



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 03:44 am BST

PDB ID : 7AOI / pdb_00007aoi
EMDB ID : EMD-11845
Title : Trypanosoma brucei mitochondrial ribosome large subunit assembly intermediate
Authors : Tobiasson, V.; Gahura, O.; Aibara, S.; Baradaran, R.; Zikova, A.; Amunts, A.
Deposited on : 2020-10-14
Resolution : 3.50 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

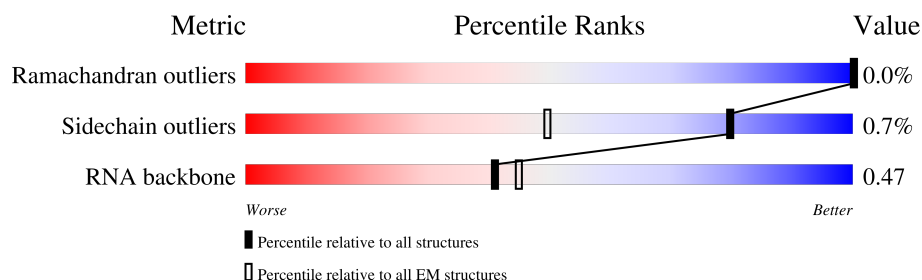
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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




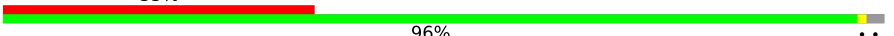
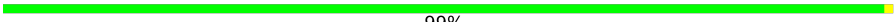


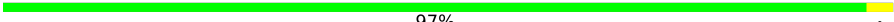


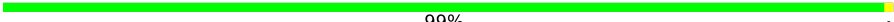
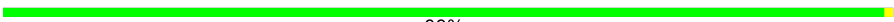




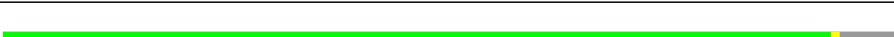






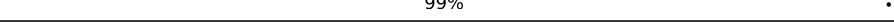
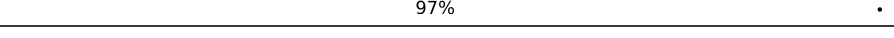


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A1	217	 98%
2	A2	463	 97%
3	A3	150	 100%
4	A5	55	 100%
5	A8	142	 100%
6	AA	758	 70% 30%
7	AE	367	 98%
8	AF	442	 99%

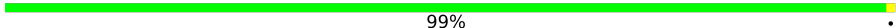

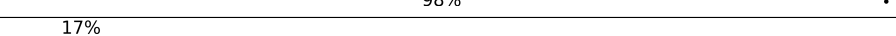


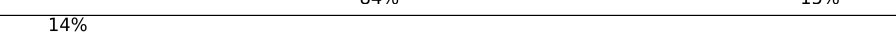
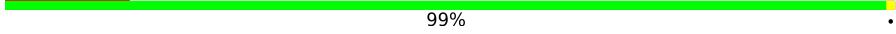

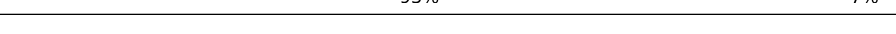
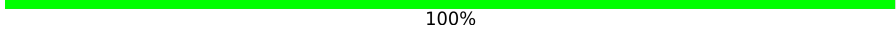

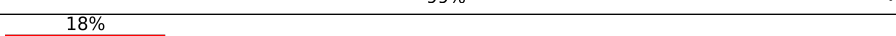
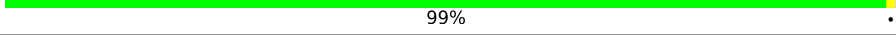

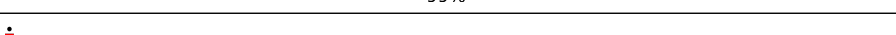
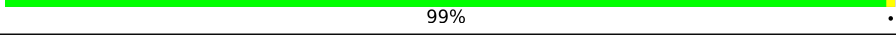


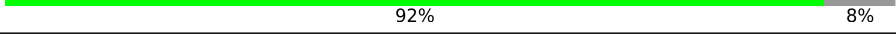
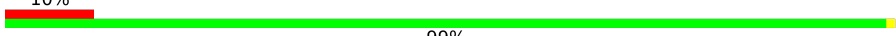
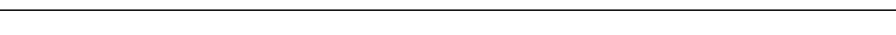
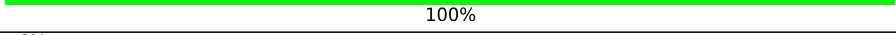
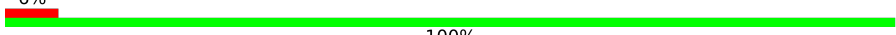
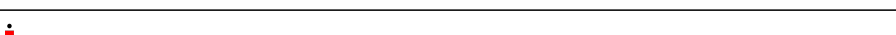
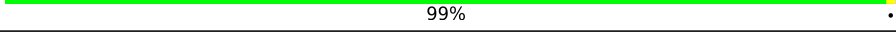
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Mol	Chain	Length	Quality of chain
9	AI	212	 100%
10	AK	278	 35% 96%
11	AN	171	 99%
12	AP	354	 87% 12%
13	AR	256	 100%
14	AT	138	 97%
15	AU	196	 89% 11%
16	AV	180	 100%
17	AW	277	 99%
18	AX	165	 99%
19	AY	340	 98%
20	Ae	116	 99%
21	Af	133	 100%
22	Ag	185	 100%
23	Al	182	 93% 7%
24	Ao	133	 100%
25	Ap	288	 100%
26	At	145	 9% 99%
27	Av	197	 98%
28	BA	798	 91% 9%
29	BB	371	 19% 99%
30	BD	417	 9% 97%
31	BE	438	 91% 8%
32	BF	421	 80% 19%
33	BH	225	 100%

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Mol	Chain	Length	Quality of chain
34	BI	323	 99%
35	BJ	161	 11% 98%
36	BK	273	 17% 89% 11%
37	BL	276	 84% 15%
38	BN	214	 14% 99%
39	BO	227	 93% 7%
40	BQ	185	 100%
41	BR	195	 99%
42	BS	144	 18% 99%
43	BT	167	 99%
44	BU	82	 99%
45	BW	187	 100%
46	BX	116	 27% 92% 8%
47	BZ	189	 10% 99%
48	Ba	135	 100%
49	Bb	103	 6% 100%
50	Bc	137	 99%
51	Bf	86	 93% 7%
52	Bg	82	 10% 100%
53	Bh	92	 98% ..
54	UA	46	 13% 100%
55	UB	9	 100%
56	UC	14	 100%
57	UD	8	 100%
58	UE	12	 100%

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Mol	Chain	Length	Quality of chain
59	UF	139	 6% 100%
60	UG	19	 100%
61	UH	17	 100%
62	UI	39	 21% 100%
63	UJ	25	 100%
64	UK	47	 100%
65	XA	155	 99%
66	XB	668	 91% 8%
67	XC	616	 94% 5%
68	XD	83	 41% 96%
68	XE	83	 5% 99%
69	XF	198	 81% 19%
70	XG	170	 96%
71	XH	533	 75% 25%
72	XI	703	 84% 15%
73	XJ	150	 99%
74	XL	528	 99%
75	XM	91	 99%
76	XN	620	 87% 13%
77	XO	428	 93% 7%
78	XP	371	 99%
79	XQ	305	 7% 92% 7%
80	XR	161	 6% 81% 15%
81	XS	182	 37% 99%
82	XT	97	 100%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 156070 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 bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	217	Total	C	N	O	S	0	0
			1788	1138	324	317	9		

- Molecule 2 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	449	Total	C	N	O	S	0	0
			3638	2324	631	670	13		

- Molecule 3 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	150	Total	C	N	O	S	0	0
			1229	782	236	205	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	198	ASP	ALA	variant	UNP A0A3L6L456

- Molecule 4 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5	55	Total	C	N	O	S	0	0
			483	311	90	76	6		

- Molecule 5 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A8	142	Total	C	N	O	S	0	0
			1203	753	243	198	9		

- Molecule 6 is a RNA chain called mt-LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	758	Total	C	N	O	P	0	0
			16041	7218	2743	5322	758		

- Molecule 7 is a protein called Ribosomal protein L3 mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AE	361	Total	C	N	O	S	0	0
			2955	1897	502	540	16		

- Molecule 8 is a protein called Ribosomal protein L4/L1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AF	442	Total	C	N	O	S	0	0
			3597	2294	624	654	25		

- Molecule 9 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	212	Total	C	N	O	S	0	0
			1790	1153	316	312	9		

- Molecule 10 is a protein called Ribosomal protein L11,uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	272	Total	C	N	O	S	0	0
			2034	1295	372	357	10		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AN	171	Total	C	N	O	S	0	0
			1432	922	261	240	9		

- Molecule 12 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AP	310	Total	C	N	O	S	0	0
			2565	1633	474	446	12		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AR	256	Total	C	N	O	S	0	0
			2144	1359	399	372	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	24	TRP	TYR	variant	UNP A0A3L6LAG5

- Molecule 14 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AT	138	Total	C	N	O	S	0	0
			1136	717	212	201	6		

- Molecule 15 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AU	175	Total	C	N	O	S	0	0
			1423	895	280	243	5		

- Molecule 16 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AV	180	Total	C	N	O	S	0	0
			1419	906	256	251	6		

- Molecule 17 is a protein called Ribosomal protein L22p/L17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AW	277	Total	C	N	O	S	0	0
			2243	1422	416	392	13		

- Molecule 18 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	165	Total	C	N	O	S	0	0
			1391	898	245	243	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	126	TYR	HIS	variant	UNP A0A3L6KW11

- Molecule 19 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AY	334	Total	C	N	O	S	0	0
			2741	1711	488	527	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	6	THR	ARG	variant	UNP C9ZK52

- Molecule 20 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ae	116	Total	C	N	O	S	0	0
			927	594	170	158	5		

- Molecule 21 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Af	133	Total	C	N	O	S	0	0
			1068	670	203	190	5		

- Molecule 22 is a protein called Mitochondrial ribosomal protein L51 / S25 / CI-B8 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ag	185	Total	C	N	O	S	0	0
			1557	974	294	282	7		

- Molecule 23 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Al	170	Total	C	N	O	S	0	0
			1356	885	235	230	6		

- Molecule 24 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ao	133	Total	C	N	O	S	0	0
			1058	672	193	190	3		

- Molecule 25 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ap	288	Total	C	N	O	S	0	0
			2347	1519	413	403	12		

- Molecule 26 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	At	145	Total	C	N	O	S	0	0
			1203	752	235	212	4		

- Molecule 27 is a protein called mL64,mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Av	196	Total	C	N	O	S	0	0
			1661	1052	312	285	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Av	163	ARG	ILE	variant	UNP A0A3L6KTC7

- Molecule 28 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	727	Total	C	N	O	S	0	0
			5779	3673	1022	1050	34		

- Molecule 29 is a protein called mL68,mL68,mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	371	Total	C	N	O	S	0	0
			2862	1819	514	517	12		

- Molecule 30 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BD	417	Total	C	N	O	S	0	0
			3339	2128	584	607	20		

- Molecule 31 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BE	401	Total	C	N	O	S	0	0
			3178	2014	552	599	13		

- Molecule 32 is a protein called Tetratricopeptide repeat.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BF	341	Total	C	N	O	S	0	0
			2805	1778	510	504	13		

- Molecule 33 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	225	Total	C	N	O	S	0	0
			1831	1171	330	327	3		

- Molecule 34 is a protein called Mitochondrial RNA binding complex 1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	323	Total	C	N	O	S	0	0
			2641	1681	483	461	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	variant	UNP A0A3L6KZH2

- Molecule 35 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	161	Total	C	N	O	S	0	0
			1329	826	257	240	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP A0A3L6KX00

- Molecule 36 is a protein called Chaperone protein DNAj, putative,mL77,Chaperone protein DNAj, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	242	Total	C	N	O	S	0	0
			1922	1193	367	354	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	348	THR	LEU	variant	UNP C9ZQR6

- Molecule 37 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	234	Total	C	N	O	S	0	0
			1887	1158	370	349	10		

- Molecule 38 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	214	Total	C	N	O	S	0	0
			1793	1126	331	330	6		

- Molecule 39 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	211	Total	C	N	O	S	0	0
			1665	1043	293	316	13		

- Molecule 40 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BQ	185	Total	C	N	O	S	0	0
			1429	908	247	267	7		

- Molecule 41 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BR	195	Total	C	N	O	S	0	0
			1650	1059	298	284	9		

- Molecule 42 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BS	144	Total	C	N	O	S	0	0
			1185	732	225	221	7		

- Molecule 43 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BT	167	Total	C	N	O	S	0	0
			1380	848	268	258	6		

- Molecule 44 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BU	82	Total	C	N	O	S	0	0
			694	436	139	115	4		

- Molecule 45 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	187	Total	C	N	O	S	0	0
			1557	987	298	264	8		

- Molecule 46 is a protein called LIM domain containing protein,mL90.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	107	Total	C	N	O	S	0	0
			867	552	160	147	8		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BZ	189	Total	C	N	O	S	0	0
			1433	903	246	278	6		

- Molecule 48 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ba	135	Total	C	N	O	S	0	0
			1191	763	217	204	7		

- Molecule 49 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bb	103	Total	C	N	O	S	0	0
			805	504	152	147	2		

- Molecule 50 is a protein called mL95.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bc	137	Total	C	N	O	S	0	0
			1194	776	216	201	1		

- Molecule 51 is a protein called mL98.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bf	80	Total	C	N	O	S	0	0
			676	432	124	120			

- Molecule 52 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bg	82	Total	C	N	O	S	0	0
			656	412	126	116	2		

- Molecule 53 is a protein called mL100,mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bh	91	Total	C	N	O	S	0	0
			730	466	129	125	10		

- Molecule 54 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UA	46	Total	C	N	O	0	0
			230	138	46	46		

- Molecule 55 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	UB	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 56 is a protein called UNK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	UC	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 57 is a protein called UNK4.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	UD	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 58 is a protein called UNK5.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UE	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 59 is a protein called UNK6/mt-LAF15_2.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UF	139	Total	C	N	O	0	0
			695	417	139	139		

- Molecule 60 is a protein called UNK7.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	UG	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 61 is a protein called UNK8.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UH	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 62 is a protein called UNK9.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	UI	39	Total	C	N	O	0	0
			195	117	39	39		

- Molecule 63 is a protein called UNK10.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	UJ	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 64 is a protein called UNK11.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	UK	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 65 is a protein called mt-LAF7,mt-LAF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	XA	154	Total	C	N	O	S	0	0
			1295	812	256	218	9		

- Molecule 66 is a protein called DEAD-box helicase, putative,mt-LAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	XB	614	Total	C	N	O	S	0	0
			4944	3123	947	848	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XB	301	ALA	THR	conflict	UNP D0A9G9
XB	462	GLY	GLU	conflict	UNP D0A9G9

- Molecule 67 is a protein called mt-LAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	XC	584	Total	C	N	O	S	0	0
			4652	2958	831	840	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XC	69	PRO	ALA	conflict	UNP D0A7A5

- Molecule 68 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	XD	83	Total	C	N	O	P	S	0	0
			685	434	107	141	1	2		
68	XE	83	Total	C	N	O	P	S	0	0
			685	434	107	141	1	2		

- Molecule 69 is a protein called mt-LAF15_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	XF	161	Total	C	N	O	S	0	0
			1264	801	231	227	5		

- Molecule 70 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	XG	164	Total	C	N	O	S	0	0
			1330	837	270	214	9		

- Molecule 71 is a protein called mt-LAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	XH	402	Total	C	N	O	S	0	0
			3208	2029	584	581	14		

- Molecule 72 is a protein called mt-LAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	XI	597	Total	C	N	O	S	0	0
			4736	2978	858	874	26		

- Molecule 73 is a protein called RNA uridylyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	XJ	150	Total	C	N	O	S	0	0
			1212	764	211	228	9		

- Molecule 74 is a protein called GTP-binding protein, putative,mt-EngA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	XL	521	Total	C	N	O	S	0	0
			4169	2609	771	768	21		

- Molecule 75 is a protein called Complex1-LYR-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XM	91	Total	C	N	O	S	0	0
			744	462	152	127	3		

- Molecule 76 is a protein called mt-LAF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	XN	541	Total	C	N	O	S	0	0
			4358	2801	757	772	28		

- Molecule 77 is a protein called SpoU rRNA Methylase family.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	XO	398	Total	C	N	O	S	0	0
			3193	1992	603	587	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XO	337	ASP	GLY	conflict	UNP A0A3L6L241

- Molecule 78 is a protein called Pseudouridylate synthase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	XP	371	Total	C	N	O	S	0	0
			2995	1918	538	521	18		

- Molecule 79 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	XQ	283	Total	C	N	O	S	0	0
			2206	1393	397	403	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XQ	331	ALA	PHE	conflict	UNP A0A3L6L0D5

- Molecule 80 is a protein called Lipase (Class 3).

