



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:40 AM EDT

PDB ID : 9PRA / pdb_00009pra
EMDB ID : EMD-71802
Title : In Situ Structure of the Human Mitochondrial Large Subunit 39S in Complex with EF-Tu
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-23
Resolution : 2.83 Å (reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

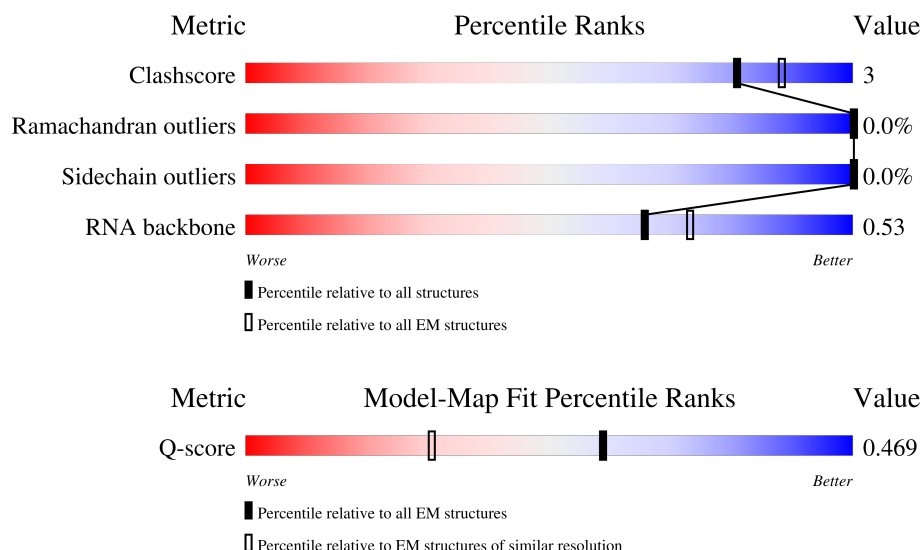
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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	11847 (2.33 - 3.33)

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.

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2	1	65	
3	2	92	

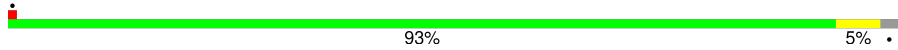
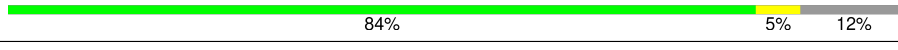
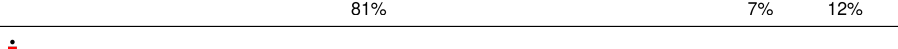
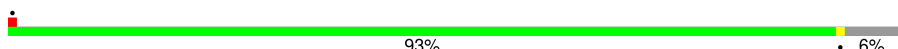
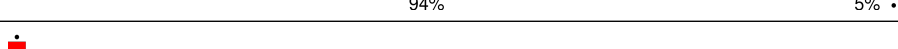
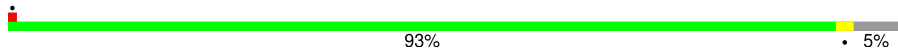
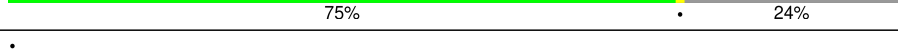
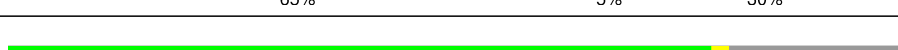
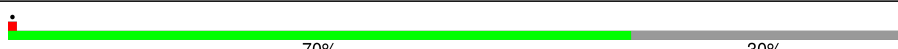
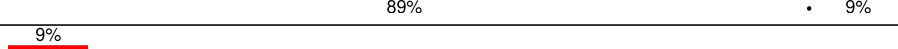
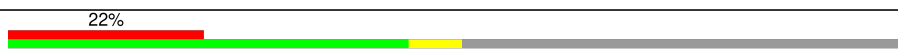
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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	d	306	
12	e	279	
13	f	212	
14	D	305	
15	E	348	
16	F	311	
17	G	198	
17	t	198	
17	u	198	
17	v	198	
17	w	198	
17	x	198	
17	y	198	
18	H	267	
19	I	261	
20	J	192	
21	K	178	
22	L	145	

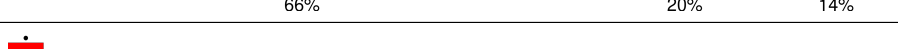
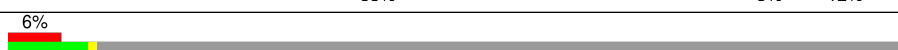
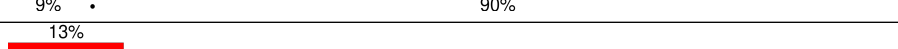
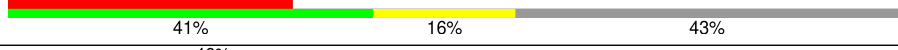
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Mol	Chain	Length	Quality of chain
23	M	296	
24	N	251	
25	O	175	
26	P	180	
27	Q	292	
28	R	149	
29	S	205	
30	T	206	
31	U	153	
32	V	216	
33	W	148	
34	X	256	
35	Y	250	
36	Z	161	
37	b	215	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	n	43	
46	o	102	
47	q	222	

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Mol	Chain	Length	Quality of chain
48	r	196	
49	z	325	
50	Ag	455	
51	A	1558	
52	c	332	
53	p	206	
54	s	439	
55	OX	435	
56	a	142	
57	Ad	234	
58	Ae	70	
59	Af	156	
60	B	72	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 115757 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
1	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

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

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

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

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

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

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

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

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

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

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

- 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	139	Total	C	N	O	S	0	0
			1179	752	207	218	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 protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L12, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL13m.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 22 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

- Molecule 45 is a protein called Nascent polypeptide.

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

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

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

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

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

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

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

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

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

- Molecule 50 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ag	393	Total	C	N	O	S	0	0
			3039	1922	535	566	16		

- Molecule 51 is a RNA chain called 16S mitochondrial rRNA.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 52 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

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

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

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

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

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

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

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

- Molecule 57 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ad	133	Total	C	N	O	S	0	0
			1092	702	181	199	10		

- Molecule 58 is a protein called Mitochondrial ribosome and complex I assembly factor Alt-MIEF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Ae	68	Total	C	N	O	0	0
			584	369	115	100		

- Molecule 59 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Af	87	Total	C	N	O	P	S	0	0
			726	463	105	150	1	7		

- Molecule 60 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	0	1	Total	Zn	0
			1	1	
61	4	1	Total	Zn	0
			1	1	

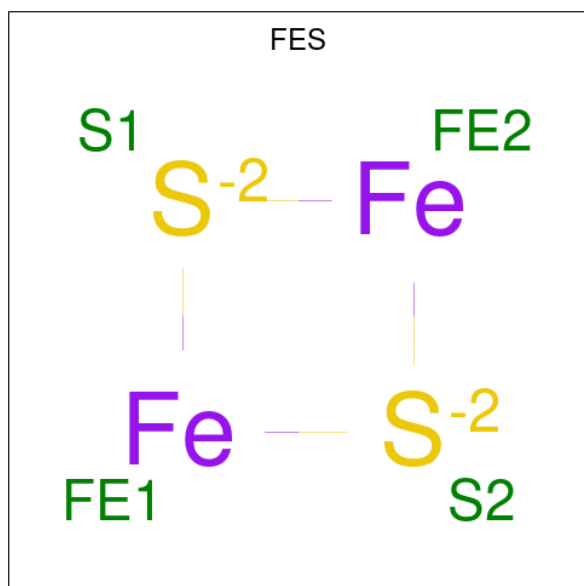
- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	K	0
			1	1	
62	6	1	Total	K	0
			1	1	
62	D	1	Total	K	0
			1	1	
62	M	1	Total	K	0
			1	1	
62	N	1	Total	K	0
			1	1	
62	W	1	Total	K	0
			1	1	
62	o	1	Total	K	0
			1	1	
62	A	29	Total	K	0
			29	29	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

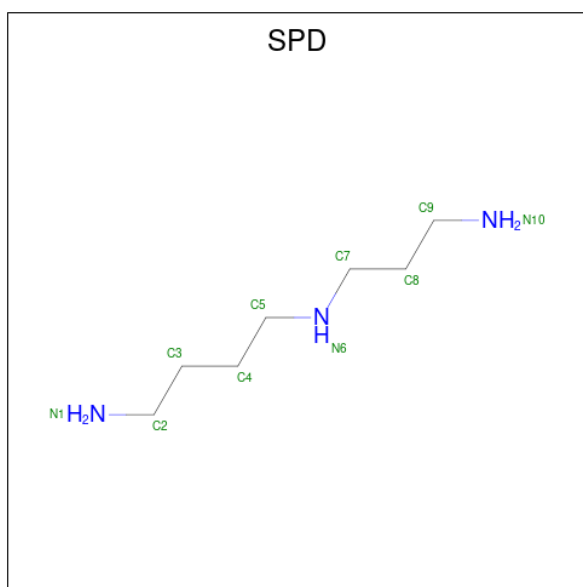
Mol	Chain	Residues	Atoms		AltConf
63	D	2	Total 2	Mg 2	0
63	E	1	Total 1	Mg 1	0
63	I	1	Total 1	Mg 1	0
63	g	1	Total 1	Mg 1	0
63	A	136	Total 136	Mg 136	0

- Molecule 64 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



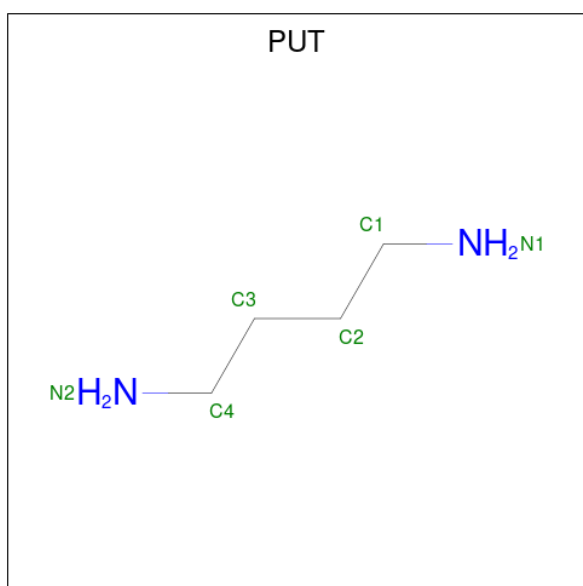
Mol	Chain	Residues	Atoms			AltConf
64	r	1	Total 4	Fe 2	S 2	0

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



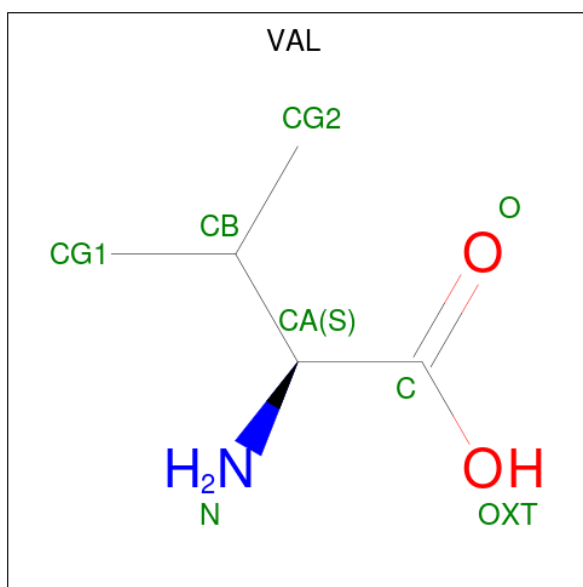
Mol	Chain	Residues	Atoms			AltConf
65	A	1	Total	C	N	0
			10	7	3	
65	A	1	Total	C	N	0
			10	7	3	

- Molecule 66 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

- Molecule 67 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

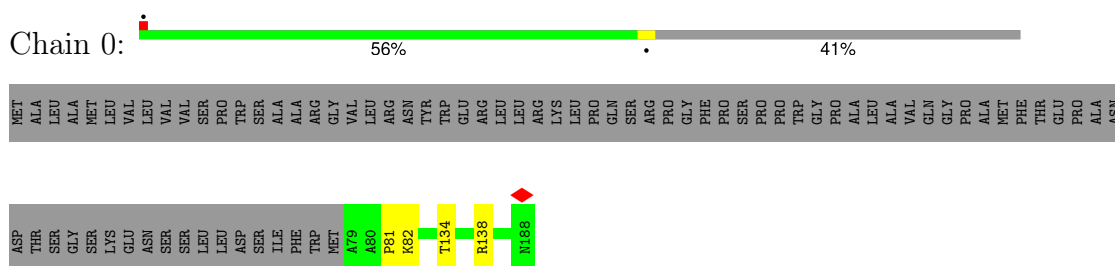


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	B	1	7	5	1	1	0

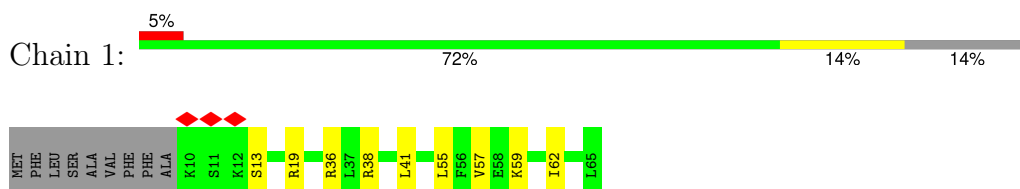
3 Residue-property plots [i](#)

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

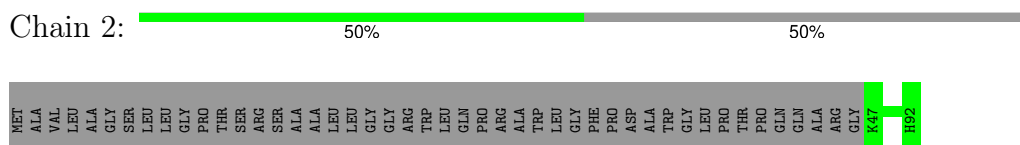
- Molecule 1: 39S ribosomal protein L32, mitochondrial



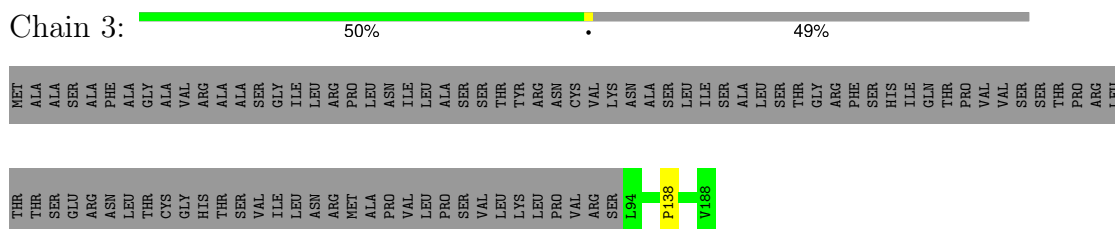
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



- Molecule 5: 39S ribosomal protein L36, mitochondrial



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

LEU PRO ALA LEU GLY P66 K69 L72 P96 M103

- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  88% 5% 7%

MET ALA LEU ALA SER GLY PRO ALA ARG ALA LEU ALA GLY SER GLY GLN LEU GLY LEU GLY PHE GLY GLY ALA PRO ARG ARG GLY A30 L55 Y82 L113 P143 H146 Q165 T175 R201 V204 R215 T232 H289 L299 R300 P301 H302

A311 L336 Q343 T362 D363 L364 L417 A423

- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  89% 7%

MET ALA ALA PRO TRP ARG ALA ALA CYS CYS ARG ARG TRP ARG GLY PHE SER THR SER ALA VAL LEU GLY R27 K81 T82 D83 P84 K85 E86 K96 R106 L161 L173 H174 V175 E181 V187 V204 H224 E227 H234 L255 P256 P257

L272 D276 T300 F319 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  80% 7% 13%

MET GLU ALA LEU ALA MET GLY SER ARG ALA ARG LEU TRP VAL LEU VAL PRO GLY GLY GLY ILE TRP ARG PHE ILE THR SER SER ALA SER Q34 R61 T77 P112 H113 D114 K117 M139 M150 I154 K159 Y162 L166 V174 Y181

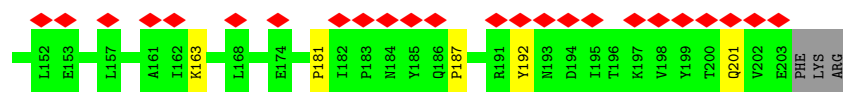
A244 R250 P267 L268 I269 T274 C275 F276 L286 R296 L302 P303 V304 D327 GLN SER LYS THR LEU GLU CYS THR THR

- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:  31% 62% 6% 33%

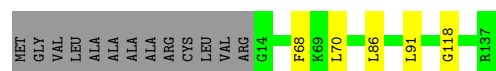
MET THR ALA SER VAL LEU ARG SER ILE SER LEU ALA LEU ARG ARG THR THR GLN THR ARG GLU THR HIS GLN ARG ALA SER LEU LEU SER PHE TRP GLU LEU ILE PRO MET ARG SER PRO LEU ARG LYS LYS LYS VAL ASP PRO LYS LYS

ASP GLN GLU ALA K65 E66 R67 L68 K69 R70 K71 I72 R73 K74 L75 E76 K77 A78 T79 Q80 E81 L82 I85 E86 D87 F88 I89 T90 P91 L92 K93 F94 L95 D96 K97 A98 R99 E100 Q103 V104 E105 L117 K125 R133 I136 R137 A138 E141 A142 E145 E149



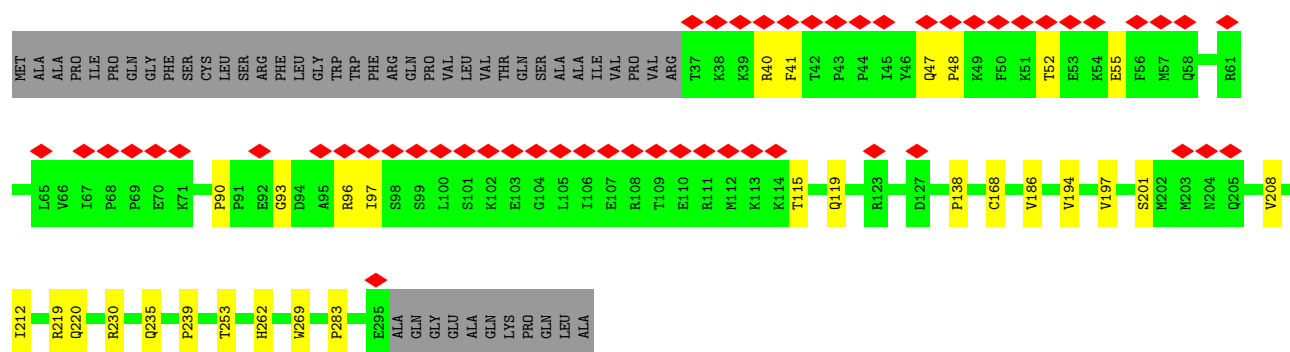
- Molecule 10: 39S ribosomal protein L41, mitochondrial

Chain 9: 87% 9%



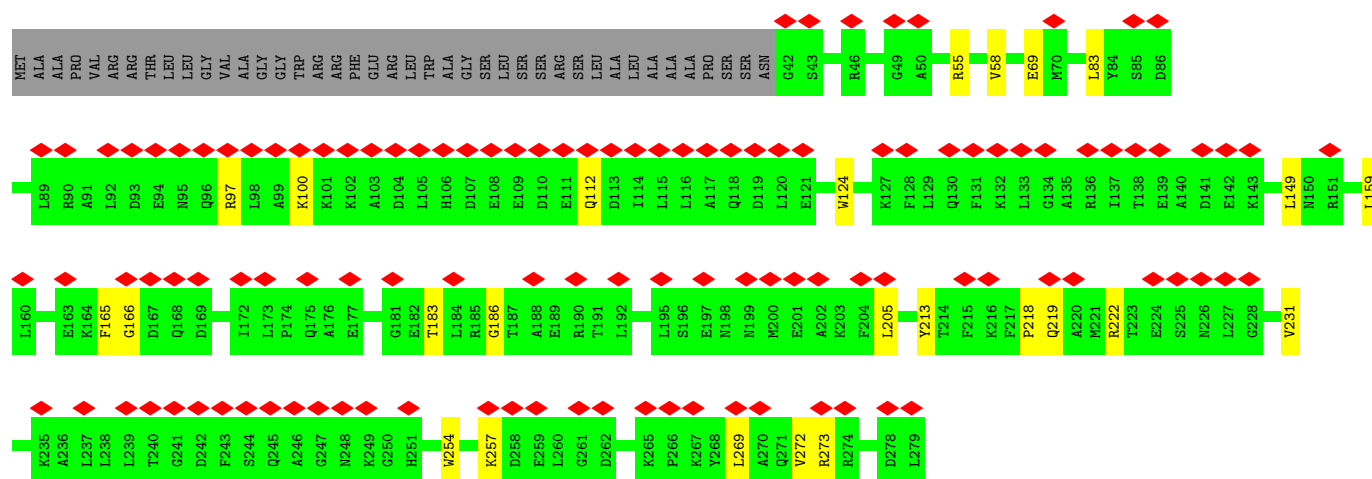
- Molecule 11: 39S ribosomal protein L45, mitochondrial

Chain d: 18% 75% 9% 15%



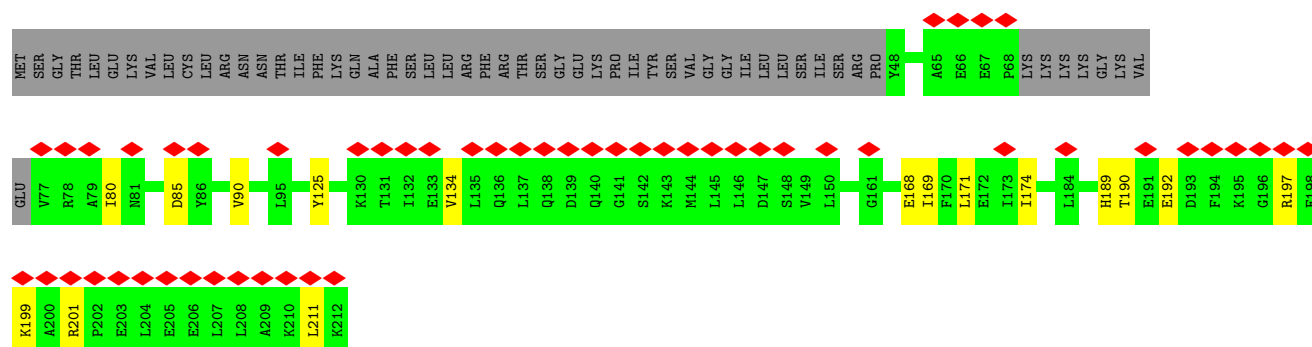
- Molecule 12: 39S ribosomal protein L46, mitochondrial

