Full wwPDB EM Validation Report ⓘ

Dec 10, 2023 – 11:26 pm GMT

PDB ID	:	8QSJ
EMDB ID	:	EMD-17720
Title	:	Human mitoribosomal large subunit assembly intermediate 2 with GTPBP7
Authors	:	Ritter, C.; Nguyen, T.G.; Kummer, E.
Deposited on	:	2023-10-10
Resolution	:	3.00 Å(reported)

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

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

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

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

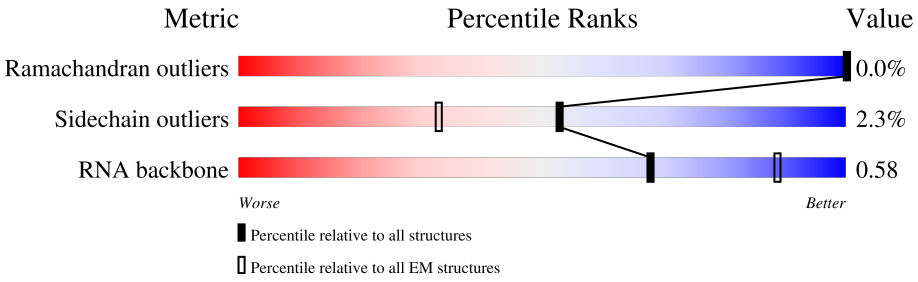
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	188	57% · 41%
2	1	65	5% 83% · 15%
3	2	92	50% 50%
4	3	188	51% 49%
5	4	103	36% 64%
6	5	423	92% · 7%
7	6	380	12% 92% · 7%
8	7	338	5% 86% · 13%

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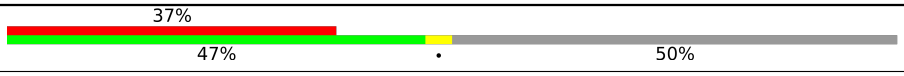
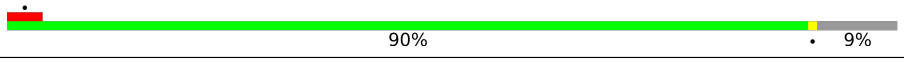
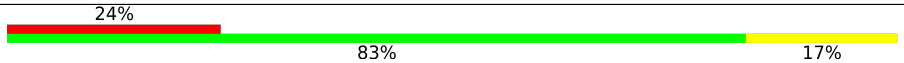
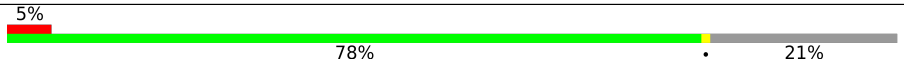
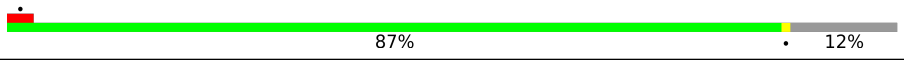
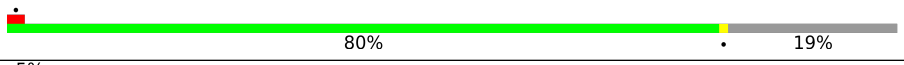
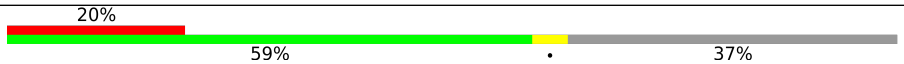
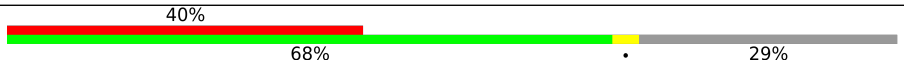
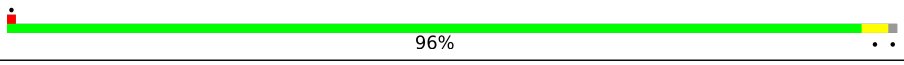
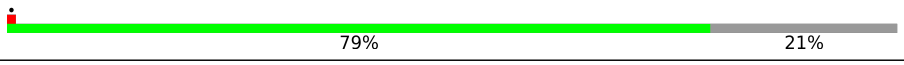
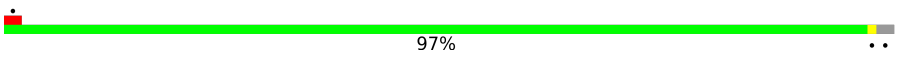
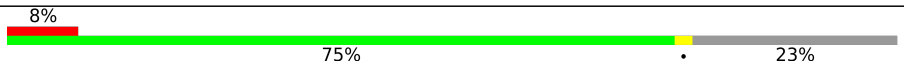
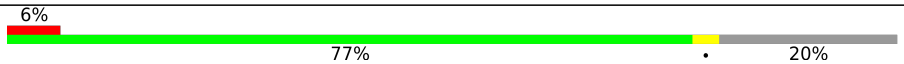
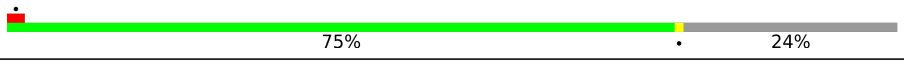
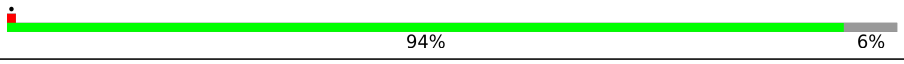
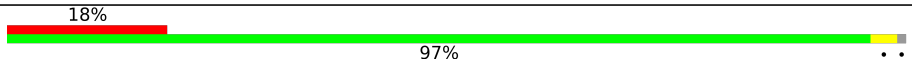
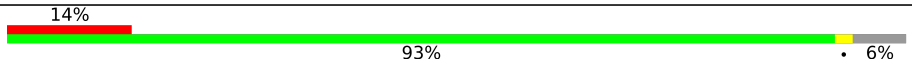
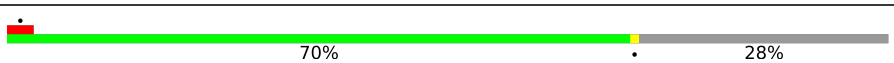
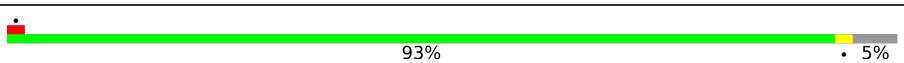
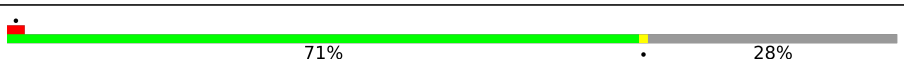
Mol	Chain	Length	Quality of chain
9	8	206	
10	9	137	
11	A	1603	
12	B	72	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	180	
25	Q	292	
26	R	149	
27	S	205	
28	T	206	
29	U	153	
30	V	216	
31	W	148	
32	X	256	
33	Y	250	

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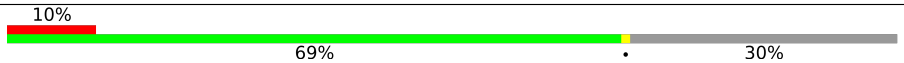
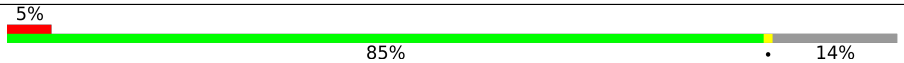
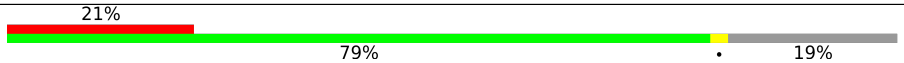
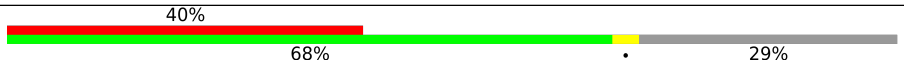
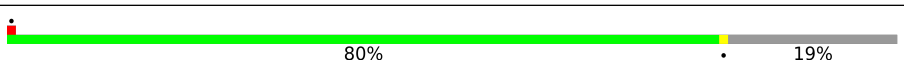
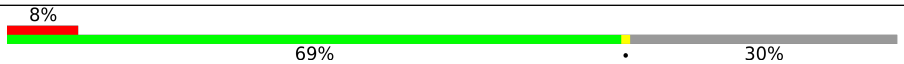
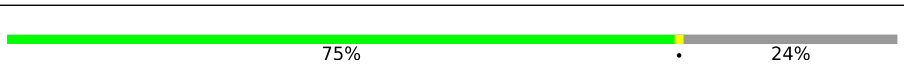
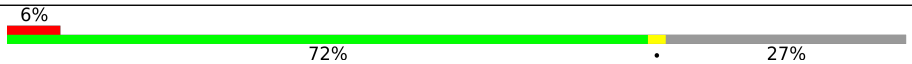
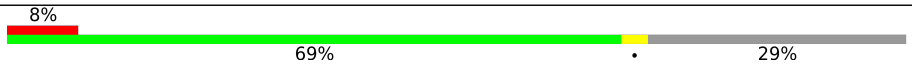
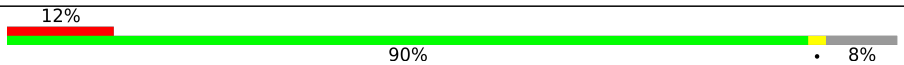
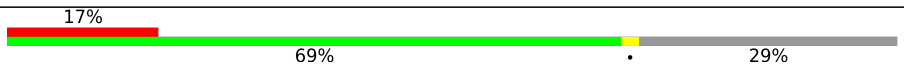
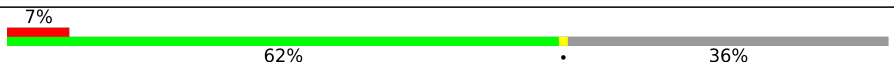
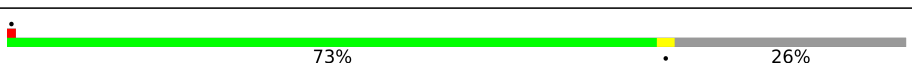
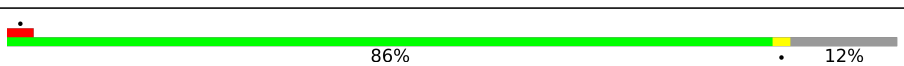
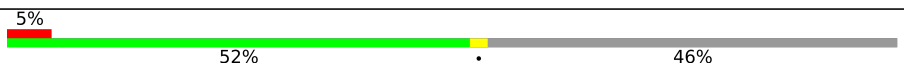
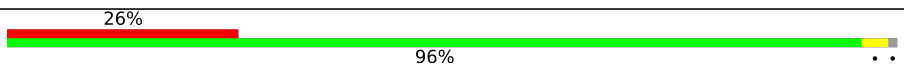
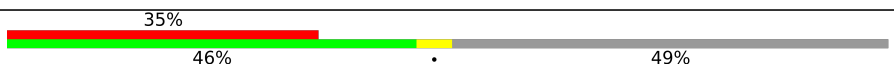
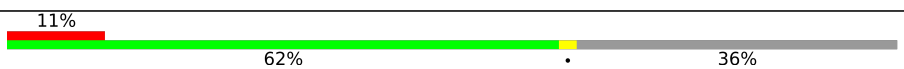
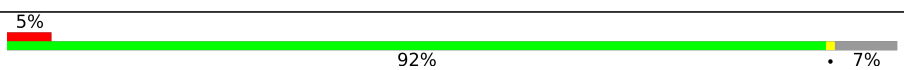
Mol	Chain	Length	Quality of chain
34	Z	161	
35	a	142	
36	b	215	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	u	234	
54	v	70	
55	w	156	
56	x	384	
57	y	381	
58	z	334	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 108265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	55	455	290	87	76	2	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	333	212	71	47	3	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	102	Total	C	N	O	S	0	0
			860	543	152	163	2		

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

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

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1418	Total	C	N	O	P	0	0
			30108	13514	5446	9730	1418		

- Molecule 12 is a RNA chain called tRNA-Val.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	72	Total	C	N	O	P	0	0
			1522	683	269	498	72		

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	240	Total	C	N	O	S	0	0
			1872	1165	378	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	97	Total	C	N	O	0	0
			802	508	155	139		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	165	Total	C	N	O	S	0	0
			1338	863	242	223	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	137	Total	C	N	O	S	0	0
			1040	665	189	184	2		

- Molecule 19 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	177	Total	C	N	O	S	0	0
			1455	936	259	253	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	194	Total	C	N	O	S	0	0
			1583	1014	291	269	9		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	221	Total	C	N	O	S	0	0
			1843	1179	327	328	9		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	152	Total	C	N	O	S	0	0
			1251	788	234	226	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	204	Total	C	N	O	S	0	0
			1667	1062	296	301	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	S	0	0
			835	536	157	139	3		

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

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

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

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

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

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

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	149	Total	C	N	O	S	0	0
			1189	739	230	217	3		

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	249	Total	C	N	O	S	0	0
			2039	1306	352	367	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	228	Total	C	N	O	S	0	0
			1848	1174	326	342	6		

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	150	Total	C	N	O	S	0	0
			1196	764	197	231	4		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	90	Total	C	N	O	S	0	0
			722	449	140	131	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	35	Total	C	N	O	S	0	0
			292	187	55	48	2		

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	141	Total	C	N	O	S	0	0
			1177	732	229	211	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	126	Total	C	N	O	S	0	0
			1044	671	172	191	10		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	69	Total	C	N	O	0	0
			588	372	116	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 56 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	338	Total	C	N	O	S	0	0
			2676	1703	467	489	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	244	Total	C	N	O	S	0	0
			1980	1264	342	362	12		

- Molecule 58 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	311	Total	C	N	O	S	0	0
			2443	1549	445	433	16		

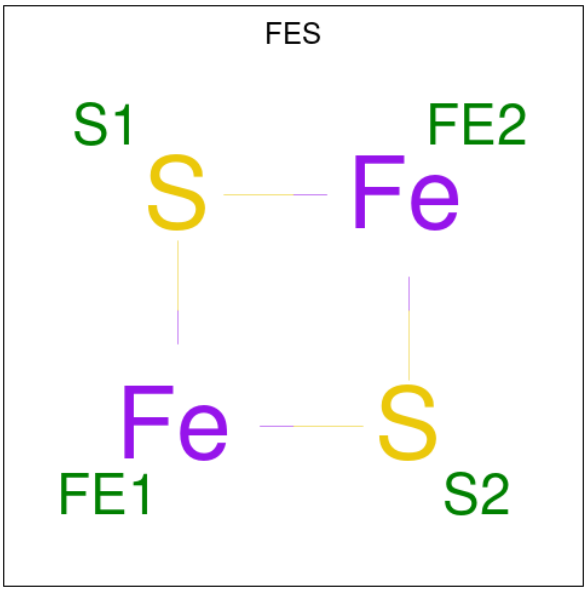
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	Zn	0
			1	1	
59	4	1	Total	Zn	0
			1	1	

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

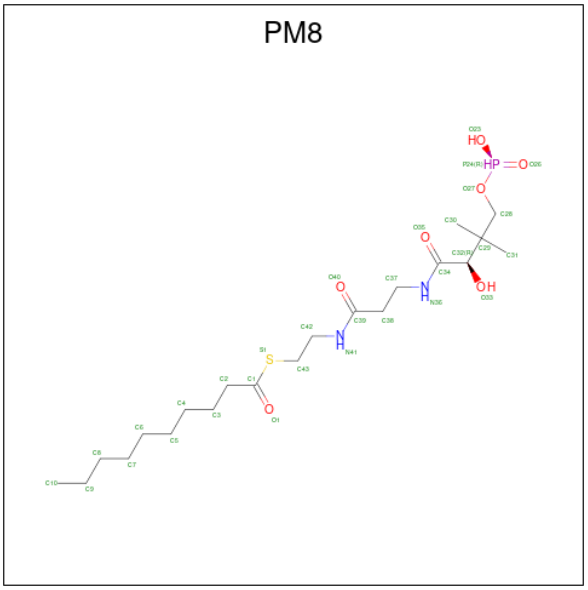
Mol	Chain	Residues	Atoms		AltConf
60	A	35	Total	Mg	0
			35	35	
60	M	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	z	1	Total	Mg	0
			1	1	

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



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

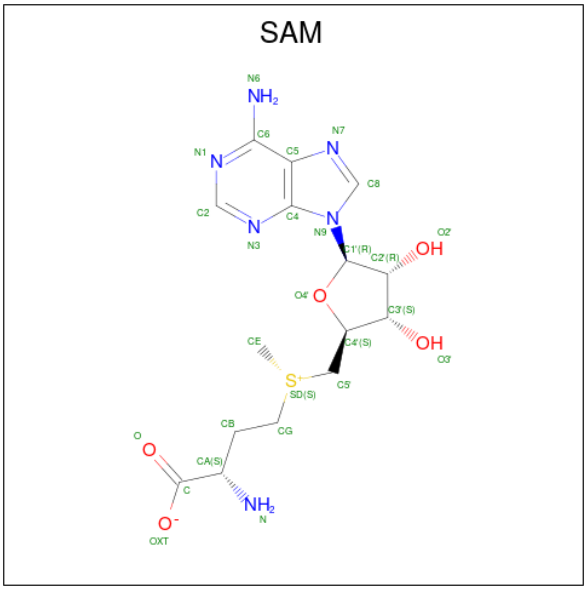
- Molecule 62 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: $C_{21}H_{41}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
62	w	1	32	21	2	7	1	1	0

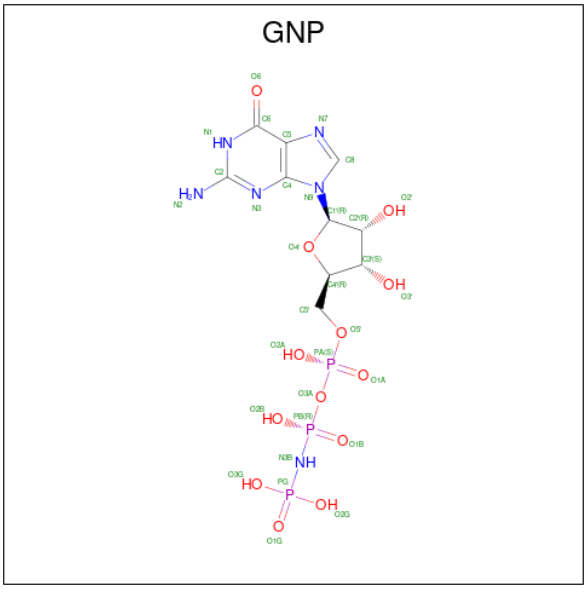
- Molecule 63 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
63	x	1	Total	C	N	O	S	0
			27	15	6	5	1	

- Molecule 64 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



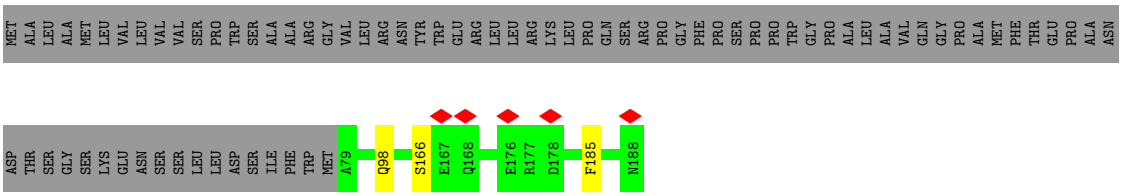
Mol	Chain	Residues	Atoms					AltConf
64	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

