



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:49 am GMT

PDB ID : 6HIW
EMDB ID : EMD-0230
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the complete small mitoribosomal subunit in complex with mt-IF-3
Authors : Ramrath, D.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.37 Å(reported)

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

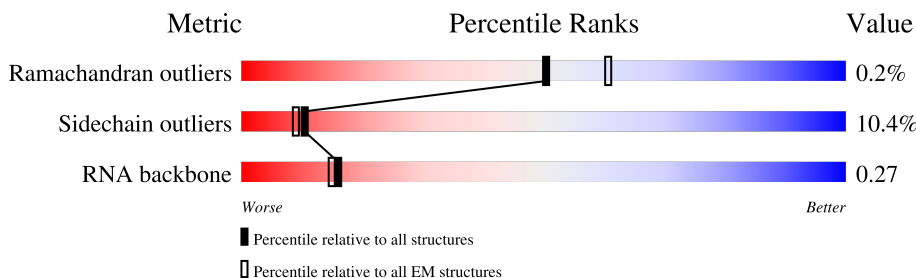
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	DA	1788	
2	DD	812	
3	DI	407	
4	DL	307	
5	DM	294	
6	DN	293	
7	DO	282	
8	DP	274	

























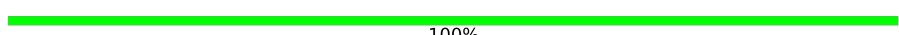
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Mol	Chain	Length	Quality of chain
9	DQ	268	92% . .
10	DR	270	82% 10% 7%
11	DS	261	84% 7% 9%
12	DU	228	85% 8% 7%
13	DZ	94	83% . 13%
14	Da	64	73% 12% 14%
15	DB	1181	86% 8% 6%
16	DC	1165	86% 8% 6%
17	DE	747	72% 7% 21%
18	DF	666	80% 8% 11%
19	DG	631	80% 9% 10%
20	DH	581	88% 9% .
21	DJ	396	72% 8% 20%
22	DK	324	73% 6% 21%
23	DT	247	86% 11% .
24	DV	183	79% 8% 13%
25	DW	179	82% 8% 10%
26	DX	169	76% 7% 17%
27	DY	163	82% 12% 6%
28	CC	74	88% 12%
29	CE	435	85% 11% .
30	CF	160	. 89% 10% .
31	CH	282	84% 12% .
32	CI	443	89% 7% .
33	CJ	817	88% 10% .






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Mol	Chain	Length	Quality of chain
34	CK	326	 80% 10% 10%
35	CL	87	 79% 18%
36	CN	166	 84% 11% 5%
37	CO	429	 74% 9% 16%
38	CP	188	 90% 6%
39	CQ	307	 53% 9% 38%
40	CR	320	 89% 8%
41	CS	244	 55% 42%
42	CU	193	 90% 6% 5%
43	CZ	360	 38% 58%
44	Ca	602	 89% 9%
45	Cb	325	 70% 7% 22%
46	Cd	440	 59% 8% 34%
47	Cg	498	 90% 7%
48	Ci	181	 78% 13% 9%
49	Cj	257	 80% 8% 12%
50	Ck	874	 73% 7% 20%
51	Cm	215	 80% 11% 9%
52	Cn	250	 39% 5% 56%
53	Cp	187	 85% 9% 6%
54	Cq	263	 87% 9%
55	Cr	439	 52% 6% 41%
56	Cv	1211	 79% 8% 13%
57	CA	621	 52% 46%
58	UO	5	 100%

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Mol	Chain	Length	Quality of chain
59	UP	7	 100%
60	UQ	32	 100%
61	UR	8	 100%
62	US	54	 100%
63	UT	44	 100%

2 Entry composition [i](#)

There are 70 unique types of molecules in this entry. The entry contains 177122 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 mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DA	1557	12482	7881	2226	2337	38	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DD	791	6523	4127	1184	1171	41	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	371	PRO	SER	conflict	UNP Q385L8
DD	599	ALA	VAL	conflict	UNP Q385L8

- Molecule 3 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	DI	390	3182	2020	554	594	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	92	GLU	GLY	conflict	UNP Q587C2
DI	116	ASP	GLU	conflict	UNP Q587C2

- Molecule 4 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	DL	283	2287	1451	423	401	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 5 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	DM	294	2430	1533	459	426	12	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	69	PHE	TYR	conflict	UNP Q57XL2
DM	97	ASN	SER	conflict	UNP Q57XL2
DM	138	SER	PRO	conflict	UNP Q57XL2
DM	173	ALA	THR	conflict	UNP Q57XL2
DM	206	ALA	THR	conflict	UNP Q57XL2

- Molecule 6 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	DN	257	2091	1331	379	371	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DN	51	GLY	SER	conflict	UNP Q38D60

- Molecule 7 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	DO	222	1804	1127	327	340	10	0	0

- Molecule 8 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	DP	189	1613	1037	290	277	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP	3	HIS	ARG	conflict	UNP Q38F25

- Molecule 9 is a protein called mS64.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	DQ	256	2061	1293	389	370	9	0	0

- Molecule 10 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	DR	251	2025	1304	369	342	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DR	65	GLY	SER	conflict	UNP Q57UA2
DR	94	GLY	GLU	conflict	UNP Q57UA2
DR	128	PRO	SER	conflict	UNP Q57UA2
DR	229	ARG	GLN	conflict	UNP Q57UA2

- Molecule 11 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	DS	238	1904	1185	356	348	15	0	0

- Molecule 12 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	DU	213	1754	1103	310	335	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DU	119	ILE	LEU	conflict	UNP Q582T9
DU	152	ILE	VAL	conflict	UNP Q582T9

- Molecule 13 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	DZ	82	697	457	113	123	4	0	0

- Molecule 14 is a protein called mS74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Da	55	501	315	109	74	3	0	0

- Molecule 15 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	DB	1111	9148	5691	1717	1711	29	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	conflict	UNP Q586P5
DB	359	ILE	THR	conflict	UNP Q586P5
DB	384	GLN	HIS	conflict	UNP Q586P5
DB	402	THR	ILE	conflict	UNP Q586P5
DB	423	THR	ALA	conflict	UNP Q586P5
DB	586	ARG	HIS	conflict	UNP Q586P5
DB	593	ARG	LYS	conflict	UNP Q586P5
DB	647	SER	GLY	conflict	UNP Q586P5

- Molecule 16 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	DC	1095	8748	5519	1544	1654	31	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	conflict	UNP Q57YB5
DC	365	LYS	GLU	conflict	UNP Q57YB5
DC	385	THR	ALA	conflict	UNP Q57YB5
DC	405	ILE	VAL	conflict	UNP Q57YB5
DC	641	SER	PRO	conflict	UNP Q57YB5
DC	651	LYS	GLU	conflict	UNP Q57YB5
DC	731	GLU	ASP	conflict	UNP Q57YB5
DC	814	GLN	HIS	conflict	UNP Q57YB5
DC	1097	ALA	VAL	conflict	UNP Q57YB5
DC	1113	THR	ILE	conflict	UNP Q57YB5

- Molecule 17 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	DE	590	4831	3075	874	863	19	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	514	THR	SER	conflict	UNP Q386Q7

- Molecule 18 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DF	590	4747	2979	896	847	25	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1

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Chain	Residue	Modelled	Actual	Comment	Reference
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

- Molecule 19 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	DG	566	4575	2875	835	834	31	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

- Molecule 20 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	DH	564	4578	2872	850	834	22	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP Q580V1
DH	194	PRO	ARG	conflict	UNP Q580V1
DH	488	GLY	SER	conflict	UNP Q580V1

- Molecule 21 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DJ	315	2572	1646	452	460	14	0	0

- Molecule 22 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	DK	255	2007	1260	365	377	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

- Molecule 23 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	DT	239	2058	1321	364	362	11	0	0

- Molecule 24 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	DV	160	1346	855	252	235	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 25 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	DW	161	1359	866	260	228	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	conflict	UNP Q383N9

- Molecule 26 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	DX	141	1196	762	226	201	7	0	0

- Molecule 27 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	DY	154	1293	827	245	216	5	0	0

- Molecule 28 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CC	74	646	451	96	98	1	0	0

- Molecule 29 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CE	417	3399	2151	632	600	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	341	ARG	LYS	conflict	UNP Q38AX6

- Molecule 30 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CF	159	1292	821	228	237	6	0	0

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	CH	273	2228	1387	432	398	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	74	ASN	SER	conflict	UNP Q388R7

- Molecule 32 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CI	424	3386	2136	611	622	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 33 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	CJ	800	6516	4119	1151	1216	30	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP Q57Z45
CJ	484	HIS	ARG	conflict	UNP Q57Z45
CJ	488	SER	ASN	conflict	UNP Q57Z45
CJ	594	GLU	VAL	conflict	UNP Q57Z45
CJ	629	ARG	LYS	conflict	UNP Q57Z45

- Molecule 34 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	CK	293	2418	1506	458	437	17	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 35 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	CL	87	733	503	113	107	10	0	0

- Molecule 36 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	CN	157	1322	843	251	220	8	0	0

- Molecule 37 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	CO	361	3003	1907	560	520	16	0	0

- Molecule 38 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	CP	180	1489	956	274	250	9	0	0

- Molecule 39 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	CQ	190	1584	1015	302	259	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CQ	138	ALA	VAL	conflict	UNP Q38DP8

- Molecule 40 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	CR	314	2567	1623	471	465	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 41 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	CS	142	1175	761	210	198	6	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP Q584T8
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP Q584T8
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

- Molecule 42 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	CU	184	1538	965	307	254	12	0	0

- Molecule 43 is a protein called mt-IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	CZ	151	1212	759	231	215	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CZ	6	SER	GLY	conflict	UNP Q57WU2
CZ	30	THR	ILE	conflict	UNP Q57WU2
CZ	172	THR	ALA	conflict	UNP Q57WU2

- Molecule 44 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ca	592	5004	3201	898	882	23	0	0

- Molecule 45 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Cb	252	2056	1300	368	380	8	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cb	244	SER	ASN	conflict	UNP Q57VB2
Cb	?	-	GLU	deletion	UNP Q57VB2
Cb	312	ALA	-	expression tag	UNP Q57VB2
Cb	313	CYS	-	expression tag	UNP Q57VB2
Cb	314	SER	-	expression tag	UNP Q57VB2
Cb	315	ARG	-	expression tag	UNP Q57VB2
Cb	316	ASP	-	expression tag	UNP Q57VB2
Cb	317	GLY	-	expression tag	UNP Q57VB2
Cb	318	PHE	-	expression tag	UNP Q57VB2
Cb	319	ALA	-	expression tag	UNP Q57VB2
Cb	320	LEU	-	expression tag	UNP Q57VB2
Cb	321	MET	-	expression tag	UNP Q57VB2
Cb	322	LYS	-	expression tag	UNP Q57VB2
Cb	323	ALA	-	expression tag	UNP Q57VB2
Cb	324	ASN	-	expression tag	UNP Q57VB2
Cb	325	LYS	-	expression tag	UNP Q57VB2

- Molecule 46 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Cd	291	2386	1491	442	443	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cd	299	UNK	GLY	conflict	UNP Q38DK6

- Molecule 47 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Cg	482	3904	2499	684	701	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	-	expression tag	UNP Q585C2

- Molecule 48 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Ci	165	1348	848	247	244	9	0	0

- Molecule 49 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Cj	226	1792	1138	310	340	4	0	0

- Molecule 50 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ck	703	5596	3503	1017	1050	26	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 51 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Cm	196	1577	975	304	289	9	0	0

- Molecule 52 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Cn	110	912	585	181	143	3	0	0

- Molecule 53 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Cp	175	1483	937	268	273	5	0	0

- Molecule 54 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Cq	252	2005	1285	342	369	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cq	48	THR	ALA	conflict	UNP Q586A1
Cq	167	MET	VAL	conflict	UNP Q586A1

- Molecule 55 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Cr	257	1999	1261	368	356	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cr	351	LYS	GLU	conflict	UNP Q585I1

- Molecule 56 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Cv	1059	8557	5387	1535	1596	39	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	718	THR	ALA	conflict	UNP Q383R4
Cv	1179	GLU	GLY	conflict	UNP Q383R4

- Molecule 57 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	CA	621	13122	5906	2227	4368	621	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	298	U	C	conflict	GB 343546
CA	473	U	G	conflict	GB 343546
CA	614	U	-	insertion	GB 343546
CA	615	U	-	insertion	GB 343546
CA	616	U	-	insertion	GB 343546
CA	617	U	-	insertion	GB 343546
CA	618	U	-	insertion	GB 343546
CA	619	U	-	insertion	GB 343546
CA	620	U	-	insertion	GB 343546
CA	621	U	-	insertion	GB 343546

- Molecule 58 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	UO	5	30	20	5	5	0	0

- Molecule 59 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
59	UP	7	42	28	7	7	0	0

- Molecule 60 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	UQ	32	192	128	32	32	0	0

- Molecule 61 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	UR	8	48	32	8	8	0	0

- Molecule 62 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	US	54	324	216	54	54	0	0

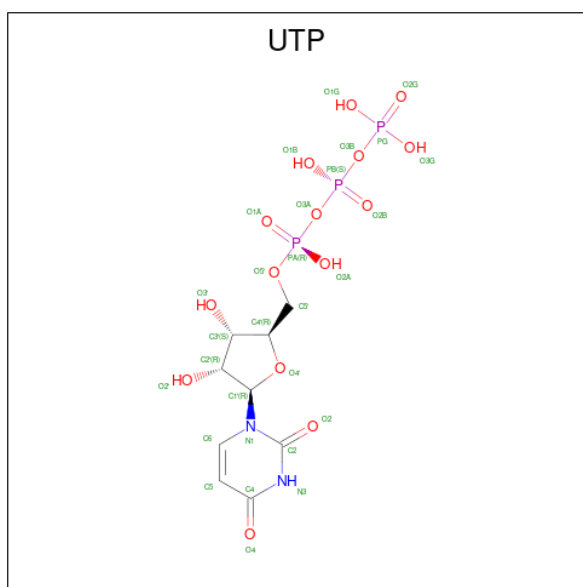
- Molecule 63 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
63	UT	44	264	176	44	44	0	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	DA	1	1	1	0
64	DS	2	2	2	0
64	Cr	1	1	1	0

- Molecule 65 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).