Mol	Chain	Residues	Atoms					AltConf	Trace
80	XR	137	Total	C	N	O	S	0	0
			1135	702	220	210	3		

- Molecule 81 is a protein called mL101.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	XS	182	Total	C	N	O	S	0	0
			1532	971	282	274	5		

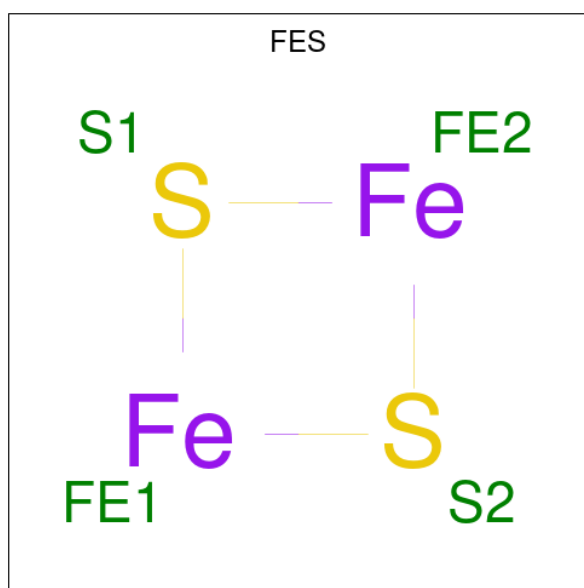
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XS	163	VAL	LEU	conflict	UNP Q4GZ80

- Molecule 82 is a protein called mt-LAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	XT	97	Total	C	N	O	S	0	0
			801	505	156	136	4		

- Molecule 83 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
83	A5	1	Total	Fe	S	0
			4	2	2	

- Molecule 84 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
84	Av	1	Total	C	N	O	P	0
			44	21	7	14	2	

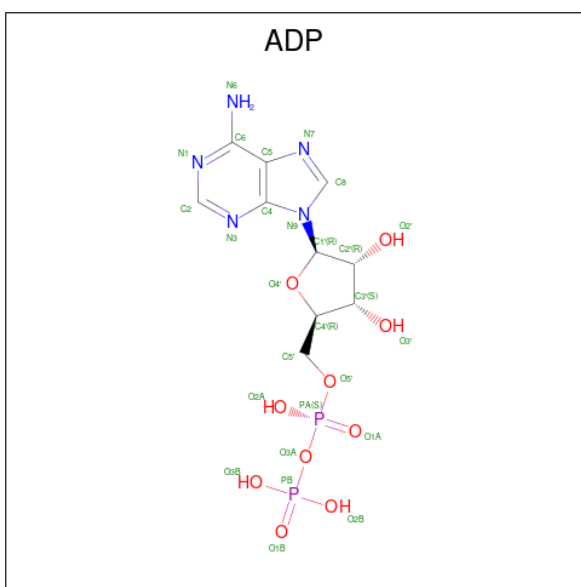
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	BX	2	Total	Zn	0
			2	2	
85	Bh	1	Total	Zn	0
			1	1	
85	XA	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

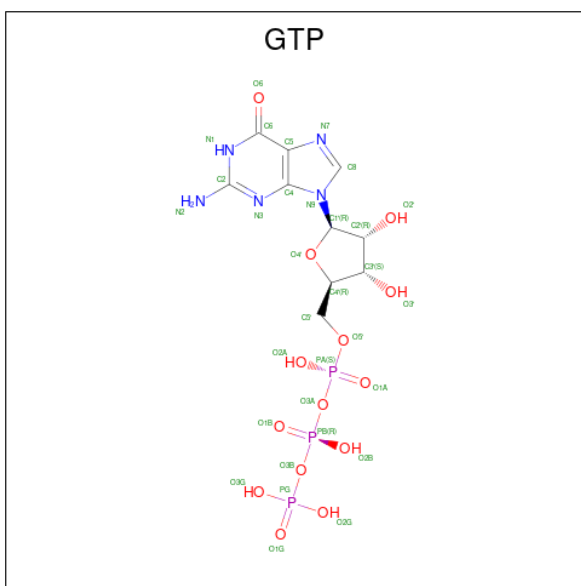
Mol	Chain	Residues	Atoms		AltConf
86	XB	1	Total	Mg	0
			1	1	

- Molecule 87 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
87	XB	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 88 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



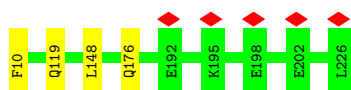
Mol	Chain	Residues	Atoms					AltConf
88	XL	1	Total 32	C 10	N 5	O 14	P 3	0
88	XL	1	Total 32	C 10	N 5	O 14	P 3	0

3 Residue-property plots [i](#)

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

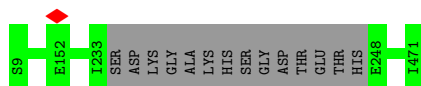
- Molecule 1: bL28m

Chain A1:  98%



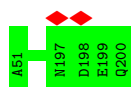
- Molecule 2: uL29m

Chain A2:  97%



- Molecule 3: uL30m

Chain A3:  100%



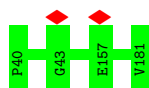
- Molecule 4: bL32m

Chain A5:  100%

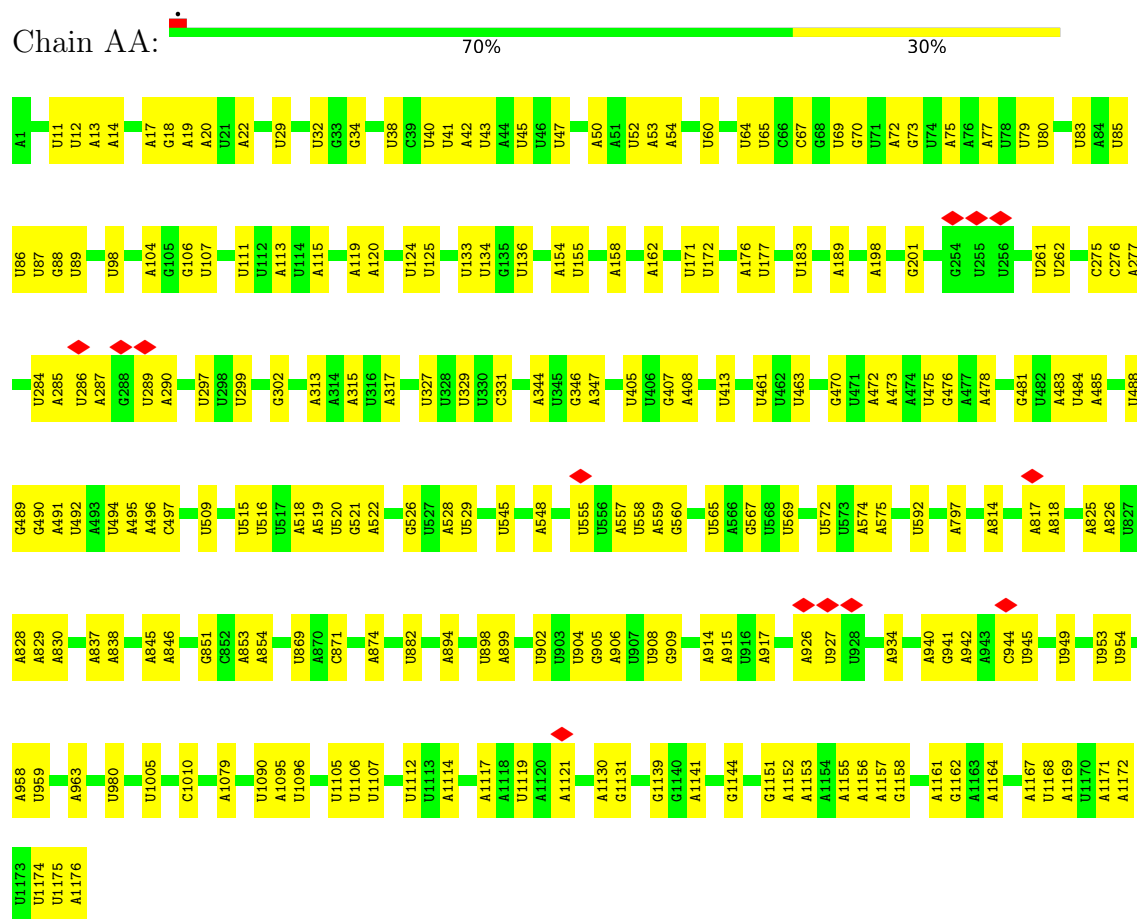
There are no outlier residues recorded for this chain.

- Molecule 5: bL33m

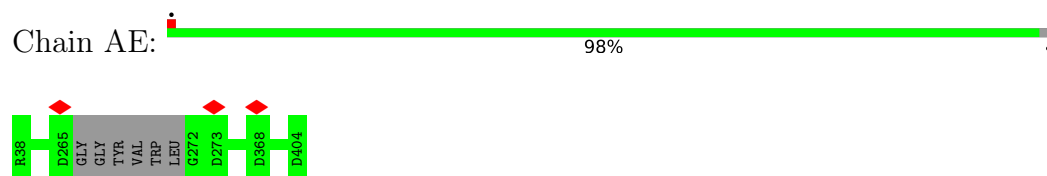
Chain A8:  100%



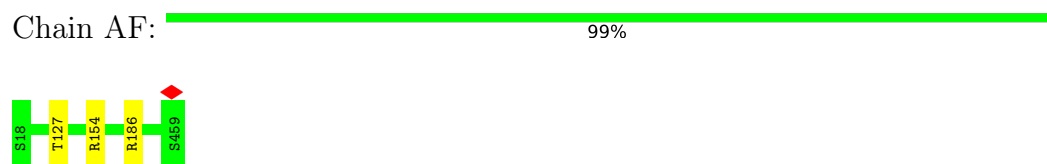
- Molecule 6: mt-LSU rRNA



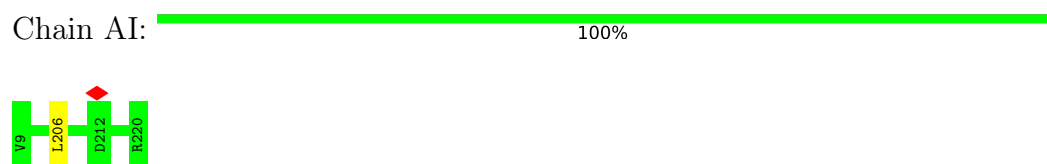
- Molecule 7: Ribosomal protein L3 mitochondrial, putative



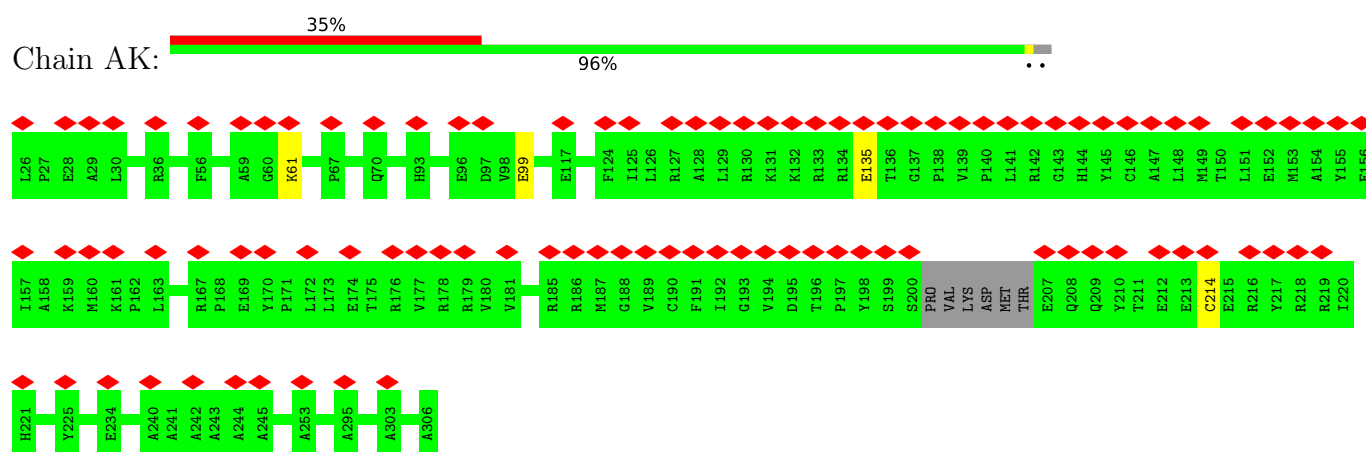
- Molecule 8: Ribosomal protein L4/L1 family



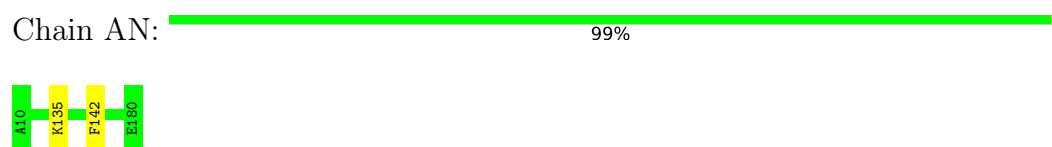
- Molecule 9: RIBOSOMAL_L9 domain-containing protein



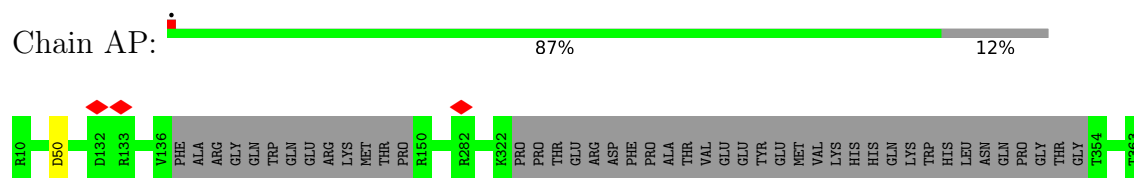
- Molecule 10: Ribosomal protein L11,uL11m



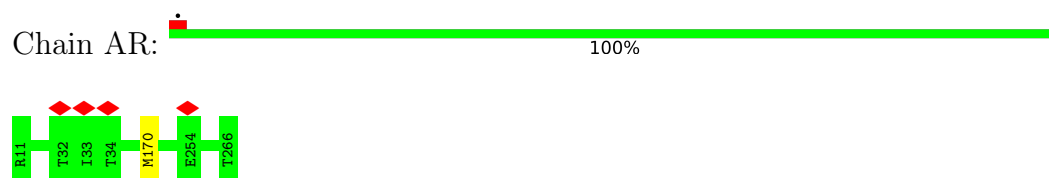
- Molecule 11: 50S ribosomal protein L13



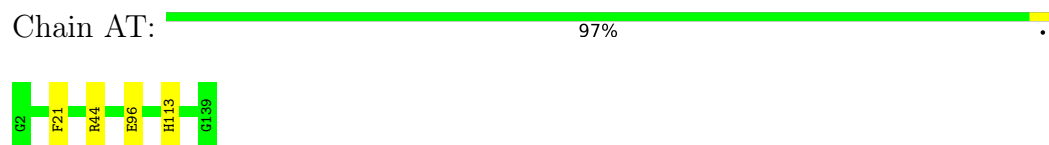
- Molecule 12: Ribosomal_L18e/L15P domain-containing protein



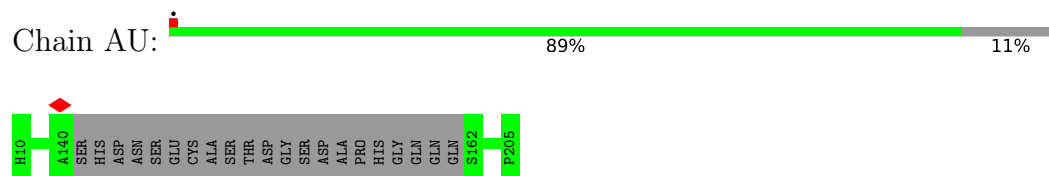
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: bL19m



- Molecule 15: bL20m



- Molecule 16: Ribosomal protein L21

Chain AV:  100%



- Molecule 17: Ribosomal protein L22p/L17e

Chain AW:  99%



- Molecule 18: Ribosomal protein L23

Chain AX:  99%



- Molecule 19: uL24m

Chain AY:  98%



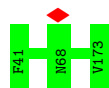
- Molecule 20: mL41

Chain Ae:  99%



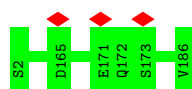
- Molecule 21: mL42

Chain Af:  100%



- Molecule 22: Mitochondrial ribosomal protein L51 / S25 / CI-B8 domain containing protein

Chain Ag:  100%



- Molecule 23: mL49

S37
R88
Q101
ARG
CYS
GLN
GLU
GLU
PRO
GLU
ALA
VAL
GLY
VAL
VAL
G114
F218

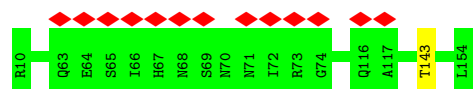
- Chain Ao: 100%

- Molecule 25: mL53

Chain Ap: 100%



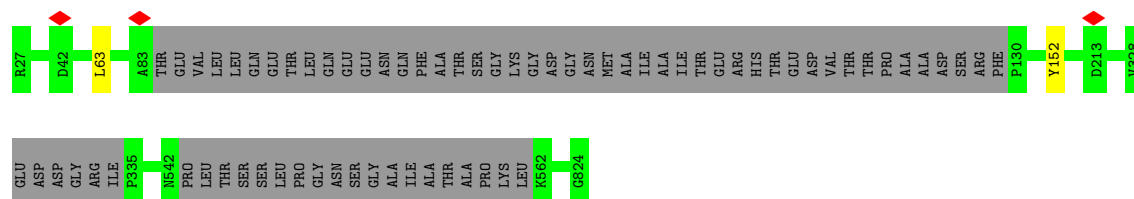
- Chain At:  9% 99%



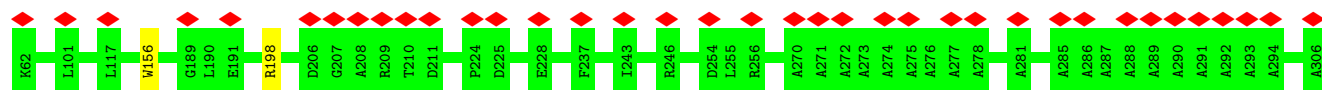
- Chain Av: 98%

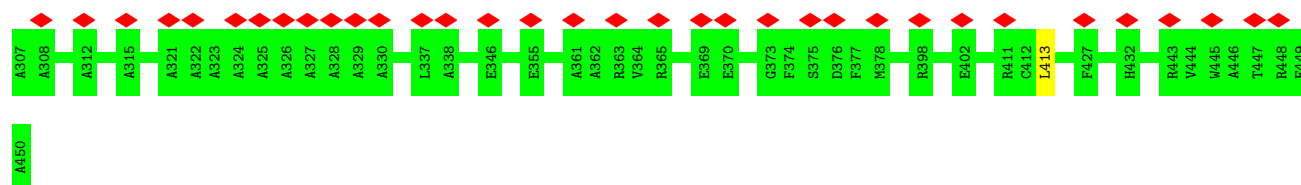


- Chain BA:  91% 9%

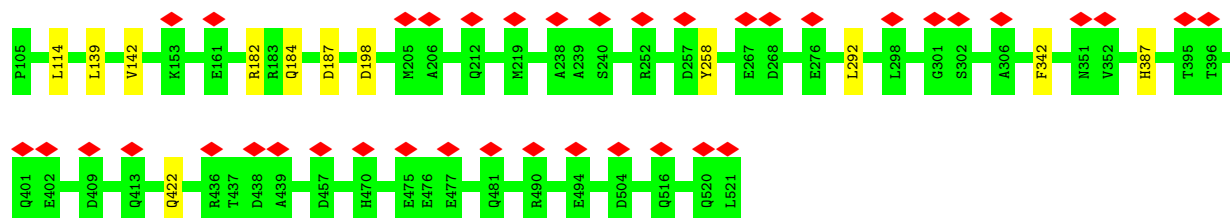


- Chain BB:  19% 99%

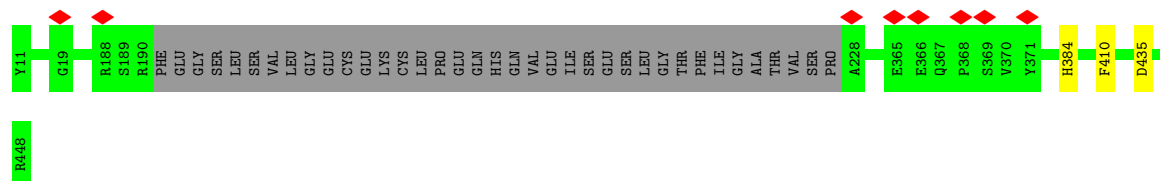




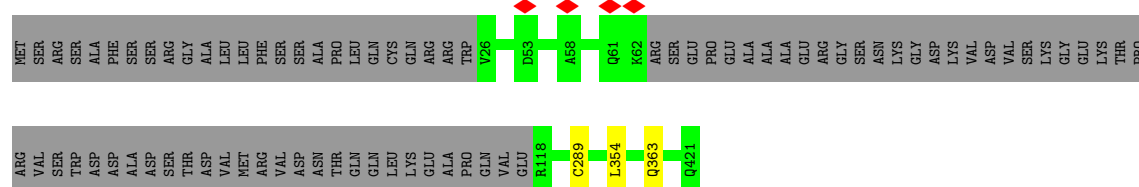
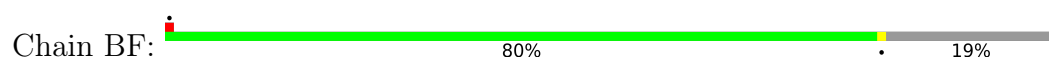
- Molecule 30: mL70



