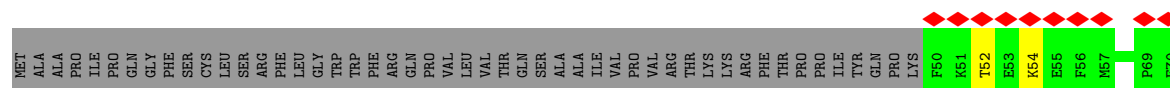


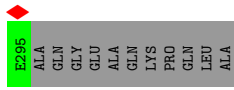
Chain 7:

Amino Acid	Frequency (%)
SER	5%
LYS	76%
ALA	11%
THR	13%
GLU	5%
CYS	5%
THR	5%
SER	5%
THR	5%
VAL	5%
LEU	5%
ARG	5%
MET	5%
GLY	5%
SER	5%
ARG	5%
ALA	5%
LEU	5%
ARG	5%
LEU	5%
TRP	5%
VAL	5%
ALA	5%
PRO	5%
GLY	5%
GLY	5%
ILE	5%
LYS	5%
TRP	5%
ARG	5%
PHE	5%
ILE	5%
THR	5%
SER	5%
SER	5%
ALA	5%
SER	5%
Q34	5%
L35	5%
S36	5%
P37	5%
L58	5%
R61	5%
T73	5%
T87	5%
S90	5%
Y99	5%
S103	5%
D114	5%
K117	5%
M143	5%
M148	5%

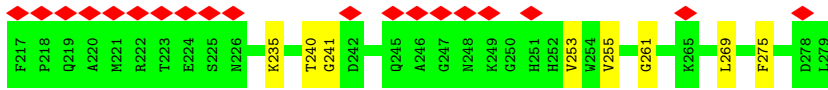
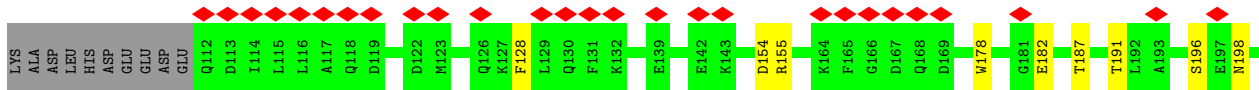
Chain 8:  18% 65% 33%

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

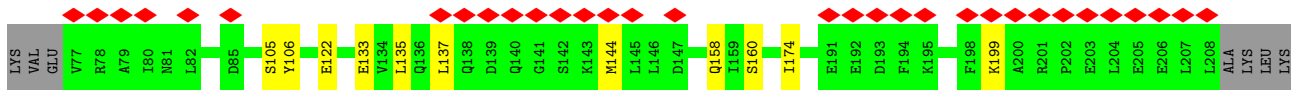




- | | |
|------|------|
| NET | ALA | ALA | PRO | VAL | ARG | ARG | THR | LEU | LEU | GLY | VAL | ALA | GLY | GLY | TRP | ARG | ARG | PHE | GLU | ARG | LEU | TRP | ALA | GLY | SER | SER | SER | ARG | SER | LEU | ALA | LEU | ALA | ALA | PRO | SER | SER | ASN | G42 | S43 | R46 | L73 | R90 | A91 | L92 | D93 | E94 | N95 | Q96 | R97 | L98 | A99 | K100 | K101 |
|------|------|



- MET SER GLY THR LEU GLU VAL LEU CYS LEU ARG ASN THR ILE PHE LYS GLN ALA PHE SER LEU ARG PHE ARG THR SER GLY LYS PRO ILE TYR SER SER VAL GLY GLY ILE LEU LEU SER ILE SER SER ARG PRO Y48 R60 A65 E66 F67 F68 LYS LYS LYS LYS GLY

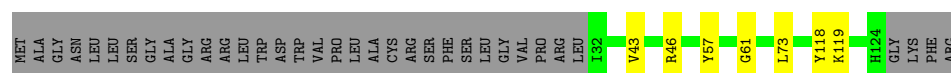


- | | | | |
|------|------|------|------|
| MET | ALA | ALA | THR | MET | PHE | ARG | ALA | THR | LEU | ARG | GLY | GLY | TRP | ARG | THR | GLY | VAL | GLN | ARG | GLY | CYS | LEU | ARG | LEU | LEU | SER | GLN | THR | GLN | GLY | P33 | D34 | E40 | S41 | V42 | E43 | E44 | M51 | S129 | P130 | E142 | F168 |
|------|------|------|------|

- | Position | Residue | Score | Conservation |
|----------|---------|-------|--------------|
| 1 | Met | 1.49 | High |
| 2 | Ala | 1.64 | High |
| 3 | Ala | 1.65 | High |
| 4 | Arg | 1.80 | High |
| 5 | Arg | 1.81 | High |
| 6 | Val | 1.82 | High |
| 7 | Ser | 1.83 | High |
| 8 | Gly | 1.84 | High |
| 9 | Ile | 1.85 | High |
| 10 | Thr | 1.86 | High |
| 11 | Arg | 1.87 | High |
| 12 | Val | 1.88 | High |
| 13 | Phe | 1.89 | High |
| 14 | Met | 1.90 | High |
| 15 | Trp | 1.91 | High |
| 16 | Thr | 1.92 | High |
| 17 | Val | 1.93 | High |
| 18 | Ser | 1.94 | High |
| 19 | Gly | 1.95 | High |
| 20 | Pro | 1.96 | High |
| 21 | Arg | 1.97 | High |
| 22 | Cys | 1.98 | High |
| 23 | Glu | 1.99 | High |
| 24 | Phe | 2.00 | High |
| 25 | Trp | 2.01 | High |
| 26 | Ser | 2.02 | High |
| 27 | Arg | 2.03 | High |
| 28 | Phe | 2.04 | High |
| 29 | Arg | 2.05 | High |
| 30 | Lys | 2.06 | High |
| 31 | Glu | 2.07 | High |
| 32 | Lys | 2.08 | High |
| 33 | Glu | 2.09 | High |
| 34 | Val | 2.10 | High |
| 35 | Val | 2.11 | High |
| 36 | Glu | 2.12 | High |
| 37 | Thr | 2.13 | High |
| 38 | Val | 2.14 | High |
| 39 | Glu | 2.15 | High |
| 40 | Lys | 2.16 | High |
| 41 | Lys | 2.17 | High |
| 42 | Glu | 2.18 | High |
| 43 | Pro | 2.19 | High |
| 44 | Pro | 2.20 | High |
| 45 | Pro | 2.21 | High |
| 46 | Pro | 2.22 | High |
| 47 | Pro | 2.23 | High |
| 48 | Pro | 2.24 | High |
| 49 | Pro | 2.25 | High |
| 50 | Pro | 2.26 | High |
| 51 | Pro | 2.27 | High |
| 52 | Pro | 2.28 | High |
| 53 | Pro | 2.29 | High |
| 54 | Pro | 2.30 | High |
| 55 | Pro | 2.31 | High |
| 56 | Pro | 2.32 | High |
| 57 | Pro | 2.33 | High |
| 58 | Pro | 2.34 | High |
| 59 | Pro | 2.35 | High |
| 60 | Pro | 2.36 | High |
| 61 | Pro | 2.37 | High |
| 62 | Pro | 2.38 | High |
| 63 | Pro | 2.39 | High |
| 64 | Pro | 2.40 | High |
| 65 | Pro | 2.41 | High |
| 66 | Pro | 2.42 | High |
| 67 | Pro | 2.43 | High |
| 68 | Pro | 2.44 | High |
| 69 | Pro | 2.45 | High |
| 70 | Pro | 2.46 | High |
| 71 | Pro | 2.47 | High |
| 72 | Pro | 2.48 | High |
| 73 | Pro | 2.49 | High |
| 74 | Pro | 2.50 | High |
| 75 | Pro | 2.51 | High |
| 76 | Pro | 2.52 | High |
| 77 | Pro | 2.53 | High |
| 78 | Pro | 2.54 | High |
| 79 | Pro | 2.55 | High |
| 80 | Pro | 2.56 | High |
| 81 | Pro | 2.57 | High |
| 82 | Pro | 2.58 | High |
| 83 | Pro | 2.59 | High |
| 84 | Pro | 2.60 | High |
| 85 | Pro | 2.61 | High |
| 86 | Pro | 2.62 | High |
| 87 | Pro | 2.63 | High |
| 88 | Pro | 2.64 | High |
| 89 | Pro | 2.65 | High |
| 90 | Pro | 2.66 | High |
| 91 | Pro | 2.67 | High |
| 92 | Pro | 2.68 | High |
| 93 | Pro | 2.69 | High |
| 94 | Pro | 2.70 | High |
| 95 | Pro | 2.71 | High |
| 96 | Pro | 2.72 | High |
| 97 | Pro | 2.73 | High |
| 98 | Pro | 2.74 | High |
| 99 | Pro | 2.75 | High |
| 100 | Pro | 2.76 | High |

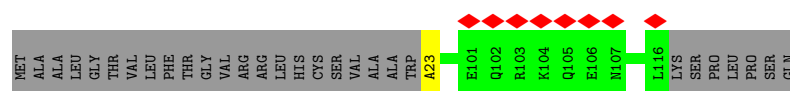
- 

Chain i: 



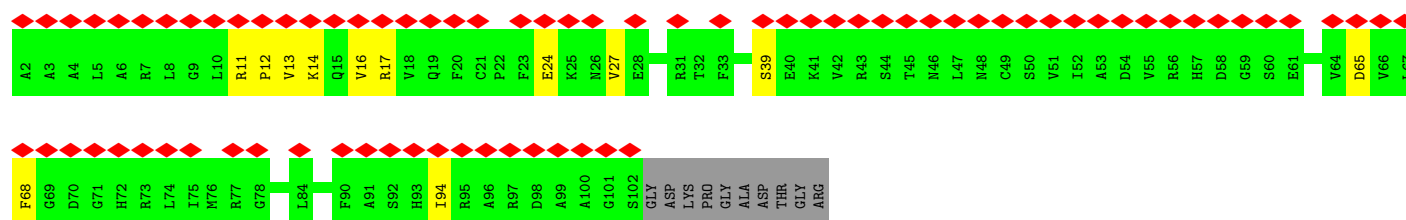
- Molecule 43: 39S ribosomal protein L52, mitochondrial

Chain j: 



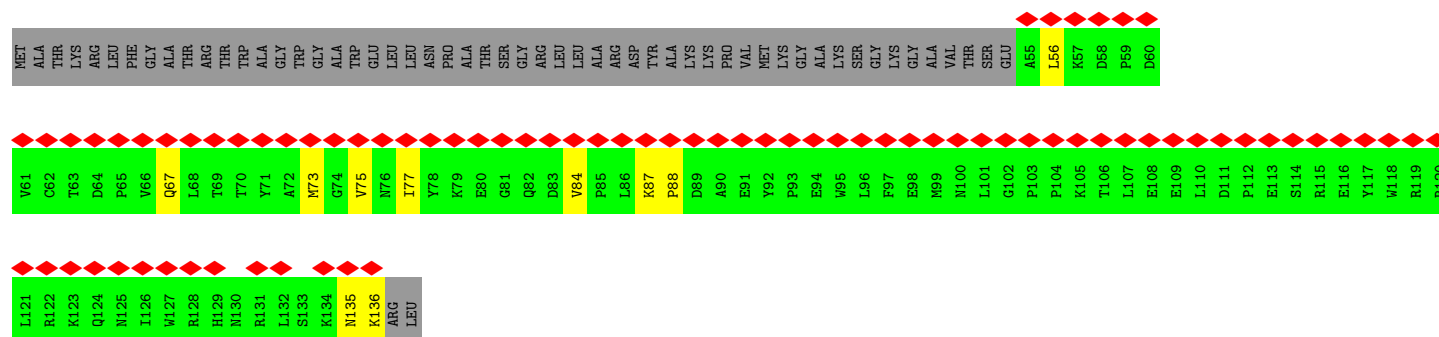
- Molecule 44: 39S ribosomal protein L53, mitochondrial

Chain k: 



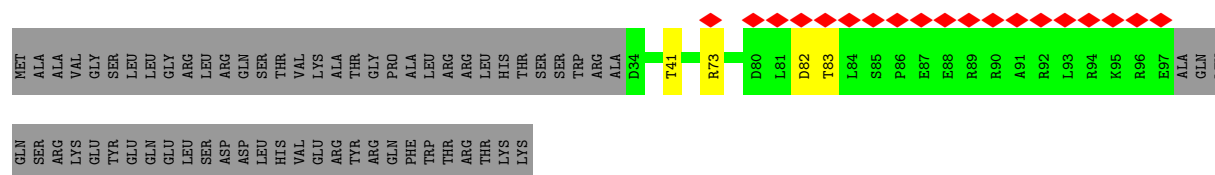
- Molecule 45: 39S ribosomal protein L54, mitochondrial

Chain l: 

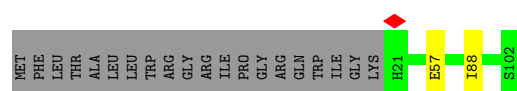
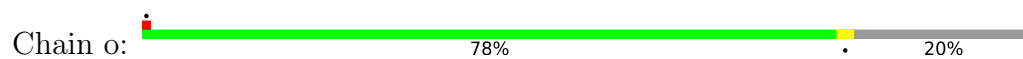


- Molecule 46: 39S ribosomal protein L55, mitochondrial

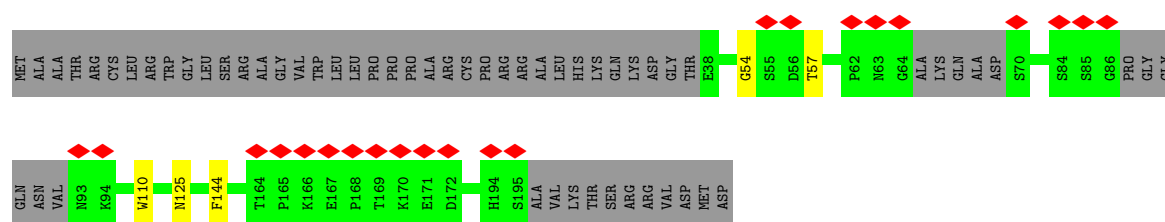
Chain m: 



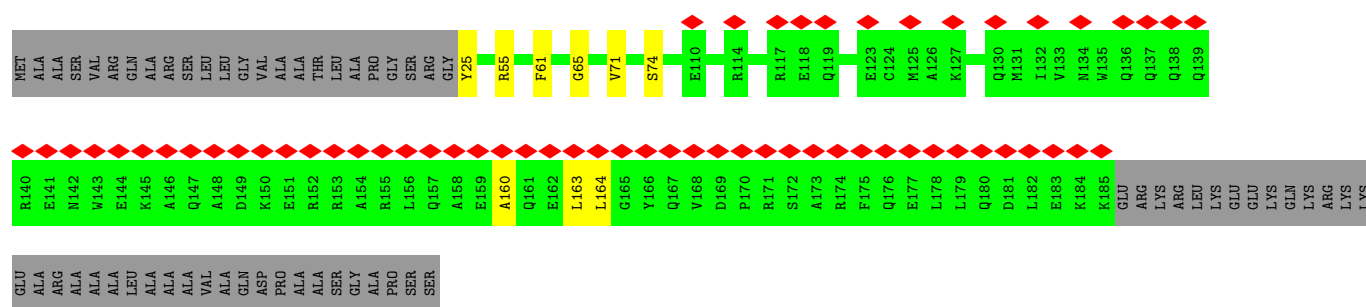
- Molecule 47: Ribosomal protein 63, mitochondrial