Chain e: 41% 76% 9% 15%



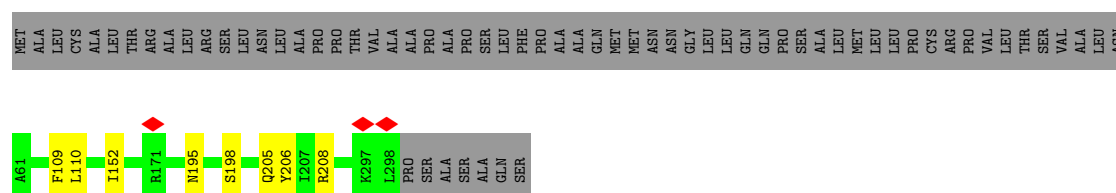
- Molecule 13: 39S ribosomal protein L48, mitochondrial

Chain f: 25% 67% 8% 26%



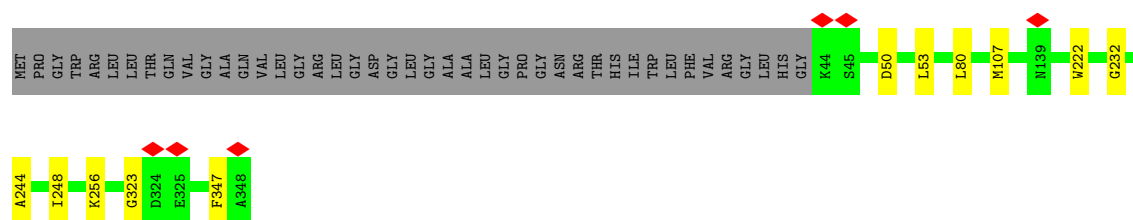
- Molecule 14: 39S ribosomal protein L2, mitochondrial

Chain D: 75% 22%



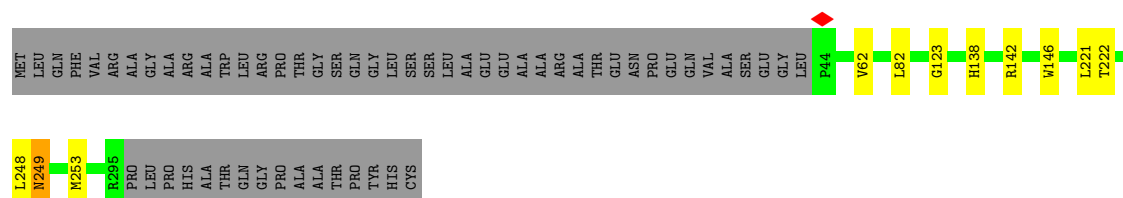
- Molecule 15: 39S ribosomal protein L3, mitochondrial

Chain E: 84% 12%



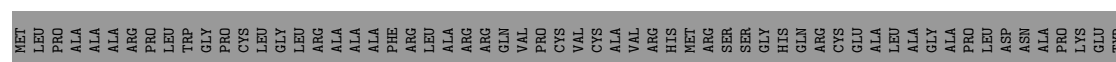
- Molecule 16: 39S ribosomal protein L4, mitochondrial

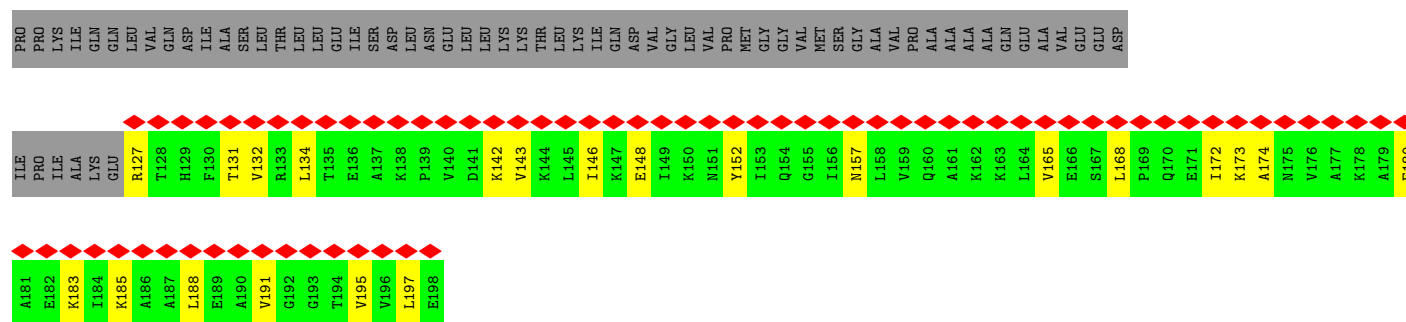
Chain F: 77% 19%



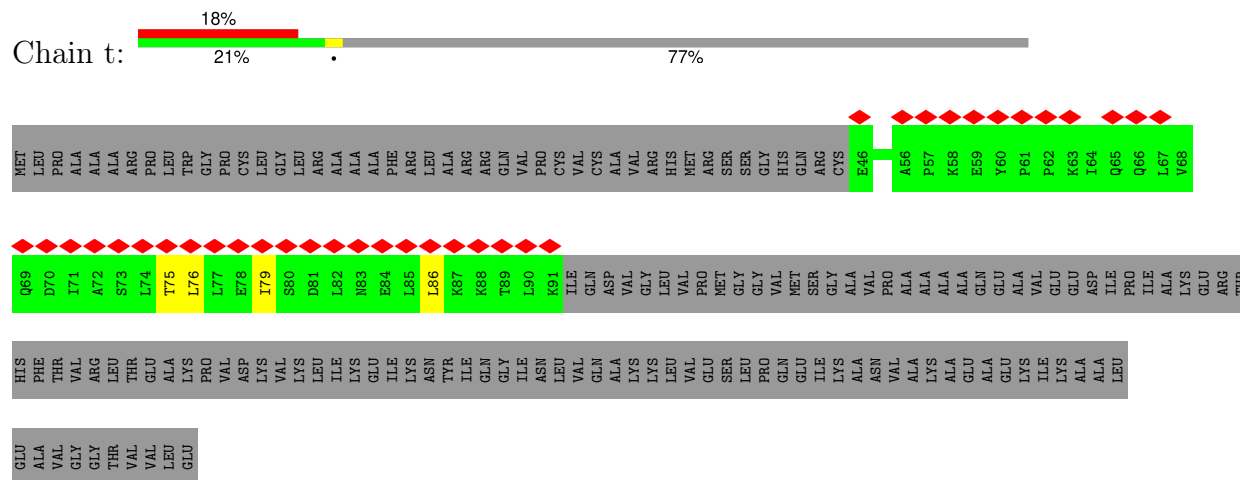
- Molecule 17: 39S ribosomal protein L12, mitochondrial

Chain G: 36% 25% 11% 64%

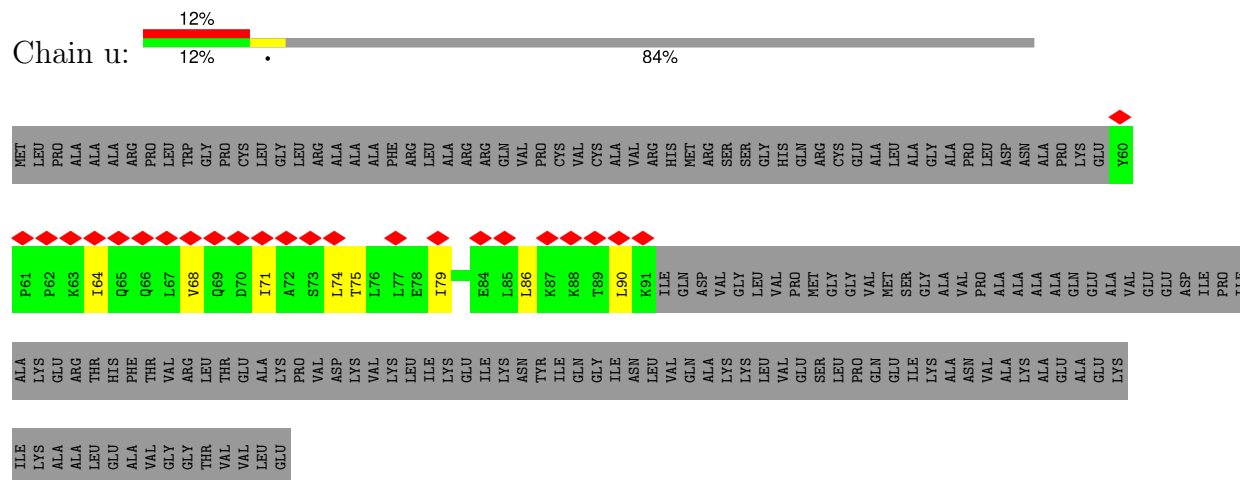




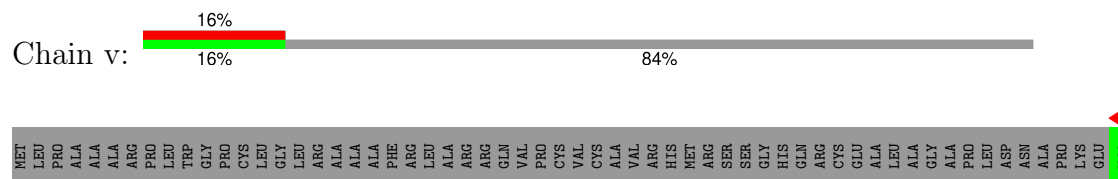
- Molecule 17: 39S ribosomal protein L12, mitochondrial

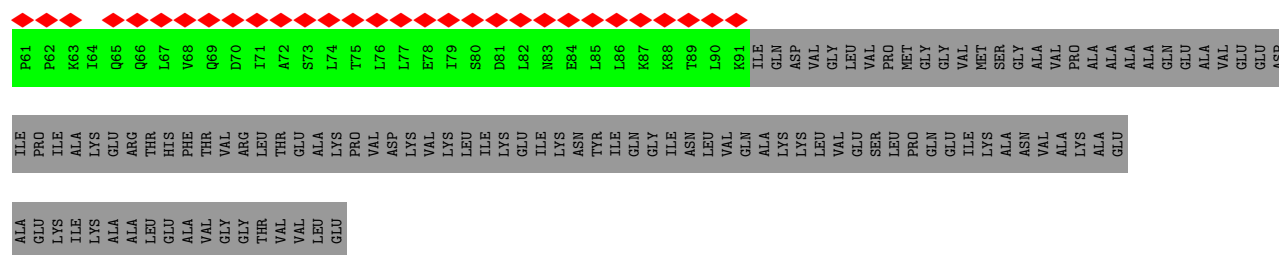


- Molecule 17: 39S ribosomal protein L12, mitochondrial

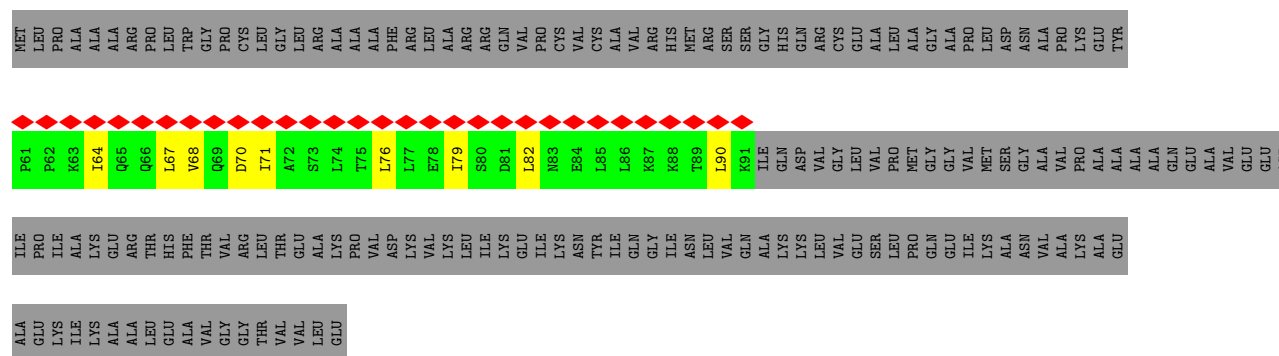


- Molecule 17: 39S ribosomal protein L12, mitochondrial

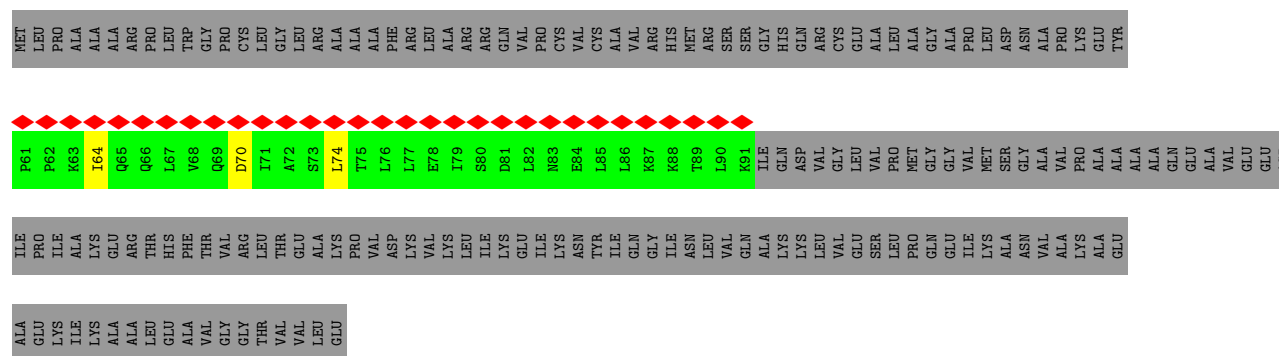




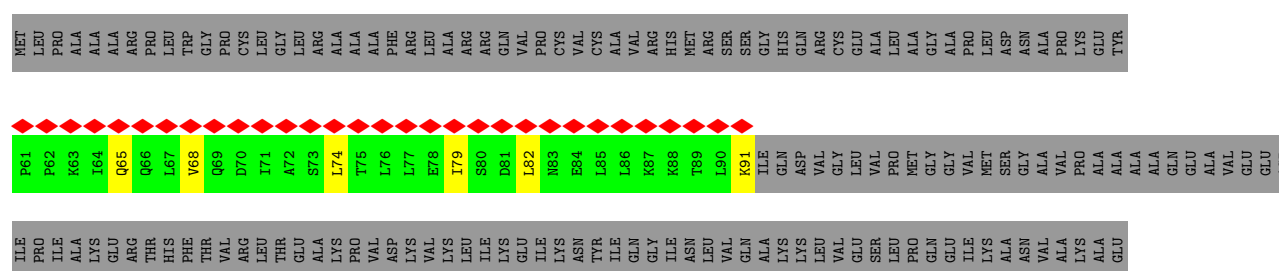
• Molecule 17: 39S ribosomal protein L12, mitochondrial



• Molecule 17: 39S ribosomal protein L12, mitochondrial



• Molecule 17: 39S ribosomal protein L12, mitochondrial



- Molecule 23: 39S ribosomal protein L15, mitochondrial

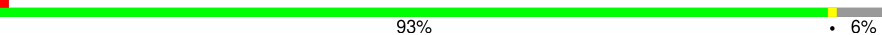
- Molecule 24: 39S ribosomal protein L16, mitochondrial

- Molecule 25: 39S ribosomal protein L17, mitochondrial

- Molecule 26: 39S ribosomal protein L18, mitochondrial

- Molecule 27: 39S ribosomal protein L19, mitochondrial

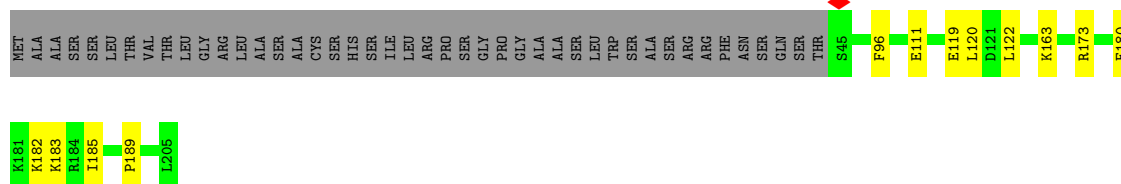
- Molecule 28: 39S ribosomal protein L20, mitochondrial

Chain R:  93% 6%



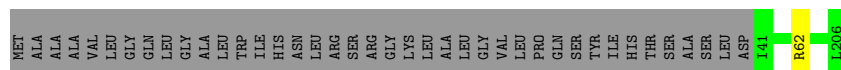
- Molecule 29: 39S ribosomal protein L21, mitochondrial

Chain S:  73% 6% 21%

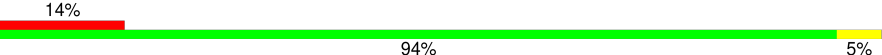


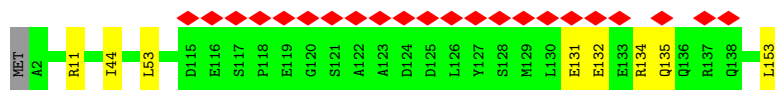
- Molecule 30: 39S ribosomal protein L22, mitochondrial

Chain T:  80% 19%



- Molecule 31: 39S ribosomal protein L23, mitochondrial

Chain U:  14% 94% 5%



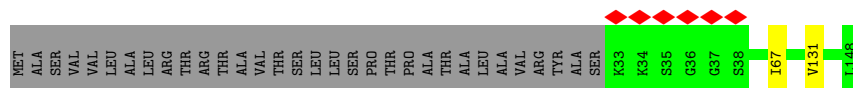
- Molecule 32: 39S ribosomal protein L24, mitochondrial

Chain V:  88% 6% 5%

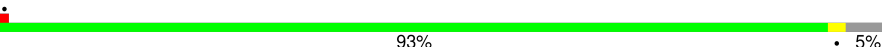


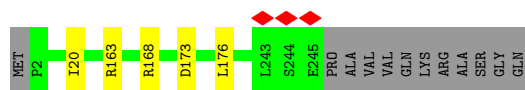
- Molecule 33: 39S ribosomal protein L27, mitochondrial

Chain W:  77% 22%

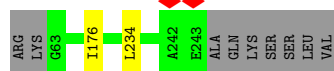
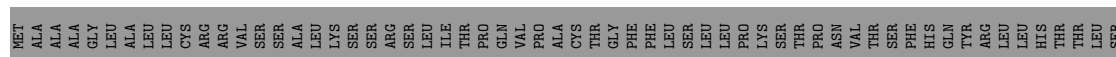


- Molecule 34: 39S ribosomal protein L28, mitochondrial

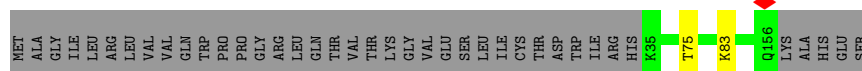
Chain X:  93% 5%



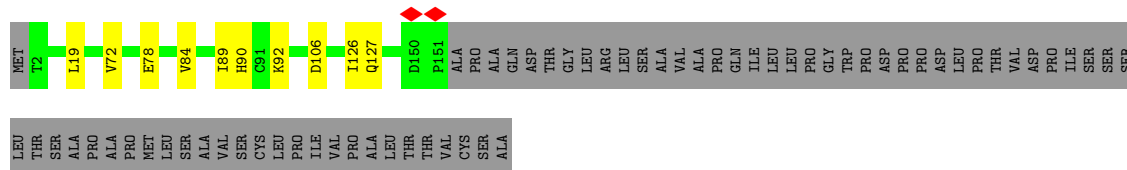
- Molecule 35: 39S ribosomal protein L47, mitochondrial



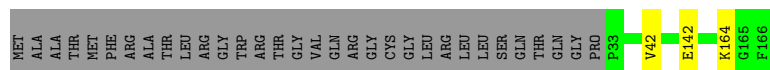
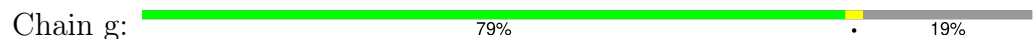
- Molecule 36: 39S ribosomal protein L30, mitochondrial



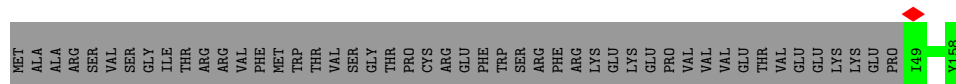
- Molecule 37: 39S ribosomal protein L43, mitochondrial



- Molecule 38: 39S ribosomal protein L49, mitochondrial



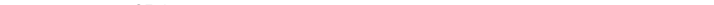
- Molecule 39: 39S ribosomal protein L50, mitochondrial

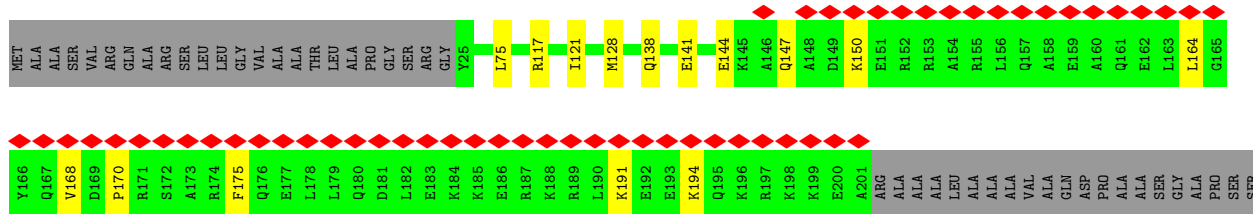


- Molecule 40: 39S ribosomal protein L51, mitochondrial

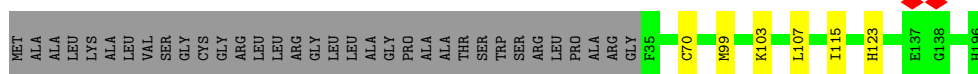


MET PHE LEU THR ALA LEU LEU TRP R9 I12 R15 I18 R23 I88 S102

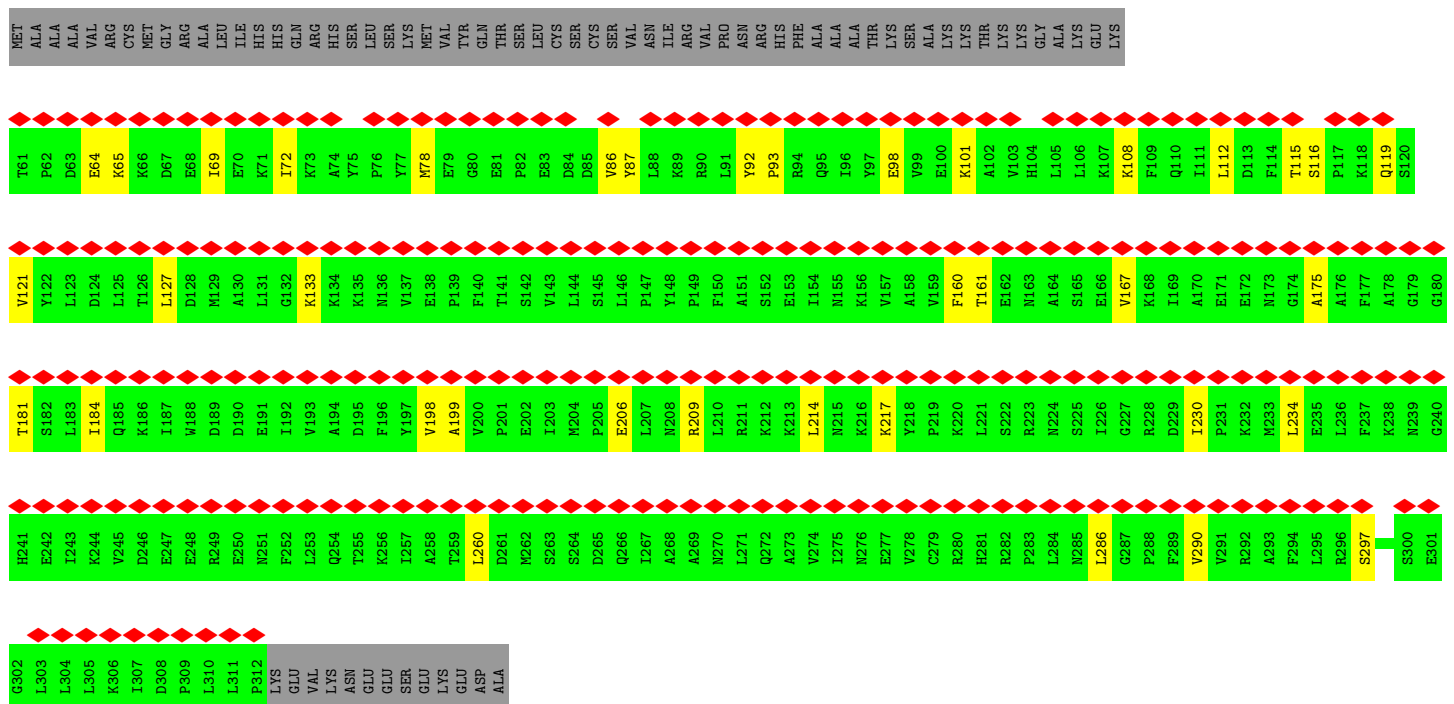
- Chain q: 