3 Residue-property plots (i)

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

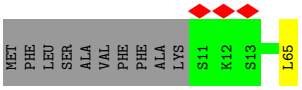
• Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:



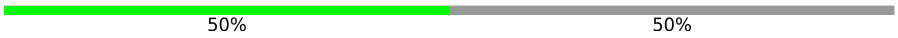
• Molecule 2: 39S ribosomal protein L33, mitochondrial

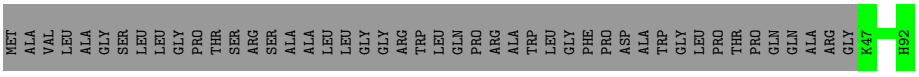
Chain 1:



• Molecule 3: 39S ribosomal protein L34, mitochondrial

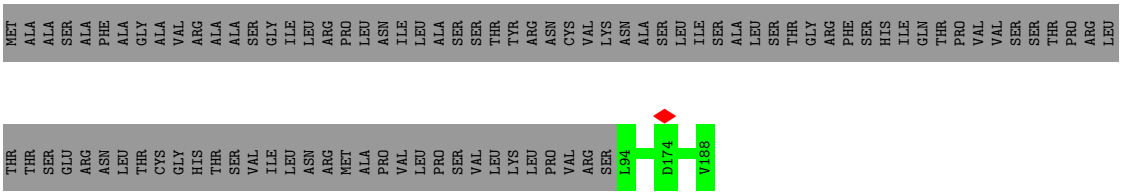
Chain 2:





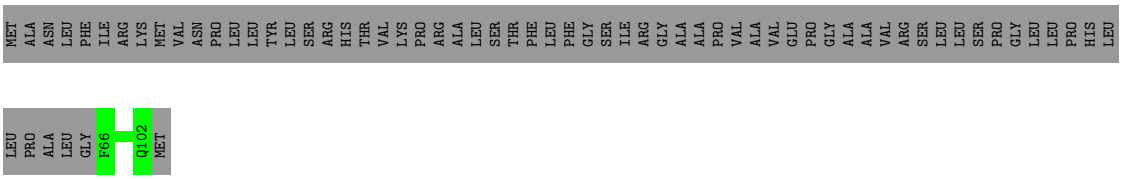
• Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3:



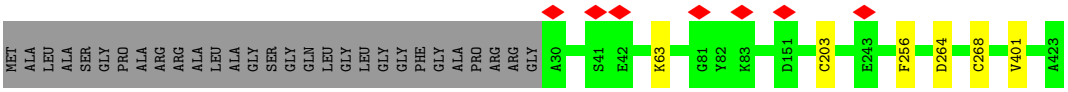
• Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:



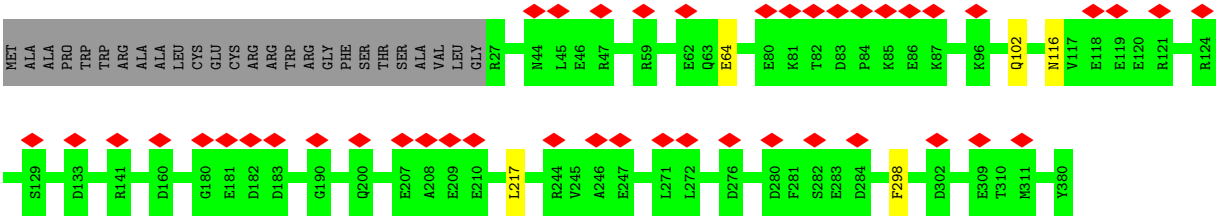
• Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:



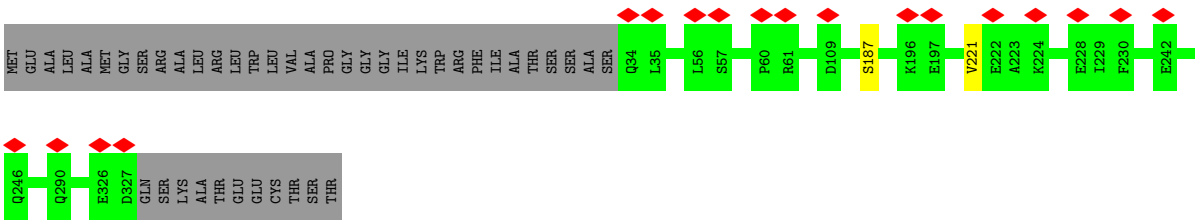
• Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:



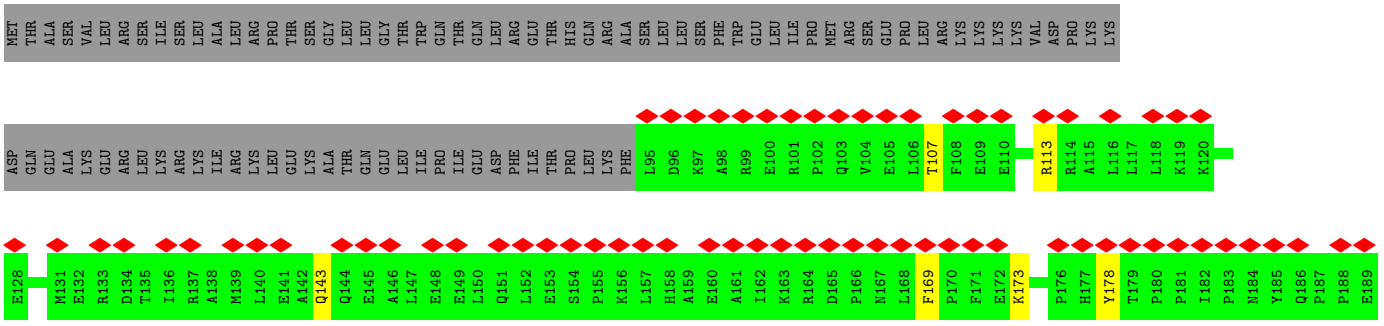
• Molecule 8: 39S ribosomal protein L39, mitochondrial

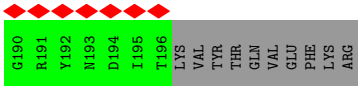
Chain 7:



• Molecule 9: 39S ribosomal protein L40, mitochondrial

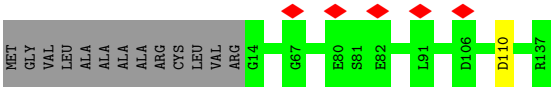
Chain 8:





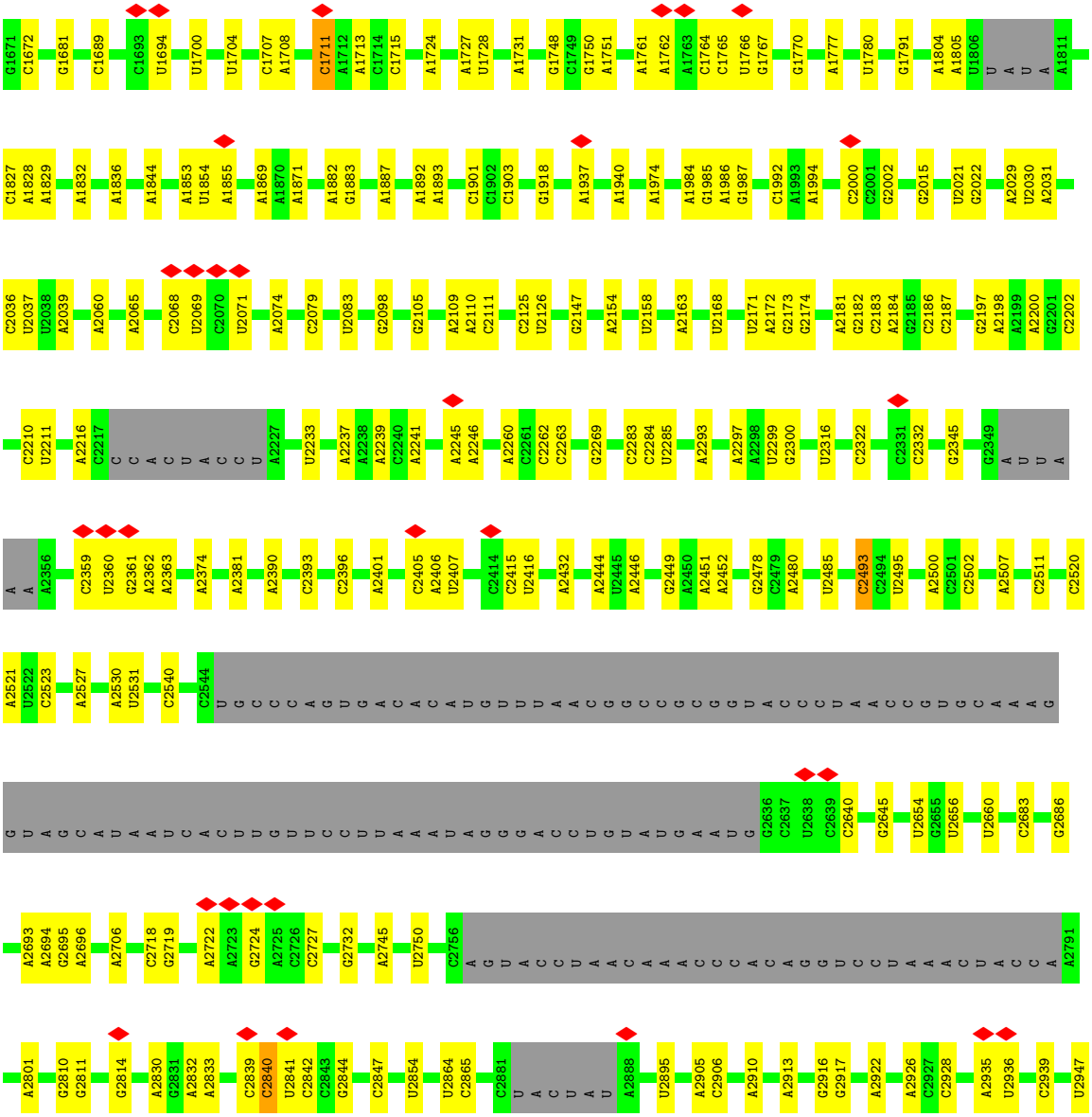
• Molecule 10: 39S ribosomal protein L41, mitochondrial

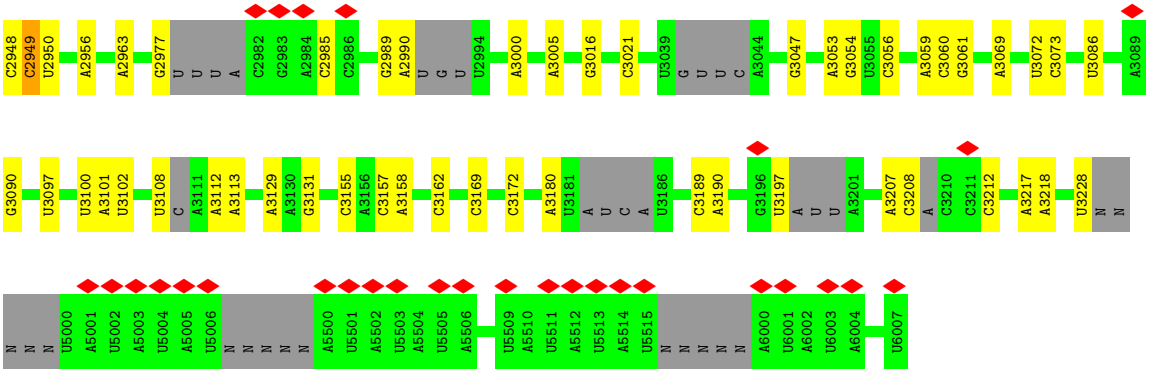
Chain 9:



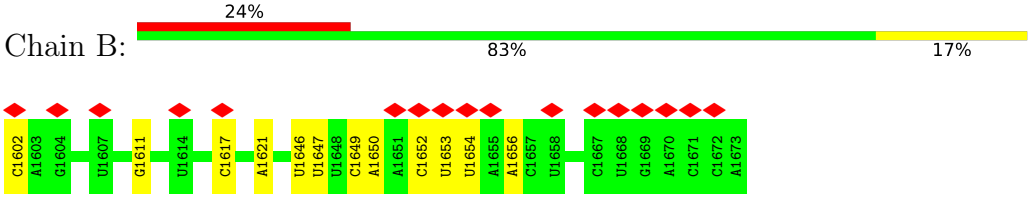
• Molecule 11: 16S rRNA

Chain A:

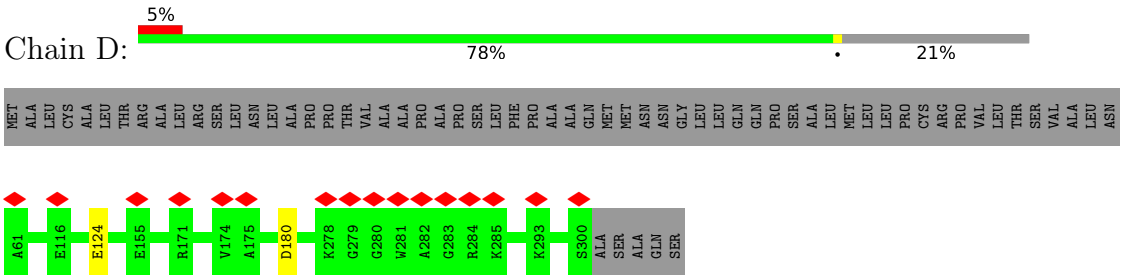




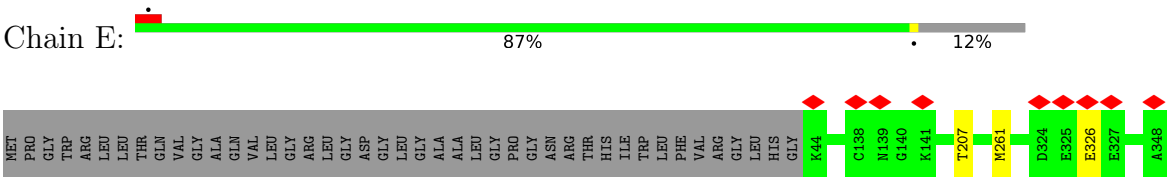
• Molecule 12: tRNA-Val



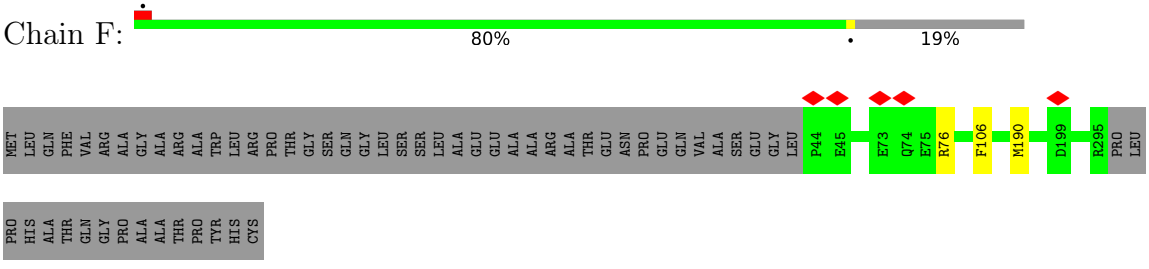
• Molecule 13: 39S ribosomal protein L2, mitochondrial



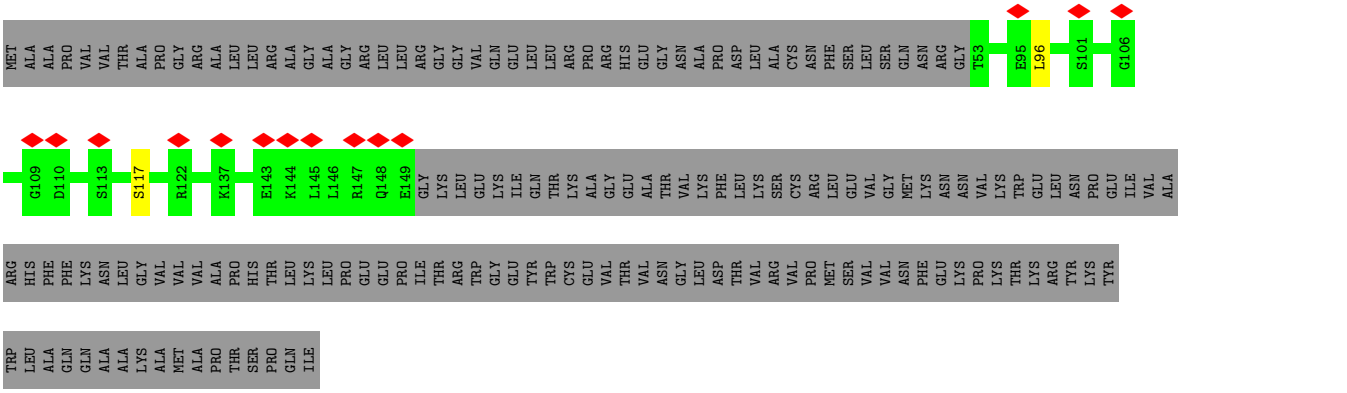
• Molecule 14: 39S ribosomal protein L3, mitochondrial



• Molecule 15: 39S ribosomal protein L4, mitochondrial

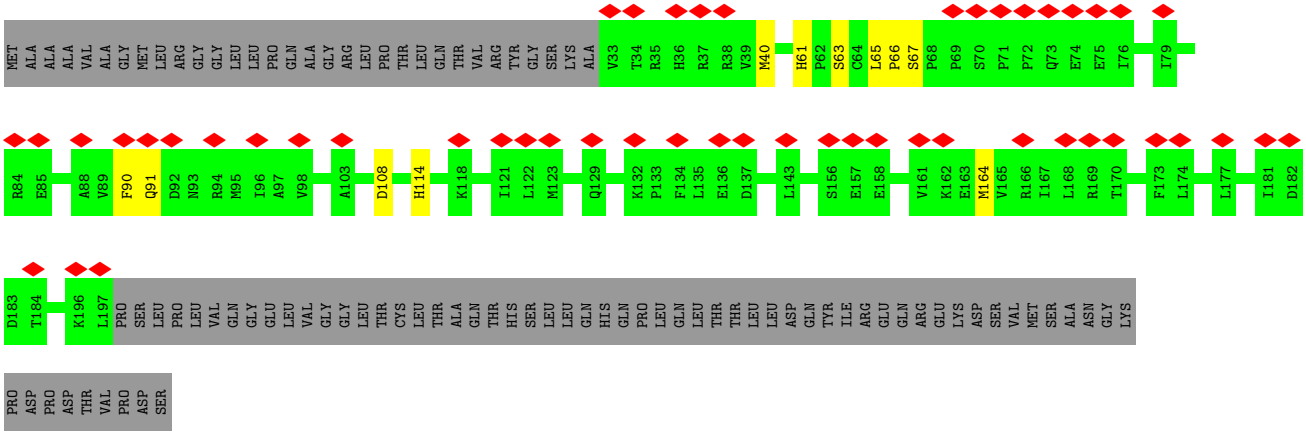


• Molecule 16: 39S ribosomal protein L9, mitochondrial



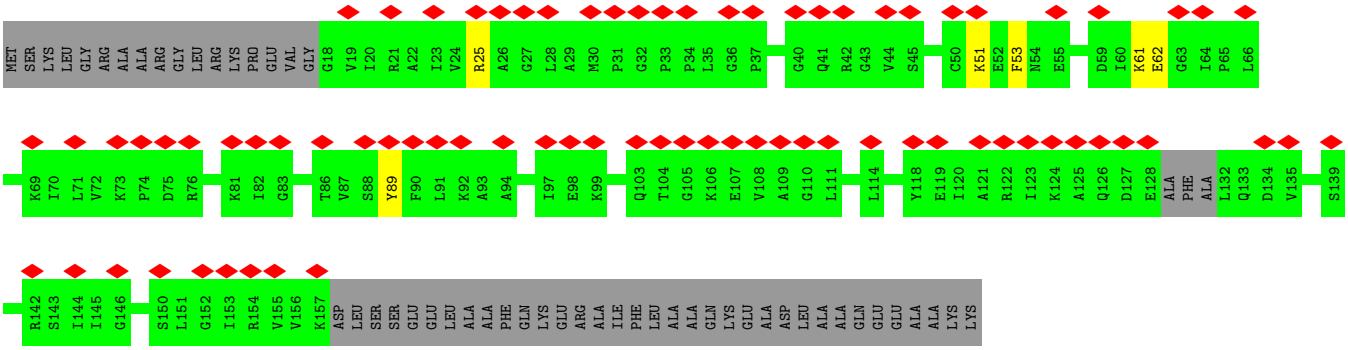
• Molecule 17: 39S ribosomal protein L10, mitochondrial