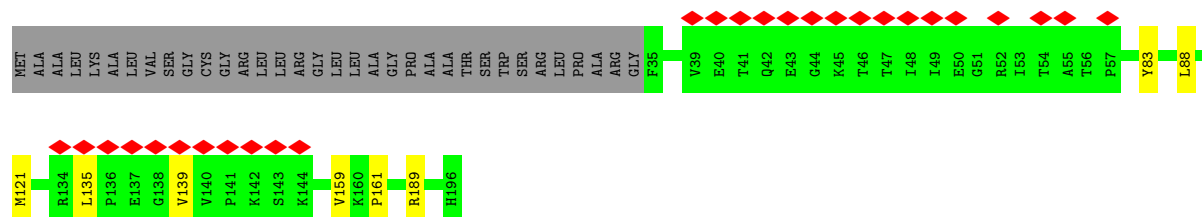
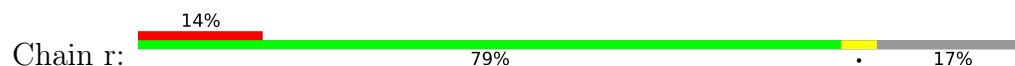
- Molecule 48: Peptidyl-tRNA hydrolase ICT1, mitochondrial



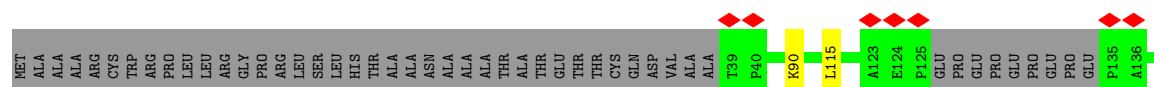
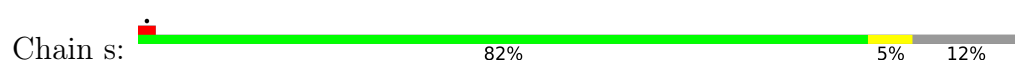
- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1



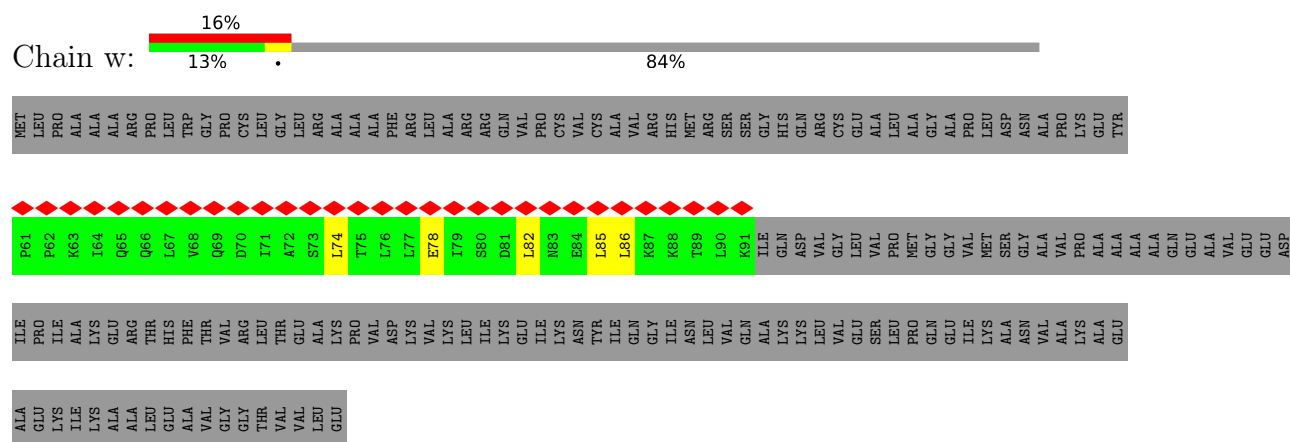
- Molecule 50: 39S ribosomal protein S18a, mitochondrial



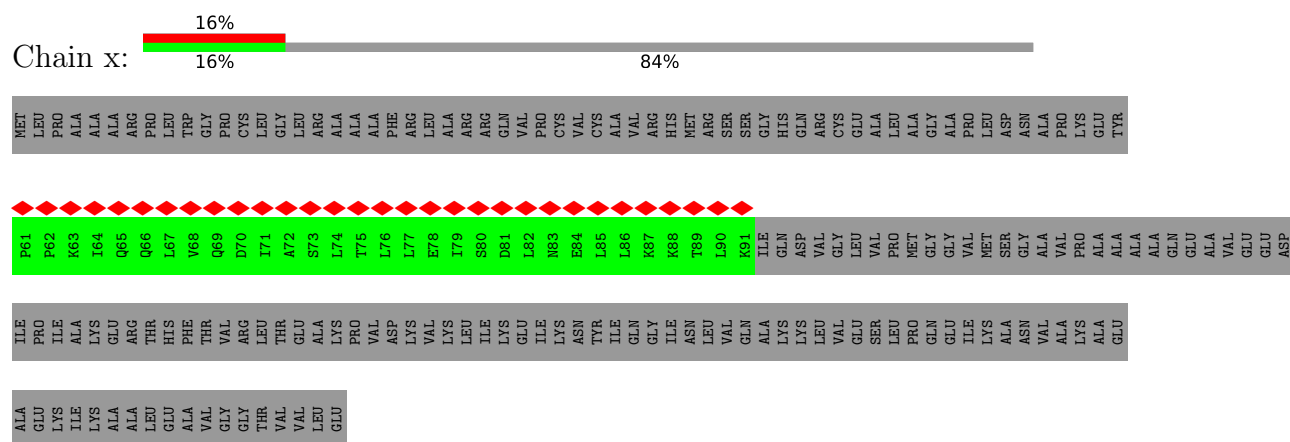
- Molecule 51: 39S ribosomal protein S30, mitochondrial



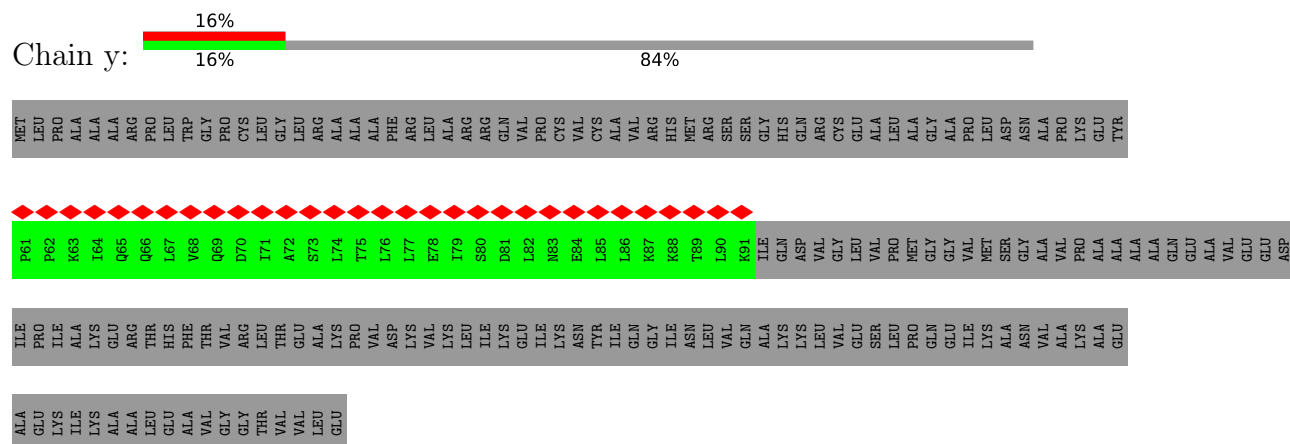
• Molecule 52: 39S ribosomal protein L12, mitochondrial



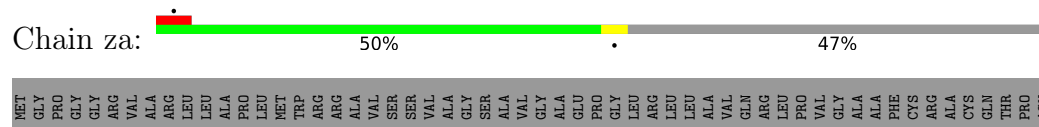
• Molecule 52: 39S ribosomal protein L12, mitochondrial

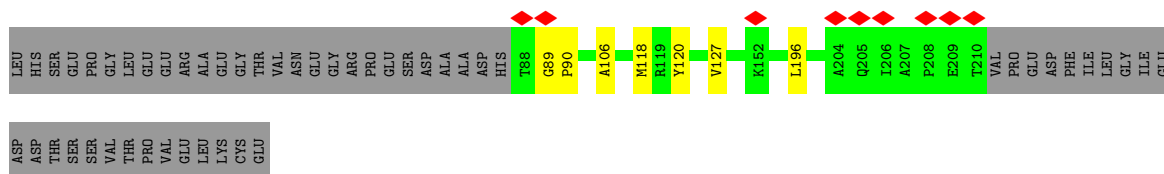


• Molecule 52: 39S ribosomal protein L12, mitochondrial

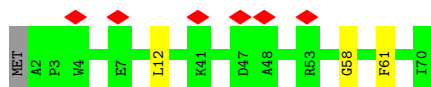


• Molecule 53: Mitochondrial assembly of ribosomal large subunit protein 1

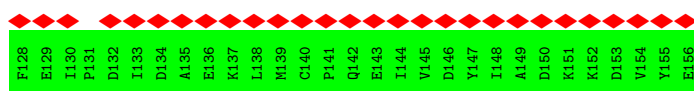
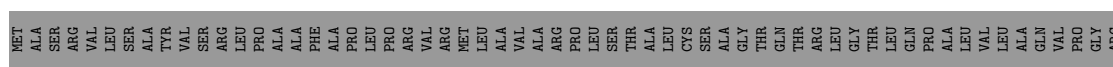




- Molecule 54: MIEF1 upstream open reading frame protein



- Molecule 55: Acyl carrier protein, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.930	Depositor
Minimum map value	-0.865	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5625, 0.5625, 0.5625	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, SAC, 2MG, AYA, FES, 8Q1, K, PSU, MG, ZN, THC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/27190	0.22	0/42294
2	B	0.09	0/1627	0.17	0/2527
3	D	0.12	0/1685	0.30	0/2265
4	E	0.13	0/2321	0.30	0/3144
5	F	0.13	0/2069	0.33	0/2813
6	H	0.12	0/816	0.27	0/1097
7	I	0.11	0/1693	0.27	0/2294
8	J	0.11	0/1348	0.27	0/1813
9	K	0.12	0/1490	0.30	0/2021
10	L	0.13	0/905	0.30	0/1218
11	M	0.12	0/2200	0.31	0/2976
12	N	0.10	0/1593	0.26	0/2144
13	O	0.13	0/1283	0.31	0/1727
14	P	0.13	0/1199	0.32	0/1623
15	Q	0.13	0/1875	0.29	0/2523
16	R	0.14	0/1175	0.31	0/1572
17	S	0.12	0/1320	0.33	0/1789
18	T	0.14	0/1403	0.34	0/1886
19	U	0.13	0/1274	0.32	0/1723
20	V	0.12	0/1721	0.30	0/2333
21	W	0.13	0/834	0.30	0/1126
22	X	0.11	0/2099	0.29	0/2837
23	Y	0.14	0/1593	0.29	0/2136
24	Z	0.14	0/1021	0.30	0/1378
25	0	0.12	0/913	0.30	0/1224
26	1	0.11	0/460	0.31	0/610
27	2	0.16	0/383	0.35	0/507
28	3	0.12	0/853	0.34	0/1136
29	5	0.12	0/3305	0.29	0/4502
30	6	0.13	0/3043	0.31	0/4140
31	7	0.11	0/2447	0.28	0/3310
32	8	0.12	0/1195	0.28	0/1610

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	9	0.15	0/1025	0.31	0/1379
34	a	0.12	0/866	0.31	0/1174
35	b	0.13	0/1211	0.34	0/1639
36	c	0.11	0/2347	0.28	0/3171
37	d	0.11	0/1984	0.28	0/2683
38	e	0.10	0/1885	0.26	0/2542
39	f	0.11	0/1241	0.24	0/1676
40	g	0.13	0/1151	0.30	0/1569
41	h	0.11	0/918	0.26	0/1249
42	i	0.15	0/813	0.35	0/1089
43	j	0.13	0/760	0.30	0/1023
44	k	0.10	0/777	0.27	0/1048
45	l	0.11	0/707	0.26	0/960
46	m	0.14	0/544	0.33	0/730
47	o	0.13	0/716	0.30	0/960
48	p	0.12	0/1223	0.28	0/1641
49	q	0.12	0/1384	0.28	0/1869
50	r	0.13	0/1362	0.29	0/1846
51	s	0.12	0/3239	0.31	0/4400
52	t	0.08	0/358	0.19	0/486
52	u	0.08	0/259	0.27	0/350
52	v	0.09	0/235	0.20	0/318
52	w	0.09	0/246	0.23	0/331
52	x	0.06	0/246	0.16	0/331
52	y	0.07	0/246	0.16	0/331
53	za	0.12	0/1036	0.29	0/1402
54	zb	0.13	0/598	0.31	0/796
55	zc	0.08	0/717	0.22	0/967
All	All	0.12	0/102427	0.27	0/144258