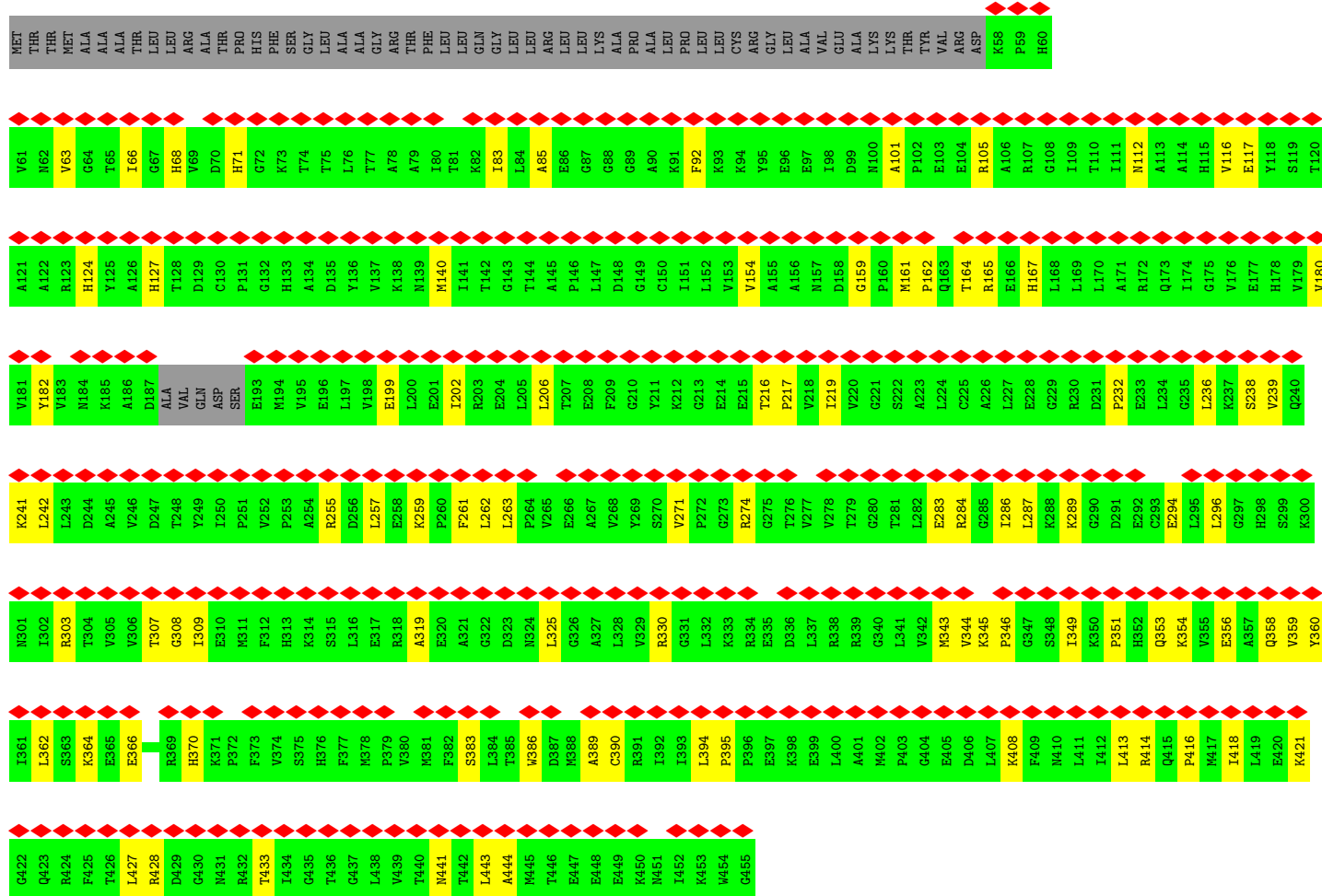
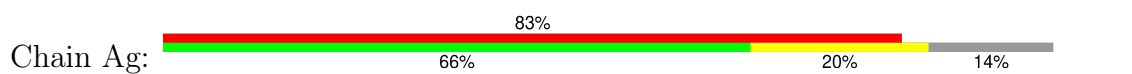
- Chain r:  80% 17%



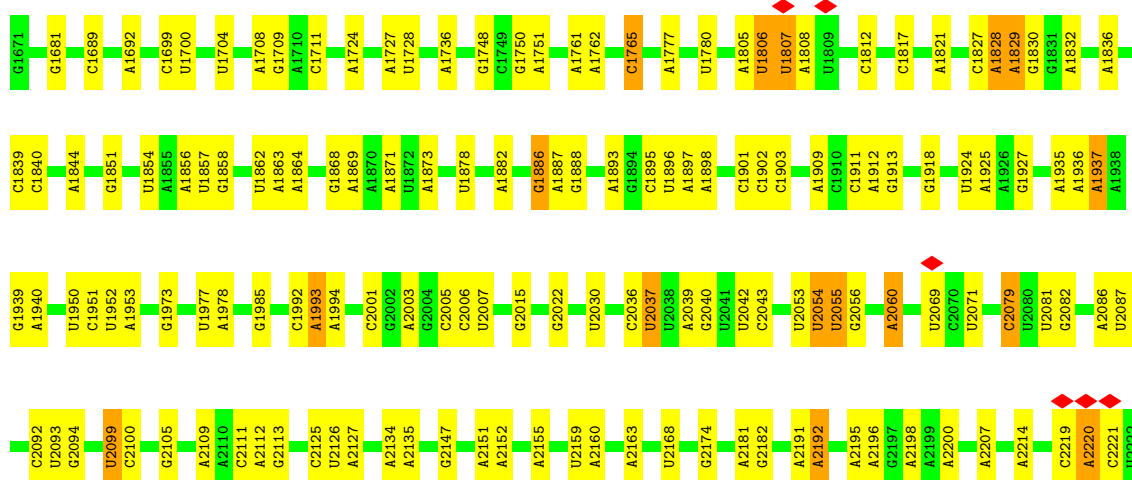
- Chain z:  75% 66% 11% 22%

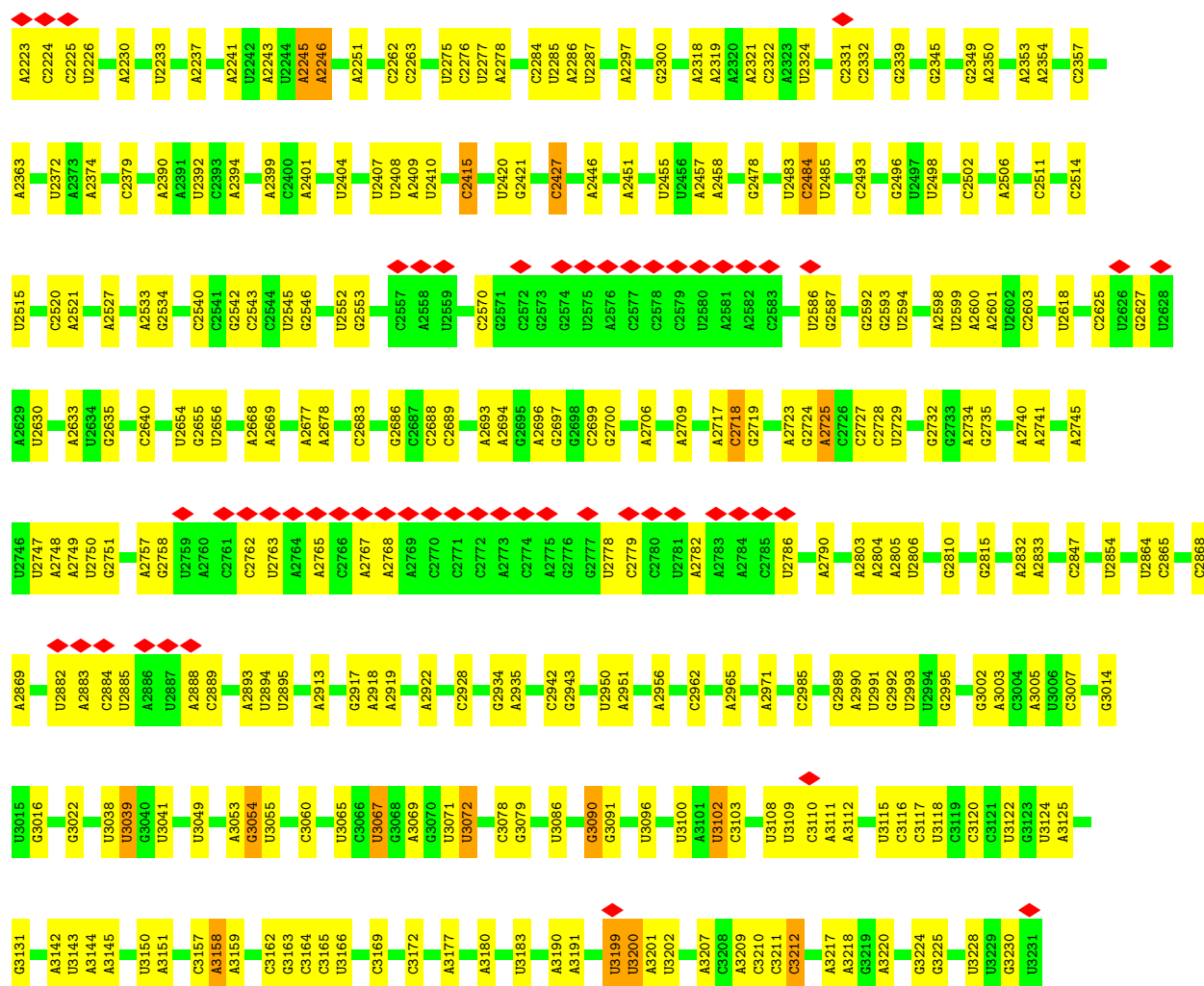


- 

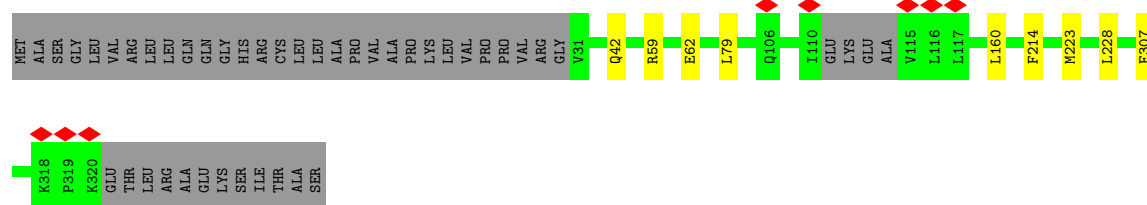
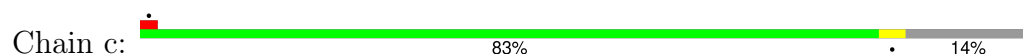


• Molecule 51: 16S mitochondrial rRNA

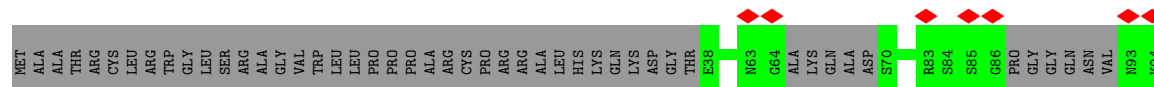




- Molecule 52: 39S ribosomal protein L44, mitochondrial

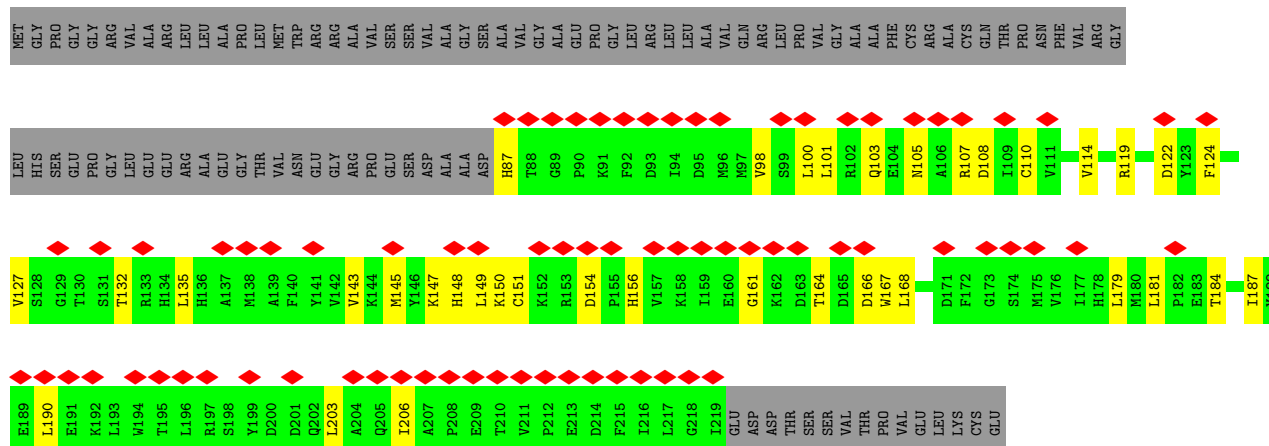
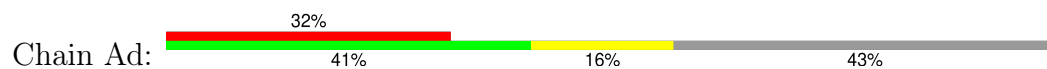


- Molecule 53: Peptidyl-tRNA hydrolase ICT1, mitochondrial

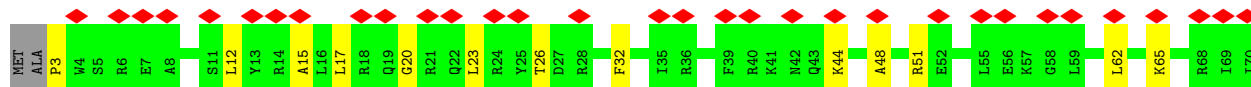
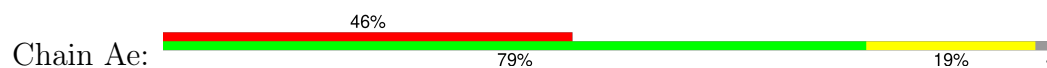




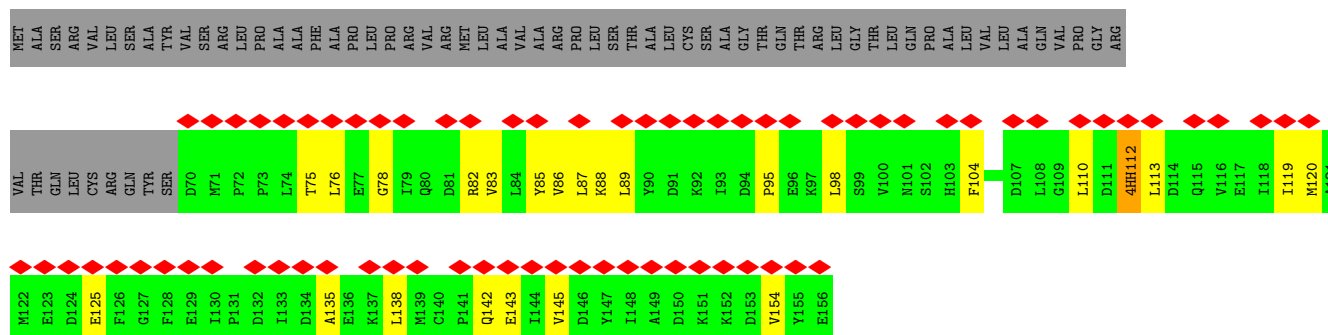
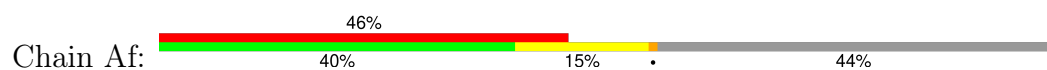
- Molecule 57: Mitochondrial assembly of ribosomal large subunit protein 1



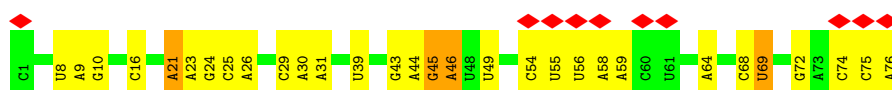
- Molecule 58: Mitochondrial ribosome and complex I assembly factor AltMIEF1



- Molecule 59: Acyl carrier protein, mitochondrial



- Molecule 60: mitochondrial tRNA^{Val}



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PUT, K, 2MG, PSU, OMU, 4HH, ACE, ZN, FES, 1MA, SPD, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.13	0/913	0.24	0/1224
2	1	0.12	0/469	0.24	0/621
3	2	0.14	0/383	0.25	0/507
4	3	0.15	0/853	0.25	0/1136
5	4	0.13	0/350	0.21	0/461
6	5	0.14	0/3305	0.28	0/4502
7	6	0.12	0/3043	0.26	0/4140
8	7	0.12	0/2447	0.25	0/3310
9	8	0.11	0/1204	0.28	0/1621
10	9	0.14	0/1025	0.29	0/1379
11	d	0.14	0/2181	0.34	0/2949
12	e	0.11	0/1970	0.29	0/2658
13	f	0.12	0/1273	0.32	0/1716
14	D	0.13	0/1896	0.25	0/2549
15	E	0.14	0/2475	0.29	0/3355
16	F	0.15	0/2090	0.27	0/2842
17	G	0.16	0/562	0.48	0/754
17	t	0.15	0/358	0.37	0/486
17	u	0.17	0/259	0.38	0/350
17	v	0.17	0/259	0.35	0/350
17	w	0.21	0/246	0.50	0/331
17	x	0.14	0/246	0.37	0/331
17	y	0.15	0/246	0.45	0/331
18	H	0.11	0/1698	0.28	0/2292
19	I	0.13	0/1731	0.31	0/2345
20	J	0.13	0/1348	0.27	0/1813
21	K	0.15	0/1497	0.27	0/2031
22	L	0.13	0/905	0.29	0/1218
23	M	0.15	0/2381	0.27	0/3212
24	N	0.13	0/1833	0.26	0/2468
25	O	0.14	0/1283	0.26	0/1727
26	P	0.12	0/1199	0.24	0/1623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	Q	0.12	0/1875	0.25	0/2523
28	R	0.15	0/1175	0.24	0/1572
29	S	0.15	0/1320	0.27	0/1789
30	T	0.13	0/1403	0.24	0/1886
31	U	0.15	0/1279	0.32	0/1730
32	V	0.11	0/1721	0.25	0/2333
33	W	0.14	0/926	0.25	0/1244
34	X	0.12	0/2099	0.23	0/2837
35	Y	0.14	0/1593	0.24	0/2136
36	Z	0.14	0/1021	0.26	0/1378
37	b	0.14	0/1218	0.27	0/1649
38	g	0.14	0/1151	0.26	0/1569
39	h	0.11	0/918	0.24	0/1249
40	i	0.15	0/850	0.25	0/1135
41	j	0.12	0/760	0.22	0/1023
42	k	0.10	0/783	0.22	0/1057
43	l	0.11	0/707	0.27	0/960
44	m	0.09	0/549	0.27	0/737
46	o	0.16	0/819	0.28	0/1097
47	q	0.12	0/1529	0.28	0/2055
48	r	0.14	0/1362	0.28	0/1846
49	z	0.13	0/2067	0.33	0/2793
50	Ag	0.12	0/3094	0.30	0/4182
51	A	0.15	0/36876	0.28	0/57402
52	c	0.12	0/2347	0.24	0/3171
53	p	0.12	0/1223	0.25	0/1641
54	s	0.14	0/3231	0.28	0/4389
55	OX	0.16	0/366	0.43	0/491
56	a	0.14	0/891	0.32	0/1208
57	Ad	0.12	0/1119	0.33	0/1516
58	Ae	0.12	0/593	0.32	0/788
59	Af	0.11	0/710	0.27	0/956
60	B	0.14	0/1626	0.26	0/2523
All	All	0.14	0/121129	0.28	0/171497

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	0	898	0	916	4	0
2	1	464	0	511	6	0
3	2	377	0	406	0	0
4	3	832	0	883	1	0
5	4	342	0	361	2	0
6	5	3210	0	3206	14	0
7	6	2948	0	2841	9	0
8	7	2390	0	2397	13	0
9	8	1179	0	1205	12	0
10	9	997	0	987	3	0
11	d	2124	0	2125	18	0
12	e	1931	0	1916	19	0
13	f	1252	0	1269	12	0
14	D	1859	0	1920	5	0
15	E	2406	0	2415	7	0
16	F	2031	0	2065	7	0
17	G	558	0	612	16	0
17	t	354	0	377	5	0
17	u	257	0	283	5	0
17	v	257	0	283	0	0
17	w	245	0	275	8	0
17	x	245	0	275	2	0
17	y	245	0	275	5	0
18	H	1661	0	1734	7	0
19	I	1695	0	1785	7	0
20	J	1330	0	1407	12	0
21	K	1455	0	1452	5	0
22	L	890	0	941	11	0
23	M	2327	0	2395	9	0
24	N	1786	0	1817	8	0
25	O	1259	0	1294	8	0
26	P	1173	0	1165	2	0
27	Q	1834	0	1872	9	0
28	R	1154	0	1214	2	0
29	S	1293	0	1365	8	0
30	T	1369	0	1410	1	0
31	U	1248	0	1228	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	V	1676	0	1687	10	0
33	W	904	0	934	1	0
34	X	2044	0	2060	4	0
35	Y	1556	0	1597	2	0
36	Z	996	0	1044	1	0
37	b	1193	0	1191	7	0
38	g	1113	0	1097	3	0
39	h	895	0	881	0	0
40	i	828	0	857	3	0
41	j	745	0	746	1	0
42	k	774	0	784	1	0
43	l	688	0	673	6	0
44	m	541	0	564	7	0
45	n	160	0	40	1	0
46	o	798	0	804	4	0
47	q	1495	0	1492	11	0
48	r	1322	0	1348	5	0
49	z	2027	0	2076	25	0
50	Ag	3039	0	3102	54	0
51	A	33070	0	16792	143	0
52	c	2299	0	2320	6	0
53	p	1205	0	1223	1	0
54	s	3148	0	3131	14	0
55	OX	359	0	355	4	0
56	a	865	0	829	0	0
57	Ad	1092	0	1084	26	0
58	Ae	584	0	600	10	0
59	Af	726	0	712	18	0
60	B	1524	0	779	11	0
61	0	1	0	0	0	0
61	4	1	0	0	0	0
62	3	1	0	0	0	0
62	6	1	0	0	0	0
62	A	29	0	0	0	0
62	D	1	0	0	0	0
62	M	1	0	0	0	0
62	N	1	0	0	0	0
62	W	1	0	0	0	0
62	o	1	0	0	0	0
63	A	136	0	0	0	0
63	D	2	0	0	0	0
63	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	I	1	0	0	0	0
63	g	1	0	0	0	0
64	r	4	0	0	1	0
65	A	20	0	38	1	0
66	A	6	0	12	0	0
67	B	7	0	8	3	0
All	All	115757	0	99742	551	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 3.