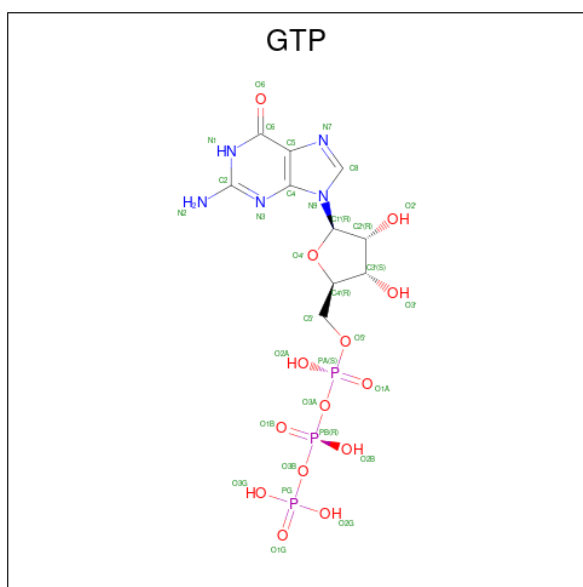


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	DJ	1	29	9	2	15	3	0

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

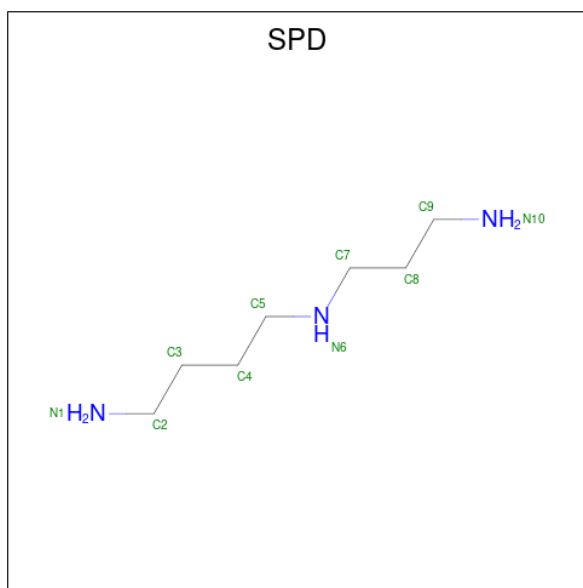
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	CQ	1	1	1	0
66	Ca	1	1	1	0
66	Cg	1	1	1	0
66	Cv	1	1	1	0
66	CA	35	35	35	0

- Molecule 67 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 68 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



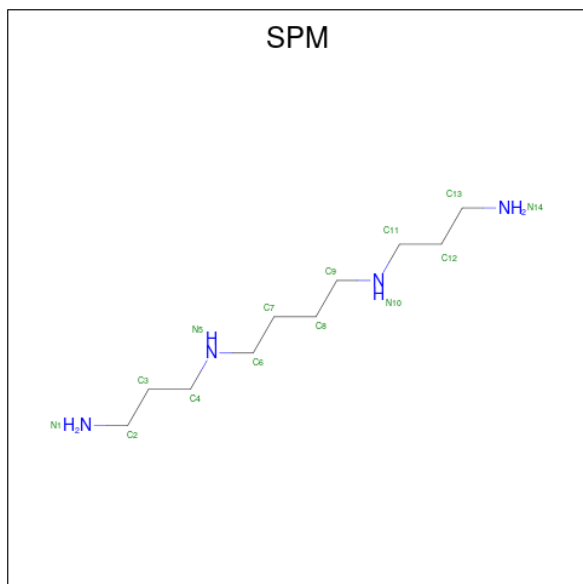
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
68	CA	1	40	28	12	0
68	CA	1	40	28	12	0
68	CA	1	40	28	12	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
68	CA	1	40	28	12	0

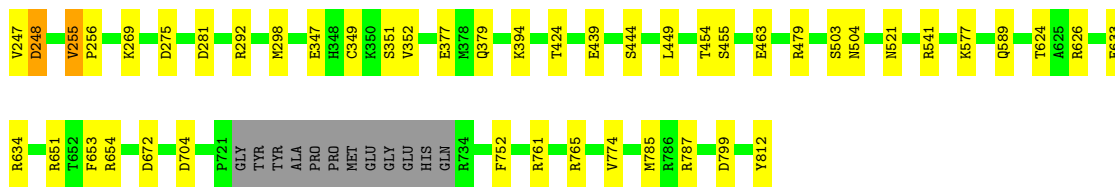
- Molecule 69 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



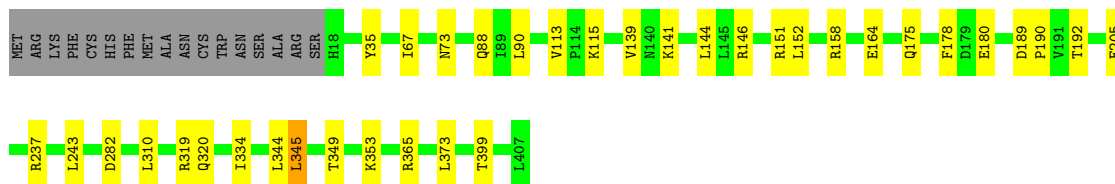
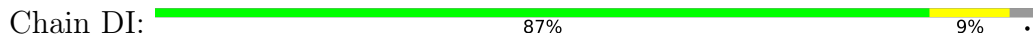
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
69	CA	1	14	10	4	0

- Molecule 70 is water.

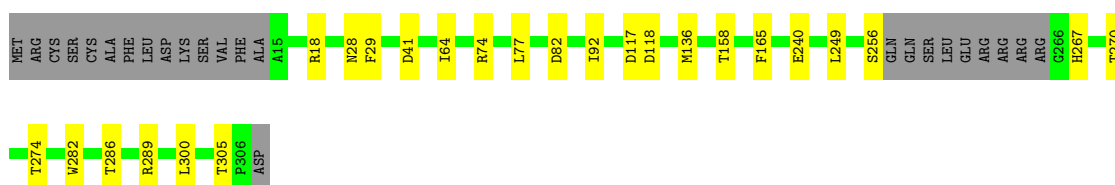
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
70	Cg	3	3	3	0



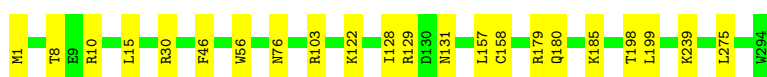
• Molecule 3: mS56



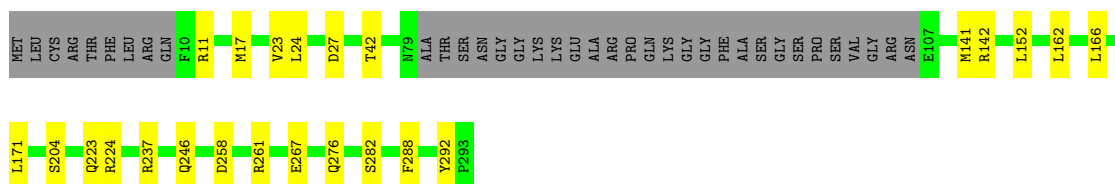
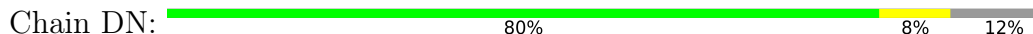
• Molecule 4: mS59



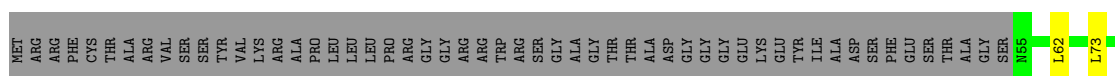
• Molecule 5: mS60



• Molecule 6: mS61

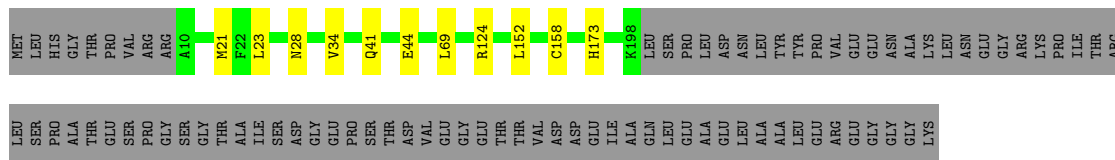


• Molecule 7: mS62





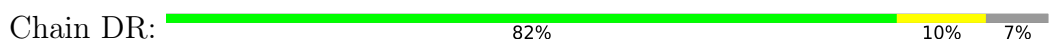
• Molecule 8: mS63



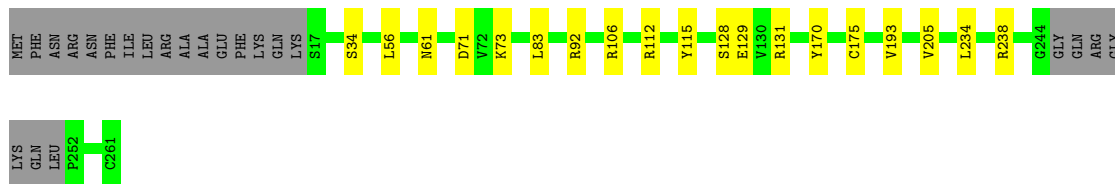
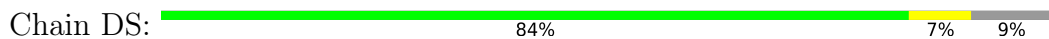
• Molecule 9: mS64



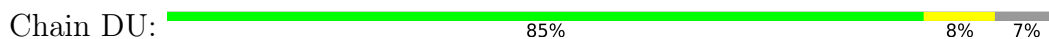
• Molecule 10: mS65



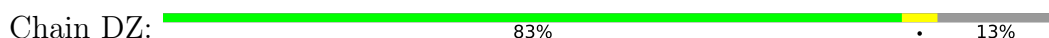
• Molecule 11: mS66



• Molecule 12: mS68

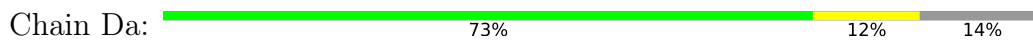


• Molecule 13: mS73

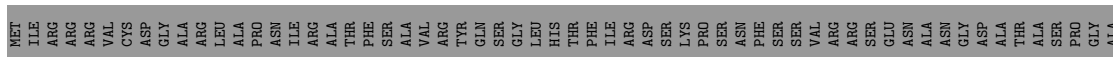
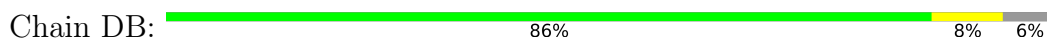




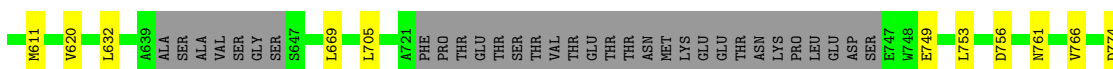
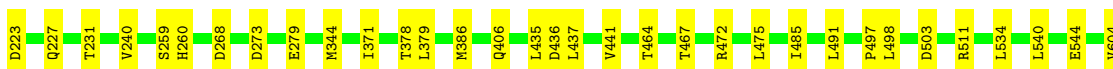
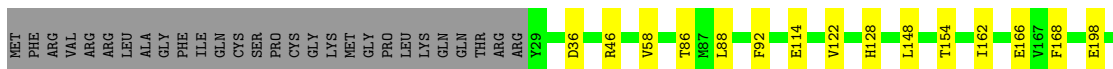
• Molecule 14: mS74