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24302	12165	12355	97	0
2	B	1524	769	780	7	0
3	D	1657	1703	1702	7	0
4	E	2257	2269	2267	20	0
5	F	2011	2042	2041	19	0
6	H	802	847	846	9	0
7	I	1657	1740	1743	13	0
8	J	1330	1408	1407	11	0
9	K	1455	1452	1452	9	0
10	L	890	942	941	4	0
11	M	2149	2208	2206	12	0
12	N	1554	1560	1557	8	0
13	O	1259	1295	1294	10	0
14	P	1173	1166	1165	2	0
15	Q	1834	1873	1872	10	0
16	R	1154	1215	1214	3	0
17	S	1293	1366	1365	8	0
18	T	1369	1411	1410	6	0
19	U	1251	1232	1232	5	0
20	V	1676	1688	1687	12	0
21	W	812	835	834	8	0
22	X	2044	2060	2060	6	0
23	Y	1556	1598	1597	8	0
24	Z	996	1045	1044	5	0
25	0	898	901	916	2	0
26	1	455	499	498	5	0
27	2	377	407	406	1	0
28	3	832	884	883	5	0
29	5	3210	3207	3206	17	0
30	6	2948	2842	2841	20	0
31	7	2390	2398	2397	21	0
32	8	1170	1193	1192	4	0
33	9	997	988	987	5	0
34	a	840	812	810	6	0
35	b	1196	1196	1190	7	0
36	c	2299	2322	2320	6	0
37	d	1933	1918	1916	9	0
38	e	1848	1851	1849	11	0
39	f	1220	1229	1227	11	0
40	g	1113	1097	1097	6	0
41	h	895	882	881	0	0
42	i	792	820	819	6	0
43	j	745	747	746	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	k	774	784	784	8	0
45	l	688	675	674	6	0
46	m	536	560	559	3	0
47	o	698	697	696	2	0
48	p	1205	1226	1223	6	0
49	q	1350	1328	1327	9	0
50	r	1322	1337	1348	6	0
51	s	3155	3141	3139	14	0
52	t	354	378	377	3	0
52	u	257	284	283	3	0
52	v	233	253	252	1	0
52	w	245	275	275	5	0
52	x	245	275	275	0	0
52	y	245	275	275	0	0
53	za	1012	1007	1006	5	0
54	zb	589	605	604	2	0
55	zc	705	692	691	4	0
56	A	33	0	0	0	0
56	B	1	0	0	0	0
56	g	1	0	0	0	0
57	6	1	0	0	0	0
57	A	7	0	0	0	0
58	0	1	0	0	0	0
59	r	4	0	0	0	0
60	zc	34	43	0	1	0
61	0	26	0	0	0	0
61	2	32	0	0	0	0
61	3	36	0	0	2	0
61	5	32	0	0	0	0
61	6	49	0	0	1	0
61	7	11	0	0	0	0
61	8	5	0	0	0	0
61	9	29	0	0	0	0
61	A	1157	0	0	11	0
61	B	26	0	0	0	0
61	D	14	0	0	0	0
61	E	77	0	0	1	0
61	F	81	0	0	0	0
61	H	7	0	0	0	0
61	K	29	0	0	1	0
61	L	38	0	0	0	0
61	M	53	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	N	1	0	0	0	0
61	O	33	0	0	0	0
61	P	52	0	0	1	0
61	Q	79	0	0	0	0
61	R	56	0	0	1	0
61	S	35	0	0	0	0
61	T	43	0	0	0	0
61	U	44	0	0	0	0
61	V	29	0	0	0	0
61	W	16	0	0	0	0
61	X	16	0	0	0	0
61	Y	46	0	0	0	0
61	Z	23	0	0	0	0
61	a	18	0	0	0	0
61	b	54	0	0	1	0
61	c	42	0	0	0	0
61	d	7	0	0	0	0
61	e	1	0	0	0	0
61	f	6	0	0	0	0
61	g	28	0	0	1	0
61	h	7	0	0	0	0
61	i	43	0	0	0	0
61	j	27	0	0	0	0
61	m	1	0	0	0	0
61	o	16	0	0	0	0
61	p	12	0	0	0	0
61	q	8	0	0	0	0
61	r	7	0	0	0	0
61	s	86	0	0	0	0
61	za	5	0	0	0	0
All	All	100401	85917	86040	426	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 (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1744:A:OP2	28:3:108:LYS:NZ	2.16	0.79
1:A:1747:G:OP2	1:A:1749:C:N4	2.17	0.78
1:A:2141:U:O4	61:A:3401:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3152:C:OP1	15:Q:141:SER:OG	2.02	0.77
1:A:2795:U:O2	6:H:87:LYS:NZ	2.17	0.77
1:A:1753:A:OP1	42:i:118:TYR:OH	2.04	0.75
1:A:3113:A:O2'	1:A:3114:U:O5'	2.05	0.75
33:9:16:ASP:OD1	33:9:25:ARG:NH1	2.22	0.73
1:A:1749:C:OP2	1:A:2899:C:O2'	2.05	0.72
1:A:2166:C:O2'	1:A:2214:A:N6	2.23	0.72
1:A:2165:C:N4	1:A:2212:C:OP1	2.24	0.71
39:f:106:TYR:OH	39:f:174:ILE:O	2.07	0.70
8:J:114:LEU:HD23	8:J:155:VAL:HG11	1.75	0.68
2:B:38:C:OP1	30:6:56:ARG:NH1	2.26	0.68
1:A:1777:A:N6	1:A:1780:U:OP2	2.29	0.66
1:A:2458:A:O2'	4:E:215:PHE:O	2.11	0.66
11:M:162:LEU:HD11	48:p:144:PHE:CB	2.26	0.65
1:A:3147:G:H5'	4:E:210:THR:HG21	1.79	0.65
39:f:199:LYS:HZ2	49:q:164:LEU:HD13	1.60	0.65
35:b:105:ALA:O	61:b:301:HOH:O	2.15	0.64
1:A:2019:G:OP1	61:A:3402:HOH:O	2.15	0.63
1:A:2310:G:O2'	1:A:2675:G:O6	2.14	0.63
1:A:3113:A:OP2	1:A:3167:U:O2'	2.16	0.63
1:A:2261:C:O2'	17:S:184:ARG:NH1	2.32	0.63
1:A:1749:C:O2'	11:M:80:LYS:NZ	2.24	0.63
1:A:2103:A:HO2'	24:Z:35:LYS:N	1.97	0.62
1:A:2865:C:N4	1:A:2869:A:N1	2.48	0.62
40:g:43:ASP:OD1	40:g:44:GLU:N	2.33	0.62
9:K:52:ASP:N	61:K:202:HOH:O	2.33	0.62
1:A:2298:A:N7	61:A:3420:HOH:O	2.31	0.61
1:A:3181:U:OP2	1:A:3182:A:O2'	2.17	0.61
9:K:28:PRO:HG3	9:K:65:ILE:HD12	1.80	0.61
7:I:86:ILE:HD11	7:I:131:LEU:HD12	1.84	0.60
44:k:68:PHE:HE2	44:k:94:ILE:HG22	1.67	0.60
45:l:67:GLN:NE2	45:l:73:MET:SD	2.75	0.59
22:X:95:ASP:O	22:X:98:SER:OG	2.19	0.59
20:V:112:GLU:OE1	20:V:112:GLU:N	2.35	0.59
1:A:2374:A:OP1	51:s:305:LYS:NZ	2.35	0.58
2:B:53:A:N6	2:B:58:A:N7	2.51	0.58
1:A:2754:A:OP1	6:H:91:LYS:NZ	2.37	0.58
1:A:2395:A:O2'	29:5:384:GLN:OE1	2.22	0.58
55:zc:93:ILE:HG23	55:zc:110:LEU:HD21	1.86	0.57
1:A:2177:U:N3	1:A:2180:A:OP2	2.38	0.57
37:d:189:LEU:HD12	37:d:217:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1805:A:OP2	20:V:94:HIS:NE2	2.34	0.57
30:6:196:THR:OG1	30:6:324:ASP:OD2	2.18	0.57
26:1:50:VAL:HG21	26:1:54:VAL:HG21	1.87	0.56
8:J:121:ALA:HB1	8:J:140:VAL:HG12	1.87	0.56
29:5:355:LEU:HD12	29:5:376:VAL:HG22	1.88	0.56
46:m:82:ASP:OD1	46:m:83:THR:N	2.39	0.56
29:5:105:TYR:CE2	29:5:262:ILE:HD13	2.41	0.56
29:5:262:ILE:C	29:5:262:ILE:HD12	2.31	0.56
39:f:199:LYS:NZ	49:q:164:LEU:HD13	2.21	0.56
1:A:2279:U:OP2	42:i:46:ARG:NH2	2.37	0.56
1:A:1718:A:N3	1:A:1911:C:O2'	2.33	0.55
4:E:61:ILE:HD11	13:O:149:LEU:HD22	1.89	0.55
28:3:170:ASN:O	61:3:201:HOH:O	2.18	0.55
29:5:216:GLU:OE2	29:5:367:ASN:ND2	2.40	0.55
34:a:45:CYS:HA	34:a:65:VAL:HG23	1.88	0.55
35:b:34:SER:OG	35:b:36:ASP:O	2.24	0.55
20:V:133:ILE:C	20:V:133:ILE:HD12	2.32	0.55
6:H:99:THR:HG22	6:H:140:PHE:CZ	2.43	0.54
30:6:120:GLU:OE2	30:6:124:ARG:NH2	2.40	0.54
31:7:73:THR:OG1	31:7:99:TYR:OH	2.23	0.54
1:A:1672:C:OP2	18:T:48:SER:OG	2.21	0.54
28:3:94:LEU:HD12	61:3:222:HOH:O	2.07	0.54
31:7:73:THR:HG1	31:7:99:TYR:HH	1.51	0.54
1:A:2150:U:OP2	43:j:23:ALA:N	2.40	0.54
1:A:1867:A:N1	1:A:2019:G:O2'	2.29	0.54
40:g:142:GLU:HB3	47:o:88:ILE:HG13	1.89	0.54
7:I:89:VAL:HG22	7:I:124:LYS:HZ1	1.73	0.54
8:J:25:ARG:HG2	45:l:56:LEU:HD22	1.90	0.54
29:5:140:VAL:O	29:5:140:VAL:HG12	2.08	0.54
1:A:1915:C:OP1	61:A:3404:HOH:O	2.18	0.53
31:7:154:ILE:HD12	31:7:183:VAL:HG21	1.90	0.53
52:w:85:LEU:HD13	52:w:85:LEU:C	2.34	0.53
7:I:103:ALA:HB1	44:k:39:SER:HA	1.91	0.53
11:M:162:LEU:HD11	48:p:144:PHE:HB2	1.90	0.53
30:6:303:PHE:CE2	30:6:311:MET:HE1	2.43	0.53
17:S:172:MET:HE1	17:S:180:PHE:HA	1.90	0.53
55:zc:91:ASP:OD1	55:zc:92:LYS:N	2.42	0.53
20:V:62:VAL:HB	20:V:120:VAL:HG13	1.91	0.53
26:1:16:ILE:HD11	26:1:61:LYS:HD2	1.91	0.53
21:W:53:ILE:HD11	21:W:75:TRP:CE2	2.45	0.52
38:e:196:SER:O	38:e:198:ASN:ND2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2011:G:N7	61:A:3428:HOH:O	2.34	0.52
5:F:281:ARG:NH2	11:M:128:THR:OG1	2.41	0.52
23:Y:191:ASN:O	23:Y:195:ASN:ND2	2.43	0.52
4:E:45:SER:O	31:7:307:ARG:NH2	2.43	0.52
1:A:1787:G:N2	1:A:1790:A:OP2	2.40	0.52
37:d:242:VAL:HG12	37:d:244:GLU:HG3	1.91	0.52
51:s:378:ALA:HB1	51:s:383:ALA:HB1	1.92	0.52
5:F:237:LEU:O	49:q:25:TYR:N	2.43	0.52
1:A:2134:A:N6	1:A:2135:A:H62	2.08	0.52
5:F:72:PHE:HA	5:F:206:LEU:HD13	1.91	0.52
37:d:263:THR:HG22	37:d:264:LYS:N	2.24	0.52
1:A:2458:A:OP2	13:O:9:ILE:N	2.43	0.52
5:F:49:ARG:NH2	5:F:81:ASP:O	2.41	0.52
12:N:105:MET:SD	12:N:183:LEU:HD21	2.50	0.51
12:N:124:VAL:CG1	12:N:152:THR:HG21	2.40	0.51
11:M:162:LEU:HD11	48:p:144:PHE:HB3	1.91	0.51
21:W:148:LEU:HD11	48:p:125:ASN:O	2.10	0.51
31:7:262:ASP:OD1	31:7:263:VAL:N	2.44	0.51
52:t:85:LEU:HD23	52:u:68:VAL:HG21	1.92	0.51
1:A:1792:G:N7	27:2:87:ARG:NH2	2.52	0.51
1:A:2875:A:N7	61:A:3429:HOH:O	2.34	0.51
47:o:57:GLU:OE1	47:o:57:GLU:N	2.41	0.51
38:e:261:GLY:HA2	38:e:269:LEU:HD22	1.92	0.51
30:6:235:TRP:CZ2	30:6:237:LEU:HD11	2.46	0.51
7:I:47:LEU:HD22	12:N:226:ILE:HG12	1.93	0.51
24:Z:132:GLU:OE1	24:Z:132:GLU:N	2.41	0.51
13:O:75:MET:HE1	15:Q:267:PHE:HA	1.92	0.51
14:P:69:THR:OG1	61:P:201:HOH:O	2.13	0.51
22:X:116:SER:O	22:X:120:ASP:N	2.44	0.51
7:I:225:GLN:HB2	7:I:226:PRO:HD3	1.93	0.50
30:6:179:VAL:HG23	30:6:179:VAL:O	2.11	0.50
1:A:1731:A:O2'	1:A:1732:C:O4'	2.14	0.50
12:N:123:ARG:O	12:N:158:ARG:NH2	2.44	0.50
55:zc:110:LEU:HD22	55:zc:114:ASP:OD2	2.11	0.50
4:E:111:THR:OG1	4:E:113:ASP:OD1	2.25	0.50
30:6:179:VAL:HG23	30:6:183:ASP:HB2	1.94	0.50
30:6:307:HIS:HB2	30:6:311:MET:HE2	1.92	0.50
36:c:287:GLU:HG2	36:c:288:THR:HG23	1.93	0.50
10:L:113:ASN:OD1	10:L:136:LYS:NZ	2.45	0.50
30:6:217:LEU:HD11	30:6:271:LEU:HD12	1.93	0.50
1:A:1701:U:O4	33:9:33:ARG:NE	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:A:OP1	61:A:3405:HOH:O	2.18	0.50
31:7:99:TYR:O	31:7:103:SER:OG	2.21	0.50
31:7:279:GLU:HG2	31:7:317:LEU:HD21	1.92	0.50
24:Z:61:GLN:OE1	24:Z:61:GLN:N	2.41	0.50
50:r:88:LEU:HD23	50:r:88:LEU:C	2.37	0.50
28:3:186:LEU:HG	28:3:188:VAL:HG23	1.94	0.50
20:V:65:LEU:HD11	20:V:121:LYS:HD2	1.92	0.50
15:Q:116:ILE:C	15:Q:117:LEU:HD23	2.37	0.49
20:V:54:TRP:NE1	20:V:56:LEU:O	2.45	0.49
29:5:222:VAL:O	29:5:222:VAL:HG13	2.11	0.49
11:M:287:ASP:OD1	11:M:289:ASN:N	2.45	0.49
29:5:212:THR:HG21	29:5:273:VAL:HG13	1.94	0.49
35:b:47:VAL:O	35:b:51:VAL:HG12	2.12	0.49
7:I:96:ILE:HD11	7:I:153:LEU:HD22	1.94	0.49
35:b:80:LEU:HD11	36:c:78:ARG:HD3	1.93	0.49
38:e:154:ASP:OD1	38:e:155:ARG:N	2.45	0.49
5:F:128:TRP:O	5:F:130:GLN:NE2	2.45	0.49
31:7:276:PHE:HB2	31:7:304:VAL:HG22	1.94	0.49
29:5:201:ARG:NH1	29:5:418:TYR:O	2.39	0.49
51:s:332:LEU:HD21	51:s:359:ALA:HB2	1.95	0.49
42:i:43:VAL:HG23	42:i:43:VAL:O	2.13	0.49
45:l:87:LYS:HB3	45:l:88:PRO:HD2	1.95	0.49
54:zb:12:LEU:HD21	54:zb:58:GLY:HA3	1.95	0.49
5:F:214:ASP:OD1	5:F:215:SER:N	2.46	0.49
8:J:75:ASP:O	8:J:76:ARG:HB2	2.13	0.49
21:W:103:VAL:HG11	30:6:61:ALA:HB1	1.95	0.49
26:1:19:ARG:HB2	26:1:62:ILE:HD11	1.95	0.49
9:K:3:SER:O	36:c:302:ARG:NH2	2.45	0.49
1:A:1734:C:OP2	6:H:72:ARG:NH2	2.46	0.48
1:A:1900:A:N7	61:A:3431:HOH:O	2.34	0.48
1:A:2865:C:O2'	1:A:2866:A:OP2	2.26	0.48
8:J:130:PHE:O	8:J:134:ASP:N	2.44	0.48
20:V:167:PRO:O	33:9:77:LEU:HD21	2.13	0.48
21:W:103:VAL:HG13	21:W:125:VAL:CG1	2.43	0.48
1:A:2864:U:OP1	21:W:50:ARG:NE	2.46	0.48
4:E:282:ILE:HD13	15:Q:94:ILE:HD13	1.95	0.48
8:J:121:ALA:HB1	8:J:140:VAL:CG1	2.43	0.48
20:V:48:PRO:HG3	23:Y:234:LEU:HD21	1.95	0.48
3:D:201:GLY:O	29:5:30:ALA:N	2.47	0.48
6:H:99:THR:HG22	6:H:140:PHE:HZ	1.78	0.48
7:I:142:ASN:HB2	7:I:185:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:150:LEU:HD21	51:s:402:TYR:CD1	2.47	0.48
49:q:71:VAL:O	49:q:74:SER:OG	2.32	0.48
17:S:135:LEU:HD12	17:S:144:LEU:HD21	1.95	0.48
26:l:16:ILE:HD11	26:l:61:LYS:CD	2.43	0.48
53:za:196:LEU:HD21	54:zb:61:PHE:HB2	1.95	0.48
1:A:1938:A:H4'	1:A:1939:G:OP1	2.14	0.48
7:I:161:VAL:HG13	7:I:191:PHE:CE1	2.48	0.48
1:A:2282:C:OP1	35:b:34:SER:OG	2.31	0.47
17:S:109:THR:HG22	17:S:112:ASP:OD2	2.14	0.47
1:A:2708:C:O2'	25:0:96:ASN:OD1	2.32	0.47
8:J:133:GLN:O	8:J:134:ASP:OD1	2.31	0.47
1:A:2364:C:OP2	19:U:78:LYS:NZ	2.44	0.47
11:M:193:PHE:O	61:M:301:HOH:O	2.20	0.47
49:q:160:ALA:HB1	49:q:163:LEU:HG	1.97	0.47
1:A:2075:U:OP2	24:Z:40:ARG:NH2	2.40	0.47
19:U:48:MET:HE2	19:U:53:LEU:HA	1.94	0.47
1:A:1798:A:N3	20:V:42:ARG:NH2	2.62	0.47
60:zc:201:8Q1:O40	60:zc:201:8Q1:N36	2.46	0.47
1:A:2052:A:H2'	1:A:2053:U:O4'	2.15	0.47
5:F:66:VAL:O	5:F:77:VAL:HG12	2.14	0.47
8:J:117:VAL:HG12	8:J:141:VAL:HG13	1.97	0.47
12:N:82:PHE:CE2	12:N:195:LEU:HD23	2.49	0.47
31:7:36:SER:HB2	31:7:37:PRO:HD2	1.97	0.47
31:7:87:THR:O	31:7:90:SER:OG	2.31	0.47
45:l:135:ASN:OD1	45:l:136:LYS:N	2.47	0.47
4:E:334:ASP:HB3	4:E:337:VAL:HG23	1.97	0.47
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.96	0.47
16:R:62:LYS:NZ	61:R:201:HOH:O	2.24	0.47
31:7:148:MET:HE2	31:7:257:ILE:HG13	1.96	0.47
30:6:215:THR:OG1	30:6:275:GLN:NE2	2.48	0.47
19:U:21:ARG:NH2	23:Y:143:ASP:OD1	2.46	0.47
52:w:74:LEU:HD13	52:w:82:LEU:CD1	2.44	0.47
1:A:2013:U:OP1	42:i:119:LYS:NZ	2.46	0.46
9:K:91:THR:HG22	50:r:161:PRO:HB3	1.96	0.46
31:7:189:LEU:O	31:7:295:ARG:NH1	2.48	0.46
18:T:57:ILE:O	37:d:227:ARG:NH2	2.44	0.46
1:A:2032:G:H1	1:A:2043:C:H42	1.62	0.46
6:H:53:THR:OG1	22:X:83:GLU:OE2	2.27	0.46
22:X:125:VAL:HG23	22:X:127:VAL:HG13	1.98	0.46
34:a:52:THR:OG1	34:a:54:ASP:OD1	2.30	0.46
52:v:65:GLN:HE21	52:w:86:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:153:VAL:HG13	31:7:205:ASP:HB2	1.97	0.46
1:A:1886:G:H1	42:i:61:GLY:HA3	1.80	0.46
1:A:1906:G:N7	61:A:3440:HOH:O	2.36	0.46
1:A:2036:C:N4	1:A:2918:A:OP1	2.49	0.46
35:b:43:ALA:HB2	35:b:89:ILE:HD12	1.97	0.46
44:k:13:VAL:HG12	44:k:14:LYS:N	2.31	0.46
7:I:147:PHE:O	7:I:148:VAL:HG23	2.15	0.46
51:s:174:LEU:HB3	51:s:175:PRO:HD3	1.98	0.46
1:A:1720:C:N4	1:A:1730:U:O4	2.49	0.45
5:F:253:MET:HE3	5:F:259:LEU:HD22	1.96	0.45
15:Q:155:ILE:HD12	15:Q:155:ILE:N	2.30	0.45
31:7:290:GLN:HB2	31:7:291:PRO:HD3	1.98	0.45
37:d:89:VAL:HG23	37:d:89:VAL:O	2.15	0.45
19:U:28:LEU:O	23:Y:114:THR:HG23	2.16	0.45
48:p:110:TRP:H	48:p:110:TRP:CD1	2.32	0.45
49:q:160:ALA:HA	49:q:163:LEU:HD23	1.99	0.45
38:e:235:LYS:NZ	38:e:275:PHE:O	2.43	0.45
49:q:163:LEU:HD12	49:q:163:LEU:O	2.17	0.45
13:O:77:ASP:HA	13:O:86:ILE:HD11	1.98	0.45
6:H:79:VAL:HG11	22:X:91:TYR:CE2	2.51	0.45
30:6:141:ARG:NH2	61:6:502:HOH:O	2.48	0.45
42:i:57:TYR:O	42:i:73:LEU:HD11	2.16	0.45
44:k:17:ARG:N	44:k:65:ASP:O	2.48	0.45
4:E:47:THR:OG1	4:E:51:GLU:OE2	2.27	0.45
4:E:208:ALA:HB2	4:E:297:VAL:HG12	1.98	0.45
1:A:2145:G:N3	17:S:104:ARG:NH1	2.59	0.45
3:D:139:ILE:HD12	3:D:150:TRP:CE3	2.52	0.45
20:V:48:PRO:HD3	23:Y:234:LEU:HD21	1.98	0.45
40:g:129:SER:OG	40:g:130:PRO:HD3	2.17	0.45
52:t:74:LEU:HD11	52:u:67:LEU:HD11	1.99	0.45
1:A:1990:G:OP1	3:D:269:ARG:NH1	2.50	0.45
7:I:221:LEU:HD13	52:w:86:LEU:HD23	1.98	0.45
13:O:38:ARG:NE	13:O:82:GLU:OE1	2.49	0.45
17:S:143:LEU:HD13	17:S:153:LEU:HD21	1.99	0.45
39:f:137:LEU:HD23	39:f:144:MET:HG2	1.99	0.45
53:za:106:ALA:HB1	53:za:127:VAL:HG13	1.99	0.45
23:Y:91:ARG:NH1	33:9:83:GLU:OE2	2.45	0.44
1:A:1719:G:H2'	1:A:1720:C:O4'	2.16	0.44
1:A:2466:A:O2'	1:A:3155:C:OP1	2.35	0.44
1:A:2906:C:N3	26:1:19:ARG:NH1	2.65	0.44
17:S:102:ALA:O	17:S:103:SER:OG	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:245:LEU:HD12	36:c:253:PRO:HD3	2.00	0.44
51:s:145:VAL:HG21	51:s:187:LEU:HD11	1.99	0.44
1:A:3113:A:HO2'	1:A:3114:U:P	2.37	0.44
