



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:33 am GMT

PDB ID : 6SGA
EMDB ID : EMD-10177
Title : Body domain of the mt-SSU assemblosome from *Trypanosoma brucei*
Authors : Saurer, M.; Ramrath, D.J.F.; Niemann, M.; Calderaro, S.; Prange, C.; Mattei, S.; Scaiola, A.; Leitner, A.; Bieri, P.; Horn, E.K.; Leibundgut, M.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2019-08-03
Resolution : 3.10 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:

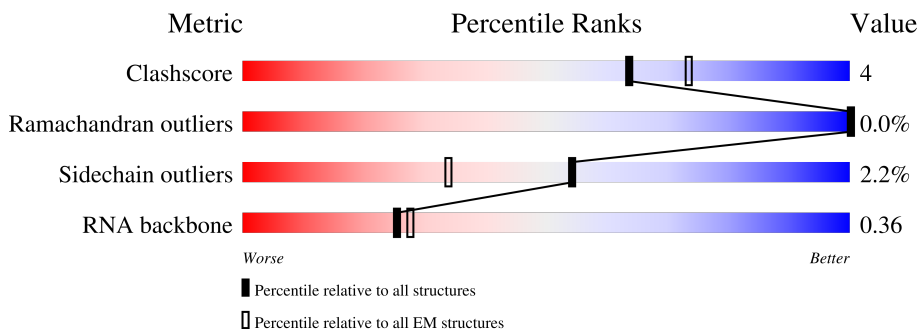
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



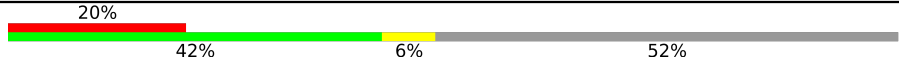
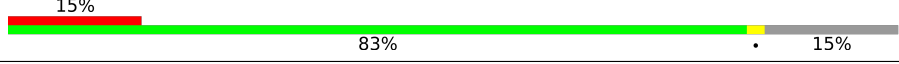



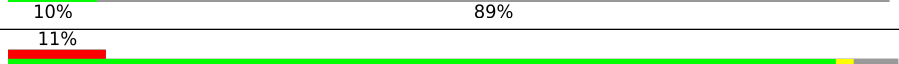
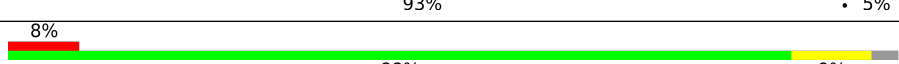
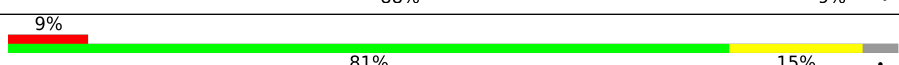
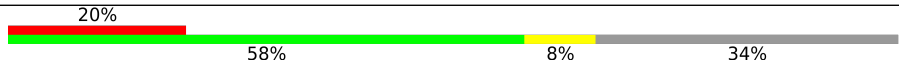


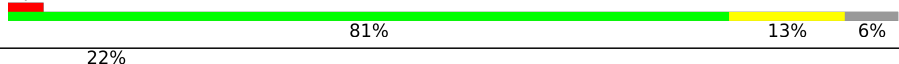
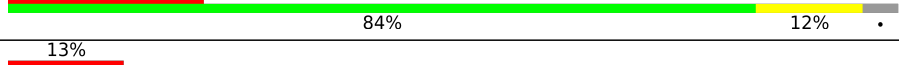

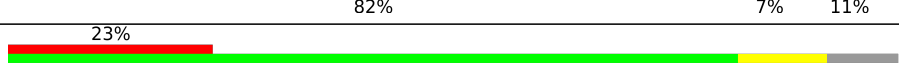







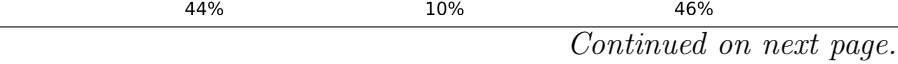


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	CE	435	 20% 81% 9% 10%
2	CF	160	 11% 86% 13% .
3	CH	282	 10% 68% 10% 21%
4	CK	326	 23% 48% . 48%
5	CO	429	 8% 73% 10% 17%
6	CP	188	 . 86% 10% .
7	CQ	336	 12% 54% 11% 35%