All (551) 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)
12:e:183:THR:HG23	12:e:186:GLY:H	1.49	0.77
14:D:205:GLN:HA	14:D:208:ARG:HH21	1.54	0.73
17:x:64:ILE:HG21	17:y:82:LEU:HD21	1.69	0.72
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.73	0.71
50:Ag:263:LEU:HB2	50:Ag:343:MET:HB3	1.71	0.71
22:L:118:ARG:HH12	22:L:120:LYS:HB2	1.58	0.69
50:Ag:154:VAL:HB	50:Ag:159:GLY:HA2	1.74	0.69
50:Ag:359:VAL:HG11	50:Ag:427:LEU:HD12	1.76	0.68
50:Ag:289:LYS:HE3	50:Ag:308:GLY:HA2	1.77	0.67
11:d:230:ARG:HD2	30:T:62:ARG:HE	1.59	0.67
32:V:79:VAL:HG12	32:V:86:VAL:HG12	1.77	0.67
49:z:184:ILE:HD13	49:z:206:GLU:HB2	1.77	0.66
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.77	0.66
58:Ae:48:ALA:HA	58:Ae:51:ARG:HD2	1.78	0.66
49:z:127:LEU:HD22	49:z:290:VAL:HG13	1.79	0.65
50:Ag:390:CYS:HB3	50:Ag:413:LEU:HD13	1.77	0.65
9:8:99:ARG:HG2	12:e:83:LEU:HB3	1.78	0.65
48:r:70:CYS:HB3	64:r:201:FES:S2	2.37	0.65
4:3:138:PRO:HG2	51:A:2854:U:H4'	1.78	0.64
50:Ag:389:ALA:HB3	50:Ag:414:ARG:HE	1.62	0.64
11:d:208:VAL:HG22	11:d:253:THR:HG23	1.79	0.64
17:y:79:ILE:HA	17:y:82:LEU:HB2	1.79	0.63
59:Af:95:PRO:HA	59:Af:98:LEU:HB3	1.81	0.63
17:t:76:LEU:HD23	17:w:68:VAL:HG13	1.81	0.63
9:8:68:LEU:HD21	13:f:211:LEU:HB2	1.81	0.62
50:Ag:162:PRO:HA	50:Ag:165:ARG:HB2	1.81	0.62
49:z:181:THR:HA	49:z:184:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:163:THR:HG21	49:z:86:VAL:HG23	1.82	0.61
9:8:136:ILE:HD11	13:f:169:ILE:HG23	1.82	0.61
49:z:161:THR:HB	49:z:167:VAL:HG22	1.81	0.61
51:A:1857:U:H2'	51:A:1858:G:C8	2.37	0.60
51:A:2740:A:H2'	51:A:2741:A:C8	2.36	0.60
58:Ae:20:GLY:HA2	58:Ae:23:LEU:HD13	1.84	0.60
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.84	0.59
51:A:2740:A:H2'	51:A:2741:A:H8	1.67	0.59
12:e:166:GLY:HA3	67:B:101:VAL:HG12	1.85	0.59
31:U:11:ARG:HH11	32:V:213:VAL:HG12	1.68	0.59
34:X:20:ILE:HG22	55:OX:434:LEU:HD23	1.83	0.59
12:e:205:LEU:HB3	13:f:168:GLU:HB2	1.83	0.59
57:Ad:184:THR:HA	57:Ad:187:ILE:HG12	1.84	0.58
57:Ad:132:THR:HA	57:Ad:135:LEU:HD12	1.85	0.58
57:Ad:166:ASP:HA	57:Ad:181:LEU:HD23	1.85	0.58
51:A:2545:U:H5''	51:A:2546:G:H5'	1.85	0.58
50:Ag:344:VAL:HG11	50:Ag:349:ILE:HD11	1.84	0.58
17:G:132:VAL:HG23	17:G:172:ILE:HB	1.84	0.58
49:z:108:LYS:O	49:z:112:LEU:HB2	2.03	0.58
50:Ag:358:GLN:HA	50:Ag:408:LYS:HA	1.86	0.58
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.86	0.58
22:L:114:PRO:HD3	22:L:136:LYS:HB3	1.86	0.57
15:E:244:ALA:HB1	15:E:248:ILE:HD11	1.85	0.57
17:t:75:THR:OG1	17:w:68:VAL:HG12	2.04	0.57
57:Ad:105:ASN:HB3	57:Ad:107:ARG:HH22	1.69	0.57
9:8:117:LEU:HD11	12:e:69:GLU:HB3	1.86	0.57
22:L:111:ASN:HB2	57:Ad:164:THR:HG22	1.87	0.57
13:f:90:VAL:HG13	13:f:189:HIS:HB3	1.86	0.57
51:A:2055:U:H2'	51:A:2056:G:H8	1.70	0.56
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.88	0.56
51:A:1862:U:H2'	51:A:1863:A:H8	1.70	0.56
54:s:63:ILE:HA	54:s:66:TRP:CD1	2.40	0.56
9:8:125:LYS:HD3	60:B:29:C:H5''	1.88	0.56
51:A:2006:C:H2'	51:A:2007:U:C6	2.41	0.56
49:z:69:ILE:HD12	49:z:72:ILE:HD11	1.87	0.56
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.71	0.55
50:Ag:66:ILE:HD12	50:Ag:140:MET:HE1	1.88	0.55
37:b:72:VAL:HG13	37:b:90:HIS:HB2	1.88	0.55
24:N:218:ILE:HG23	24:N:223:MET:HB2	1.88	0.55
49:z:115:THR:HG22	51:A:2778:U:H5''	1.87	0.55
6:5:289:HIS:O	6:5:343:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:3158:A:H2'	51:A:3159:A:C8	2.42	0.55
50:Ag:428:ARG:HG2	50:Ag:433:THR:HA	1.88	0.55
18:H:201:VAL:HA	49:z:86:VAL:HG12	1.88	0.55
50:Ag:362:LEU:HD12	50:Ag:366:GLU:HG2	1.89	0.55
60:B:30:A:H2'	60:B:31:A:H8	1.71	0.55
46:o:15:ARG:HB3	46:o:18:ILE:HG12	1.88	0.54
17:w:67:LEU:HA	17:w:70:ASP:HB2	1.90	0.54
51:A:2093:U:H2'	51:A:2094:G:C8	2.42	0.54
17:w:64:ILE:O	17:w:68:VAL:HG23	2.08	0.54
50:Ag:296:LEU:HD11	50:Ag:418:ILE:HD11	1.89	0.54
17:G:157:ASN:HD22	50:Ag:161:MET:HG3	1.72	0.54
51:A:2099:U:H2'	51:A:2100:C:C6	2.41	0.54
51:A:2718:C:H2'	51:A:2991:U:H4'	1.90	0.54
57:Ad:143:VAL:HG22	57:Ad:147:LYS:HE3	1.90	0.54
20:J:140:VAL:O	20:J:144:ILE:HG12	2.08	0.53
1:0:138:ARG:HB3	51:A:2321:A:C8	2.43	0.53
23:M:281:LYS:HG2	38:g:42:VAL:HG22	1.90	0.53
50:Ag:354:LYS:HG2	50:Ag:443:LEU:HD13	1.89	0.53
50:Ag:262:LEU:HA	50:Ag:344:VAL:HG12	1.91	0.53
17:G:132:VAL:HG12	17:G:197:LEU:HB3	1.90	0.53
17:G:134:LEU:HA	17:G:195:VAL:HA	1.89	0.53
11:d:138:PRO:HG3	11:d:194:VAL:HG23	1.91	0.53
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.73	0.53
50:Ag:303:ARG:HH21	50:Ag:346:PRO:HG2	1.74	0.53
59:Af:119:ILE:HD13	59:Af:135:ALA:HB1	1.89	0.53
51:A:2727:C:H2'	51:A:2728:C:C6	2.44	0.52
51:A:3211:C:H4'	51:A:3212:C:H5	1.74	0.52
40:i:61:GLY:HA3	51:A:1886:G:H1	1.74	0.52
51:A:3158:A:H2'	51:A:3159:A:H8	1.74	0.52
51:A:3224:G:H2'	51:A:3225:G:H8	1.75	0.52
60:B:23:A:H2'	60:B:24:G:C8	2.45	0.52
11:d:48:PRO:HG2	32:V:102:MET:HE3	1.92	0.52
12:e:183:THR:HG23	12:e:186:GLY:N	2.21	0.52
49:z:198:VAL:HB	49:z:230:ILE:HG23	1.92	0.52
15:E:50:ASP:HA	15:E:53:LEU:HG	1.91	0.52
18:H:98:LEU:HD11	18:H:105:VAL:HG23	1.90	0.52
19:I:47:LEU:HD22	24:N:226:ILE:HG12	1.92	0.52
23:M:44:ARG:HG3	23:M:45:ARG:HG3	1.90	0.52
29:S:96:PHE:HB3	37:b:126:ILE:HD13	1.90	0.52
51:A:2409:A:H2'	51:A:2410:U:C6	2.45	0.52
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:88:SER:HA	20:J:151:LEU:HD11	1.91	0.52
47:q:168:VAL:HG12	47:q:175:PHE:HB2	1.92	0.52
11:d:115:THR:O	11:d:119:GLN:HG2	2.10	0.52
6:5:299:LEU:HB2	6:5:302:HIS:HD2	1.74	0.51
11:d:52:THR:HG23	11:d:55:GLU:H	1.75	0.51
19:I:116:LEU:HG	19:I:121:ILE:HB	1.92	0.51
54:s:145:VAL:HG21	54:s:187:LEU:HD11	1.91	0.51
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.25	0.51
40:i:75:ARG:HH22	51:A:1765:C:H5'	1.75	0.51
47:q:191:LYS:HA	47:q:194:LYS:HG2	1.91	0.51
50:Ag:360:TYR:HE2	50:Ag:362:LEU:HD13	1.75	0.51
51:A:2086:A:H2'	51:A:2087:U:C6	2.45	0.51
54:s:84:THR:HB	54:s:280:ASN:HB2	1.93	0.51
59:Af:88:LYS:HB2	59:Af:95:PRO:HG3	1.91	0.51
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.91	0.51
24:N:124:VAL:HG12	24:N:158:ARG:HE	1.76	0.51
12:e:219:GLN:HA	12:e:222:ARG:HB2	1.93	0.51
15:E:80:LEU:HD12	15:E:323:GLY:HA3	1.93	0.51
50:Ag:353:GLN:H	50:Ag:444:ALA:HA	1.76	0.51
7:6:173:LEU:HD13	7:6:272:LEU:HD22	1.92	0.51
54:s:243:ILE:HD13	54:s:296:HIS:HD2	1.75	0.51
58:Ae:3:PRO:HB3	59:Af:112:4HH:HS2	1.92	0.51
57:Ad:145:MET:HE3	57:Ad:149:LEU:HD11	1.92	0.51
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.92	0.51
58:Ae:17:LEU:HB2	59:Af:120:MET:HE1	1.92	0.51
9:8:192:TYR:HE1	13:f:134:VAL:HG22	1.75	0.51
23:M:261:ASP:HB3	23:M:264:GLN:HB2	1.93	0.51
51:A:2081:U:H2'	51:A:2082:G:C8	2.45	0.51
59:Af:112:4HH:HL22	59:Af:113:LEU:HD11	1.93	0.51
48:r:99:MET:HE1	48:r:115:ILE:HG22	1.93	0.51
49:z:119:GLN:HB2	49:z:260:LEU:HD12	1.93	0.51
17:G:148:GLU:O	17:G:152:TYR:HB3	2.11	0.50
25:O:50:ASP:HB2	25:O:107:MET:HE1	1.92	0.50
51:A:1952:U:H2'	51:A:1953:A:C8	2.46	0.50
9:8:187:PRO:HG2	44:m:79:ILE:HD11	1.92	0.50
58:Ae:15:ALA:HB3	58:Ae:62:LEU:HD11	1.92	0.50
51:A:2408:U:H2'	51:A:2409:A:H8	1.76	0.50
51:A:2727:C:H2'	51:A:2728:C:H6	1.75	0.50
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.93	0.50
49:z:184:ILE:HG22	49:z:209:ARG:HH21	1.76	0.50
54:s:137:LEU:HD21	54:s:422:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.93	0.50
25:O:10:SER:HB2	51:A:2457:A:H3'	1.93	0.50
17:u:74:LEU:HD23	17:u:79:ILE:HG12	1.93	0.50
50:Ag:364:LYS:HG2	50:Ag:370:HIS:HA	1.93	0.50
51:A:2392:U:H2'	51:A:2394:A:H62	1.75	0.50
51:A:2598:A:H3'	51:A:2625:C:H42	1.76	0.50
12:e:269:LEU:HA	12:e:272:VAL:HG12	1.94	0.50
50:Ag:271:VAL:HB	50:Ag:274:ARG:HB2	1.93	0.50
22:L:75:LEU:HD11	22:L:105:VAL:HG21	1.94	0.49
50:Ag:356:GLU:HB3	50:Ag:441:ASN:HB3	1.94	0.49
8:7:244:ALA:HB1	8:7:250:ARG:HE	1.77	0.49
19:I:154:LEU:HD12	19:I:164:MET:HE3	1.94	0.49
27:Q:148:THR:HG22	27:Q:165:GLU:HG2	1.94	0.49
29:S:173:ARG:HB2	29:S:182:LYS:HG3	1.94	0.49
17:y:65:GLN:HA	17:y:68:VAL:HG12	1.94	0.49
51:A:2339:G:H21	51:A:2427:C:H5'	1.77	0.49
57:Ad:124:PHE:HE2	57:Ad:190:LEU:HD13	1.76	0.49
50:Ag:351:PRO:HB2	50:Ag:416:PRO:HB2	1.94	0.49
20:J:114:LEU:HB3	43:l:96:LEU:HD21	1.94	0.49
51:A:1828:A:H4'	51:A:1829:A:C8	2.47	0.49
51:A:2734:A:H2'	51:A:2735:G:H8	1.77	0.49
57:Ad:151:CYS:HB3	57:Ad:154:ASP:HB2	1.94	0.49
59:Af:85:TYR:O	59:Af:88:LYS:HG3	2.11	0.49
9:8:201:GLN:HB3	13:f:201:ARG:HG3	1.94	0.49
22:L:32:ILE:HD11	22:L:103:ASN:HB3	1.95	0.49
17:t:86:LEU:HG	17:u:71:ILE:HD11	1.94	0.49
51:A:2151:A:H2'	51:A:2152:A:C8	2.48	0.49
51:A:3143:U:H2'	51:A:3144:A:H8	1.78	0.49
13:f:190:THR:HG23	13:f:192:GLU:HG3	1.95	0.49
51:A:2514:C:H2'	51:A:2515:U:H6	1.78	0.49
51:A:2894:U:H5''	51:A:2895:U:O4'	2.13	0.49
51:A:3163:G:H2'	51:A:3164:C:H6	1.77	0.49
58:Ae:12:LEU:HD12	58:Ae:62:LEU:HD13	1.95	0.49
7:6:161:LEU:HD23	7:6:300:THR:HG21	1.95	0.48
17:t:76:LEU:HA	17:t:79:ILE:HB	1.95	0.48
49:z:78:MET:HE1	49:z:93:PRO:HD2	1.95	0.48
51:A:3120:C:H5'	57:Ad:156:HIS:CE1	2.48	0.48
16:F:249:ASN:N	16:F:249:ASN:HD22	2.11	0.48
23:M:177:ALA:HB1	23:M:203:ARG:HH12	1.78	0.48
24:N:36:VAL:HG11	43:l:124:GLN:HB3	1.95	0.48
51:A:3071:U:H2'	51:A:3072:U:H2'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:69:LYS:HB2	5:4:72:LEU:HD23	1.96	0.48
51:A:2318:A:H2'	51:A:2319:A:C8	2.48	0.48
51:A:3102:U:H2'	51:A:3103:C:H6	1.78	0.48
57:Ad:110:CYS:HA	58:Ae:26:THR:HG23	1.94	0.48
51:A:1862:U:H2'	51:A:1863:A:C8	2.48	0.48
51:A:3115:U:H2'	51:A:3116:C:H6	1.79	0.48
11:d:186:VAL:HG21	11:d:239:PRO:HB3	1.95	0.48
12:e:165:PHE:O	67:B:101:VAL:N	2.46	0.48
18:H:174:VAL:HG12	18:H:192:HIS:HB3	1.94	0.48
19:I:203:VAL:HA	19:I:206:GLU:HB2	1.95	0.48
23:M:40:PRO:HG3	51:A:1868:G:H2'	1.96	0.48
29:S:163:LYS:HB2	37:b:106:ASP:HB3	1.94	0.48
59:Af:82:ARG:HH21	59:Af:125:GLU:HG2	1.79	0.48
12:e:124:TRP:CD2	44:m:72:ARG:HG2	2.48	0.48
17:G:165:VAL:HA	17:G:168:LEU:HG	1.96	0.48
34:X:168:ARG:HH11	34:X:176:LEU:HB2	1.79	0.48
12:e:218:PRO:HG2	67:B:101:VAL:HG22	1.95	0.48
35:Y:176:ILE:HG21	55:OX:430:TRP:CG	2.48	0.48
57:Ad:150:LYS:HG2	57:Ad:154:ASP:HB3	1.96	0.48
6:5:204:VAL:HG13	54:s:152:GLN:HE21	1.78	0.48
59:Af:104:PHE:HB3	59:Af:110:LEU:HD12	1.96	0.48
8:7:302:LEU:HD23	25:O:144:LEU:HD23	1.94	0.47
47:q:138:GLN:O	47:q:141:GLU:HG3	2.14	0.47
51:A:3054:G:H2'	51:A:3055:U:C6	2.49	0.47
20:J:151:LEU:HD23	51:A:2174:G:H4'	1.95	0.47
32:V:55:TYR:HB2	32:V:133:ILE:HD11	1.96	0.47
51:A:2668:A:H2'	51:A:2669:A:C8	2.49	0.47
16:F:123:GLY:HA3	16:F:142:ARG:HG2	1.97	0.47
51:A:1829:A:H2'	51:A:1830:G:H8	1.78	0.47
51:A:2127:A:H4'	51:A:2251:A:C5	2.49	0.47
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.50	0.47
32:V:16:PRO:HD2	32:V:19:TYR:HB2	1.95	0.47
51:A:2677:A:H2'	51:A:2678:A:C8	2.49	0.47
51:A:3038:U:H2'	51:A:3039:OMU:H6	1.96	0.47
51:A:3115:U:H2'	51:A:3116:C:C6	2.49	0.47
60:B:74:C:H2'	60:B:75:C:O4'	2.14	0.47
49:z:116:SER:HB2	51:A:2778:U:O2'	2.15	0.47
6:5:30:ALA:HB2	14:D:110:LEU:HD22	1.96	0.47
25:O:46:TRP:CD1	25:O:121:ALA:HB2	2.49	0.47
51:A:3150:U:H2'	51:A:3151:A:H8	1.79	0.47
50:Ag:261:PHE:CZ	50:Ag:345:LYS:HE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:c:79:LEU:HD13	52:c:214:PHE:HE2	1.78	0.47
60:B:68:C:H2'	60:B:69:U:C6	2.50	0.47
27:Q:117:LEU:HD12	27:Q:151:LEU:HD21	1.96	0.47
51:A:2803:A:H2'	51:A:2804:A:O4'	2.15	0.47
47:q:147:GLN:O	47:q:150:LYS:HG3	2.14	0.47
50:Ag:85:ALA:HB2	50:Ag:92:PHE:HB3	1.97	0.47
60:B:29:C:H2'	60:B:30:A:H8	1.80	0.47
7:6:224:HIS:CE1	7:6:227:GLU:H	2.32	0.46
12:e:257:LYS:HE2	12:e:273:ARG:HE	1.79	0.46
34:X:168:ARG:HG3	34:X:173:ASP:HB3	1.97	0.46
51:A:1750:G:H2'	51:A:1751:A:C8	2.50	0.46
27:Q:126:ALA:HB1	57:Ad:119:ARG:HB3	1.96	0.46
50:Ag:206:LEU:HD13	50:Ag:216:THR:HG21	1.96	0.46
50:Ag:287:LEU:H	50:Ag:319:ALA:HB3	1.79	0.46
20:J:117:VAL:HG21	20:J:145:ILE:HG13	1.96	0.46
22:L:136:LYS:HG3	57:Ad:167:TRP:CD2	2.51	0.46
29:S:111:GLU:HG2	37:b:19:LEU:HD11	1.96	0.46
48:r:103:LYS:NZ	51:A:2220:A:H5''	2.31	0.46
17:u:86:LEU:O	17:u:90:LEU:HB2	2.15	0.46
51:A:1911:C:H2'	51:A:1912:A:H8	1.78	0.46
51:A:1935:A:C2	51:A:1936:A:H1'	2.50	0.46
51:A:2804:A:H2'	51:A:2805:A:H8	1.80	0.46
38:g:142:GLU:HB3	46:o:88:ILE:HG13	1.97	0.46
51:A:2092:C:H2'	51:A:2093:U:C6	2.50	0.46
51:A:2277:U:H2'	51:A:2278:A:H8	1.80	0.46
16:F:138:HIS:CD2	16:F:146:TRP:HE1	2.34	0.46
24:N:227:ARG:HA	24:N:230:LEU:HB2	1.97	0.46
25:O:44:ALA:HB3	25:O:49:VAL:HG23	1.98	0.46
50:Ag:307:THR:HG21	50:Ag:330:ARG:HD2	1.98	0.46
51:A:2037:U:H4'	51:A:2040:G:N1	2.31	0.46
51:A:2483:U:H2'	51:A:2484:C:O4'	2.15	0.46
37:b:78:GLU:HG3	37:b:84:VAL:HG22	1.97	0.46
45:n:73:UNK:HA	51:A:2725:A:N1	2.30	0.46
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.97	0.46
19:I:140:TYR:HB3	19:I:143:LEU:HD12	1.97	0.46
51:A:3163:G:H2'	51:A:3164:C:C6	2.51	0.46
12:e:159:LEU:HD12	12:e:254:TRP:CH2	2.51	0.46
44:m:51:LEU:HD12	44:m:67:ARG:HB3	1.97	0.46
49:z:175:ALA:HA	49:z:234:LEU:HD23	1.98	0.46
50:Ag:63:VAL:O	50:Ag:127:HIS:HA	2.16	0.46
51:A:1839:C:H2'	51:A:1840:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:2408:U:H2'	51:A:2409:A:C8	2.51	0.46
51:A:2420:U:H2'	51:A:2421:G:H8	1.81	0.46
11:d:93:GLY:HA3	11:d:96:ARG:HB3	1.96	0.46
12:e:55:ARG:NH1	12:e:58:VAL:HG23	2.31	0.46
16:F:62:VAL:HG23	16:F:82:LEU:HB2	1.97	0.46
29:S:183:LYS:HE2	29:S:185:ILE:HD11	1.98	0.46
17:u:75:THR:O	17:u:79:ILE:HG13	2.16	0.46
17:w:79:ILE:HA	17:w:82:LEU:HD12	1.98	0.46
51:A:3090:G:H2'	51:A:3091:G:H8	1.81	0.46
52:c:228:LEU:HB2	52:c:307:PHE:HD2	1.81	0.46
12:e:55:ARG:HG3	12:e:149:LEU:HD22	1.98	0.45
22:L:125:THR:HG22	22:L:144:PHE:HB3	1.97	0.45
51:A:2942:C:H2'	51:A:2943:G:H8	1.80	0.45
51:A:3117:C:H2'	51:A:3118:U:H6	1.81	0.45
51:A:1911:C:H2'	51:A:1912:A:C8	2.51	0.45
59:Af:83:VAL:HG21	59:Af:145:VAL:HG12	1.97	0.45
59:Af:112:4HH:HO3	59:Af:112:4HH:HL3	1.52	0.45
49:z:160:PHE:HD2	49:z:199:ALA:HB2	1.82	0.45
50:Ag:263:LEU:HD11	50:Ag:287:LEU:HD21	1.97	0.45
50:Ag:294:GLU:HB2	50:Ag:346:PRO:HG3	1.97	0.45
9:8:181:PRO:HB3	44:m:60:ASP:HB2	1.99	0.45
11:d:96:ARG:HG2	11:d:97:ILE:H	1.81	0.45
33:W:67:ILE:HG21	33:W:131:VAL:HG21	1.97	0.45
17:G:134:LEU:HD13	17:G:195:VAL:HG22	1.98	0.45
47:q:141:GLU:HA	47:q:144:GLU:HG3	1.97	0.45
17:t:76:LEU:HD22	17:w:71:ILE:HG21	1.99	0.45
49:z:64:GLU:HG2	49:z:65:LYS:N	2.32	0.45
51:A:1829:A:H2'	51:A:1830:G:C8	2.51	0.45
6:5:55:LEU:HD11	34:X:163:ARG:HE	1.82	0.45
17:G:188:LEU:HA	17:G:191:VAL:HG12	1.98	0.45
32:V:139:GLU:H	55:OX:399:GLN:NE2	2.15	0.45
50:Ag:259:LYS:HB3	50:Ag:284:ARG:HH11	1.82	0.45
2:1:55:LEU:HB2	47:q:128:MET:HE1	1.99	0.45
6:5:299:LEU:HB3	6:5:301:PRO:HD2	1.99	0.45
22:L:73:ILE:HD11	22:L:105:VAL:HG11	1.99	0.45
60:B:21:A:H61	60:B:46:A:H2'	1.82	0.45
11:d:197:VAL:HG22	11:d:212:ILE:HG23	1.98	0.45
12:e:213:TYR:HB3	12:e:231:VAL:HB	1.98	0.45
51:A:2805:A:H2'	51:A:2806:U:C6	2.51	0.45
54:s:119:PRO:HG3	54:s:394:TRP:CD2	2.51	0.45
6:5:82:TYR:HE1	31:U:11:ARG:HH21	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:106:ARG:HG2	26:P:110:TRP:CE2	2.52	0.45
11:d:40:ARG:HG3	11:d:41:PHE:H	1.82	0.45
51:A:2111:C:H2'	51:A:2112:A:C8	2.51	0.45
51:A:2245:A:H4'	51:A:2246:A:OP1	2.17	0.45
57:Ad:161:GLY:HA3	57:Ad:168:LEU:HA	1.99	0.45
51:A:1895:C:H2'	51:A:1896:U:C6	2.52	0.44
51:A:1952:U:H2'	51:A:1953:A:H8	1.82	0.44
21:K:20:LEU:HD22	21:K:141:LEU:HD13	1.99	0.44
51:A:2552:U:C2	51:A:2553:G:C8	3.05	0.44
13:f:80:ILE:HG23	13:f:90:VAL:HG12	1.99	0.44
25:O:38:ARG:HB2	25:O:85:LEU:HD11	1.98	0.44
58:Ae:20:GLY:HA3	58:Ae:32:PHE:CE1	2.53	0.44
19:I:82:LEU:HB3	19:I:130:VAL:HG21	1.99	0.44
20:J:161:SER:HA	43:l:69:THR:HG21	1.99	0.44
23:M:274:VAL:HG11	47:q:75:LEU:HD13	1.98	0.44
27:Q:96:ARG:HA	27:Q:99:MET:HE3	1.98	0.44
51:A:2586:U:H2'	51:A:2587:G:H8	1.83	0.44
57:Ad:108:ASP:O	57:Ad:127:VAL:HA	2.17	0.44
59:Af:76:LEU:HB2	59:Af:154:VAL:HG11	2.00	0.44
27:Q:129:LYS:HB2	57:Ad:119:ARG:HA	1.99	0.44
50:Ag:117:GLU:HG3	50:Ag:124:HIS:CE1	2.52	0.44
51:A:1897:A:H2'	51:A:1898:A:H8	1.83	0.44
53:p:133:LEU:HD21	53:p:157:MET:HE1	1.98	0.44
11:d:220:GLN:HB2	31:U:153:LEU:HD21	2.00	0.44
49:z:98:GLU:HB3	49:z:101:LYS:HB2	2.00	0.44
51:A:2053:U:HO2'	51:A:2054:U:H6	1.63	0.44
51:A:2275:U:H2'	51:A:2276:C:C6	2.53	0.44
51:A:2868:C:H2'	51:A:2869:A:O4'	2.18	0.44
12:e:97:ARG:HA	12:e:100:LYS:HG2	1.98	0.44
24:N:104:MET:HE3	24:N:104:MET:HB3	1.87	0.44
48:r:70:CYS:HB2	48:r:107:LEU:HA	2.00	0.44
50:Ag:219:ILE:HG12	50:Ag:241:LYS:HB3	2.00	0.44
50:Ag:394:LEU:HD12	50:Ag:395:PRO:HD2	2.00	0.44
51:A:1939:G:O2'	51:A:1973:G:H4'	2.18	0.44
6:5:113:LEU:HD12	6:5:311:ALA:HB1	2.00	0.44
9:8:201:GLN:HB2	13:f:199:LYS:HE2	1.99	0.44
12:e:124:TRP:CE2	44:m:72:ARG:HG2	2.53	0.44
17:G:127:ARG:HA	17:G:127:ARG:HD2	1.80	0.44
20:J:58:LYS:HA	20:J:58:LYS:HD2	1.78	0.44
49:z:214:LEU:HB3	49:z:217:LYS:HB3	2.00	0.44
59:Af:83:VAL:O	59:Af:87:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:B:25:C:H2'	60:B:26:A:H8	1.83	0.44
27:Q:100:LEU:HD21	27:Q:286:ILE:HG12	1.98	0.44
17:u:64:ILE:O	17:u:68:VAL:HG23	2.18	0.44
51:A:3002:G:H2'	51:A:3003:A:H8	1.82	0.44
1:0:81:PRO:HA	51:A:3102:U:C2	2.53	0.43
50:Ag:219:ILE:HD13	50:Ag:242:LEU:HD22	1.99	0.43
51:A:2728:C:H2'	51:A:2729:U:H6	1.82	0.43
17:G:131:THR:HA	17:G:174:ALA:HA	2.00	0.43
22:L:142:GLN:HG3	57:Ad:203:LEU:HD11	2.00	0.43
25:O:47:ALA:HB3	51:A:2455:U:H5'	2.00	0.43
51:A:1863:A:H2'	51:A:1864:A:C8	2.53	0.43
7:6:175:VAL:HG22	7:6:204:VAL:HG22	2.00	0.43
12:e:97:ARG:HH11	12:e:112:GLN:HE22	1.66	0.43
27:Q:146:GLY:O	51:A:3151:A:H4'	2.18	0.43
47:q:117:ARG:O	47:q:121:ILE:HG12	2.19	0.43
49:z:133:LYS:HE3	49:z:286:LEU:HD13	2.00	0.43
51:A:1936:A:H4'	51:A:1937:A:C8	2.53	0.43
51:A:2950:U:H2'	51:A:2951:A:H8	1.83	0.43
29:S:119:GLU:HG2	29:S:189:PRO:HB2	1.99	0.43
50:Ag:105:ARG:HB3	57:Ad:148:HIS:CE1	2.54	0.43
51:A:2275:U:H2'	51:A:2276:C:H6	1.83	0.43
51:A:2995:G:H1	51:A:3067:PSU:HN3	1.66	0.43
57:Ad:135:LEU:HD11	57:Ad:181:LEU:HD22	2.00	0.43
2:1:55:LEU:H	47:q:128:MET:HE2	1.84	0.43
8:7:286:LEU:HD11	8:7:296:ARG:HB2	2.01	0.43
50:Ag:255:ARG:HH22	50:Ag:257:LEU:HD21	1.82	0.43
51:A:2286:A:H2'	51:A:2287:U:C6	2.54	0.43
46:o:12:ILE:HG13	46:o:23:ARG:HB2	2.01	0.43
50:Ag:199:GLU:HA	50:Ag:202:ILE:HD12	2.01	0.43
54:s:142:LEU:HD13	54:s:422:VAL:HG21	1.99	0.43
21:K:5:SER:HB2	21:K:8:PRO:HD2	2.01	0.43
51:A:2415:C:H3'	54:s:165:ARG:NH2	2.34	0.43
51:A:3201:A:H2'	51:A:3202:U:O4'	2.19	0.43
60:B:43:G:H2'	60:B:44:A:C8	2.53	0.43
14:D:109:PHE:CE1	14:D:208:ARG:HD3	2.54	0.43
16:F:249:ASN:N	16:F:249:ASN:ND2	2.67	0.43
51:A:1924:U:H2'	51:A:1925:A:C8	2.54	0.43
54:s:65:ARG:O	54:s:69:THR:HG23	2.19	0.43
1:0:134:THR:HG23	25:O:130:LEU:HD22	2.01	0.43
50:Ag:286:ILE:HG23	50:Ag:319:ALA:H	1.84	0.43
51:A:1806:U:H4'	51:A:1807:U:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:s:152:GLN:HA	54:s:156:TYR:HB2	2.00	0.43
58:Ae:65:LYS:HA	58:Ae:65:LYS:HD2	1.89	0.43
21:K:60:MET:HE2	21:K:133:ILE:HD11	2.00	0.42
50:Ag:309:ILE:HG22	50:Ag:325:LEU:HD12	2.00	0.42
51:A:1897:A:H2'	51:A:1898:A:C8	2.54	0.42
54:s:105:TRP:CG	54:s:271:LEU:HD13	2.54	0.42
57:Ad:127:VAL:HG23	57:Ad:179:LEU:HD13	2.00	0.42
11:d:219:ARG:HD3	11:d:239:PRO:HB2	2.00	0.42
14:D:152:ILE:HB	14:D:195:ASN:HD21	1.83	0.42
15:E:107:MET:HE3	27:Q:145:LEU:HD12	2.01	0.42
17:G:152:TYR:OH	17:G:173:LYS:HG3	2.19	0.42
17:G:180:GLU:O	17:G:183:LYS:HG3	2.19	0.42
23:M:116:ILE:HD12	23:M:152:VAL:HB	2.01	0.42
17:w:76:LEU:HD23	17:w:76:LEU:H	1.84	0.42
51:A:2815:OMG:HM23	51:A:2815:OMG:H1'	1.77	0.42
17:G:185:LYS:HD2	17:G:188:LEU:HD11	2.00	0.42
23:M:139:GLN:HB3	23:M:158:LEU:HB2	2.02	0.42
32:V:80:ILE:HB	32:V:85:TRP:HB2	2.01	0.42
43:l:87:LYS:HB3	43:l:91:GLU:OE2	2.19	0.42
50:Ag:232:PRO:HA	50:Ag:236:LEU:HD13	2.01	0.42
5:4:96:PRO:HB2	51:A:3014:G:H5''	2.00	0.42
15:E:222:TRP:CD1	15:E:256:LYS:HB3	2.55	0.42
50:Ag:182:TYR:HE1	50:Ag:238:SER:HB2	1.84	0.42
51:A:3143:U:H2'	51:A:3144:A:C8	2.53	0.42
49:z:87:TYR:CD2	49:z:92:TYR:HB2	2.54	0.42
51:A:2748:A:H2'	51:A:2749:A:H8	1.85	0.42
8:7:269:ILE:HD12	8:7:274:ILE:HB	2.02	0.42
50:Ag:262:LEU:HB3	50:Ag:283:GLU:OE2	2.20	0.42
51:A:3199:U:H5''	51:A:3200:U:H4'	2.01	0.42
11:d:168:CYS:HB2	11:d:262:HIS:O	2.19	0.42
22:L:118:ARG:NH1	57:Ad:206:ILE:HD13	2.34	0.42
58:Ae:44:LYS:H	59:Af:112:4HH:HP3	1.85	0.42
59:Af:138:LEU:HD23	59:Af:143:GLU:HB3	2.02	0.42
60:B:9:1MA:N3	60:B:45:G:H2'	2.35	0.42
8:7:77:THR:HG23	11:d:283:PRO:HA	2.02	0.42
51:A:1977:U:H2'	51:A:1978:A:H8	1.85	0.42
51:A:3144:A:H2'	51:A:3145:A:H8	1.85	0.42
11:d:201:SER:O	11:d:208:VAL:HG12	2.20	0.42
20:J:113:THR:HG23	20:J:115:LYS:H	1.83	0.42
42:k:18:VAL:HG11	42:k:34:LEU:HB2	2.01	0.42
51:A:2042:U:H2'	51:A:2043:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:2748:A:H2'	51:A:2749:A:C8	2.55	0.42
51:A:3124:U:H2'	51:A:3125:A:H8	1.85	0.42
8:7:61:ARG:CZ	11:d:235:GLN:HE22	2.33	0.42
20:J:122:ARG:HD2	20:J:137:LEU:HD21	2.02	0.42
22:L:127:LEU:HB2	22:L:138:LEU:HD21	2.02	0.42
29:S:120:LEU:HB3	29:S:122:LEU:HD12	2.01	0.42
6:5:215:ARG:HD2	6:5:364:LEU:O	2.20	0.41
11:d:90:PRO:HB2	11:d:269:TRP:HZ2	1.84	0.41
15:E:347:PHE:CE2	27:Q:170:ARG:HG2	2.55	0.41
32:V:136:ARG:NH2	55:OX:403:HIS:HB2	2.35	0.41
50:Ag:116:VAL:HG13	50:Ag:127:HIS:HB3	2.01	0.41
51:A:1912:A:H2'	51:A:1913:G:C8	2.55	0.41
14:D:198:SER:HB3	14:D:206:TYR:HE2	1.85	0.41
16:F:248:LEU:HG	16:F:253:MET:HE2	2.01	0.41
18:H:118:LEU:HD11	18:H:122:ARG:HH21	1.85	0.41
51:A:1761:A:H2'	51:A:1762:A:C8	2.55	0.41
51:A:2134:A:N6	51:A:2135:A:H62	2.19	0.41
54:s:243:ILE:HD13	54:s:296:HIS:CD2	2.55	0.41
54:s:332:LEU:HD13	54:s:372:TYR:HB2	2.01	0.41
1:0:82:LYS:HE2	51:A:2717:A:H2'	2.02	0.41
2:1:57:VAL:HG23	2:1:59:LYS:HE3	2.01	0.41
10:9:118:GLY:HA3	32:V:191:LEU:HD12	2.01	0.41
24:N:109:ILE:HD13	24:N:161:VAL:HG11	2.03	0.41
28:R:91:VAL:HG11	41:j:24:GLY:HA3	2.02	0.41
48:r:123:HIS:HB3	51:A:3191:A:H4'	2.02	0.41
51:A:2533:A:H2'	51:A:2534:G:C8	2.55	0.41
20:J:61:LYS:HD3	43:l:79:LYS:HG2	2.02	0.41
20:J:102:ARG:NH2	20:J:178:GLN:HE22	2.18	0.41
29:S:173:ARG:HB3	29:S:180:PHE:HE2	1.84	0.41
31:U:44:ILE:HG21	31:U:53:LEU:HD22	2.01	0.41
51:A:2006:C:H2'	51:A:2007:U:H6	1.81	0.41
51:A:2060:A:C8	51:A:2079:C:C4	3.08	0.41
51:A:3090:G:H2'	51:A:3091:G:C8	2.56	0.41
13:f:171:LEU:HD13	13:f:174:ILE:HD11	2.03	0.41
16:F:221:LEU:HG	16:F:222:THR:HG23	2.02	0.41
17:w:90:LEU:HA	17:y:74:LEU:HD21	2.03	0.41
50:Ag:383:SER:HB2	50:Ag:386:TRP:CZ2	2.56	0.41
51:A:3165:C:H2'	51:A:3166:U:C6	2.55	0.41
7:6:173:LEU:HD22	7:6:272:LEU:HB2	2.01	0.41
8:7:166:LEU:HB3	8:7:181:TYR:HE2	1.86	0.41
9:8:91:PRO:HD2	9:8:94:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:125:TYR:CD2	13:f:197:ARG:HD3	2.56	0.41
19:I:235:GLN:OE1	17:y:91:LYS:HA	2.20	0.41
51:A:1950:U:H2'	51:A:1951:C:C6	2.56	0.41
57:Ad:98:VAL:HA	57:Ad:101:LEU:HD12	2.02	0.41
57:Ad:100:LEU:O	57:Ad:103:GLN:HG2	2.21	0.41
38:g:164:LYS:HD2	38:g:164:LYS:HA	1.91	0.41
43:l:96:LEU:HA	43:l:99:MET:HE3	2.02	0.41
59:Af:142:GLN:HA	59:Af:145:VAL:HG22	2.03	0.41
15:E:232:GLY:HA2	51:A:1953:A:OP1	2.20	0.41
17:G:143:VAL:HA	17:G:146:ILE:HG12	2.03	0.41
28:R:111:LYS:HD3	37:b:127:GLN:HB3	2.03	0.41
31:U:132:GLU:HA	31:U:135:GLN:HB3	2.01	0.41
49:z:116:SER:HB3	51:A:2779:C:H5'	2.03	0.41
50:Ag:274:ARG:HA	50:Ag:274:ARG:HD2	1.83	0.41
59:Af:75:THR:HG23	59:Af:78:GLY:H	1.86	0.41
8:7:159:LYS:HE2	8:7:162:TYR:HE2	1.86	0.41
9:8:163:LYS:HD3	13:f:85:ASP:OD1	2.21	0.41
20:J:135:VAL:HG11	51:A:2192:A:O2'	2.21	0.41
21:K:4:PHE:HB2	21:K:9:GLN:HB2	2.03	0.41
24:N:133:ARG:HD3	51:A:2109:A:H5'	2.02	0.41
36:Z:75:THR:HB	36:Z:83:LYS:HG2	2.03	0.41
44:m:69:ARG:HG3	44:m:70:GLU:HG2	2.02	0.41
50:Ag:83:ILE:HD13	50:Ag:239:VAL:HG21	2.03	0.41
51:A:2699:C:H2'	51:A:2700:G:H8	1.86	0.41
51:A:2747:U:H2'	51:A:2748:A:H8	1.85	0.41
51:A:3142:A:H2'	51:A:3143:U:C6	2.56	0.41
52:c:160:LEU:HD21	52:c:223:MET:HG3	2.03	0.41
59:Af:86:VAL:HA	59:Af:89:LEU:HD12	2.02	0.41
60:B:29:C:C2	60:B:30:A:C8	3.09	0.41
2:1:13:SER:HB2	2:1:36:ARG:HH21	1.86	0.41
6:5:417:LEU:HD23	6:5:417:LEU:HA	1.86	0.41
8:7:150:MET:O	8:7:154:ILE:HG12	2.21	0.41
10:9:68:PHE:CE2	10:9:70:LEU:HB2	2.56	0.41
17:G:148:GLU:HB2	17:G:191:VAL:HG21	2.02	0.41
18:H:174:VAL:HG23	18:H:237:VAL:HA	2.02	0.41
21:K:67:PHE:HB3	21:K:71:LYS:HB2	2.03	0.41
40:i:38:LEU:HG	52:c:42:GLN:HG3	2.03	0.41
44:m:59:GLN:OE1	44:m:79:ILE:HG13	2.21	0.41
17:x:70:ASP:O	17:x:74:LEU:HG	2.21	0.41
18:H:176:MET:HE1	18:H:188:ILE:HD11	2.03	0.40
50:Ag:105:ARG:HG3	57:Ad:87:HIS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:1863:A:H2'	51:A:1864:A:H8	1.85	0.40
51:A:2697:G:OP2	65:A:3303:SPD:H31	2.21	0.40
51:A:3144:A:H2'	51:A:3145:A:C8	2.56	0.40
57:Ad:114:VAL:HB	57:Ad:122:ASP:HA	2.03	0.40
26:P:52:ASN:HB3	26:P:55:ASN:HB2	2.03	0.40
32:V:48:PRO:HD3	35:Y:234:LEU:HD22	2.03	0.40
46:o:12:ILE:HD13	46:o:12:ILE:HA	1.94	0.40
47:q:170:PRO:HA	47:q:175:PHE:CD1	2.56	0.40
49:z:69:ILE:HA	49:z:72:ILE:HG12	2.02	0.40
51:A:2005:C:H2'	51:A:2006:C:C6	2.55	0.40
51:A:2750:U:H2'	51:A:2751:G:H8	1.86	0.40
51:A:2804:A:H2'	51:A:2805:A:C8	2.56	0.40
31:U:131:GLU:O	31:U:134:ARG:HG3	2.20	0.40
50:Ag:68:HIS:HB3	50:Ag:71:HIS:CE1	2.57	0.40
50:Ag:101:ALA:HB3	50:Ag:112:ASN:HB3	2.04	0.40
50:Ag:421:LYS:HE3	50:Ag:421:LYS:HB3	1.84	0.40
51:A:1851:G:H2'	51:A:2693:A:N7	2.36	0.40
51:A:2134:A:H62	51:A:2135:A:H62	1.67	0.40
23:M:97:SER:HB2	23:M:143:GLU:HB3	2.03	0.40
37:b:89:ILE:HA	37:b:92:LYS:HD2	2.04	0.40
50:Ag:164:THR:O	50:Ag:167:HIS:HB2	2.22	0.40
51:A:1993:A:H8	51:A:2498:U:O2'	2.04	0.40
51:A:2688:C:H2'	51:A:2689:C:C6	2.56	0.40
17:G:142:LYS:O	17:G:146:ILE:HG12	2.22	0.40
49:z:121:VAL:HA	49:z:297:SER:HA	2.02	0.40
49:z:198:VAL:HG12	49:z:230:ILE:HG12	2.04	0.40
50:Ag:180:VAL:HG13	50:Ag:217:PRO:HG2	2.02	0.40
51:A:2542:G:H2'	51:A:2543:C:C6	2.55	0.40
51:A:3078:C:H2'	51:A:3079:G:H8	1.85	0.40
51:A:3117:C:H2'	51:A:3118:U:C6	2.57	0.40
52:c:59:ARG:HB2	52:c:62:GLU:HG2	2.03	0.40
52:c:79:LEU:HD13	52:c:214:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	385 (98%)	7 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	137/206 (66%)	135 (98%)	2 (2%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
11	d	257/306 (84%)	239 (93%)	17 (7%)	1 (0%)	30	48
12	e	236/279 (85%)	227 (96%)	9 (4%)	0	100	100
13	f	153/212 (72%)	147 (96%)	6 (4%)	0	100	100
14	D	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
15	E	303/348 (87%)	292 (96%)	11 (4%)	0	100	100
16	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
17	G	70/198 (35%)	67 (96%)	3 (4%)	0	100	100
17	t	44/198 (22%)	44 (100%)	0	0	100	100
17	u	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
17	v	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
17	w	29/198 (15%)	27 (93%)	2 (7%)	0	100	100
17	x	29/198 (15%)	28 (97%)	1 (3%)	0	100	100
17	y	29/198 (15%)	27 (93%)	2 (7%)	0	100	100
18	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
19	I	210/261 (80%)	205 (98%)	5 (2%)	0	100	100
20	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
21	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
22	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
23	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	N	220/251 (88%)	220 (100%)	0	0	100	100
25	O	152/175 (87%)	147 (97%)	5 (3%)	0	100	100
26	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
27	Q	218/292 (75%)	212 (97%)	6 (3%)	0	100	100
28	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
29	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
30	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
31	U	150/153 (98%)	145 (97%)	5 (3%)	0	100	100
32	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
33	W	114/148 (77%)	111 (97%)	3 (3%)	0	100	100
34	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
35	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
36	Z	120/161 (74%)	117 (98%)	3 (2%)	0	100	100
37	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
38	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
39	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
40	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
41	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
42	k	100/112 (89%)	100 (100%)	0	0	100	100
43	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
44	m	63/128 (49%)	61 (97%)	2 (3%)	0	100	100
46	o	92/102 (90%)	92 (100%)	0	0	100	100
47	q	175/222 (79%)	175 (100%)	0	0	100	100
48	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
49	z	250/325 (77%)	235 (94%)	15 (6%)	0	100	100
50	Ag	389/455 (86%)	382 (98%)	7 (2%)	0	100	100
52	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
53	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
54	s	381/439 (87%)	375 (98%)	6 (2%)	0	100	100
55	OX	38/435 (9%)	35 (92%)	3 (8%)	0	100	100
56	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	Ad	131/234 (56%)	126 (96%)	5 (4%)	0	100	100
58	Ae	66/70 (94%)	63 (96%)	3 (4%)	0	100	100
59	Af	84/156 (54%)	84 (100%)	0	0	100	100
All	All	9794/13730 (71%)	9572 (98%)	221 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	d	47	GLN