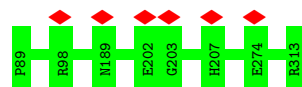
- Molecule 31: mL71



- Molecule 32: Tetratricopeptide repeat



- Molecule 33: mL74



- Molecule 34: Mitochondrial RNA binding complex 1 subunit

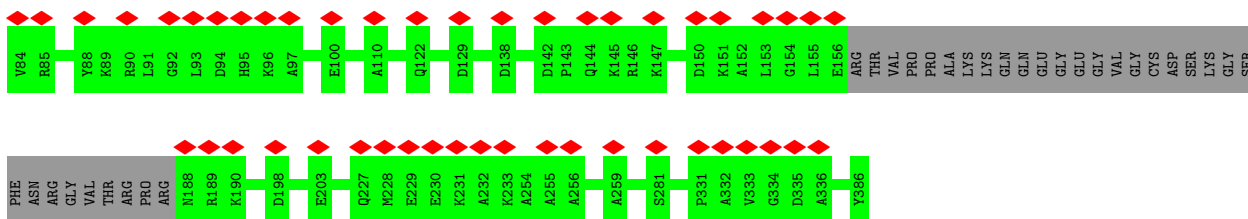
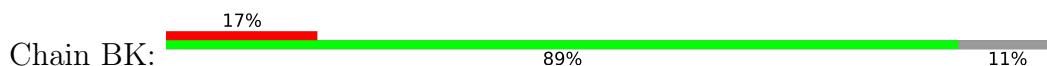




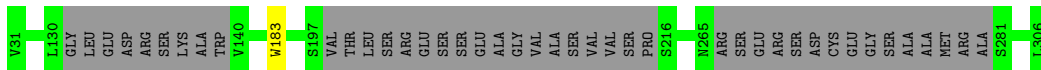
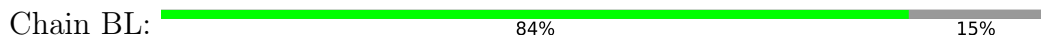
- Molecule 35: mL76



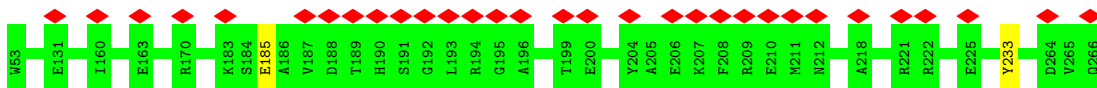
- Molecule 36: Chaperone protein DNAj, putative, mL77, Chaperone protein DNAj, putative



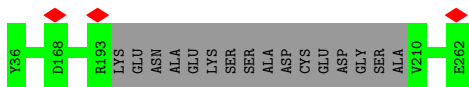
- Molecule 37: mL78



- Molecule 38: mL80



- Molecule 39: mL81



- Molecule 40: Peptidyl-prolyl cis-trans isomerase



There are no outlier residues recorded for this chain.

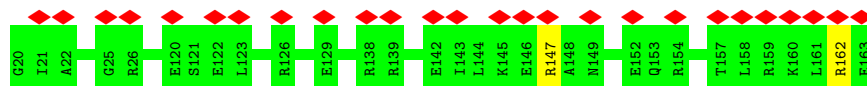
- Molecule 41: mL84

Chain BR:  99%



- Molecule 42: mL85

Chain BS:  18% 99%



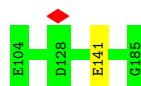
- Molecule 43: mL86

Chain BT:  99%



- Molecule 44: mL87

Chain BU:  99%



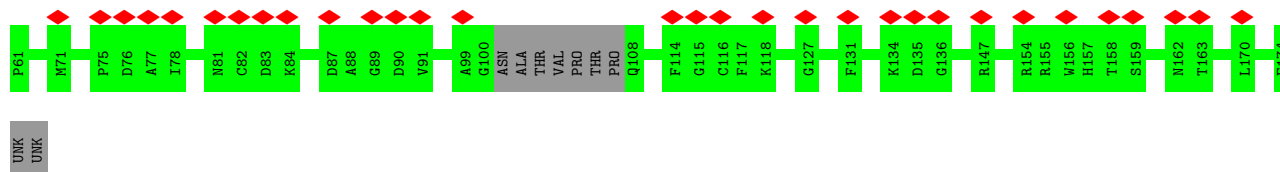
- Molecule 45: mL89

Chain BW:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: LIM domain containing protein, mL90

Chain BX:  27% 92% 8%



- Molecule 47: Peptidyl-prolyl cis-trans isomerase

Chain BZ:  10% 99%



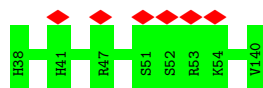
- Molecule 48: mL93

Chain Ba:  100%

There are no outlier residues recorded for this chain.

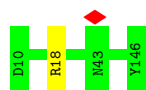
- Molecule 49: mL94

Chain Bb:  6% 100%



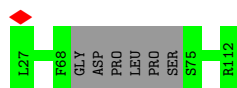
- Molecule 50: mL95

Chain Bc:  99%



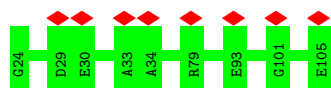
- Molecule 51: mL98

Chain Bf:  93% 7%



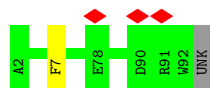
- Molecule 52: mL99

Chain Bg:  10% 100%



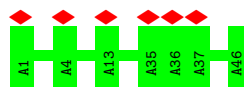
- Molecule 53: mL100,mL100

Chain Bh:  98%



- Molecule 54: UNK1

Chain UA:  13% 100%



- Molecule 55: UNK2

Chain UB:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: UNK3

Chain UC:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: UNK4

Chain UD:  100%

There are no outlier residues recorded for this chain.

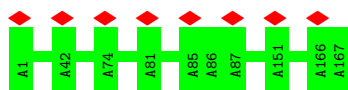
- Molecule 58: UNK5

Chain UE:  100%

There are no outlier residues recorded for this chain.

- Molecule 59: UNK6/mt-LAF15_2

Chain UF:  6% 100%



- Molecule 60: UNK7

Chain UG:  100%

There are no outlier residues recorded for this chain.

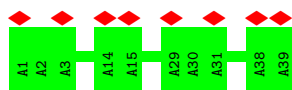
- Molecule 61: UNK8

Chain UH:  100%

There are no outlier residues recorded for this chain.

- Molecule 62: UNK9

Chain UI:  21% 100%

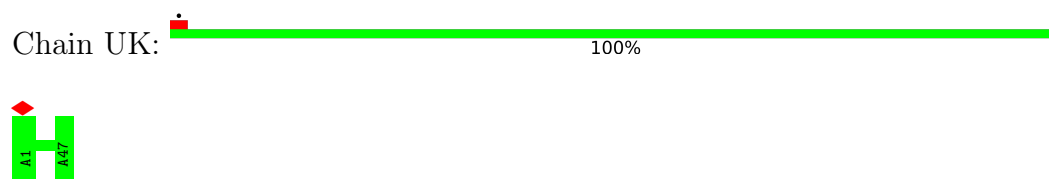


- Molecule 63: UNK10

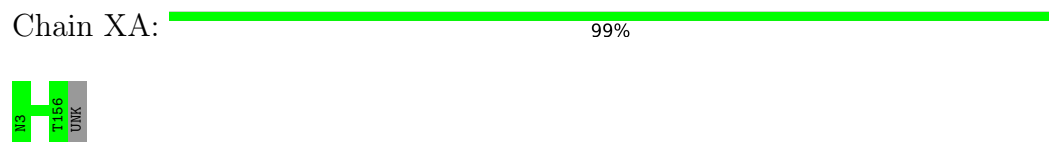
Chain UJ:  100%

There are no outlier residues recorded for this chain.

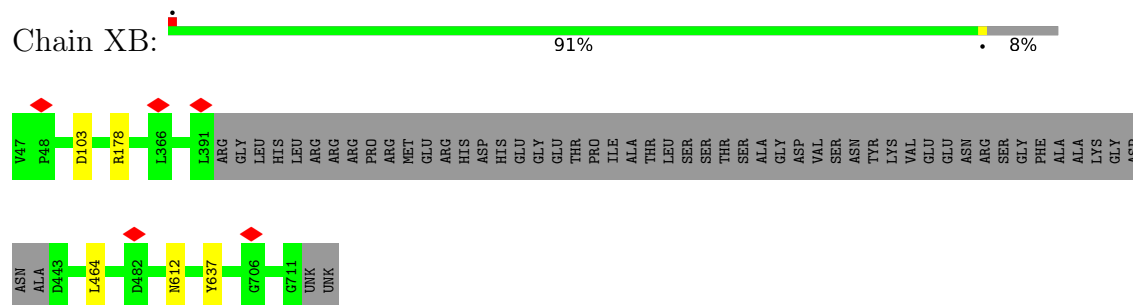
- Molecule 64: UNK11



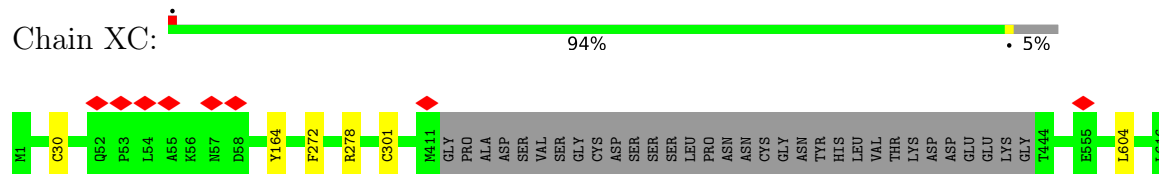
- Molecule 65: mt-LAF7,mt-LAF7



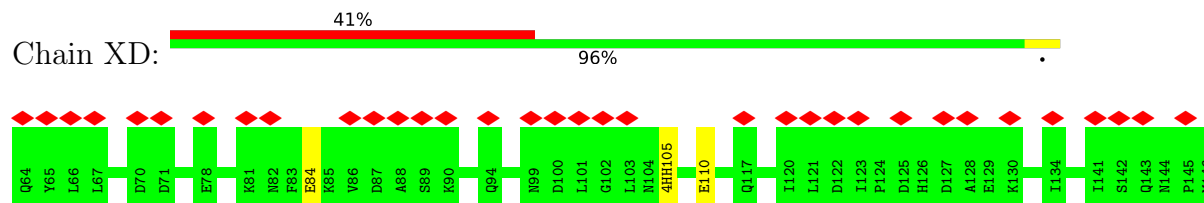
- Molecule 66: DEAD-box helicase, putative,mt-LAF2



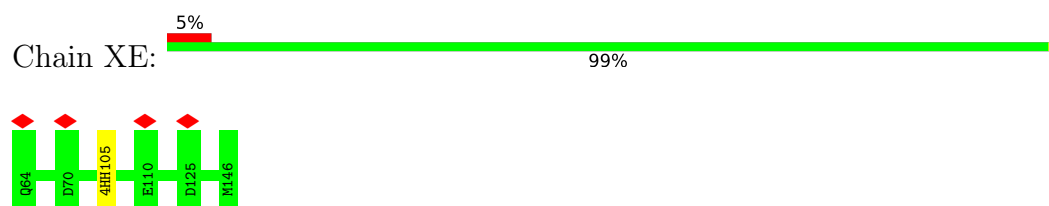
- Molecule 67: mt-LAF4




- Molecule 68: Acyl carrier protein

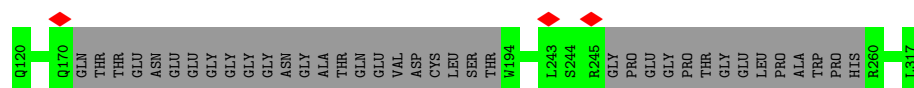


- Molecule 68: Acyl carrier protein



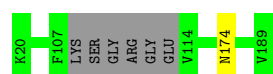
- Molecule 69: mt-LAF15_1

Chain XF:  81% 19%




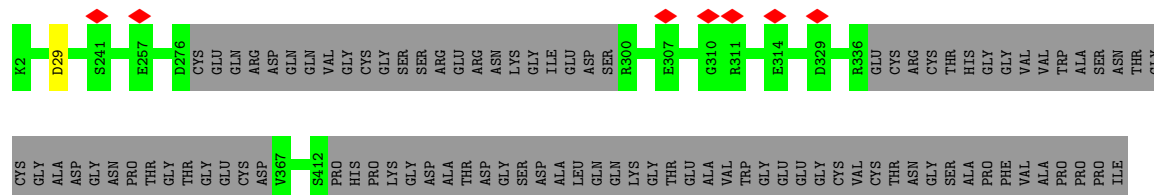
- Molecule 70: 50S ribosomal protein L14

Chain XG:  96%




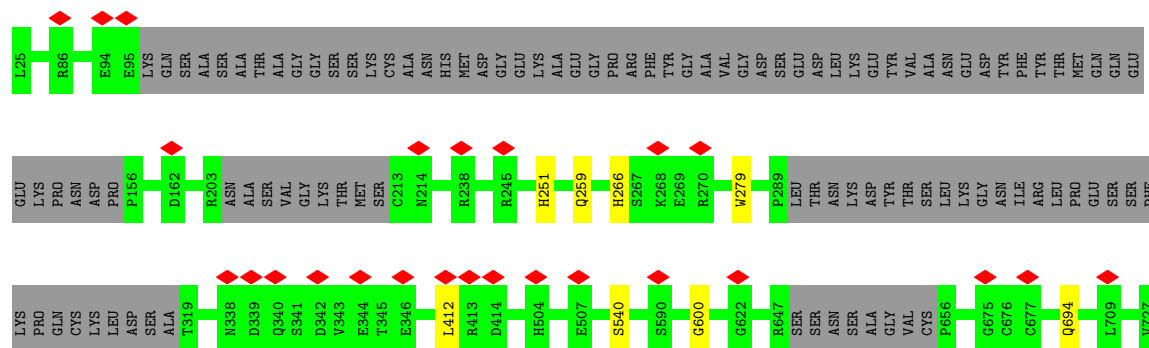
- Molecule 71: mt-LAF8

Chain XH:  75% 25%

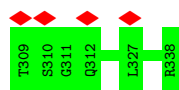


- Molecule 72: mt-LAF14

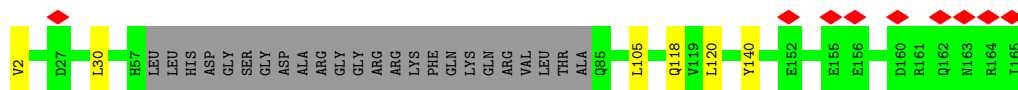
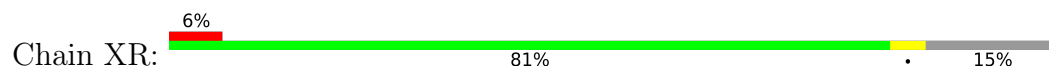
Chain XI:  84% 15%