4:E:310:LEU:HD12	4:E:310:LEU:C	2.43	0.44
31:7:242:GLU:O	31:7:245:SER:OG	2.35	0.44
1:A:2472:A:OP1	10:L:56:ARG:NH1	2.50	0.44
8:J:101:ALA:HB2	8:J:109:ALA:HB2	1.99	0.44
17:S:135:LEU:HD23	17:S:135:LEU:C	2.43	0.44
19:U:19:VAL:O	19:U:19:VAL:HG13	2.17	0.44
10:L:128:ARG:NH2	53:za:120:TYR:O	2.51	0.44
7:I:101:ASN:O	7:I:152:MET:HE1	2.17	0.44
51:s:160:ARG:NE	51:s:160:ARG:HA	2.33	0.44
18:T:73:ILE:HD12	18:T:73:ILE:N	2.33	0.44
39:f:105:SER:OG	46:m:41:THR:HG21	2.17	0.44
44:k:16:VAL:HG12	44:k:17:ARG:N	2.33	0.44
1:A:1883:G:H5'	40:g:91:MET:HG3	1.99	0.44
1:A:2244:U:H4'	50:r:189:ARG:HD3	2.00	0.44
5:F:136:ALA:O	5:F:137:ARG:C	2.61	0.44
49:q:61:PHE:O	49:q:65:GLY:N	2.44	0.44
6:H:93:ASN:ND2	6:H:113:SER:O	2.51	0.44
8:J:159:LEU:C	8:J:159:LEU:HD12	2.43	0.44
28:3:162:THR:O	28:3:167:LYS:NZ	2.50	0.44
1:A:1732:C:H5''	1:A:1733:C:OP2	2.17	0.43
15:Q:227:LYS:HB3	15:Q:228:PRO:HA	2.00	0.43
32:8:117:LEU:HD23	38:e:73:LEU:HD22	1.99	0.43
1:A:2135:A:N3	1:A:2135:A:H2'	2.33	0.43
2:B:24:G:H2'	2:B:25:C:O4'	2.17	0.43
52:t:68:VAL:HG13	52:u:86:LEU:HD23	2.01	0.43
2:B:5:G:N2	2:B:69:U:O2	2.51	0.43
15:Q:79:GLU:OE2	15:Q:79:GLU:N	2.43	0.43
52:w:78:GLU:O	52:w:82:LEU:HG	2.17	0.43
1:A:2181:A:H2'	1:A:2207:A:H5'	1.99	0.43
1:A:2257:C:N4	61:A:3503:HOH:O	2.47	0.43
4:E:123:GLN:HG2	4:E:125:GLN:HG3	2.01	0.43
4:E:282:ILE:CD1	15:Q:94:ILE:HD13	2.48	0.43
18:T:52:GLU:OE1	18:T:52:GLU:N	2.51	0.43
30:6:62:GLU:HA	30:6:62:GLU:OE1	2.18	0.43
39:f:135:LEU:HD12	39:f:135:LEU:N	2.34	0.43
1:A:2449:G:OP2	51:s:225:ARG:NH2	2.46	0.43
11:M:250:ASP:OD1	11:M:251:GLU:N	2.51	0.43
38:e:178:TRP:NE1	38:e:182:GLU:O	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1737:A:N6	1:A:1760:G:O2'	2.44	0.43
1:A:2127:A:H4'	1:A:2251:A:C5	2.53	0.43
1:A:2260:A:OP1	1:A:2260:A:H8	2.01	0.43
38:e:253:VAL:O	38:e:253:VAL:HG13	2.19	0.43
9:K:74:GLN:HG3	50:r:159:VAL:HG11	1.99	0.43
29:5:289:HIS:ND1	29:5:290:THR:OG1	2.38	0.43
33:9:53:ILE:HD12	33:9:56:MET:SD	2.58	0.43
4:E:303:LYS:HD3	4:E:303:LYS:C	2.44	0.43
5:F:95:ILE:HD13	5:F:172:LEU:CD2	2.49	0.43
5:F:128:TRP:N	5:F:129:PRO:CD	2.82	0.43
29:5:161:ALA:O	29:5:165:GLN:NE2	2.52	0.43
44:k:68:PHE:CE2	44:k:94:ILE:HG22	2.52	0.43
51:s:115:LEU:HD23	51:s:259:ILE:HD12	2.01	0.43
13:O:38:ARG:NH2	13:O:82:GLU:OE1	2.48	0.43
30:6:215:THR:HG23	30:6:238:THR:HG22	2.00	0.43
3:D:253:ASN:OD1	3:D:254:LYS:N	2.52	0.43
5:F:95:ILE:HD13	5:F:172:LEU:HD23	2.01	0.43
34:a:104:GLU:HB2	34:a:107:PRO:HD2	2.01	0.43
36:c:259:ARG:HB2	36:c:271:PHE:HB2	2.01	0.43
50:r:83:TYR:HB3	50:r:121:MET:HE3	1.99	0.43
4:E:109:LEU:N	4:E:117:HIS:O	2.45	0.42
29:5:56:GLU:O	29:5:56:GLU:HG3	2.18	0.42
1:A:2406:A:O2'	1:A:2407:U:O5'	2.37	0.42
15:Q:181:LYS:O	15:Q:218:ASN:N	2.50	0.42
51:s:271:LEU:N	51:s:272:PRO:HA	2.33	0.42
1:A:3227:U:O2'	1:A:3230:G:OP1	2.25	0.42
9:K:15:ALA:CB	36:c:269:LEU:HD22	2.49	0.42
10:L:94:PRO:O	10:L:97:THR:OG1	2.27	0.42
13:O:16:ARG:NH2	13:O:50:ASP:OD2	2.42	0.42
13:O:140:SER:O	13:O:146:ASN:ND2	2.52	0.42
21:W:103:VAL:HG13	21:W:125:VAL:HG13	2.01	0.42
35:b:26:LEU:HD22	35:b:105:ALA:HA	2.01	0.42
44:k:11:ARG:HB2	44:k:12:PRO:HD3	2.02	0.42
1:A:1822:U:O2	1:A:2707:A:O2'	2.37	0.42
9:K:177:ARG:O	9:K:178:LEU:CB	2.67	0.42
11:M:149:THR:HG22	11:M:149:THR:O	2.19	0.42
32:8:194:ASP:OD1	32:8:196:THR:HG23	2.19	0.42
53:za:118:MET:SD	53:za:118:MET:N	2.92	0.42
1:A:1760:G:N7	49:q:55:ARG:NH2	2.61	0.42
1:A:2289:G:OP1	11:M:34:LYS:NZ	2.52	0.42
20:V:47:GLU:HG3	23:Y:241:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:265:ILE:N	30:6:265:ILE:HD12	2.34	0.42
39:f:122:GLU:OE2	39:f:160:SER:OG	2.27	0.42
1:A:2511:C:OP1	3:D:263:ASN:ND2	2.46	0.42
1:A:2321:A:C2	25:0:142:GLY:HA3	2.55	0.42
11:M:107:LEU:HD13	61:g:321:HOH:O	2.20	0.42
18:T:61:PRO:CG	37:d:180:THR:HG21	2.50	0.42
23:Y:238:PHE:HB2	23:Y:241:LEU:HD12	2.02	0.42
1:A:2006:C:H2'	1:A:2007:U:C6	2.54	0.42
2:B:9:1MA:C2	2:B:45:G:C4	3.08	0.42
51:s:282:ILE:HD13	51:s:341:MET:SD	2.60	0.42
1:A:1937:A:O2'	1:A:1938:A:H5'	2.20	0.42
12:N:96:TYR:HB3	12:N:151:VAL:HB	2.02	0.42
12:N:224:LEU:N	12:N:224:LEU:HD12	2.35	0.42
30:6:270:PHE:N	30:6:317:SER:O	2.47	0.42
31:7:185:LEU:HD12	31:7:295:ARG:HD2	2.02	0.42
31:7:270:PRO:HG2	31:7:274:ILE:HD11	2.02	0.42
51:s:207:HIS:ND1	51:s:234:ASP:OD1	2.49	0.42
1:A:2098:G:O2'	1:A:2099:U:OP2	2.28	0.42
1:A:2718:C:H2'	1:A:2719:G:O4'	2.19	0.42
20:V:62:VAL:HG12	20:V:122:LEU:HD12	2.02	0.42
29:5:112:ARG:HG2	29:5:304:LEU:HD21	2.01	0.42
39:f:122:GLU:N	39:f:158:GLN:O	2.52	0.42
4:E:58:VAL:HB	4:E:59:PRO:HD3	2.01	0.41
5:F:206:LEU:HD11	5:F:210:ARG:NE	2.34	0.41
48:p:54:GLY:O	48:p:57:THR:HG22	2.20	0.41
31:7:203:THR:HG22	31:7:280:VAL:H	1.85	0.41
32:8:195:ILE:HD11	39:f:133:GLU:OE1	2.20	0.41
7:I:185:ILE:O	7:I:185:ILE:HG13	2.20	0.41
12:N:240:LYS:NZ	12:N:251:VAL:O	2.54	0.41
13:O:86:ILE:HB	13:O:87:PRO:HD3	2.02	0.41
16:R:141:ILE:HG22	34:a:51:LEU:HD12	2.02	0.41
30:6:224:HIS:HA	30:6:232:TYR:CE2	2.55	0.41
37:d:189:LEU:HD12	37:d:217:HIS:HD2	1.84	0.41
38:e:253:VAL:HG22	38:e:255:VAL:HG13	2.02	0.41
30:6:323:TRP:NE1	30:6:339:GLU:OE2	2.46	0.41
38:e:187:THR:O	38:e:191:THR:HG23	2.20	0.41
51:s:150:LEU:HG	51:s:405:ILE:HD11	2.01	0.41
1:A:2327:U:H2'	1:A:2328:C:O4'	2.20	0.41
1:A:2756:C:O2'	1:A:2791:A:N6	2.53	0.41
5:F:218:LEU:HD13	5:F:260:VAL:HB	2.02	0.41
21:W:139:GLU:OE1	21:W:139:GLU:N	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:r:135:LEU:HD22	50:r:139:VAL:HG21	2.01	0.41
1:A:2028:G:O6	61:A:3406:HOH:O	2.22	0.41
4:E:144:THR:HB	4:E:178:ILE:HG23	2.03	0.41
32:8:191:ARG:NE	39:f:144:MET:SD	2.94	0.41
1:A:2392:U:H2'	1:A:2394:A:H62	1.85	0.41
2:B:14:A:N1	2:B:21:A:O2'	2.44	0.41
6:H:102:VAL:HG12	6:H:104:ASN:H	1.85	0.41
11:M:283:LEU:HD22	40:g:40:GLU:HG2	2.03	0.41
31:7:114:ASP:HB2	31:7:117:LYS:HB2	2.02	0.41
31:7:186:ASP:OD1	31:7:187:SER:N	2.54	0.41
1:A:2744:U:O2'	1:A:2746:U:O4	2.30	0.41
15:Q:155:ILE:HG22	15:Q:156:GLU:HG2	2.02	0.41
37:d:169:PHE:HB3	37:d:170:PRO:HD3	2.01	0.41
38:e:128:PHE:HB2	46:m:73:ARG:HB2	2.03	0.41
38:e:240:THR:HG22	38:e:241:GLY:N	2.35	0.41
44:k:24:GLU:O	44:k:27:VAL:HG22	2.20	0.41
1:A:2473:A:H2'	1:A:2473:A:N3	2.36	0.41
3:D:217:LEU:HD12	3:D:233:GLN:OE1	2.21	0.41
5:F:284:TYR:HB2	5:F:285:PRO:CD	2.51	0.41
18:T:157:ARG:HG3	18:T:158:TYR:H	1.86	0.41
24:Z:155:GLU:O	24:Z:156:GLN:C	2.64	0.41
29:5:296:LYS:O	29:5:296:LYS:HG3	2.21	0.41
34:a:78:PRO:O	34:a:79:ASP:C	2.63	0.41
40:g:41:SER:OG	40:g:43:ASP:OD1	2.38	0.41
55:zc:87:LEU:O	55:zc:93:ILE:HD11	2.20	0.41
4:E:48:TRP:CD1	4:E:50:ASP:OD1	2.74	0.41
5:F:101:MET:N	5:F:101:MET:HE2	2.36	0.41
30:6:217:LEU:C	30:6:217:LEU:HD12	2.46	0.41
5:F:110:SER:O	5:F:158:PRO:HA	2.21	0.40
16:R:83:TYR:CZ	16:R:87:ILE:HG13	2.56	0.40
30:6:82:THR:HG22	30:6:83:ASP:N	2.36	0.40
3:D:79:MET:HE1	3:D:134:CYS:SG	2.61	0.40
4:E:285:VAL:HB	61:E:469:HOH:O	2.21	0.40
9:K:156:ASP:OD1	9:K:157:GLU:N	2.54	0.40
21:W:67:ILE:HG21	21:W:131:VAL:HG21	2.02	0.40
1:A:3148:C:H5'	4:E:290:PRO:HA	2.04	0.40
7:I:100:GLN:HB2	7:I:177:LEU:HD11	2.03	0.40
8:J:85:PRO:HG2	45:l:77:ILE:HG21	2.04	0.40
22:X:20:ILE:HG21	22:X:212:ILE:HG23	2.03	0.40
31:7:205:ASP:OD1	34:a:95:ARG:NE	2.51	0.40
1:A:2067:C:H5''	39:f:60:LYS:HZ2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:271:LEU:HB3	4:E:285:VAL:HG13	2.04	0.40
13:O:64:LYS:NZ	13:O:100:GLN:O	2.54	0.40
53:za:89:GLY:N	53:za:90:PRO:HD3	2.36	0.40
1:A:1935:A:H4'	1:A:1937:A:H62	1.86	0.40
1:A:2409:A:O2'	29:5:270:ILE:O	2.39	0.40
2:B:16:C:OP2	2:B:59:A:N6	2.51	0.40
5:F:69:LEU:HD21	5:F:212:TRP:HH2	1.86	0.40
5:F:127:PRO:HG3	5:F:141:ILE:HG23	2.04	0.40
14:P:36:ASP:N	14:P:37:PRO:CD	2.84	0.40
29:5:178:PRO:HG3	29:5:296:LYS:HD3	2.04	0.40
37:d:52:THR:HG22	37:d:54:LYS:H	1.86	0.40
45:l:75:VAL:HG11	45:l:84:VAL:HB	2.04	0.40
51:s:90:LYS:O	51:s:275:LYS:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	212/305 (70%)	210 (99%)	2 (1%)	0	100	100
4	E	280/348 (80%)	278 (99%)	2 (1%)	0	100	100
5	F	245/311 (79%)	240 (98%)	5 (2%)	0	100	100
6	H	95/267 (36%)	91 (96%)	4 (4%)	0	100	100
7	I	204/261 (78%)	202 (99%)	2 (1%)	0	100	100
8	J	173/192 (90%)	166 (96%)	7 (4%)	0	100	100
9	K	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
10	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
11	M	265/296 (90%)	263 (99%)	2 (1%)	0	100	100
12	N	185/251 (74%)	182 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
14	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
15	Q	218/292 (75%)	218 (100%)	0	0	100	100
16	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
17	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
18	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
19	U	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
20	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
21	W	100/148 (68%)	99 (99%)	1 (1%)	0	100	100
22	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
23	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
24	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
25	0	108/188 (57%)	108 (100%)	0	0	100	100
26	1	53/65 (82%)	51 (96%)	2 (4%)	0	100	100
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	5	392/423 (93%)	387 (99%)	5 (1%)	0	100	100
30	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
31	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
32	8	136/206 (66%)	132 (97%)	4 (3%)	0	100	100
33	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
34	a	96/142 (68%)	92 (96%)	4 (4%)	0	100	100
35	b	148/214 (69%)	144 (97%)	4 (3%)	0	100	100
36	c	282/332 (85%)	281 (100%)	1 (0%)	0	100	100
37	d	232/306 (76%)	230 (99%)	2 (1%)	0	100	100
38	e	224/279 (80%)	222 (99%)	2 (1%)	0	100	100
39	f	149/212 (70%)	149 (100%)	0	0	100	100
40	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
41	h	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
42	i	91/128 (71%)	91 (100%)	0	0	100	100
43	j	92/123 (75%)	89 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	k	99/111 (89%)	92 (93%)	7 (7%)	0	100	100
45	l	80/138 (58%)	80 (100%)	0	0	100	100
46	m	62/128 (48%)	62 (100%)	0	0	100	100
47	o	80/102 (78%)	80 (100%)	0	0	100	100
48	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
49	q	159/222 (72%)	157 (99%)	2 (1%)	0	100	100
50	r	160/196 (82%)	157 (98%)	3 (2%)	0	100	100
51	s	382/439 (87%)	371 (97%)	11 (3%)	0	100	100
52	t	44/198 (22%)	44 (100%)	0	0	100	100
52	u	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
52	v	27/198 (14%)	27 (100%)	0	0	100	100
52	w	29/198 (15%)	28 (97%)	1 (3%)	0	100	100
52	x	29/198 (15%)	29 (100%)	0	0	100	100
52	y	29/198 (15%)	29 (100%)	0	0	100	100
53	za	121/234 (52%)	112 (93%)	9 (7%)	0	100	100
54	zb	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
55	zc	85/156 (54%)	79 (93%)	6 (7%)	0	100	100
All	All	8684/12210 (71%)	8545 (98%)	139 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	172/245 (70%)	172 (100%)	0	100	100
4	E	246/290 (85%)	245 (100%)	1 (0%)	84	89
5	F	217/262 (83%)	217 (100%)	0	100	100
6	H	88/228 (39%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	190/232 (82%)	190 (100%)	0	100	100
8	J	138/150 (92%)	138 (100%)	0	100	100
9	K	154/154 (100%)	154 (100%)	0	100	100
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	230/249 (92%)	230 (100%)	0	100	100
12	N	164/211 (78%)	164 (100%)	0	100	100
13	O	134/150 (89%)	134 (100%)	0	100	100
14	P	126/155 (81%)	126 (100%)	0	100	100
15	Q	202/256 (79%)	202 (100%)	0	100	100
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	146 (100%)	0	100	100
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	134/134 (100%)	134 (100%)	0	100	100
20	V	183/191 (96%)	183 (100%)	0	100	100
21	W	84/119 (71%)	84 (100%)	0	100	100
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	163 (100%)	0	100	100
24	Z	113/147 (77%)	113 (100%)	0	100	100
25	0	99/164 (60%)	99 (100%)	0	100	100
26	1	52/60 (87%)	52 (100%)	0	100	100
27	2	40/72 (56%)	40 (100%)	0	100	100
28	3	88/166 (53%)	88 (100%)	0	100	100
29	5	353/368 (96%)	353 (100%)	0	100	100
30	6	313/332 (94%)	313 (100%)	0	100	100
31	7	270/303 (89%)	269 (100%)	1 (0%)	84	89
32	8	128/190 (67%)	128 (100%)	0	100	100
33	9	104/112 (93%)	104 (100%)	0	100	100
34	a	96/133 (72%)	96 (100%)	0	100	100
35	b	131/184 (71%)	131 (100%)	0	100	100
36	c	251/288 (87%)	251 (100%)	0	100	100
37	d	215/274 (78%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	e	198/236 (84%)	198 (100%)	0	100	100
39	f	136/188 (72%)	136 (100%)	0	100	100
40	g	124/148 (84%)	124 (100%)	0	100	100
41	h	104/148 (70%)	104 (100%)	0	100	100
42	i	83/110 (76%)	83 (100%)	0	100	100
43	j	74/97 (76%)	74 (100%)	0	100	100
44	k	83/89 (93%)	83 (100%)	0	100	100
45	l	76/116 (66%)	76 (100%)	0	100	100
46	m	58/113 (51%)	58 (100%)	0	100	100
47	o	71/87 (82%)	71 (100%)	0	100	100
48	p	135/181 (75%)	135 (100%)	0	100	100
49	q	138/178 (78%)	138 (100%)	0	100	100
50	r	147/169 (87%)	147 (100%)	0	100	100
51	s	340/381 (89%)	340 (100%)	0	100	100
52	t	40/158 (25%)	40 (100%)	0	100	100
52	u	31/158 (20%)	31 (100%)	0	100	100
52	v	28/158 (18%)	28 (100%)	0	100	100
52	w	30/158 (19%)	30 (100%)	0	100	100
52	x	30/158 (19%)	30 (100%)	0	100	100
52	y	30/158 (19%)	30 (100%)	0	100	100
53	za	114/200 (57%)	114 (100%)	0	100	100
54	zb	59/60 (98%)	59 (100%)	0	100	100
55	zc	81/136 (60%)	81 (100%)	0	100	100
All	All	7816/10462 (75%)	7814 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	303	LYS
31	7	143	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	195	ASN
3	D	252	HIS
5	F	98	GLN
5	F	138	HIS
7	I	142	ASN
8	J	54	ASN
9	K	89	GLN
10	L	104	ASN
11	M	276	ASN
12	N	237	HIS
14	P	114	HIS
15	Q	237	ASN
16	R	89	ASN
17	S	140	ASN
18	T	75	HIS
21	W	65	ASN
21	W	80	HIS
22	X	93	ASN
24	Z	62	ASN
24	Z	126	GLN
25	0	115	HIS
27	2	54	GLN
28	3	178	GLN
29	5	119	GLN
29	5	183	ASN
29	5	195	HIS
29	5	266	HIS
30	6	308	GLN
31	7	69	HIS
32	8	158	HIS
35	b	16	HIS
35	b	25	GLN
36	c	73	GLN
36	c	118	ASN
36	c	168	HIS
38	e	75	GLN
38	e	118	GLN
39	f	111	HIS
39	f	189	HIS
45	l	76	ASN
48	p	93	ASN
48	p	176	HIS
49	q	60	GLN