• Molecule 15: mS49




• Molecule 16: mS50




• Molecule 17: mS52

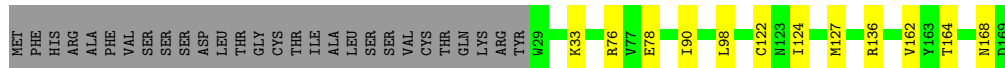
• Molecule 25: mS70

Chain DW:  82% 8% 10%




• Molecule 26: mS71

Chain DX:  76% 7% 17%



• Molecule 27: mS72

Chain DY:  82% 12% 6%




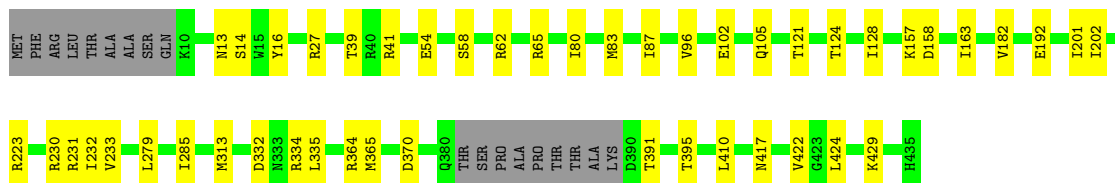
• Molecule 28: uS3m

Chain CC:  88% 12%




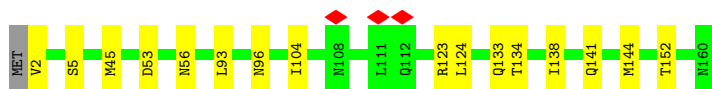
• Molecule 29: uS5m

Chain CE:  85% 11%




• Molecule 30: bS6m

Chain CF:  89% 10%

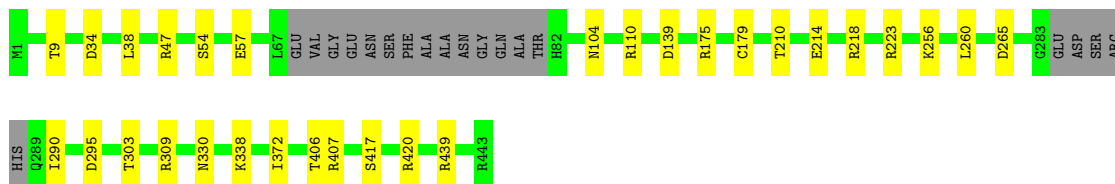
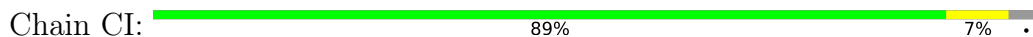


• Molecule 31: uS8m

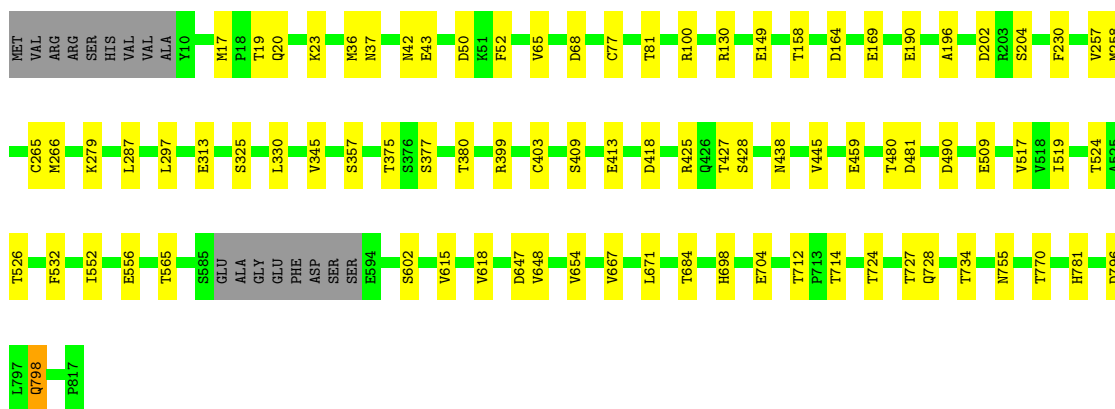
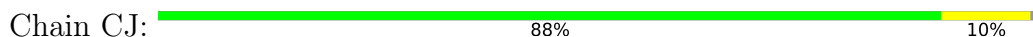
Chain CH:  84% 12%



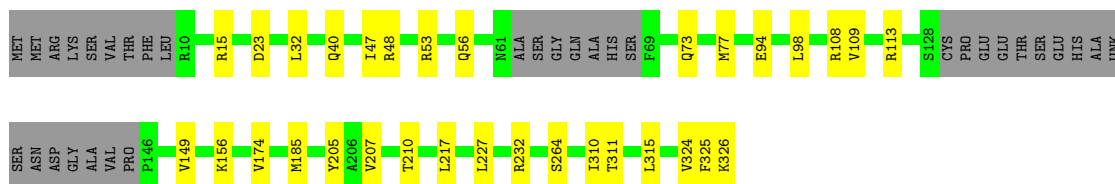
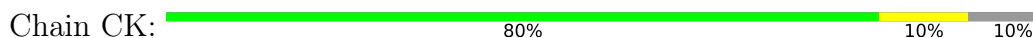
• Molecule 32: uS9m



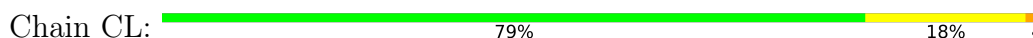
• Molecule 33: uS10m



• Molecule 34: uS11m

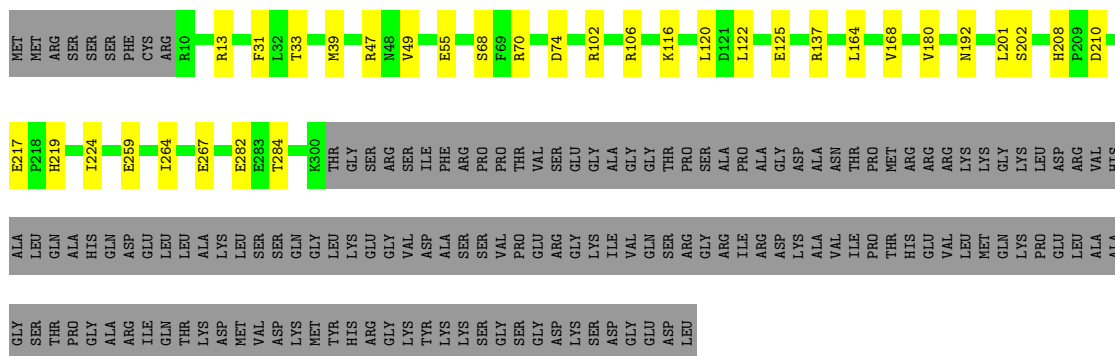


• Molecule 35: uS12m



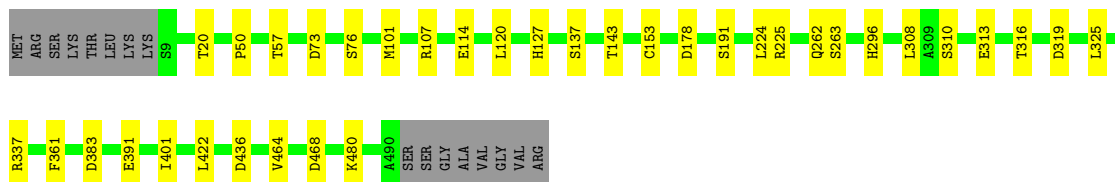
• Molecule 36: uS14m

Chain Cd:  59% 8% 34%




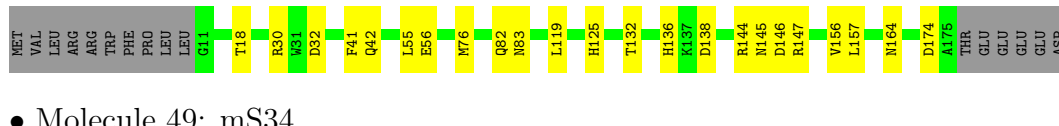
• Molecule 47: mS29

Chain Cg:  90% 7%




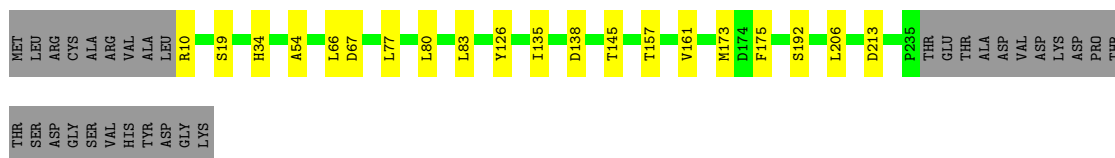
• Molecule 48: mS33

Chain Ci:  78% 13% 9%



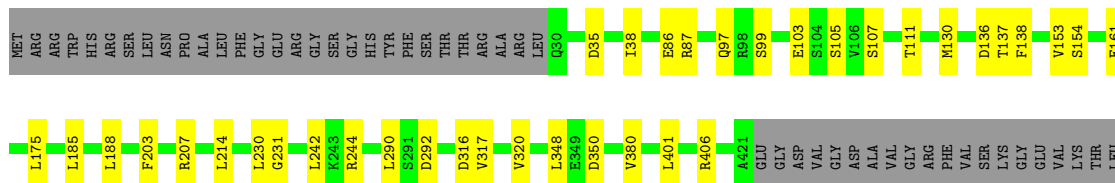
• Molecule 49: mS34

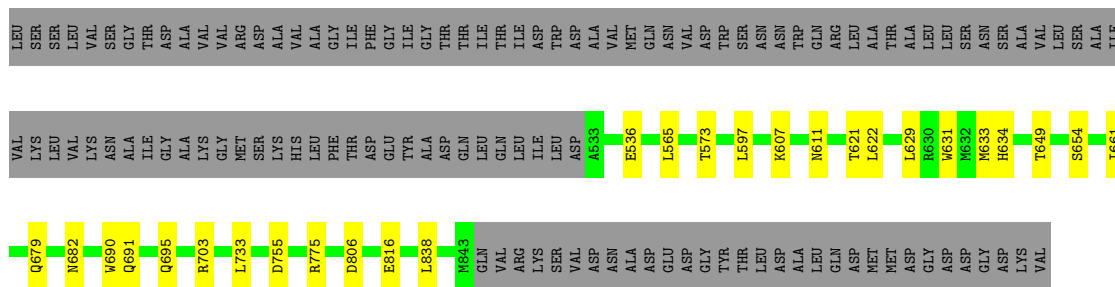
Chain Cj:  80% 8% 12%



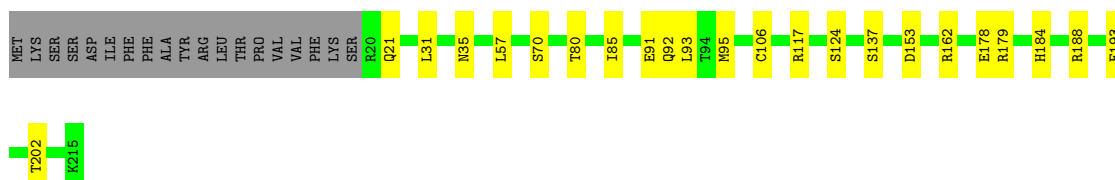
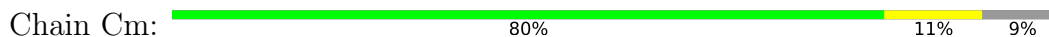
• Molecule 50: mS35

Chain Ck:  73% 7% 20%

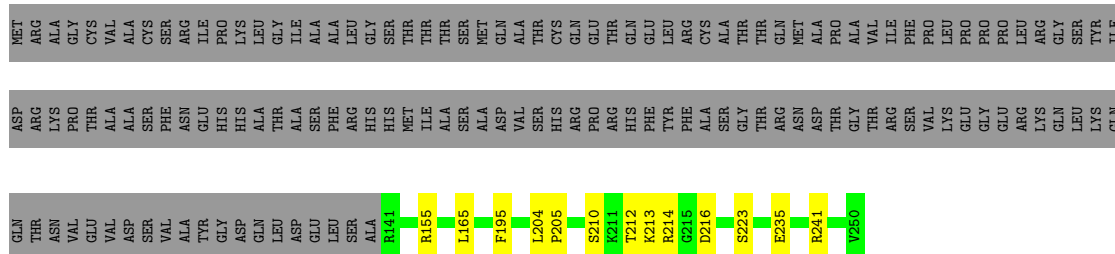
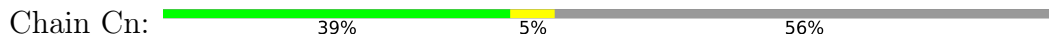




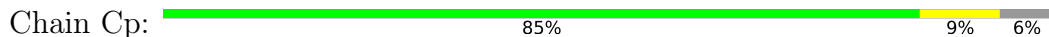
• Molecule 51: mS37



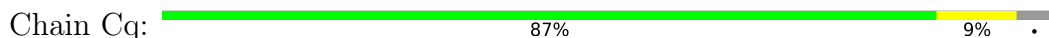
• Molecule 52: mS38



• Molecule 53: mS41

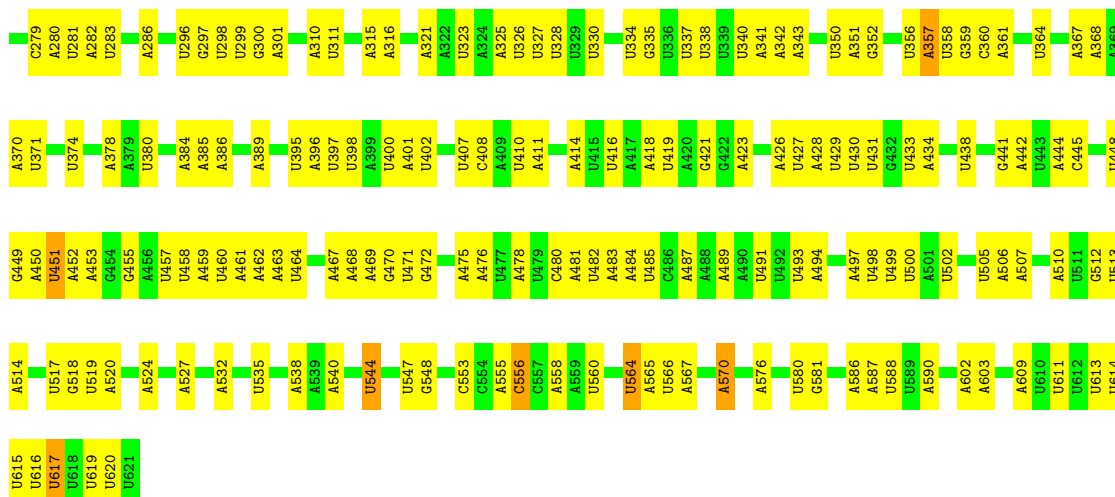


• Molecule 54: mS42



• Molecule 55: mS43





- Molecule 58: Unknown Protein

Chain UO:  100%

There are no outlier residues recorded for this chain.

