



## wwPDB EM Validation Summary Report ⓘ

Apr 26, 2022 – 01:51 pm BST

PDB ID : 7PUB  
EMDB ID : EMD-13661  
Title : Late assembly intermediate of the Trypanosoma brucei mitoribosomal small subunit  
Authors : Lenarcic, T.; Leibundgut, M.; Saurer, M.; Ramrath, D.J.F.; Fluegel, T.; Boehringer, D.; Ban, N.  
Deposited on : 2021-09-29  
Resolution : 3.70 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](mailto: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.

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

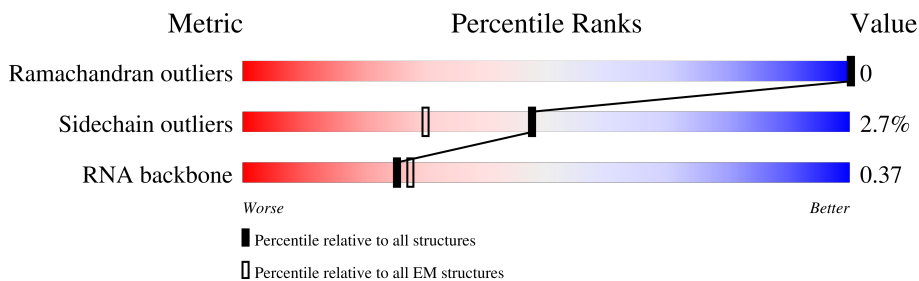
EMDB validation analysis : 0.0.1.dev7  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28

# 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 3.70 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.



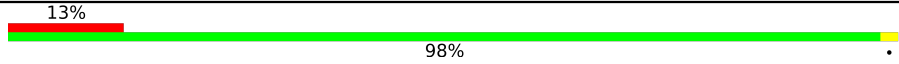
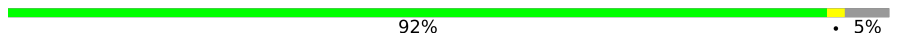

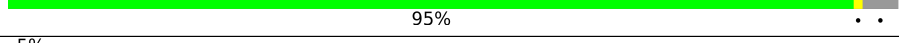

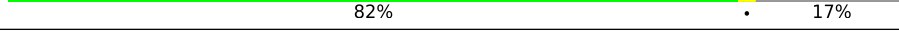
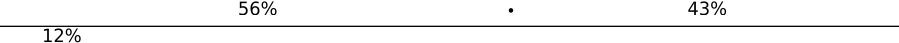
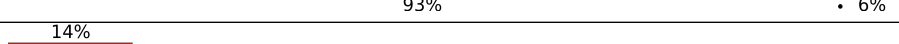
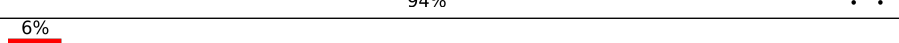
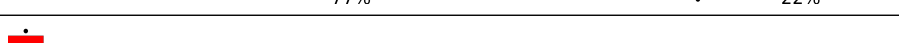


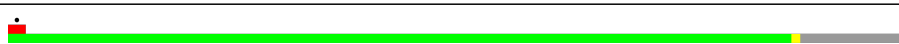




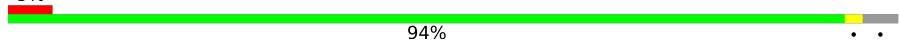



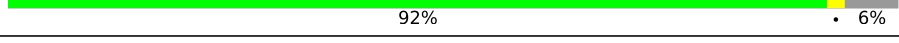
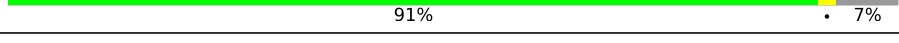
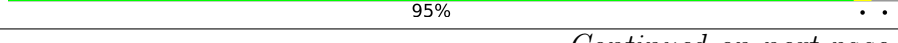

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	CA	621	13% (red), 59% (green), 41% (yellow)
2	CC	74	11% (red), 95% (green), 5% (yellow)
3	CE	435	9% (red), 95% (green), 5% (yellow)
4	CF	160	91% (green), 7% (yellow), 2% (grey)
5	CH	282	8% (red), 96% (green), 2% (yellow), 2% (grey)
6	CI	443	7% (red), 94% (green), 2% (yellow), 2% (grey)
7	CJ	817	96% (green), 2% (yellow), 2% (grey)
8	CK	326	7% (red), 90% (green), 9% (yellow)

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Mol	Chain	Length	Quality of chain
9	CL	87	
10	CN	166	
11	CO	429	
12	CP	188	
13	CQ	307	
14	CR	320	
15	CS	244	
16	CU	193	
17	Ca	602	
18	Cb	325	
19	Cd	440	
20	Cg	498	
21	Ci	181	
22	Cj	257	
23	Ck	874	
24	Cm	215	
25	Cn	250	
26	Cp	187	
27	Cq	263	
28	Cr	439	
29	Cv	1211	
30	DA	1788	
31	DB	1181	
32	DC	1165	
33	DD	812	

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Mol	Chain	Length	Quality of chain
34	DE	747	77% 21%
35	DF	666	86% 12%
36	DG	631	85% 13%
37	DH	581	93%
38	DI	407	94%
39	DJ	396	88% 10%
40	DK	324	78% 19%
41	DL	307	93% 5%
42	DM	294	99%
43	DN	293	84% 14%
44	DO	282	78% 22%
45	DP	274	74% 24%
46	DQ	268	92% 5%
47	DR	270	89% 7%
48	DS	261	92% 7%
49	DT	247	92%
50	DU	228	91% 7%
51	DV	183	84% 13%
52	DW	179	89% 10%
53	DX	169	80% 18%
54	DY	163	93% 6%
55	DZ	94	84% 13%
56	Da	64	52% 47%
57	F3	966	74% 26%
58	F6	676	59% 38%

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Mol	Chain	Length	Quality of chain
59	F7	679	55% 82% 15%
60	F9	608	6% 55% 44%
61	FO	334	5% 77% 20%
62	Ff	848	• 70% 28%
63	Fg	550	8% 91% 7%
64	Fh	318	15% 84% 14%
65	Fi	629	14% 73% 25%
66	IA	787	5% 86% 12%
67	IB	803	5% 62% 36%
68	U6	21	48% 100%
68	UJ	21	10% 100%
69	U7	40	15% 100%
70	UE	53	19% 100%
71	UF	39	44% 100%
72	UG	13	15% 100%
73	UI	10	20% 100%
74	UK	3	100%
75	UL	20	20% 100%

## 2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 212864 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 RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	CA	621	12330	5513	1927	4269	621	0	0

- Molecule 2 is a protein called uS3m.

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

- Molecule 3 is a protein called Ribosomal\_S5\_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CE	426	3459	2188	642	613	16	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CF	149	1240	791	217	226	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	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	variant	UNP Q388R7

- Molecule 6 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CI	427	3410	2148	615	630	17	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CJ	803	6535	4133	1152	1221	29	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 8 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CK	298	2447	1520	465	445	17	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 9 is a protein called uS12m.

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

- Molecule 10 is a protein called uS14m.

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

- Molecule 11 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	CO	308	2552	1615	476	448	13	0	0

- Molecule 12 is a protein called bS16m.

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

- Molecule 13 is a protein called 30S Ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CQ	226	1866	1186	355	317	8	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 14 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	CR	267	2210	1398	405	402	5	0	0

There is a discrepancy between the modelled and reference sequences:

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



- Molecule 15 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	CS	139	1149	743	205	195	6	0	0

- Molecule 16 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CU	181	1522	957	303	250	12	0	0

- Molecule 17 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Ca	575	4911	3146	875	867	23	0	0

- Molecule 18 is a protein called mS23.

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

- Molecule 19 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Cd	230	1961	1242	358	350	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cd	299	UNK	GLY	conflict	UNP Q38DK6
Cd	364	UNK	GLY	conflict	UNP Q38DK6

- Molecule 20 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Cg	480	3895	2494	682	699	20	0	0

- Molecule 21 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Ci	164	1343	845	246	243	9	0	0

- Molecule 22 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Cj	227	1799	1142	311	342	4	0	0

- Molecule 23 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Ck	682	5442	3411	990	1016	25	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	variant	UNP Q387C7
Ck	144	PHE	LEU	variant	UNP Q387C7
Ck	253	TYR	PHE	variant	UNP Q387C7
Ck	339	GLU	VAL	variant	UNP Q387C7
Ck	815	GLY	ARG	variant	UNP Q387C7
Ck	871	GLY	GLU	variant	UNP Q387C7

- Molecule 24 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Cm	145	1184	735	230	210	9	0	0

- Molecule 25 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Cn	62	528	345	105	75	3	0	0

- Molecule 26 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Cp	173	1466	928	265	268	5	0	0

- Molecule 27 is a protein called Superoxide dismutase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	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	variant	UNP Q586A1
Cq	167	MET	VAL	variant	UNP Q586A1

- Molecule 28 is a protein called Sod\_Fe\_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Cr	267	2083	1317	382	369	15	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 29 is a protein called ECH\_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Cv	1040	8404	5291	1508	1568	37	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	1179	GLU	GLY	variant	UNP Q383R4

- Molecule 30 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	DA	1552	12448	7861	2220	2329	38	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 31 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	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	variant	UNP Q586P5
DB	359	ILE	THR	variant	UNP Q586P5
DB	384	GLN	HIS	variant	UNP Q586P5
DB	402	THR	ILE	variant	UNP Q586P5
DB	423	THR	ALA	variant	UNP Q586P5
DB	586	ARG	HIS	variant	UNP Q586P5
DB	593	ARG	LYS	variant	UNP Q586P5
DB	647	SER	GLY	variant	UNP Q586P5

- Molecule 32 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	DC	1089	8709	5498	1538	1642	31	0	0

There are 10 discrepancies between the modelled and reference sequences:

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

- Molecule 33 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	DD	790	6513	4121	1181	1170	41	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 34 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	DE	588	4798	3052	868	859	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	378	UNK	LYS	variant	UNP Q386Q7
DE	384	UNK	THR	variant	UNP Q386Q7

- Molecule 35 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	DF	589	4738	2974	895	844	25	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	variant	UNP Q38ET1
DF	258	ASP	ASN	variant	UNP Q38ET1
DF	372	ASN	ASP	variant	UNP Q38ET1
DF	406	ASN	SER	variant	UNP Q38ET1
DF	510	ASP	GLY	variant	UNP Q38ET1
DF	577	ALA	VAL	variant	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	variant	UNP Q38ET1

- Molecule 36 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	DG	552	4482	2820	818	813	31	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 37 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	DH	559	4541	2849	843	828	21	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 38 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	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	variant	UNP Q587C2
DI	116	ASP	GLU	variant	UNP Q587C2

- Molecule 39 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	DJ	357	2914	1858	512	530	14	0	0

- Molecule 40 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	DK	263	2083	1312	374	392	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 41 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	DL	291	2360	1495	441	412	12	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 42 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	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	variant	UNP Q57XL2
DM	97	ASN	SER	variant	UNP Q57XL2
DM	138	SER	PRO	variant	UNP Q57XL2
DM	173	ALA	THR	variant	UNP Q57XL2
DM	206	ALA	THR	variant	UNP Q57XL2

- Molecule 43 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	DN	253	2062	1313	374	365	10	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 44 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	DO	221	1796	1123	325	338	10	0	0

- Molecule 45 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	DP	207	1760	1132	312	307	9	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called AKAP7\_NLS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	DQ	255	2055	1290	388	368	9	0	0

- Molecule 47 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	DR	250	2019	1301	368	340	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 48 is a protein called mS66.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	DS	243	1950	1216	364	356	14	0	0

- Molecule 49 is a protein called Rhodanese domain-containing protein.

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

- Molecule 50 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	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	variant	UNP Q582T9
DU	152	ILE	VAL	variant	UNP Q582T9

- Molecule 51 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	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	variant	UNP Q57UZ6

- Molecule 52 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	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	variant	UNP Q383N9

- Molecule 53 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	DX	139	1174	747	223	197	7	0	0

- Molecule 54 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	DY	154	1295	829	247	214	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DY	34	HIS	ASP	variant	UNP Q57YD4

- Molecule 55 is a protein called mS73.

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

- Molecule 56 is a protein called mS74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Da	34	305	193	67	43	2	0	0

- Molecule 57 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	F3	252	2003	1259	354	378	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	44	THR	ALA	variant	UNP Q38E61
F3	190	VAL	ILE	variant	UNP Q38E61
F3	303	ALA	SER	variant	UNP Q38E61
F3	418	ASP	ASN	variant	UNP Q38E61

- Molecule 58 is a protein called mt-SAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	F6	416	3358	2124	580	636	18	0	0

- Molecule 59 is a protein called mt-SAF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	F7	576	4584	2922	792	837	33	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F7	36	ILE	THR	variant	UNP Q57UW6
F7	470	GLU	LYS	variant	UNP Q57UW6
F7	474	VAL	ALA	variant	UNP Q57UW6

- Molecule 60 is a protein called mt-SAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	F9	342	2815	1736	530	539	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F9	117	ALA	SER	variant	UNP Q57YC0
F9	145	TYR	HIS	variant	UNP Q57YC0
F9	316	LYS	GLU	variant	UNP Q57YC0
F9	412	GLY	VAL	variant	UNP Q57YC0
F9	449	VAL	ALA	variant	UNP Q57YC0
F9	537	GLY	SER	variant	UNP Q57YC0

- Molecule 61 is a protein called mt-SAF22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	FO	267	2236	1407	432	385	12	0	0

- Molecule 62 is a protein called DNA photolyase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	Ff	614	4941	3135	885	898	23	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ff	109	ALA	VAL	variant	UNP Q382U6
Ff	127	UNK	TYR	conflict	UNP Q382U6
Ff	138	GLN	ARG	variant	UNP Q382U6
Ff	200	CYS	SER	variant	UNP Q382U6
Ff	319	ALA	THR	variant	UNP Q382U6
Ff	334	ASN	THR	variant	UNP Q382U6
Ff	350	ILE	THR	variant	UNP Q382U6
Ff	362	ALA	VAL	variant	UNP Q382U6
Ff	844	THR	SER	variant	UNP Q382U6

- Molecule 63 is a protein called Acyl transferase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Fg	513	3994	2512	698	754	30	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fg	90	LYS	ARG	variant	UNP Q38DK4
Fg	152	VAL	LEU	variant	UNP Q38DK4
Fg	159	ILE	VAL	variant	UNP Q38DK4
Fg	363	MET	ARG	variant	UNP Q38DK4
Fg	399	UNK	GLU	conflict	UNP Q38DK4
Fg	525	LYS	ARG	variant	UNP Q38DK4

- Molecule 64 is a protein called mt-SAF37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Fh	274	2230	1384	420	411	15	0	0

- Molecule 65 is a protein called mt-SAF38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Fi	469	3734	2363	683	665	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fi	35	THR	SER	variant	UNP Q57ZP1
Fi	69	GLY	SER	variant	UNP Q57ZP1
Fi	185	PRO	HIS	variant	UNP Q57ZP1

- Molecule 66 is a protein called Translation initiation factor IF-2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	IA	693	5414	3397	972	1018	27	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IA	373	LYS	GLU	variant	UNP Q57WE3
IA	451	ILE	VAL	variant	UNP Q57WE3
IA	584	ASN	SER	variant	UNP Q57WE3
IA	679	ASP	VAL	variant	UNP Q57WE3

- Molecule 67 is a protein called mt-SAF39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	IB	511	4103	2561	764	760	18	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IB	136	LYS	GLU	variant	UNP Q387Q6
IB	226	ASP	ASN	variant	UNP Q387Q6
IB	237	CYS	SER	variant	UNP Q387Q6
IB	259	THR	ARG	variant	UNP Q387Q6
IB	268	GLU	LYS	variant	UNP Q387Q6
IB	275	CYS	TYR	variant	UNP Q387Q6
IB	312	THR	SER	variant	UNP Q387Q6
IB	459	ASP	ALA	variant	UNP Q387Q6
IB	572	HIS	ARG	variant	UNP Q387Q6

- Molecule 68 is a protein called Unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	U6	21	105	63	21	21	0	0
68	UJ	21	105	63	21	21	0	0

- Molecule 69 is a protein called Unk7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
69	U7	40	200	120	40	40	0	0

- Molecule 70 is a protein called UnkE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
70	UE	53	265	159	53	53	0	0

- Molecule 71 is a protein called UnkF.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
71	UF	39	195	117	39	39	0	0

- Molecule 72 is a protein called UnkG.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	UG	13	65	39	13	13	0	0

- Molecule 73 is a protein called UnkI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
73	UI	10	50	30	10	10	0	0

- Molecule 74 is a protein called UnkK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
74	UK	3	15	9	3	3	0	0