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Mol	Chain	Res	Type
49	q	100	GLN
51	s	107	GLN
52	v	65	GLN
55	zc	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1133/1561 (72%)	223 (19%)	0
2	B	71/72 (98%)	11 (15%)	0
All	All	1204/1633 (73%)	234 (19%)	0

All (234) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1674	A
1	A	1678	C
1	A	1679	U
1	A	1681	G
1	A	1688	A
1	A	1689	C
1	A	1690	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1711	C
1	A	1713	A
1	A	1721	C
1	A	1722	A
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1731	A
1	A	1733	C
1	A	1735	A
1	A	1737	A
1	A	1748	G
1	A	1749	C

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Mol	Chain	Res	Type
1	A	1764	C
1	A	1765	C
1	A	1777	A
1	A	1805	A
1	A	1807	U
1	A	1810	A
1	A	1817	C
1	A	1821	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1857	U
1	A	1858	G
1	A	1868	G
1	A	1869	A
1	A	1882	A
1	A	1883	G
1	A	1886	G
1	A	1887	A
1	A	1893	A
1	A	1901	C
1	A	1902	C
1	A	1903	C
1	A	1918	G
1	A	1919	C
1	A	1934	U
1	A	1935	A
1	A	1936	A
1	A	1937	A
1	A	1939	G
1	A	1940	A
1	A	1941	G
1	A	1985	G
1	A	1992	C
1	A	1994	A
1	A	1999	A
1	A	2000	C
1	A	2013	U
1	A	2022	G

Continued on next page...

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Mol	Chain	Res	Type
1	A	2033	A
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2055	U
1	A	2060	A
1	A	2066	C
1	A	2068	C
1	A	2069	U
1	A	2070	C
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2098	G
1	A	2099	U
1	A	2105	G
1	A	2109	A
1	A	2111	C
1	A	2113	G
1	A	2132	A
1	A	2141	U
1	A	2142	A
1	A	2147	G
1	A	2155	A
1	A	2156	A
1	A	2159	U
1	A	2160	A
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2167	A
1	A	2168	U
1	A	2171	U
1	A	2172	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2188	A
1	A	2190	C
1	A	2192	A
1	A	2194	U
1	A	2197	G

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Mol	Chain	Res	Type
1	A	2198	A
1	A	2199	A
1	A	2200	A
1	A	2201	G
1	A	2202	C
1	A	2204	U
1	A	2207	A
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2245	A
1	A	2246	A
1	A	2262	C
1	A	2263	C
1	A	2284	C
1	A	2285	U
1	A	2294	A
1	A	2297	A
1	A	2331	C
1	A	2332	C
1	A	2345	G
1	A	2350	A
1	A	2351	U
1	A	2363	A
1	A	2374	A
1	A	2381	A
1	A	2390	A
1	A	2399	A
1	A	2401	A
1	A	2404	U
1	A	2407	U
1	A	2415	C
1	A	2427	C
1	A	2431	C
1	A	2432	A
1	A	2433	C
1	A	2434	A
1	A	2435	G
1	A	2446	A
1	A	2451	A
1	A	2473	A
1	A	2475	U

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Mol	Chain	Res	Type
1	A	2476	C
1	A	2478	G
1	A	2497	U
1	A	2502	C
1	A	2503	A
1	A	2520	C
1	A	2521	A
1	A	2523	C
1	A	2527	A
1	A	2539	A
1	A	2648	U
1	A	2656	U
1	A	2660	U
1	A	2686	G
1	A	2694	A
1	A	2706	A
1	A	2721	G
1	A	2726	C
1	A	2727	C
1	A	2731	U
1	A	2732	G
1	A	2735	G
1	A	2738	U
1	A	2740	A
1	A	2798	A
1	A	2847	C
1	A	2848	A
1	A	2851	A
1	A	2854	U
1	A	2864	U
1	A	2865	C
1	A	2882	U
1	A	2907	U
1	A	2910	A
1	A	2911	C
1	A	2916	G
1	A	2917	G
1	A	2918	A
1	A	2928	C
1	A	2932	G
1	A	3108	U
1	A	3110	C

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Mol	Chain	Res	Type
1	A	3112	A
1	A	3113	A
1	A	3114	U
1	A	3122	U
1	A	3135	A
1	A	3137	G
1	A	3141	A
1	A	3147	G
1	A	3150	U
1	A	3157	C
1	A	3160	A
1	A	3162	C
1	A	3175	A
1	A	3180	A
1	A	3188	U
1	A	3193	U
1	A	3194	U
1	A	3197	U
1	A	3199	U
1	A	3200	U
1	A	3201	A
1	A	3208	C
1	A	3211	C
1	A	3212	C
1	A	3217	A
1	A	3218	A
1	A	3228	U
1	A	3229	U
1	A	3231	U
2	B	11	C
2	B	14	A
2	B	16	C
2	B	20	A
2	B	21	A
2	B	48	U
2	B	54	C
2	B	55	U
2	B	59	A
2	B	63	G
2	B	64	A

There are no RNA pucker outliers to report.