- Molecule 59: Unknown Protein

Chain UP:  100%

There are no outlier residues recorded for this chain.

- Molecule 60: Unknown Protein

Chain UQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 61: Unknown Protein

Chain UR:  100%

There are no outlier residues recorded for this chain.

- Molecule 62: Unknown Protein

Chain US:  100%

There are no outlier residues recorded for this chain.

- Molecule 63: Unknown Protein

Chain UT:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31911	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.538	Depositor
Minimum map value	-0.316	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0114	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, SPM, SPD, ZN, GTP

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	DA	0.37	0/12780	0.55	3/17297 (0.0%)
2	DD	0.38	0/6710	0.57	1/9087 (0.0%)
3	DI	0.37	0/3248	0.57	1/4401 (0.0%)
4	DL	0.42	0/2346	0.60	0/3164
5	DM	0.40	0/2488	0.58	0/3362
6	DN	0.40	0/2148	0.59	0/2916
7	DO	0.38	0/1840	0.60	0/2482
8	DP	0.34	0/1662	0.50	0/2249
9	DQ	0.37	0/2111	0.59	0/2863
10	DR	0.35	0/2090	0.58	0/2849
11	DS	0.35	0/1950	0.54	0/2633
12	DU	0.37	0/1799	0.54	0/2438
13	DZ	0.39	0/725	0.57	0/984
14	Da	0.42	0/520	0.58	0/694
15	DB	0.36	0/9369	0.53	0/12692
16	DC	0.34	0/8952	0.51	0/12145
17	DE	0.32	0/4955	0.51	0/6708
18	DF	0.35	0/4856	0.54	2/6581 (0.0%)
19	DG	0.35	0/4674	0.53	0/6333
20	DH	0.35	0/4684	0.53	1/6347 (0.0%)
21	DJ	0.35	0/2649	0.53	0/3598
22	DK	0.34	0/2045	0.50	0/2759
23	DT	0.35	0/2133	0.53	0/2889
24	DV	0.38	0/1382	0.58	0/1871
25	DW	0.36	0/1407	0.54	0/1916
26	DX	0.36	0/1231	0.54	0/1654
27	DY	0.41	0/1334	0.58	0/1810
28	CC	0.39	0/666	0.59	0/900
29	CE	0.42	0/3484	0.60	0/4708
30	CF	0.39	0/1319	0.57	0/1783
31	CH	0.46	0/2276	0.59	0/3071
32	CI	0.41	0/3453	0.56	0/4655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	CJ	0.42	0/6705	0.58	0/9124
34	CK	0.38	0/2472	0.58	0/3315
35	CL	0.43	0/759	0.63	0/1026
36	CN	0.42	0/1361	0.57	0/1840
37	CO	0.41	0/3085	0.58	0/4165
38	CP	0.43	0/1533	0.61	0/2074
39	CQ	0.48	0/1631	0.66	0/2203
40	CR	0.42	0/2640	0.60	0/3572
41	CS	0.38	0/1209	0.54	0/1626
42	CU	0.38	0/1576	0.55	0/2115
43	CZ	0.35	0/1237	0.55	1/1659 (0.1%)
44	Ca	0.42	0/5159	0.59	3/6980 (0.0%)
45	Cb	0.42	0/2105	0.60	1/2842 (0.0%)
46	Cd	0.41	0/2438	0.56	0/3288
47	Cg	0.38	0/4025	0.57	0/5467
48	Ci	0.39	0/1388	0.64	1/1878 (0.1%)
49	Cj	0.35	0/1842	0.54	0/2511
50	Ck	0.37	0/5696	0.56	0/7705
51	Cm	0.47	0/1616	0.65	0/2175
52	Cn	0.41	0/934	0.58	0/1248
53	Cp	0.36	0/1528	0.55	0/2072
54	Cq	0.42	0/2066	0.58	0/2815
55	Cr	0.34	0/2038	0.56	3/2759 (0.1%)
56	Cv	0.40	0/8780	0.59	1/11901 (0.0%)
57	CA	0.49	1/14679 (0.0%)	1.01	30/22827 (0.1%)
All	All	0.39	1/181788 (0.0%)	0.62	48/249026 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DA	0	2
2	DD	0	3
6	DN	0	1
7	DO	0	2
10	DR	0	2
16	DC	0	2
19	DG	0	2
21	DJ	0	1
23	DT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	DX	0	1
31	CH	0	2
33	CJ	0	2
35	CL	0	3
37	CO	0	2
46	Cd	0	1
47	Cg	0	1
50	Ck	0	1
56	Cv	0	2
All	All	0	31

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	357	A	N9-C4	-5.86	1.34	1.37

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	451	U	N1-C2-O2	7.12	127.78	122.80
57	CA	493	U	C2-N1-C1'	7.02	126.12	117.70
57	CA	188	U	C2-N1-C1'	6.84	125.91	117.70
57	CA	63	G	N3-C4-C5	6.75	131.97	128.60
57	CA	188	U	N3-C2-O2	-6.65	117.55	122.20

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DA	166	TYR	Peptide
1	DA	273	ASP	Peptide
2	DD	247	VAL	Peptide
2	DD	255	VAL	Peptide
2	DD	351	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	1551/1788 (87%)	1490 (96%)	59 (4%)	2 (0%)	51	82
2	DD	787/812 (97%)	740 (94%)	44 (6%)	3 (0%)	34	68
3	DI	388/407 (95%)	365 (94%)	22 (6%)	1 (0%)	41	73
4	DL	279/307 (91%)	261 (94%)	18 (6%)	0	100	100
5	DM	292/294 (99%)	280 (96%)	12 (4%)	0	100	100
6	DN	253/293 (86%)	238 (94%)	15 (6%)	0	100	100
7	DO	220/282 (78%)	209 (95%)	10 (4%)	1 (0%)	29	63
8	DP	187/274 (68%)	176 (94%)	11 (6%)	0	100	100
9	DQ	254/268 (95%)	244 (96%)	9 (4%)	1 (0%)	34	68
10	DR	247/270 (92%)	236 (96%)	10 (4%)	1 (0%)	34	68
11	DS	234/261 (90%)	222 (95%)	11 (5%)	1 (0%)	34	68
12	DU	211/228 (92%)	198 (94%)	11 (5%)	2 (1%)	17	51
13	DZ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
14	Da	53/64 (83%)	52 (98%)	1 (2%)	0	100	100
15	DB	1109/1181 (94%)	1073 (97%)	35 (3%)	1 (0%)	51	82
16	DC	1087/1165 (93%)	1053 (97%)	33 (3%)	1 (0%)	51	82
17	DE	576/747 (77%)	564 (98%)	12 (2%)	0	100	100
18	DF	586/666 (88%)	568 (97%)	18 (3%)	0	100	100
19	DG	558/631 (88%)	543 (97%)	15 (3%)	0	100	100
20	DH	560/581 (96%)	539 (96%)	21 (4%)	0	100	100
21	DJ	313/396 (79%)	299 (96%)	13 (4%)	1 (0%)	41	73
22	DK	249/324 (77%)	238 (96%)	11 (4%)	0	100	100
23	DT	237/247 (96%)	232 (98%)	5 (2%)	0	100	100
24	DV	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
25	DW	159/179 (89%)	153 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DX	139/169 (82%)	130 (94%)	9 (6%)	0	100	100
27	DY	152/163 (93%)	147 (97%)	5 (3%)	0	100	100
28	CC	72/74 (97%)	67 (93%)	5 (7%)	0	100	100
29	CE	413/435 (95%)	386 (94%)	26 (6%)	1 (0%)	47	78
30	CF	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
31	CH	271/282 (96%)	259 (96%)	11 (4%)	1 (0%)	34	68
32	CI	418/443 (94%)	405 (97%)	13 (3%)	0	100	100
33	CJ	796/817 (97%)	755 (95%)	39 (5%)	2 (0%)	41	73
34	CK	287/326 (88%)	267 (93%)	20 (7%)	0	100	100
35	CL	85/87 (98%)	79 (93%)	5 (6%)	1 (1%)	13	44
36	CN	155/166 (93%)	148 (96%)	7 (4%)	0	100	100
37	CO	359/429 (84%)	342 (95%)	16 (4%)	1 (0%)	41	73
38	CP	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
39	CQ	188/307 (61%)	178 (95%)	10 (5%)	0	100	100
40	CR	312/320 (98%)	297 (95%)	14 (4%)	1 (0%)	41	73
41	CS	140/244 (57%)	132 (94%)	8 (6%)	0	100	100
42	CU	182/193 (94%)	173 (95%)	8 (4%)	1 (0%)	29	63
43	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	22	56
44	Ca	590/602 (98%)	551 (93%)	34 (6%)	5 (1%)	19	53
45	Cb	248/325 (76%)	241 (97%)	7 (3%)	0	100	100
46	Cd	288/440 (66%)	277 (96%)	10 (4%)	1 (0%)	41	73
47	Cg	480/498 (96%)	462 (96%)	18 (4%)	0	100	100
48	Ci	163/181 (90%)	154 (94%)	9 (6%)	0	100	100
49	Cj	224/257 (87%)	215 (96%)	8 (4%)	1 (0%)	34	68
50	Ck	699/874 (80%)	676 (97%)	22 (3%)	1 (0%)	51	82
51	Cm	194/215 (90%)	182 (94%)	12 (6%)	0	100	100
52	Cn	108/250 (43%)	103 (95%)	5 (5%)	0	100	100
53	Cp	173/187 (92%)	167 (96%)	6 (4%)	0	100	100
54	Cq	250/263 (95%)	242 (97%)	8 (3%)	0	100	100
55	Cr	253/439 (58%)	241 (95%)	11 (4%)	1 (0%)	34	68
56	Cv	1051/1211 (87%)	1010 (96%)	41 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	19802/22847 (87%)	18951 (96%)	818 (4%)	33 (0%)	50	78