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	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	129/190 (68%)	129 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
11	d	237/274 (86%)	237 (100%)	0	100	100
12	e	207/236 (88%)	207 (100%)	0	100	100
13	f	139/188 (74%)	139 (100%)	0	100	100
14	D	192/245 (78%)	192 (100%)	0	100	100
15	E	260/290 (90%)	260 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	F	219/262 (84%)	218 (100%)	1 (0%)	81	90
17	G	60/158 (38%)	60 (100%)	0	100	100
17	t	40/158 (25%)	40 (100%)	0	100	100
17	u	31/158 (20%)	31 (100%)	0	100	100
17	v	31/158 (20%)	31 (100%)	0	100	100
17	w	30/158 (19%)	30 (100%)	0	100	100
17	x	30/158 (19%)	30 (100%)	0	100	100
17	y	30/158 (19%)	30 (100%)	0	100	100
18	H	182/228 (80%)	182 (100%)	0	100	100
19	I	194/232 (84%)	194 (100%)	0	100	100
20	J	138/150 (92%)	137 (99%)	1 (1%)	76	88
21	K	155/155 (100%)	155 (100%)	0	100	100
22	L	98/124 (79%)	98 (100%)	0	100	100
23	M	246/249 (99%)	246 (100%)	0	100	100
24	N	189/211 (90%)	189 (100%)	0	100	100
25	O	134/150 (89%)	134 (100%)	0	100	100
26	P	126/155 (81%)	126 (100%)	0	100	100
27	Q	202/256 (79%)	202 (100%)	0	100	100
28	R	118/126 (94%)	118 (100%)	0	100	100
29	S	146/180 (81%)	146 (100%)	0	100	100
30	T	146/176 (83%)	146 (100%)	0	100	100
31	U	134/135 (99%)	134 (100%)	0	100	100
32	V	183/191 (96%)	183 (100%)	0	100	100
33	W	94/119 (79%)	94 (100%)	0	100	100
34	X	220/229 (96%)	220 (100%)	0	100	100
35	Y	163/223 (73%)	163 (100%)	0	100	100
36	Z	113/147 (77%)	113 (100%)	0	100	100
37	b	132/186 (71%)	132 (100%)	0	100	100
38	g	124/148 (84%)	124 (100%)	0	100	100
39	h	104/148 (70%)	104 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	j	74/97 (76%)	74 (100%)	0	100	100
42	k	83/89 (93%)	83 (100%)	0	100	100
43	l	76/116 (66%)	76 (100%)	0	100	100
44	m	58/113 (51%)	58 (100%)	0	100	100
46	o	80/87 (92%)	80 (100%)	0	100	100
47	q	153/178 (86%)	153 (100%)	0	100	100
48	r	147/169 (87%)	147 (100%)	0	100	100
49	z	226/287 (79%)	226 (100%)	0	100	100
50	Ag	327/374 (87%)	327 (100%)	0	100	100
52	c	251/288 (87%)	251 (100%)	0	100	100
53	p	135/181 (75%)	135 (100%)	0	100	100
54	s	339/381 (89%)	339 (100%)	0	100	100
55	OX	38/372 (10%)	38 (100%)	0	100	100
56	a	99/133 (74%)	99 (100%)	0	100	100
57	Ad	123/200 (62%)	123 (100%)	0	100	100
58	Ae	59/60 (98%)	59 (100%)	0	100	100
59	Af	80/135 (59%)	80 (100%)	0	100	100
All	All	8767/11745 (75%)	8765 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
16	F	249	ASN
20	J	178	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	15	ASN
4	3	178	GLN
4	3	185	ASN
6	5	150	GLN
6	5	214	ASN
6	5	269	ASN
6	5	353	HIS