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

7 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	$\# Z > 2$
2	2MG	B	10	2	23,26,27	0.24	0	33,38,41	0.34	0
35	THC	b	2	35	8,9,10	0.31	0	10,11,13	0.55	0
2	1MA	B	9	2	21,25,26	0.79	1 (4%)	30,37,40	0.72	1 (3%)
2	PSU	B	39	2	18,21,22	0.47	0	21,30,33	0.55	0
44	AYA	k	2	44	6,7,8	0.84	0	6,8,10	0.47	0
19	AYA	U	2	19	6,7,8	0.80	0	6,8,10	0.49	0
9	SAC	K	2	9	7,8,9	0.26	0	7,9,11	0.67	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
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
35	THC	b	2	35	-	0/9/10/12	-
2	1MA	B	9	2	-	0/7/25/26	0/3/3/3
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
44	AYA	k	2	44	-	0/5/6/8	-
19	AYA	U	2	19	-	1/5/6/8	-
9	SAC	K	2	9	-	0/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	1MA	C6-N6	3.29	1.35	1.28

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	1MA	N1-C6-N6	2.99	127.23	119.71

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	U	2	AYA	C-CA-N-CT

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9	1MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 44 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	8Q1	zc	201	55	28,33,34	0.11	0	32,40,43	0.25	0
59	FES	r	201	7,50	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	8Q1	zc	201	55	-	3/38/40/41	-
59	FES	r	201	7,50	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

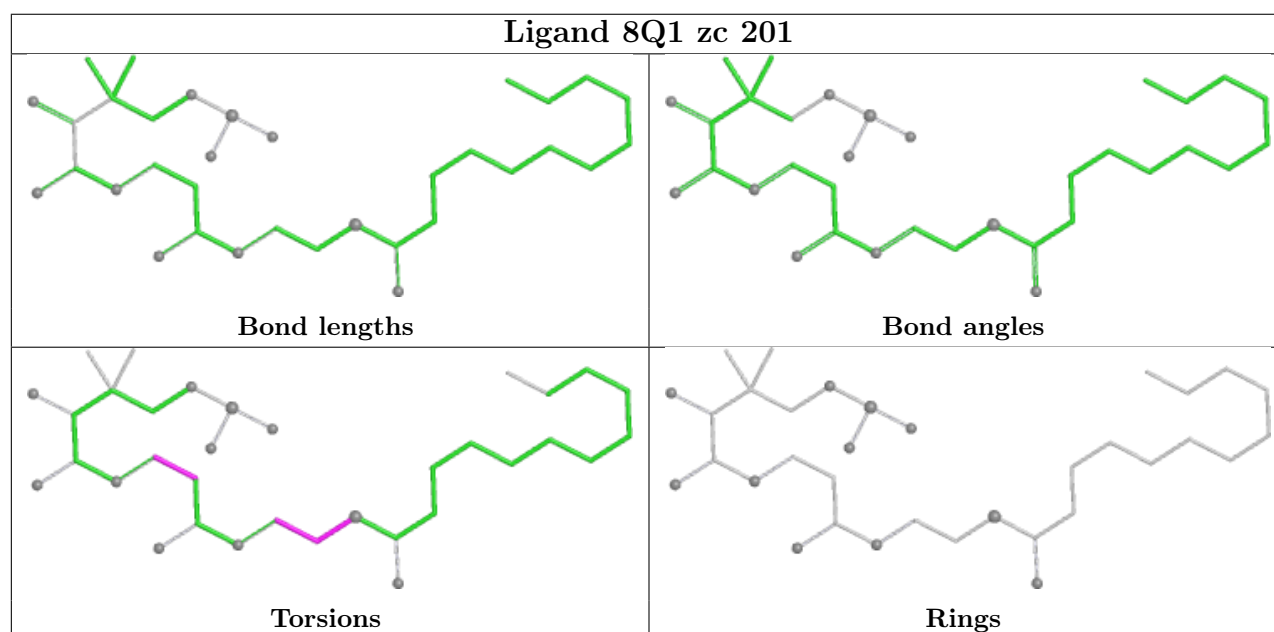
Mol	Chain	Res	Type	Atoms
60	zc	201	8Q1	N41-C42-C43-S44
60	zc	201	8Q1	N36-C37-C38-C39
60	zc	201	8Q1	C42-C43-S44-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	zc	201	8Q1	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

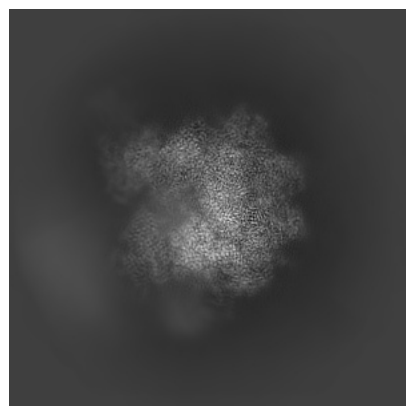
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13562. These allow visual inspection of the internal detail of the map and identification of artifacts.

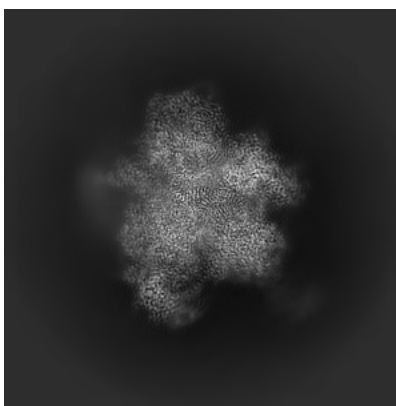
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

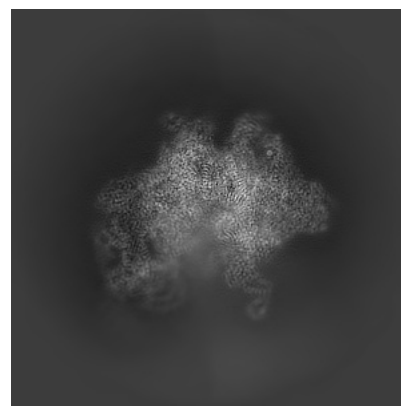
6.1.1 Primary map



X

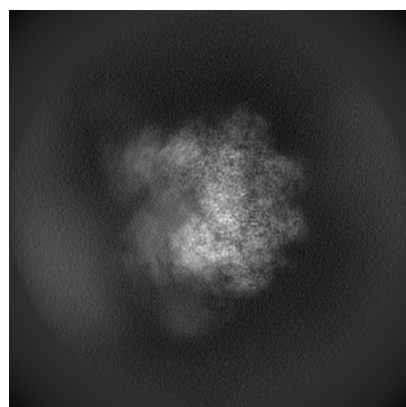


Y

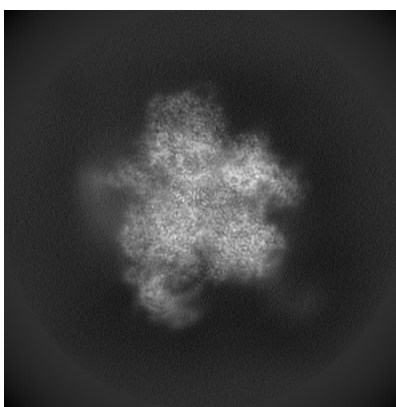


Z

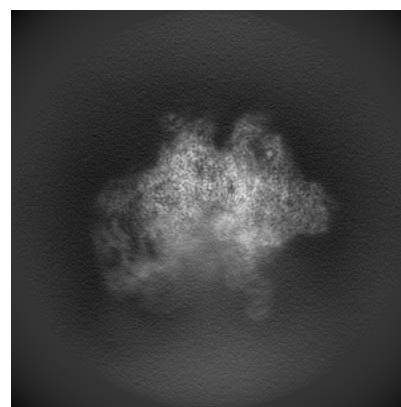
6.1.2 Raw map



X



Y

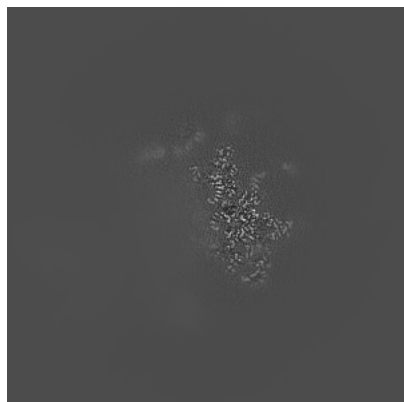


Z

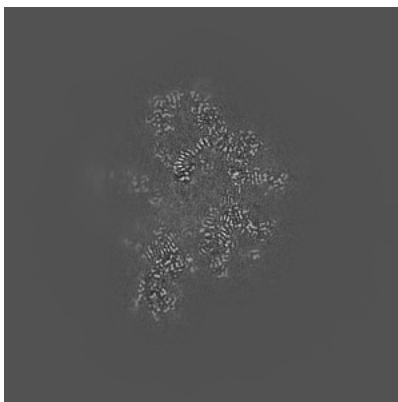
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

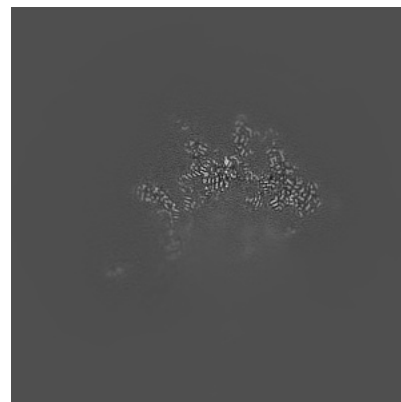
6.2.1 Primary map



X Index: 360

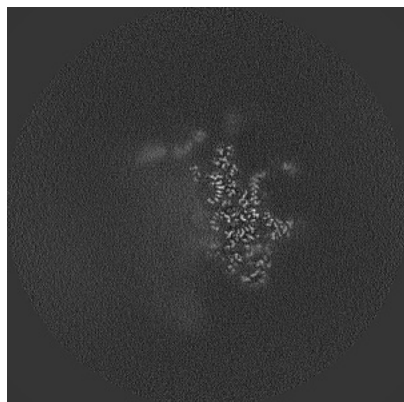


Y Index: 360

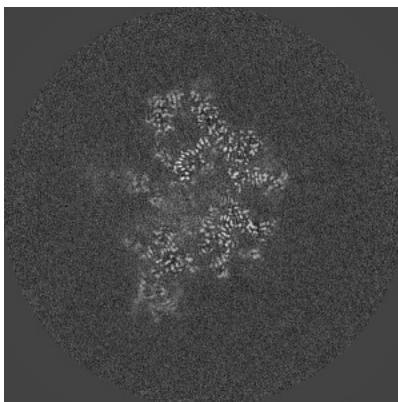


Z Index: 360

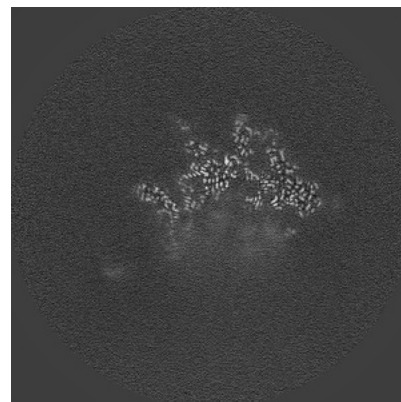
6.2.2 Raw map



X Index: 250



Y Index: 250



Z Index: 250

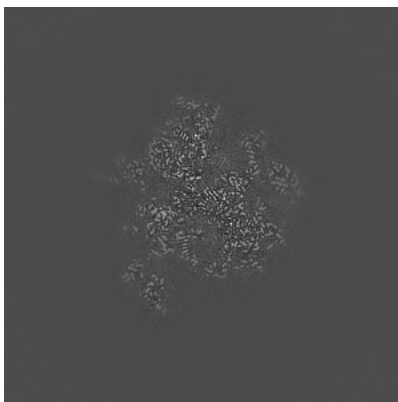
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

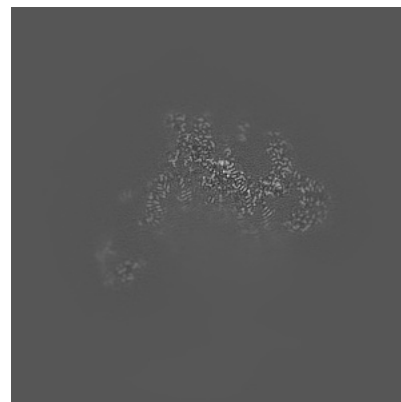
6.3.1 Primary map



X Index: 420

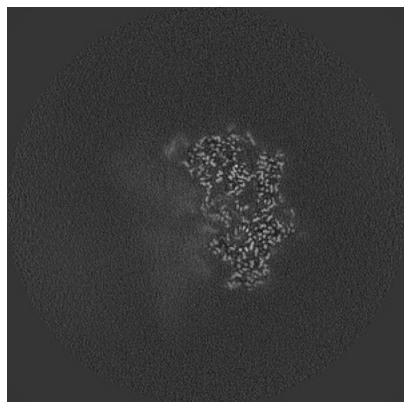


Y Index: 405

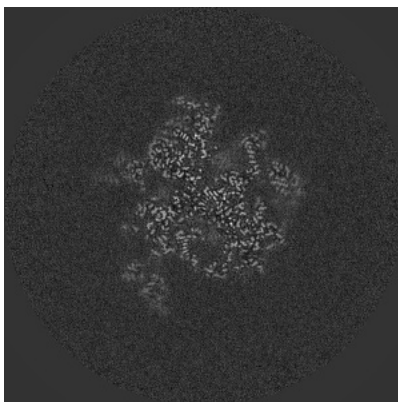


Z Index: 335

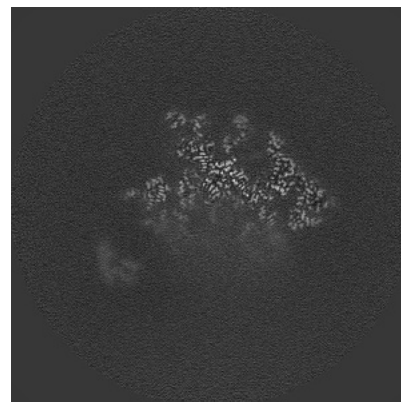
6.3.2 Raw map



X Index: 225



Y Index: 281

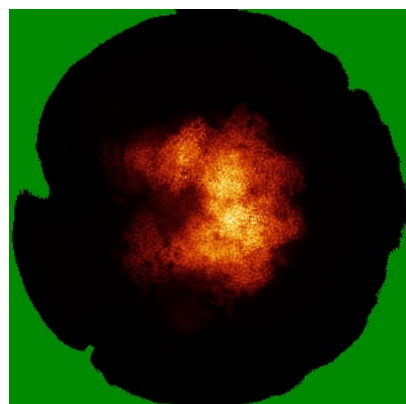


Z Index: 238

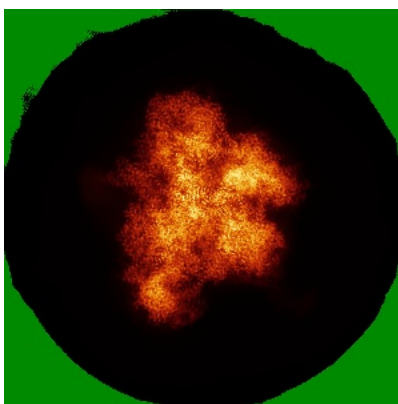
The images above show the largest variance slices of the map in three orthogonal directions.