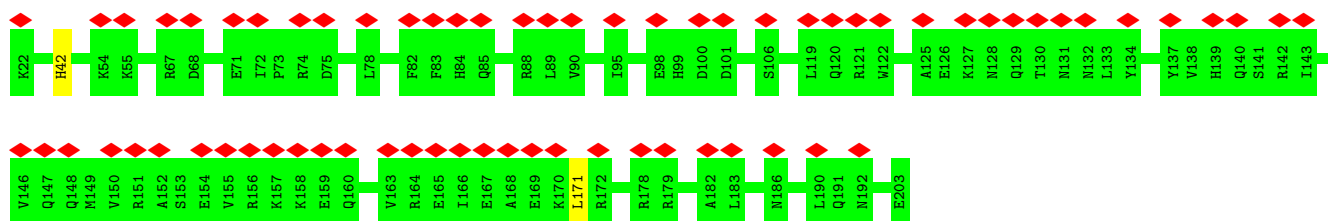
-
- | Amino Acid | Percentage (%) | Category | Property |
|------------|----------------|-------------|-------------|
| S44 | ~1.5 | Hydrophilic | Red Diamond |
| D81 | ~1.5 | Hydrophilic | Red Diamond |
| L93 | ~1.5 | Hydrophobic | Red Diamond |
| I106 | ~1.5 | Hydrophobic | Red Diamond |
| I107 | ~1.5 | Hydrophobic | Red Diamond |
| D108 | ~1.5 | Hydrophilic | Red Diamond |
| E134 | ~1.5 | Hydrophilic | Red Diamond |
| R135 | ~1.5 | Hydrophilic | Red Diamond |
| K146 | ~1.5 | Hydrophilic | Red Diamond |
| R147 | ~1.5 | Hydrophilic | Red Diamond |
| S148 | ~1.5 | Hydrophilic | Red Diamond |
| D151 | ~1.5 | Hydrophilic | Red Diamond |
| E154 | ~1.5 | Hydrophilic | Red Diamond |
| N183 | ~1.5 | Hydrophilic | Red Diamond |
| N191 | ~1.5 | Hydrophilic | Red Diamond |
| E198 | ~1.5 | Hydrophilic | Red Diamond |
| Y199 | ~1.5 | Hydrophilic | Red Diamond |
| Q200 | ~1.5 | Hydrophilic | Red Diamond |
| F201 | ~1.5 | Hydrophobic | Red Diamond |
| H202 | ~1.5 | Hydrophilic | Red Diamond |
| ARG | ~1.5 | Charged | |
| GLU | ~1.5 | Hydrophilic | |
| ASP | ~1.5 | Charged | |
| PHE | ~1.5 | Hydrophobic | |
| ARG | ~1.5 | Charged | |
| ARG | ~1.5 | Charged | |
| ARG | ~1.5 | Charged | |
| PRO | ~1.5 | Hydrophobic | |
| THR | ~1.5 | Hydrophilic | |
| PRO | ~1.5 | Hydrophobic | |
| GLU | ~1.5 | Hydrophilic | |
| ALA | ~1.5 | Hydrophobic | |
| VAL | ~1.5 | Hydrophobic | |
| SER | ~1.5 | Hydrophilic | |
| ILE | ~1.5 | Hydrophobic | |
| ALA | ~1.5 | Hydrophobic | |
| PRO | ~1.5 | Hydrophobic | |
| GLY | ~1.5 | Hydrophilic | |
| THR | ~1.5 | Hydrophilic | |
| THR | ~1.5 | Hydrophilic | |
| ARG | ~1.5 | Charged | |
| GLY | ~1.5 | Hydrophilic | |
| V215 | ~1.5 | Hydrophobic | Red Diamond |
| L261 | ~1.5 | Hydrophobic | |
| D272 | ~1.5 | Hydrophilic | Red Diamond |
| H288 | ~1.5 | Hydrophobic | Red Diamond |



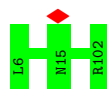
- Molecule 80: Lipase (Class 3)



- Molecule 81: mL101



- Molecule 82: mt-LAF19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.143	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	642.00006, 642.00006, 642.00006	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, NAD, ZN, ADP, 4HH, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A1	0.25	0/1828	0.39	0/2466
2	A2	0.24	0/3740	0.38	0/5094
3	A3	0.24	0/1255	0.39	0/1692
4	A5	0.26	0/498	0.39	0/663
5	A8	0.24	0/1231	0.40	0/1648
6	AA	0.18	0/17938	0.67	1/27870 (0.0%)
7	AE	0.27	0/3053	0.41	0/4149
8	AF	0.25	0/3706	0.40	0/5029
9	AI	0.25	0/1850	0.38	0/2515
10	AK	0.25	0/2077	0.40	0/2815
11	AN	0.24	0/1481	0.40	0/2016
12	AP	0.24	0/2642	0.41	0/3581
13	AR	0.25	0/2210	0.39	0/2988
14	AT	0.24	0/1166	0.41	0/1576
15	AU	0.24	0/1456	0.39	0/1971
16	AV	0.25	0/1449	0.45	0/1966
17	AW	0.24	0/2299	0.41	0/3108
18	AX	0.25	0/1436	0.39	0/1952
19	AY	0.24	0/2794	0.39	0/3775
20	Ae	0.24	0/960	0.42	0/1304
21	Af	0.23	0/1095	0.41	0/1484
22	Ag	0.24	0/1600	0.39	0/2168
23	Al	0.26	0/1398	0.40	0/1901
24	Ao	0.25	0/1094	0.39	0/1489
25	Ap	0.24	0/2421	0.39	0/3289
26	At	0.24	0/1235	0.39	0/1674
27	Av	0.25	0/1706	0.39	0/2299
28	BA	0.24	0/5907	0.39	0/8009
29	BB	0.24	0/2930	0.38	0/3984
30	BD	0.24	0/3408	0.38	0/4615
31	BE	0.25	0/3259	0.39	0/4413
32	BF	0.25	0/2866	0.39	0/3863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BH	0.24	0/1883	0.39	0/2567
34	BI	0.24	0/2717	0.39	0/3674
35	BJ	0.23	0/1356	0.38	0/1830
36	BK	0.24	0/1963	0.36	0/2647
37	BL	0.23	0/1924	0.38	0/2596
38	BN	0.24	0/1837	0.39	0/2484
39	BO	0.25	0/1693	0.40	0/2290
40	BQ	0.26	0/1466	0.42	0/1987
41	BR	0.24	0/1693	0.41	0/2284
42	BS	0.23	0/1202	0.39	0/1618
43	BT	0.24	0/1408	0.39	0/1895
44	BU	0.24	0/711	0.38	0/955
45	BW	0.25	0/1604	0.38	0/2167
46	BX	0.24	0/897	0.41	0/1215
47	BZ	0.24	0/1460	0.43	0/1975
48	Ba	0.25	0/1233	0.38	0/1667
49	Bb	0.23	0/822	0.40	0/1113
50	Bc	0.25	0/1238	0.39	0/1685
51	Bf	0.26	0/697	0.40	0/938
52	Bg	0.24	0/671	0.40	0/905
53	Bh	0.25	0/752	0.40	0/1015
54	UA	0.28	0/229	0.34	0/319
55	UB	0.37	0/44	0.51	0/60
56	UC	0.33	0/69	0.46	0/95
57	UD	0.35	0/39	0.43	0/53
58	UE	0.33	0/59	0.41	0/81
59	UF	0.26	0/688	0.31	0/952
60	UG	0.30	0/94	0.31	0/130
61	UH	0.32	0/84	0.43	0/116
62	UI	0.29	0/194	0.46	0/270
63	UJ	0.31	0/124	0.43	0/172
64	UK	0.29	0/234	0.46	0/326
65	XA	0.26	0/1331	0.43	0/1784
66	XB	0.24	0/5052	0.42	0/6829
67	XC	0.24	0/4763	0.41	0/6454
68	XD	0.23	0/667	0.36	0/906
68	XE	0.23	0/667	0.37	0/906
69	XF	0.23	0/1288	0.36	0/1747
70	XG	0.24	0/1362	0.43	0/1835
71	XH	0.24	0/3277	0.39	0/4441
72	XI	0.23	0/4820	0.38	0/6535
73	XJ	0.23	0/1234	0.38	0/1670
74	XL	0.24	0/4237	0.40	0/5715

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	XM	0.22	0/757	0.36	0/1018
76	XN	0.25	0/4487	0.39	0/6111
77	XO	0.23	0/3254	0.40	0/4400
78	XP	0.25	0/3080	0.41	0/4177
79	XQ	0.24	0/2248	0.40	0/3042
80	XR	0.24	0/1150	0.36	0/1546
81	XS	0.23	0/1557	0.36	0/2099
82	XT	0.24	0/819	0.37	0/1097
All	All	0.24	0/161123	0.44	1/221759 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AA	284	U	C2-N1-C1'	5.47	124.26	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
2	A2	445/463 (96%)	438 (98%)	7 (2%)	0	100	100
3	A3	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
4	A5	53/55 (96%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A8	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
7	AE	357/367 (97%)	344 (96%)	13 (4%)	0	100	100
8	AF	440/442 (100%)	421 (96%)	19 (4%)	0	100	100
9	AI	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
10	AK	266/278 (96%)	259 (97%)	7 (3%)	0	100	100
11	AN	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
12	AP	304/354 (86%)	298 (98%)	6 (2%)	0	100	100
13	AR	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
14	AT	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
15	AU	171/196 (87%)	162 (95%)	9 (5%)	0	100	100
16	AV	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
17	AW	275/277 (99%)	272 (99%)	3 (1%)	0	100	100
18	AX	163/165 (99%)	159 (98%)	4 (2%)	0	100	100
19	AY	330/340 (97%)	322 (98%)	8 (2%)	0	100	100
20	Ae	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
21	Af	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
22	Ag	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
23	Al	166/182 (91%)	161 (97%)	5 (3%)	0	100	100
24	Ao	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
25	Ap	286/288 (99%)	272 (95%)	14 (5%)	0	100	100
26	At	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
27	Av	194/197 (98%)	186 (96%)	8 (4%)	0	100	100
28	BA	719/798 (90%)	692 (96%)	27 (4%)	0	100	100
29	BB	363/371 (98%)	354 (98%)	9 (2%)	0	100	100
30	BD	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
31	BE	397/438 (91%)	374 (94%)	23 (6%)	0	100	100
32	BF	337/421 (80%)	329 (98%)	8 (2%)	0	100	100
33	BH	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
34	BI	321/323 (99%)	312 (97%)	9 (3%)	0	100	100
35	BJ	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
36	BK	234/273 (86%)	228 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	226/276 (82%)	217 (96%)	9 (4%)	0	100	100
38	BN	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
39	BO	207/227 (91%)	203 (98%)	4 (2%)	0	100	100
40	BQ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
41	BR	193/195 (99%)	188 (97%)	5 (3%)	0	100	100
42	BS	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
43	BT	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
44	BU	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
45	BW	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
46	BX	103/116 (89%)	96 (93%)	7 (7%)	0	100	100
47	BZ	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
48	Ba	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
49	Bb	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
50	Bc	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
51	Bf	76/86 (88%)	72 (95%)	4 (5%)	0	100	100
52	Bg	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
53	Bh	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
54	UA	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
55	UB	7/9 (78%)	7 (100%)	0	0	100	100
56	UC	12/14 (86%)	12 (100%)	0	0	100	100
57	UD	6/8 (75%)	6 (100%)	0	0	100	100
58	UE	10/12 (83%)	10 (100%)	0	0	100	100
59	UF	125/139 (90%)	125 (100%)	0	0	100	100
60	UG	17/19 (90%)	16 (94%)	1 (6%)	0	100	100
61	UH	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
62	UI	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
63	UJ	23/25 (92%)	23 (100%)	0	0	100	100
64	UK	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
65	XA	152/155 (98%)	145 (95%)	7 (5%)	0	100	100
66	XB	610/668 (91%)	584 (96%)	26 (4%)	0	100	100
67	XC	580/616 (94%)	556 (96%)	24 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	XD	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
68	XE	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
69	XF	155/198 (78%)	154 (99%)	1 (1%)	0	100	100
70	XG	160/170 (94%)	156 (98%)	4 (2%)	0	100	100
71	XH	388/533 (73%)	374 (96%)	14 (4%)	0	100	100
72	XI	587/703 (84%)	568 (97%)	18 (3%)	1 (0%)	44	75
73	XJ	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
74	XL	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
75	XM	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
76	XN	535/620 (86%)	507 (95%)	28 (5%)	0	100	100
77	XO	392/428 (92%)	379 (97%)	13 (3%)	0	100	100
78	XP	369/371 (100%)	351 (95%)	18 (5%)	0	100	100
79	XQ	279/305 (92%)	265 (95%)	14 (5%)	0	100	100
80	XR	133/161 (83%)	132 (99%)	1 (1%)	0	100	100
81	XS	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
82	XT	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	17137/18343 (93%)	16559 (97%)	577 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	XI	600	GLY

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	A1	195/195 (100%)	191 (98%)	4 (2%)	48	71
2	A2	394/405 (97%)	394 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A3	135/135 (100%)	135 (100%)	0	100	100
4	A5	52/52 (100%)	52 (100%)	0	100	100
5	A8	126/126 (100%)	126 (100%)	0	100	100
7	AE	312/316 (99%)	312 (100%)	0	100	100
8	AF	394/394 (100%)	391 (99%)	3 (1%)	79	88
9	AI	192/192 (100%)	191 (100%)	1 (0%)	86	93
10	AK	179/185 (97%)	175 (98%)	4 (2%)	47	70
11	AN	152/152 (100%)	150 (99%)	2 (1%)	65	81
12	AP	275/314 (88%)	274 (100%)	1 (0%)	89	95
13	AR	222/222 (100%)	221 (100%)	1 (0%)	86	93
14	AT	119/119 (100%)	115 (97%)	4 (3%)	32	60
15	AU	151/168 (90%)	151 (100%)	0	100	100
16	AV	153/153 (100%)	153 (100%)	0	100	100
17	AW	245/245 (100%)	243 (99%)	2 (1%)	79	88
18	AX	153/153 (100%)	152 (99%)	1 (1%)	81	89
19	AY	299/305 (98%)	298 (100%)	1 (0%)	91	96
20	Ae	100/100 (100%)	99 (99%)	1 (1%)	73	84
21	Af	116/116 (100%)	116 (100%)	0	100	100
22	Ag	169/169 (100%)	169 (100%)	0	100	100
23	Al	146/156 (94%)	145 (99%)	1 (1%)	81	89
24	Ao	107/107 (100%)	107 (100%)	0	100	100
25	Ap	249/249 (100%)	249 (100%)	0	100	100
26	At	132/132 (100%)	131 (99%)	1 (1%)	79	88
27	Av	172/172 (100%)	170 (99%)	2 (1%)	67	82
28	BA	641/698 (92%)	639 (100%)	2 (0%)	91	96
29	BB	266/266 (100%)	263 (99%)	3 (1%)	70	83
30	BD	356/356 (100%)	344 (97%)	12 (3%)	32	60
31	BE	343/375 (92%)	340 (99%)	3 (1%)	75	86
32	BF	295/363 (81%)	292 (99%)	3 (1%)	73	84
33	BH	194/194 (100%)	194 (100%)	0	100	100
34	BI	271/271 (100%)	268 (99%)	3 (1%)	70	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BJ	140/140 (100%)	136 (97%)	4 (3%)	37	64
36	BK	198/223 (89%)	198 (100%)	0	100	100
37	BL	201/234 (86%)	200 (100%)	1 (0%)	86	93
38	BN	189/189 (100%)	187 (99%)	2 (1%)	70	83
39	BO	181/193 (94%)	181 (100%)	0	100	100
40	BQ	155/155 (100%)	155 (100%)	0	100	100
41	BR	171/171 (100%)	170 (99%)	1 (1%)	84	91
42	BS	128/128 (100%)	126 (98%)	2 (2%)	58	76
43	BT	146/146 (100%)	144 (99%)	2 (1%)	62	79
44	BU	71/71 (100%)	70 (99%)	1 (1%)	62	79
45	BW	163/163 (100%)	163 (100%)	0	100	100
46	BX	92/98 (94%)	92 (100%)	0	100	100
47	BZ	159/159 (100%)	158 (99%)	1 (1%)	84	91
48	Ba	128/128 (100%)	128 (100%)	0	100	100
49	Bb	88/88 (100%)	88 (100%)	0	100	100
50	Bc	127/127 (100%)	126 (99%)	1 (1%)	79	88
51	Bf	71/76 (93%)	71 (100%)	0	100	100
52	Bg	65/65 (100%)	65 (100%)	0	100	100
53	Bh	79/79 (100%)	78 (99%)	1 (1%)	65	81
65	XA	134/134 (100%)	134 (100%)	0	100	100
66	XB	535/577 (93%)	530 (99%)	5 (1%)	75	86
67	XC	517/544 (95%)	511 (99%)	6 (1%)	67	82
68	XD	77/77 (100%)	75 (97%)	2 (3%)	41	66
68	XE	77/77 (100%)	77 (100%)	0	100	100
69	XF	134/161 (83%)	134 (100%)	0	100	100
70	XG	142/146 (97%)	141 (99%)	1 (1%)	81	89
71	XH	352/454 (78%)	349 (99%)	3 (1%)	75	86
72	XI	531/618 (86%)	524 (99%)	7 (1%)	65	81
73	XJ	134/134 (100%)	133 (99%)	1 (1%)	81	89
74	XL	452/457 (99%)	452 (100%)	0	100	100
75	XM	76/76 (100%)	75 (99%)	1 (1%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	XN	472/538 (88%)	472 (100%)	0	100	100
77	XO	348/373 (93%)	348 (100%)	0	100	100
78	XP	326/326 (100%)	324 (99%)	2 (1%)	84	91
79	XQ	239/257 (93%)	236 (99%)	3 (1%)	65	81
80	XR	120/138 (87%)	114 (95%)	6 (5%)	20	49
81	XS	169/169 (100%)	167 (99%)	2 (1%)	67	82
82	XT	84/84 (100%)	84 (100%)	0	100	100
All	All	14776/15528 (95%)	14666 (99%)	110 (1%)	80	89

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	10	PHE
1	A1	119	GLN
1	A1	148	LEU
1	A1	176	GLN
8	AF	127	THR
8	AF	154	ARG
8	AF	186	ARG
9	AI	206	LEU
10	AK	61	LYS
10	AK	99	GLU
10	AK	135	GLU
10	AK	214	CYS
11	AN	135	LYS
11	AN	142	PHE
12	AP	50	ASP
13	AR	170	MET
14	AT	21	PHE
14	AT	44	ARG
14	AT	96	GLU
14	AT	113	HIS
17	AW	133	LEU
17	AW	248	LEU
18	AX	197	ARG
19	AY	125	ILE
20	Ae	153	PHE
23	Al	88	ARG
26	At	143	THR
27	Av	29	MET