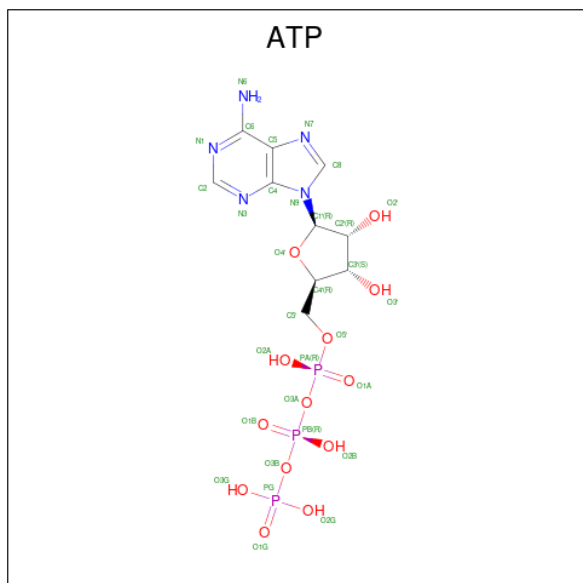
- Molecule 75 is a protein called UnkL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
75	UL	20	100	60	20	20	0	0

- Molecule 76 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
76	CA	3	3	3	0
76	CQ	1	1	1	0
76	Cg	1	1	1	0
76	IA	1	1	1	0

- Molecule 77 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

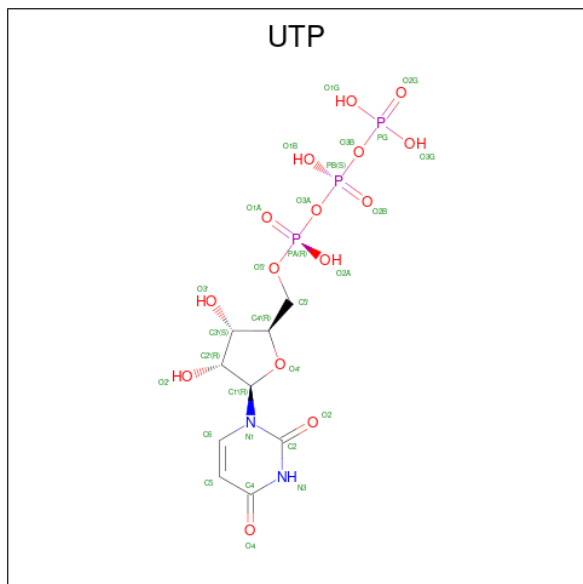


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
77	Cg	1	31	10	5	13	3	0

- Molecule 78 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

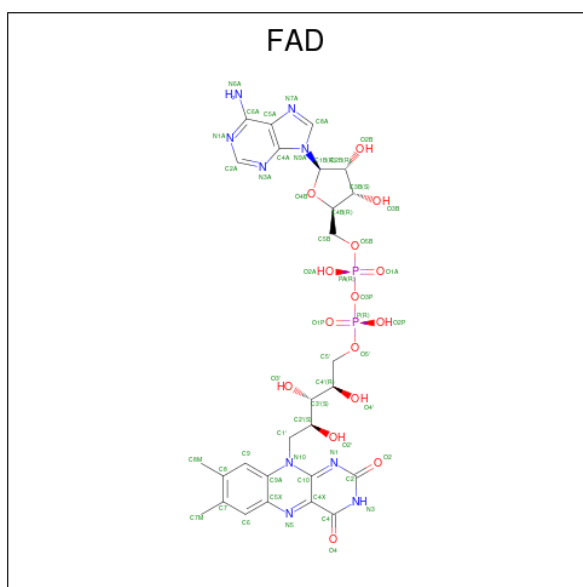
- Molecule 79 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).



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

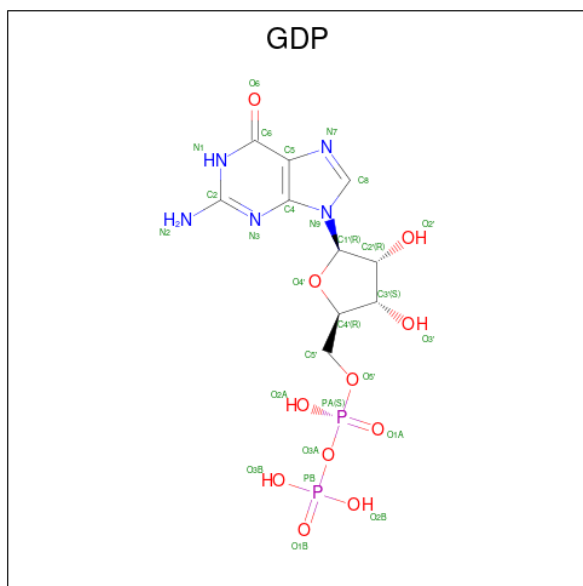
- Molecule 80 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





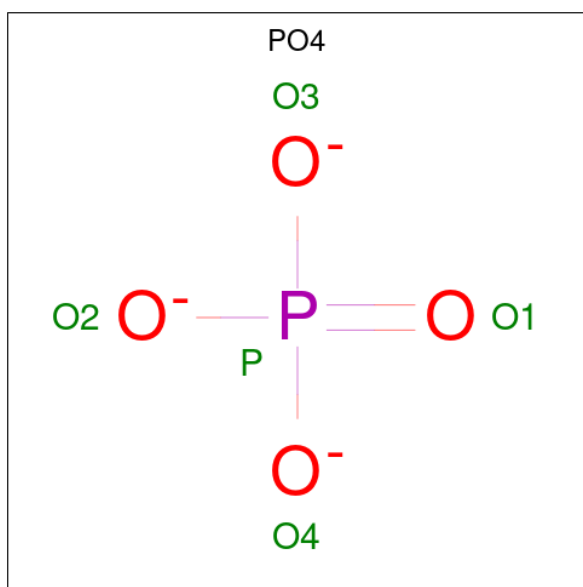
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
80	Ff	1	53	27	9	15	2	0

- Molecule 81 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
81	IA	1	28	10	5	11	2	0

- Molecule 82 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			AltConf
82	IA	1	Total	O	P	0
			5	4	1	

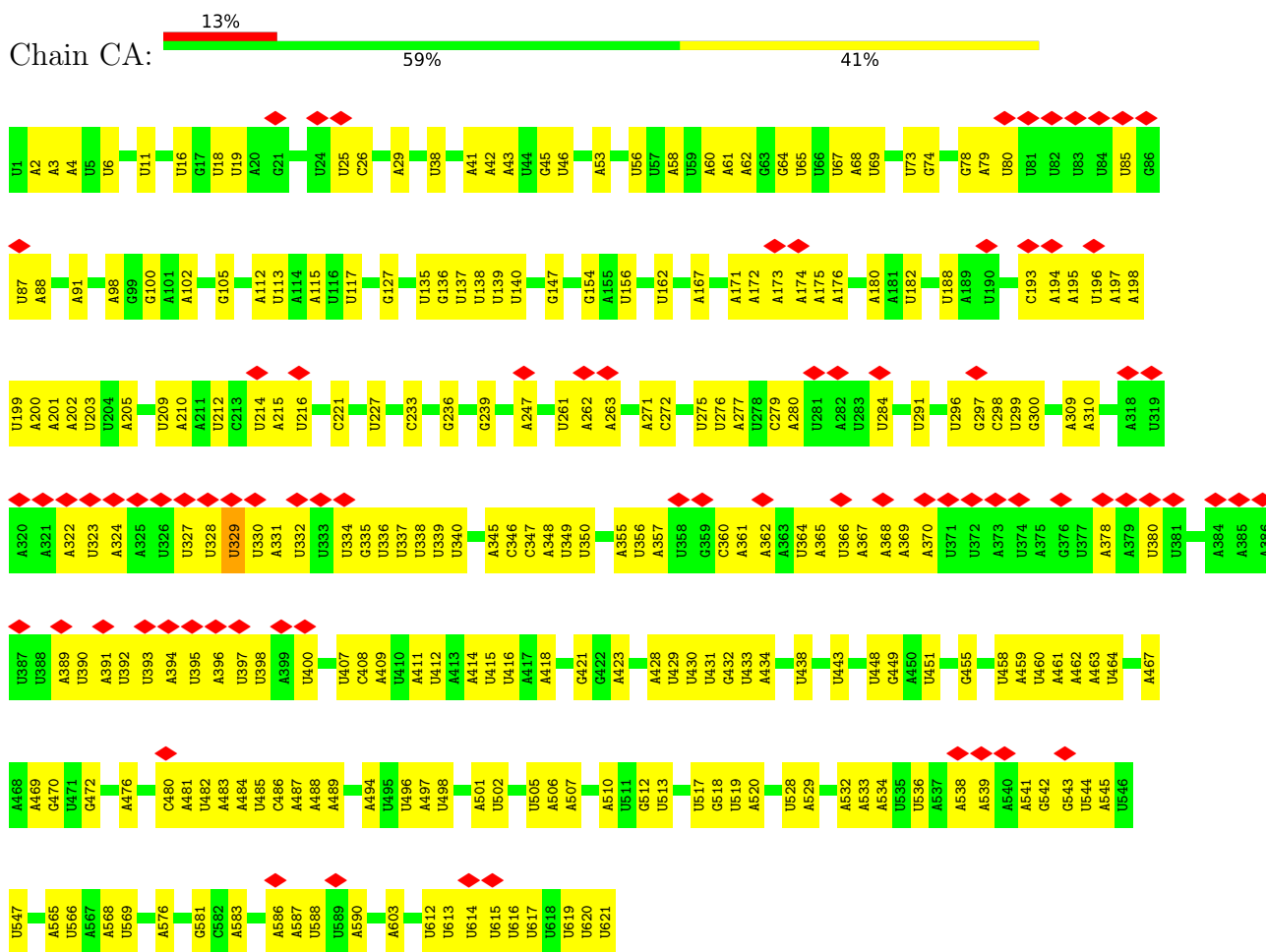
- Molecule 83 is water.

Mol	Chain	Residues	Atoms		AltConf
83	Cg	3	Total	O	0
			3	3	
83	IA	2	Total	O	0
			2	2	

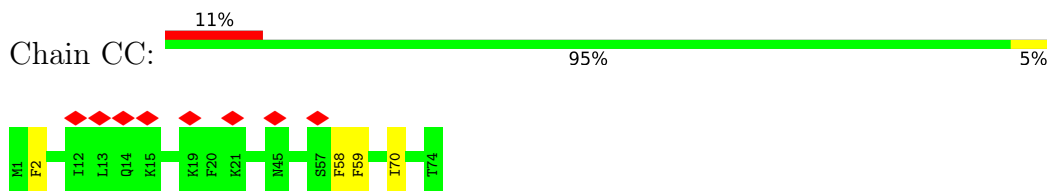
### 3 Residue-property plots

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

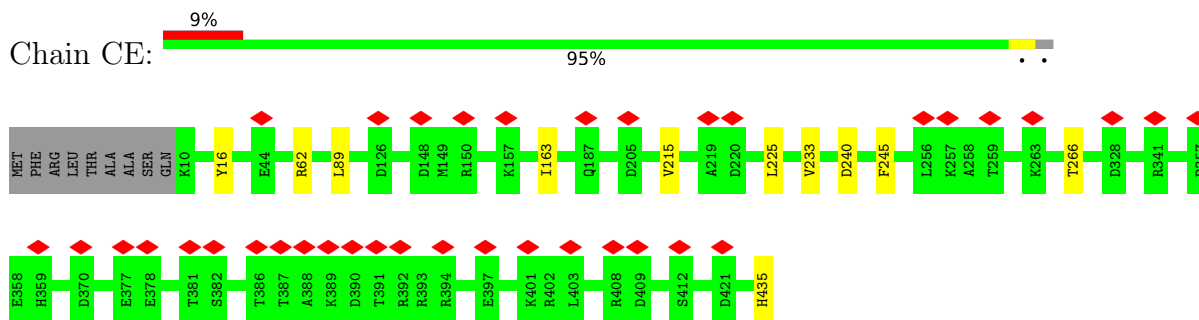
- Molecule 1: 9S rRNA



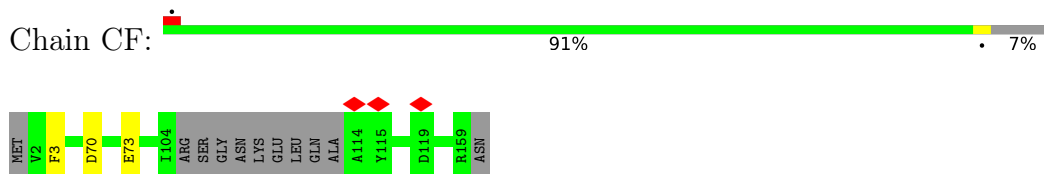
- Molecule 2: uS3m



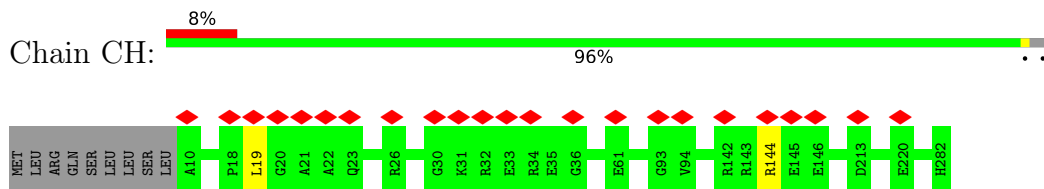
- Molecule 3: Ribosomal\_S5\_C domain-containing protein



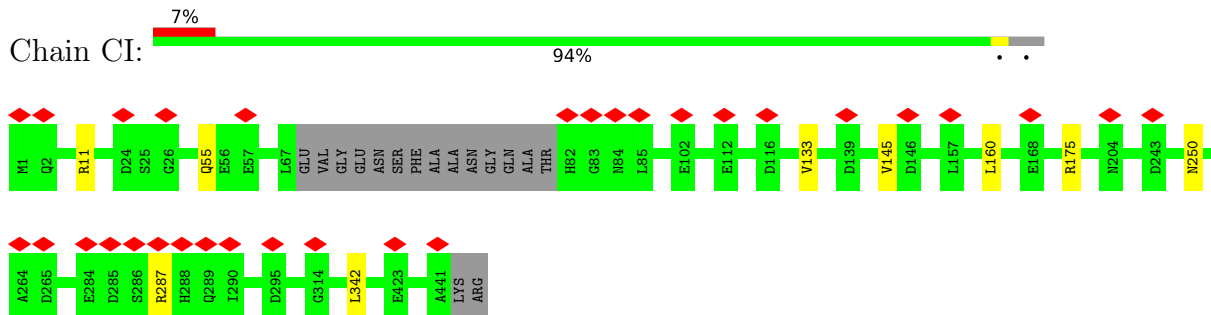
- Molecule 4: bS6m



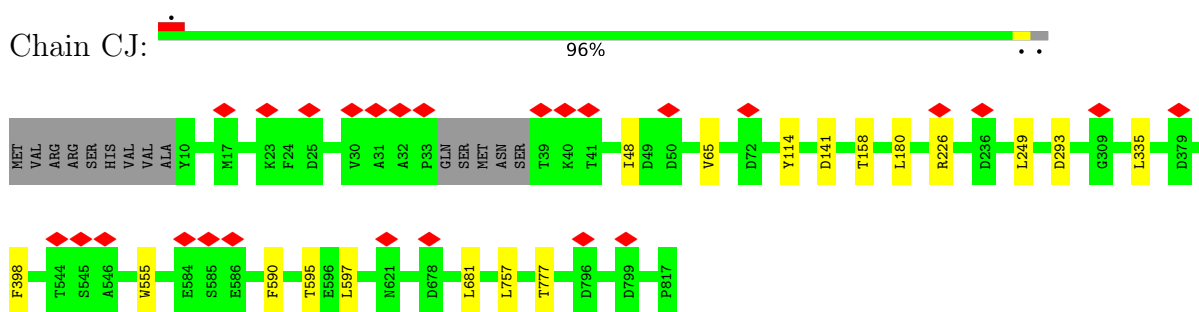
- Molecule 5: 30S ribosomal protein S8, putative



- Molecule 6: uS9m

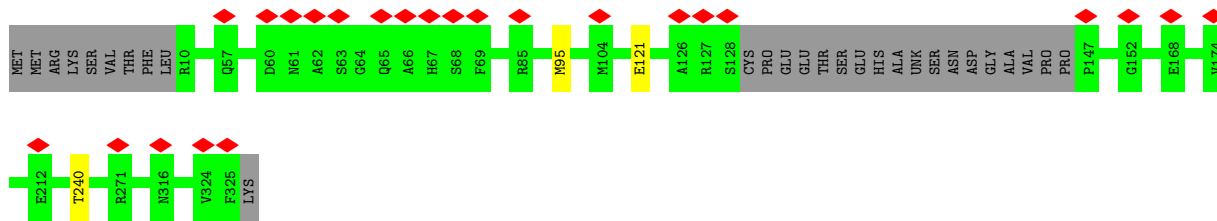


- Molecule 7: LysM domain-containing protein



- Molecule 8: uS11m

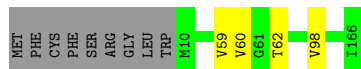




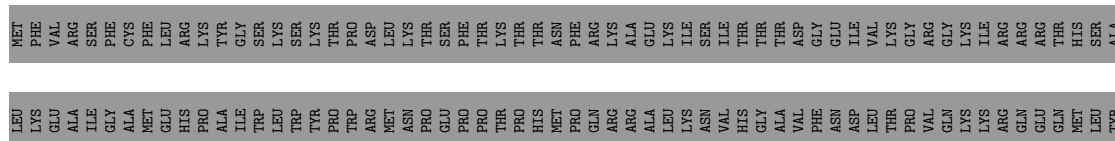
• Molecule 9: uS12m



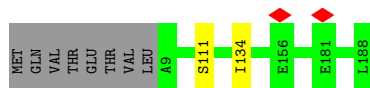
• Molecule 10: uS14m



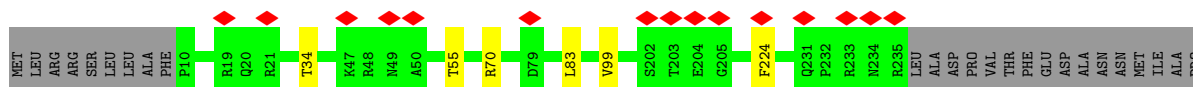
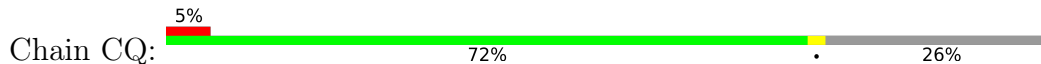
• Molecule 11: uS15m