Chain I:



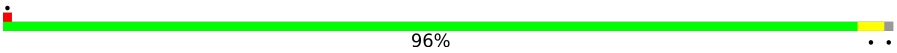
• Molecule 18: 39S ribosomal protein L11, mitochondrial

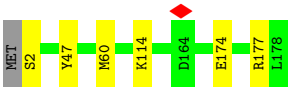
Chain J:



• Molecule 19: 39S ribosomal protein L13, mitochondrial

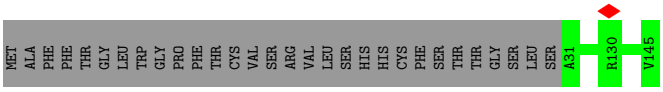
Chain K:





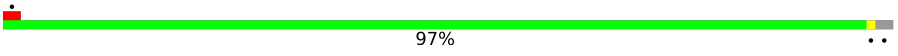
• Molecule 20: 39S ribosomal protein L14, mitochondrial

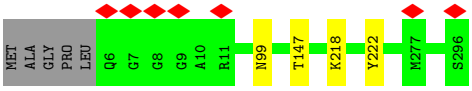
Chain L:



• Molecule 21: 39S ribosomal protein L15, mitochondrial

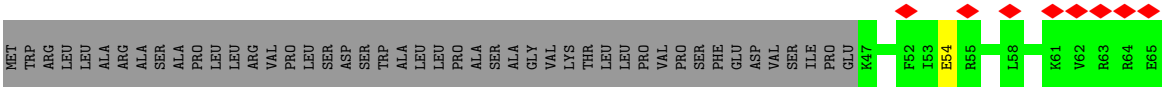
Chain M:

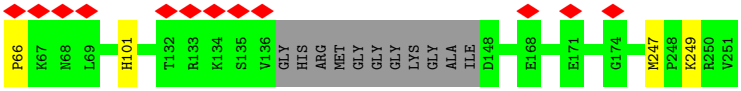




• Molecule 22: 39S ribosomal protein L16, mitochondrial

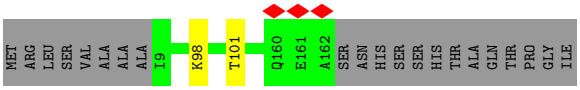
Chain N:





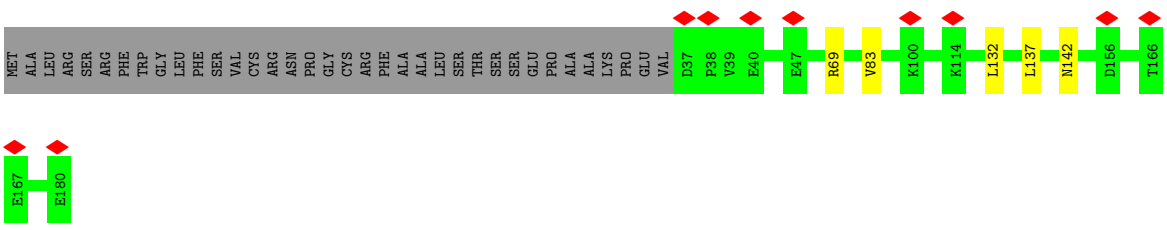
• Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:



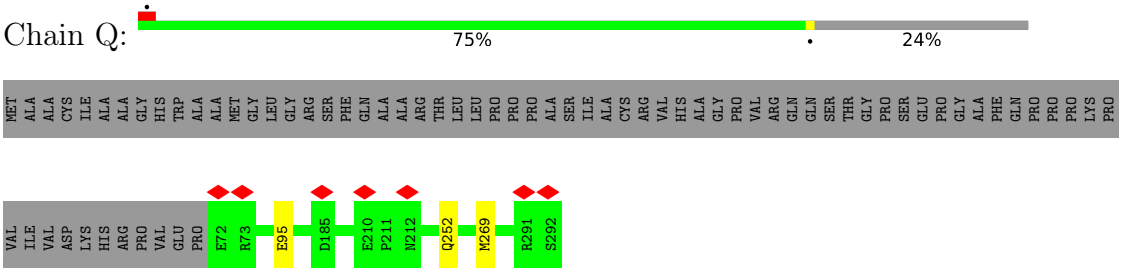
• Molecule 24: 39S ribosomal protein L18, mitochondrial

Chain P:



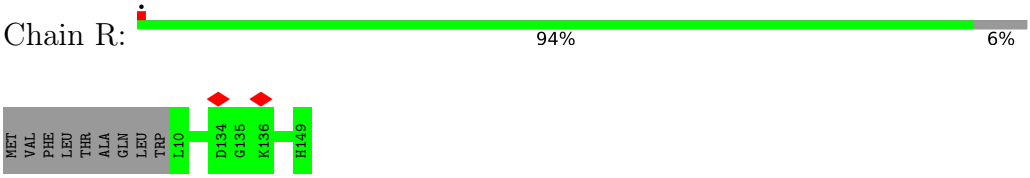
• Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q:



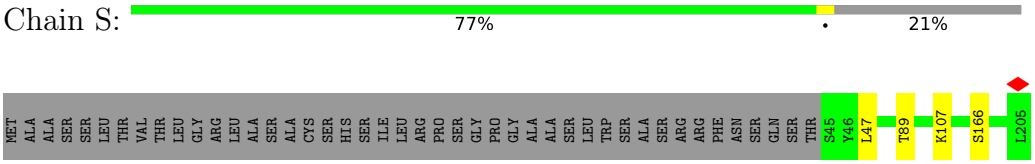
• Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R:



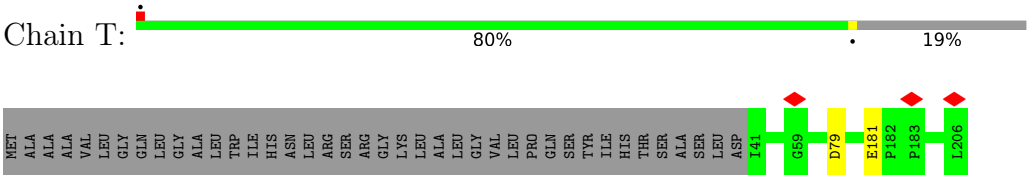
• Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S:



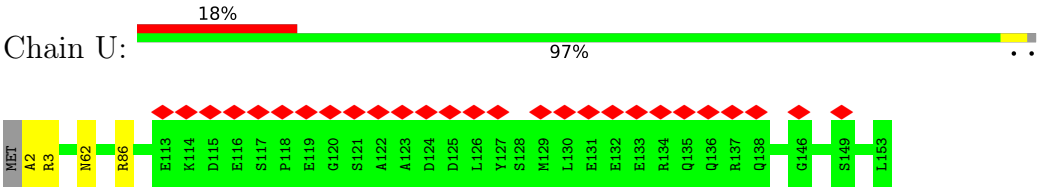
• Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T:



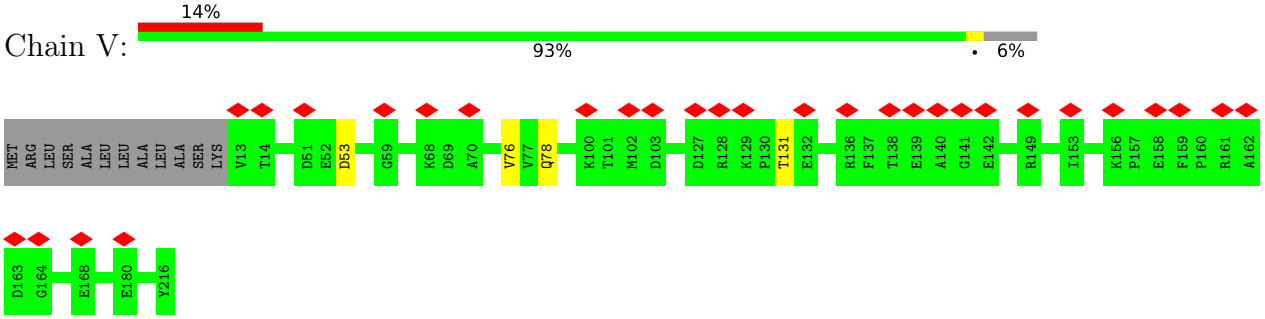
• Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U:



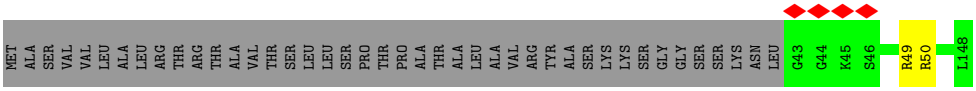
• Molecule 30: 39S ribosomal protein L24, mitochondrial

Chain V:



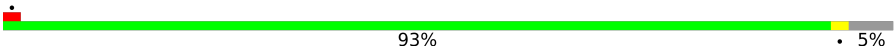
• Molecule 31: 39S ribosomal protein L27, mitochondrial

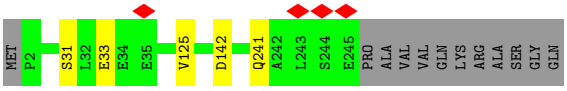
Chain W:



• Molecule 32: 39S ribosomal protein L28, mitochondrial

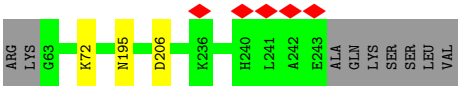
Chain X:





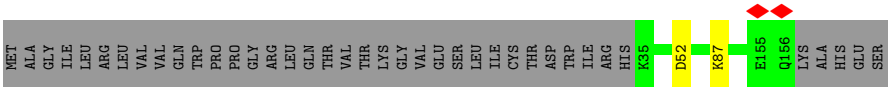
• Molecule 33: 39S ribosomal protein L47, mitochondrial

Chain Y:



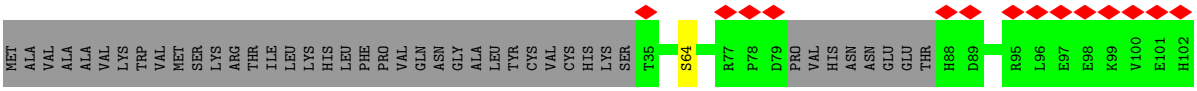
• Molecule 34: 39S ribosomal protein L30, mitochondrial

Chain Z:



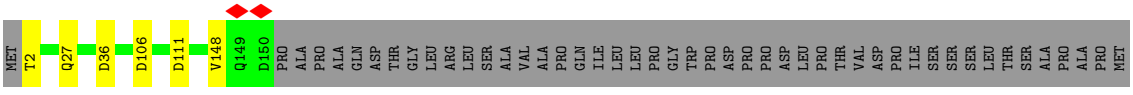
• Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a:

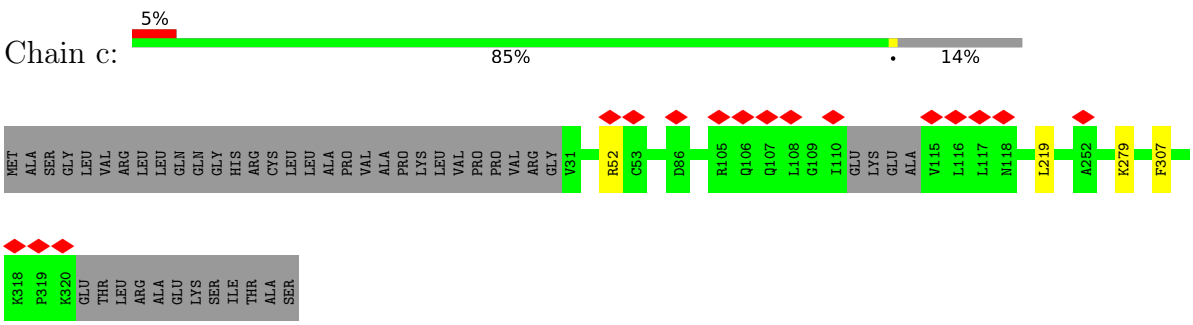


• Molecule 36: 39S ribosomal protein L43, mitochondrial

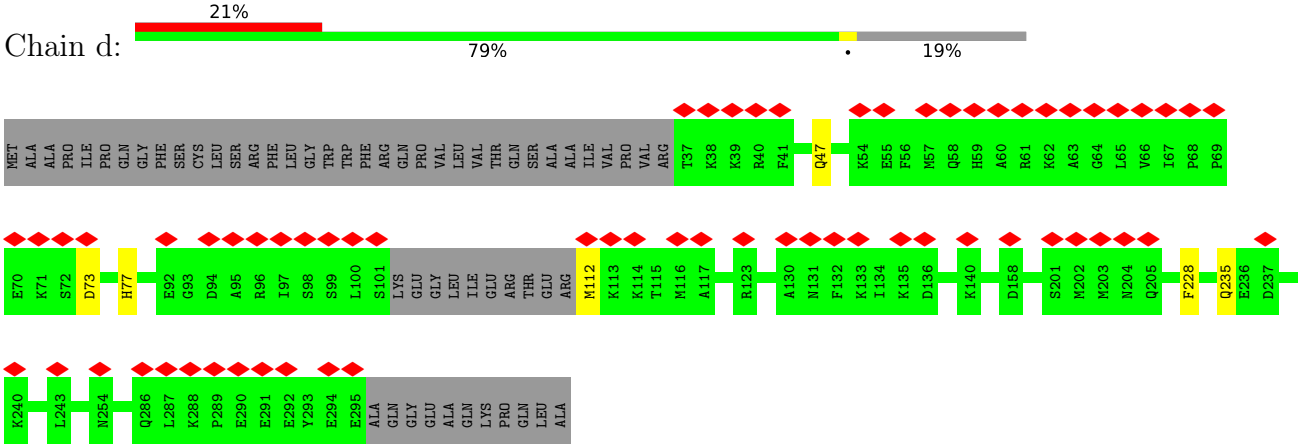
Chain b:



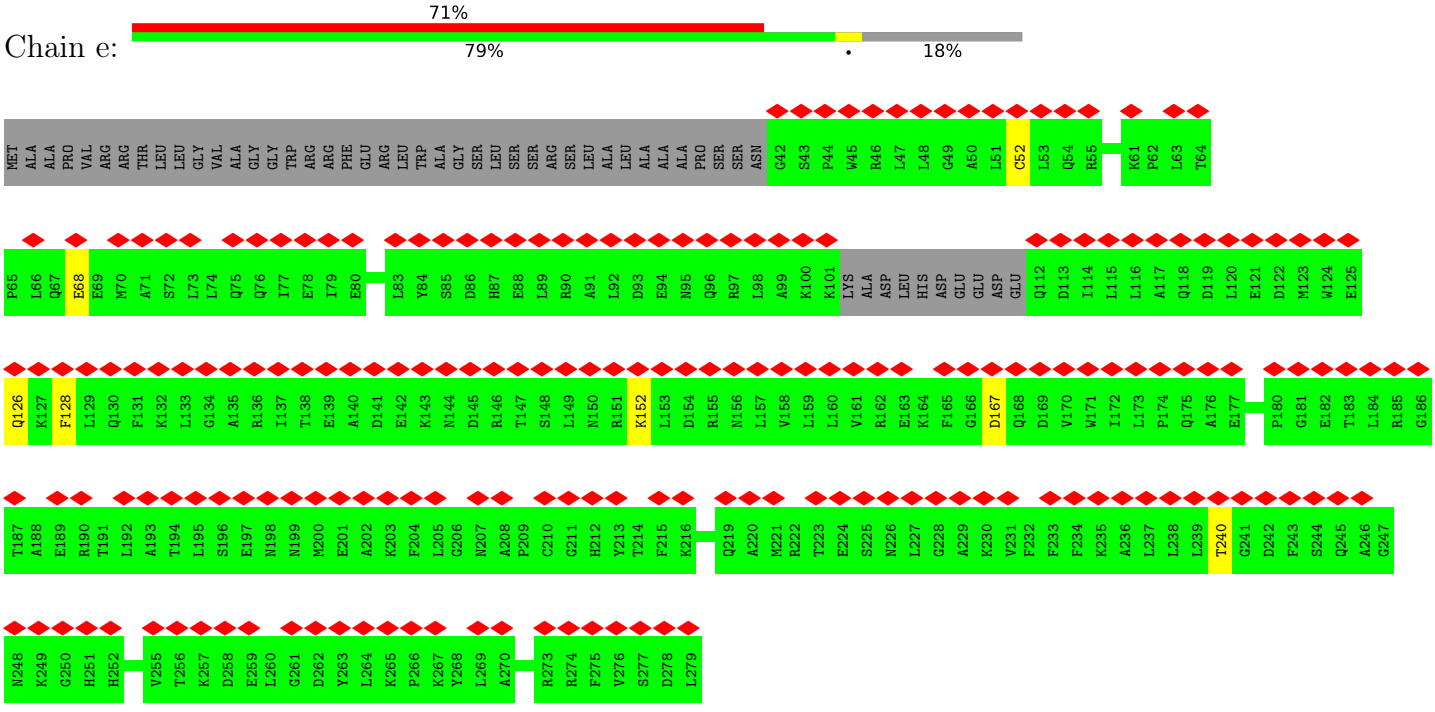
• Molecule 37: 39S ribosomal protein L44, mitochondrial



• Molecule 38: 39S ribosomal protein L45, mitochondrial



• Molecule 39: 39S ribosomal protein L46, mitochondrial

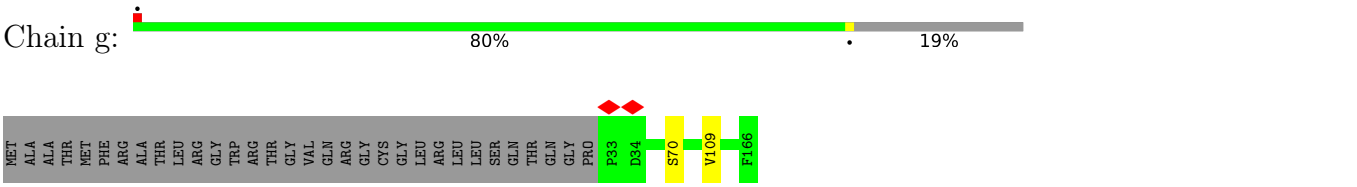


• Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f:

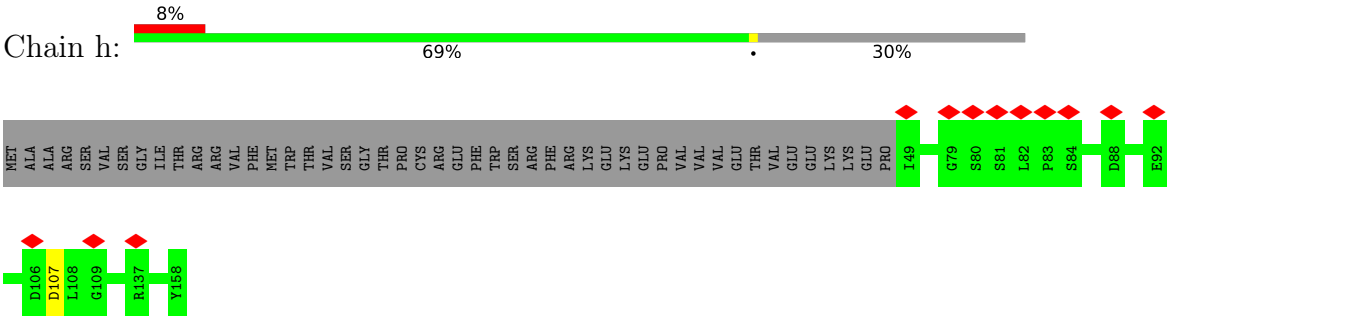
• Molecule 41: 39S ribosomal protein L49, mitochondrial

Chain g:



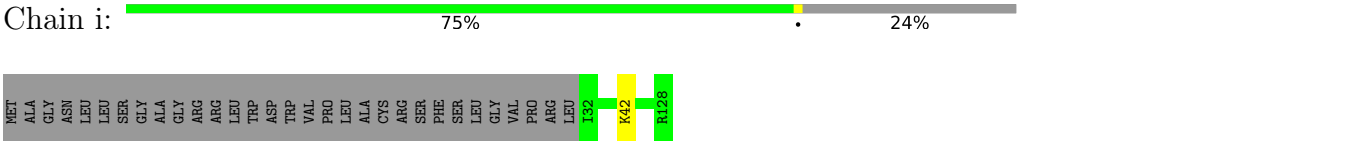
• Molecule 42: 39S ribosomal protein L50, mitochondrial

Chain h:



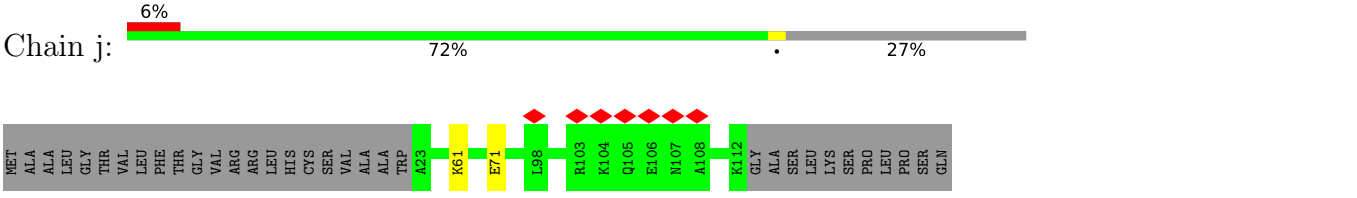
• Molecule 43: 39S ribosomal protein L51, mitochondrial

Chain i:



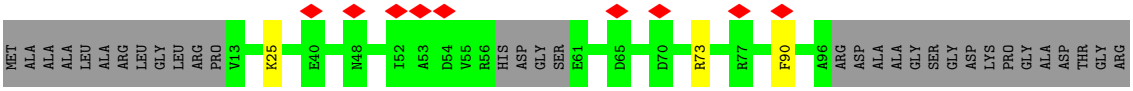
• Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain j:



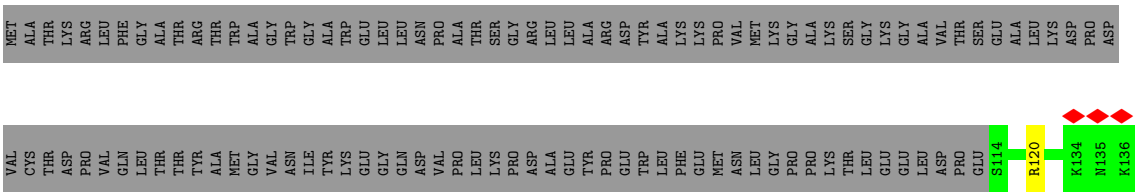
• Molecule 45: 39S ribosomal protein L53, mitochondrial

Chain k:



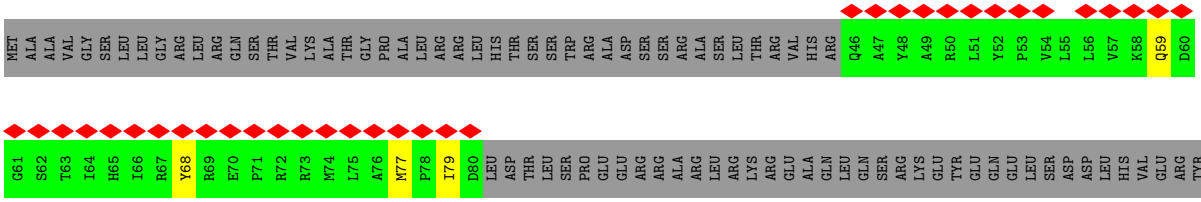
• Molecule 46: 39S ribosomal protein L54, mitochondrial

Chain l:



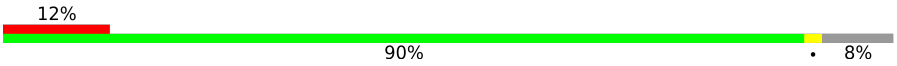
• Molecule 47: 39S ribosomal protein L55, mitochondrial

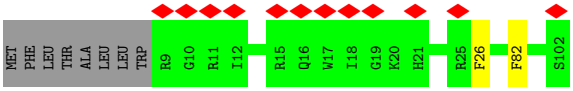
Chain m:



• Molecule 48: Ribosomal protein 63, mitochondrial

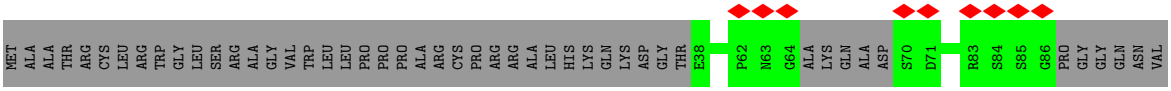
Chain o:





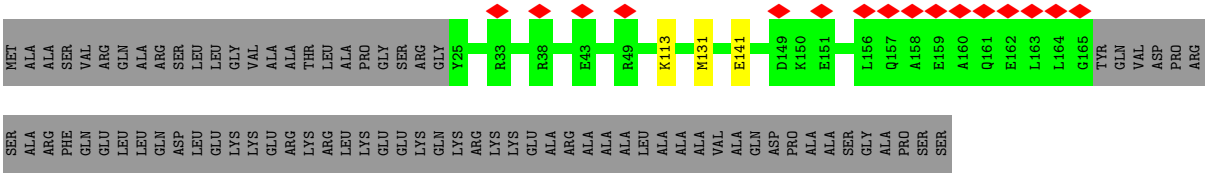
• Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



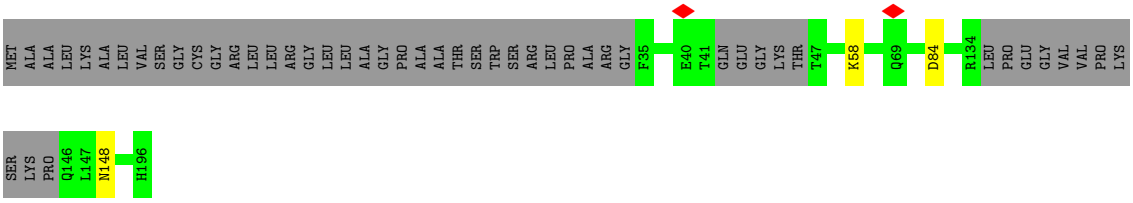
• Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



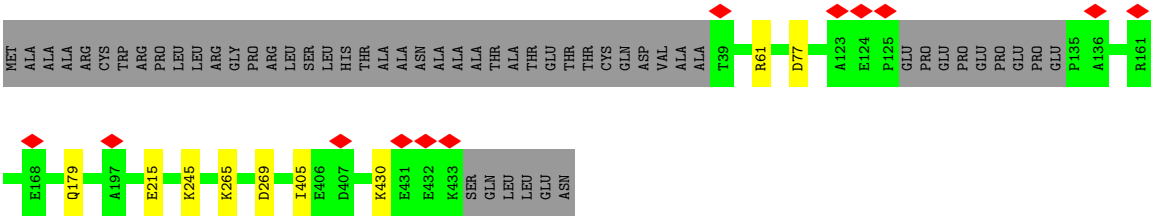
• Molecule 51: 39S ribosomal protein S18a, mitochondrial

Chain r:



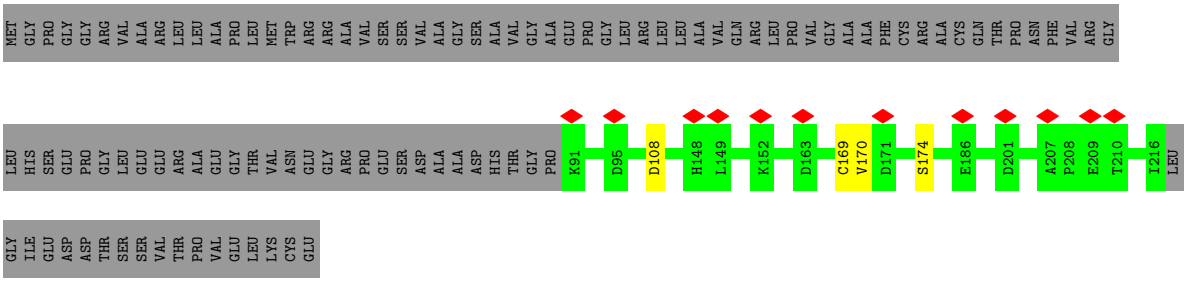
• Molecule 52: 39S ribosomal protein S30, mitochondrial

Chain s:



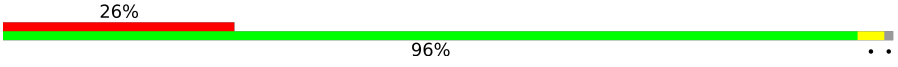
• Molecule 53: Mitochondrial assembly of ribosomal large subunit protein 1

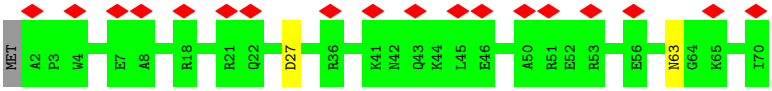
Chain u:



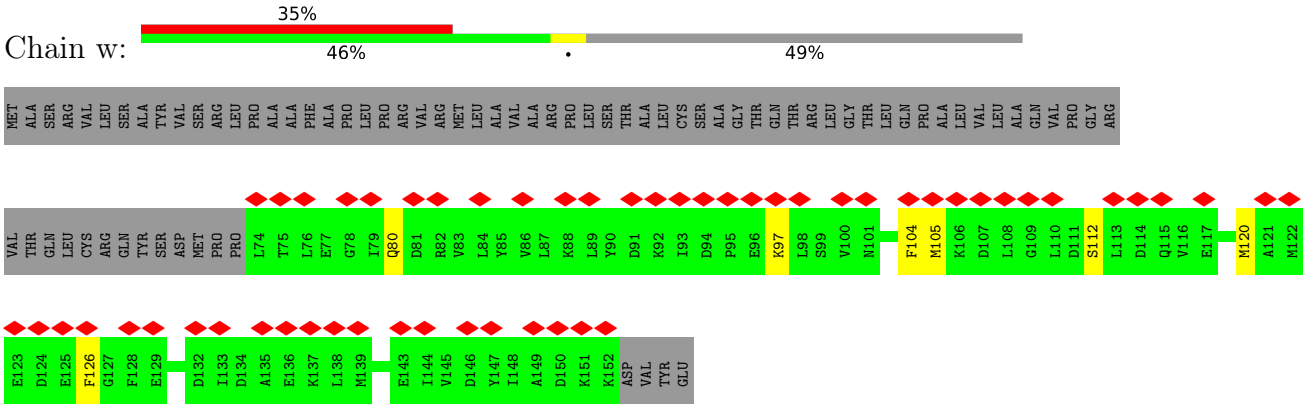
• Molecule 54: MIEF1 upstream open reading frame protein

Chain v:

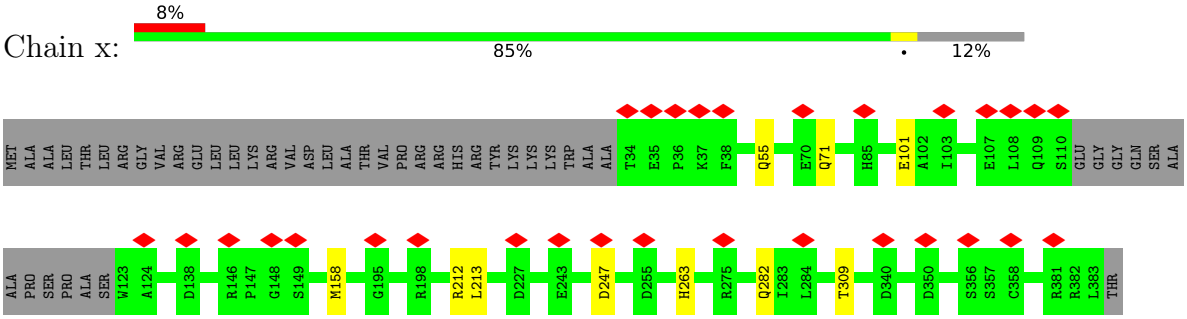




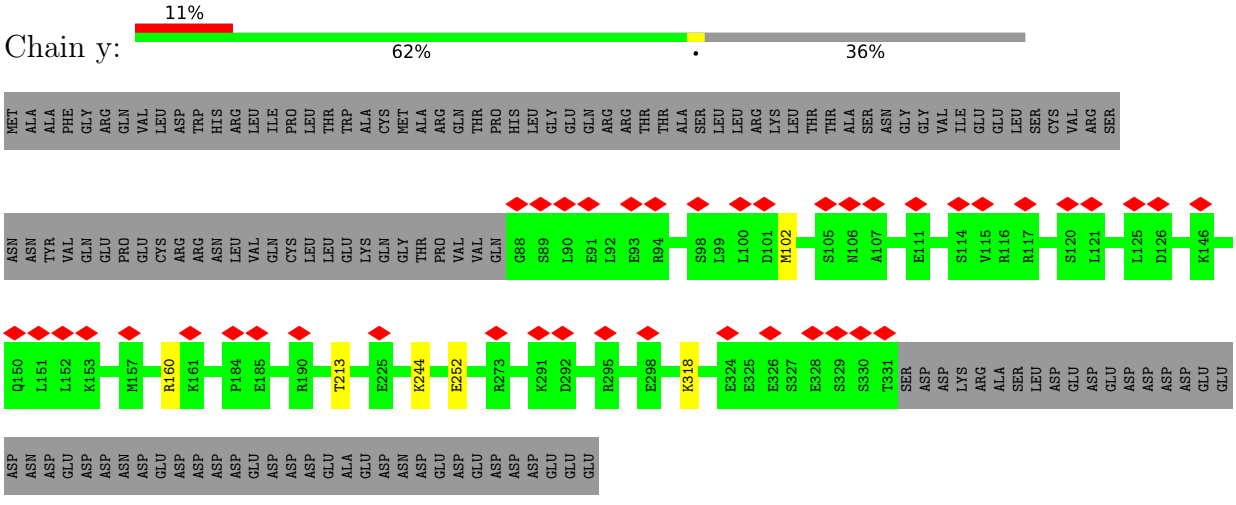
• Molecule 55: Acyl carrier protein, mitochondrial



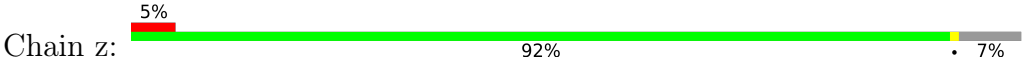
• Molecule 56: 5-methylcytosine rRNA methyltransferase NSUN4