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Mol	Chain	Res	Type
27	Av	45	LEU
28	BA	63	LEU
28	BA	152	TYR
29	BB	156	TRP
29	BB	198	ARG
29	BB	413	LEU
30	BD	114	LEU
30	BD	139	LEU
30	BD	142	VAL
30	BD	182	ARG
30	BD	184	GLN
30	BD	187	ASP
30	BD	198	ASP
30	BD	258	TYR
30	BD	292	LEU
30	BD	342	PHE
30	BD	387	HIS
30	BD	422	GLN
31	BE	384	HIS
31	BE	410	PHE
31	BE	435	ASP
32	BF	289	CYS
32	BF	354	LEU
32	BF	363	GLN
34	BI	108	GLU
34	BI	119	GLU
34	BI	133	PHE
35	BJ	180	GLU
35	BJ	203	LEU
35	BJ	216	HIS
35	BJ	256	LEU
37	BL	183	TRP
38	BN	185	GLU
38	BN	233	TYR
41	BR	133	GLN
42	BS	147	ARG
42	BS	162	ARG
43	BT	34	ARG
43	BT	104	ARG
44	BU	141	GLU
47	BZ	36	ASN
50	Bc	18	ARG

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Mol	Chain	Res	Type
53	Bh	7	PHE
66	XB	103	ASP
66	XB	178	ARG
66	XB	464	LEU
66	XB	612	ASN
66	XB	637	TYR
67	XC	30	CYS
67	XC	164	TYR
67	XC	272	PHE
67	XC	278	ARG
67	XC	301	CYS
67	XC	604	LEU
68	XD	84	GLU
68	XD	110	GLU
70	XG	174	ASN
71	XH	29	ASP
71	XH	497	ASP
71	XH	544	LEU
72	XI	251	HIS
72	XI	259	GLN
72	XI	266	HIS
72	XI	279	TRP
72	XI	412	LEU
72	XI	540	SER
72	XI	694	GLN
73	XJ	249	GLN
75	XM	67	GLN
78	XP	178	MET
78	XP	196	TRP
79	XQ	93	LEU
79	XQ	183	ASN
79	XQ	261	LEU
80	XR	2	VAL
80	XR	30	LEU
80	XR	105	LEU
80	XR	118	GLN
80	XR	120	LEU
80	XR	140	TYR
81	XS	42	HIS
81	XS	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
5	A8	161	ASN
11	AN	63	GLN
12	AP	81	HIS
17	AW	75	GLN
66	XB	352	GLN
70	XG	105	GLN
74	XL	450	GLN
75	XM	67	GLN
81	XS	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	AA	744/758 (98%)	219 (29%)	8 (1%)

All (219) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	AA	11	U
6	AA	12	U
6	AA	13	A
6	AA	14	A
6	AA	17	A
6	AA	18	G
6	AA	20	A
6	AA	22	A
6	AA	29	U
6	AA	32	U
6	AA	34	G
6	AA	38	U
6	AA	40	U
6	AA	41	U
6	AA	42	A
6	AA	43	U
6	AA	45	U
6	AA	47	U
6	AA	50	A
6	AA	52	U
6	AA	53	A
6	AA	54	A
6	AA	60	U
6	AA	64	U

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Mol	Chain	Res	Type
6	AA	65	U
6	AA	67	C
6	AA	70	G
6	AA	72	A
6	AA	73	G
6	AA	75	A
6	AA	77	A
6	AA	79	U
6	AA	80	U
6	AA	83	U
6	AA	85	U
6	AA	86	U
6	AA	87	U
6	AA	88	G
6	AA	89	U
6	AA	98	U
6	AA	104	A
6	AA	106	G
6	AA	107	U
6	AA	111	U
6	AA	113	A
6	AA	115	A
6	AA	119	A
6	AA	120	A
6	AA	124	U
6	AA	125	U
6	AA	133	U
6	AA	134	U
6	AA	136	U
6	AA	154	A
6	AA	155	U
6	AA	158	A
6	AA	162	A
6	AA	171	U
6	AA	172	U
6	AA	176	A
6	AA	177	U
6	AA	183	U
6	AA	189	A
6	AA	198	A
6	AA	201	G
6	AA	261	U

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Mol	Chain	Res	Type
6	AA	262	U
6	AA	275	C
6	AA	276	C
6	AA	277	A
6	AA	285	A
6	AA	286	U
6	AA	287	A
6	AA	289	U
6	AA	290	A
6	AA	297	U
6	AA	299	U
6	AA	302	G
6	AA	313	A
6	AA	315	A
6	AA	317	A
6	AA	327	U
6	AA	329	U
6	AA	331	C
6	AA	344	A
6	AA	346	G
6	AA	347	A
6	AA	405	U
6	AA	407	G
6	AA	408	A
6	AA	413	U
6	AA	461	U
6	AA	463	U
6	AA	470	G
6	AA	472	A
6	AA	473	A
6	AA	475	U
6	AA	476	G
6	AA	478	A
6	AA	481	G
6	AA	483	A
6	AA	485	A
6	AA	488	U
6	AA	489	G
6	AA	490	G
6	AA	491	A
6	AA	492	U
6	AA	494	U

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Mol	Chain	Res	Type
6	AA	495	A
6	AA	496	A
6	AA	497	C
6	AA	509	U
6	AA	515	U
6	AA	516	U
6	AA	518	A
6	AA	519	A
6	AA	520	U
6	AA	521	G
6	AA	522	A
6	AA	526	G
6	AA	528	A
6	AA	529	U
6	AA	545	U
6	AA	548	A
6	AA	555	U
6	AA	557	A
6	AA	558	U
6	AA	559	A
6	AA	560	G
6	AA	565	U
6	AA	567	G
6	AA	569	U
6	AA	572	U
6	AA	574	A
6	AA	575	A
6	AA	592	U
6	AA	797	A
6	AA	814	A
6	AA	817	A
6	AA	818	A
6	AA	825	A
6	AA	826	A
6	AA	828	A
6	AA	829	A
6	AA	830	A
6	AA	837	A
6	AA	838	A
6	AA	845	A
6	AA	846	A
6	AA	851	G

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Mol	Chain	Res	Type
6	AA	853	A
6	AA	854	A
6	AA	869	U
6	AA	871	C
6	AA	874	A
6	AA	882	U
6	AA	894	A
6	AA	898	U
6	AA	899	A
6	AA	902	U
6	AA	904	U
6	AA	905	G
6	AA	906	A
6	AA	908	U
6	AA	909	G
6	AA	914	A
6	AA	915	A
6	AA	917	A
6	AA	926	A
6	AA	927	U
6	AA	934	A
6	AA	940	A
6	AA	941	G
6	AA	942	A
6	AA	944	C
6	AA	945	U
6	AA	949	U
6	AA	953	U
6	AA	954	U
6	AA	958	A
6	AA	959	U
6	AA	963	A
6	AA	980	U
6	AA	1005	U
6	AA	1010	C
6	AA	1079	A
6	AA	1090	U
6	AA	1096	U
6	AA	1105	U
6	AA	1106	U
6	AA	1107	U
6	AA	1112	U

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Mol	Chain	Res	Type
6	AA	1114	A
6	AA	1117	A
6	AA	1119	U
6	AA	1121	A
6	AA	1130	A
6	AA	1131	G
6	AA	1139	G
6	AA	1141	A
6	AA	1144	G
6	AA	1151	G
6	AA	1152	A
6	AA	1153	A
6	AA	1155	A
6	AA	1156	A
6	AA	1157	A
6	AA	1158	G
6	AA	1161	A
6	AA	1162	G
6	AA	1164	A
6	AA	1167	A
6	AA	1168	U
6	AA	1169	A
6	AA	1171	A
6	AA	1172	A
6	AA	1174	U
6	AA	1175	U
6	AA	1176	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	AA	19	A
6	AA	41	U
6	AA	69	U
6	AA	171	U
6	AA	484	U
6	AA	490	G
6	AA	515	U
6	AA	1095	A

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

2 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	$\# Z > 2$
68	4HH	XE	105	68	21,26,27	1.98	4 (19%)	27,35,37	1.10	2 (7%)
68	4HH	XD	105	68	21,26,27	1.97	4 (19%)	27,35,37	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	4HH	XE	105	68	-	6/32/35/37	-
68	4HH	XD	105	68	-	12/32/35/37	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	XE	105	4HH	CL3-NN	5.47	1.45	1.33
68	XD	105	4HH	CL3-NN	5.44	1.45	1.33
68	XE	105	4HH	CQ-NR	5.40	1.45	1.33
68	XD	105	4HH	CQ-NR	5.40	1.45	1.33
68	XD	105	4HH	ON-CL3	-2.25	1.18	1.23
68	XE	105	4HH	ON-CL3	-2.23	1.19	1.23
68	XE	105	4HH	OR-CQ	-2.17	1.18	1.23
68	XD	105	4HH	OR-CQ	-2.11	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	XE	105	4HH	OG-CB-CA	2.40	110.48	108.14
68	XE	105	4HH	CP-CQ-NR	2.01	119.81	116.42

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	XD	105	4HH	N-CA-CB-OG
68	XD	105	4HH	CJ-CK-CM-CL3
68	XD	105	4HH	CJ-CK-CM-OM
68	XD	105	4HH	CL1-CK-CM-CL3
68	XD	105	4HH	CL1-CK-CM-OM
68	XD	105	4HH	CL2-CK-CM-CL3
68	XD	105	4HH	CL2-CK-CM-OM
68	XD	105	4HH	CJ-O3P-P-OG
68	XD	105	4HH	NR-CS-CT-SU
68	XE	105	4HH	CB-OG-P-O2P
68	XE	105	4HH	CB-OG-P-O3P
68	XE	105	4HH	NR-CS-CT-SU
68	XD	105	4HH	NN-CO-CP-CQ
68	XE	105	4HH	CJ-O3P-P-OG
68	XE	105	4HH	CL2-CK-CM-OM
68	XD	105	4HH	CK-CJ-O3P-P
68	XD	105	4HH	CJ-O3P-P-O1P
68	XE	105	4HH	CJ-CK-CM-CL3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 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
88	GTP	XL	602	-	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
88	GTP	XL	601	-	26,34,34	1.13	2 (7%)	32,54,54	1.66	7 (21%)
84	NAD	Av	301	-	42,48,48	5.07	16 (38%)	50,73,73	2.31	8 (16%)
83	FES	A5	101	4	0,4,4	-	-	-	-	-
87	ADP	XB	902	86	24,29,29	3.34	10 (41%)	29,45,45	3.55	6 (20%)

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
88	GTP	XL	602	-	-	4/18/38/38	0/3/3/3
88	GTP	XL	601	-	-	2/18/38/38	0/3/3/3
84	NAD	Av	301	-	-	5/26/62/62	0/5/5/5
83	FES	A5	101	4	-	-	0/1/1/1
87	ADP	XB	902	86	-	1/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Av	301	NAD	C2D-C1D	-15.03	1.31	1.53
84	Av	301	NAD	O4B-C1B	14.88	1.61	1.41
84	Av	301	NAD	O4D-C1D	14.87	1.61	1.41
84	Av	301	NAD	C2B-C1B	-14.35	1.32	1.53
87	XB	902	ADP	C3'-C4'	-8.37	1.31	1.53
87	XB	902	ADP	O4'-C4'	7.74	1.62	1.45
87	XB	902	ADP	O4'-C1'	-7.64	1.30	1.41
84	Av	301	NAD	O4B-C4B	-7.31	1.28	1.45
84	Av	301	NAD	O4D-C4D	-5.60	1.32	1.45
84	Av	301	NAD	C7N-N7N	4.48	1.41	1.33
87	XB	902	ADP	C6-N6	4.10	1.49	1.34
88	XL	601	GTP	C5-C6	-4.01	1.39	1.47
88	XL	602	GTP	C5-C6	-3.98	1.39	1.47
84	Av	301	NAD	O3D-C3D	-3.68	1.34	1.43
84	Av	301	NAD	O2B-C2B	3.58	1.51	1.43
87	XB	902	ADP	O2'-C2'	-3.57	1.34	1.43
84	Av	301	NAD	C6A-N6A	3.40	1.46	1.34
87	XB	902	ADP	C2-N3	3.20	1.37	1.32
87	XB	902	ADP	O3'-C3'	3.01	1.50	1.43
84	Av	301	NAD	C5A-C4A	-2.91	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Av	301	NAD	O2D-C2D	2.72	1.49	1.43
87	XB	902	ADP	PB-O2B	-2.61	1.44	1.54
84	Av	301	NAD	C5B-C4B	2.43	1.59	1.51
87	XB	902	ADP	C5-C4	-2.26	1.35	1.40
84	Av	301	NAD	PA-O5B	2.25	1.68	1.59
88	XL	601	GTP	C2-N3	2.20	1.38	1.33
88	XL	602	GTP	C2-N3	2.20	1.38	1.33
84	Av	301	NAD	C2A-N3A	2.11	1.35	1.32
87	XB	902	ADP	C2-N1	2.09	1.37	1.33
84	Av	301	NAD	C2A-N1A	2.03	1.37	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	XB	902	ADP	C1'-N9-C4	-11.54	106.37	126.64
84	Av	301	NAD	C5A-C6A-N6A	11.13	137.27	120.35
87	XB	902	ADP	C5-C6-N6	10.83	136.81	120.35
87	XB	902	ADP	N6-C6-N1	-7.70	102.59	118.57
84	Av	301	NAD	N6A-C6A-N1A	-7.58	102.83	118.57
84	Av	301	NAD	N3A-C2A-N1A	-5.54	120.03	128.68
87	XB	902	ADP	N3-C2-N1	-5.52	120.04	128.68
88	XL	601	GTP	PB-O3B-PG	-4.14	118.61	132.83
88	XL	602	GTP	PA-O3A-PB	-4.02	119.03	132.83
88	XL	601	GTP	PA-O3A-PB	-3.94	119.32	132.83
84	Av	301	NAD	C3D-C2D-C1D	3.34	106.01	100.98
88	XL	602	GTP	PB-O3B-PG	-3.27	121.61	132.83
88	XL	601	GTP	C5-C6-N1	3.23	119.66	113.95
88	XL	602	GTP	C5-C6-N1	3.22	119.64	113.95
88	XL	601	GTP	C8-N7-C5	3.13	108.95	102.99
88	XL	602	GTP	C8-N7-C5	3.10	108.90	102.99
88	XL	601	GTP	C3'-C2'-C1'	2.99	105.47	100.98
88	XL	602	GTP	C3'-C2'-C1'	2.94	105.41	100.98
88	XL	601	GTP	C2-N1-C6	-2.88	119.80	125.10
84	Av	301	NAD	PN-O3-PA	-2.87	122.97	132.83
88	XL	602	GTP	C2-N1-C6	-2.87	119.82	125.10
87	XB	902	ADP	PA-O3A-PB	-2.71	123.54	132.83
88	XL	602	GTP	O6-C6-C5	-2.17	120.14	124.37
88	XL	601	GTP	O6-C6-C5	-2.11	120.25	124.37
84	Av	301	NAD	C3N-C7N-N7N	2.06	120.22	117.75
84	Av	301	NAD	C6N-N1N-C2N	-2.05	120.10	121.97
87	XB	902	ADP	C3'-C2'-C1'	2.01	104.01	100.98
84	Av	301	NAD	O7N-C7N-N7N	-2.01	119.73	122.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

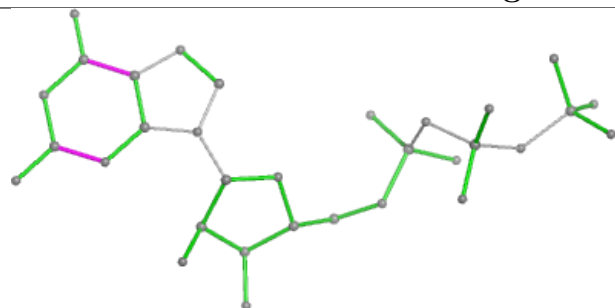
Mol	Chain	Res	Type	Atoms
87	XB	902	ADP	C5'-O5'-PA-O1A
88	XL	602	GTP	C5'-O5'-PA-O2A
84	Av	301	NAD	O4B-C4B-C5B-O5B
88	XL	601	GTP	C3'-C4'-C5'-O5'
84	Av	301	NAD	C3B-C4B-C5B-O5B
88	XL	601	GTP	O4'-C4'-C5'-O5'
84	Av	301	NAD	C5B-O5B-PA-O3
88	XL	602	GTP	C5'-O5'-PA-O3A
84	Av	301	NAD	C5B-O5B-PA-O1A
88	XL	602	GTP	C5'-O5'-PA-O1A
88	XL	602	GTP	PG-O3B-PB-O2B
84	Av	301	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

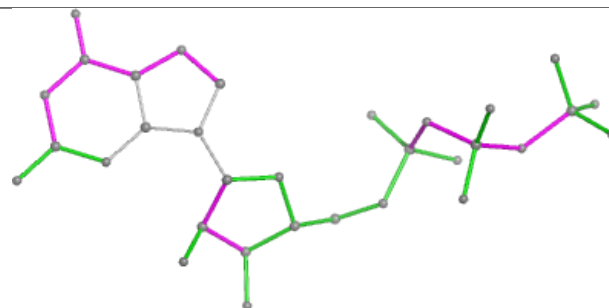
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