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

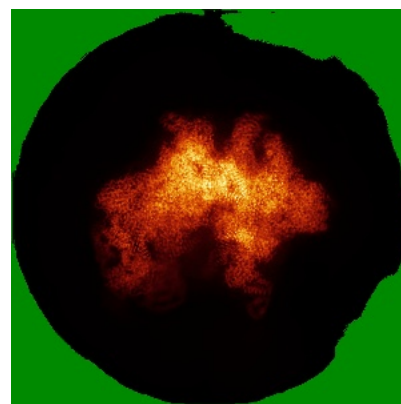
6.4.1 Primary map



X

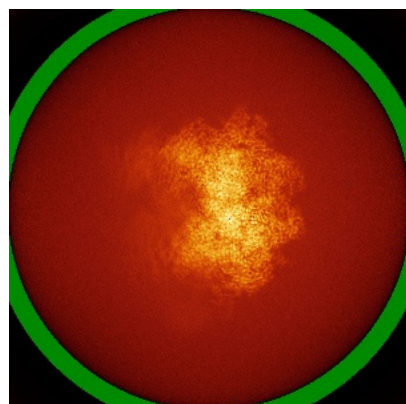


Y

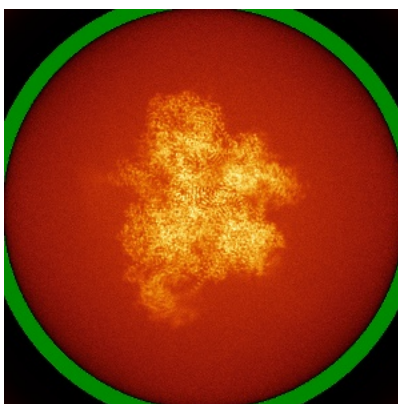


Z

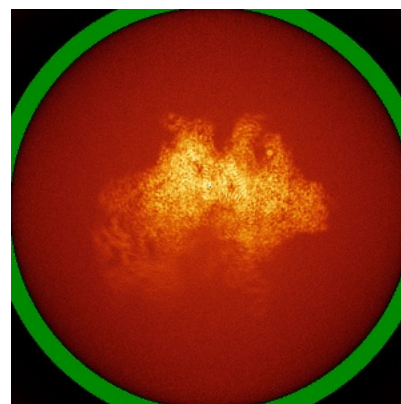
6.4.2 Raw map



X



Y



Z

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

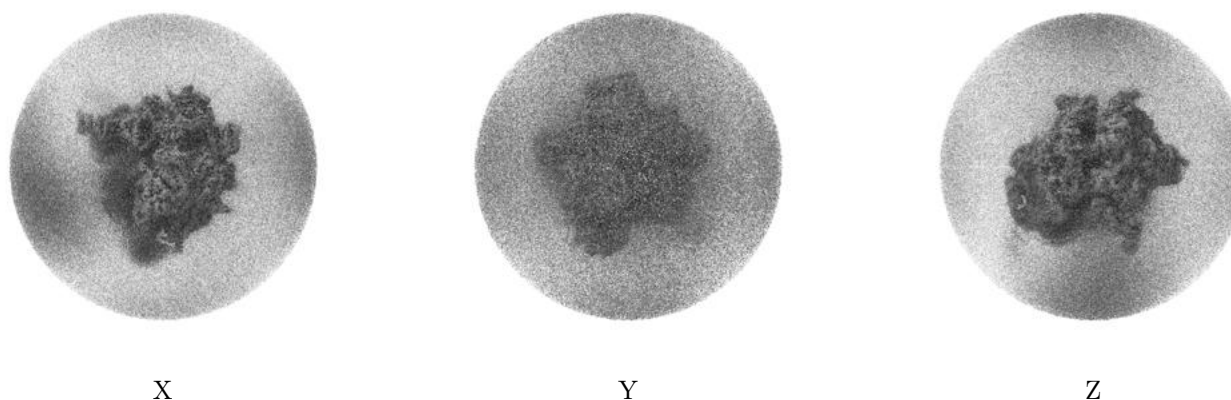
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

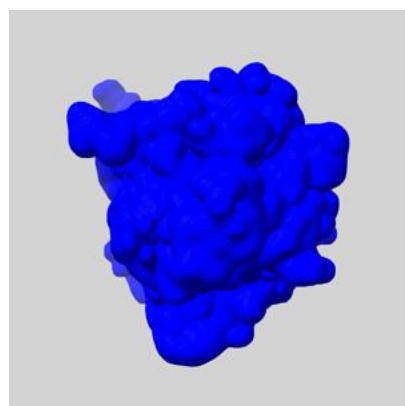
6.6 Mask visualisation [i](#)

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

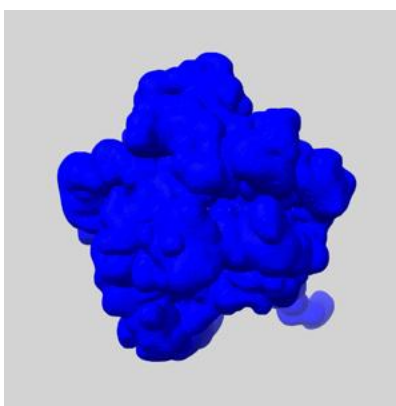
A mask typically either:

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

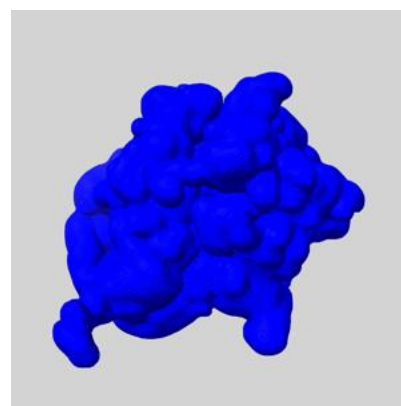
6.6.1 emd_13562_msk_1.map [i](#)



X



Y

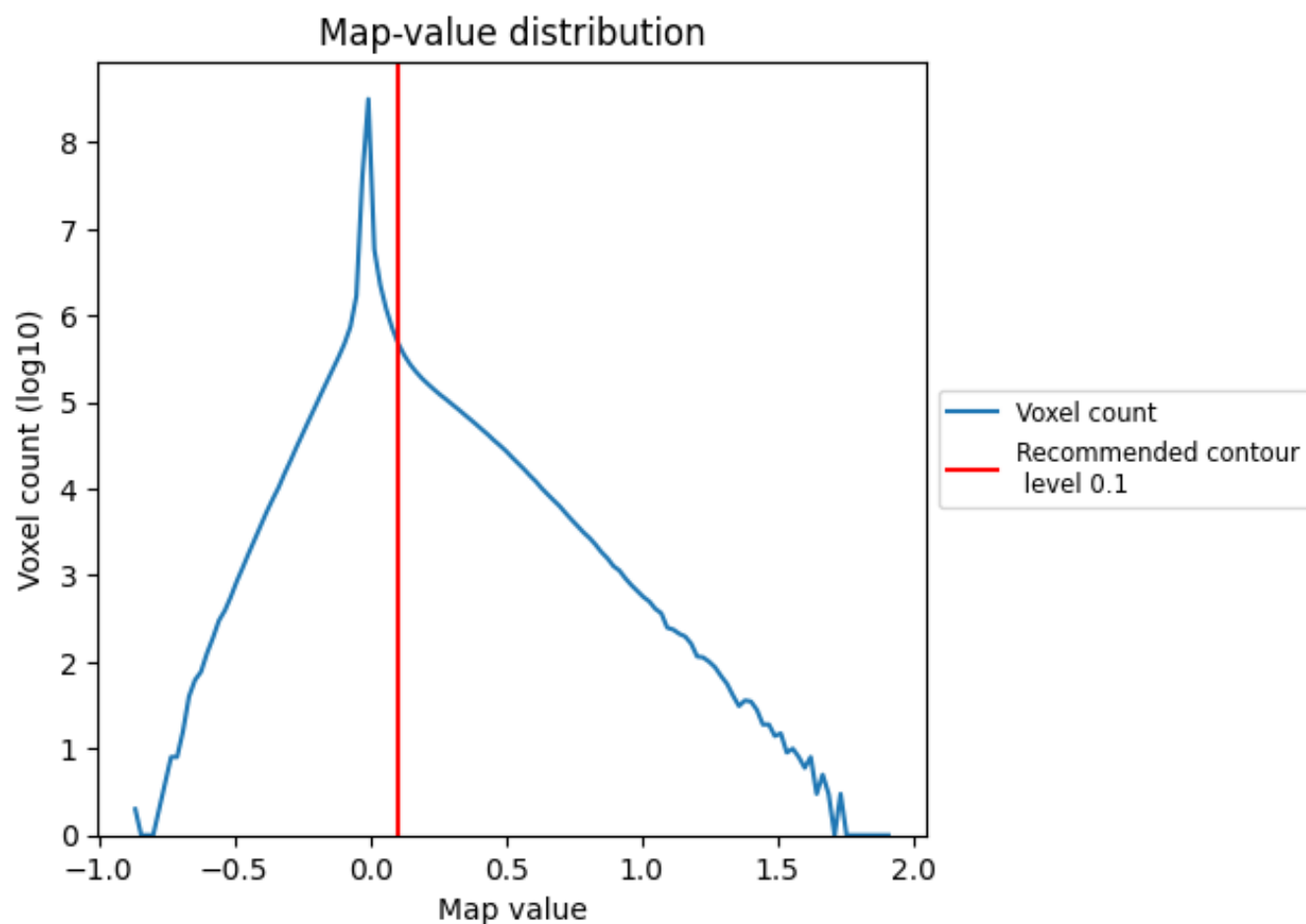


Z

7 Map analysis [i](#)

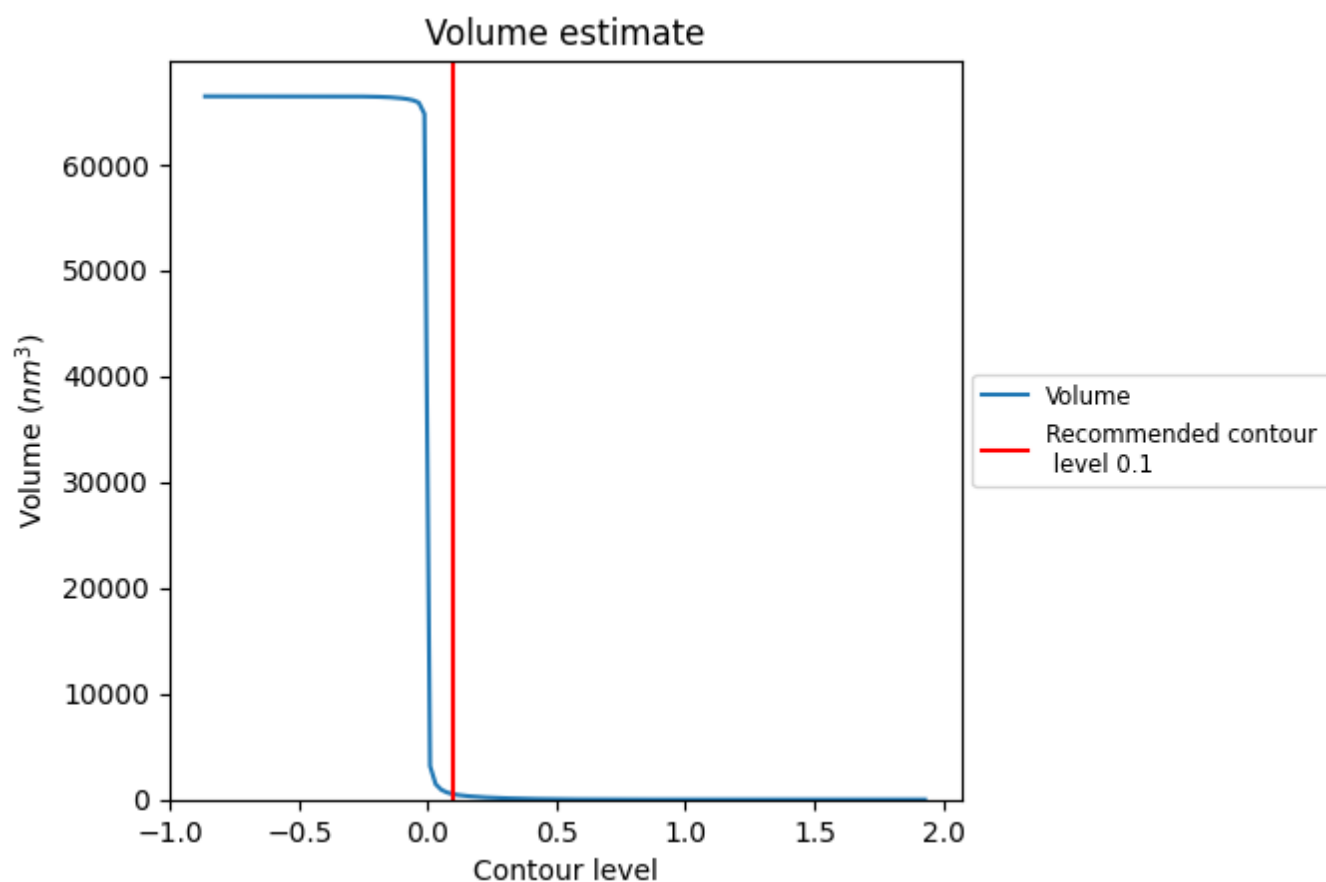
This section contains the results of statistical analysis of the map.

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.

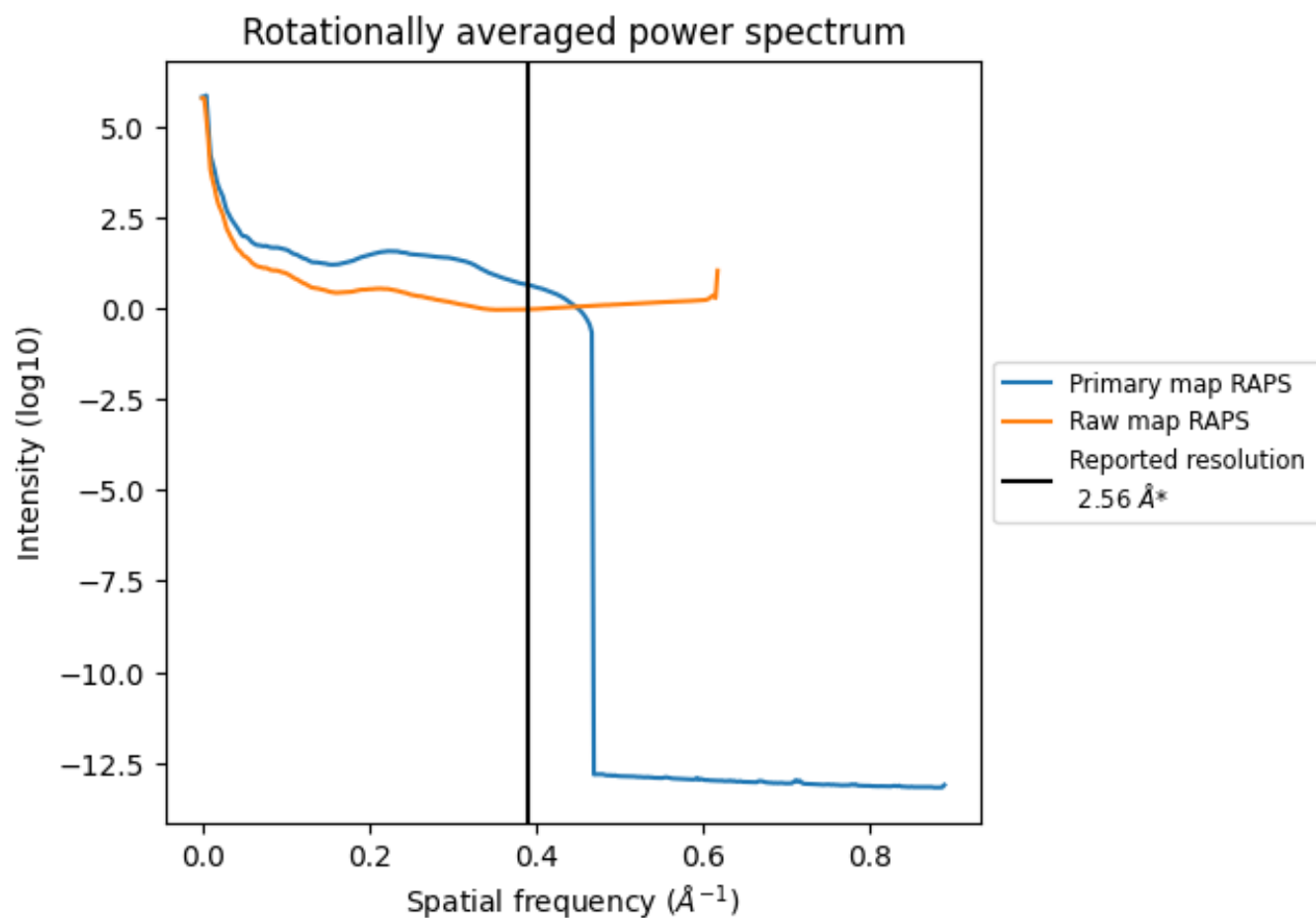
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 509 nm^3 ; this corresponds to an approximate mass of 459 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