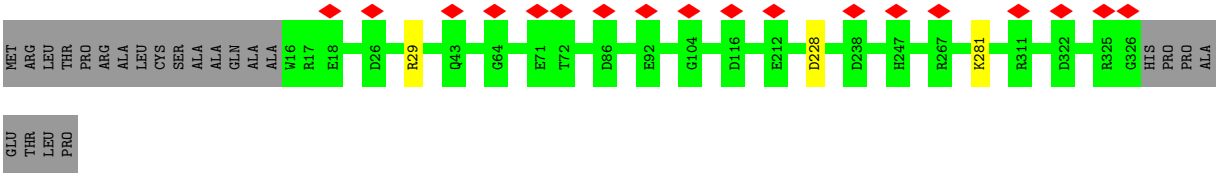


• Molecule 57: Transcription termination factor 4, mitochondrial



• Molecule 58: Mitochondrial ribosome-associated GTPase 1




MET
ARG
LEU
THR
PRO
ARG
ALA
LEU
CYS
SER
ALA
ALA
GLN
ALA
ALA
W16
R17
E18
D26
R29
Q43
G64
E71
T72
D86
E92
G104
D116
E212
D228
D238
H247
R267
K281
R311
D322
R325
G326
HIS
PRO
PRO
ALA
GLU
THR
LEU
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.009	Depositor
Minimum map value	-2.665	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.204	Depositor
Recommended contour level	0.814	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, THC, SAM, PM8, ZN, MG, AYA, GNP, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.24	0/913	0.50	0/1224
2	1	0.24	0/460	0.55	0/610
3	2	0.23	0/383	0.52	0/507
4	3	0.23	0/853	0.51	0/1136
5	4	0.24	0/341	0.57	0/451
6	5	0.24	0/3305	0.45	0/4502
7	6	0.24	0/3043	0.49	0/4140
8	7	0.24	0/2447	0.44	0/3310
9	8	0.25	0/880	0.52	0/1188
10	9	0.26	0/1025	0.48	0/1379
11	A	0.19	0/33679	0.76	16/52392 (0.0%)
12	B	0.30	1/1700 (0.1%)	0.73	0/2641
13	D	0.25	0/1910	0.55	0/2569
14	E	0.24	0/2475	0.44	0/3355
15	F	0.24	0/2090	0.48	0/2842
16	H	0.23	0/816	0.53	0/1097
17	I	0.26	0/1368	0.54	0/1849
18	J	0.24	0/1054	0.50	0/1419
19	K	0.24	0/1490	0.46	0/2021
20	L	0.24	0/905	0.53	0/1218
21	M	0.25	0/2381	0.50	0/3212
22	N	0.25	0/1624	0.52	0/2185
23	O	0.23	0/1283	0.51	0/1727
24	P	0.24	0/1199	0.53	0/1623
25	Q	0.24	0/1884	0.49	0/2535
26	R	0.24	0/1175	0.50	0/1572
27	S	0.24	0/1320	0.49	0/1789
28	T	0.25	0/1403	0.47	0/1886
29	U	0.25	0/1274	0.51	0/1723
30	V	0.24	0/1712	0.50	0/2322
31	W	0.24	0/857	0.48	0/1155
32	X	0.24	0/2099	0.44	0/2837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.23	0/1593	0.49	0/2136
34	Z	0.23	0/1021	0.46	0/1378
35	a	0.24	0/866	0.49	0/1174
36	b	0.24	0/1203	0.53	0/1627
37	c	0.24	0/2347	0.45	0/3171
38	d	0.25	0/2095	0.47	0/2834
39	e	0.24	0/1885	0.47	0/2542
40	f	0.24	0/1216	0.45	0/1638
41	g	0.25	0/1151	0.50	0/1569
42	h	0.24	0/918	0.47	0/1249
43	i	0.24	0/850	0.50	0/1135
44	j	0.24	0/737	0.48	0/992
45	k	0.25	0/635	0.52	0/855
46	l	0.22	0/226	0.56	0/299
47	m	0.25	0/298	0.59	0/402
48	o	0.23	0/819	0.52	0/1097
49	p	0.23	0/1223	0.50	0/1641
50	q	0.24	0/1208	0.51	0/1633
51	r	0.25	0/1238	0.53	0/1676
52	s	0.24	0/3239	0.48	0/4400
53	u	0.24	0/1069	0.48	0/1447
54	v	0.24	0/597	0.59	0/796
55	w	0.25	0/647	0.44	0/871
56	x	0.24	0/2737	0.46	0/3714
57	y	0.24	0/2011	0.47	0/2702
58	z	0.24	0/2484	0.49	0/3349
All	All	0.23	1/113661 (0.0%)	0.60	16/160743 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	8	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1602	C	OP3-P	-10.57	1.48	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1711	C	C2-N1-C1'	8.13	127.74	118.80
11	A	1711	C	N1-C2-O2	8.06	123.74	118.90
11	A	2840	C	C2-N1-C1'	7.37	126.91	118.80
11	A	1728	U	N3-C4-O4	7.33	124.53	119.40
11	A	1711	C	N3-C2-O2	-6.50	117.35	121.90
11	A	1728	U	C2-N1-C1'	6.04	124.94	117.70
11	A	1728	U	C5-C4-O4	-5.76	122.44	125.90
11	A	2840	C	C6-N1-C1'	-5.67	114.00	120.80
11	A	1711	C	C6-N1-C1'	-5.59	114.09	120.80
11	A	2495	U	C5-C6-N1	5.59	125.50	122.70
11	A	1728	U	C5-C6-N1	5.56	125.48	122.70
11	A	1711	C	C6-N1-C2	-5.37	118.15	120.30
11	A	2949	C	C2-N1-C1'	5.27	124.60	118.80
11	A	2495	U	C2-N1-C1'	5.22	123.96	117.70
11	A	2495	U	N3-C4-O4	5.10	122.97	119.40
11	A	2493	C	C2-N1-C1'	5.09	124.40	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	8	169	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	53/65 (82%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	35/103 (34%)	35 (100%)	0	0	100	100
6	5	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	100/206 (48%)	96 (96%)	4 (4%)	0	100	100
10	9	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
13	D	238/305 (78%)	235 (99%)	3 (1%)	0	100	100
14	E	303/348 (87%)	298 (98%)	5 (2%)	0	100	100
15	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
16	H	95/267 (36%)	95 (100%)	0	0	100	100
17	I	163/261 (62%)	151 (93%)	11 (7%)	1 (1%)	25	64
18	J	133/192 (69%)	120 (90%)	13 (10%)	0	100	100
19	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
20	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
21	M	289/296 (98%)	288 (100%)	1 (0%)	0	100	100
22	N	190/251 (76%)	181 (95%)	8 (4%)	1 (0%)	29	68
23	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
24	P	142/180 (79%)	142 (100%)	0	0	100	100
25	Q	219/292 (75%)	216 (99%)	3 (1%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
27	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
28	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
29	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
30	V	202/216 (94%)	200 (99%)	2 (1%)	0	100	100
31	W	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
32	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
33	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
34	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
35	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	b	147/215 (68%)	144 (98%)	3 (2%)	0	100	100
37	c	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
38	d	245/306 (80%)	239 (98%)	6 (2%)	0	100	100
39	e	224/279 (80%)	217 (97%)	7 (3%)	0	100	100
40	f	146/212 (69%)	139 (95%)	7 (5%)	0	100	100
41	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
42	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
43	i	95/128 (74%)	95 (100%)	0	0	100	100
44	j	88/123 (72%)	87 (99%)	1 (1%)	0	100	100
45	k	76/112 (68%)	74 (97%)	2 (3%)	0	100	100
46	l	21/138 (15%)	21 (100%)	0	0	100	100
47	m	33/128 (26%)	32 (97%)	1 (3%)	0	100	100
48	o	92/102 (90%)	92 (100%)	0	0	100	100
49	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
50	q	139/222 (63%)	139 (100%)	0	0	100	100
51	r	140/196 (71%)	132 (94%)	8 (6%)	0	100	100
52	s	382/439 (87%)	377 (99%)	5 (1%)	0	100	100
53	u	124/234 (53%)	121 (98%)	3 (2%)	0	100	100
54	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
55	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
56	x	334/384 (87%)	323 (97%)	11 (3%)	0	100	100
57	y	242/381 (64%)	240 (99%)	2 (1%)	0	100	100
58	z	309/334 (92%)	301 (97%)	8 (3%)	0	100	100
All	All	9251/12228 (76%)	9060 (98%)	189 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	N	66	PRO
17	I	66	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	99/164 (60%)	96 (97%)	3 (3%)	41 75
2	1	52/60 (87%)	51 (98%)	1 (2%)	57 84
3	2	40/72 (56%)	40 (100%)	0	100 100
4	3	88/166 (53%)	88 (100%)	0	100 100
5	4	36/89 (40%)	36 (100%)	0	100 100
6	5	353/368 (96%)	347 (98%)	6 (2%)	60 85
7	6	313/332 (94%)	308 (98%)	5 (2%)	62 86
8	7	270/303 (89%)	268 (99%)	2 (1%)	84 94
9	8	93/190 (49%)	88 (95%)	5 (5%)	22 57
10	9	104/112 (93%)	103 (99%)	1 (1%)	76 91
13	D	194/245 (79%)	192 (99%)	2 (1%)	76 91
14	E	260/290 (90%)	257 (99%)	3 (1%)	71 90
15	F	219/262 (84%)	216 (99%)	3 (1%)	67 88
16	H	88/228 (39%)	86 (98%)	2 (2%)	50 80
17	I	153/232 (66%)	143 (94%)	10 (6%)	17 50
18	J	112/150 (75%)	106 (95%)	6 (5%)	22 57
19	K	154/155 (99%)	149 (97%)	5 (3%)	39 74
20	L	98/124 (79%)	98 (100%)	0	100 100
21	M	246/249 (99%)	242 (98%)	4 (2%)	62 86
22	N	167/211 (79%)	163 (98%)	4 (2%)	49 79
23	O	134/150 (89%)	132 (98%)	2 (2%)	65 87
24	P	126/155 (81%)	121 (96%)	5 (4%)	31 68
25	Q	203/256 (79%)	200 (98%)	3 (2%)	65 87
26	R	118/126 (94%)	118 (100%)	0	100 100
27	S	146/180 (81%)	142 (97%)	4 (3%)	44 77
28	T	146/176 (83%)	144 (99%)	2 (1%)	67 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	U	134/135 (99%)	131 (98%)	3 (2%)	52 81
30	V	182/191 (95%)	178 (98%)	4 (2%)	52 81
31	W	86/119 (72%)	84 (98%)	2 (2%)	50 80
32	X	220/229 (96%)	215 (98%)	5 (2%)	50 80
33	Y	163/223 (73%)	160 (98%)	3 (2%)	59 85
34	Z	113/147 (77%)	111 (98%)	2 (2%)	59 85
35	a	96/133 (72%)	94 (98%)	2 (2%)	53 82
36	b	130/185 (70%)	125 (96%)	5 (4%)	33 69
37	c	251/288 (87%)	247 (98%)	4 (2%)	62 86
38	d	228/274 (83%)	222 (97%)	6 (3%)	46 78
39	e	198/236 (84%)	191 (96%)	7 (4%)	36 71
40	f	133/188 (71%)	127 (96%)	6 (4%)	27 64
41	g	124/148 (84%)	122 (98%)	2 (2%)	62 86
42	h	104/148 (70%)	103 (99%)	1 (1%)	76 91
43	i	86/110 (78%)	85 (99%)	1 (1%)	71 90
44	j	72/97 (74%)	70 (97%)	2 (3%)	43 77
45	k	71/90 (79%)	68 (96%)	3 (4%)	30 66
46	l	23/116 (20%)	22 (96%)	1 (4%)	29 66
47	m	31/113 (27%)	27 (87%)	4 (13%)	4 19
48	o	80/87 (92%)	78 (98%)	2 (2%)	47 79
49	p	135/181 (75%)	130 (96%)	5 (4%)	34 70
50	q	119/178 (67%)	116 (98%)	3 (2%)	47 79
51	r	133/169 (79%)	130 (98%)	3 (2%)	50 80
52	s	340/381 (89%)	331 (97%)	9 (3%)	46 78
53	u	118/200 (59%)	114 (97%)	4 (3%)	37 72
54	v	59/60 (98%)	57 (97%)	2 (3%)	37 72
55	w	73/136 (54%)	66 (90%)	7 (10%)	8 32
56	x	293/328 (89%)	283 (97%)	10 (3%)	37 72
57	y	226/350 (65%)	220 (97%)	6 (3%)	44 77
58	z	270/287 (94%)	267 (99%)	3 (1%)	73 90
All	All	8303/10572 (78%)	8108 (98%)	195 (2%)	53 80

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	98	GLN
1	0	166	SER
1	0	185	PHE
2	1	65	LEU
6	5	63	LYS
6	5	203	CYS
6	5	256	PHE
6	5	264	ASP
6	5	268	CYS
6	5	401	VAL
7	6	64	GLU
7	6	102	GLN
7	6	116	ASN
7	6	217	LEU
7	6	298	PHE
8	7	187	SER
8	7	221	VAL
9	8	107	THR
9	8	113	ARG
9	8	143	GLN
9	8	173	LYS
9	8	178	TYR
10	9	110	ASP
13	D	124	GLU
13	D	180	ASP
14	E	207	THR
14	E	261	MET
14	E	326	GLU
15	F	76	ARG
15	F	106	PHE
15	F	190	MET
16	H	96	LEU
16	H	117	SER
17	I	40	MET
17	I	61	HIS
17	I	63	SER
17	I	65	LEU
17	I	67	SER
17	I	90	PHE
17	I	91	GLN
17	I	108	ASP
17	I	114	HIS

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Mol	Chain	Res	Type
17	I	164	MET
18	J	25	ARG
18	J	51	LYS
18	J	53	PHE
18	J	61	LYS
18	J	62	GLU
18	J	89	TYR
19	K	47	TYR
19	K	60	MET
19	K	114	LYS
19	K	174	GLU
19	K	177	ARG
21	M	99	ASN
21	M	147	THR
21	M	218	LYS
21	M	222	TYR
22	N	54	GLU
22	N	101	HIS
22	N	247	MET
22	N	249	LYS
23	O	98	LYS
23	O	101	THR
24	P	69	ARG
24	P	83	VAL
24	P	132	LEU
24	P	137	LEU
24	P	142	ASN
25	Q	95	GLU
25	Q	252	GLN
25	Q	269	MET
27	S	47	LEU
27	S	89	THR
27	S	107	LYS
27	S	166	SER
28	T	79	ASP
28	T	181	GLU
29	U	3	ARG
29	U	62	ASN
29	U	86	ARG
30	V	53	ASP
30	V	76	VAL
30	V	78	GLN

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Mol	Chain	Res	Type
30	V	131	THR
31	W	49	ARG
31	W	50	ARG
32	X	31	SER
32	X	33	GLU
32	X	125	VAL
32	X	142	ASP
32	X	241	GLN
33	Y	72	LYS
33	Y	195	ASN
33	Y	206	ASP
34	Z	52	ASP
34	Z	87	LYS
35	a	64	SER
35	a	115	MET
36	b	27	GLN
36	b	36	ASP
36	b	106	ASP
36	b	111	ASP
36	b	148	VAL
37	c	52	ARG
37	c	219	LEU
37	c	279	LYS
37	c	307	PHE
38	d	47	GLN
38	d	73	ASP
38	d	77	HIS
38	d	112	MET
38	d	228	PHE
38	d	235	GLN
39	e	52	CYS
39	e	68	GLU
39	e	126	GLN
39	e	128	PHE
39	e	152	LYS
39	e	167	ASP
39	e	240	THR
40	f	84	THR
40	f	124	SER
40	f	125	TYR
40	f	168	GLU
40	f	187	LYS

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Mol	Chain	Res	Type
40	f	194	PHE
41	g	70	SER
41	g	109	VAL
42	h	107	ASP
43	i	42	LYS
44	j	61	LYS
44	j	71	GLU
45	k	25	LYS
45	k	73	ARG
45	k	90	PHE
46	l	120	ARG
47	m	59	GLN
47	m	68	TYR
47	m	77	MET
47	m	79	ILE
48	o	26	PHE
48	o	82	PHE
49	p	116	ARG
49	p	122	THR
49	p	124	LYS
49	p	125	ASN
49	p	190	GLN
50	q	113	LYS
50	q	131	MET
50	q	141	GLU
51	r	58	LYS
51	r	84	ASP
51	r	148	ASN
52	s	61	ARG
52	s	77	ASP
52	s	179	GLN
52	s	215	GLU
52	s	245	LYS
52	s	265	LYS
52	s	269	ASP
52	s	405	ILE
52	s	430	LYS
53	u	108	ASP
53	u	169	CYS
53	u	170	VAL
53	u	174	SER
54	v	27	ASP

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Mol	Chain	Res	Type
54	v	63	ASN
55	w	80	GLN
55	w	97	LYS
55	w	104	PHE
55	w	105	MET
55	w	112	SER
55	w	120	MET
55	w	126	PHE
56	x	55	GLN
56	x	71	GLN
56	x	101	GLU
56	x	158	MET
56	x	212	ARG
56	x	213	LEU
56	x	247	ASP
56	x	263	HIS
56	x	282	GLN
56	x	309	THR
57	y	102	MET
57	y	160	ARG
57	y	213	THR
57	y	244	LYS
57	y	252	GLU
57	y	318	LYS
58	z	29	ARG
58	z	228	ASP
58	z	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	83	ASN
5	4	68	ASN
7	6	239	ASN
7	6	275	GLN
15	F	103	GLN
17	I	93	ASN
18	J	48	GLN
22	N	98	HIS
38	d	211	GLN
49	p	176	HIS
50	q	142	ASN

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Mol	Chain	Res	Type
54	v	42	ASN
56	x	78	ASN
56	x	193	GLN
57	y	110	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1401/1603 (87%)	260 (18%)	5 (0%)
12	B	71/72 (98%)	11 (15%)	0
All	All	1472/1675 (87%)	271 (18%)	5 (0%)

All (271) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1681	G
11	A	1689	C
11	A	1694	U
11	A	1700	U
11	A	1704	U
11	A	1707	C
11	A	1708	A
11	A	1711	C
11	A	1713	A
11	A	1715	C
11	A	1724	A
11	A	1727	A
11	A	1731	A
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1762	A
11	A	1764	C
11	A	1765	C
11	A	1766	U
11	A	1767	G
11	A	1770	G
11	A	1777	A
11	A	1780	U

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Mol	Chain	Res	Type
11	A	1791	G
11	A	1804	A
11	A	1805	A
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1853	A
11	A	1854	U
11	A	1855	A
11	A	1869	A
11	A	1871	A
11	A	1882	A
11	A	1883	G
11	A	1887	A
11	A	1892	A
11	A	1893	A
11	A	1901	C
11	A	1903	C
11	A	1918	G
11	A	1937	A
11	A	1940	A
11	A	1974	A
11	A	1984	A
11	A	1985	G
11	A	1986	A
11	A	1987	G
11	A	1992	C
11	A	1994	A
11	A	2000	C
11	A	2002	G
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2029	A
11	A	2030	U
11	A	2031	A
11	A	2036	C
11	A	2037	U
11	A	2039	A

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Mol	Chain	Res	Type
11	A	2060	A
11	A	2065	A
11	A	2068	C
11	A	2069	U
11	A	2071	U
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2098	G
11	A	2105	G
11	A	2109	A
11	A	2110	A
11	A	2111	C
11	A	2125	C
11	A	2126	U
11	A	2147	G
11	A	2154	A
11	A	2158	U
11	A	2163	A
11	A	2168	U
11	A	2171	U
11	A	2172	A
11	A	2173	G
11	A	2174	G
11	A	2181	A
11	A	2182	G
11	A	2183	C
11	A	2184	A
11	A	2187	C
11	A	2197	G
11	A	2198	A
11	A	2200	A
11	A	2202	C
11	A	2210	C
11	A	2211	U
11	A	2216	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2245	A
11	A	2246	A

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Mol	Chain	Res	Type
11	A	2260	A
11	A	2262	C
11	A	2263	C
11	A	2269	G
11	A	2283	C
11	A	2284	C
11	A	2285	U
11	A	2293	A
11	A	2297	A
11	A	2299	U
11	A	2300	G
11	A	2316	U
11	A	2322	C
11	A	2332	C
11	A	2345	G
11	A	2359	C
11	A	2360	U
11	A	2361	G
11	A	2362	A
11	A	2363	A
11	A	2374	A
11	A	2381	A
11	A	2390	A
11	A	2393	C
11	A	2396	C
11	A	2401	A
11	A	2405	C
11	A	2406	A
11	A	2407	U
11	A	2415	C
11	A	2416	U
11	A	2432	A
11	A	2444	A
11	A	2446	A
11	A	2449	G
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2480	A
11	A	2485	U
11	A	2493	C
11	A	2500	A

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Mol	Chain	Res	Type
11	A	2502	C
11	A	2507	A
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2523	C
11	A	2527	A
11	A	2531	U
11	A	2540	C
11	A	2640	C
11	A	2645	G
11	A	2654	U
11	A	2656	U
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2693	A
11	A	2694	A
11	A	2695	G
11	A	2696	A
11	A	2706	A
11	A	2718	C
11	A	2719	G
11	A	2722	A
11	A	2724	G
11	A	2727	C
11	A	2732	G
11	A	2745	A
11	A	2750	U
11	A	2801	A
11	A	2810	G
11	A	2811	G
11	A	2814	G
11	A	2830	A
11	A	2832	A
11	A	2833	A
11	A	2839	C
11	A	2840	C
11	A	2841	U
11	A	2842	C
11	A	2844	G
11	A	2847	C