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Mol	Chain	Res	Type
7	6	292	GLN
7	6	295	GLN
8	7	165	ASN
8	7	287	GLN
11	d	47	GLN
11	d	77	HIS
11	d	149	HIS
13	f	111	HIS
14	D	194	ASN
14	D	195	ASN
21	K	9	GLN
21	K	40	GLN
22	L	113	ASN
26	P	142	ASN
27	Q	132	GLN
27	Q	237	ASN
30	T	56	GLN
30	T	145	GLN
31	U	41	GLN
32	V	117	HIS
34	X	93	ASN
34	X	177	HIS
35	Y	189	HIS
36	Z	98	GLN
37	b	123	ASN
39	h	110	HIS
43	l	124	GLN
43	l	125	ASN
44	m	44	HIS
47	q	60	GLN
47	q	130	GLN
47	q	134	ASN
47	q	195	GLN
48	r	79	HIS
49	z	136	ASN
50	Ag	313	HIS
50	Ag	376	HIS
50	Ag	415	GLN
53	p	117	GLN
53	p	184	ASN
53	p	194	HIS
54	s	107	GLN

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Mol	Chain	Res	Type
54	s	152	GLN
55	OX	399	GLN
56	a	126	HIS
58	Ae	22	GLN
58	Ae	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	A	1556/1558 (99%)	257 (16%)	2 (0%)
60	B	70/72 (97%)	16 (22%)	0
All	All	1626/1630 (99%)	273 (16%)	2 (0%)

All (273) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	A	1681	G
51	A	1689	C
51	A	1692	A
51	A	1699	C
51	A	1700	U
51	A	1704	U
51	A	1708	A
51	A	1709	G
51	A	1711	C
51	A	1724	A
51	A	1727	A
51	A	1728	U
51	A	1736	A
51	A	1748	G
51	A	1765	C
51	A	1777	A
51	A	1780	U
51	A	1805	A
51	A	1806	U
51	A	1807	U
51	A	1808	A
51	A	1812	C
51	A	1817	C
51	A	1821	A
51	A	1827	C

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Mol	Chain	Res	Type
51	A	1828	A
51	A	1829	A
51	A	1832	A
51	A	1836	A
51	A	1844	A
51	A	1854	U
51	A	1856	A
51	A	1869	A
51	A	1871	A
51	A	1873	A
51	A	1878	U
51	A	1882	A
51	A	1886	G
51	A	1887	A
51	A	1888	G
51	A	1893	A
51	A	1901	C
51	A	1902	C
51	A	1903	C
51	A	1909	A
51	A	1918	G
51	A	1927	G
51	A	1937	A
51	A	1940	A
51	A	1985	G
51	A	1992	C
51	A	1993	A
51	A	1994	A
51	A	2001	C
51	A	2003	A
51	A	2015	G
51	A	2022	G
51	A	2030	U
51	A	2036	C
51	A	2037	U
51	A	2039	A
51	A	2054	U
51	A	2055	U
51	A	2060	A
51	A	2069	U
51	A	2071	U
51	A	2079	C

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Mol	Chain	Res	Type
51	A	2099	U
51	A	2105	G
51	A	2113	G
51	A	2125	C
51	A	2126	U
51	A	2147	G
51	A	2155	A
51	A	2159	U
51	A	2160	A
51	A	2163	A
51	A	2168	U
51	A	2181	A
51	A	2182	G
51	A	2191	A
51	A	2192	A
51	A	2195	A
51	A	2196	A
51	A	2198	A
51	A	2200	A
51	A	2207	A
51	A	2214	A
51	A	2219	C
51	A	2220	A
51	A	2221	C
51	A	2223	A
51	A	2224	C
51	A	2225	C
51	A	2226	U
51	A	2230	A
51	A	2233	U
51	A	2237	A
51	A	2241	A
51	A	2243	A
51	A	2245	A
51	A	2246	A
51	A	2262	C
51	A	2263	C
51	A	2284	C
51	A	2285	U
51	A	2297	A
51	A	2300	G
51	A	2322	C

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Mol	Chain	Res	Type
51	A	2324	U
51	A	2331	C
51	A	2332	C
51	A	2345	G
51	A	2349	G
51	A	2350	A
51	A	2353	A
51	A	2354	A
51	A	2357	C
51	A	2363	A
51	A	2372	U
51	A	2374	A
51	A	2379	C
51	A	2390	A
51	A	2399	A
51	A	2401	A
51	A	2404	U
51	A	2407	U
51	A	2415	C
51	A	2427	C
51	A	2446	A
51	A	2451	A
51	A	2458	A
51	A	2478	G
51	A	2485	U
51	A	2493	C
51	A	2496	G
51	A	2502	C
51	A	2506	A
51	A	2511	C
51	A	2520	C
51	A	2521	A
51	A	2527	A
51	A	2540	C
51	A	2570	C
51	A	2592	G
51	A	2593	G
51	A	2594	U
51	A	2599	U
51	A	2600	A
51	A	2601	A
51	A	2603	C

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Mol	Chain	Res	Type
51	A	2618	U
51	A	2627	G
51	A	2630	U
51	A	2633	A
51	A	2635	G
51	A	2640	C
51	A	2654	U
51	A	2655	G
51	A	2656	U
51	A	2683	C
51	A	2686	G
51	A	2694	A
51	A	2696	A
51	A	2706	A
51	A	2709	A
51	A	2718	C
51	A	2719	G
51	A	2723	A
51	A	2724	G
51	A	2725	A
51	A	2732	G
51	A	2745	A
51	A	2757	A
51	A	2758	G
51	A	2762	C
51	A	2763	U
51	A	2765	A
51	A	2767	A
51	A	2768	A
51	A	2782	A
51	A	2786	U
51	A	2790	A
51	A	2810	G
51	A	2832	A
51	A	2833	A
51	A	2847	C
51	A	2864	U
51	A	2865	C
51	A	2882	U
51	A	2883	A
51	A	2884	C
51	A	2885	U

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Mol	Chain	Res	Type
51	A	2888	A
51	A	2889	C
51	A	2893	A
51	A	2913	A
51	A	2917	G
51	A	2918	A
51	A	2919	A
51	A	2922	A
51	A	2928	C
51	A	2934	G
51	A	2935	A
51	A	2956	A
51	A	2962	C
51	A	2965	A
51	A	2971	A
51	A	2985	C
51	A	2989	G
51	A	2990	A
51	A	2992	G
51	A	2993	U
51	A	3005	A
51	A	3007	C
51	A	3016	G
51	A	3022	G
51	A	3041	U
51	A	3049	U
51	A	3053	A
51	A	3054	G
51	A	3060	C
51	A	3065	U
51	A	3069	A
51	A	3072	U
51	A	3086	U
51	A	3090	G
51	A	3096	U
51	A	3100	U
51	A	3102	U
51	A	3108	U
51	A	3109	U
51	A	3110	C
51	A	3111	A
51	A	3112	A

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Mol	Chain	Res	Type
51	A	3122	U
51	A	3131	G
51	A	3157	C
51	A	3158	A
51	A	3162	C
51	A	3169	C
51	A	3172	C
51	A	3177	A
51	A	3180	A
51	A	3183	U
51	A	3190	A
51	A	3199	U
51	A	3200	U
51	A	3207	A
51	A	3209	A
51	A	3210	C
51	A	3212	C
51	A	3217	A
51	A	3218	A
51	A	3220	A
51	A	3228	U
51	A	3230	G
60	B	8	U
60	B	10	2MG
60	B	16	C
60	B	21	A
60	B	45	G
60	B	46	A
60	B	49	U
60	B	54	C
60	B	55	U
60	B	56	U
60	B	58	A
60	B	59	A
60	B	64	A
60	B	69	U
60	B	72	G
60	B	76	A

All (2) RNA pucker outliers are listed below:

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

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

9 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$
60	1MA	B	9	60	21,25,26	0.36	0	30,37,40	0.65	0
60	2MG	B	10	60	23,26,27	0.36	0	33,38,41	0.41	0
59	4HH	Af	112	59	22,26,27	0.44	0	27,35,37	1.04	3 (11%)
60	PSU	B	39	60	18,21,22	1.04	1 (5%)	21,30,33	0.71	0
51	OMG	A	3040	51	23,26,27	0.33	0	32,38,41	0.45	0
51	OMU	A	3039	62,51	19,22,23	0.31	0	25,31,34	0.77	1 (4%)
51	1MA	A	2617	51	21,25,26	0.37	0	30,37,40	0.60	0
51	OMG	A	2815	62,51	23,26,27	0.34	0	32,38,41	0.41	0
51	PSU	A	3067	51	18,21,22	1.07	2 (11%)	21,30,33	0.79	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	1MA	B	9	60	-	0/7/25/26	0/3/3/3
60	2MG	B	10	60	-	0/9/27/28	0/3/3/3
59	4HH	Af	112	59	-	11/33/35/37	-
60	PSU	B	39	60	-	0/7/25/26	0/2/2/2
51	OMG	A	3040	51	-	0/9/27/28	0/3/3/3
51	OMU	A	3039	62,51	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	1MA	A	2617	51	-	0/7/25/26	0/3/3/3
51	OMG	A	2815	62,51	-	0/9/27/28	0/3/3/3
51	PSU	A	3067	51	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	B	39	PSU	C6-C5	3.69	1.39	1.35
51	A	3067	PSU	C6-C5	3.50	1.39	1.35
51	A	3067	PSU	O4'-C1'	-2.38	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Af	112	4HH	OG-CB-CA	2.99	111.05	108.14
51	A	3039	OMU	C2'-C1'-N1	-2.80	108.93	114.24
59	Af	112	4HH	OG-P-O2P	2.67	119.54	108.94
51	A	3067	PSU	O4'-C1'-C2'	2.44	108.52	105.15
59	Af	112	4HH	P-OG-CB	2.34	134.75	121.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	Af	112	4HH	CA-CB-OG-P
59	Af	112	4HH	CB-OG-P-O1P
59	Af	112	4HH	CM-CL3-NN-CO
59	Af	112	4HH	ON-CL3-NN-CO
59	Af	112	4HH	ON-CL3-CM-OM
59	Af	112	4HH	NN-CL3-CM-OM
59	Af	112	4HH	CO-CP-CQ-NR
59	Af	112	4HH	CO-CP-CQ-OR
59	Af	112	4HH	O3P-CJ-CK-CL1
59	Af	112	4HH	O3P-CJ-CK-CL2
59	Af	112	4HH	CJ-CK-CM-CL3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	Af	112	4HH	4	0
51	A	3039	OMU	1	0
51	A	2815	OMG	1	0
51	A	3067	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 179 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
67	VAL	B	101	60	4,6,7	0.80	0	6,7,9	1.13	1 (16%)
65	SPD	A	3302	-	9,9,9	0.15	0	8,8,8	0.16	0
65	SPD	A	3303	-	9,9,9	0.16	0	8,8,8	0.23	0
66	PUT	A	3304	-	5,5,5	0.15	0	4,4,4	0.23	0
64	FES	r	201	19,48	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
67	VAL	B	101	60	-	0/5/6/8	-
65	SPD	A	3302	-	-	0/7/7/7	-
65	SPD	A	3303	-	-	1/7/7/7	-
66	PUT	A	3304	-	-	0/3/3/3	-
64	FES	r	201	19,48	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	B	101	VAL	O-C-CA	-2.61	118.07	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

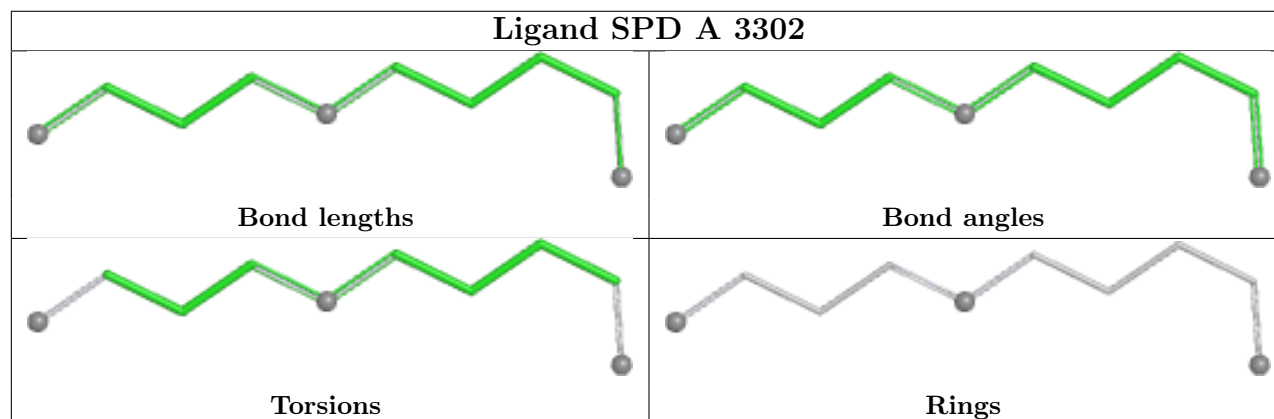
Mol	Chain	Res	Type	Atoms
65	A	3303	SPD	C2-C3-C4-C5

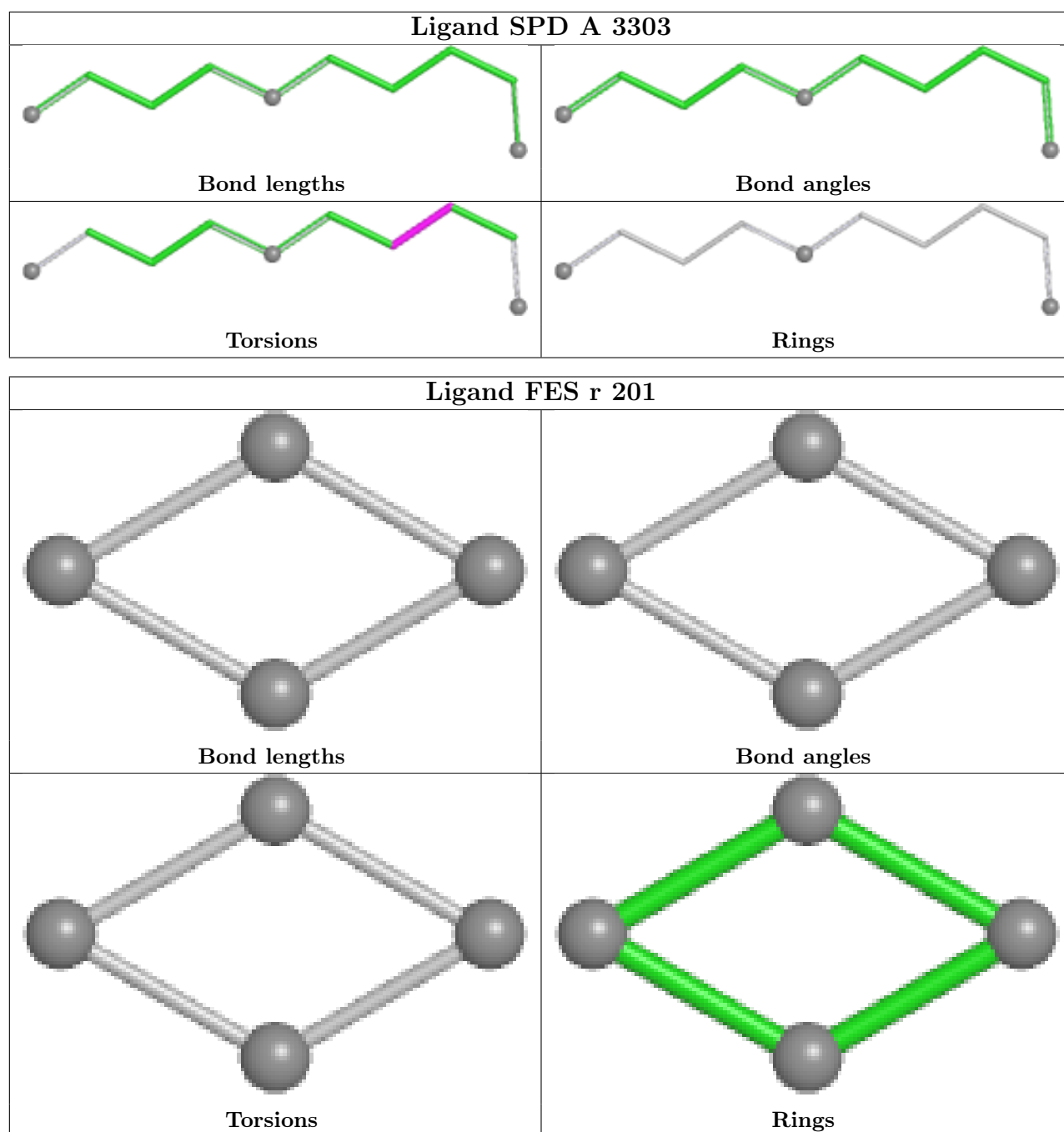
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	B	101	VAL	3	0
65	A	3303	SPD	1	0
64	r	201	FES	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	A	1
60	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	9.61
1	B	46:A	O3'	48:U	P	4.56

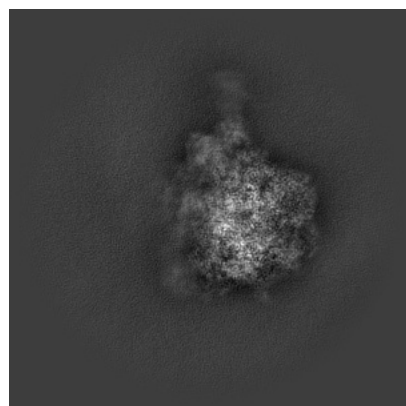
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71802. These allow visual inspection of the internal detail of the map and identification of artifacts.