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	CZ	296	PRO
44	Ca	32	PRO
44	Ca	33	PRO
44	Ca	35	PRO
2	DD	352	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	1322/1514 (87%)	1199 (91%)	123 (9%)	9	31
2	DD	694/711 (98%)	626 (90%)	68 (10%)	8	29
3	DI	350/365 (96%)	315 (90%)	35 (10%)	7	28
4	DL	241/263 (92%)	216 (90%)	25 (10%)	7	26
5	DM	252/252 (100%)	230 (91%)	22 (9%)	10	35
6	DN	229/256 (90%)	206 (90%)	23 (10%)	7	28
7	DO	186/229 (81%)	171 (92%)	15 (8%)	11	38
8	DP	170/239 (71%)	159 (94%)	11 (6%)	17	48
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	36	65
10	DR	220/235 (94%)	193 (88%)	27 (12%)	4	19
11	DS	209/228 (92%)	191 (91%)	18 (9%)	10	36
12	DU	190/201 (94%)	171 (90%)	19 (10%)	7	28
13	DZ	72/84 (86%)	68 (94%)	4 (6%)	21	52
14	Da	50/59 (85%)	42 (84%)	8 (16%)	2	11
15	DB	976/1030 (95%)	885 (91%)	91 (9%)	9	31
16	DC	927/985 (94%)	832 (90%)	95 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	DE	519/644 (81%)	467 (90%)	52 (10%)	7	28
18	DF	500/560 (89%)	446 (89%)	54 (11%)	6	25
19	DG	490/543 (90%)	433 (88%)	57 (12%)	5	21
20	DH	493/504 (98%)	439 (89%)	54 (11%)	6	24
21	DJ	275/347 (79%)	246 (90%)	29 (10%)	7	26
22	DK	209/261 (80%)	190 (91%)	19 (9%)	9	32
23	DT	220/228 (96%)	194 (88%)	26 (12%)	5	20
24	DV	145/165 (88%)	130 (90%)	15 (10%)	7	27
25	DW	148/163 (91%)	134 (90%)	14 (10%)	8	30
26	DX	124/149 (83%)	113 (91%)	11 (9%)	9	34
27	DY	137/146 (94%)	117 (85%)	20 (15%)	3	13
28	CC	73/73 (100%)	64 (88%)	9 (12%)	4	19
29	CE	358/372 (96%)	312 (87%)	46 (13%)	4	17
30	CF	136/144 (94%)	120 (88%)	16 (12%)	5	20
31	CH	237/246 (96%)	205 (86%)	32 (14%)	4	16
32	CI	357/371 (96%)	327 (92%)	30 (8%)	11	37
33	CJ	709/723 (98%)	627 (88%)	82 (12%)	5	21
34	CK	257/283 (91%)	225 (88%)	32 (12%)	4	18
35	CL	79/79 (100%)	63 (80%)	16 (20%)	1	4
36	CN	142/150 (95%)	124 (87%)	18 (13%)	4	18
37	CO	318/377 (84%)	277 (87%)	41 (13%)	4	17
38	CP	160/168 (95%)	149 (93%)	11 (7%)	15	46
39	CQ	171/270 (63%)	144 (84%)	27 (16%)	2	11
40	CR	275/279 (99%)	247 (90%)	28 (10%)	7	28
41	CS	126/220 (57%)	118 (94%)	8 (6%)	18	49
42	CU	160/169 (95%)	150 (94%)	10 (6%)	18	49
43	CZ	121/313 (39%)	108 (89%)	13 (11%)	6	25
44	Ca	516/543 (95%)	464 (90%)	52 (10%)	7	28
45	Cb	219/277 (79%)	195 (89%)	24 (11%)	6	24
46	Cd	237/381 (62%)	206 (87%)	31 (13%)	4	17
47	Cg	424/437 (97%)	389 (92%)	35 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Ci	144/160 (90%)	122 (85%)	22 (15%)	2	12
49	Cj	193/219 (88%)	174 (90%)	19 (10%)	8	29
50	Ck	608/747 (81%)	546 (90%)	62 (10%)	7	28
51	Cm	165/184 (90%)	142 (86%)	23 (14%)	3	15
52	Cn	95/210 (45%)	82 (86%)	13 (14%)	3	15
53	Cp	163/175 (93%)	147 (90%)	16 (10%)	8	29
54	Cq	210/221 (95%)	186 (89%)	24 (11%)	5	22
55	Cr	211/369 (57%)	185 (88%)	26 (12%)	4	19
56	Cv	912/1034 (88%)	813 (89%)	99 (11%)	6	24
All	All	17352/19794 (88%)	15544 (90%)	1808 (10%)	10	26

5 of 1808 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	DY	37	ARG
56	Cv	793	PHE
33	CJ	704	GLU
56	Cv	613	LEU
50	Ck	695	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 379 such sidechains are listed below:

Mol	Chain	Res	Type
33	CJ	170	HIS
42	CU	180	GLN
33	CJ	494	GLN
37	CO	111	GLN
46	Cd	37	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	CA	619/621 (99%)	287 (46%)	9 (1%)

5 of 287 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
57	CA	2	A
57	CA	3	A
57	CA	4	A
57	CA	5	U
57	CA	6	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	CA	527	A
57	CA	547	U
57	CA	275	U
57	CA	350	U
57	CA	361	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 43 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	GTP	Cg	501	66	26,34,34	1.23	1 (3%)	32,54,54	1.56	8 (25%)
68	SPD	CA	736	-	9,9,9	0.34	0	8,8,8	0.73	0
68	SPD	CA	738	-	9,9,9	0.53	0	8,8,8	0.48	0
68	SPD	CA	739	-	9,9,9	0.41	0	8,8,8	0.59	0
68	SPD	CA	737	-	9,9,9	0.35	0	8,8,8	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	SPM	CA	740	-	13,13,13	0.35	0	12,12,12	0.81	0
65	UTP	DJ	401	-	22,30,30	2.04	3 (13%)	27,47,47	1.50	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	GTP	Cg	501	66	-	4/18/38/38	0/3/3/3
68	SPD	CA	736	-	-	4/7/7/7	-
68	SPD	CA	738	-	-	3/7/7/7	-
68	SPD	CA	739	-	-	2/7/7/7	-
68	SPD	CA	737	-	-	0/7/7/7	-
69	SPM	CA	740	-	-	4/11/11/11	-
65	UTP	DJ	401	-	-	9/20/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	DJ	401	UTP	O4'-C1'	5.40	1.48	1.41
65	DJ	401	UTP	C6-N1	4.86	1.41	1.35
67	Cg	501	GTP	C5-C6	-4.32	1.38	1.47
65	DJ	401	UTP	C4-N3	3.86	1.39	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	DJ	401	UTP	PB-O3B-PG	-3.46	120.96	132.83
67	Cg	501	GTP	PB-O3B-PG	-3.34	121.38	132.83
67	Cg	501	GTP	C2-N1-C6	-3.17	119.25	125.10
67	Cg	501	GTP	C8-N7-C5	3.08	108.85	102.99
67	Cg	501	GTP	N2-C2-N1	2.90	122.89	116.71

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	DJ	401	UTP	C5'-O5'-PA-O1A
65	DJ	401	UTP	C5'-O5'-PA-O2A

Continued on next page...

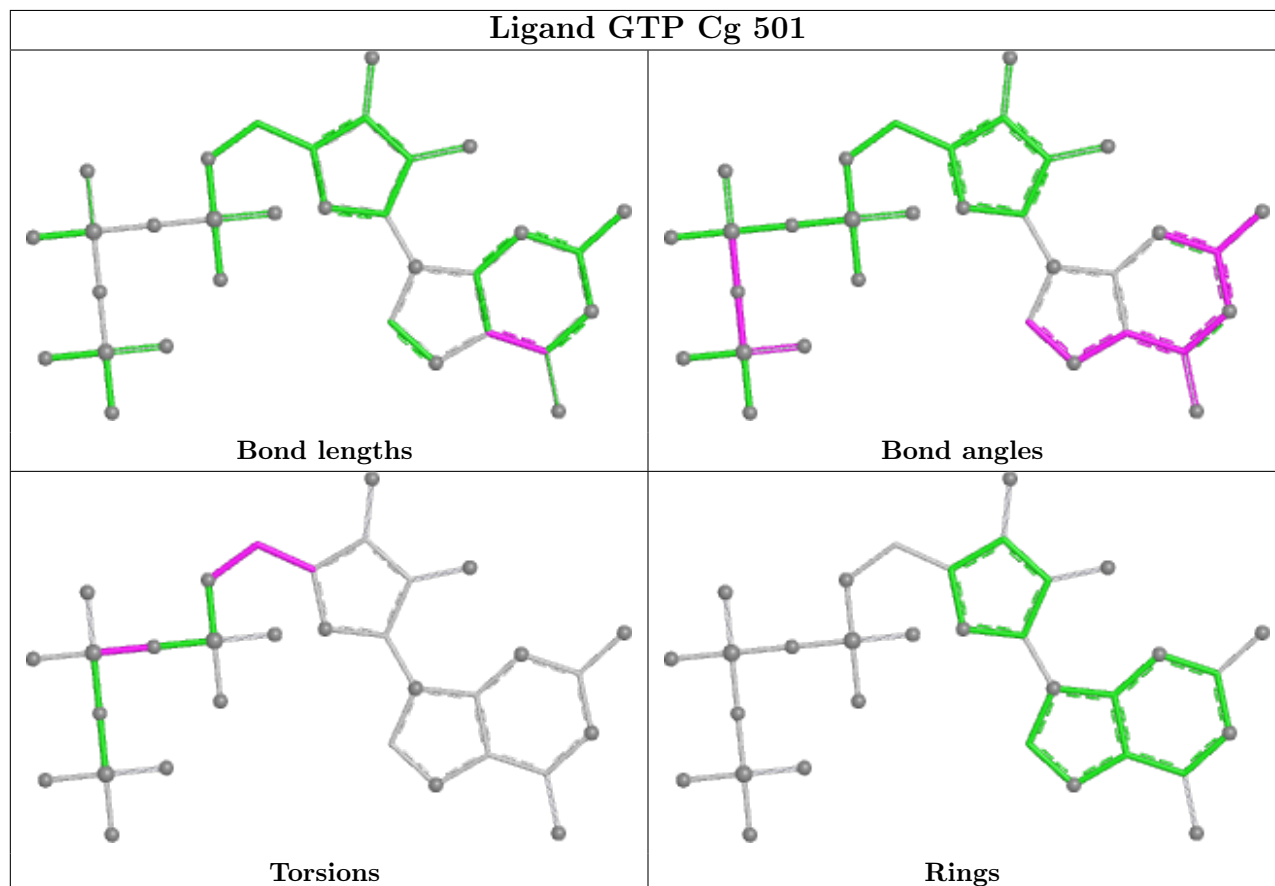
Continued from previous page...

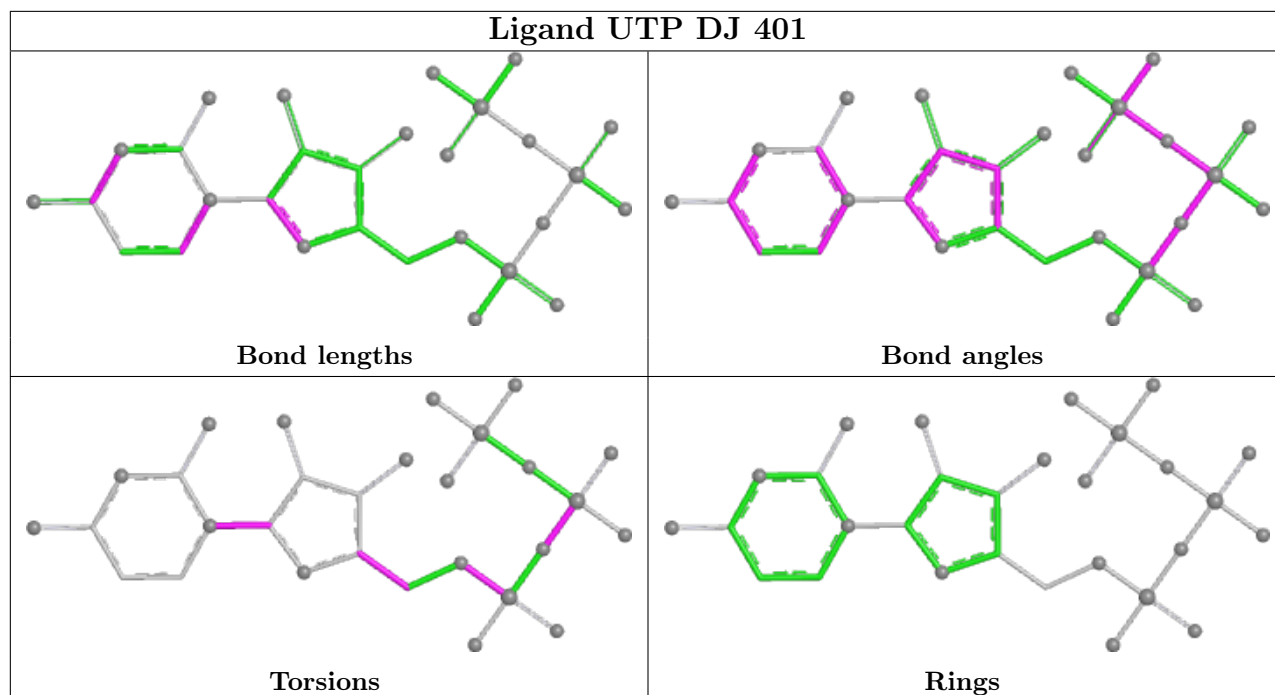
Mol	Chain	Res	Type	Atoms
65	DJ	401	UTP	C5'-O5'-PA-O3A
65	DJ	401	UTP	O4'-C4'-C5'-O5'
65	DJ	401	UTP	O4'-C1'-N1-C6

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.





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
57	CA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CA	80:U	O3'	81:U	P	6.49

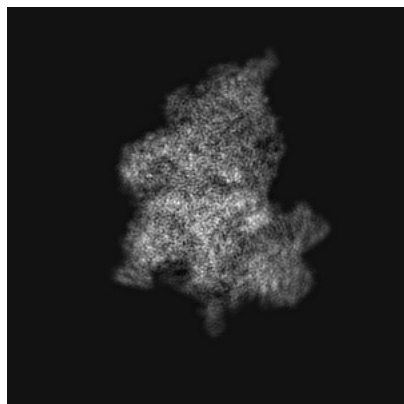
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0230. These allow visual inspection of the internal detail of the map and identification of artifacts.