• Molecule 12: bS16m

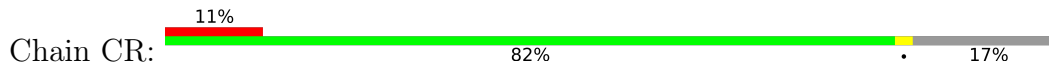


• Molecule 13: 30S Ribosomal protein S17, putative



ASN  
ALA  
PRO  
ALA  
ALA  
ALA  
LEU  
ASP  
ALA  
SER  
ASP  
PRO  
PRO  
LEU  
LEU  
ASP  
ARG  
GLY  
GLU  
TYR  
THR  
THR  
VAL  
VAL  
GLU  
GLN  
ASP  
THR  
ARG  
ASN  
LYS  
LYS  
GLY  
ASP  
ASP  
TYR  
TRP  
MET  
ASN  
LEU  
GLN  
PRO  
LYS  
GLU  
LYS  
TYR  
ASP  
PHE  
LYS  
SER  
PHE  
LYS  
SER  
PRO

• Molecule 14: bS18m



MET ASN ARG THR GLY SER I8 Y9 A10 H11 Q15 F16 A17 V18 T36 E41 E44 L80 D91 F103 D104 K108 Q111 N128 D146 A189 Y190 Q191 R219 R223 E226 S231 G232 S233 A234 S235 A236 R237 G238 S239 G240 G241 G242

T243 E257 S262 L263 H264 R266 M271 E272 D273 V274 GLY ARG SER VAL LYS ASN PRO THR PRO GLY LEU MET SER THR LYS MET LYS LYS PHE HIS ASN LEU TYR SER SER THR LYS ARG MET GLY PHE SER ASN PRO THR LEU ILE LYS VAL

• Molecule 15: uS19m



MET ALA PHE ARG ASN THR PHE THR PRO GLY LYS PHE SER THR VAL SER LYS ASN TLE VAL TRP VAL SER VAL VAL PHE LEU ARG ALA GLY PHE THR LEU HIS SER VAL LEU MET LEU PRO VAL SER TYR LEU SER LYS ILE LEU CYS ASP VAL LYS LYS

ILE VAL TYR PHE HIS THR CYS THR ARG LYS LYS MET SER LEU ARG CYS PRO CYS VAL TRP LYS SER VAL VAL ILE THR LYS ASP GLY PRO THR LYS SER VAL VAL ILE GLY THR PHE LEU GLN LYS ARG PHE LEU LYS V106 V177 L228 F243 LYS

• Molecule 16: bS21m



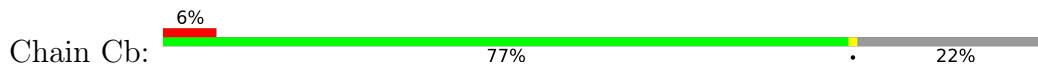
MET LEU HIS THR ARG THR LEU TRP LEU ARG GLY Y12 N51 I54 K82 K118 E121 D122 R125 T146 D147 W149 A150 R151 E152 R153 R160 Q161 V162 R163 A164 L165 P166 M167 V168 M169 Y188 R189 W190 R191 V192 ASN

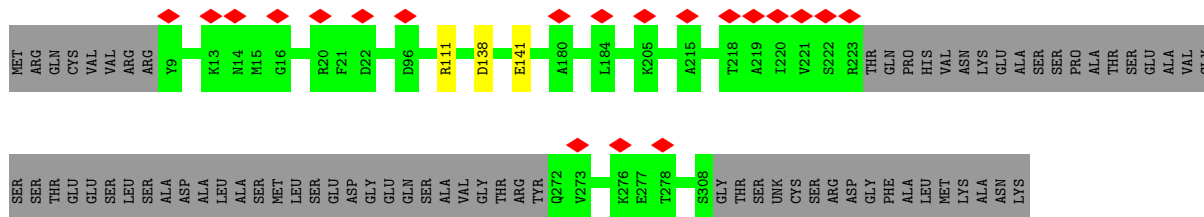
• Molecule 17: mS22



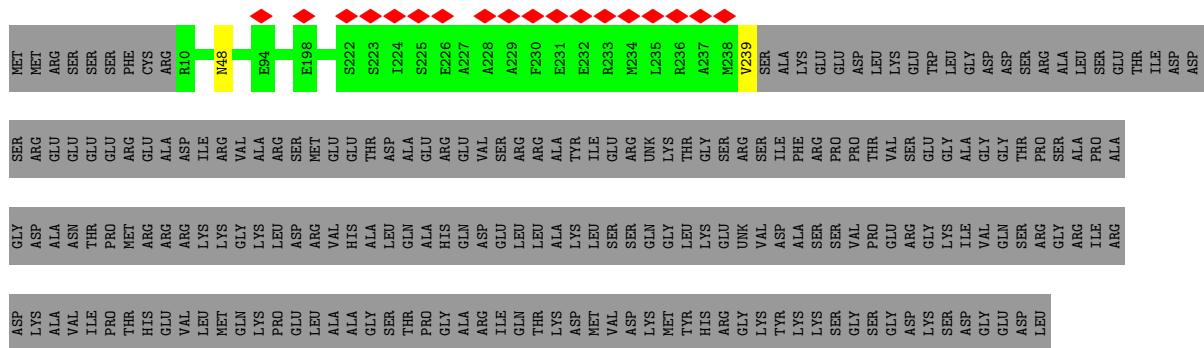
MET LEU ARG ARG ALA TYR ILE GLN ARG TYR PRO PHE ASN LYS ARG GLY PRO ARG GLU H21 H26 H27 E31 P32 P33 LYS PRO LEU GLN TRP ARG D40 P41 K42 V43 V44 T45 R46 D47 L48 S49 V50 M51 K52 S53 F54 D55 A56 D72 E73 K86 L112 K116 R132 A135 S136 G137 K138 D139 N140 T141 D145 D146 E154 N165 A166 G167 D187 E218 A219 L220 T221 Q222 N223 S224 P225 H226 N227 K228 E229 Q230 L231 Q232 R233 K234 L235 A236 F237 Q238 T239 S240 L241 G242 T243 P244 E245 F246 F247 D248 D260 L267 F272

• Molecule 18: mS23

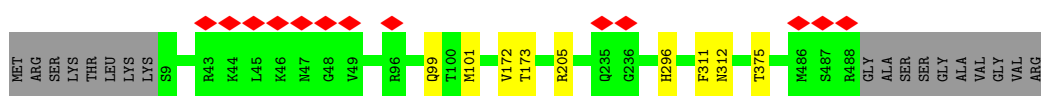




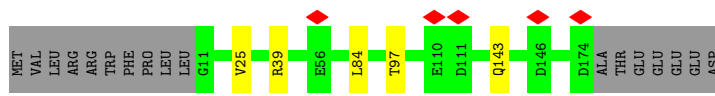
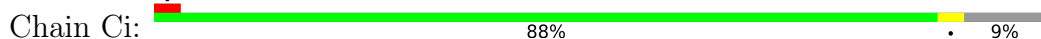
• Molecule 19: mS26



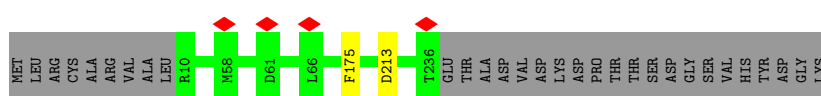
• Molecule 20: mS29



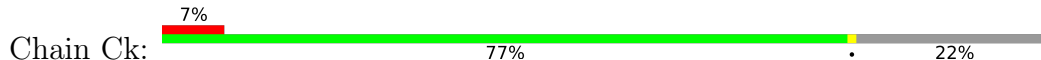
• Molecule 21: mS33

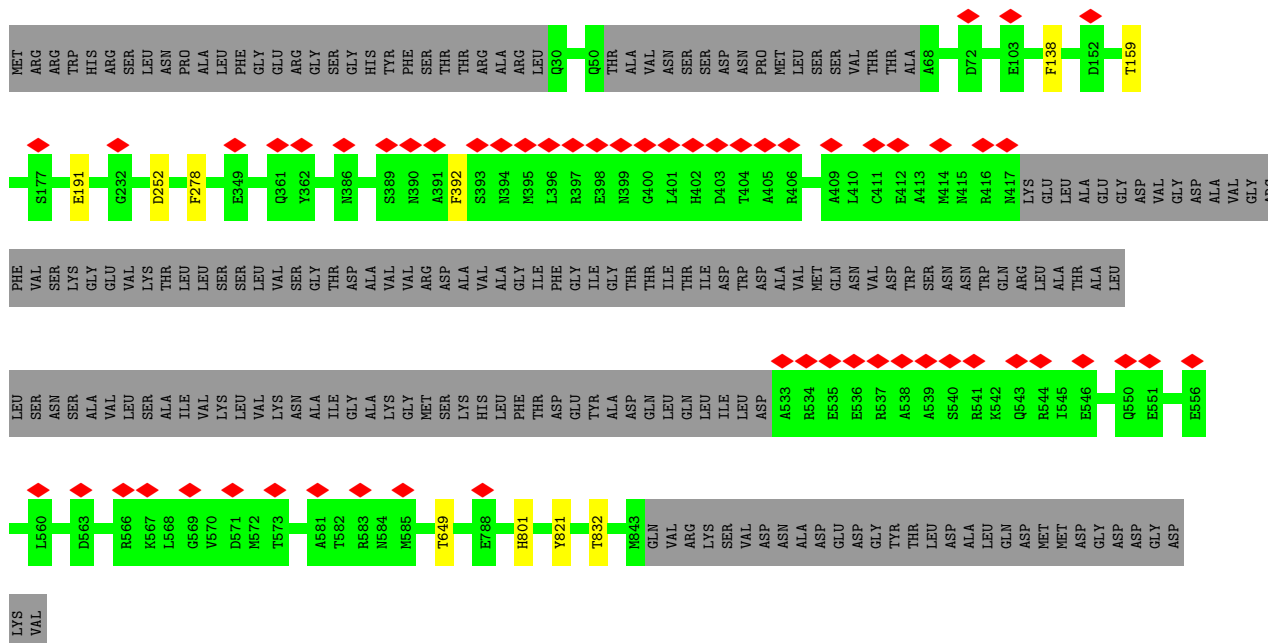


• Molecule 22: mS34

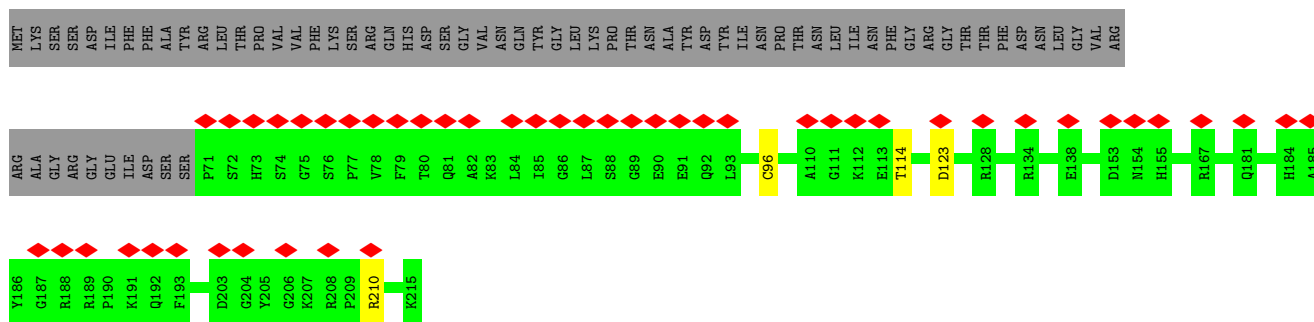


• Molecule 23: mS35

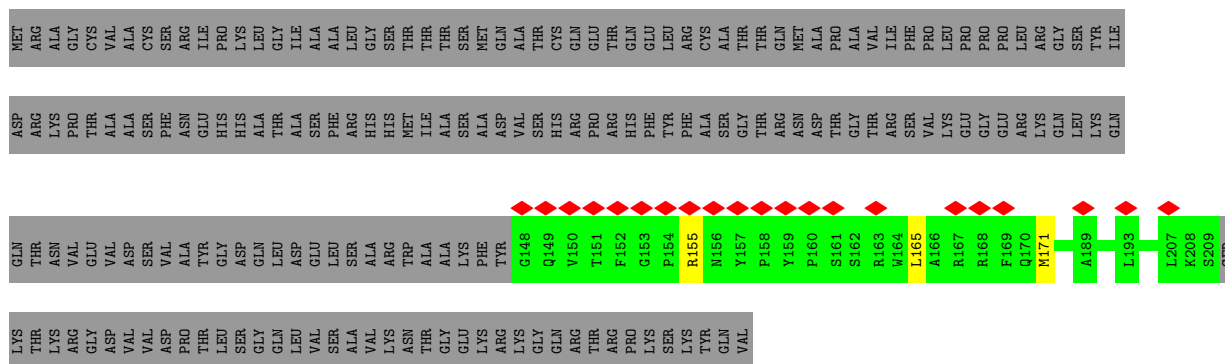




• Molecule 24: mS37

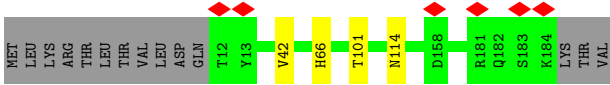


• Molecule 25: mS38

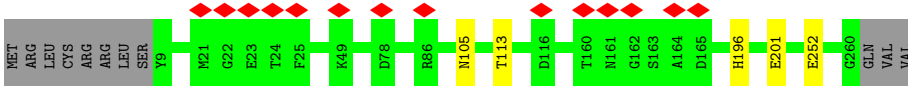


• Molecule 26: Protein FYV4, mitochondrial

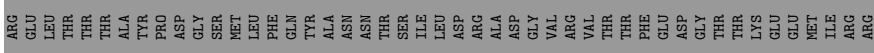
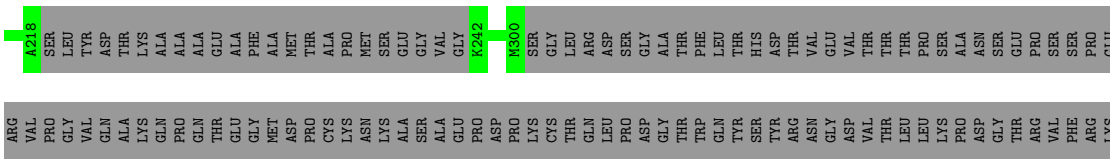
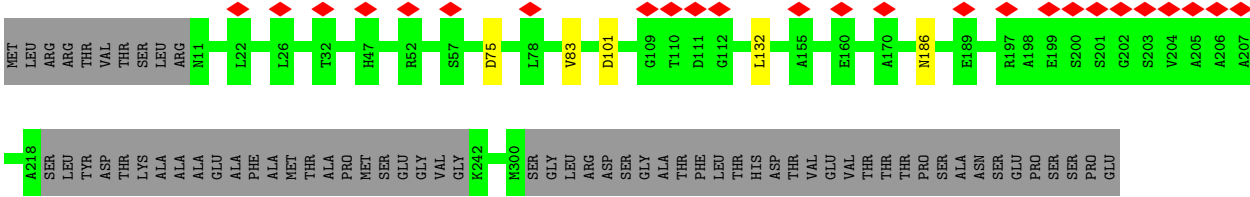