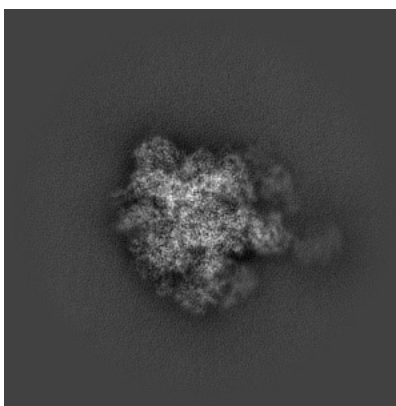
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

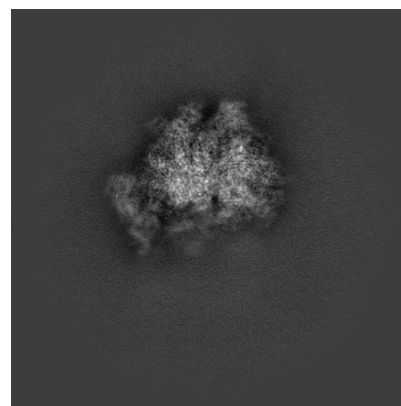
6.1.1 Primary map



X

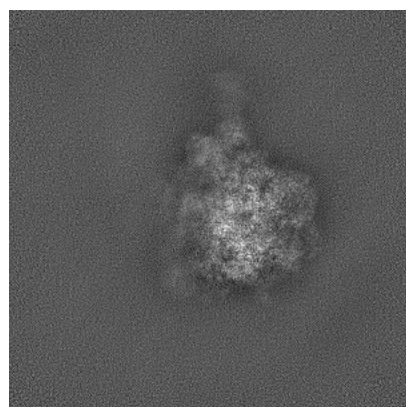


Y

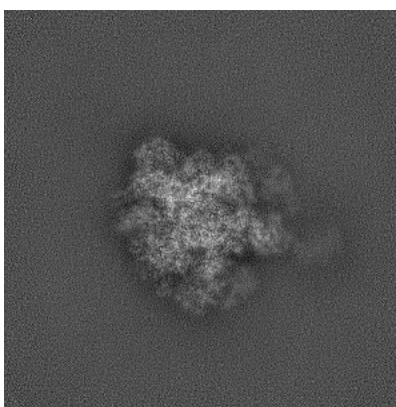


Z

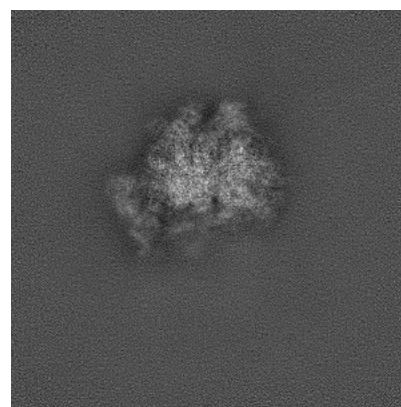
6.1.2 Raw map



X



Y

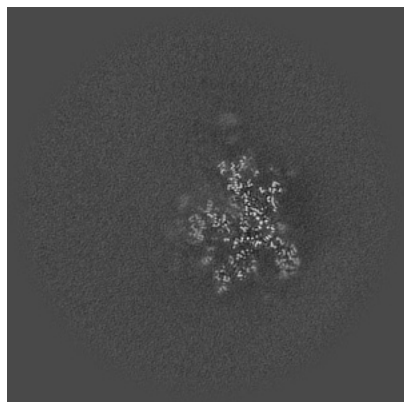


Z

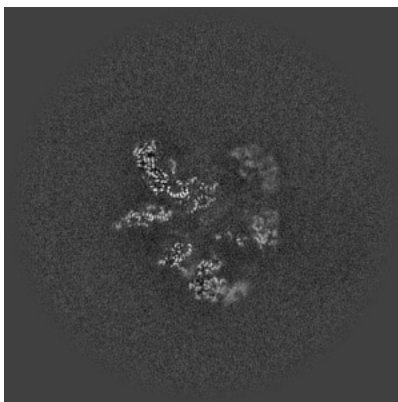
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

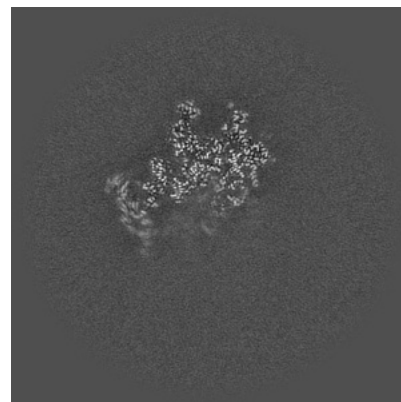
6.2.1 Primary map



X Index: 240

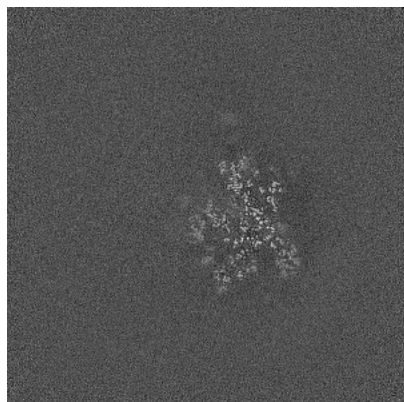


Y Index: 240

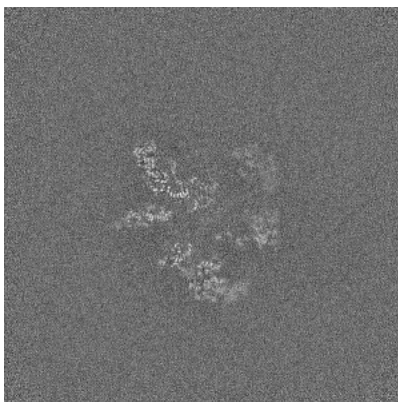


Z Index: 240

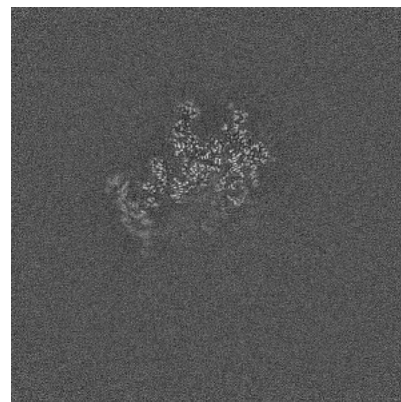
6.2.2 Raw map



X Index: 240



Y Index: 240

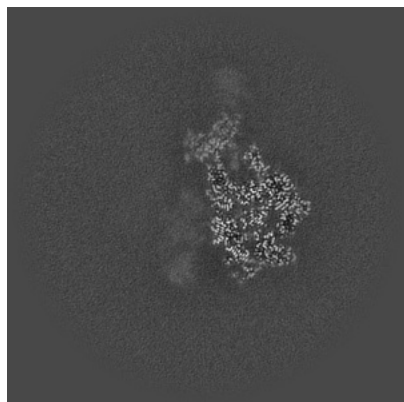


Z Index: 240

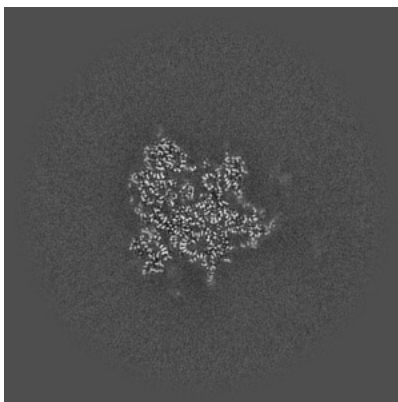
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

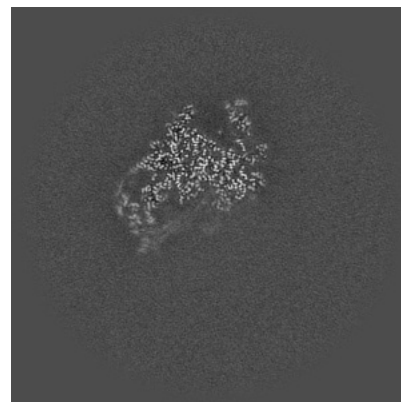
6.3.1 Primary map



X Index: 203

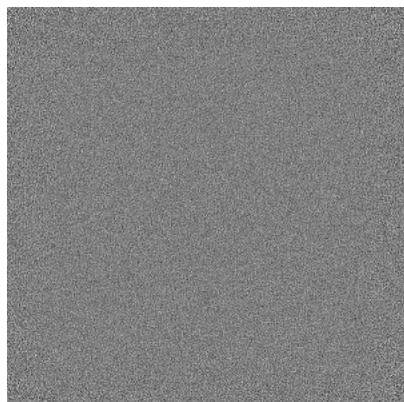


Y Index: 287

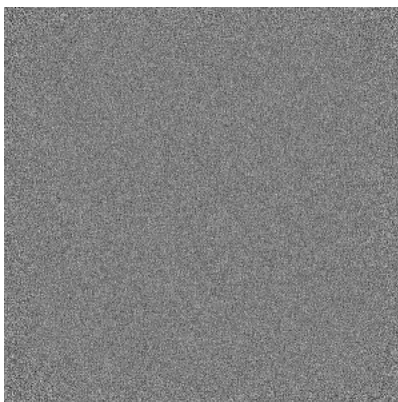


Z Index: 249

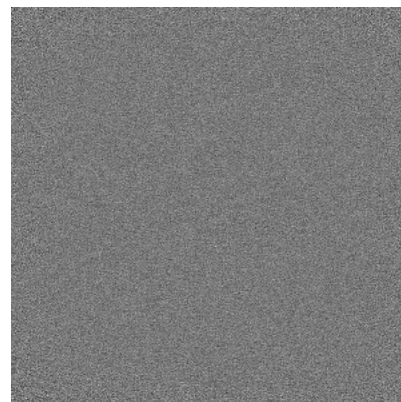
6.3.2 Raw map



X Index: 0



Y Index: 0

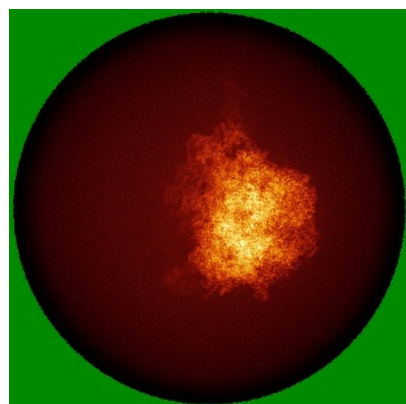


Z Index: 0

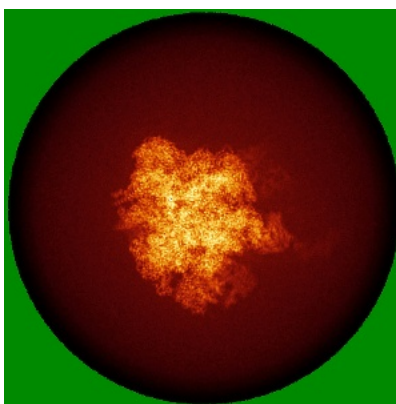
The images above show the largest variance slices of the map in three orthogonal directions.

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

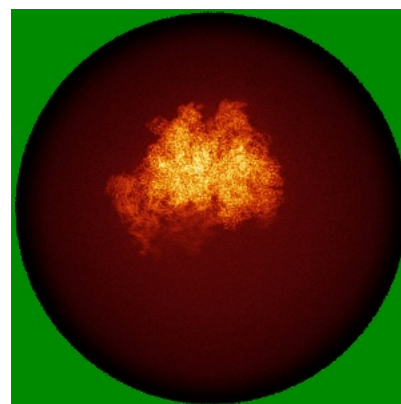
6.4.1 Primary map



X

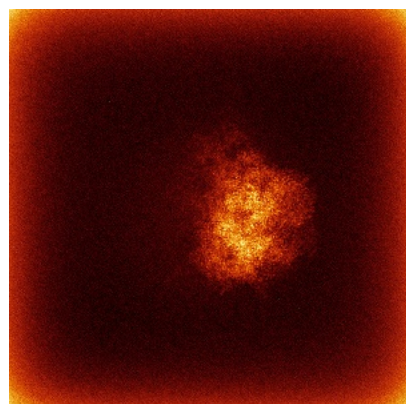


Y

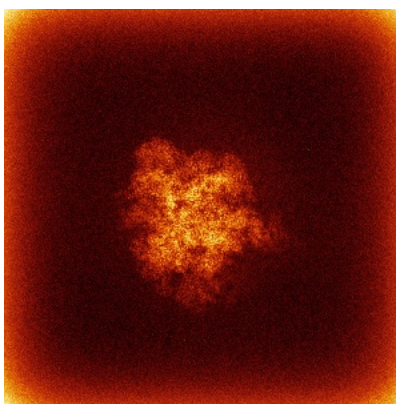


Z

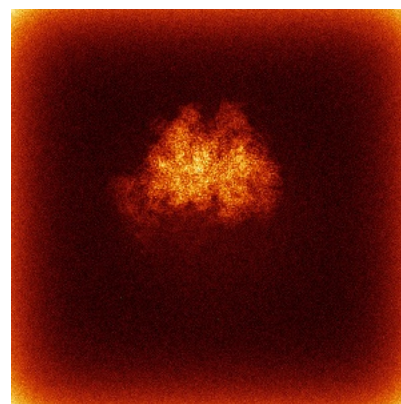
6.4.2 Raw map



X



Y

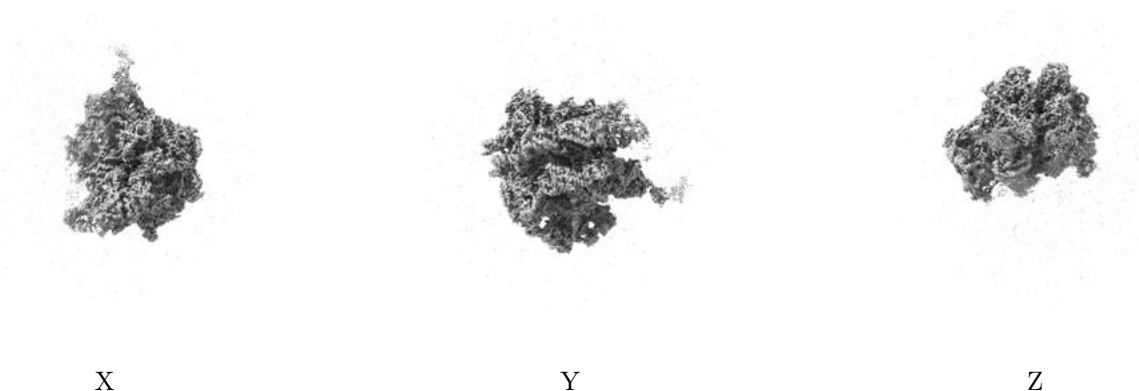


Z

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

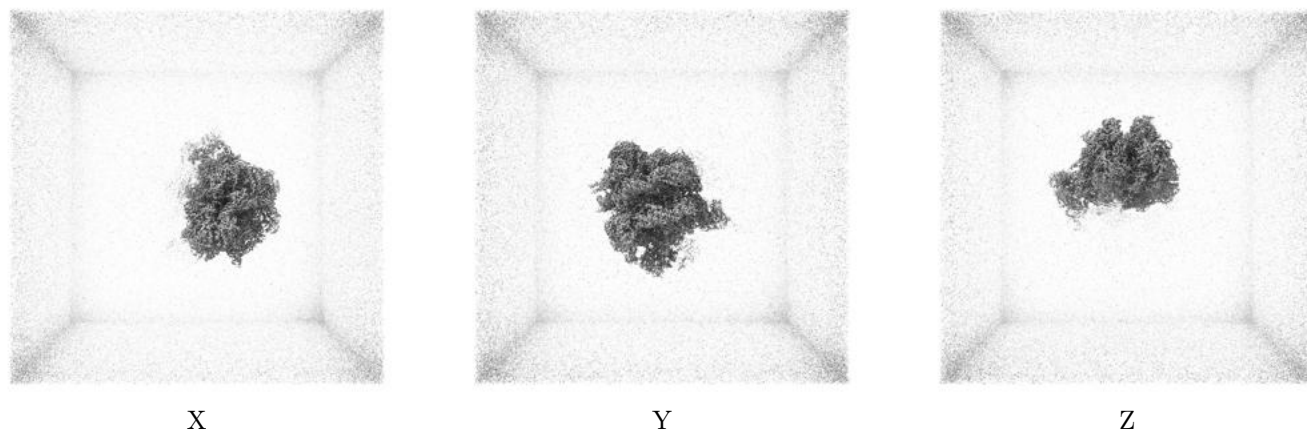
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

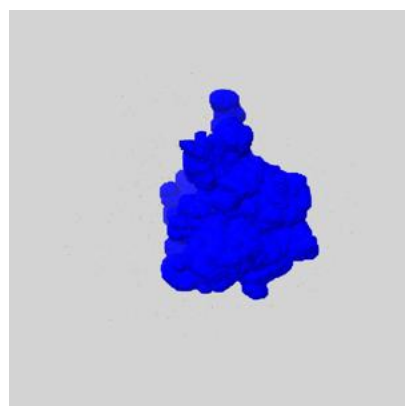
6.6 Mask visualisation [i](#)

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

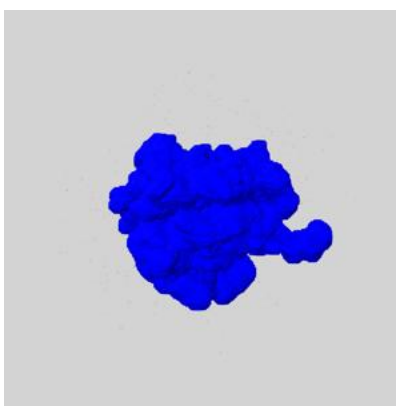
A mask typically either:

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

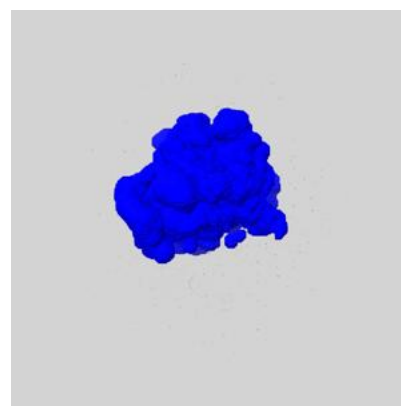
6.6.1 emd_71802_msk_1.map [i](#)