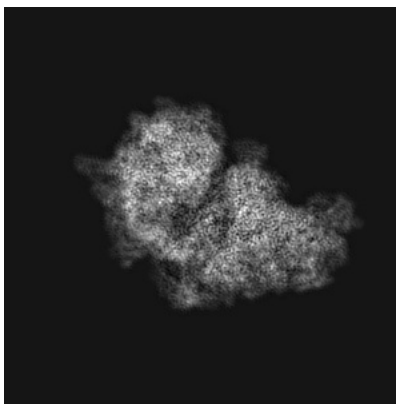
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

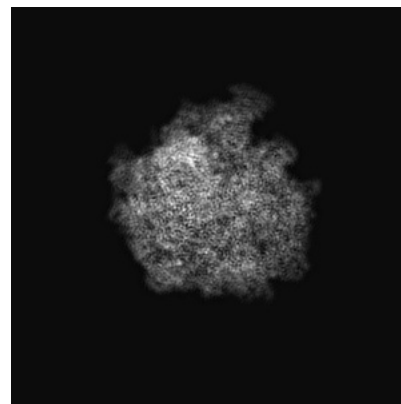
6.1.1 Primary map



X

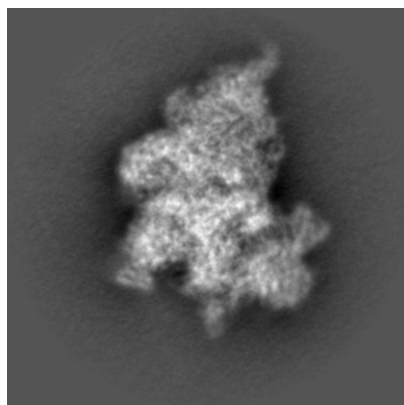


Y

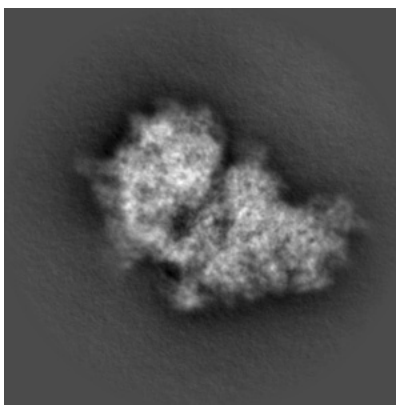


Z

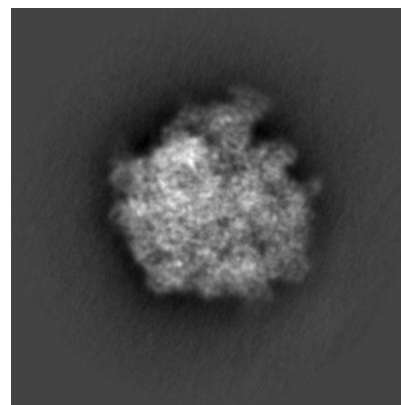
6.1.2 Raw map



X



Y

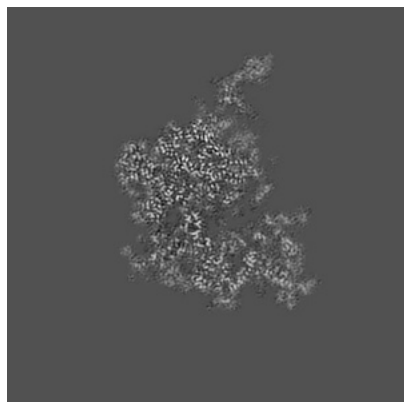


Z

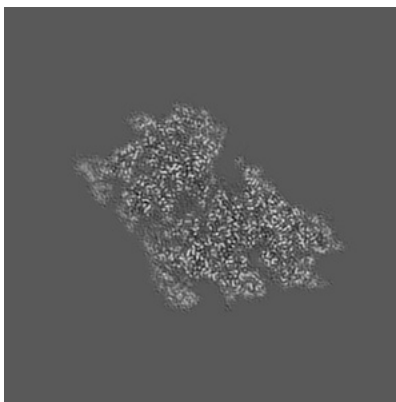
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

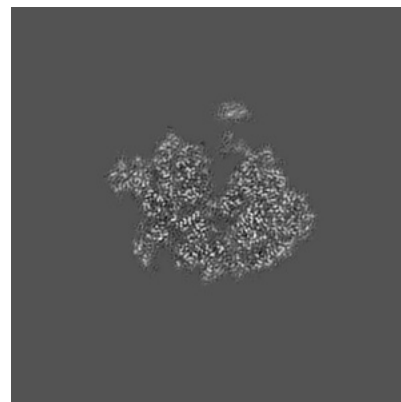
6.2.1 Primary map



X Index: 160

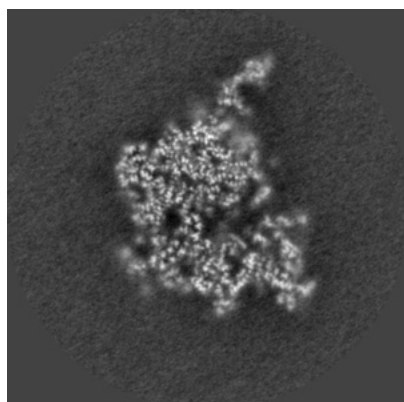


Y Index: 160

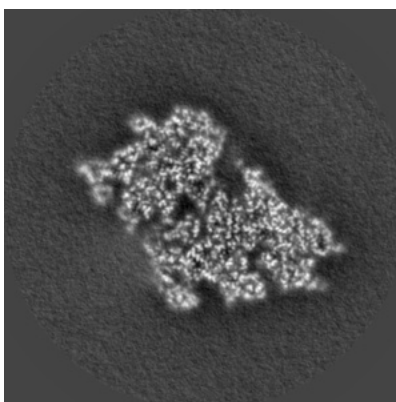


Z Index: 160

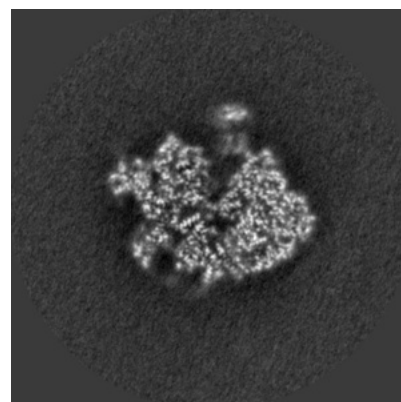
6.2.2 Raw map



X Index: 160



Y Index: 160

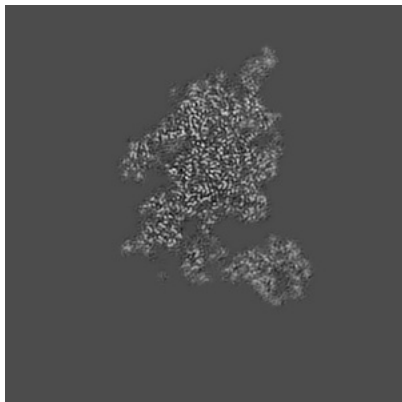


Z Index: 160

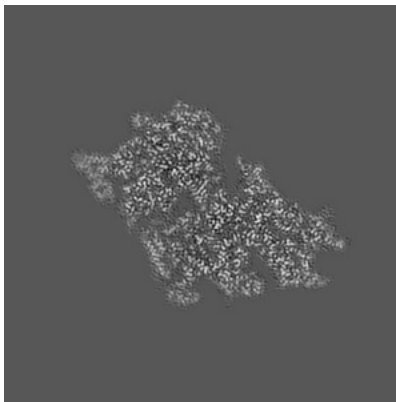
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

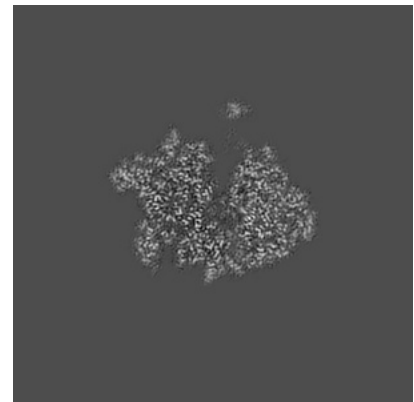
6.3.1 Primary map



X Index: 143

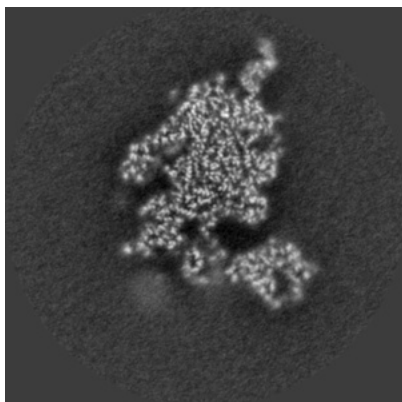


Y Index: 162

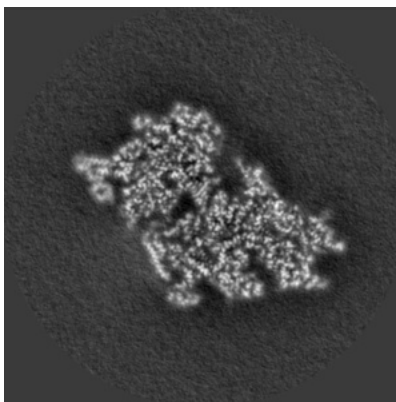


Z Index: 162

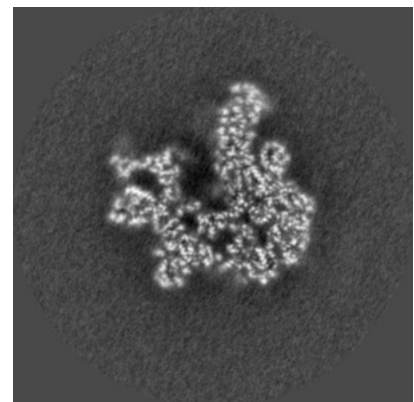
6.3.2 Raw map



X Index: 143



Y Index: 162

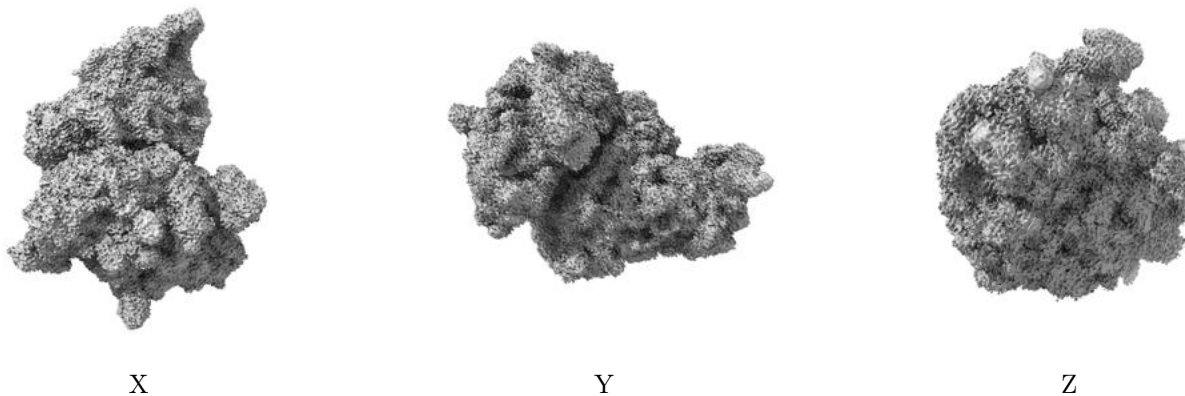


Z Index: 143

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

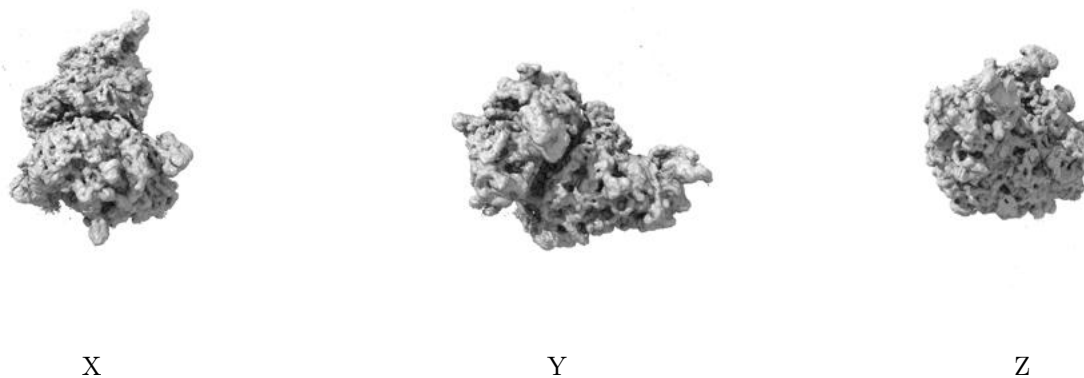
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