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Mol	Chain	Res	Type
11	A	2854	U
11	A	2864	U
11	A	2865	C
11	A	2895	U
11	A	2906	C
11	A	2910	A
11	A	2913	A
11	A	2916	G
11	A	2917	G
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2935	A
11	A	2936	U
11	A	2939	C
11	A	2947	U
11	A	2948	C
11	A	2949	C
11	A	2950	U
11	A	2956	A
11	A	2963	A
11	A	2977	G
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3021	C
11	A	3047	G
11	A	3053	A
11	A	3054	G
11	A	3056	C
11	A	3059	A
11	A	3060	C
11	A	3061	G
11	A	3069	A
11	A	3072	U
11	A	3073	C
11	A	3086	U
11	A	3090	G
11	A	3097	U

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Mol	Chain	Res	Type
11	A	3100	U
11	A	3101	A
11	A	3102	U
11	A	3108	U
11	A	3112	A
11	A	3113	A
11	A	3129	A
11	A	3131	G
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3169	C
11	A	3172	C
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3197	U
11	A	3207	A
11	A	3208	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3228	U
12	B	1611	G
12	B	1617	C
12	B	1621	A
12	B	1646	U
12	B	1647	U
12	B	1649	C
12	B	1650	A
12	B	1652	C
12	B	1653	U
12	B	1654	U
12	B	1656	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2030	U
11	A	2186	C
11	A	2245	A

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Mol	Chain	Res	Type
11	A	2530	A
11	A	2905	A

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

3 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	$\#\|Z\| > 2$
19	SAC	K	2	19	7,8,9	1.01	0	8,9,11	0.85	1 (12%)
29	AYA	U	2	29	6,7,8	1.27	1 (16%)	5,8,10	1.18	1 (20%)
36	THC	b	2	36	8,9,10	1.07	1 (12%)	9,11,13	0.78	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
19	SAC	K	2	19	-	3/7/8/10	-
29	AYA	U	2	29	-	0/4/6/8	-
36	THC	b	2	36	-	0/8/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	U	2	AYA	CA-N	-2.44	1.44	1.46
36	b	2	THC	CA-N1	-2.15	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	U	2	AYA	CB-CA-N	2.42	112.30	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	2	SAC	OG-CB-CA	-2.01	105.84	110.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	2	SAC	O-C-CA-CB
19	K	2	SAC	N-CA-CB-OG
19	K	2	SAC	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 40 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
64	GNP	z	401	60	29,34,34	1.60	7 (24%)	33,54,54	2.13	6 (18%)
63	SAM	x	401	-	24,29,29	1.21	3 (12%)	23,42,42	1.58	4 (17%)
62	PM8	w	200	55	25,31,31	1.90	6 (24%)	30,38,38	1.75	6 (20%)
61	FES	r	201	51	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
64	GNP	z	401	60	-	4/14/38/38	0/3/3/3
63	SAM	x	401	-	-	4/12/33/33	0/3/3/3
62	PM8	w	200	55	-	13/36/38/38	-
61	FES	r	201	51	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	w	200	PM8	C34-N36	5.77	1.46	1.33
62	w	200	PM8	C39-N41	5.32	1.45	1.33
64	z	401	GNP	PB-O3A	4.29	1.64	1.59
63	x	401	SAM	C2-N3	4.01	1.38	1.32
64	z	401	GNP	C6-N1	3.09	1.38	1.33
64	z	401	GNP	PB-O1B	3.04	1.51	1.46
64	z	401	GNP	PG-N3B	3.03	1.71	1.63
64	z	401	GNP	PG-O1G	2.71	1.50	1.46
62	w	200	PM8	C1-S1	2.44	1.82	1.76
63	x	401	SAM	C2-N1	2.38	1.38	1.33
64	z	401	GNP	PB-O2B	-2.27	1.50	1.56
62	w	200	PM8	C2-C1	2.27	1.53	1.50
62	w	200	PM8	O40-C39	-2.23	1.18	1.23
62	w	200	PM8	O35-C34	-2.17	1.19	1.23
63	x	401	SAM	OXT-C	-2.16	1.23	1.30
64	z	401	GNP	C5-C6	2.03	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	z	401	GNP	C5-C6-N1	-8.42	111.92	123.43
62	w	200	PM8	C2-C1-S1	5.93	120.36	113.46
64	z	401	GNP	C2-N1-C6	5.84	125.21	115.93
63	x	401	SAM	N3-C2-N1	-5.31	120.38	128.68
62	w	200	PM8	O1-C1-C2	-3.40	119.97	123.99
63	x	401	SAM	C3'-C2'-C1'	3.15	105.72	100.98
64	z	401	GNP	PB-O3A-PA	-3.08	121.76	132.62
62	w	200	PM8	C37-C38-C39	2.90	117.19	112.36
64	z	401	GNP	N3-C2-N1	-2.79	123.50	127.22
62	w	200	PM8	C38-C39-N41	2.70	120.96	116.42
63	x	401	SAM	OXT-C-O	-2.66	118.05	124.09
64	z	401	GNP	C4-C5-C6	-2.55	118.37	120.80
62	w	200	PM8	C43-S1-C1	2.28	108.98	101.87
62	w	200	PM8	O1-C1-S1	-2.27	119.67	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	x	401	SAM	OXT-C-CA	2.22	120.94	113.38
64	z	401	GNP	C2-N3-C4	-2.17	112.88	115.36

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	w	200	PM8	O27-C28-C29-C32
62	w	200	PM8	C32-C34-N36-C37
62	w	200	PM8	N36-C37-C38-C39
62	w	200	PM8	N41-C42-C43-S1
62	w	200	PM8	C42-C43-S1-C1
63	x	401	SAM	CB-CG-SD-C5'
64	z	401	GNP	PG-N3B-PB-O1B
64	z	401	GNP	PG-N3B-PB-O3A
64	z	401	GNP	PA-O3A-PB-O1B
64	z	401	GNP	PA-O3A-PB-O2B
62	w	200	PM8	C38-C39-N41-C42
62	w	200	PM8	O35-C34-N36-C37
62	w	200	PM8	O40-C39-N41-C42
62	w	200	PM8	O27-C28-C29-C30
62	w	200	PM8	O27-C28-C29-C31
63	x	401	SAM	CB-CG-SD-CE
62	w	200	PM8	C3-C4-C5-C6
63	x	401	SAM	C-CA-CB-CG
62	w	200	PM8	O33-C32-C34-O35
63	x	401	SAM	N-CA-CB-CG
62	w	200	PM8	C5-C6-C7-C8

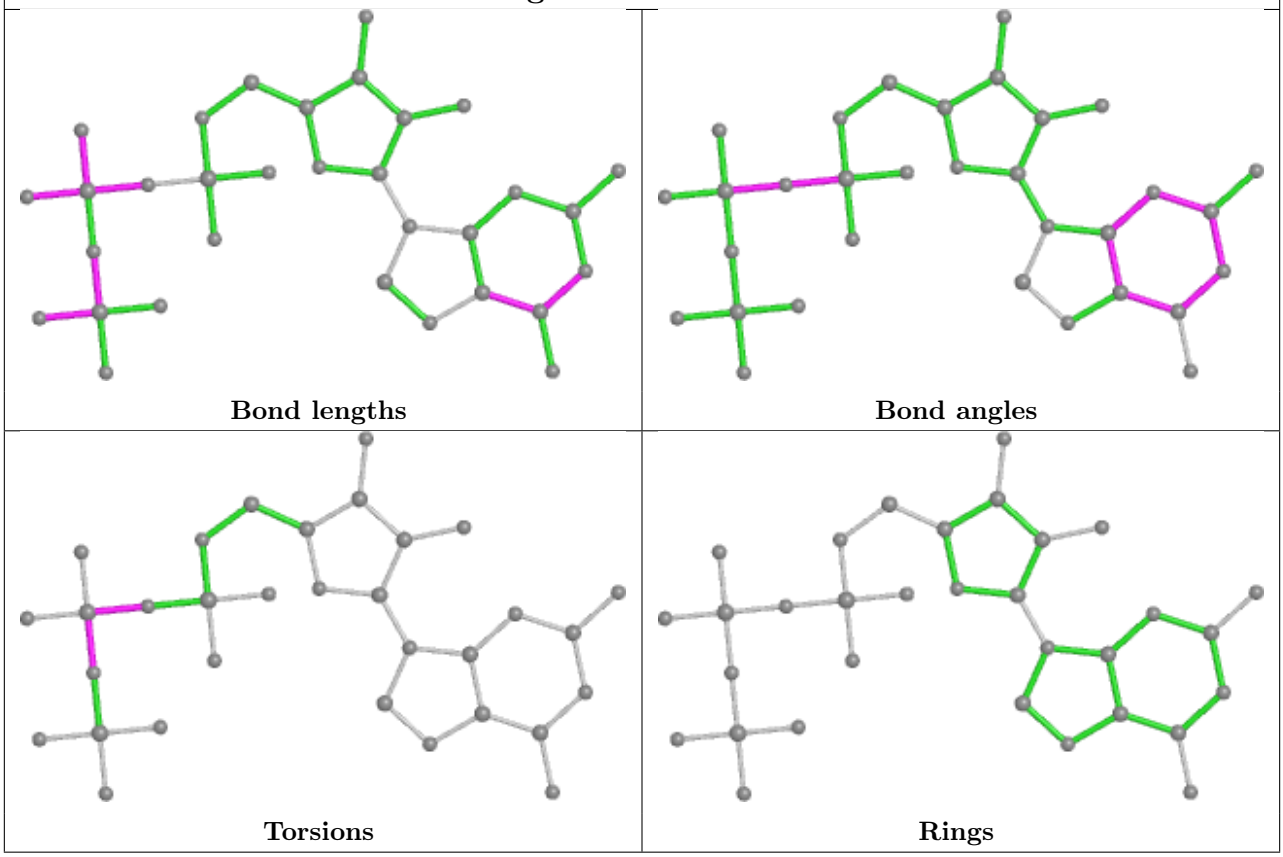
There are no ring outliers.

No monomer is involved in short contacts.

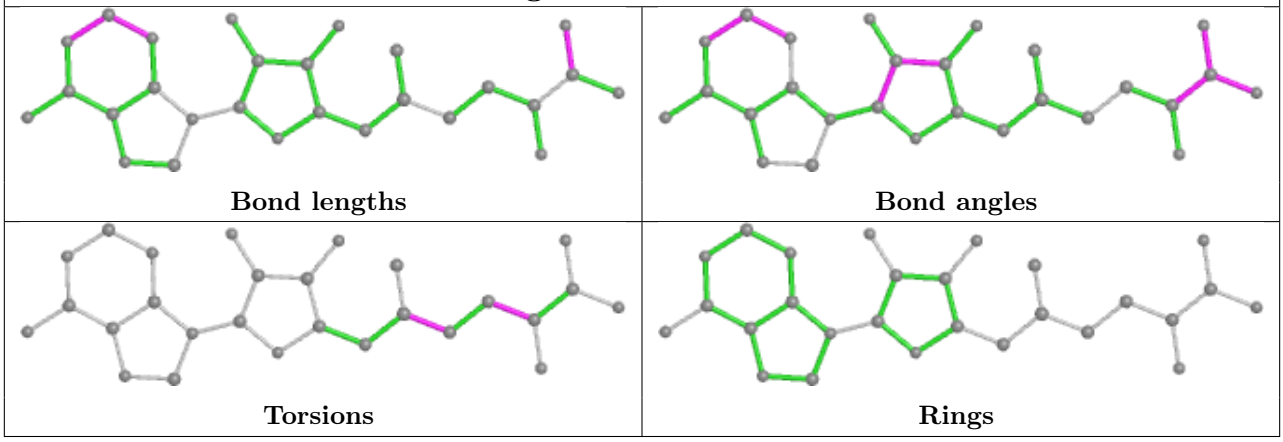
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

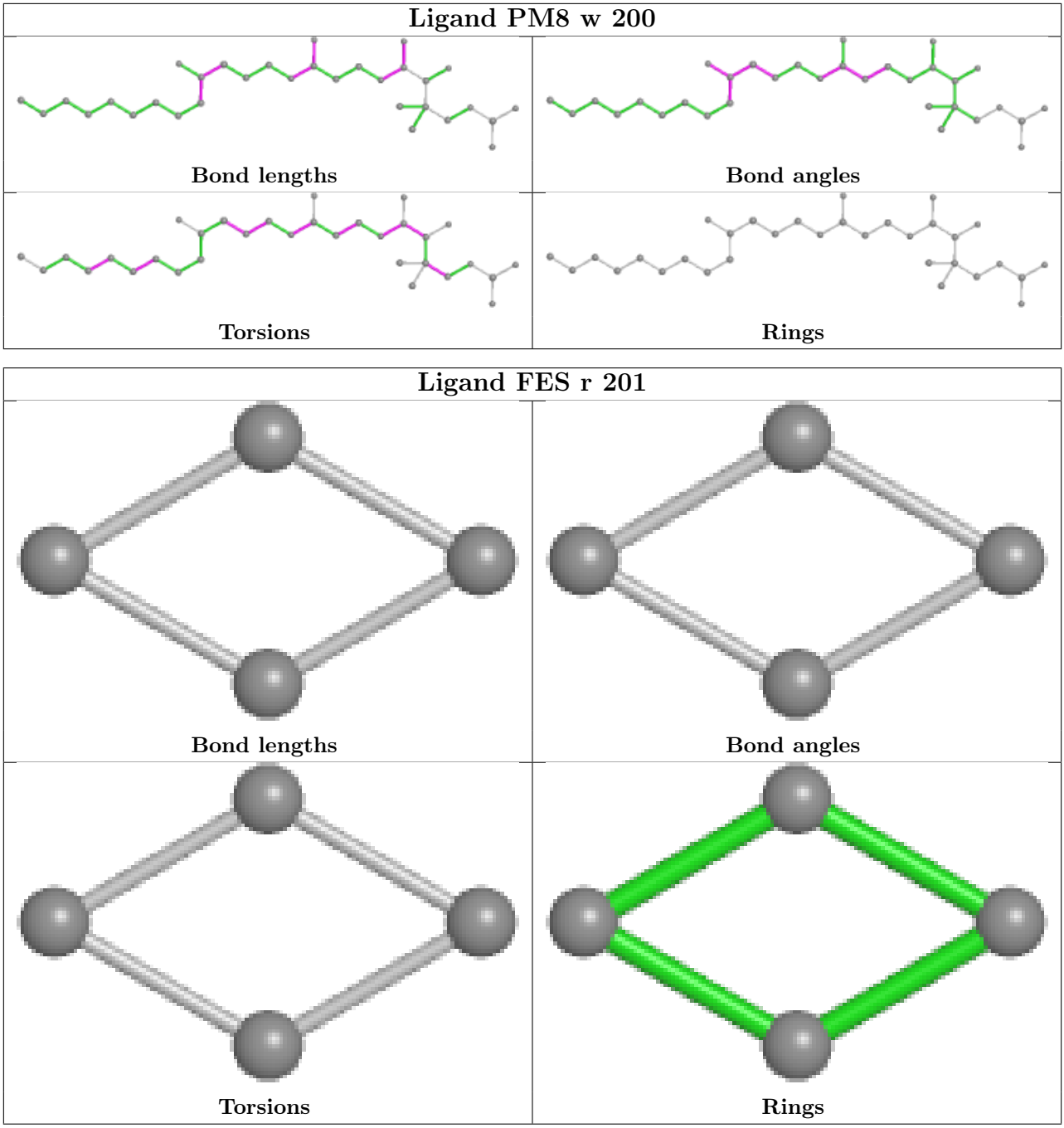
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP z 401



Ligand SAM x 401





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

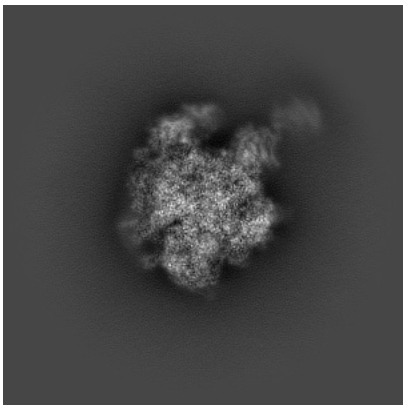
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17720. These allow visual inspection of the internal detail of the map and identification of artifacts.

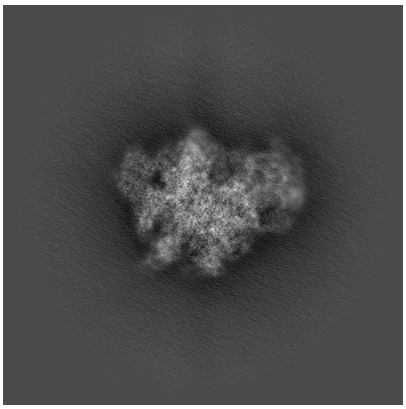
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

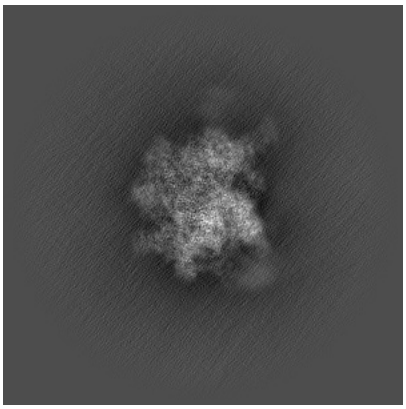
6.1.1 Primary map



X

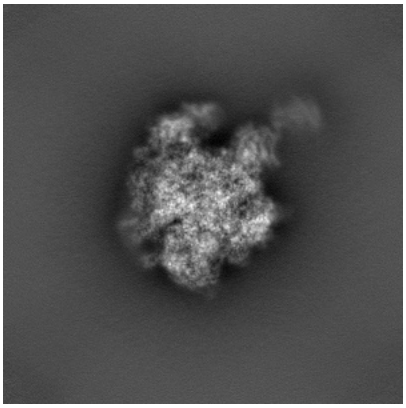


Y

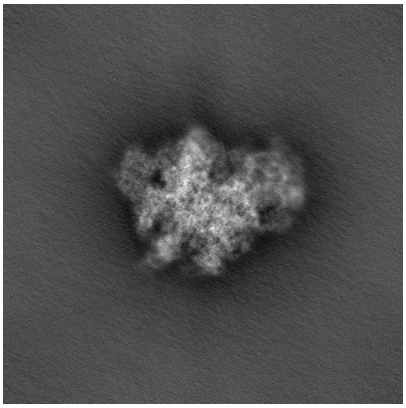


Z

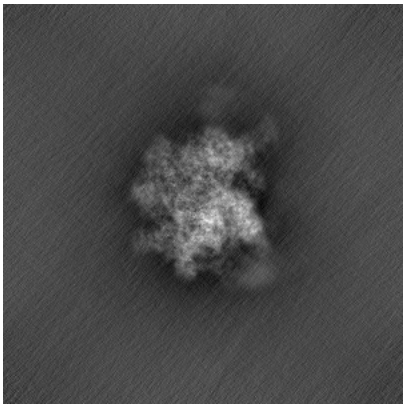
6.1.2 Raw map



X



Y

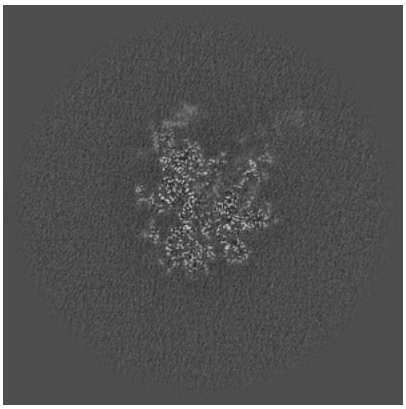


Z

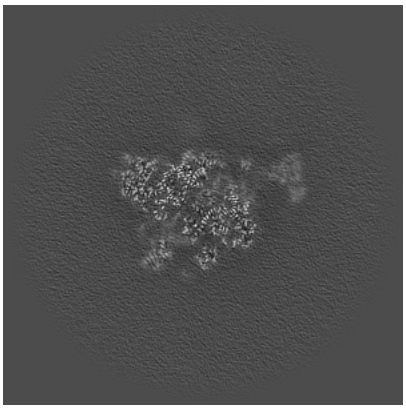
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