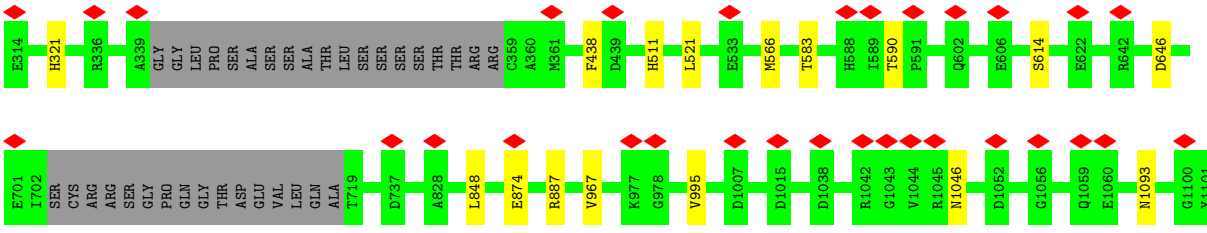
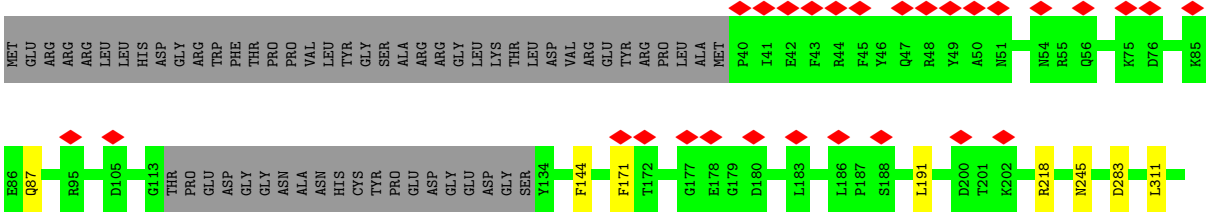
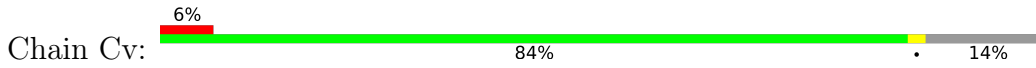
- Molecule 27: Superoxide dismutase, putative



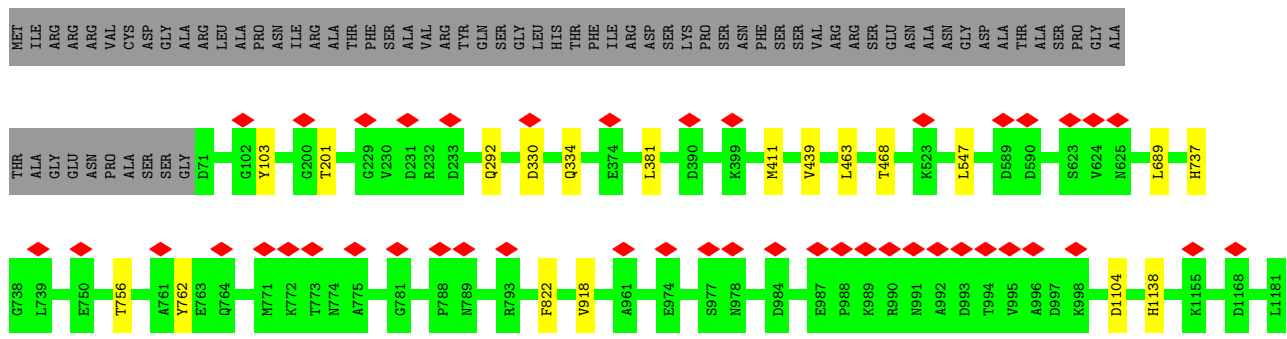
- Molecule 28: Sod\_Fe\_C domain-containing protein



- Molecule 29: ECH\_2 domain-containing protein

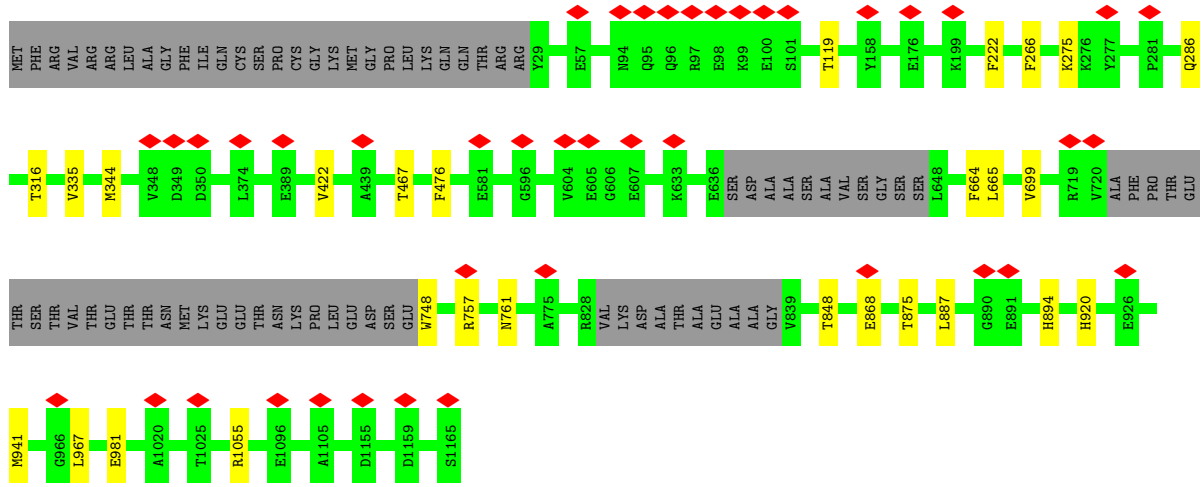






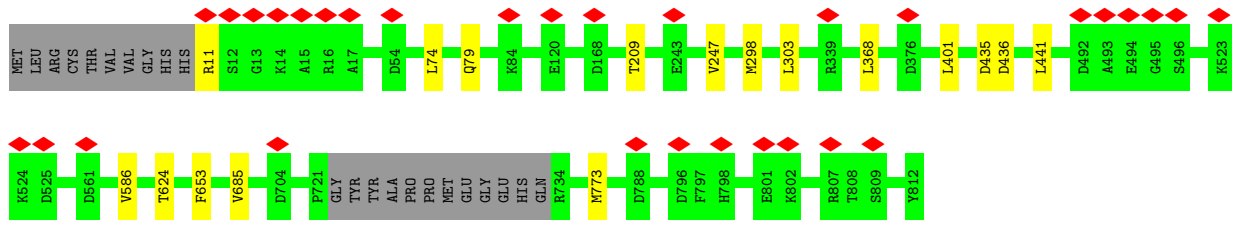
• Molecule 32: mS50

Chain DC: 91% 7%



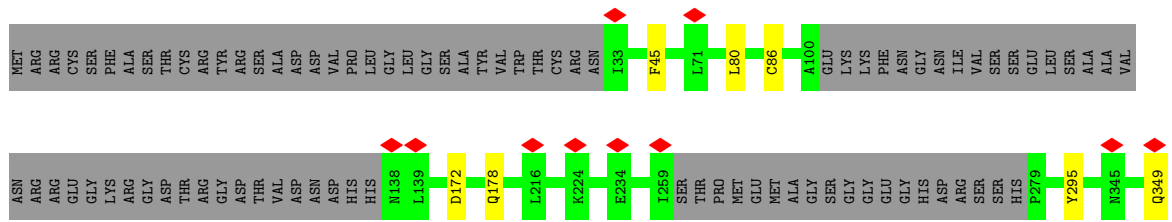
• Molecule 33: mS51

Chain DD: 95% 2%

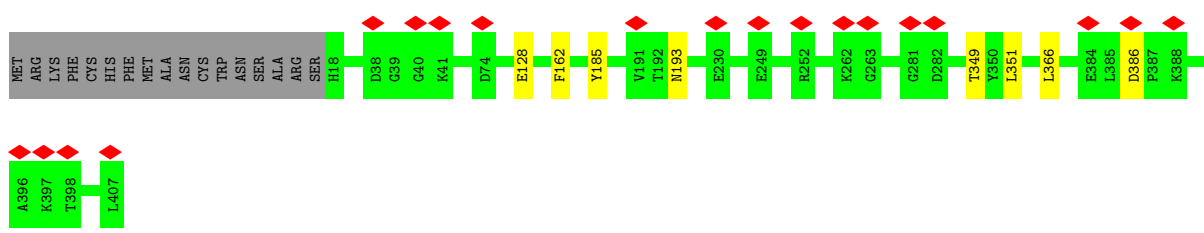


• Molecule 34: mS52

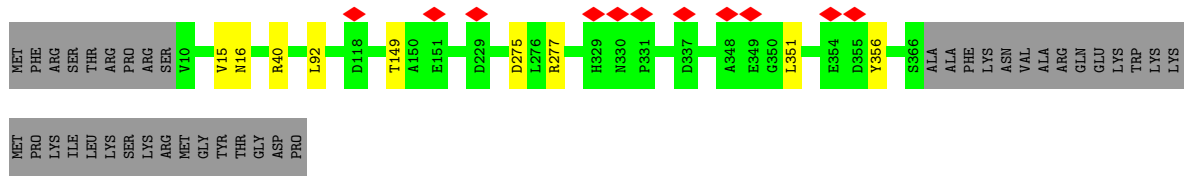
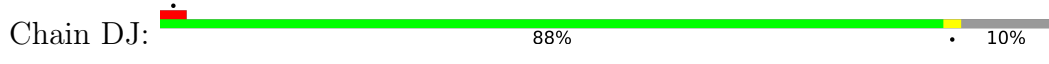
Chain DE: 77% 21%



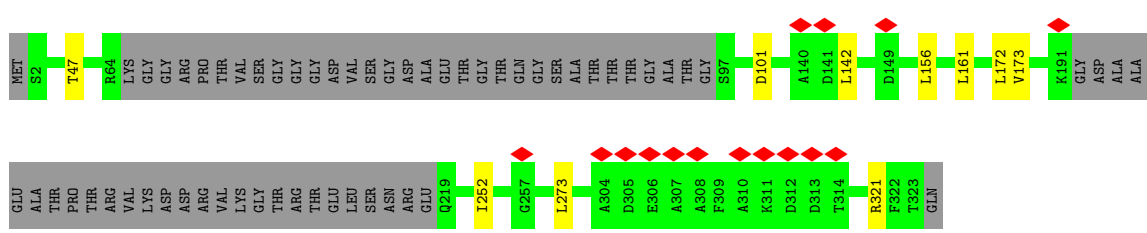
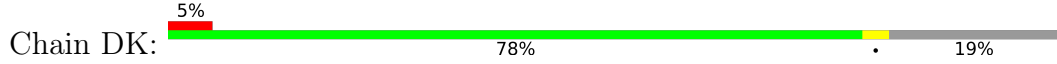




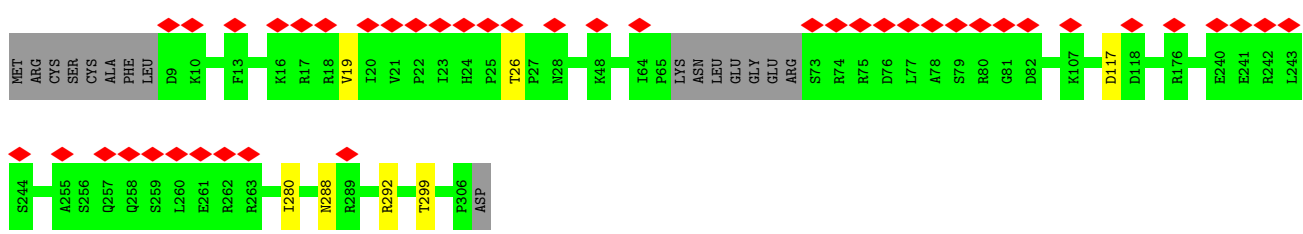
• Molecule 39: mS57



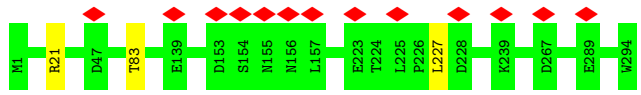
• Molecule 40: mS58



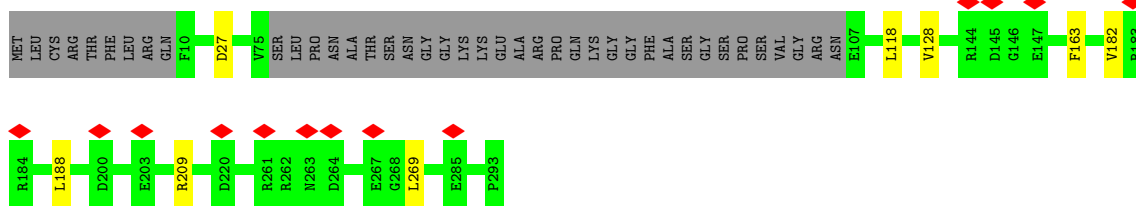
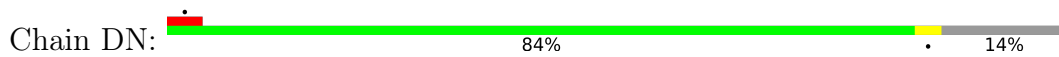
• Molecule 41: mS59



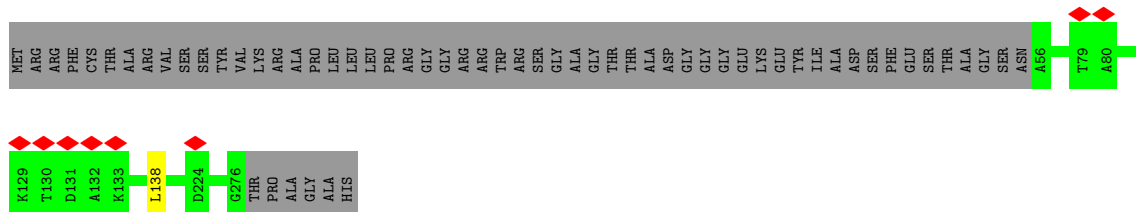
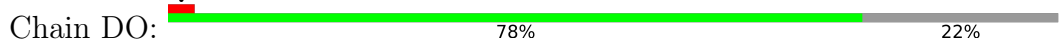
• Molecule 42: mS60



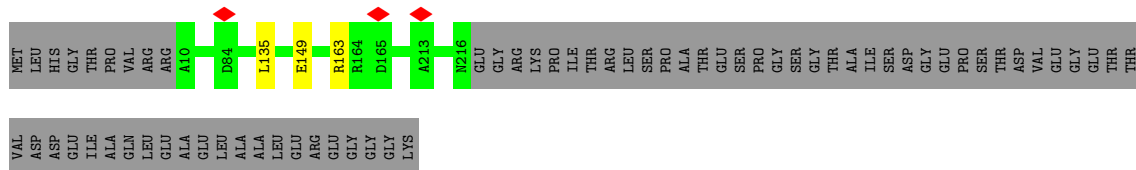
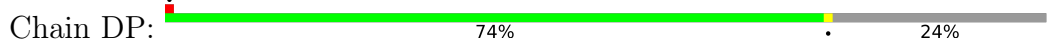
• Molecule 43: mS61



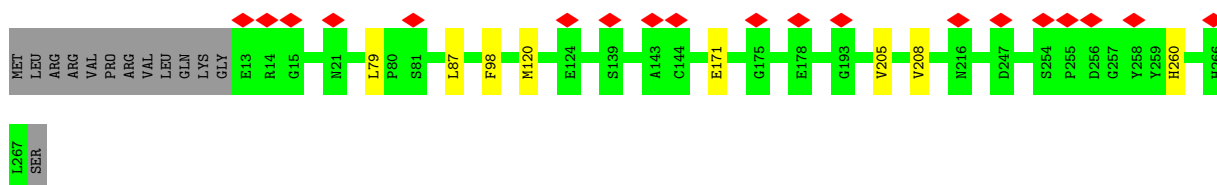
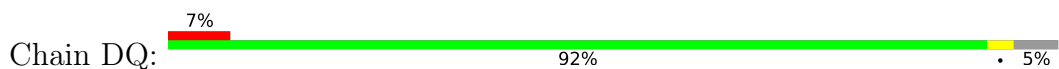
- Molecule 44: mS62



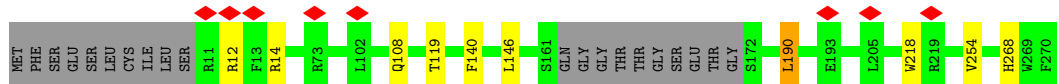
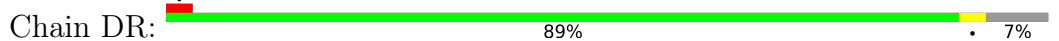
- Molecule 45: mS63



- Molecule 46: AKAP7\_NLS domain-containing protein

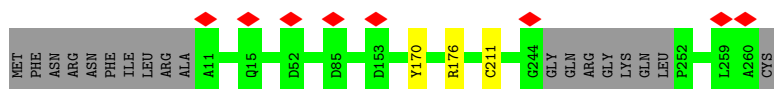


- Molecule 47: mS65



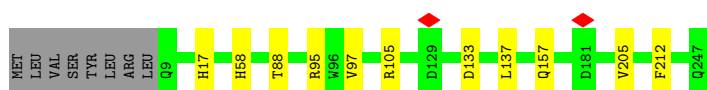
- Molecule 48: mS66

Chain DS:  92% 7%



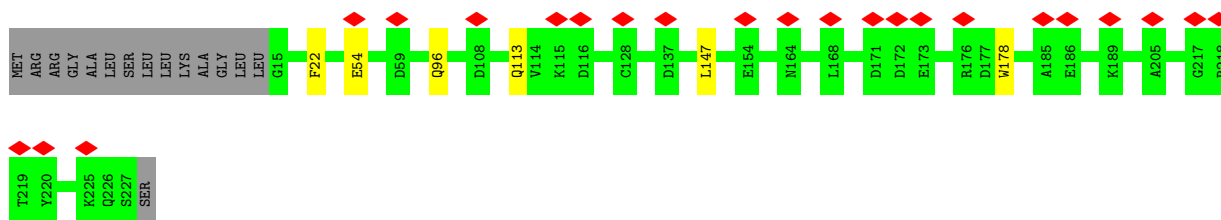
- Molecule 49: Rhodanese domain-containing protein