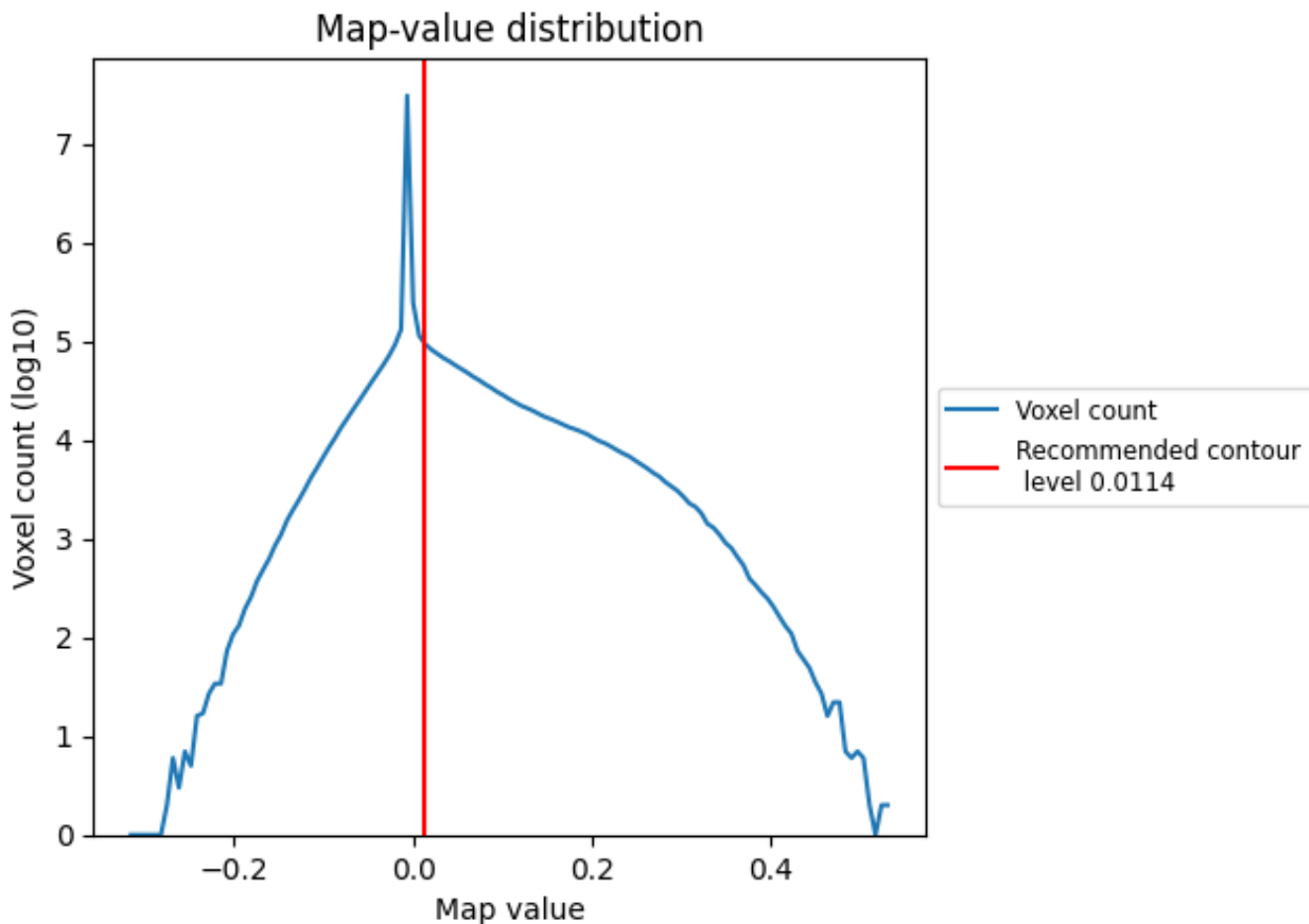
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

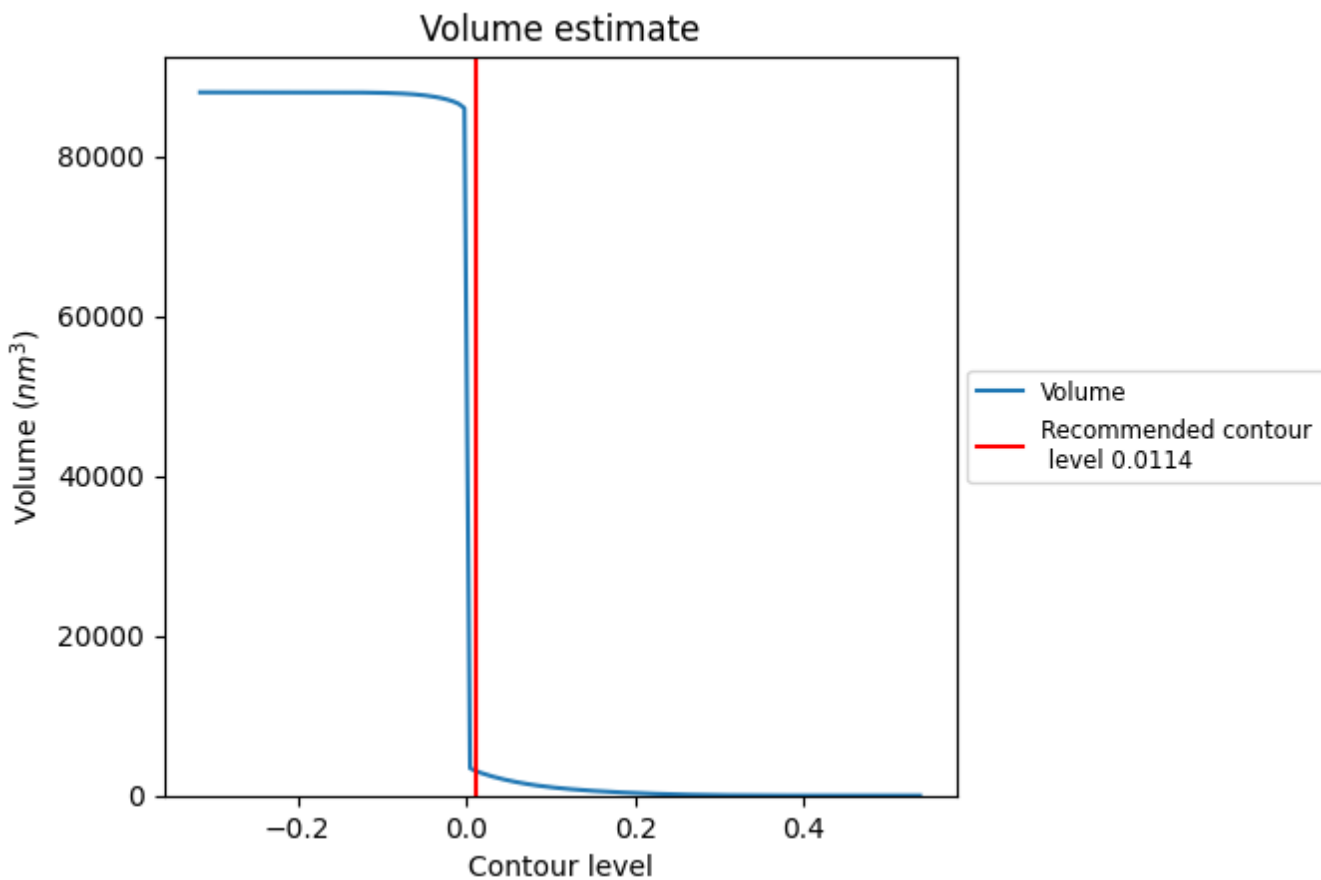
This section contains the results of statistical analysis of the map.

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.

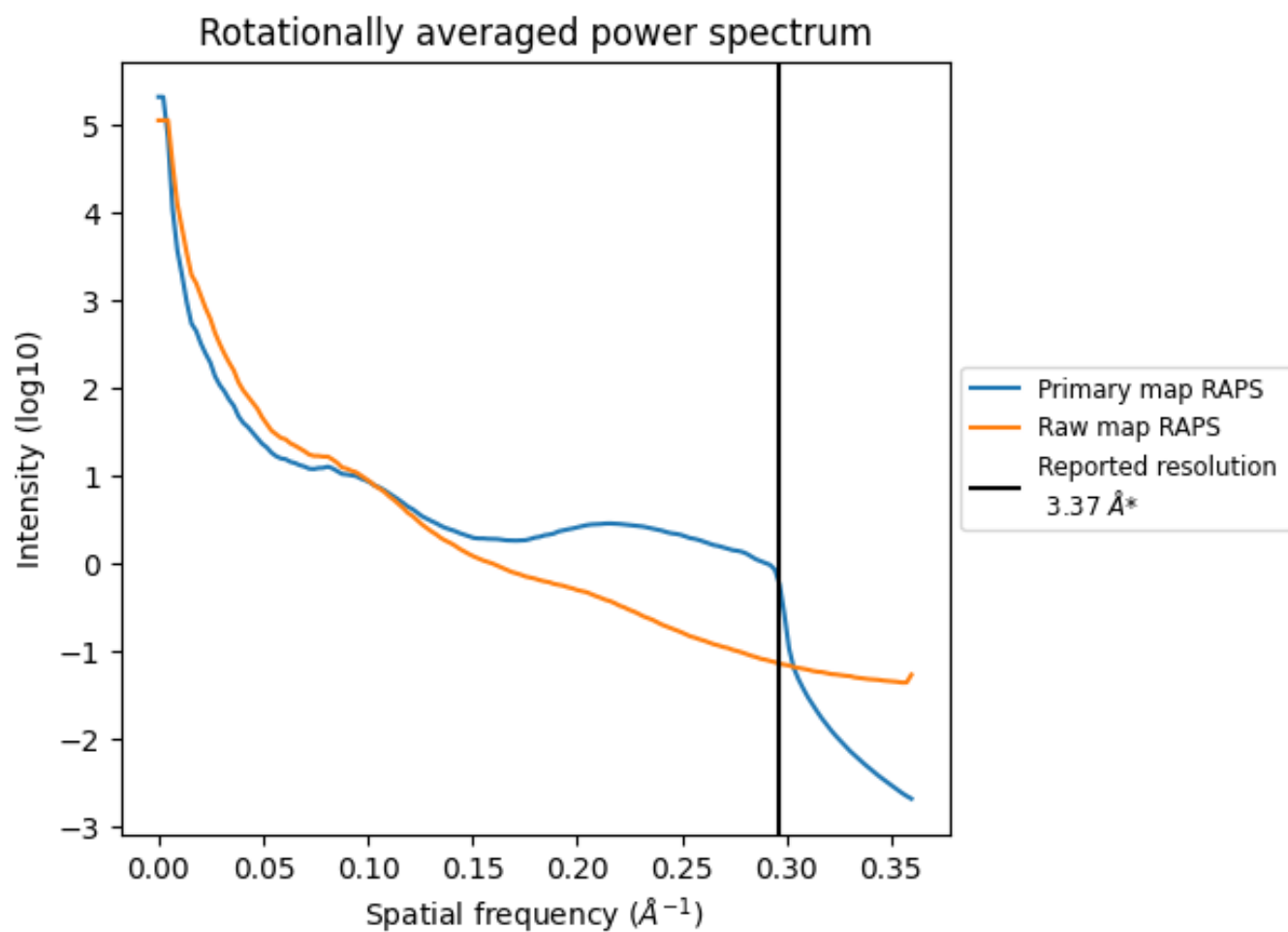
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3069 nm³; this corresponds to an approximate mass of 2773 kDa.