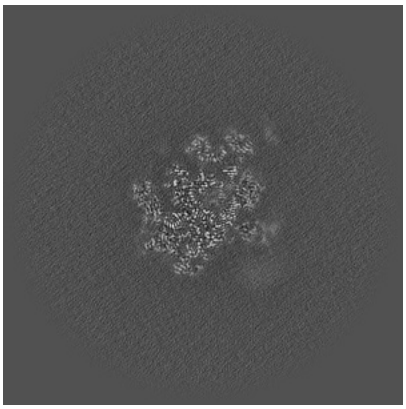
6.2.1 Primary map



X Index: 240

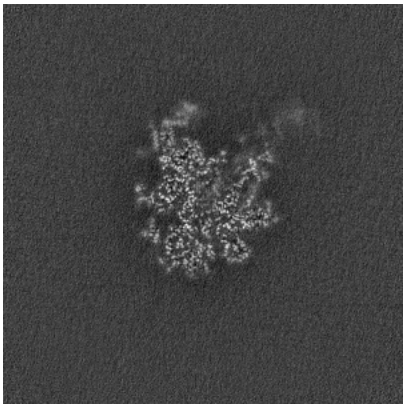


Y Index: 240

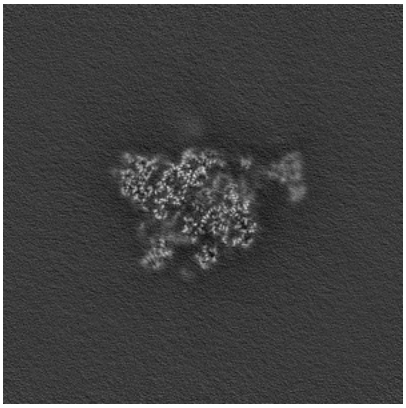


Z Index: 240

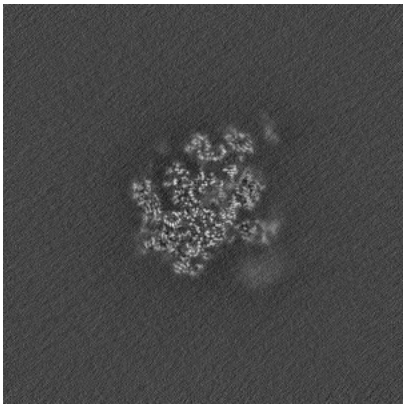
6.2.2 Raw map



X Index: 240



Y Index: 240

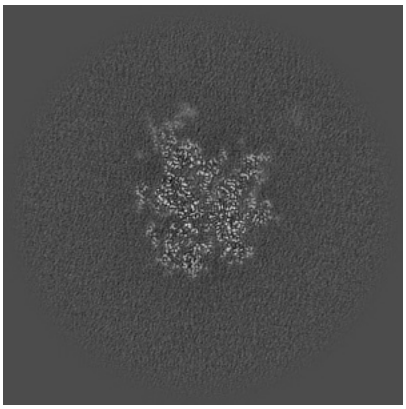


Z Index: 240

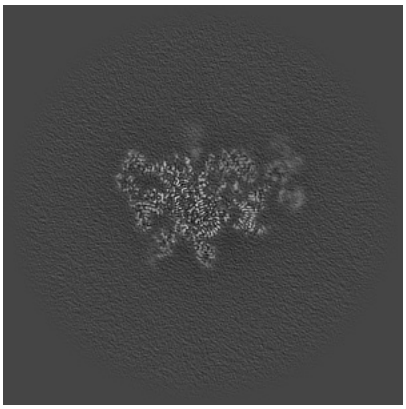
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

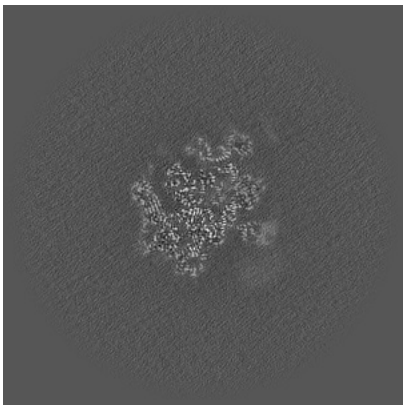
6.3.1 Primary map



X Index: 237

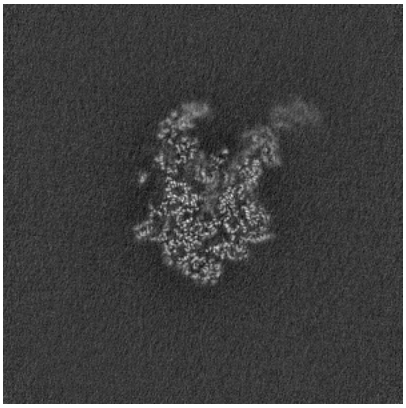


Y Index: 226

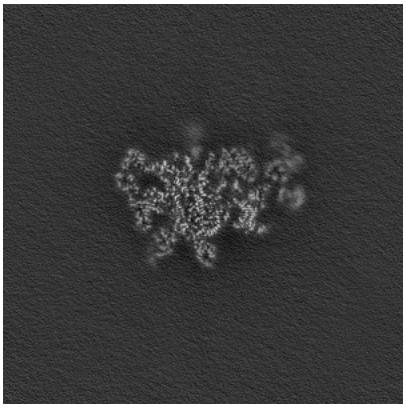


Z Index: 242

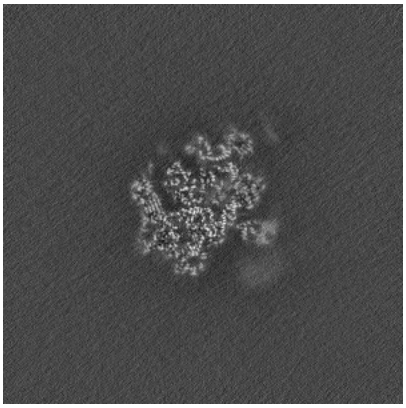
6.3.2 Raw map



X Index: 250



Y Index: 226

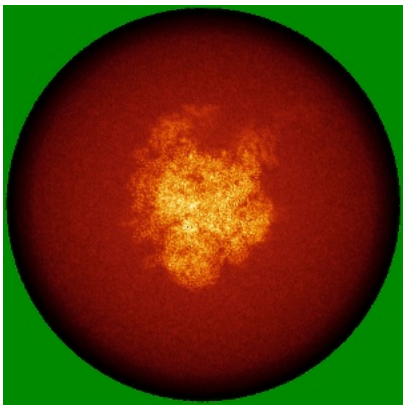


Z Index: 242

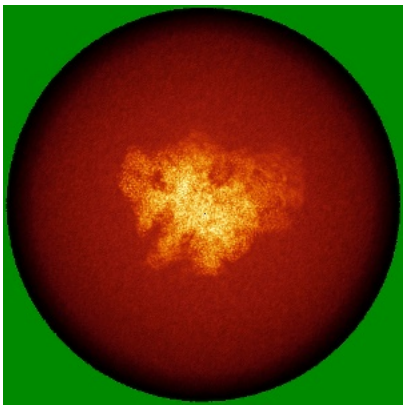
The images above show the largest variance slices of the map in three orthogonal directions.

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

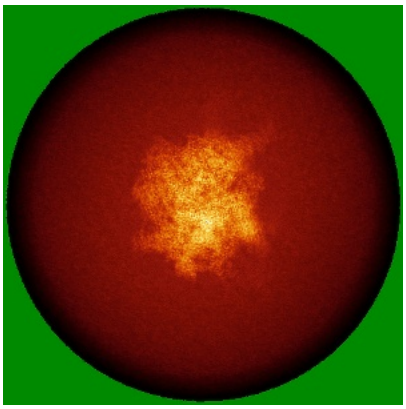
6.4.1 Primary map



X

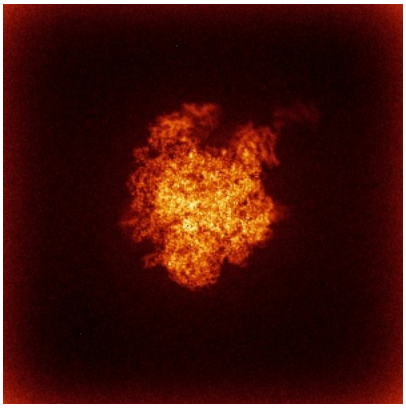


Y

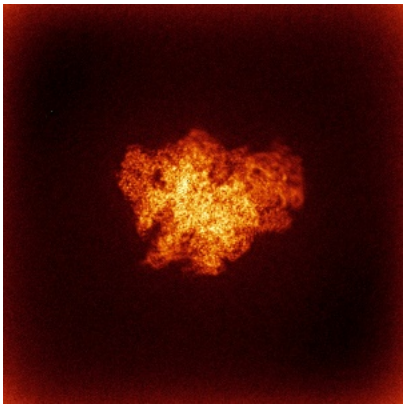


Z

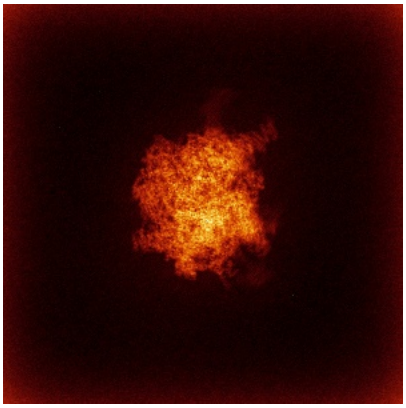
6.4.2 Raw map



X



Y

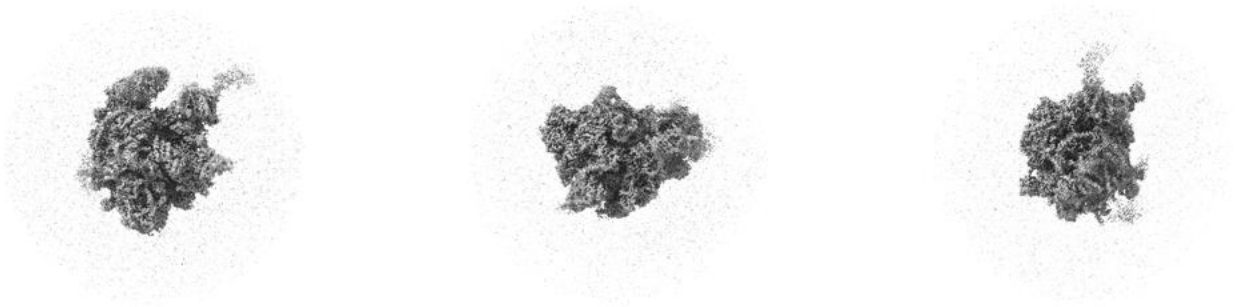


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.814. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

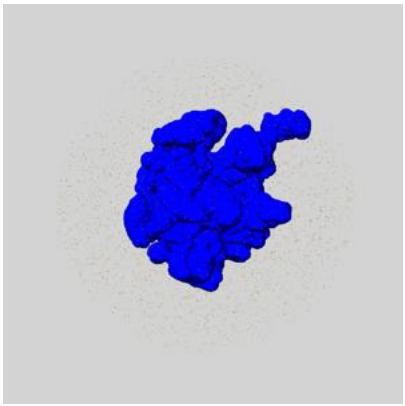
6.6 Mask visualisation (i)

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

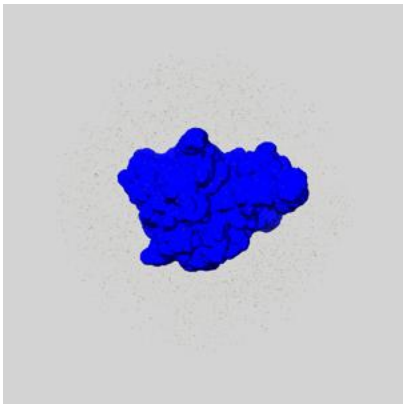
A mask typically either:

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

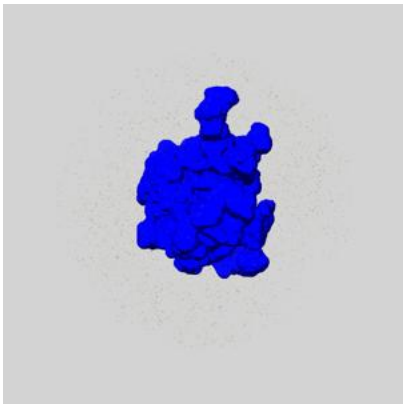
6.6.1 emd_17720_msk_1.map (i)



X



Y

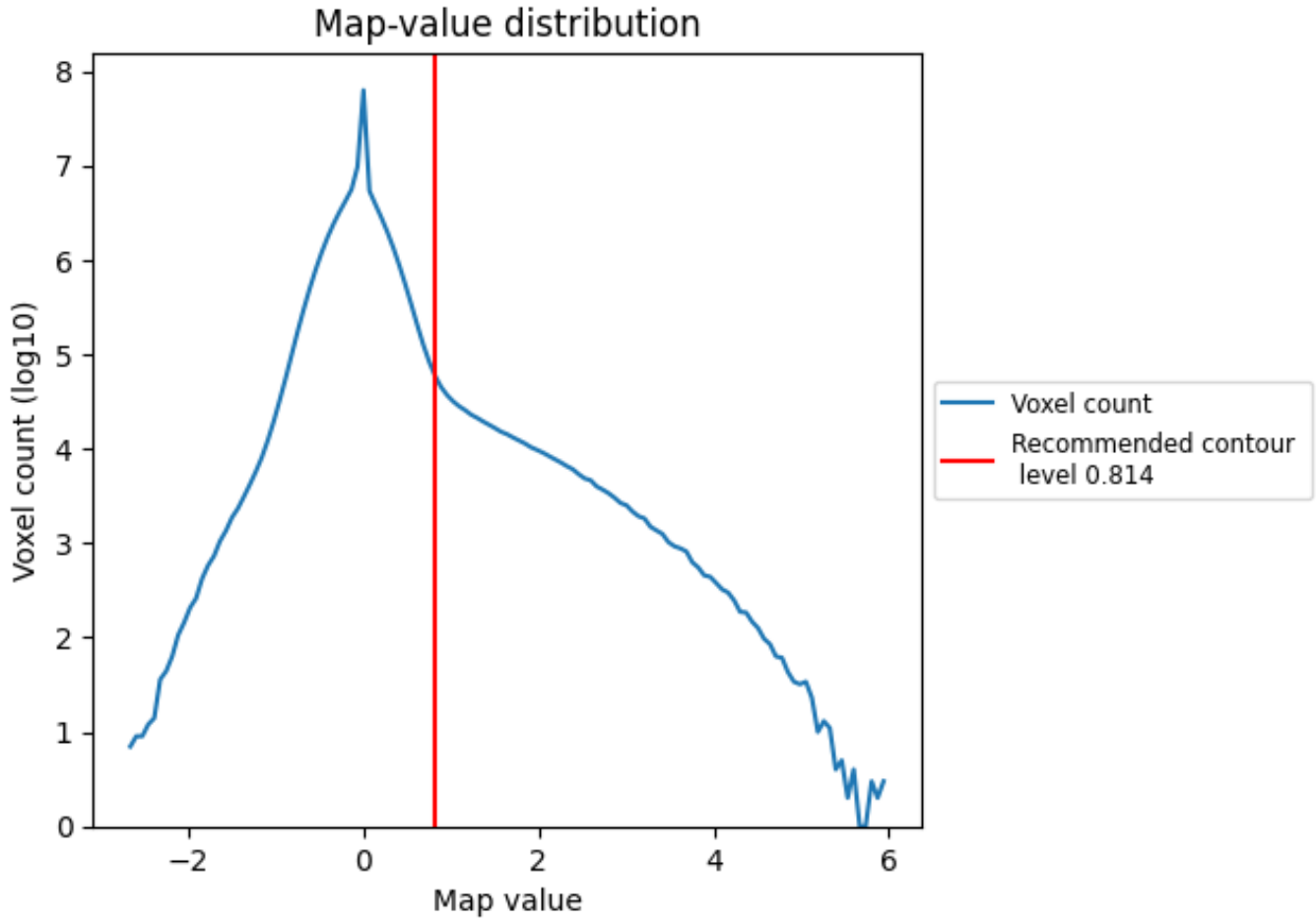


Z

7 Map analysis

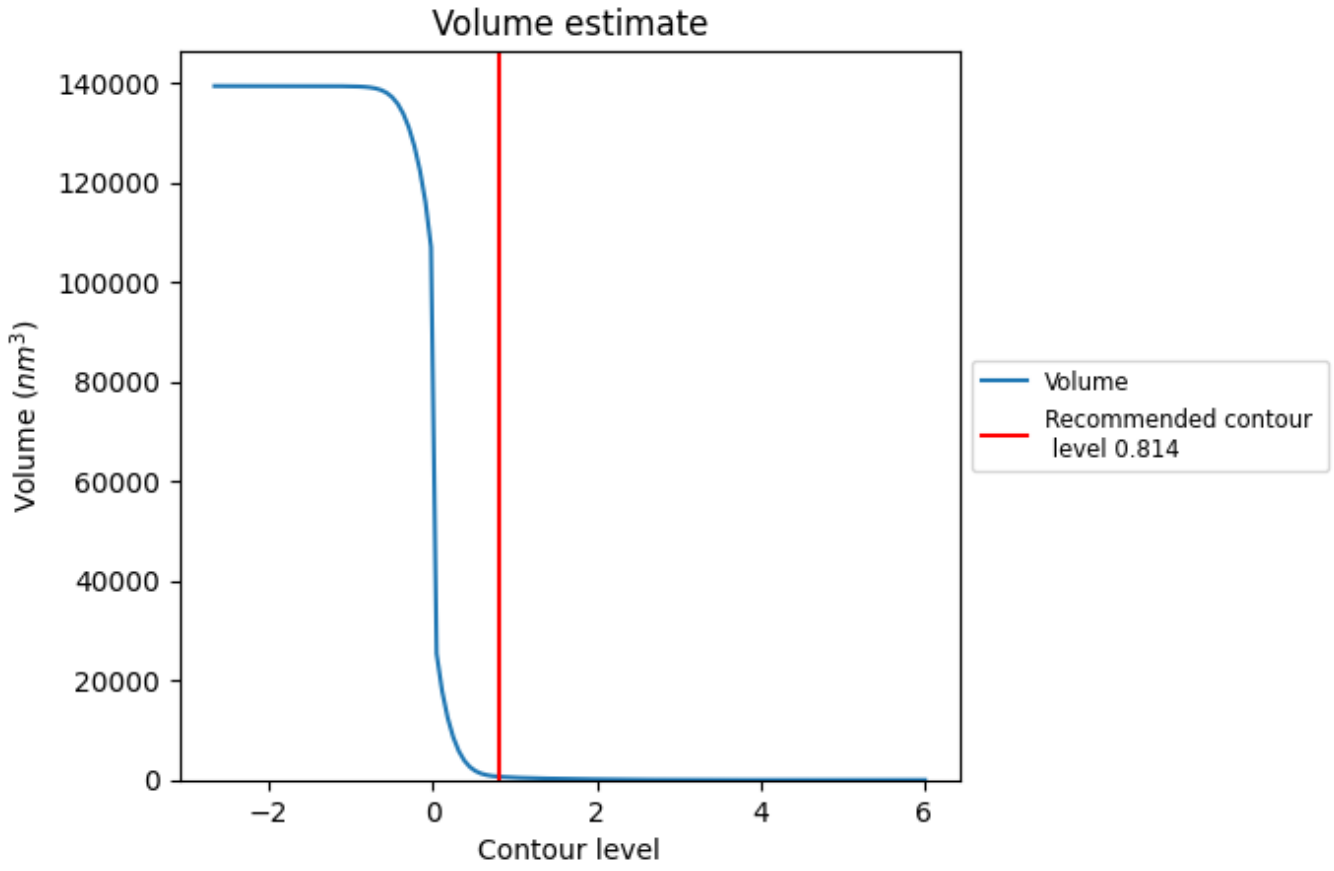
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