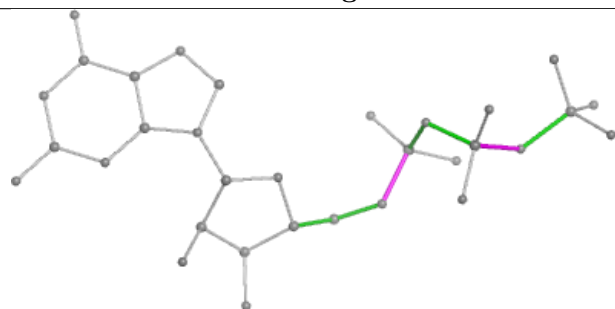
Ligand GTP XL 602



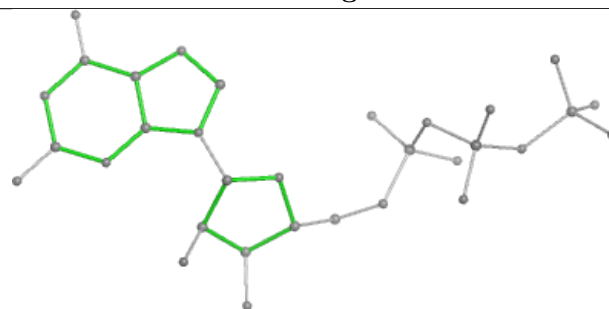
Bond lengths



Bond angles

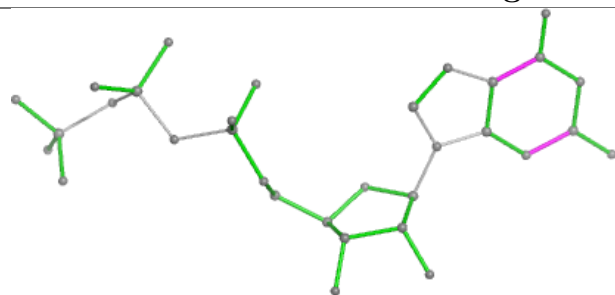


Torsions

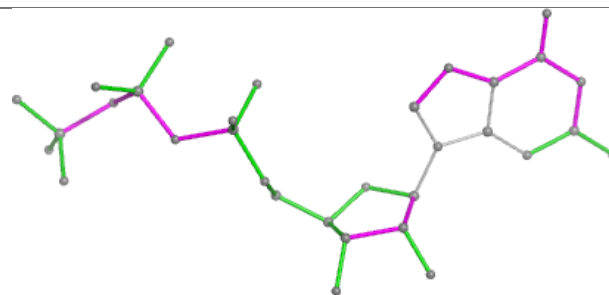


Rings

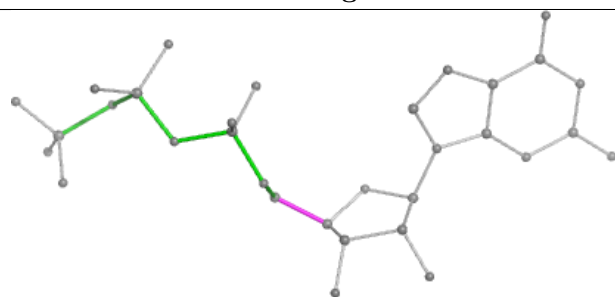
Ligand GTP XL 601



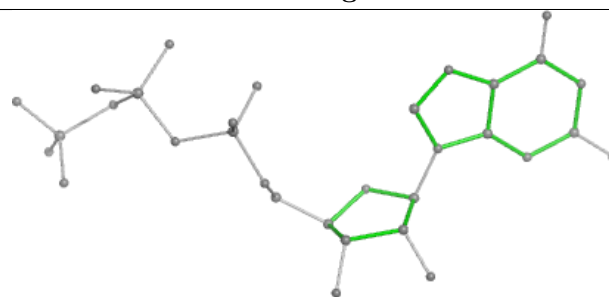
Bond lengths



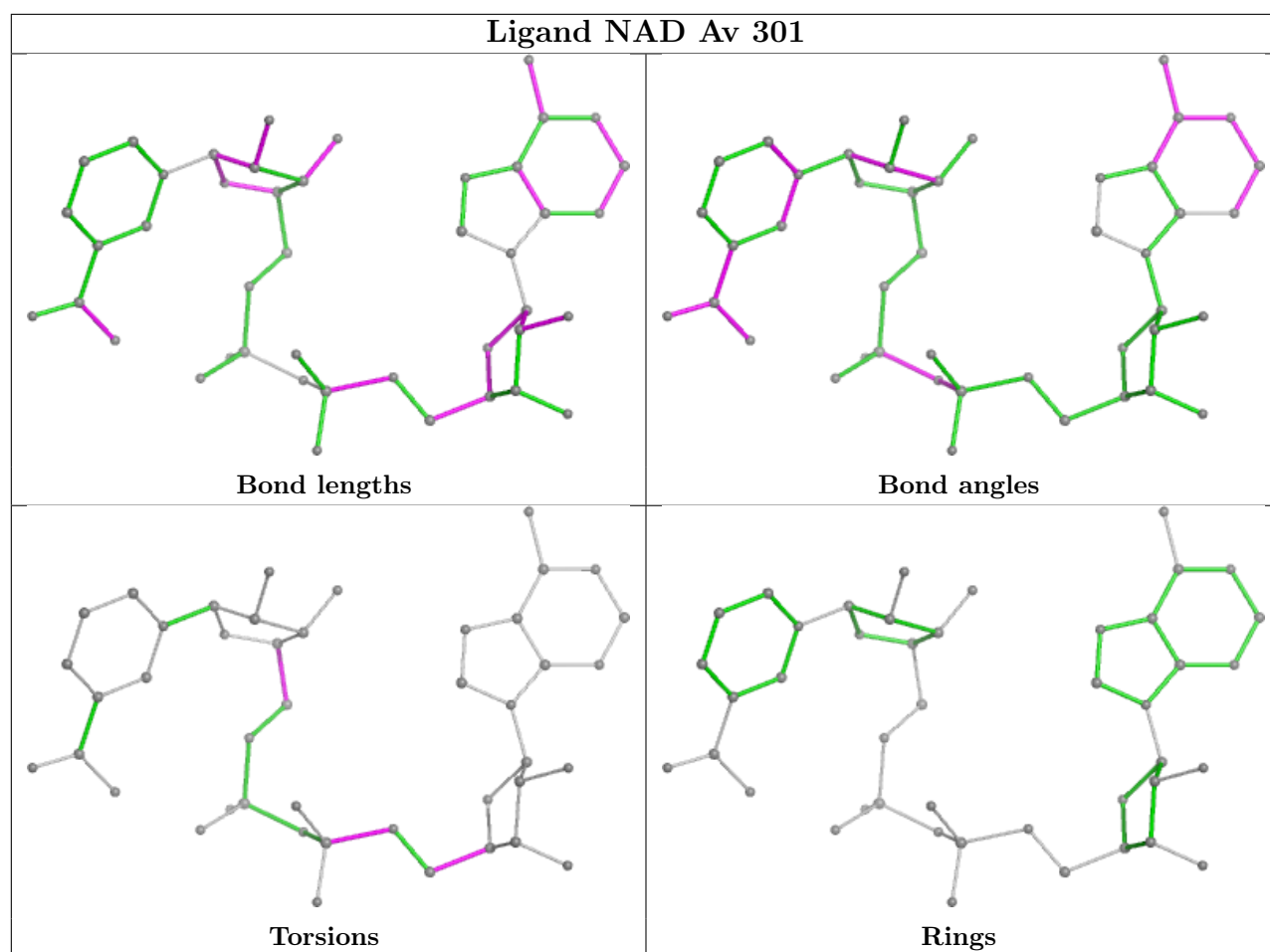
Bond angles

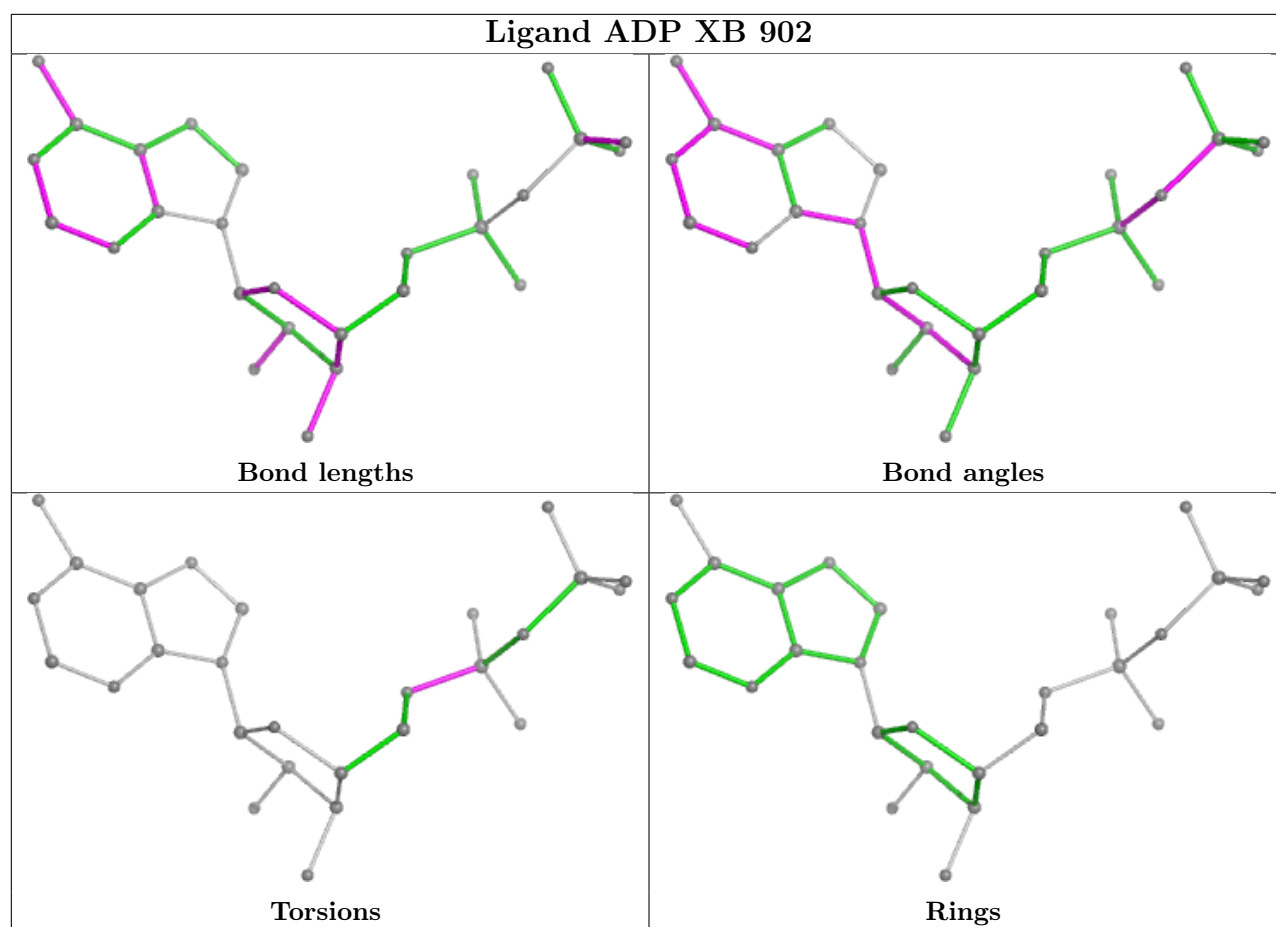


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	AA	14
59	UF	6
29	BB	3
36	BK	2
71	XH	2
10	AK	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	356:A	O3'	369:U	P	34.53
1	AA	594:A	O3'	796:A	P	31.20
1	UF	105:ALA	C	122:ALA	N	30.57
1	BK	233:LYS	C	254:ALA	N	28.37
1	UF	34:ALA	C	37:ALA	N	22.56
1	AA	380:G	O3'	404:U	P	20.97
1	AA	534:U	O3'	541:A	P	19.51
1	BK	269:ALA	C	280:LEU	N	19.38
1	UF	135:ALA	C	140:ALA	N	18.98
1	AA	989:U	O3'	1001:G	P	17.71
1	AA	582:A	O3'	591:G	P	16.56
1	AA	264:U	O3'	270:A	P	16.48
1	AA	1090:U	O3'	1095:A	P	16.18
1	AA	205:U	O3'	254:G	P	15.15
1	AA	1013:C	O3'	1071:U	P	15.08
1	AA	450:U	O3'	456:U	P	14.15
1	AA	413:U	O3'	445:U	P	12.66
1	XH	113:LEU	C	184:ILE	N	12.09
1	BB	258:PHE	C	264:ALA	N	11.96
1	AA	967:G	O3'	972:G	P	11.71
1	BB	294:ALA	C	304:ALA	N	11.57
1	UF	87:ALA	C	92:ALA	N	10.93
1	AA	883:U	O3'	887:A	P	10.10
1	AK	235:GLU	C	239:ALA	N	8.23
1	BB	341:ALA	C	346:GLU	N	7.64
1	XH	55:PRO	C	86:SER	N	7.57
1	UF	27:ALA	C	29:ALA	N	6.13
1	UF	63:ALA	C	65:ALA	N	5.33

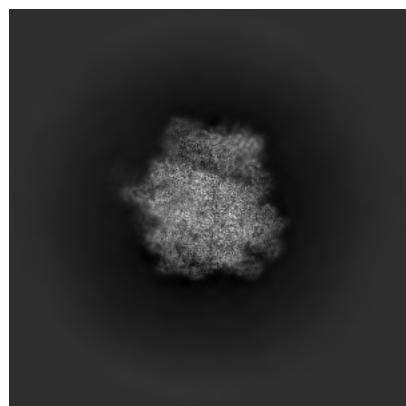
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11845. These allow visual inspection of the internal detail of the map and identification of artifacts.

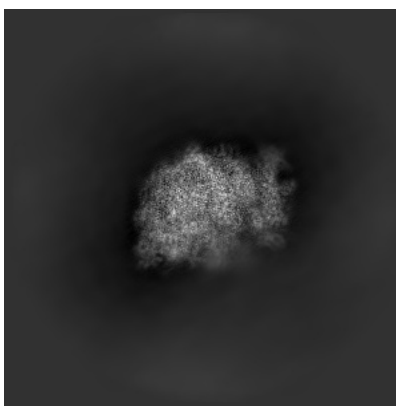
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

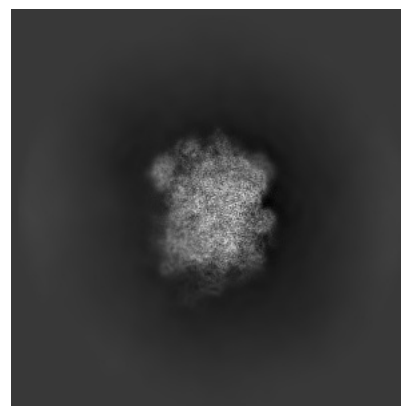
6.1.1 Primary map



X

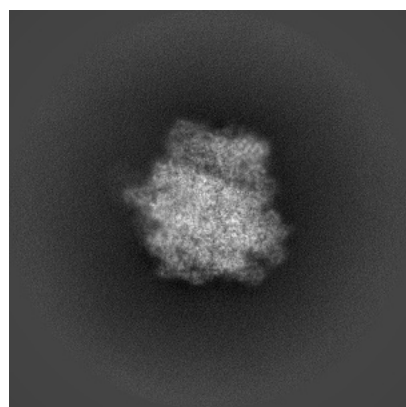


Y

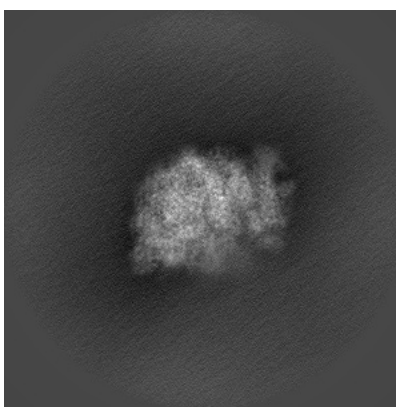


Z

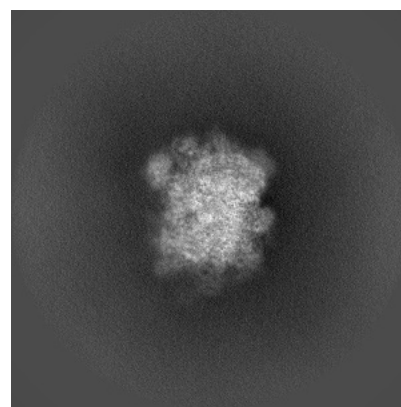
6.1.2 Raw map



X



Y

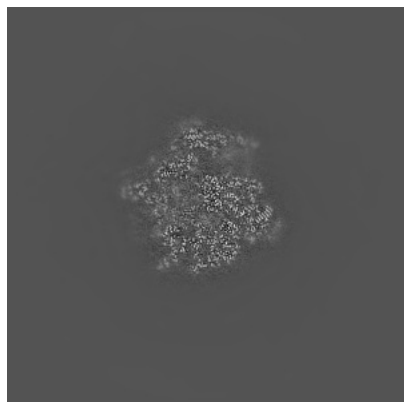


Z

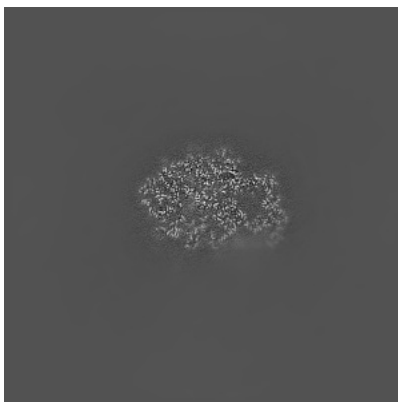
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

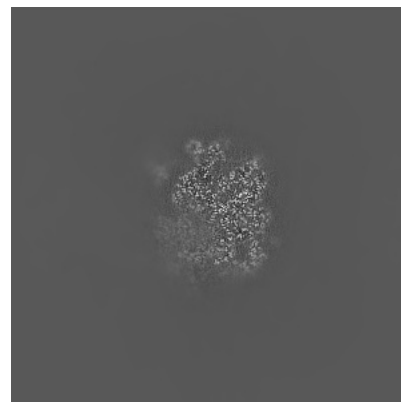
6.2.1 Primary map



X Index: 300

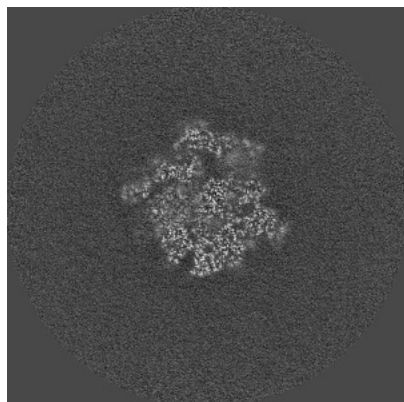


Y Index: 300

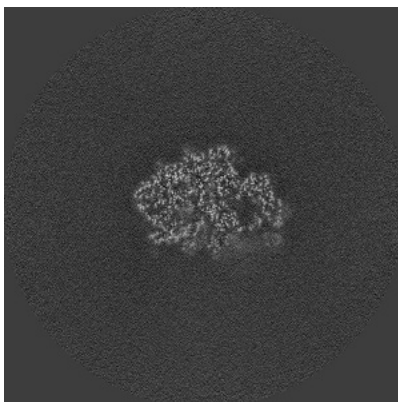


Z Index: 300

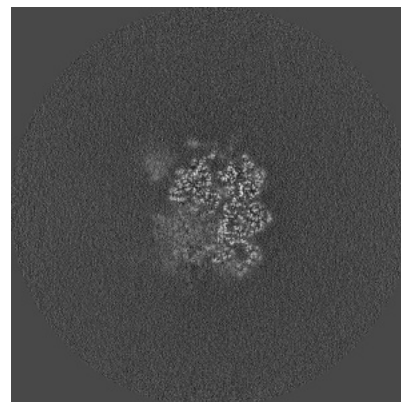
6.2.2 Raw map



X Index: 300



Y Index: 300

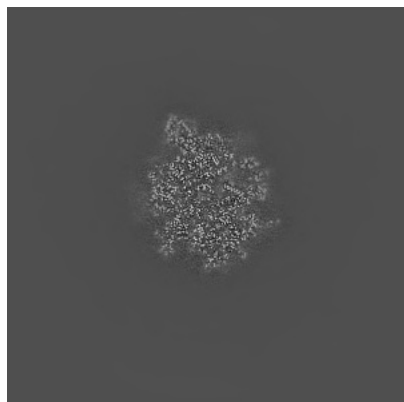


Z Index: 300

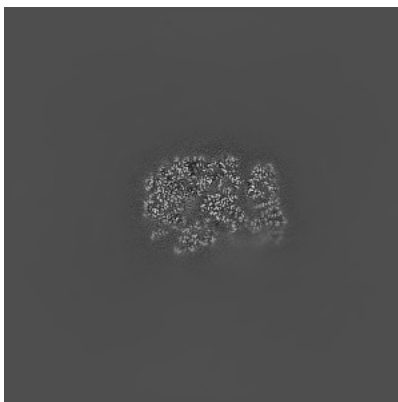
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