Chain DT:  92% 7%




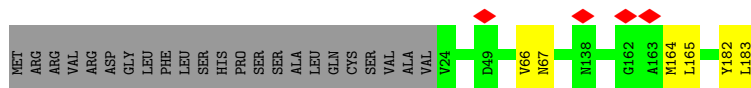
- Molecule 50: Ubiquitin-like domain-containing protein

Chain DU:  10% 91% 7%



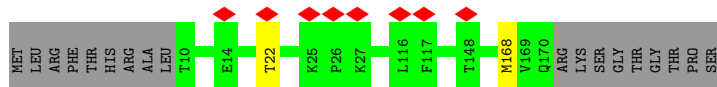
- Molecule 51: mS69

Chain DV:  84% 13%




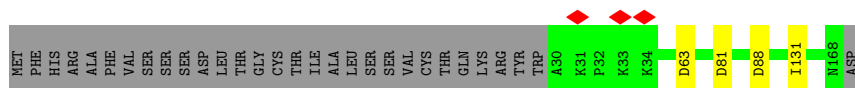
- Molecule 52: mS70

Chain DW:  89% 10%



- Molecule 53: mS71

Chain DX:  80% 18%

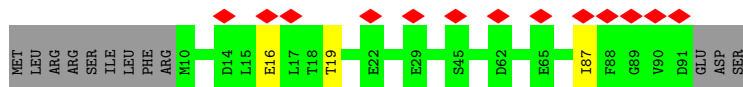
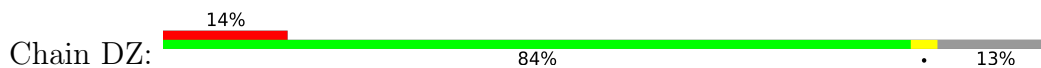


- Molecule 54: mS72

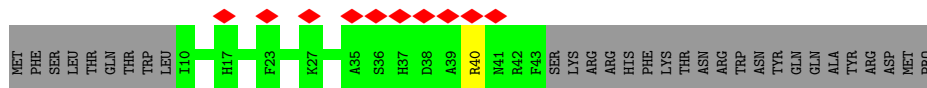
Chain DY:  93% 6%



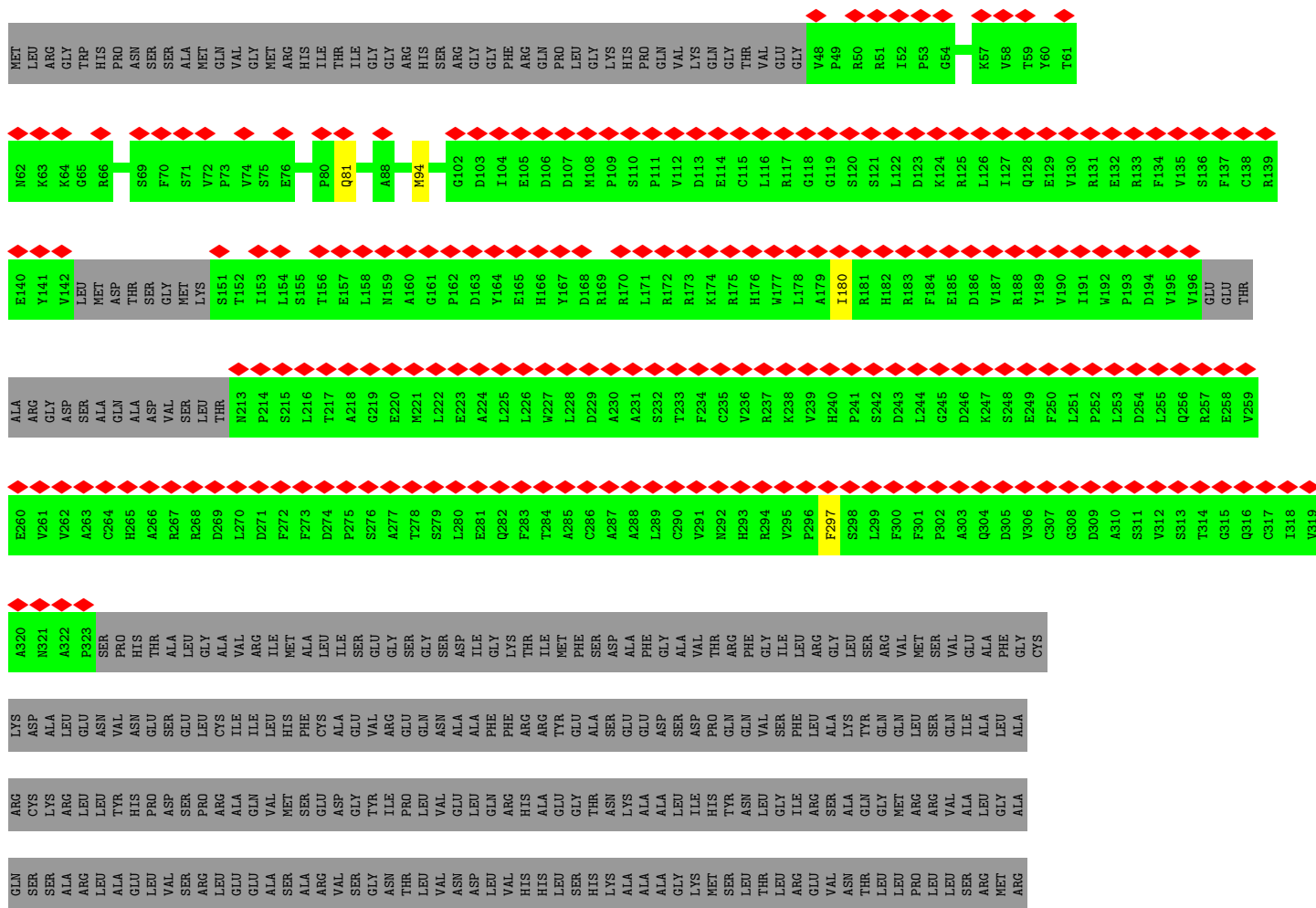
• Molecule 55: mS73



• Molecule 56: mS74

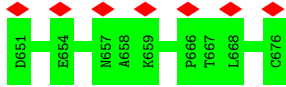


• Molecule 57: mt-SAF3

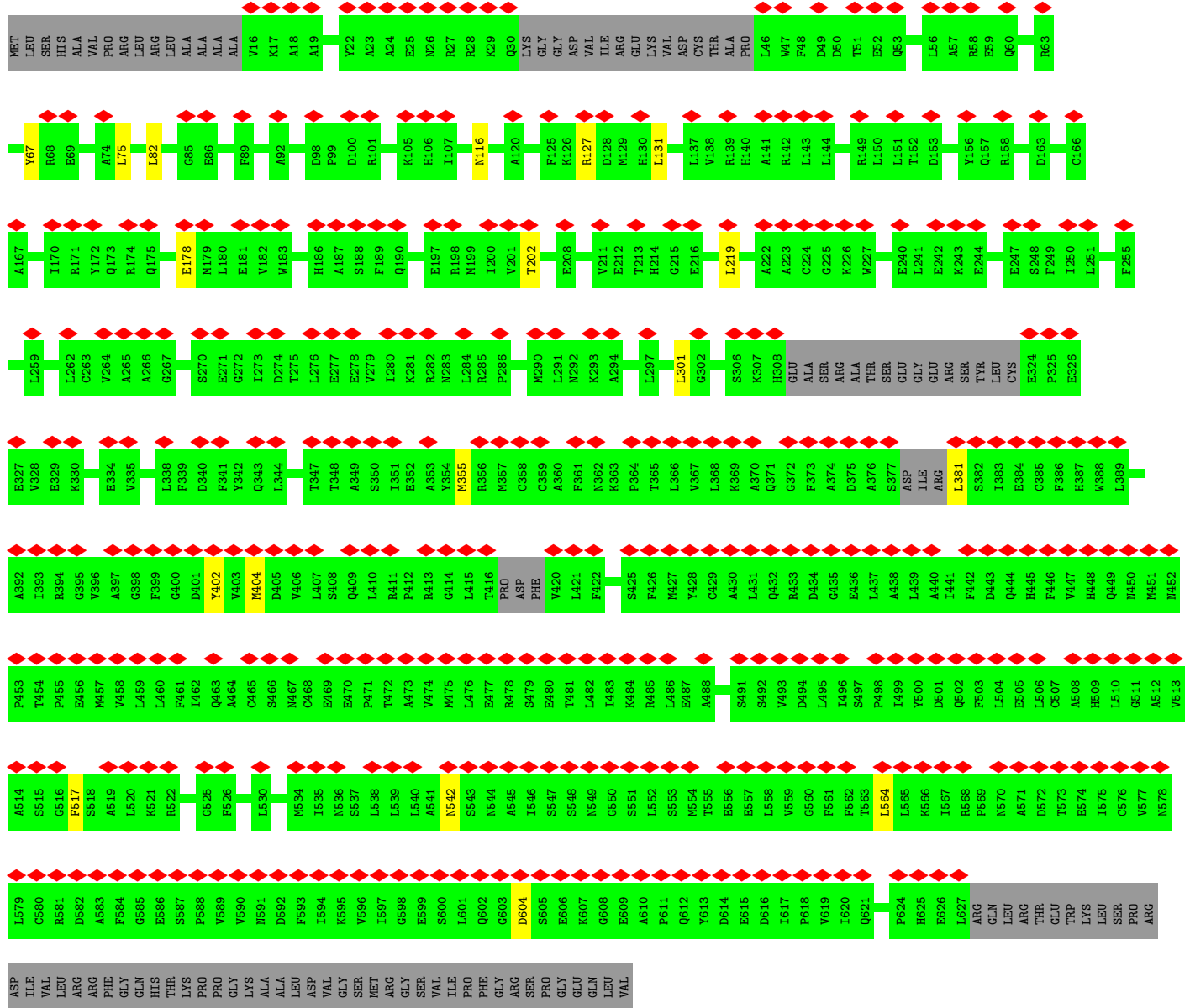
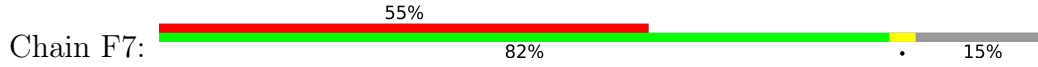




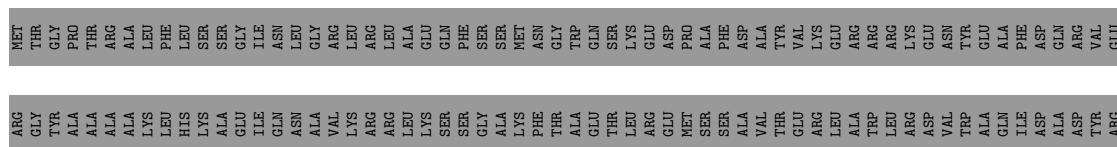


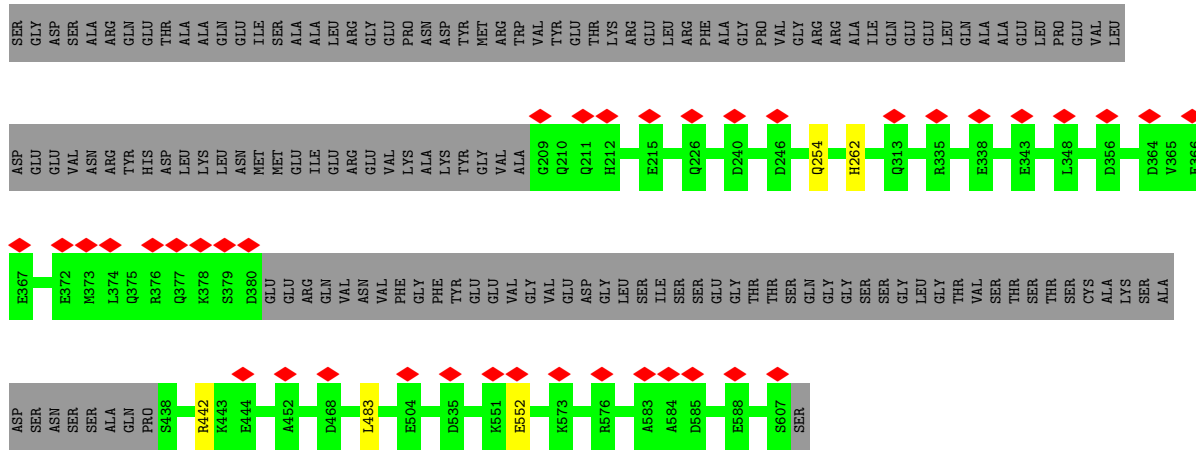


• Molecule 59: mt-SAF7

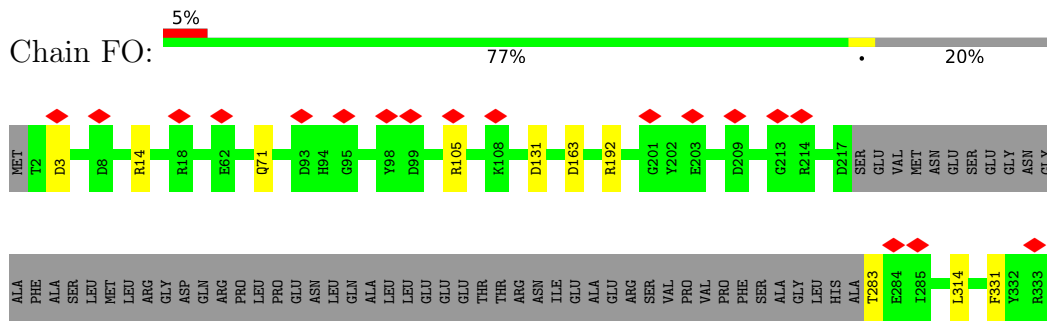


• Molecule 60: mt-SAF9

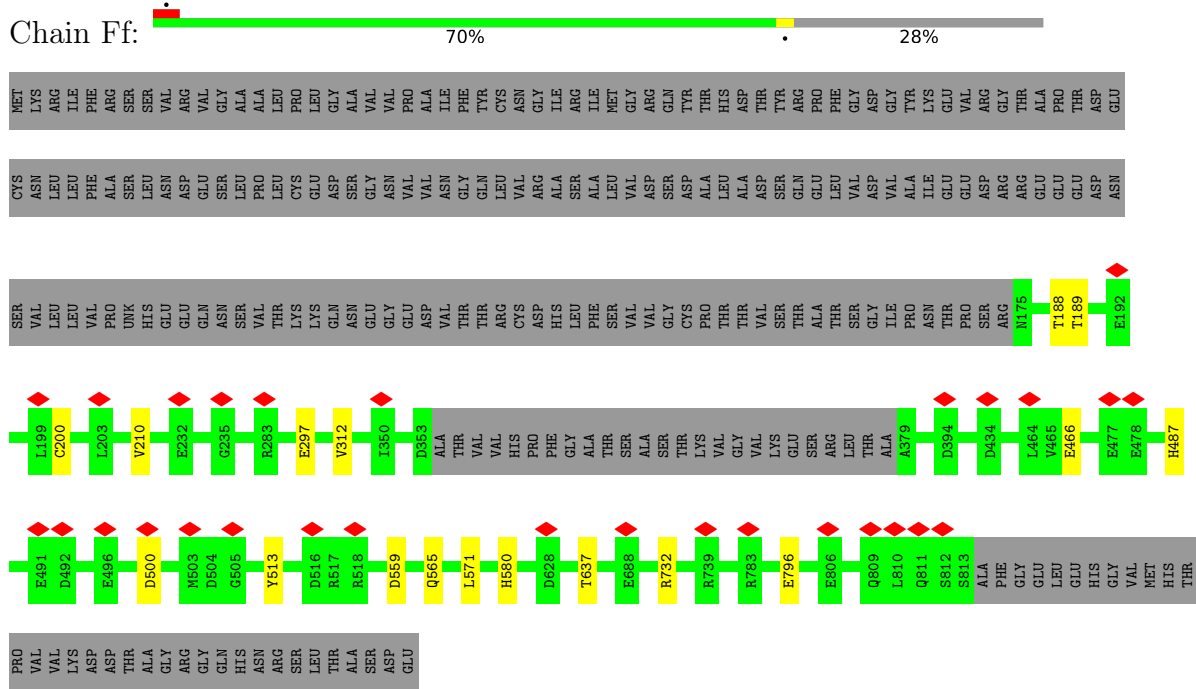




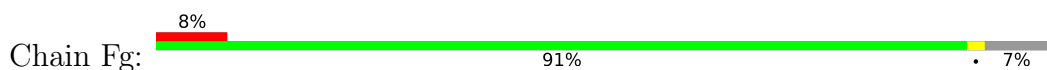
• Molecule 61: mt-SAF22



• Molecule 62: DNA photolyase, putative

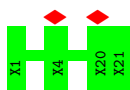


• Molecule 63: Acyl transferase-like protein

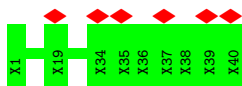




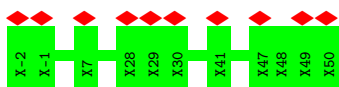




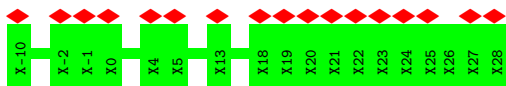
- Molecule 69: Unk7



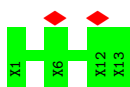
- Molecule 70: UnkE



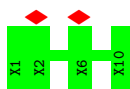
- Molecule 71: UnkF



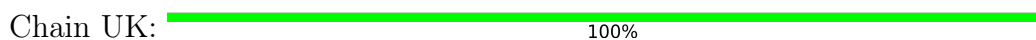
- Molecule 72: UnkG



- Molecule 73: UnkI

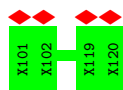


- Molecule 74: UnkK



There are no outlier residues recorded for this chain.