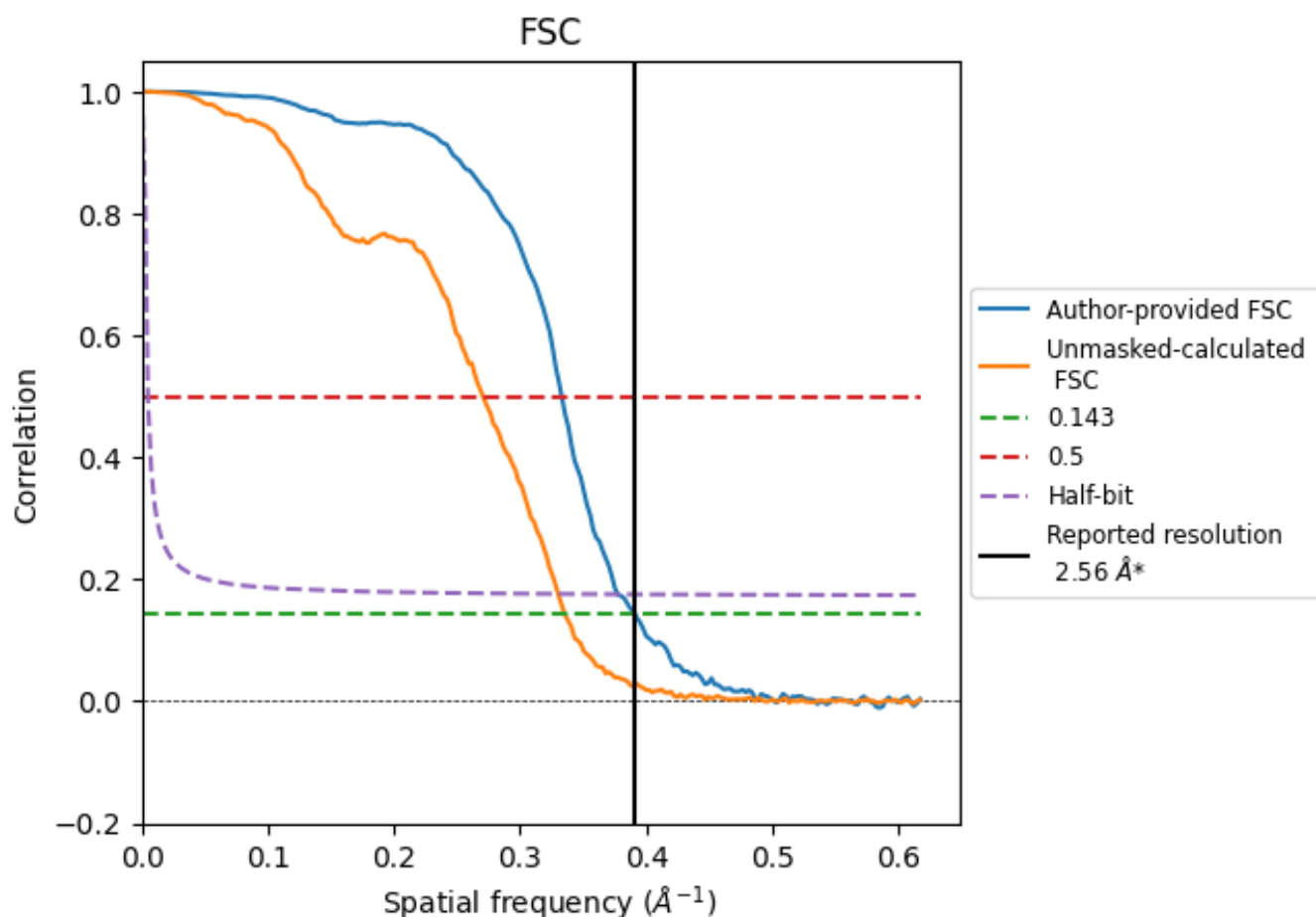


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

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 0.391 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

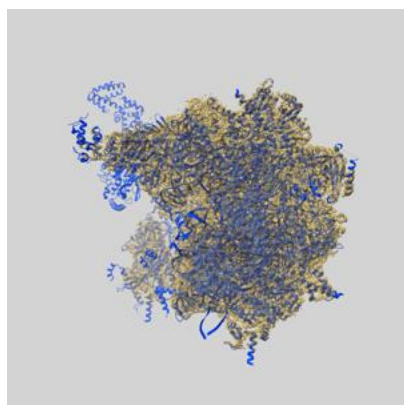
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.55	3.00	2.65
Unmasked-calculated*	2.98	3.70	3.03

*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 2.98 differs from the reported value 2.56 by more than 10 %

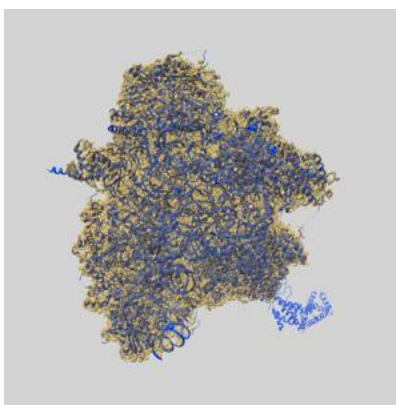
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13562 and PDB model 7PO4. Per-residue inclusion information can be found in section [3](#) on page [19](#).

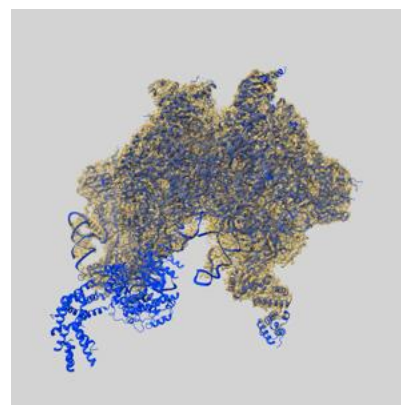
9.1 Map-model overlay [i](#)



X



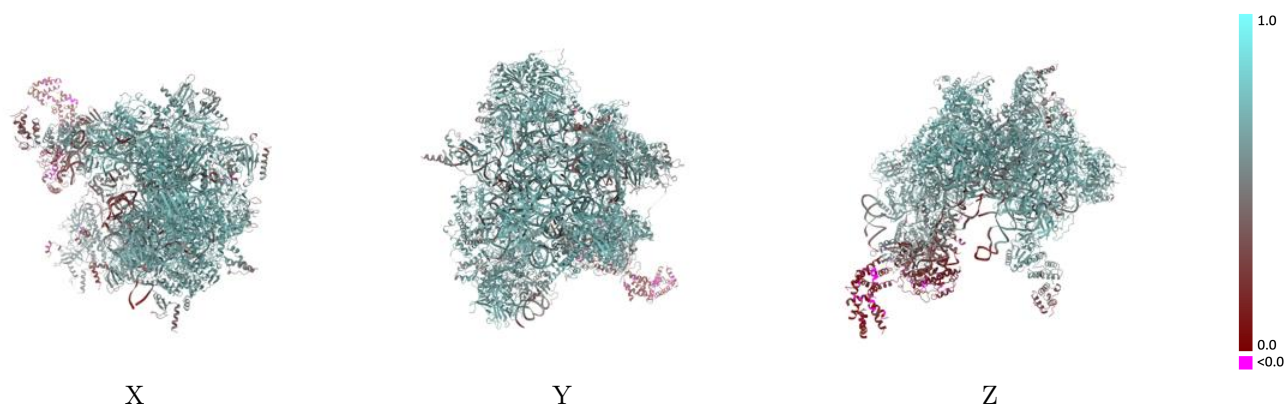
Y



Z

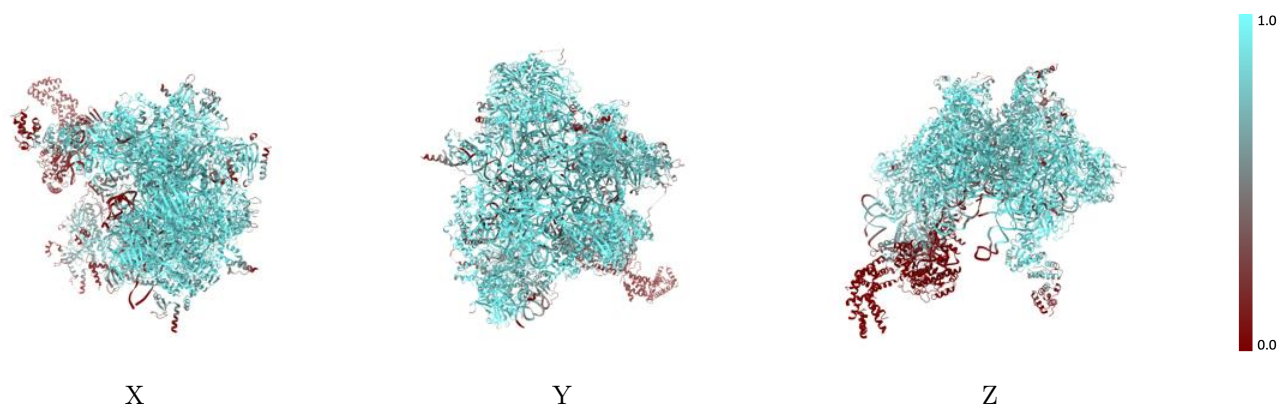
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



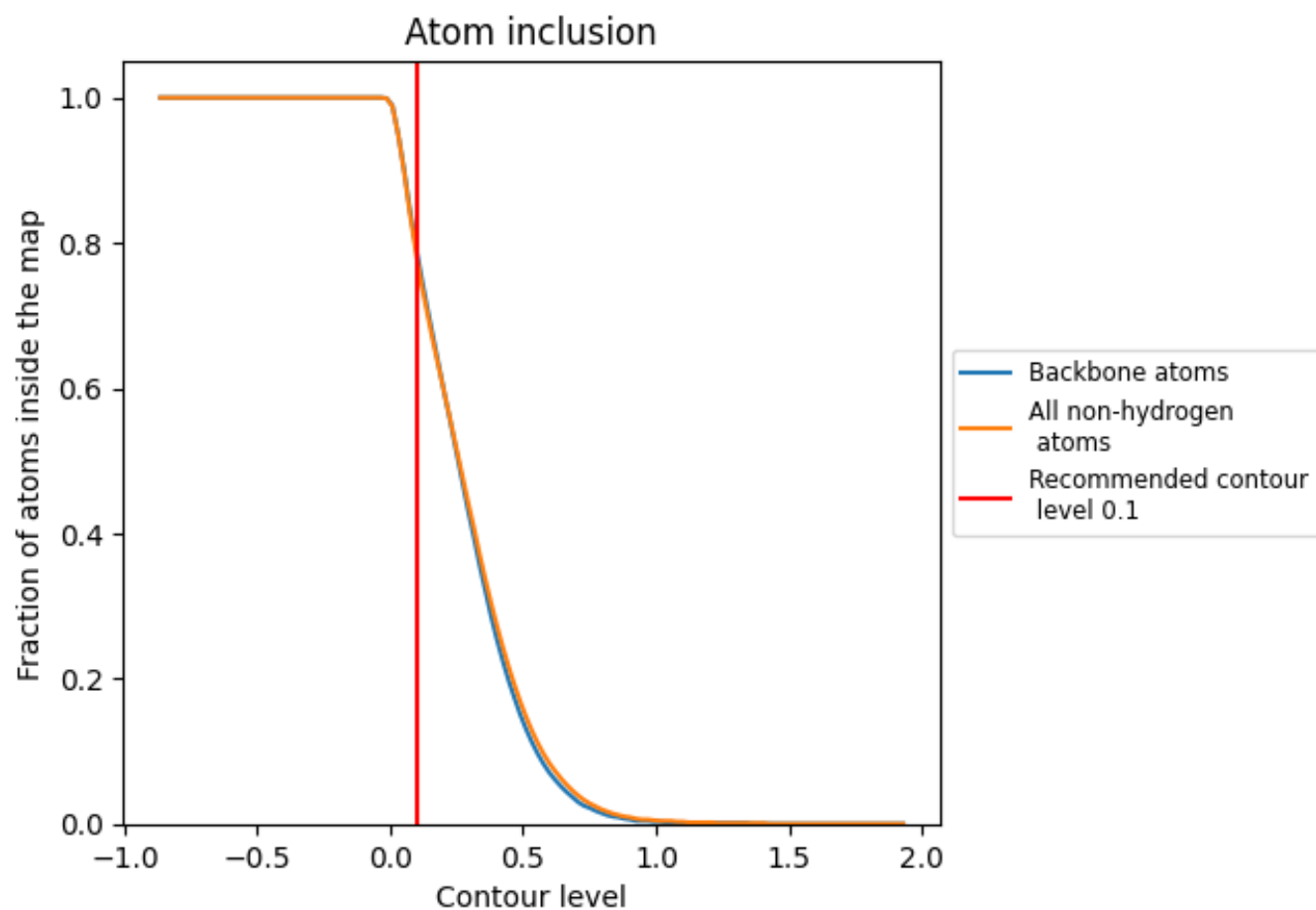
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5950
0	 0.9070	 0.6800
1	 0.4370	 0.4890
2	 0.9860	 0.7510
3	 0.9730	 0.7030
5	 0.9020	 0.6370
6	 0.9210	 0.6560
7	 0.8010	 0.5980
8	 0.5670	 0.4900
9	 0.8800	 0.6560
A	 0.7910	 0.5840
B	 0.7750	 0.5580
D	 0.8250	 0.6170
E	 0.9410	 0.6660
F	 0.9540	 0.7080
H	 0.6440	 0.5460
I	 0.1510	 0.3200
J	 0.0000	 0.1440
K	 0.9520	 0.6820
L	 0.9660	 0.6690
M	 0.9370	 0.6720
N	 0.4920	 0.4840
O	 0.9420	 0.6820
P	 0.9660	 0.6870
Q	 0.9330	 0.6600
R	 0.9680	 0.7270
S	 0.9350	 0.6820
T	 0.9510	 0.6980
U	 0.8440	 0.6480
V	 0.8450	 0.6200
W	 0.9550	 0.6760
X	 0.8650	 0.6240
Y	 0.9530	 0.6930
Z	 0.9290	 0.6780
a	 0.8450	 0.6450



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Chain	Atom inclusion	Q-score
b	 0.9640	 0.7190
c	 0.9050	 0.6630
d	 0.7530	 0.5690
e	 0.5890	 0.5300
f	 0.6520	 0.5480
g	 0.9330	 0.6840
h	 0.8420	 0.6190
i	 0.9780	 0.7380
j	 0.8490	 0.6460
k	 0.1910	 0.3970
l	 0.0570	 0.2700
m	 0.5760	 0.4850
o	 0.9420	 0.6800
p	 0.7600	 0.5770
q	 0.5440	 0.5040
r	 0.7960	 0.5830
s	 0.9270	 0.6790
t	 0.0000	 0.1930
u	 0.0000	 0.1390
v	 0.0000	 0.1330
w	 0.0000	 0.0320
x	 0.0000	 0.0900
y	 0.0000	 0.0730
za	 0.8000	 0.5840
zb	 0.6770	 0.5270
zc	 0.1580	 0.3610