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

7.3 Rotationally averaged power spectrum i

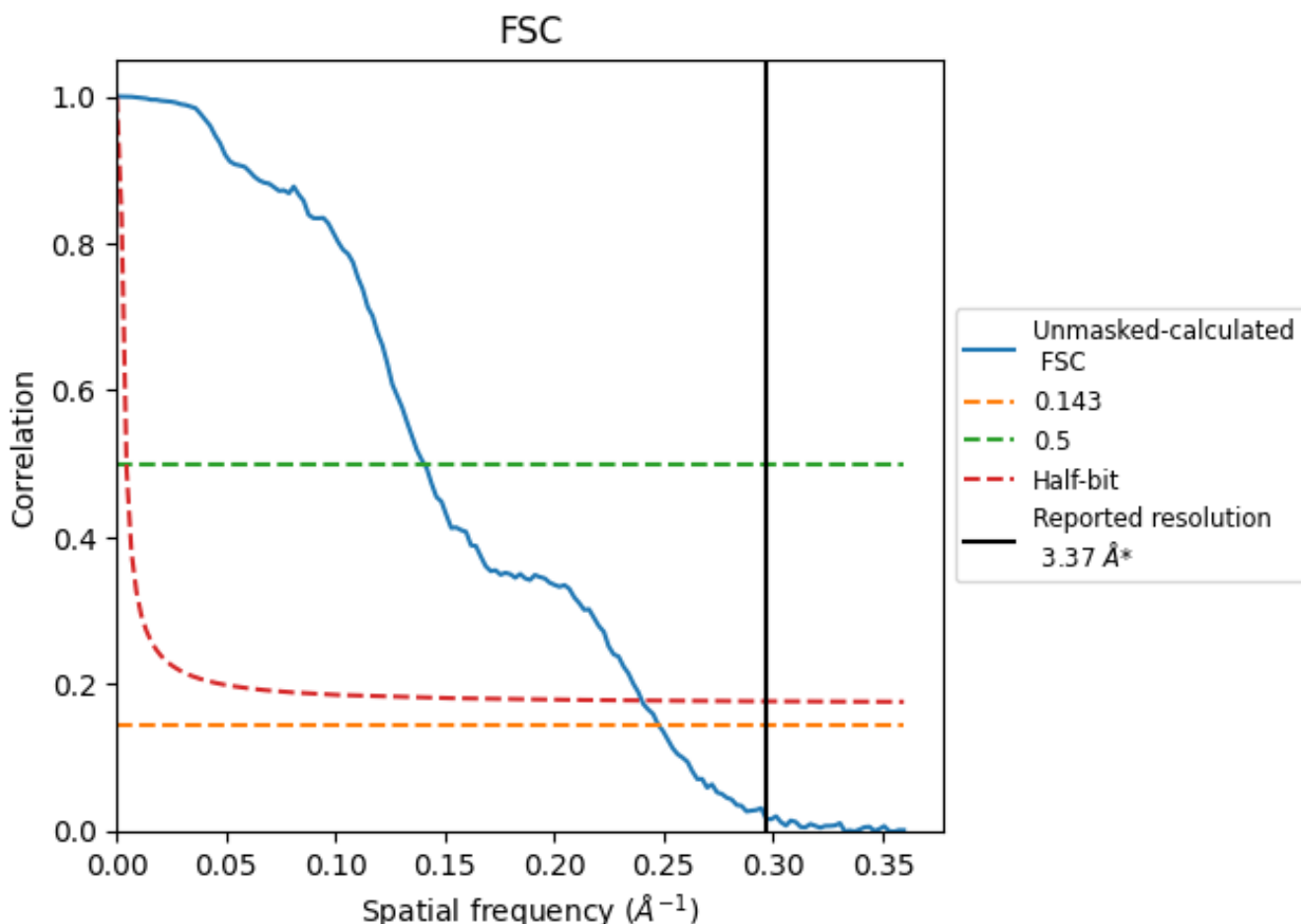


*Reported resolution corresponds to spatial frequency of 0.297 \AA^{-1}

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 0.297 Å⁻¹

8.2 Resolution estimates [i](#)

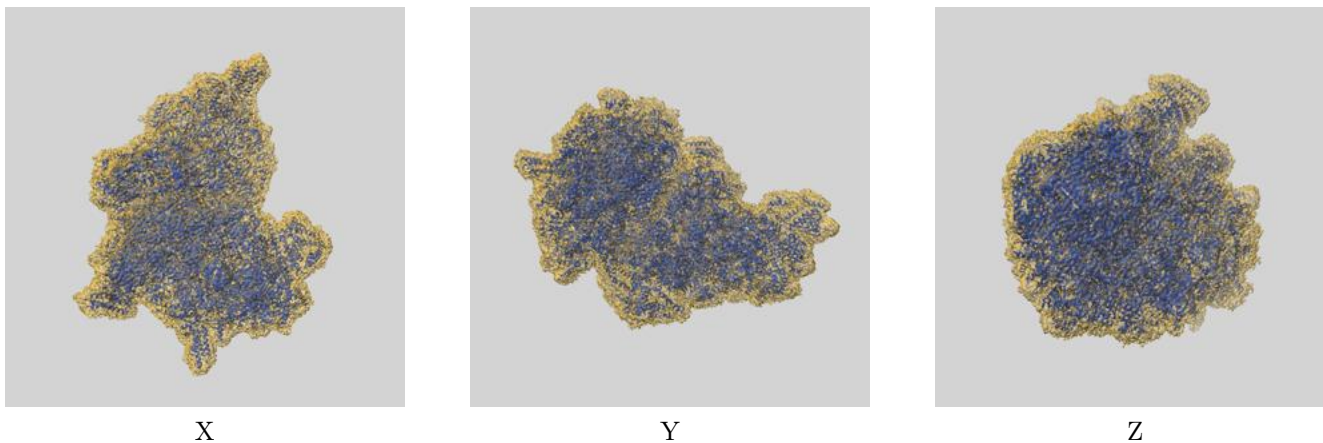
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	7.13	4.17

*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 4.04 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

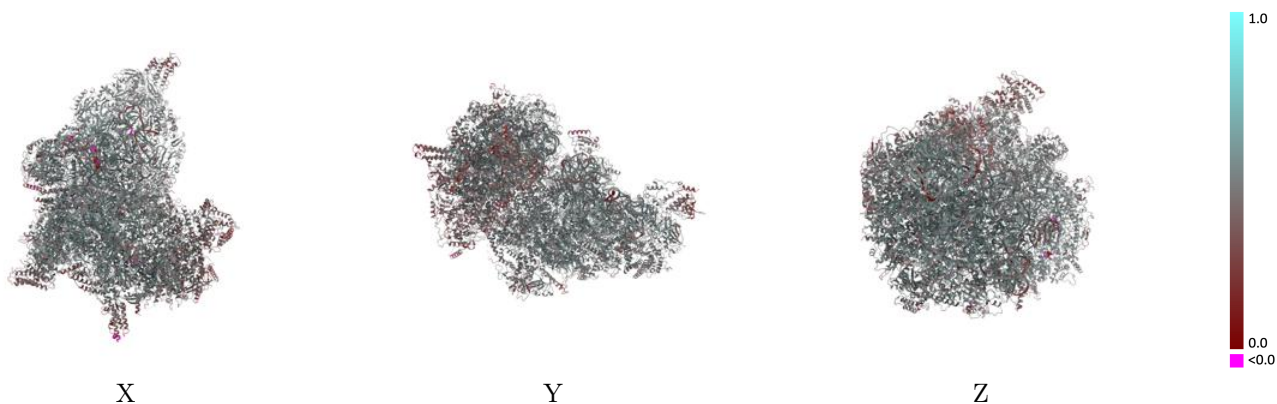
This section contains information regarding the fit between EMDB map EMD-0230 and PDB model 6HIW. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



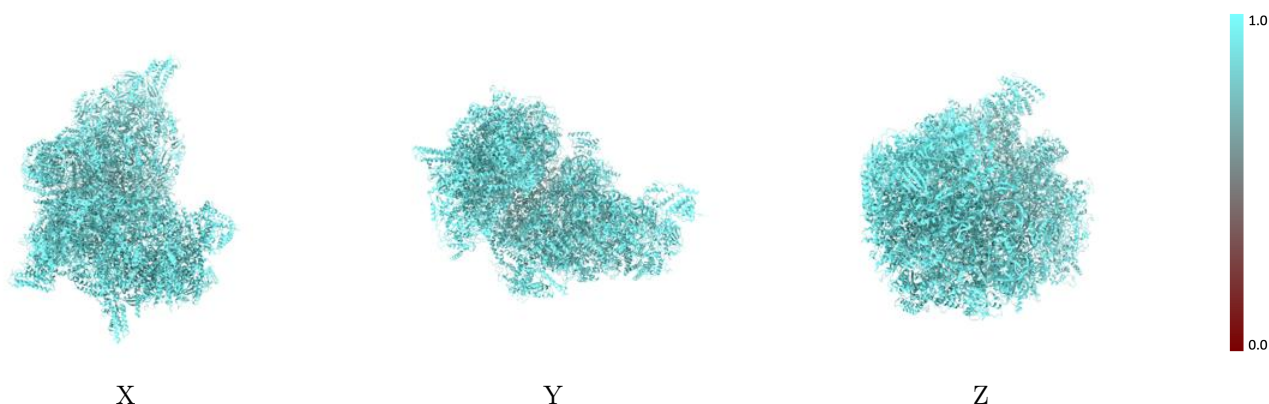
The images above show the 3D surface view of the map at the recommended contour level 0.0114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



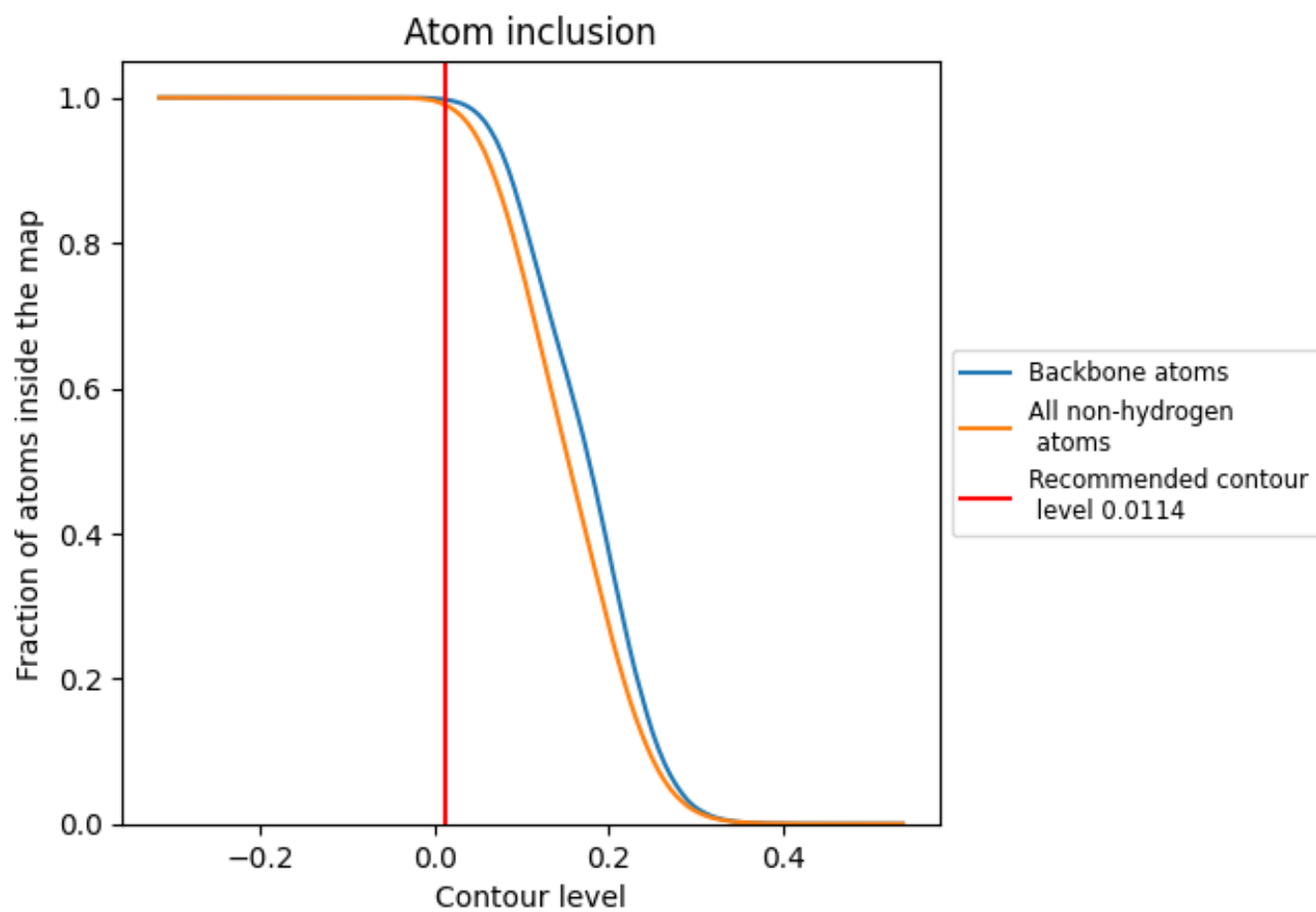
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0114).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9904	 0.4880
CA	 0.9935	 0.5000
CC	 0.9734	 0.5070
CE	 0.9918	 0.5330
CF	 0.9840	 0.4870
CH	 0.9828	 0.5160
CI	 0.9872	 0.5190
CJ	 0.9861	 0.5010
CK	 0.9944	 0.4860
CL	 0.9944	 0.5200
CN	 0.9914	 0.5310
CO	 0.9959	 0.5210
CP	 0.9958	 0.5250
CQ	 0.9974	 0.5500
CR	 0.9860	 0.5100
CS	 0.9948	 0.5120
CU	 0.9939	 0.5090
CZ	 0.9855	 0.3940
Ca	 0.9899	 0.5130
Cb	 0.9930	 0.4990
Cd	 0.9896	 0.4760
Cg	 0.9917	 0.5000
Ci	 0.9877	 0.5170
Cj	 0.9989	 0.4810
Ck	 0.9798	 0.4500
Cm	 0.9817	 0.5070
Cn	 0.9977	 0.5270
Cp	 0.9965	 0.4630
Cq	 0.9939	 0.5180
Cr	 0.9954	 0.4560
Cv	 0.9942	 0.5120
DA	 0.9920	 0.4800
DB	 0.9845	 0.4860
DC	 0.9883	 0.3980
DD	 0.9924	 0.5080



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Chain	Atom inclusion	Q-score
DE	 0.9913	 0.4280
DF	 0.9937	 0.4900
DG	 0.9887	 0.4560
DH	 0.9885	 0.4870
DI	 0.9958	 0.4970
DJ	 0.9917	 0.4820
DK	 0.9888	 0.4680
DL	 0.9751	 0.5140
DM	 0.9940	 0.5260
DN	 0.9901	 0.5130
DO	 0.9937	 0.4740
DP	 0.9974	 0.4270
DQ	 0.9960	 0.4900
DR	 0.9975	 0.4740
DS	 0.9989	 0.4800
DT	 0.9920	 0.4960
DU	 0.9918	 0.5000
DV	 0.9869	 0.5200
DW	 0.9909	 0.5100
DX	 0.9887	 0.5040
DY	 0.9887	 0.5170
DZ	 0.9883	 0.5220
Da	 1.0000	 0.5490
UO	 1.0000	 0.4330
UP	 1.0000	 0.3640
UQ	 0.9896	 0.4000
UR	 1.0000	 0.3800
US	 0.9938	 0.4110
UT	 0.9659	 0.3610