- Molecule 75: UnkL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17391	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	0.222	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	500.4, 500.4, 500.4	wwPDB
Map dimensions	360, 360, 360	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: ATP, PO4, GDP, UTP, ZN, FAD, MG

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	CA	0.17	0/13759	0.70	1/21382 (0.0%)
2	CC	0.26	0/666	0.43	0/900
3	CE	0.25	0/3547	0.50	0/4798
4	CF	0.25	0/1266	0.51	0/1708
5	CH	0.25	0/2276	0.52	0/3071
6	CI	0.25	0/3479	0.49	0/4693
7	CJ	0.25	0/6725	0.48	0/9152
8	CK	0.25	0/2502	0.51	0/3357
9	CL	0.28	0/759	0.50	0/1026
10	CN	0.25	0/1361	0.47	0/1840
11	CO	0.26	0/2614	0.49	0/3520
12	CP	0.24	0/1533	0.49	0/2074
13	CQ	0.25	0/1919	0.50	0/2595
14	CR	0.25	0/2276	0.48	0/3087
15	CS	0.26	0/1183	0.48	0/1593
16	CU	0.24	0/1560	0.51	0/2094
17	Ca	0.25	0/5066	0.47	0/6852
18	Cb	0.25	0/2105	0.48	0/2842
19	Cd	0.25	0/2016	0.44	0/2715
20	Cg	0.25	0/4016	0.46	0/5455
21	Ci	0.25	0/1383	0.49	0/1871
22	Cj	0.25	0/1849	0.48	0/2521
23	Ck	0.24	0/5540	0.49	0/7490
24	Cm	0.25	0/1215	0.49	0/1630
25	Cn	0.25	0/543	0.52	0/725
26	Cp	0.25	0/1511	0.48	0/2049
27	Cq	0.25	0/2066	0.44	0/2815
28	Cr	0.24	0/2131	0.48	0/2895
29	Cv	0.24	0/8625	0.48	0/11690
30	DA	0.24	0/12744	0.48	0/17248
31	DB	0.24	0/9369	0.50	0/12692
32	DC	0.25	0/8913	0.49	0/12092

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	DD	0.25	0/6699	0.49	0/9072
34	DE	0.25	0/4920	0.49	0/6666
35	DF	0.25	0/4847	0.51	0/6569
36	DG	0.24	0/4578	0.50	0/6202
37	DH	0.25	0/4645	0.50	0/6295
38	DI	0.25	0/3248	0.48	0/4401
39	DJ	0.25	0/2999	0.46	0/4071
40	DK	0.24	0/2123	0.47	0/2865
41	DL	0.25	0/2420	0.51	0/3262
42	DM	0.24	0/2488	0.49	0/3362
43	DN	0.24	0/2118	0.52	0/2874
44	DO	0.25	0/1832	0.50	0/2471
45	DP	0.24	0/1813	0.47	0/2457
46	DQ	0.24	0/2105	0.52	0/2855
47	DR	0.25	0/2084	0.51	1/2841 (0.0%)
48	DS	0.24	0/1997	0.50	0/2694
49	DT	0.25	0/2133	0.47	0/2889
50	DU	0.24	0/1799	0.50	0/2438
51	DV	0.25	0/1382	0.51	0/1871
52	DW	0.24	0/1407	0.49	0/1916
53	DX	0.25	0/1207	0.50	0/1620
54	DY	0.26	0/1337	0.51	0/1814
55	DZ	0.25	0/725	0.43	0/984
56	Da	0.26	0/317	0.54	0/422
57	F3	0.24	0/2049	0.48	0/2782
58	F6	0.24	0/3434	0.47	0/4661
59	F7	0.24	0/4684	0.47	0/6341
60	F9	0.24	0/2863	0.50	0/3835
61	FO	0.24	0/2292	0.52	0/3096
62	Ff	0.25	0/5082	0.48	0/6918
63	Fg	0.24	0/4074	0.48	0/5522
64	Fh	0.24	0/2278	0.50	0/3073
65	Fi	0.24	0/3833	0.50	0/5202
66	IA	0.25	0/5512	0.49	0/7462
67	IB	0.25	0/4193	0.51	0/5672
All	All	0.24	0/218034	0.51	2/297947 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	DR	190	LEU	CA-CB-CG	5.49	127.92	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	CA	329	U	OP2-P-O3'	5.33	116.94	105.20

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	
2	CC	72/74 (97%)	66 (92%)	6 (8%)	0	100	100
3	CE	424/435 (98%)	406 (96%)	18 (4%)	0	100	100
4	CF	145/160 (91%)	139 (96%)	6 (4%)	0	100	100
5	CH	271/282 (96%)	263 (97%)	8 (3%)	0	100	100
6	CI	423/443 (96%)	411 (97%)	12 (3%)	0	100	100
7	CJ	799/817 (98%)	771 (96%)	28 (4%)	0	100	100
8	CK	294/326 (90%)	284 (97%)	10 (3%)	0	100	100
9	CL	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
10	CN	155/166 (93%)	149 (96%)	6 (4%)	0	100	100
11	CO	306/429 (71%)	292 (95%)	14 (5%)	0	100	100
12	CP	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
13	CQ	224/307 (73%)	219 (98%)	5 (2%)	0	100	100
14	CR	265/320 (83%)	258 (97%)	7 (3%)	0	100	100
15	CS	137/244 (56%)	132 (96%)	5 (4%)	0	100	100
16	CU	179/193 (93%)	175 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Ca	571/602 (95%)	549 (96%)	22 (4%)	0	100	100
18	Cb	248/325 (76%)	236 (95%)	12 (5%)	0	100	100
19	Cd	228/440 (52%)	223 (98%)	5 (2%)	0	100	100
20	Cg	478/498 (96%)	473 (99%)	5 (1%)	0	100	100
21	Ci	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
22	Cj	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
23	Ck	676/874 (77%)	666 (98%)	10 (2%)	0	100	100
24	Cm	143/215 (66%)	138 (96%)	5 (4%)	0	100	100
25	Cn	60/250 (24%)	59 (98%)	1 (2%)	0	100	100
26	Cp	171/187 (91%)	167 (98%)	4 (2%)	0	100	100
27	Cq	250/263 (95%)	241 (96%)	9 (4%)	0	100	100
28	Cr	263/439 (60%)	258 (98%)	5 (2%)	0	100	100
29	Cv	1032/1211 (85%)	994 (96%)	38 (4%)	0	100	100
30	DA	1546/1788 (86%)	1513 (98%)	33 (2%)	0	100	100
31	DB	1109/1181 (94%)	1076 (97%)	33 (3%)	0	100	100
32	DC	1081/1165 (93%)	1023 (95%)	58 (5%)	0	100	100
33	DD	786/812 (97%)	758 (96%)	28 (4%)	0	100	100
34	DE	576/747 (77%)	549 (95%)	27 (5%)	0	100	100
35	DF	585/666 (88%)	559 (96%)	26 (4%)	0	100	100
36	DG	542/631 (86%)	529 (98%)	13 (2%)	0	100	100
37	DH	555/581 (96%)	530 (96%)	25 (4%)	0	100	100
38	DI	388/407 (95%)	372 (96%)	16 (4%)	0	100	100
39	DJ	355/396 (90%)	351 (99%)	4 (1%)	0	100	100
40	DK	257/324 (79%)	249 (97%)	8 (3%)	0	100	100
41	DL	287/307 (94%)	283 (99%)	4 (1%)	0	100	100
42	DM	292/294 (99%)	277 (95%)	15 (5%)	0	100	100
43	DN	249/293 (85%)	243 (98%)	6 (2%)	0	100	100
44	DO	219/282 (78%)	207 (94%)	12 (6%)	0	100	100
45	DP	205/274 (75%)	198 (97%)	7 (3%)	0	100	100
46	DQ	253/268 (94%)	249 (98%)	4 (2%)	0	100	100
47	DR	246/270 (91%)	240 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DS	239/261 (92%)	238 (100%)	1 (0%)	0	100	100
49	DT	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
50	DU	211/228 (92%)	204 (97%)	7 (3%)	0	100	100
51	DV	158/183 (86%)	144 (91%)	14 (9%)	0	100	100
52	DW	159/179 (89%)	152 (96%)	7 (4%)	0	100	100
53	DX	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
54	DY	152/163 (93%)	145 (95%)	7 (5%)	0	100	100
55	DZ	80/94 (85%)	78 (98%)	2 (2%)	0	100	100
56	Da	32/64 (50%)	31 (97%)	1 (3%)	0	100	100
57	F3	246/966 (26%)	243 (99%)	3 (1%)	0	100	100
58	F6	410/676 (61%)	402 (98%)	8 (2%)	0	100	100
59	F7	566/679 (83%)	544 (96%)	22 (4%)	0	100	100
60	F9	338/608 (56%)	329 (97%)	9 (3%)	0	100	100
61	FO	263/334 (79%)	255 (97%)	8 (3%)	0	100	100
62	Ff	610/848 (72%)	593 (97%)	17 (3%)	0	100	100
63	Fg	507/550 (92%)	487 (96%)	20 (4%)	0	100	100
64	Fh	270/318 (85%)	259 (96%)	11 (4%)	0	100	100
65	Fi	459/629 (73%)	438 (95%)	21 (5%)	0	100	100
66	IA	687/787 (87%)	668 (97%)	19 (3%)	0	100	100
67	IB	507/803 (63%)	491 (97%)	16 (3%)	0	100	100
All	All	24263/29685 (82%)	23456 (97%)	807 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	CC	73/73 (100%)	69 (94%)	4 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CE	365/372 (98%)	354 (97%)	11 (3%)	41	66
4	CF	135/144 (94%)	132 (98%)	3 (2%)	52	72
5	CH	237/246 (96%)	235 (99%)	2 (1%)	81	89
6	CI	360/371 (97%)	351 (98%)	9 (2%)	47	70
7	CJ	710/723 (98%)	692 (98%)	18 (2%)	47	70
8	CK	259/283 (92%)	256 (99%)	3 (1%)	71	84
9	CL	79/79 (100%)	77 (98%)	2 (2%)	47	70
10	CN	142/150 (95%)	138 (97%)	4 (3%)	43	67
11	CO	270/377 (72%)	263 (97%)	7 (3%)	46	69
12	CP	160/168 (95%)	158 (99%)	2 (1%)	69	83
13	CQ	201/270 (74%)	195 (97%)	6 (3%)	41	66
14	CR	233/279 (84%)	228 (98%)	5 (2%)	53	74
15	CS	123/220 (56%)	121 (98%)	2 (2%)	62	80
16	CU	159/169 (94%)	158 (99%)	1 (1%)	86	93
17	Ca	518/543 (95%)	507 (98%)	11 (2%)	53	74
18	Cb	219/277 (79%)	216 (99%)	3 (1%)	67	82
19	Cd	207/381 (54%)	205 (99%)	2 (1%)	76	86
20	Cg	424/437 (97%)	415 (98%)	9 (2%)	53	74
21	Ci	144/160 (90%)	139 (96%)	5 (4%)	36	63
22	Cj	194/219 (89%)	192 (99%)	2 (1%)	76	86
23	Ck	589/746 (79%)	579 (98%)	10 (2%)	60	79
24	Cm	124/184 (67%)	120 (97%)	4 (3%)	39	65
25	Cn	54/210 (26%)	51 (94%)	3 (6%)	21	53
26	Cp	161/175 (92%)	157 (98%)	4 (2%)	47	70
27	Cq	210/221 (95%)	205 (98%)	5 (2%)	49	71
28	Cr	223/369 (60%)	218 (98%)	5 (2%)	52	72
29	Cv	894/1033 (86%)	870 (97%)	24 (3%)	44	68
30	DA	1319/1514 (87%)	1277 (97%)	42 (3%)	39	65
31	DB	976/1030 (95%)	957 (98%)	19 (2%)	57	76
32	DC	923/985 (94%)	896 (97%)	27 (3%)	42	66
33	DD	693/711 (98%)	676 (98%)	17 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DE	514/642 (80%)	499 (97%)	15 (3%)	42	66
35	DF	499/560 (89%)	485 (97%)	14 (3%)	43	67
36	DG	481/543 (89%)	464 (96%)	17 (4%)	36	63
37	DH	489/504 (97%)	472 (96%)	17 (4%)	36	63
38	DI	350/365 (96%)	342 (98%)	8 (2%)	50	71
39	DJ	313/347 (90%)	304 (97%)	9 (3%)	42	66
40	DK	218/261 (84%)	208 (95%)	10 (5%)	27	57
41	DL	249/263 (95%)	242 (97%)	7 (3%)	43	67
42	DM	252/252 (100%)	249 (99%)	3 (1%)	71	84
43	DN	225/256 (88%)	217 (96%)	8 (4%)	35	63
44	DO	185/229 (81%)	184 (100%)	1 (0%)	88	94
45	DP	187/239 (78%)	184 (98%)	3 (2%)	62	80
46	DQ	227/239 (95%)	219 (96%)	8 (4%)	36	63
47	DR	219/235 (93%)	209 (95%)	10 (5%)	27	57
48	DS	213/228 (93%)	210 (99%)	3 (1%)	67	82
49	DT	220/228 (96%)	209 (95%)	11 (5%)	24	55
50	DU	190/201 (94%)	184 (97%)	6 (3%)	39	65
51	DV	145/165 (88%)	139 (96%)	6 (4%)	30	59
52	DW	148/163 (91%)	146 (99%)	2 (1%)	67	82
53	DX	122/149 (82%)	118 (97%)	4 (3%)	38	64
54	DY	137/146 (94%)	134 (98%)	3 (2%)	52	72
55	DZ	72/84 (86%)	69 (96%)	3 (4%)	30	59
56	Da	30/59 (51%)	29 (97%)	1 (3%)	38	64
57	F3	223/809 (28%)	219 (98%)	4 (2%)	59	77
58	F6	368/590 (62%)	350 (95%)	18 (5%)	25	56
59	F7	493/577 (85%)	475 (96%)	18 (4%)	34	61
60	F9	288/504 (57%)	283 (98%)	5 (2%)	60	79
61	FO	234/290 (81%)	224 (96%)	10 (4%)	29	58
62	Ff	519/715 (73%)	502 (97%)	17 (3%)	38	64
63	Fg	441/469 (94%)	431 (98%)	10 (2%)	50	71
64	Fh	242/281 (86%)	235 (97%)	7 (3%)	42	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	Fi	404/536 (75%)	394 (98%)	10 (2%)	47	70
66	IA	586/661 (89%)	571 (97%)	15 (3%)	46	69
67	IB	435/675 (64%)	421 (97%)	14 (3%)	39	65
All	All	21296/25584 (83%)	20728 (97%)	568 (3%)	48	68

5 of 568 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	F7	75	LEU
59	F7	517	PHE
59	F7	67	TYR
63	Fg	486	VAL
30	DA	979	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 321 such sidechains are listed below:

Mol	Chain	Res	Type
44	DO	88	GLN
62	Ff	317	GLN
46	DQ	73	HIS
54	DY	106	GLN
65	Fi	401	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	620/621 (99%)	252 (40%)	2 (0%)

5 of 252 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	CA	2	A
1	CA	3	A
1	CA	4	A
1	CA	6	U
1	CA	11	U

All (2) RNA pucker outliers are listed below:



Mol	Chain	Res	Type
1	CA	299	U
1	CA	512	G

#### 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 15 ligands modelled in this entry, 10 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
80	FAD	Ff	901	-	51,58,58	1.21	6 (11%)	60,89,89	2.23	8 (13%)
77	ATP	Cg	1000	76	26,33,33	0.61	0	31,52,52	0.75	1 (3%)
79	UTP	DJ	401	-	26,30,30	1.88	4 (15%)	34,47,47	1.10	1 (2%)
82	PO4	IA	1001	76	4,4,4	0.91	0	6,6,6	0.44	0
81	GDP	IA	1000	76	24,30,30	1.17	2 (8%)	31,47,47	1.99	8 (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
77	ATP	Cg	1000	76	-	2/18/38/38	0/3/3/3
80	FAD	Ff	901	-	-	11/30/50/50	0/6/6/6
79	UTP	DJ	401	-	-	4/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	GDP	IA	1000	76	-	3/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	DJ	401	UTP	C6-C5	-6.73	1.34	1.52
80	Ff	901	FAD	C4X-C10	5.48	1.44	1.38
79	DJ	401	UTP	C6-N1	-5.16	1.37	1.47
81	IA	1000	GDP	C5-C6	4.16	1.48	1.41
80	Ff	901	FAD	C4-N3	2.95	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Ff	901	FAD	C2-N3-C4	12.97	126.09	115.14
80	Ff	901	FAD	C4X-C4-N3	-6.98	113.88	123.43
81	IA	1000	GDP	C2-N3-C4	4.84	120.88	115.36
80	Ff	901	FAD	C10-C4X-N5	4.75	124.55	121.26
81	IA	1000	GDP	C2-N1-C6	4.04	122.34	115.93