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Mol	Chain	Length	Quality of chain
8	CR	320	
9	Ca	602	
10	Cb	311	
11	Cd	440	
12	Cj	257	
13	Cn	250	
14	Cp	187	
15	DD	812	
16	DI	407	
17	DL	307	
18	DO	282	
19	DP	274	
20	DR	270	
21	DU	228	
22	DZ	94	
23	F2	1024	
24	F3	966	
25	F5	754	
26	F6	676	
27	F7	679	
28	F8	726	
29	F9	608	
30	FA	642	
31	FB	579	
31	FC	579	

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Mol	Chain	Length	Quality of chain
32	FE	553	14% 67% 11% 22%
33	FJ	362	56% 86% 11%
34	FM	370	11% 78% 9% 12%
34	FN	370	27% 78% 8% 14%
35	FO	334	7% 81% 15%
36	FP	349	14% 92% 7%
37	FQ	307	30% 72% 11% 16%
37	FR	307	37% 67% 12% 21%
37	FS	307	49% 76% 14% 10%
37	FT	307	31% 66% 9% 24%
37	FU	307	49% 79% 9% 12%
38	FW	263	8% 83% 11% 6%
39	FX	239	85% 8% 8%
40	FY	188	16% 27% 7% 65%
41	FZ	178	74% 68% 7% 25%
42	Fa	171	37% 94% 5%
43	Fb	151	33% 84% 15%
44	Fc	148	20% 55% 43%
45	Fd	143	6% 66% 33%
46	UA	21	95% 62% 38%
47	UB	27	100% 85% 15%
48	UC	10	10% 90% 10%
49	UD	9	44% 56%
49	UM	9	33% 78% 22%
49	UQ	9	22% 89% 11%

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Mol	Chain	Length	Quality of chain
50	UE	45	98% 84% 16%
50	UP	45	80% 100%
51	UF	11	36% 82% 18%
52	UG	17	41% 88% 12%
53	UH	5	100% 80% 20%
54	UI	8	25% 62% 38%
54	UN	8	50% 38% 62%
55	UJ	16	100% 81% 19%
56	UL	22	45% 95% 5%
57	UO	30	80% 80% 20%
58	UU	24	71% 100%
59	UY	468	100% 69% 31%
60	CA	474	43% 47% 42% 9%
61	F1	1041	5% 95%
62	FF	474	97%

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 137038 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 uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CE	392	3147	1992	579	561	15	0	0

- Molecule 2 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CF	159	1317	835	234	242	6	0	0

- Molecule 3 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CH	222	1824	1144	349	321	10	0	0

- Molecule 4 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CK	171	1384	875	251	249	9	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CO	358	2979	1891	557	514	17	0	0

- Molecule 6 is a protein called bS16m.

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

- Molecule 7 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CQ	219	Total	C	N	O	S	0	0
			1805	1151	340	306	8		

- Molecule 8 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CR	153	Total	C	N	O	S	0	0
			1274	821	233	218	2		

- Molecule 9 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ca	512	Total	C	N	O	S	0	0
			4340	2778	770	771	21		

- Molecule 10 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Cb	153	Total	C	N	O	S	0	0
			1274	819	232	217	6		

- Molecule 11 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Cd	185	Total	C	N	O	S	0	0
			1616	1032	297	279	8		

- Molecule 12 is a protein called mS34.

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

- Molecule 13 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Cn	27	234	155	44	35	0	0

- Molecule 14 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Cp	178	1506	952	272	277	5	0	0

- Molecule 15 is a protein called mS51 (KRIPP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	DD	786	6488	4110	1168	1169	41	0	0

- Molecule 16 is a protein called mS56.