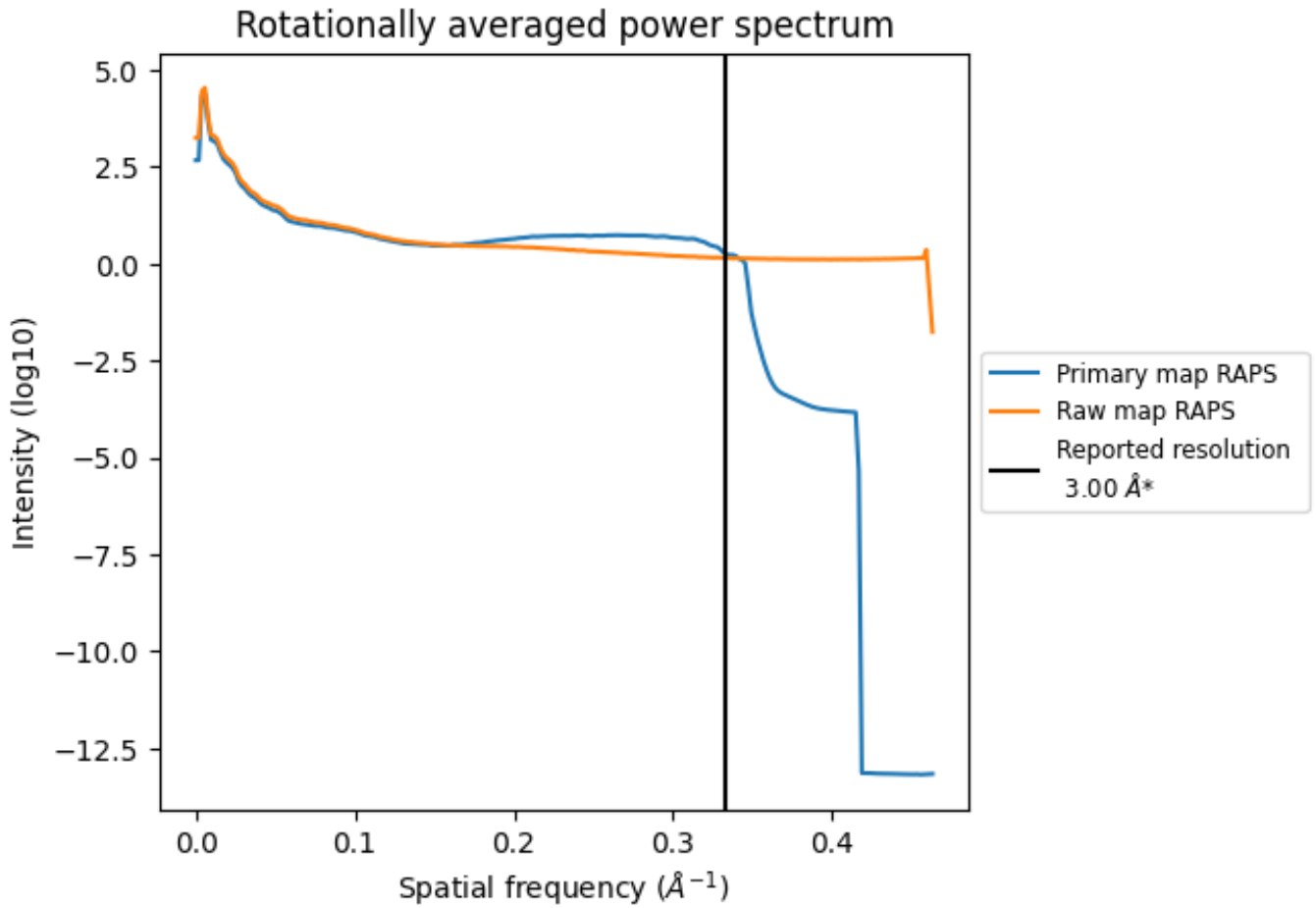
7.2 Volume estimate



The volume at the recommended contour level is 647 nm^3; this corresponds to an approximate mass of 584 kDa.

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

7.3 Rotationally averaged power spectrum (i)

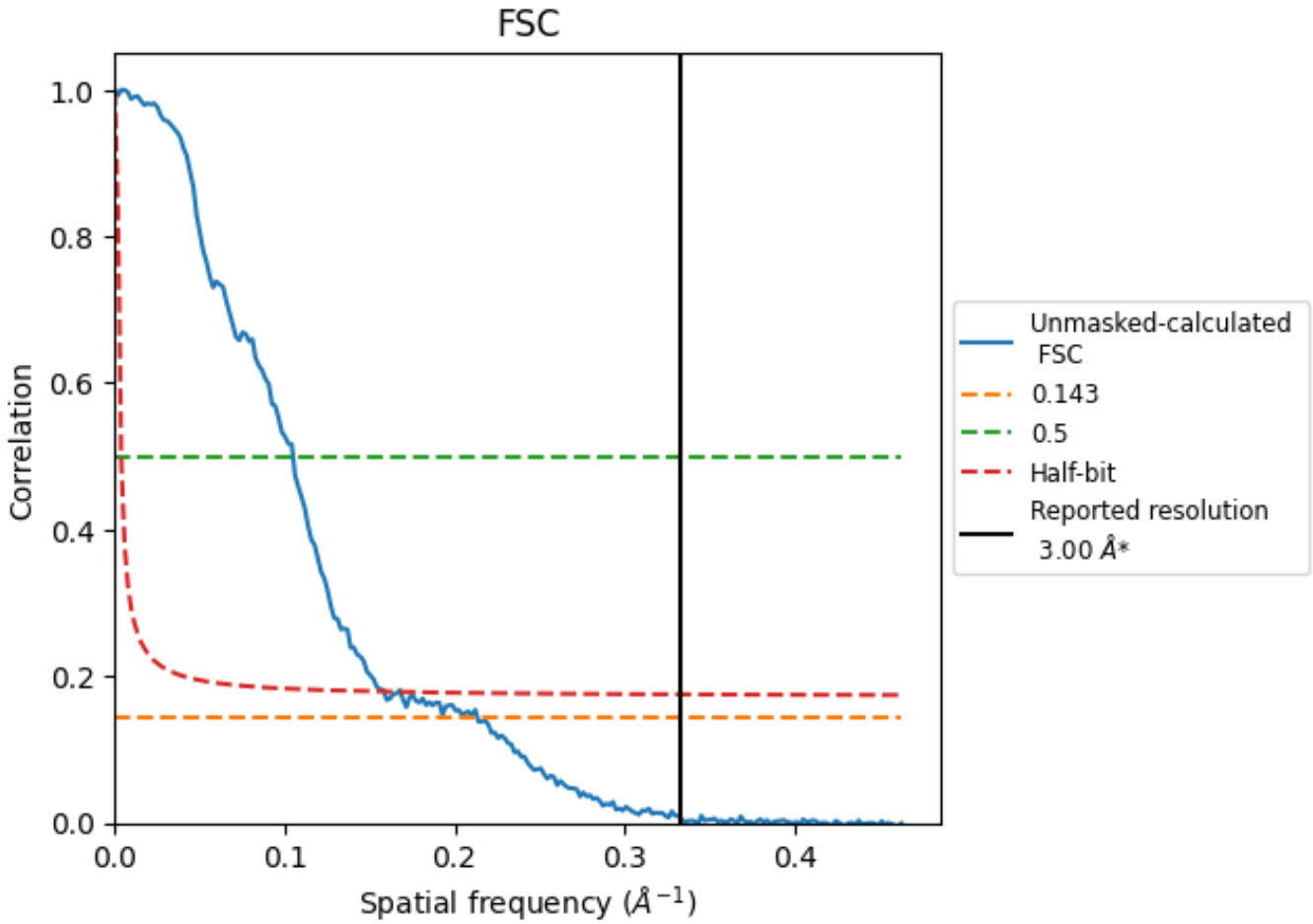


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

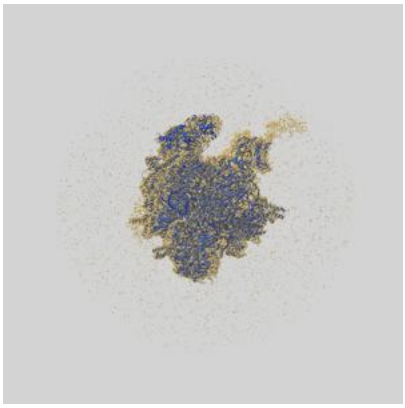
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	9.53	6.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.68 differs from the reported value 3.0 by more than 10 %

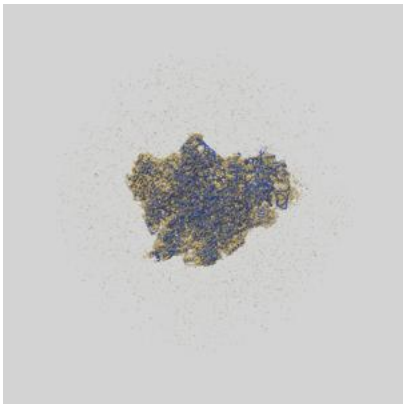
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17720 and PDB model 8QSJ. Per-residue inclusion information can be found in section 3 on page 16.

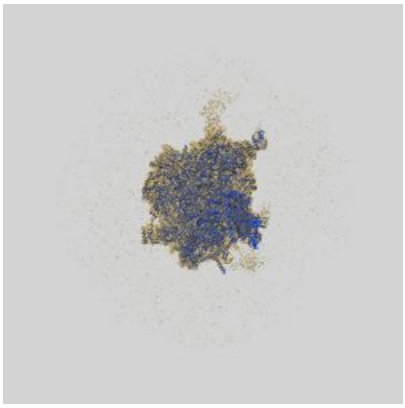
9.1 Map-model overlay



X



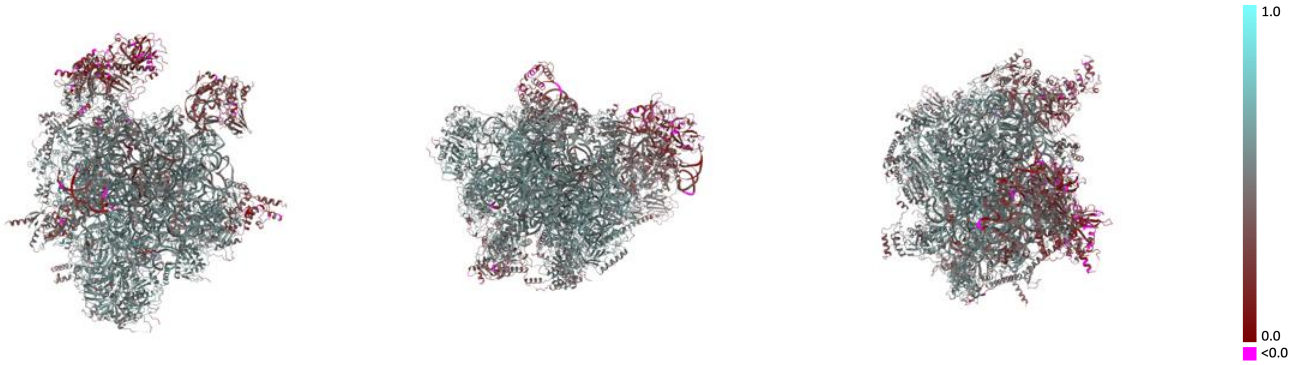
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.814 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

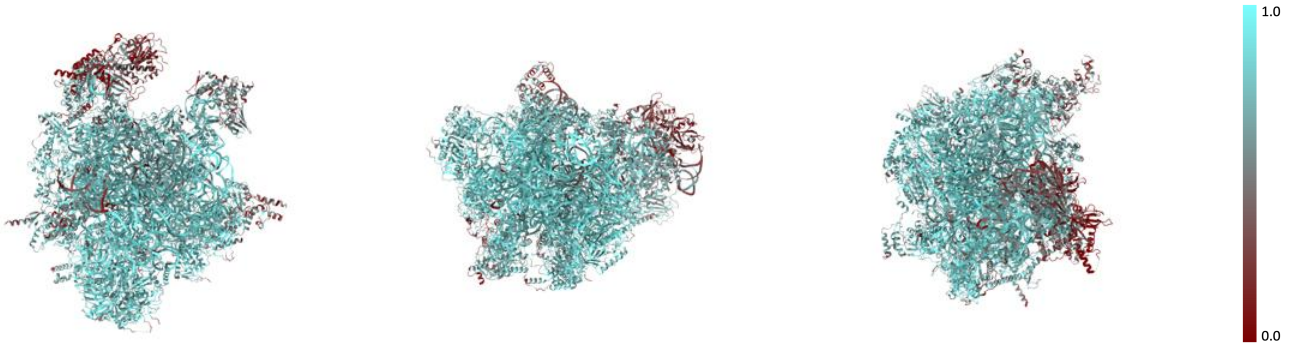
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

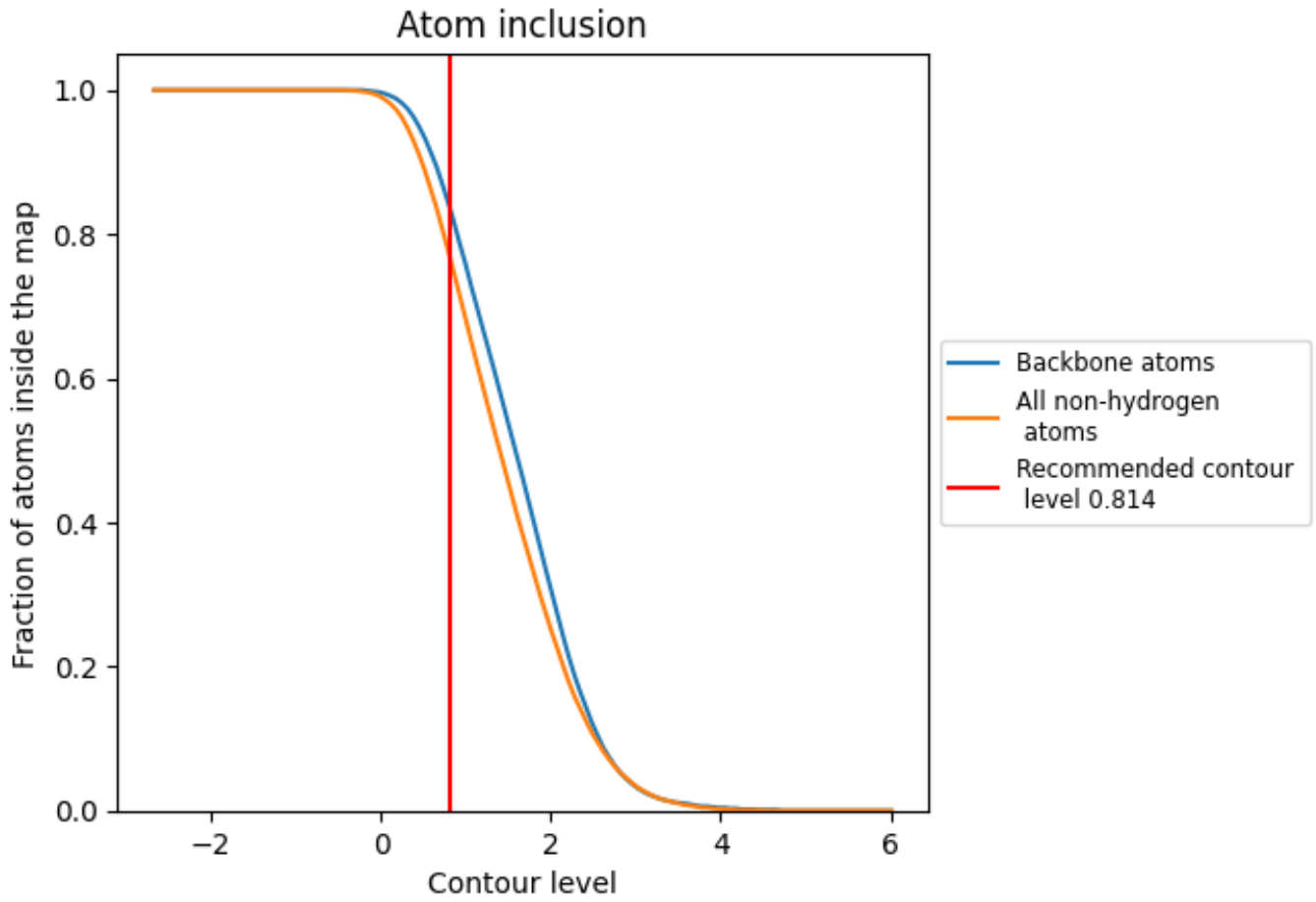
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.814).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.814) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.4930
0	0.8060	0.5410
1	0.7600	0.5180
2	0.8970	0.5980
3	0.9240	0.6070
4	0.8650	0.5570
5	0.8100	0.5290
6	0.7070	0.4530
7	0.7230	0.4500
8	0.2770	0.2360
9	0.8000	0.5130
A	0.8780	0.5350
B	0.6300	0.3020
D	0.7990	0.5340
E	0.8500	0.5550
F	0.8420	0.5390
H	0.6910	0.4750
I	0.5260	0.3510
J	0.3570	0.1980
K	0.8710	0.5760
L	0.8170	0.5460
M	0.8470	0.5590
N	0.7100	0.4730
O	0.8620	0.5680
P	0.7210	0.4550
Q	0.8000	0.5360
R	0.8750	0.5790
S	0.8330	0.5400
T	0.8370	0.5590
U	0.7380	0.5100
V	0.6800	0.4460
W	0.8480	0.5750
X	0.7950	0.5340
Y	0.8210	0.5340
Z	0.8470	0.5610

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Chain	Atom inclusion	Q-score
a	0.7220	0.4820
b	0.8500	0.5410
c	0.7640	0.4860
d	0.5670	0.3940
e	0.1930	0.1730
f	0.3710	0.2980
g	0.8400	0.5350
h	0.6950	0.4210
i	0.8770	0.5830
j	0.7950	0.5090
k	0.6480	0.3900
l	0.6800	0.3900
m	0.1150	0.1670
o	0.7520	0.5350
p	0.6320	0.4340
q	0.6860	0.4490
r	0.8400	0.5160
s	0.8310	0.5490
u	0.6710	0.4510
v	0.5750	0.3340
w	0.3040	0.2010
x	0.6750	0.4630
y	0.6250	0.4220
z	0.7060	0.4640