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

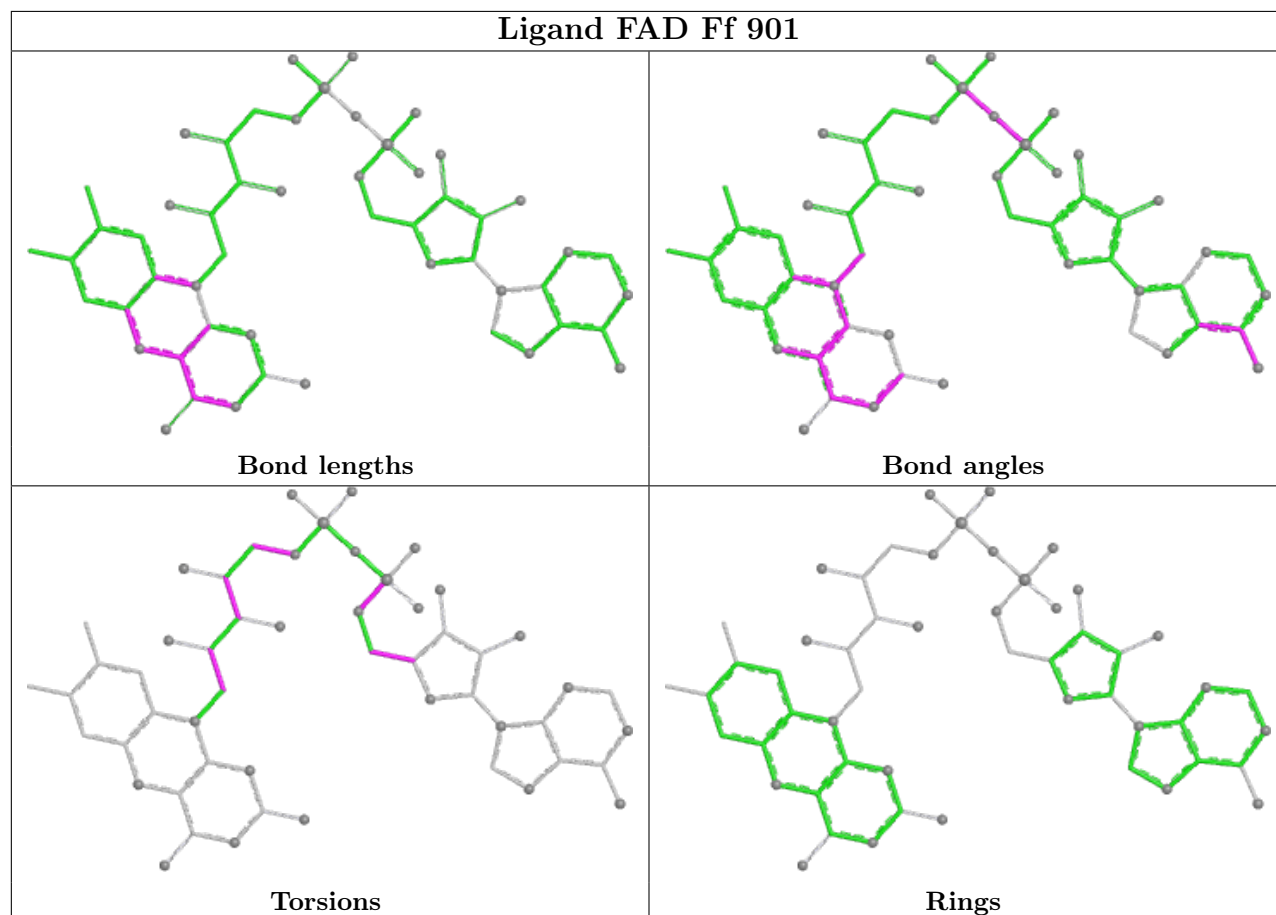
Mol	Chain	Res	Type	Atoms
79	DJ	401	UTP	O4'-C1'-N1-C6
80	Ff	901	FAD	C5B-O5B-PA-O3P
80	Ff	901	FAD	N10-C1'-C2'-O2'
80	Ff	901	FAD	C2'-C3'-C4'-O4'
80	Ff	901	FAD	C2'-C3'-C4'-C5'

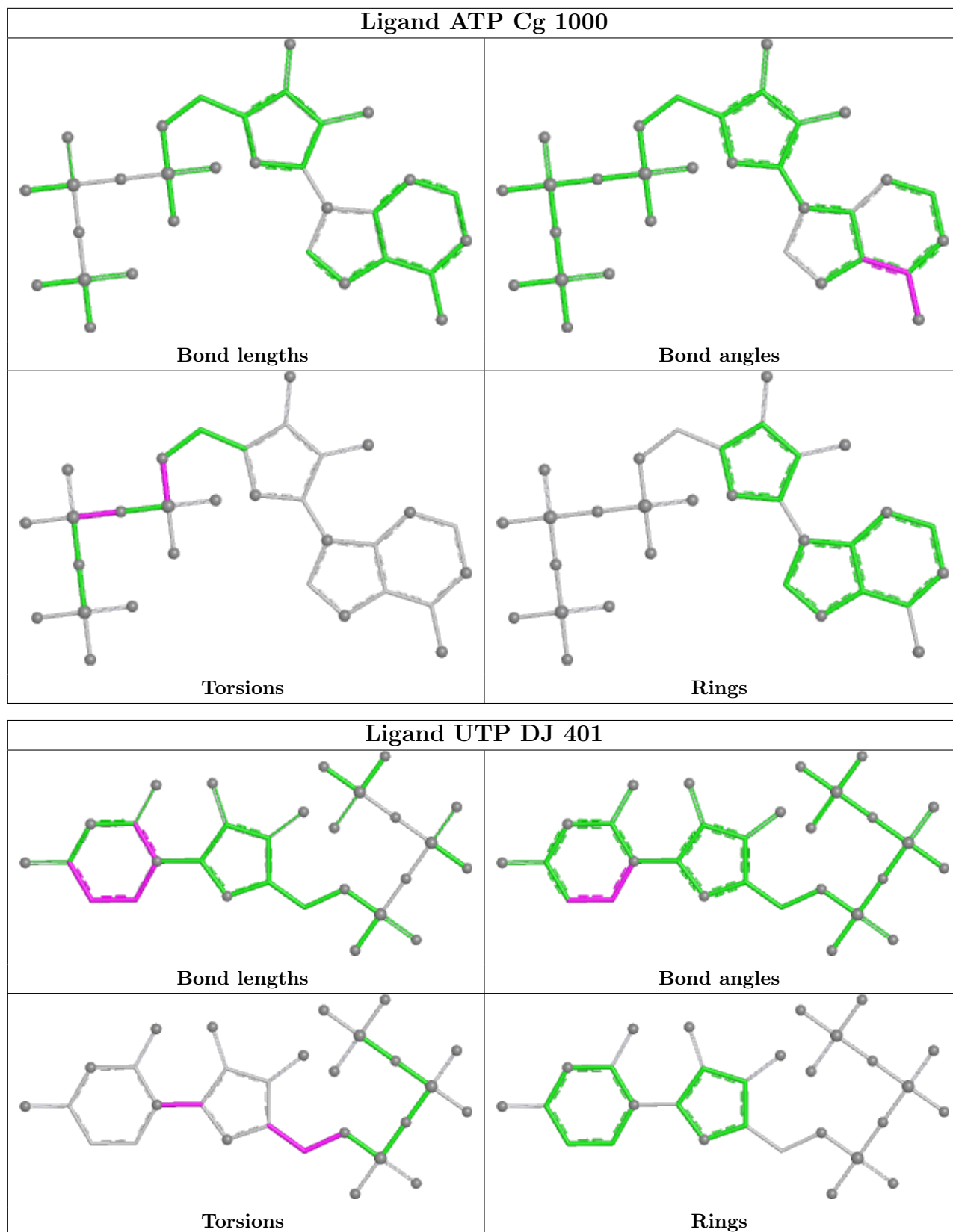
There are no ring outliers.

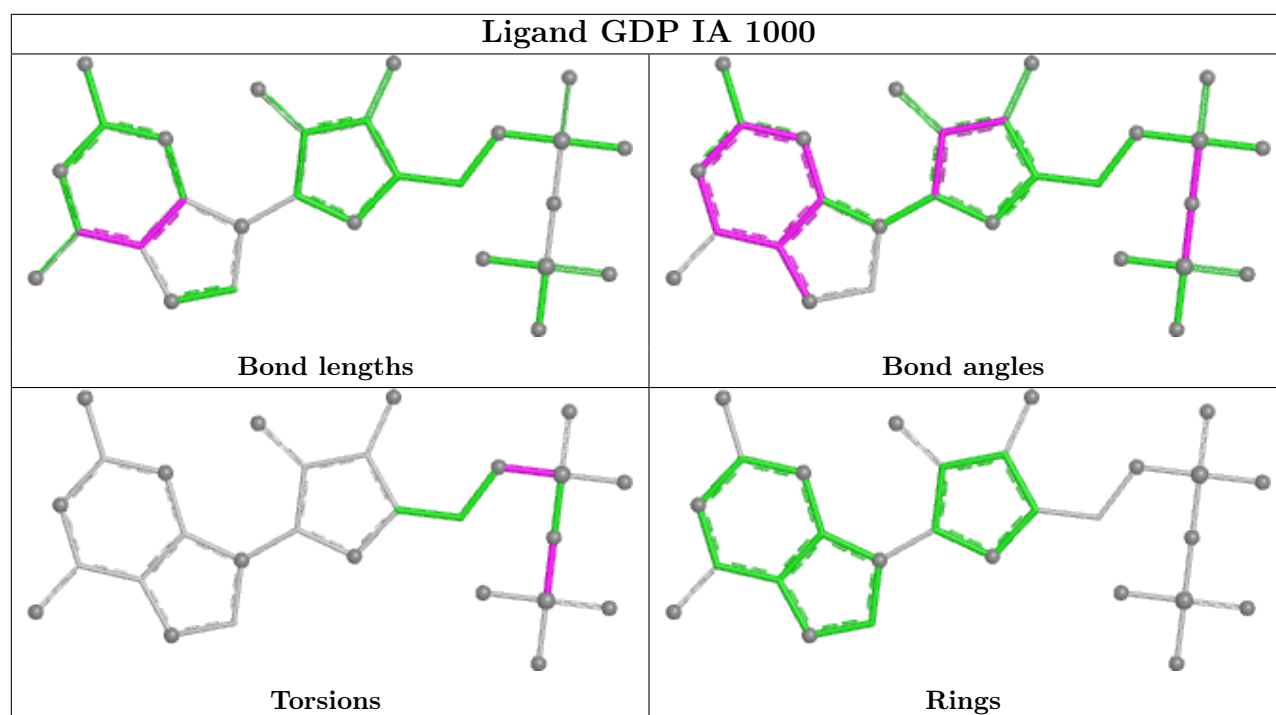
No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

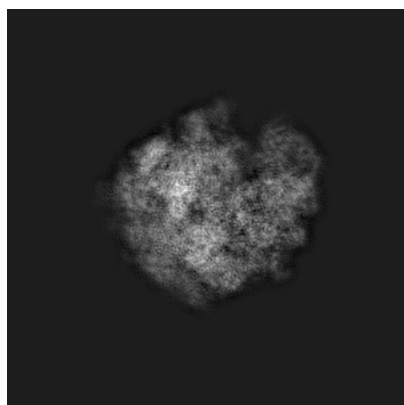
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13661. These allow visual inspection of the internal detail of the map and identification of artifacts.

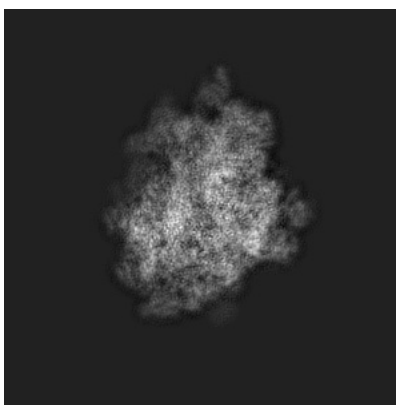
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

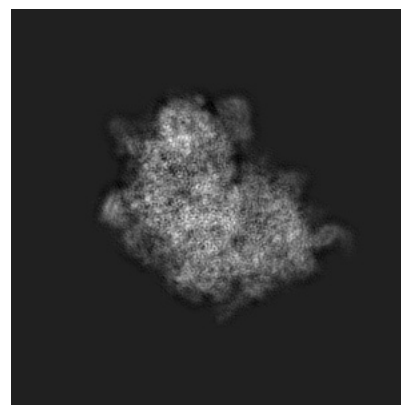
#### 6.1.1 Primary map



X



Y

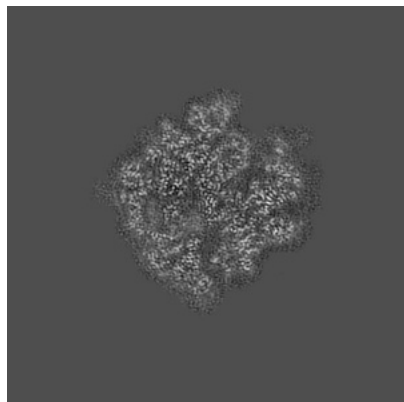


Z

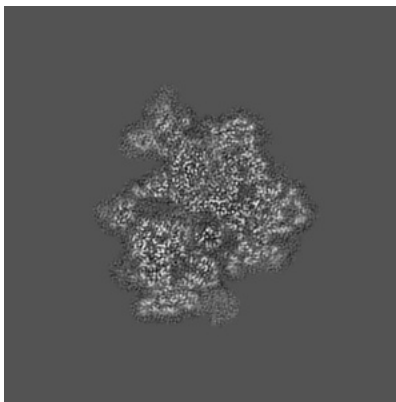
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

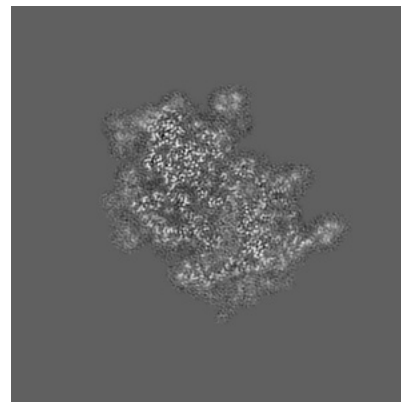
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

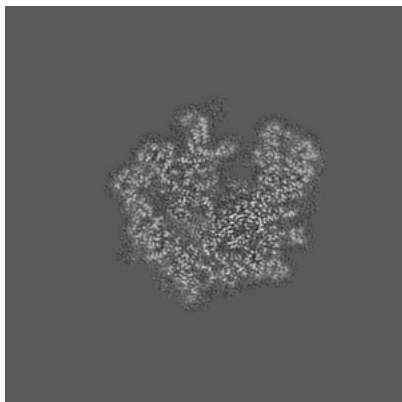


Z Index: 180

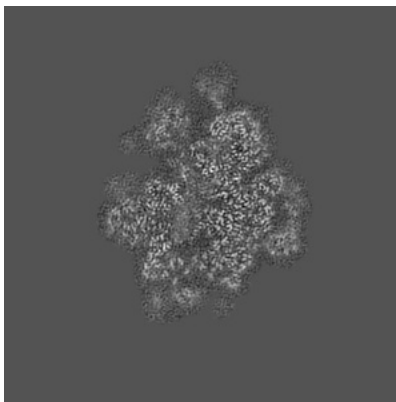
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

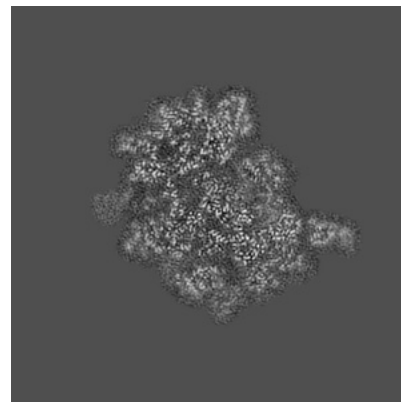
### 6.3.1 Primary map



X Index: 158



Y Index: 165

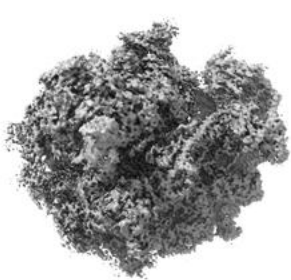


Z Index: 192

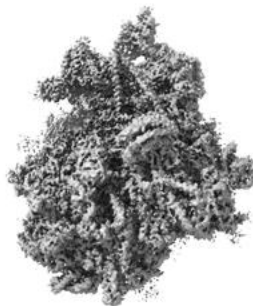
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

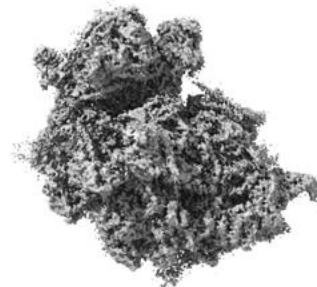
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