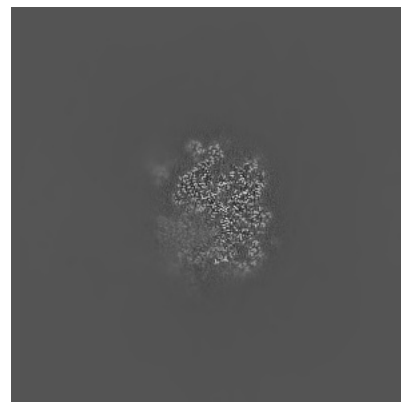
6.3.1 Primary map



X Index: 331

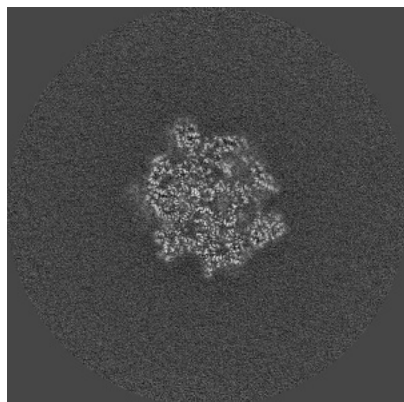


Y Index: 309

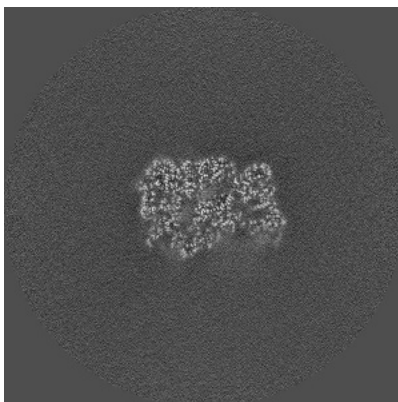


Z Index: 301

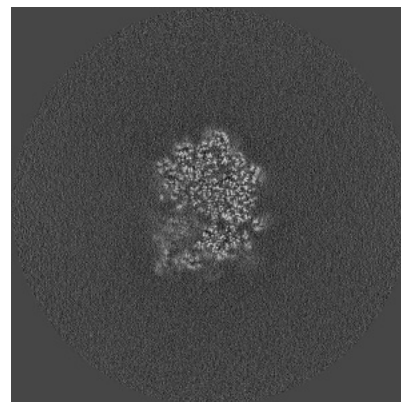
6.3.2 Raw map



X Index: 318



Y Index: 319

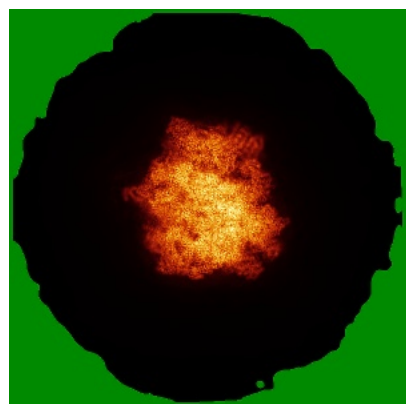


Z Index: 259

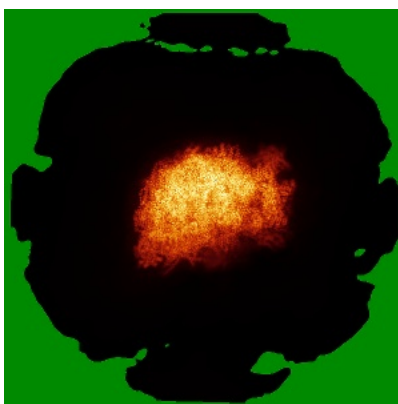
The images above show the largest variance slices of the map in three orthogonal directions.

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

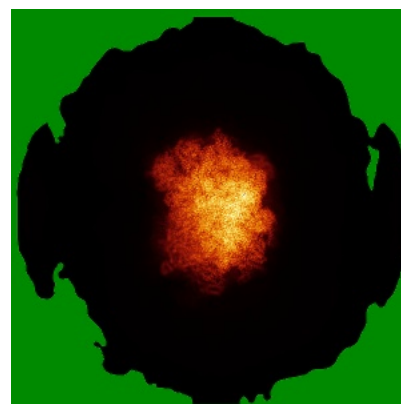
6.4.1 Primary map



X

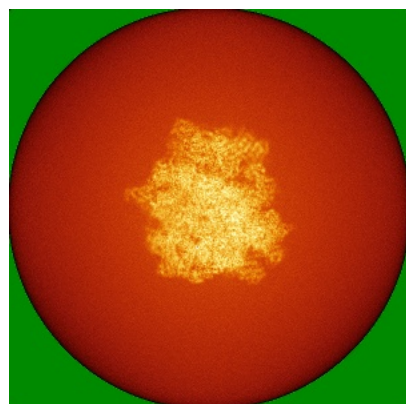


Y

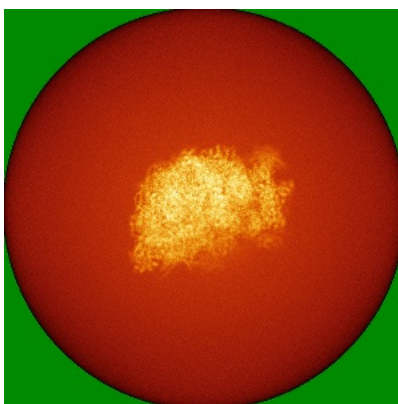


Z

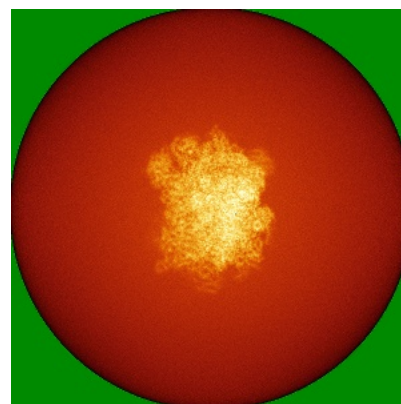
6.4.2 Raw map



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.

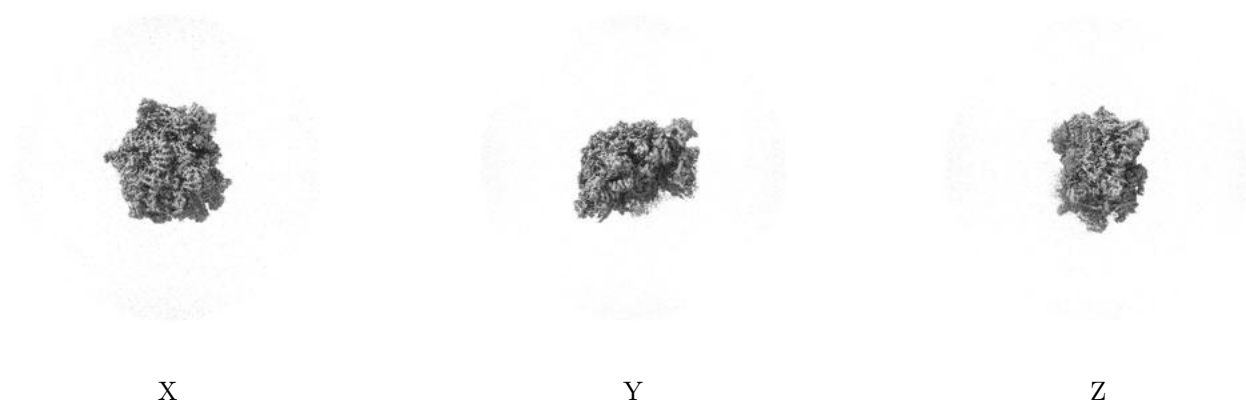
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

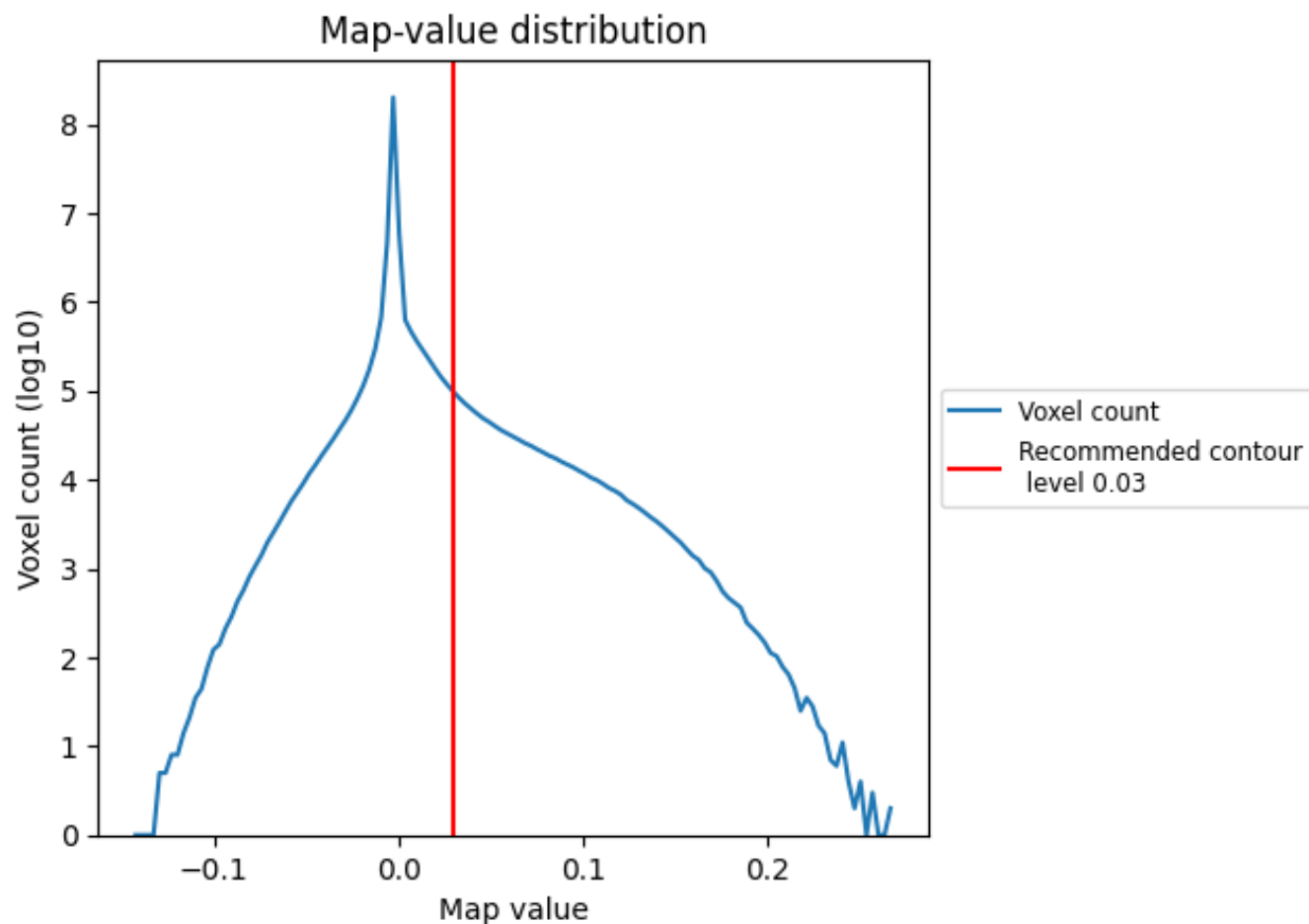
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

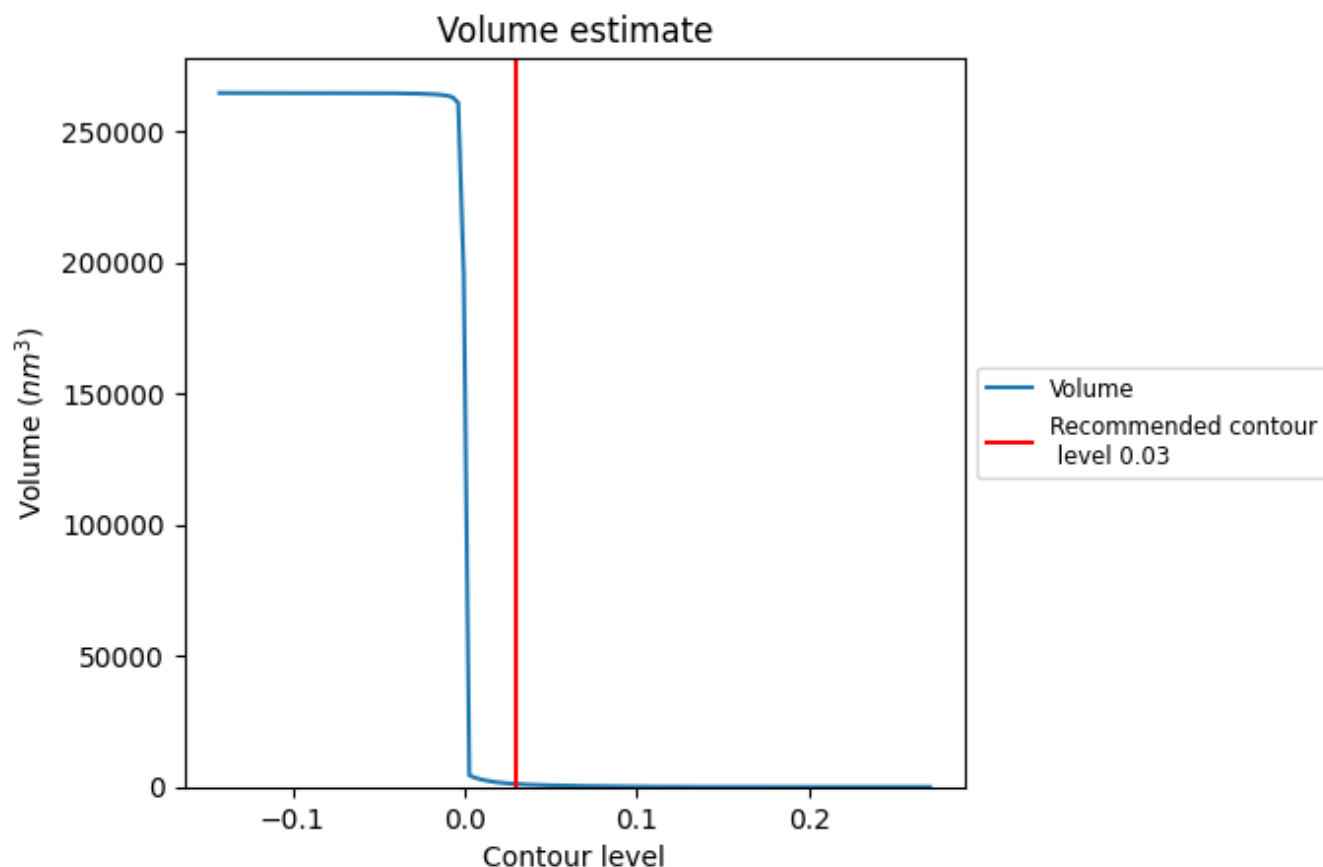
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