X



Y

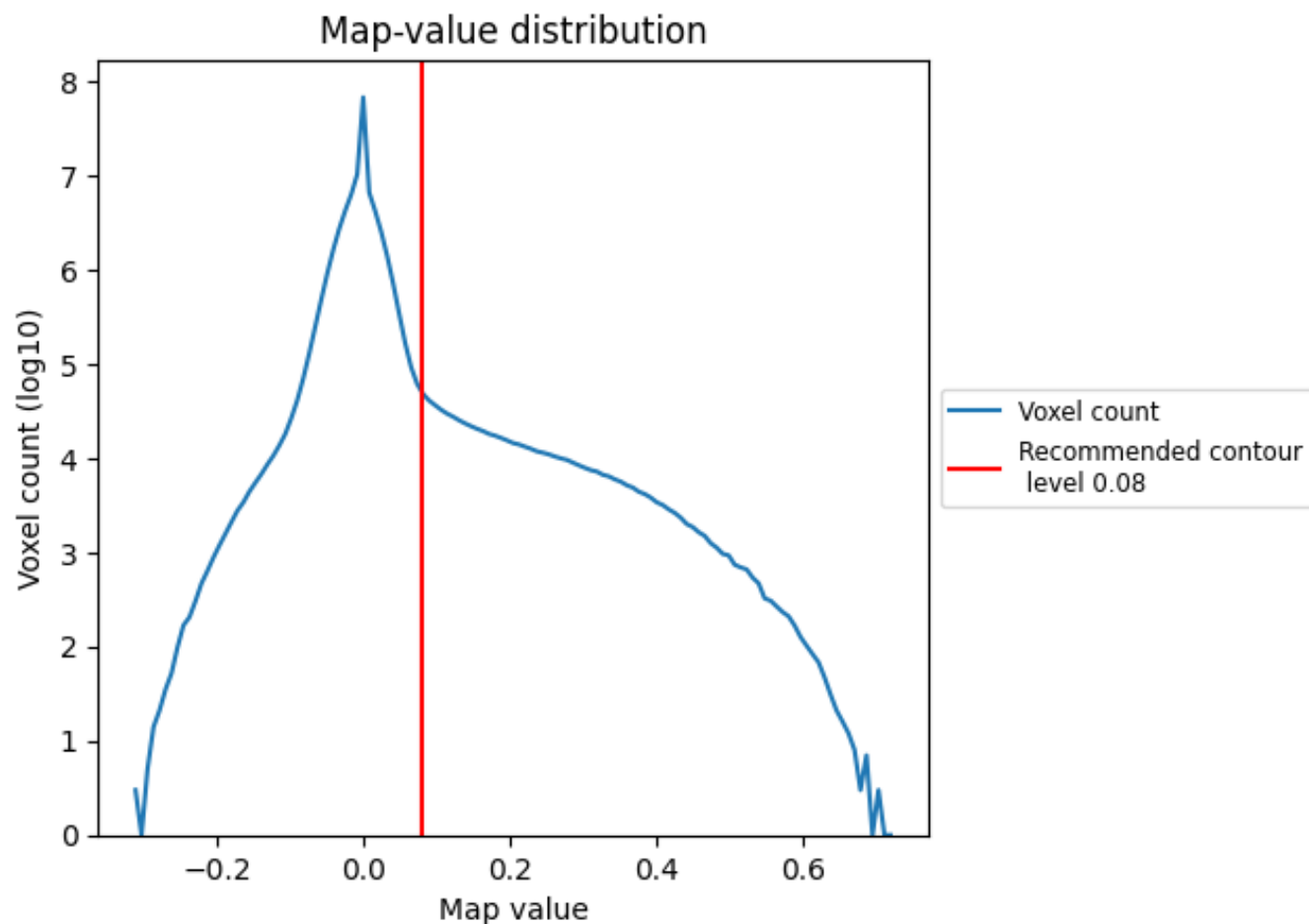


Z

7 Map analysis [i](#)

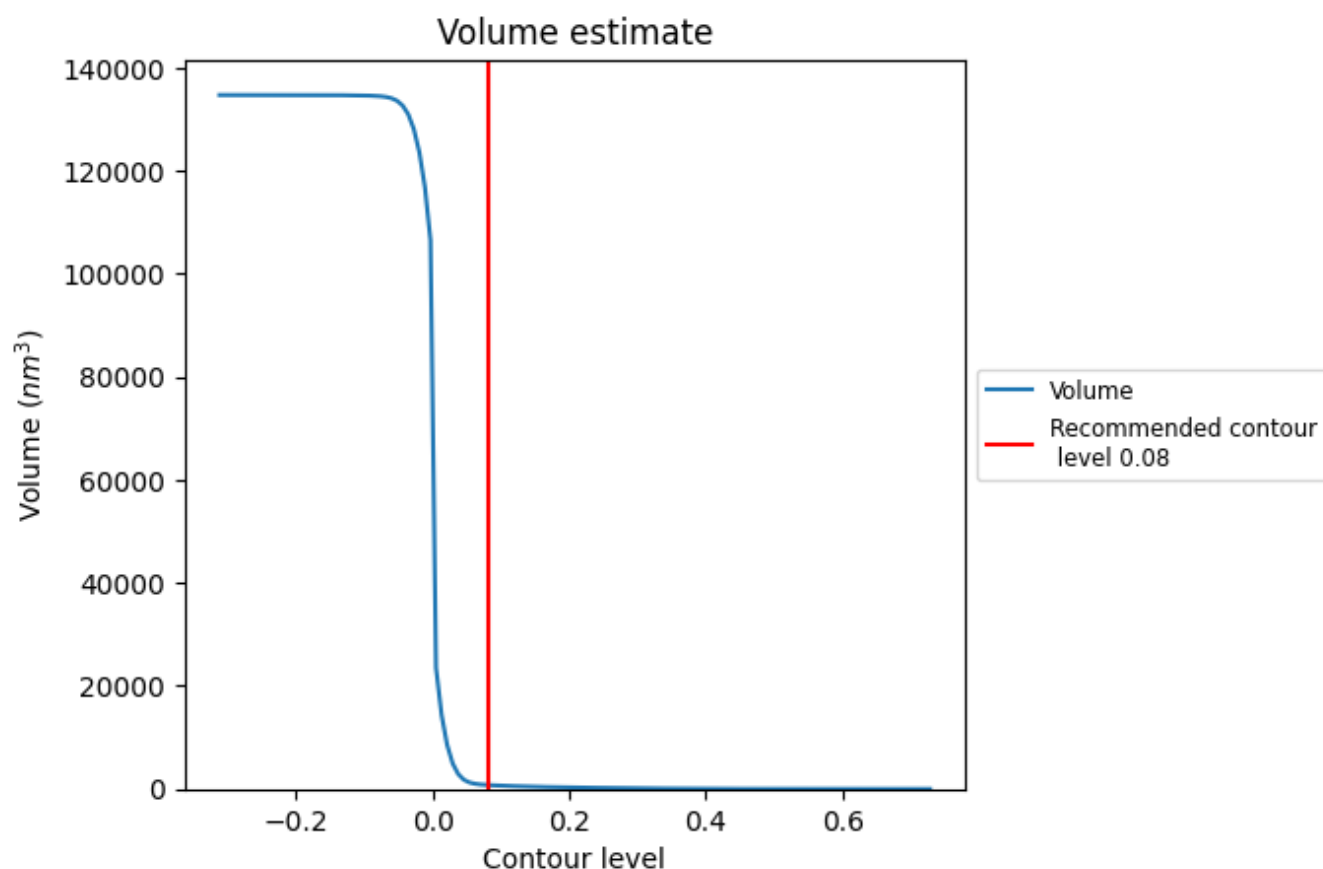
This section contains the results of statistical analysis of the map.

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.

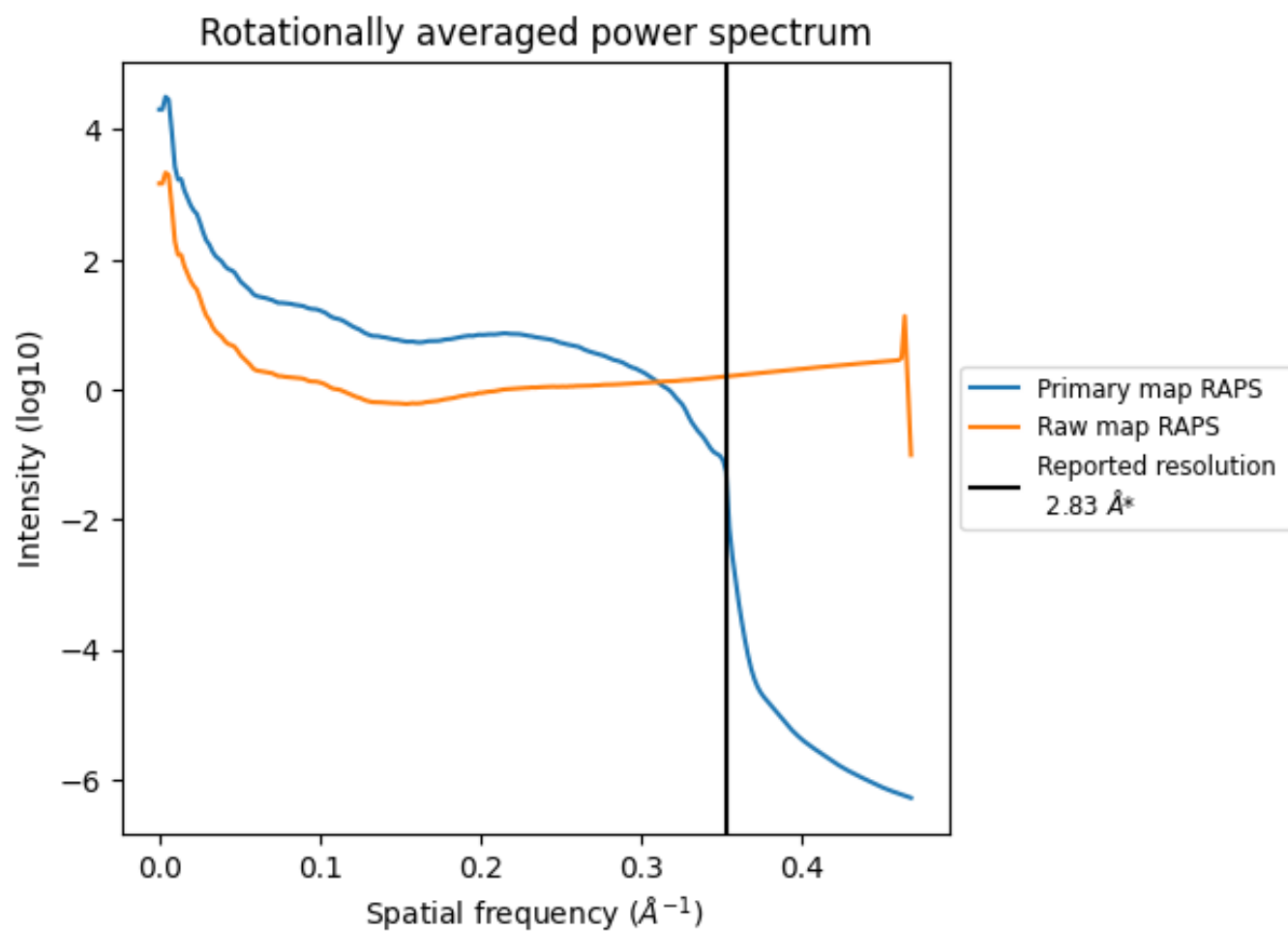
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 772 nm^3 ; this corresponds to an approximate mass of 697 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 ⓘ

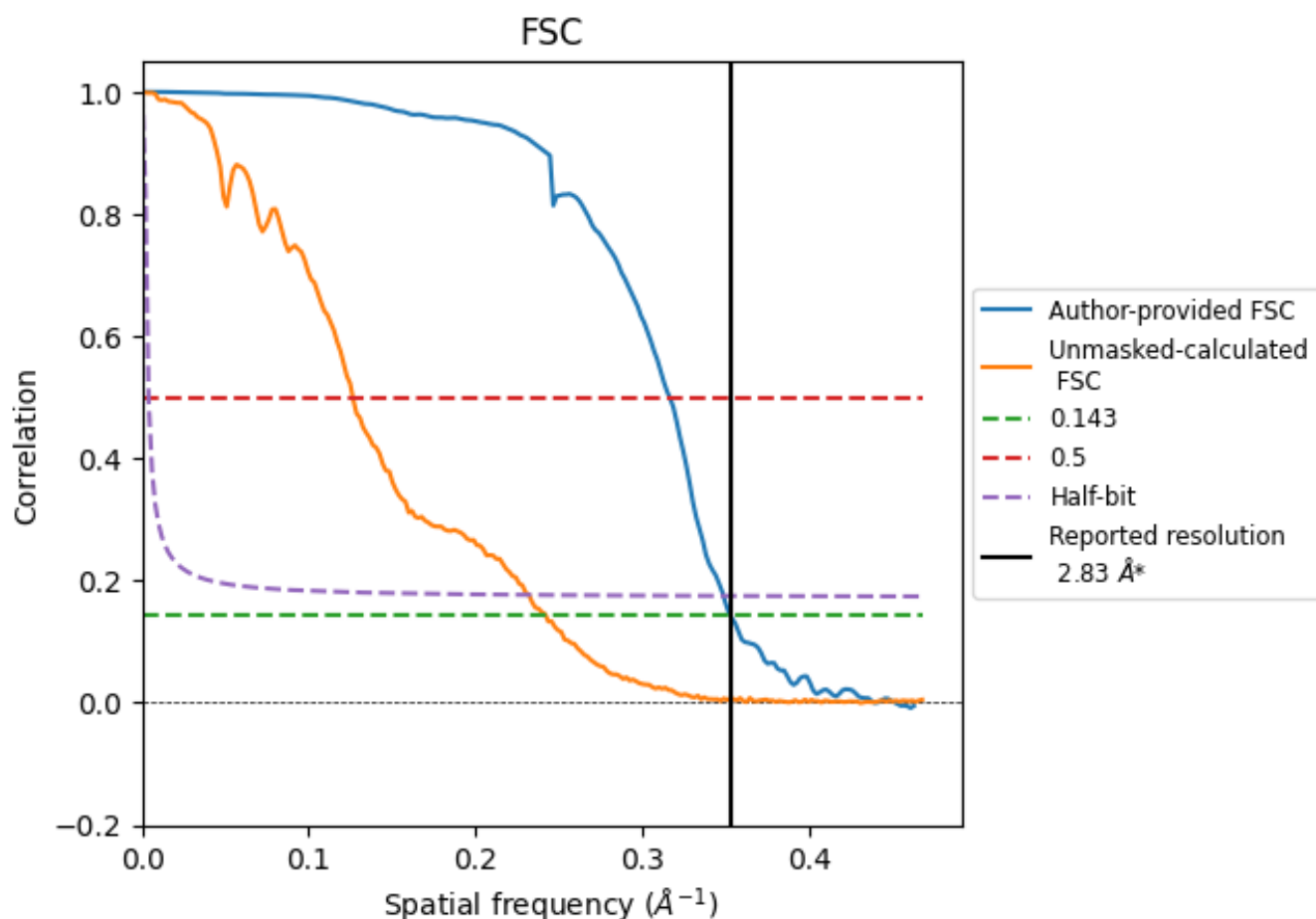


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

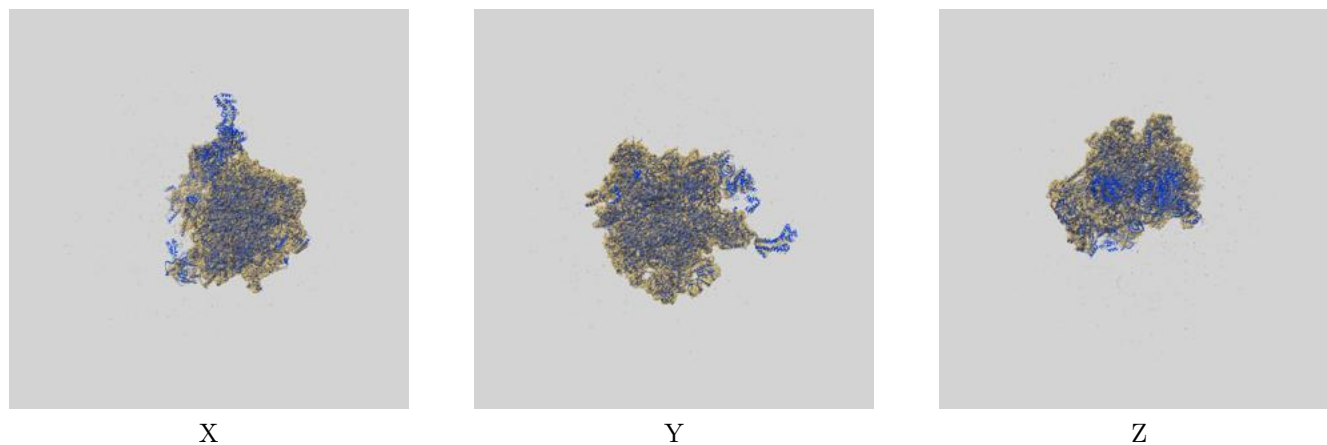
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.16	2.87
Unmasked-calculated*	4.13	7.91	4.31

*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 4.13 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

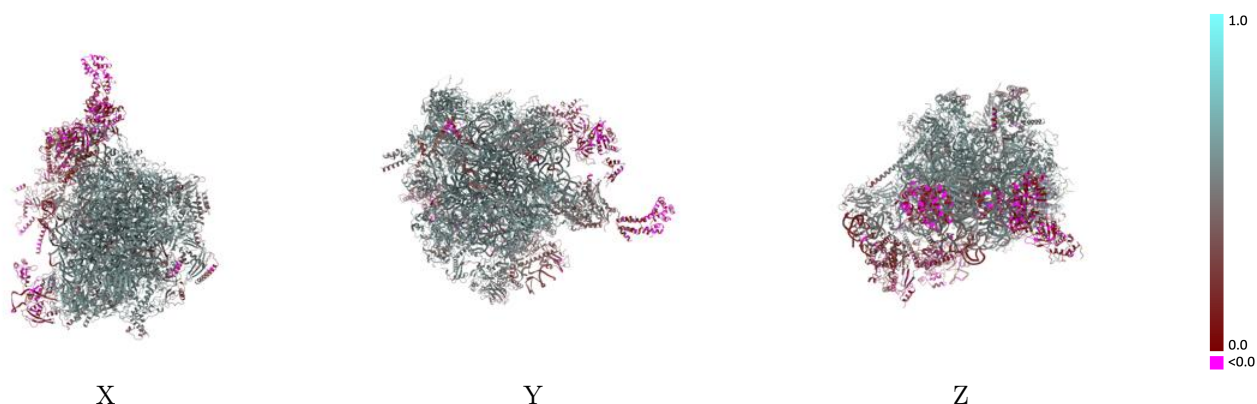
This section contains information regarding the fit between EMDB map EMD-71802 and PDB model 9PRA. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



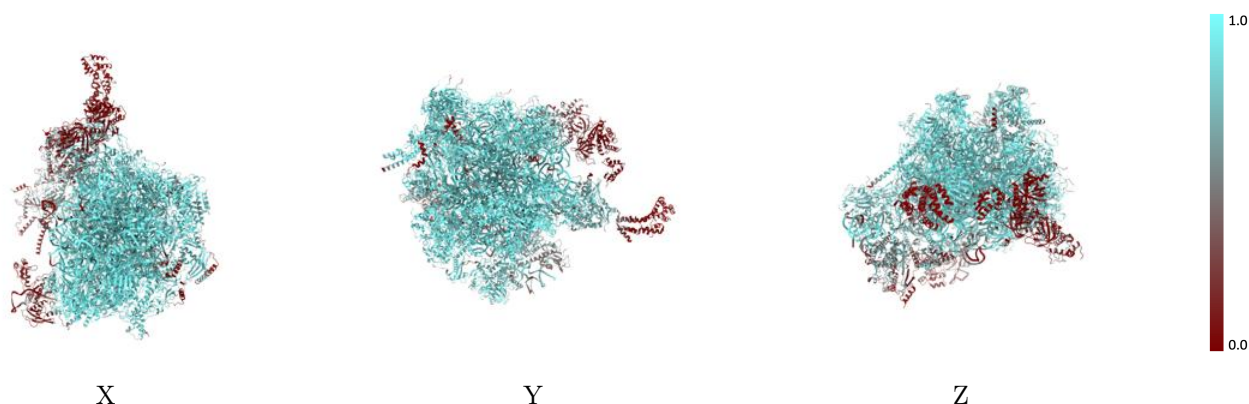
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



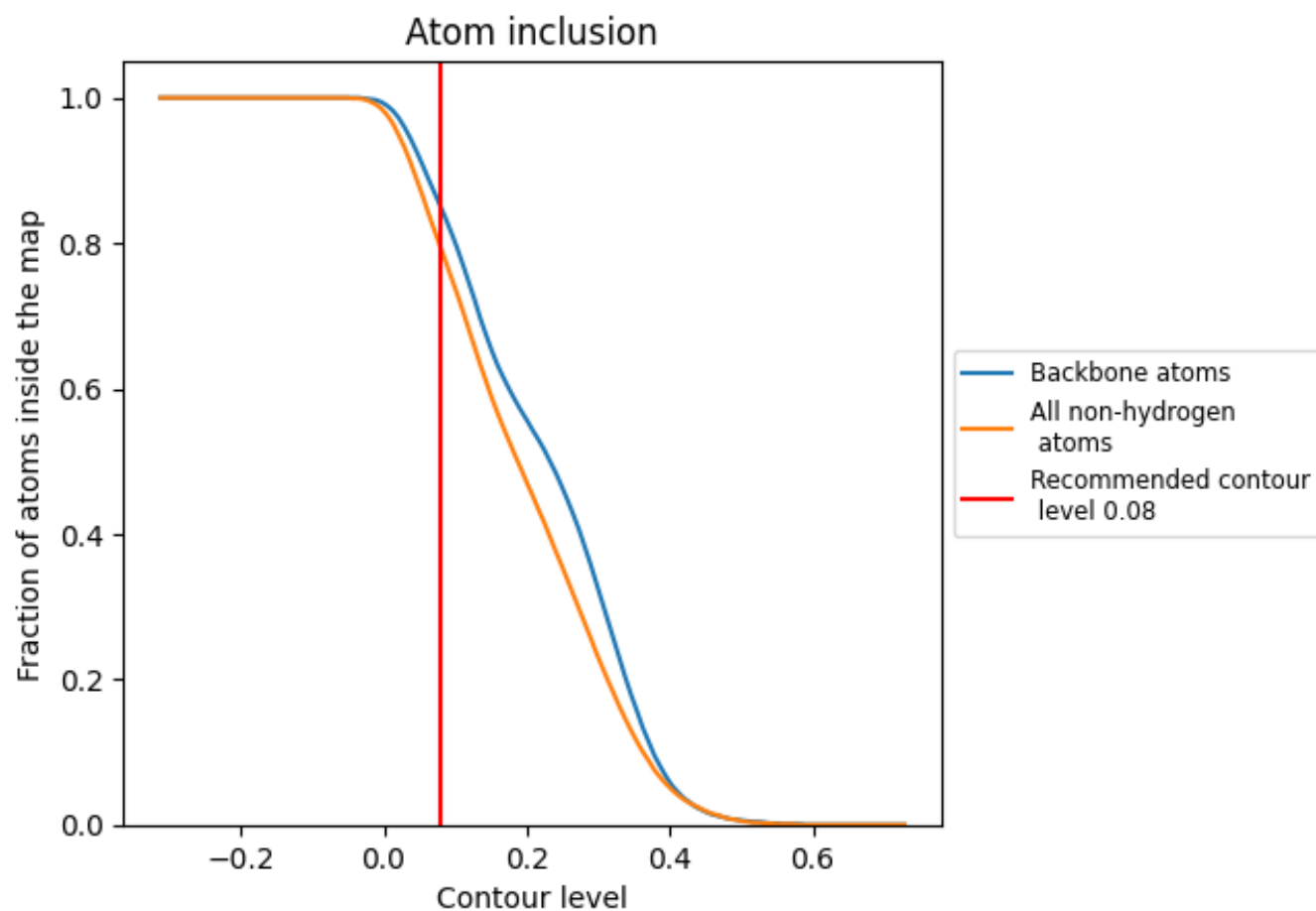
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.4690
0	 0.9010	 0.5450
1	 0.8250	 0.5170
2	 0.9530	 0.5860
3	 0.9500	 0.5880
4	 0.8930	 0.5730
5	 0.8880	 0.5400
6	 0.8380	 0.4810
7	 0.8420	 0.4910
8	 0.4280	 0.2230
9	 0.8810	 0.5300
A	 0.9310	 0.5270
Ad	 0.3620	 0.2800
Ae	 0.4260	 0.1920
Af	 0.2210	 0.1680
Ag	 0.0750	 0.1060
B	 0.7780	 0.3060
D	 0.8970	 0.5610
E	 0.9050	 0.5540
F	 0.9400	 0.5710
G	 0.0130	 0.1170
H	 0.5040	 0.3130
I	 0.6060	 0.3550
J	 0.5700	 0.2870
K	 0.9310	 0.5700
L	 0.8940	 0.5440
M	 0.9290	 0.5670
N	 0.8900	 0.5450
O	 0.9180	 0.5630
OX	 0.3290	 0.3250
P	 0.8640	 0.5210
Q	 0.8780	 0.5420
R	 0.9310	 0.5680
S	 0.9090	 0.5570
T	 0.9250	 0.5770



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Chain	Atom inclusion	Q-score
U	 0.8120	 0.4870
V	 0.8520	 0.5090
W	 0.8890	 0.5560
X	 0.8780	 0.5400
Y	 0.9050	 0.5510
Z	 0.9100	 0.5650
a	 0.7600	 0.4750
b	 0.9240	 0.5680
c	 0.8830	 0.5230
d	 0.6790	 0.4390
e	 0.4270	 0.1810
f	 0.5060	 0.2800
g	 0.9160	 0.5530
h	 0.8500	 0.4960
i	 0.9490	 0.5850
j	 0.8620	 0.5110
k	 0.7610	 0.4450
l	 0.6400	 0.3370
m	 0.4350	 0.2280
n	 0.3000	 0.2460
o	 0.9400	 0.5750
p	 0.7540	 0.4600
q	 0.5950	 0.3500
r	 0.9000	 0.5420
s	 0.9020	 0.5490
t	 0.2640	 0.1880
u	 0.2190	 0.1630
v	 0.0390	 0.0400
w	 0.0330	 0.0670
x	 0.0000	 0.0200
y	 0.0000	 0.0210
z	 0.0630	 0.0690