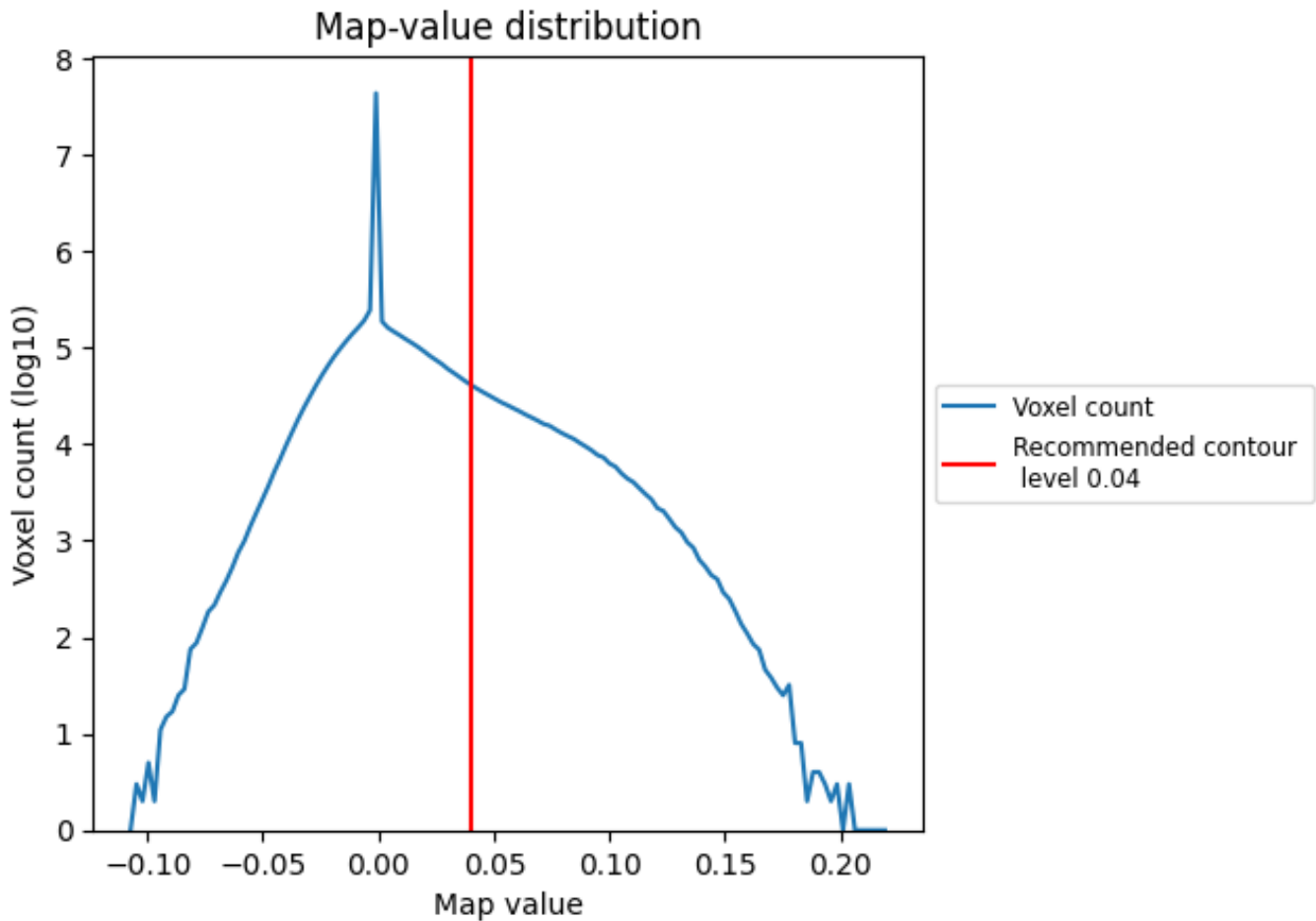
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

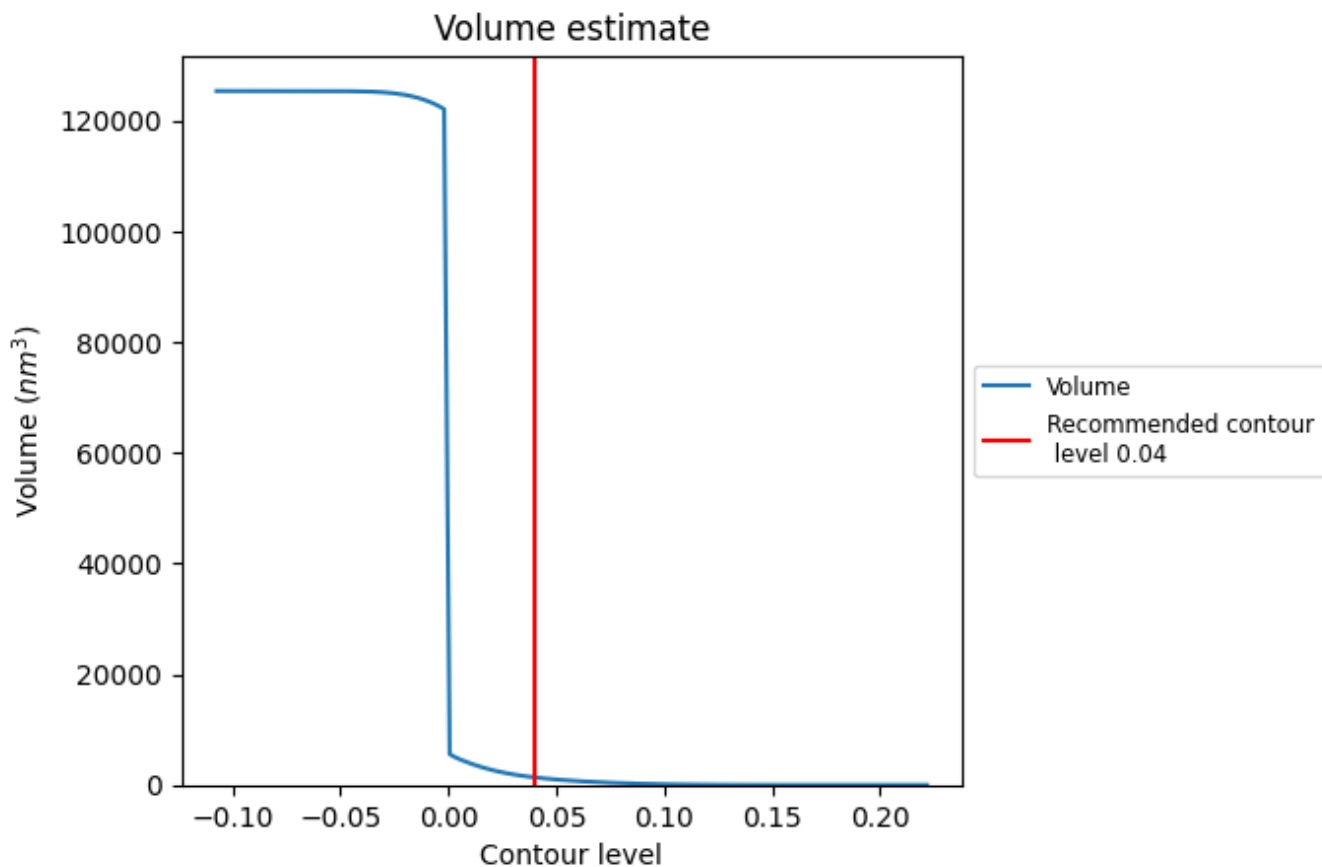
This section contains the results of statistical analysis of the map.

### 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.

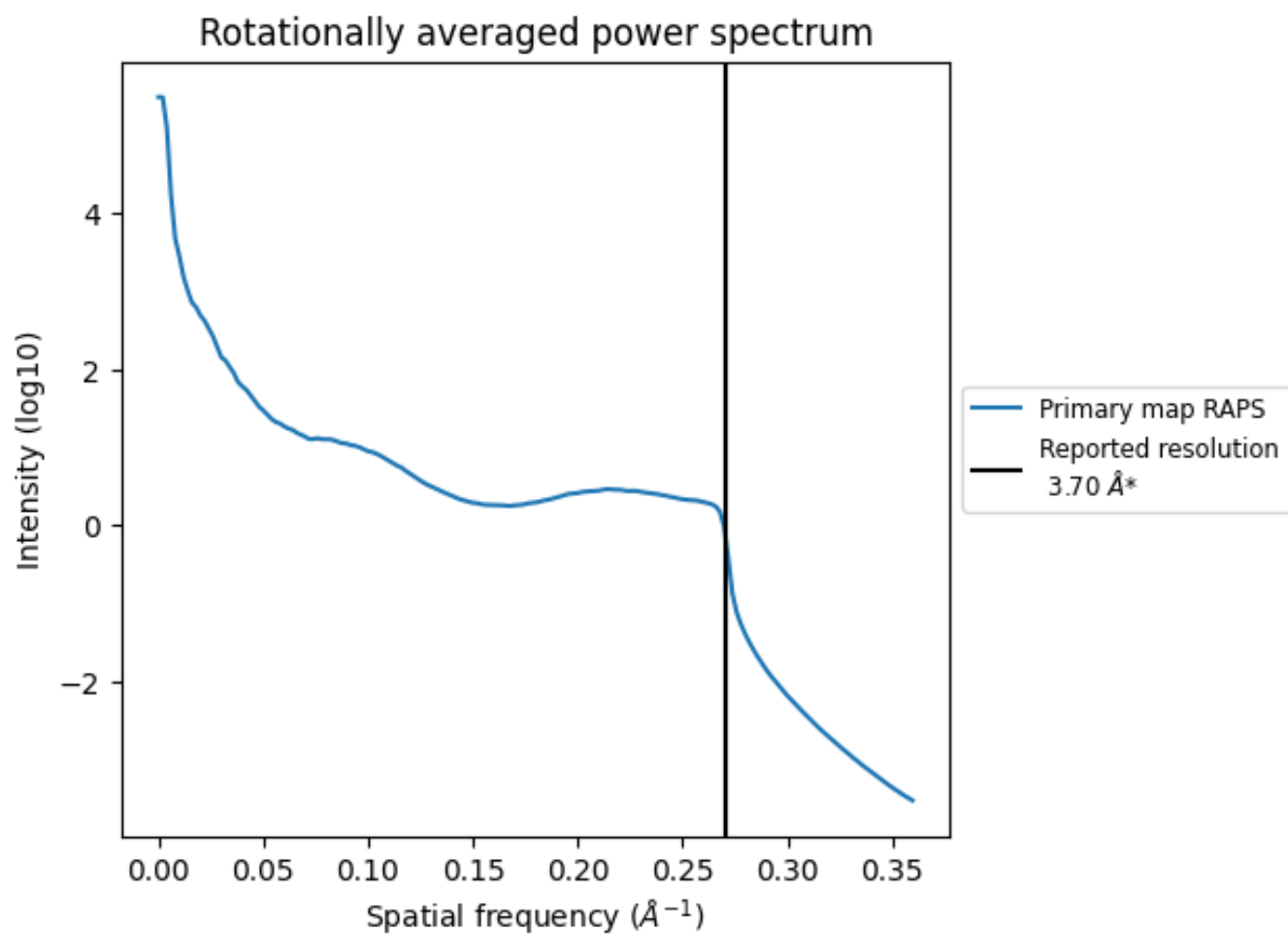
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1367 nm<sup>3</sup>; this corresponds to an approximate mass of 1235 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 0.270 Å<sup>-1</sup>

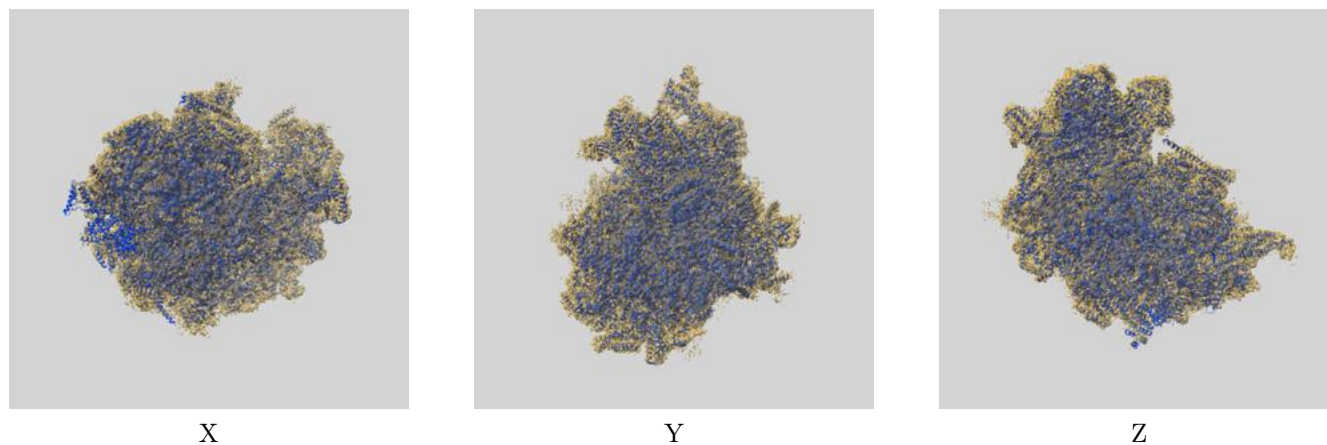
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

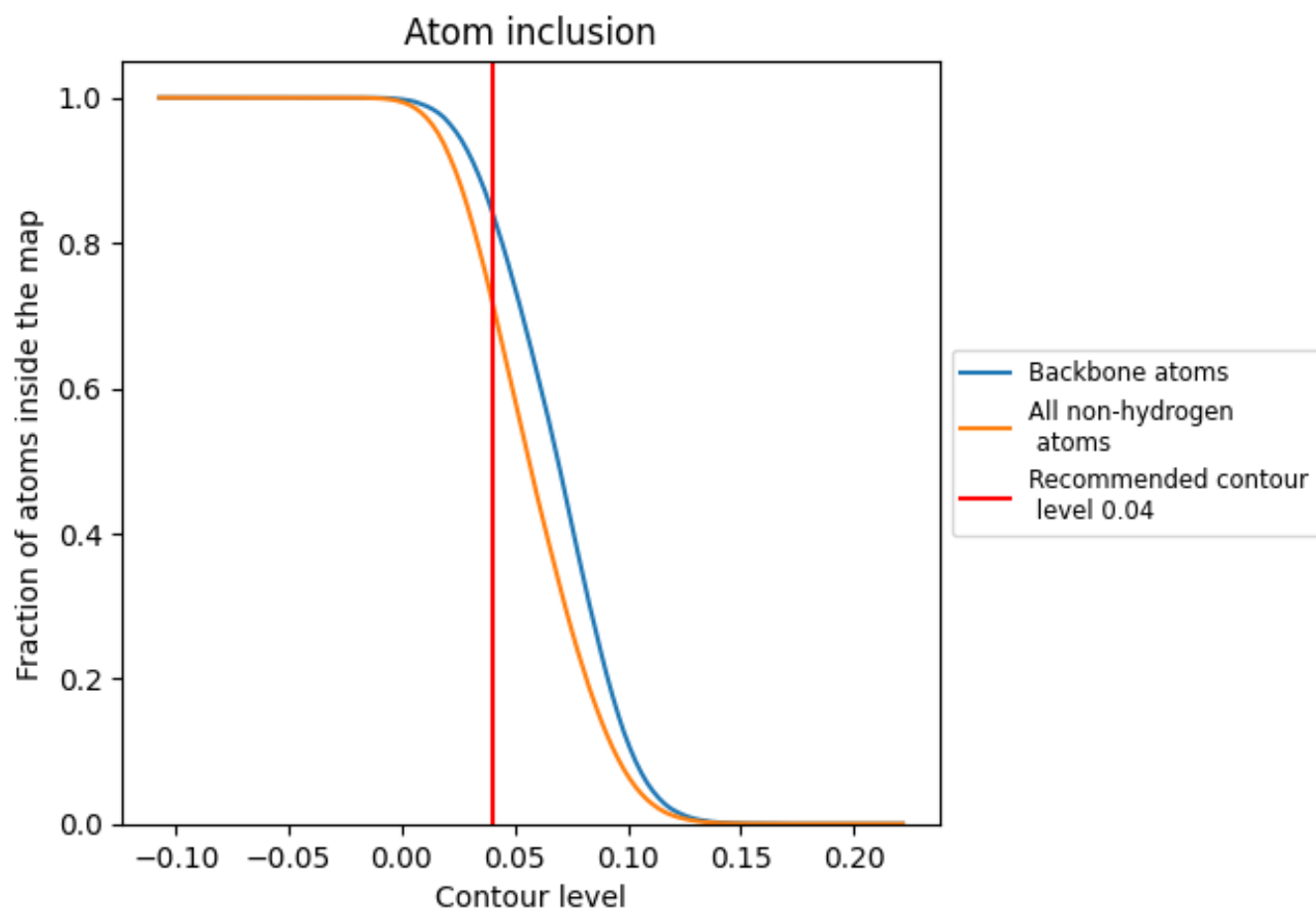
This section contains information regarding the fit between EMDB map EMD-13661 and PDB model 7PUB. Per-residue inclusion information can be found in section 3 on page 27.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.