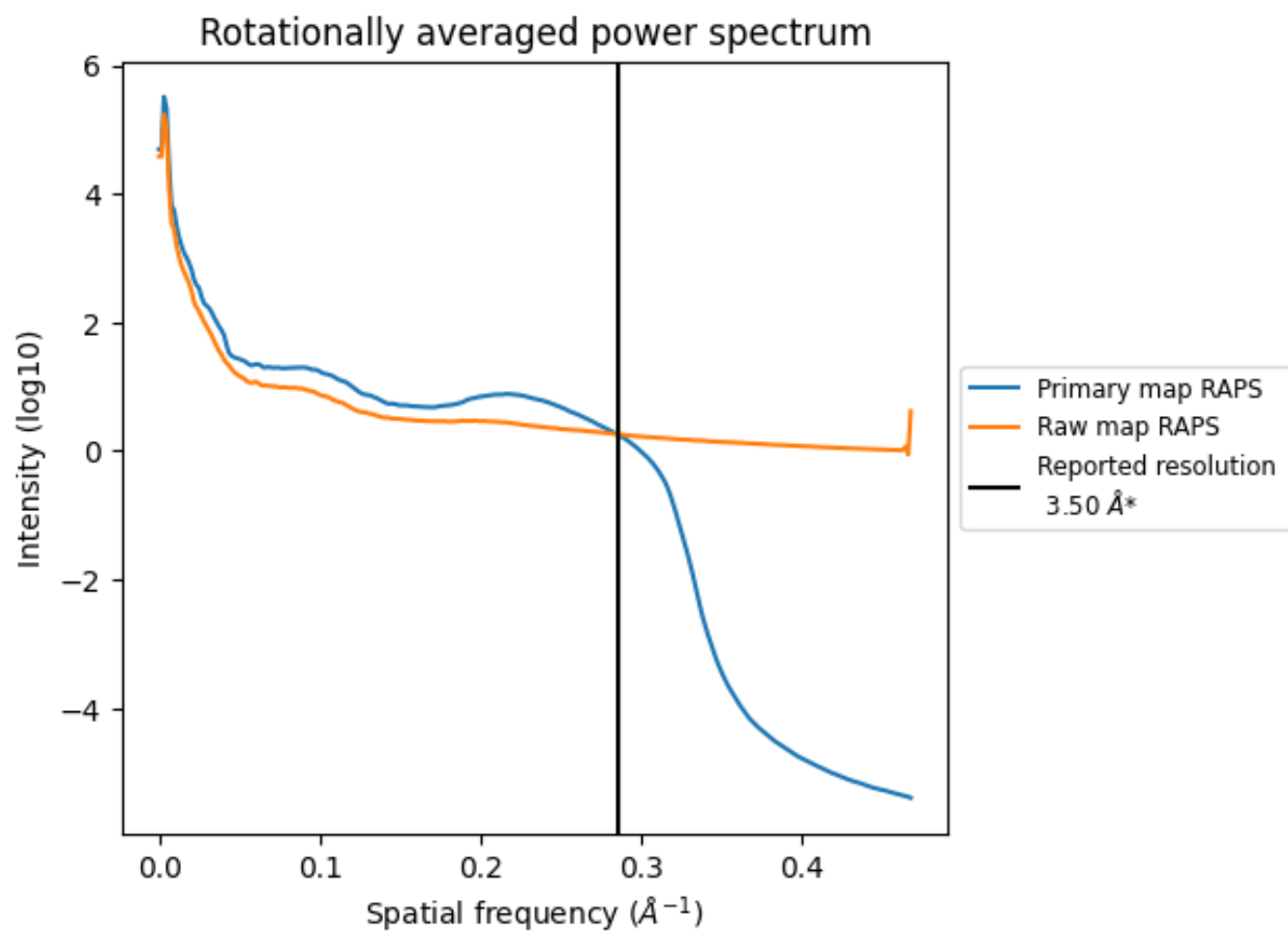
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1128 nm^3 ; this corresponds to an approximate mass of 1019 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 ⓘ

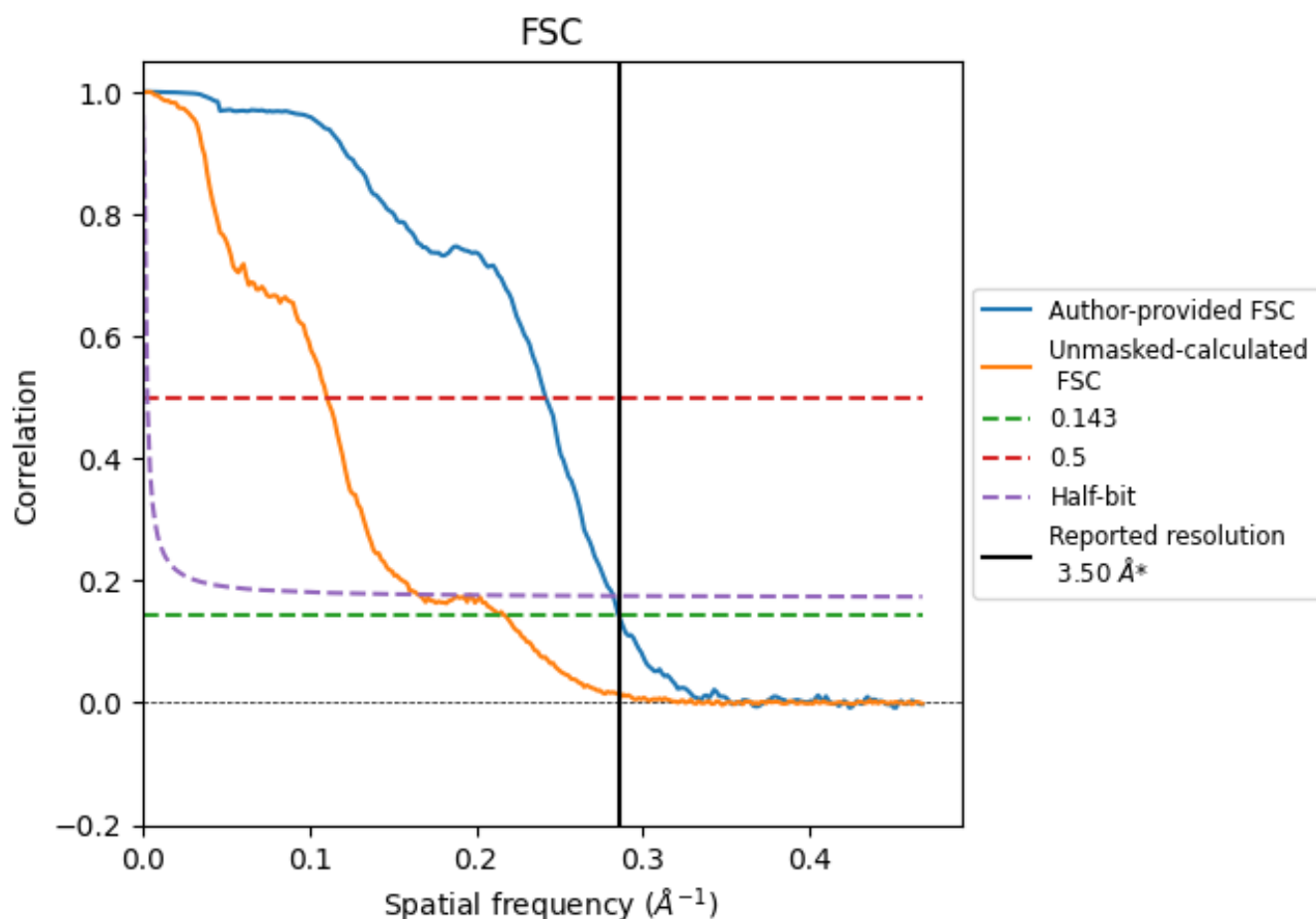


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

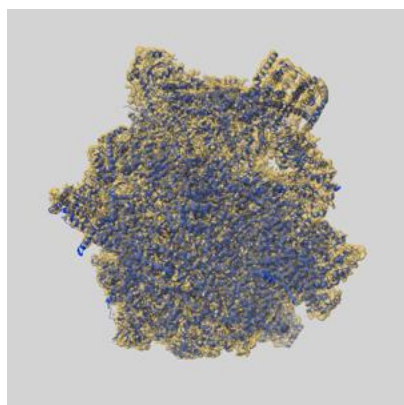
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.14	3.54
Unmasked-calculated*	4.69	9.04	6.06

*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 4.69 differs from the reported value 3.5 by more than 10 %

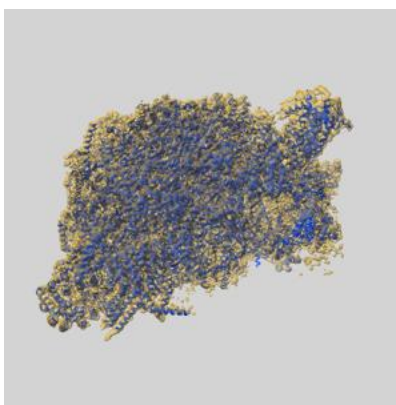
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11845 and PDB model 7AOI. Per-residue inclusion information can be found in section [3](#) on page [22](#).

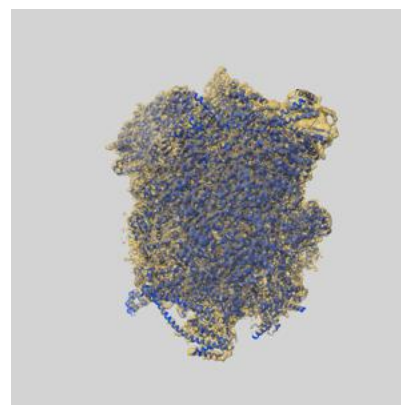
9.1 Map-model overlay [i](#)



X



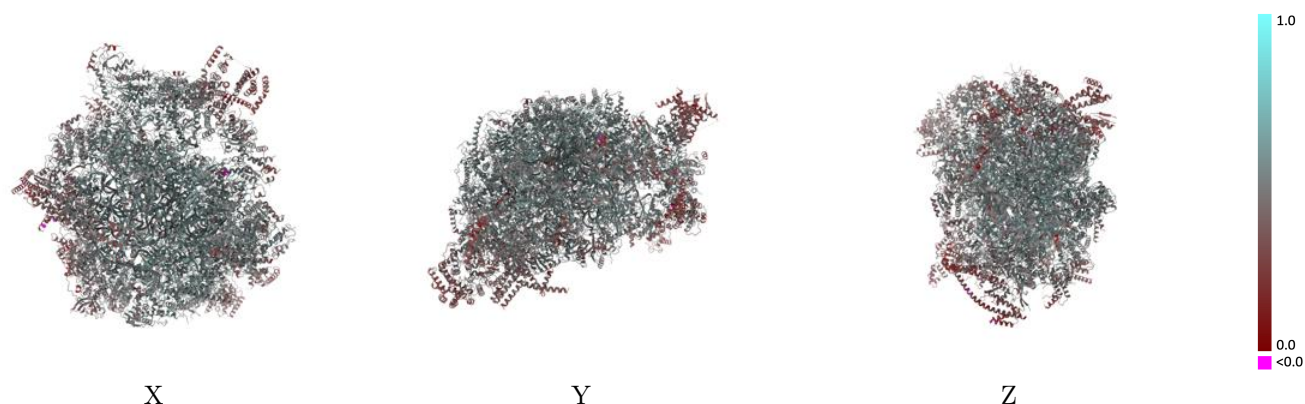
Y



Z

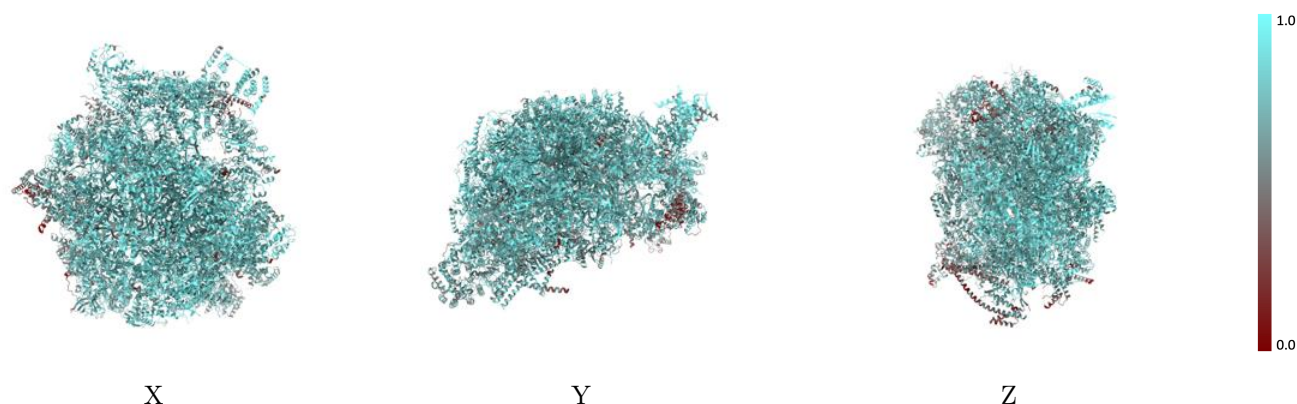
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



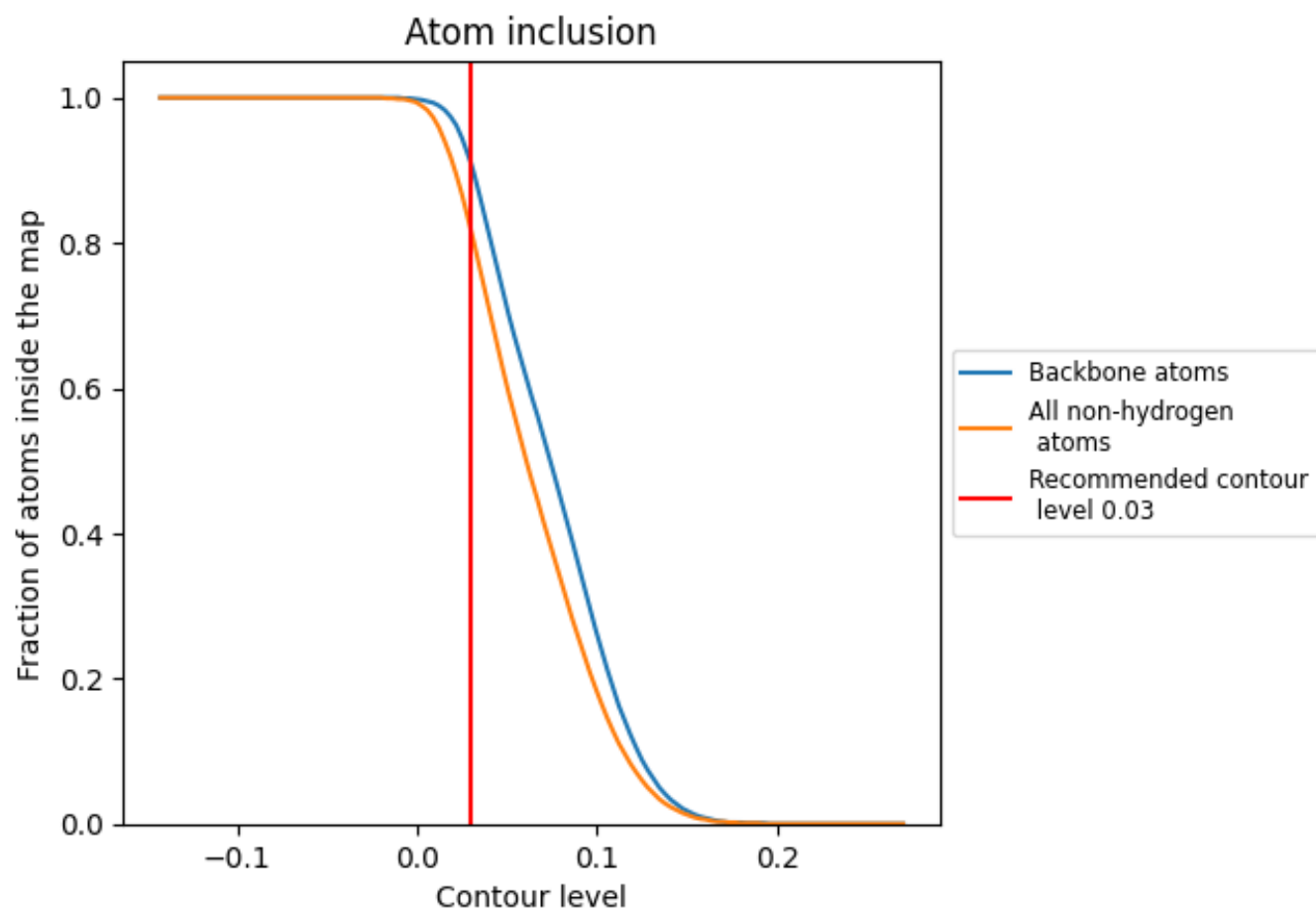
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4860
A1	 0.8050	 0.4690
A2	 0.8680	 0.5070
A3	 0.8760	 0.5420
A5	 0.8950	 0.5460
A8	 0.8730	 0.5340
AA	 0.8980	 0.5140
AE	 0.8990	 0.5550
AF	 0.8950	 0.5460
AI	 0.8390	 0.4910
AK	 0.4990	 0.3180
AN	 0.9030	 0.5550
AP	 0.8790	 0.5410
AR	 0.8400	 0.5100
AT	 0.8590	 0.5180
AU	 0.8810	 0.5360
AV	 0.8950	 0.5440
AW	 0.8730	 0.5450
AX	 0.8740	 0.5290
AY	 0.8130	 0.4830
Ae	 0.8540	 0.5080
Af	 0.8570	 0.5210
Ag	 0.8770	 0.5300
Al	 0.9000	 0.5500
Ao	 0.8860	 0.5460
Ap	 0.8630	 0.5130
At	 0.7900	 0.4790
Av	 0.8360	 0.5000
BA	 0.8740	 0.5220
BB	 0.6320	 0.3210
BD	 0.6630	 0.3580
BE	 0.8010	 0.4630
BF	 0.8670	 0.5240
BH	 0.8030	 0.4960
BI	 0.8750	 0.5200

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BJ	 0.7250	 0.3880
BK	 0.6480	 0.4040
BL	 0.8450	 0.4880
BN	 0.6630	 0.3740
BO	 0.8210	 0.4880
BQ	 0.8800	 0.5270
BR	 0.8320	 0.5050
BS	 0.7030	 0.4240
BT	 0.8780	 0.5200
BU	 0.8040	 0.4630
BW	 0.9140	 0.5380
BX	 0.5320	 0.4160
BZ	 0.7170	 0.4080
Ba	 0.8860	 0.5290
Bb	 0.7720	 0.4310
Bc	 0.8500	 0.5250
Bf	 0.8330	 0.5090
Bg	 0.7450	 0.4620
Bh	 0.7680	 0.4550
UA	 0.8040	 0.3060
UB	 0.9560	 0.5380
UC	 0.8710	 0.5040
UD	 0.8500	 0.5170
UE	 0.9170	 0.5460
UF	 0.8560	 0.3150
UG	 0.7890	 0.4900
UH	 0.8710	 0.4510
UI	 0.7540	 0.4190
UJ	 0.9440	 0.5420
UK	 0.9110	 0.5410
XA	 0.9150	 0.5670
XB	 0.8690	 0.5360
XC	 0.8510	 0.5050
XD	 0.4570	 0.2780
XE	 0.6980	 0.3850
XF	 0.7590	 0.3950
XG	 0.8380	 0.5300
XH	 0.8010	 0.4550
XI	 0.7490	 0.4340
XJ	 0.7560	 0.4880
XL	 0.7800	 0.4760
XM	 0.7150	 0.4440

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Chain	Atom inclusion	Q-score
XN	 0.8470	 0.4930
XO	 0.7620	 0.4510
XP	 0.8510	 0.5360
XQ	 0.6680	 0.4360
XR	 0.6980	 0.3790
XS	 0.4720	 0.3340
XT	 0.8570	 0.5340