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

- Molecule 17 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	DL	203	1656	1059	296	291	10	0	0

- Molecule 18 is a protein called mS62 (KRIPP14).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DO	204	1648	1031	300	307	10	0	0

- Molecule 19 is a protein called mS63 (KRIPP16).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	DP	212	1800	1156	321	314	9	0	0

- Molecule 20 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	DR	254	2042	1313	373	346	10	0	0

- Molecule 21 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DU	219	1738	1095	308	331	4	0	0

- Molecule 22 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	DZ	30	254	167	41	45	1	0	0

- Molecule 23 is a protein called mt-SAF2 (KRIPP2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	F2	915	7274	4570	1281	1384	39	0	0

- Molecule 24 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	F3	888	6879	4302	1222	1303	52	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 25 is a protein called mt-SAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	F5	480	3474	2167	646	647	14	0	0

- Molecule 26 is a protein called mt-SAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	F6	456	3646	2311	635	686	14	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F6	285	ARG	HIS	conflict	UNP Q38FQ8
F6	291	ILE	THR	conflict	UNP Q38FQ8
F6	602	ALA	VAL	conflict	UNP Q38FQ8
F6	676	CYS	PHE	conflict	UNP Q38FQ8

- Molecule 27 is a protein called mt-SAF7 (KRIPP10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	F7	662	5225	3322	918	950	35	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 28 is a protein called mt-SAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	F8	513	3934	2493	721	701	19	0	0

- Molecule 29 is a protein called mt-SAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	F9	216	1755	1088	325	337	5	0	0

- Molecule 30 is a protein called mt-SAF10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	FA	579	4421	2801	785	813	22	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FA	173	ALA	THR	conflict	UNP Q386U1
FA	352	TYR	HIS	conflict	UNP Q386U1

- Molecule 31 is a protein called mt-SAF11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	FB	377	Total	C	N	O	S	0	0
			3055	1928	574	543	10		
31	FC	311	Total	C	N	O	S	0	0
			2572	1629	488	447	8		

- Molecule 32 is a protein called mt-SAF13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FE	434	Total	C	N	O	S	0	0
			3523	2268	611	626	18		

- Molecule 33 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	FJ	353	Total	C	N	O	S	0	0
			2917	1843	550	516	8		

- Molecule 34 is a protein called mt-SAF21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	FM	326	Total	C	N	O	S	0	0
			2449	1515	449	465	20		
34	FN	319	Total	C	N	O	S	0	0
			2392	1478	436	458	20		

- Molecule 35 is a protein called mt-SAF22 (KRIPP17).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FO	324	Total	C	N	O	S	0	0
			2671	1674	509	474	14		

- Molecule 36 is a protein called mt-SAF23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	FP	348	Total	C	N	O	S	0	0
			2643	1682	464	487	10		

- Molecule 37 is a protein called mt-SAF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	FQ	257	Total	C	N	O	S	0	0
			2003	1265	358	373	7		
37	FR	243	Total	C	N	O	S	0	0
			1923	1217	344	355	7		
37	FS	277	Total	C	N	O	S	0	0
			2198	1389	397	404	8		
37	FT	233	Total	C	N	O	S	0	0
			1854	1177	331	339	7		
37	FU	270	Total	C	N	O	S	0	0
			2105	1331	380	386	8		

- Molecule 38 is a protein called mt-SAF26.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	FW	247	Total	C	N	O	S	0	0
			2034	1272	384	371	7		

- Molecule 39 is a protein called mt-SAF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	FX	220	Total	C	N	O	S	0	0
			1741	1093	318	316	14		

- Molecule 40 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	FY	65	Total	C	N	O	0	0
			544	343	102	99		

- Molecule 41 is a protein called mt-SAF29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	FZ	133	Total	C	N	O	S	0	0
			973	605	181	185	2		

- Molecule 42 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Fa	163	1323	860	236	223	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fa	73	ALA	VAL	conflict	UNP Q57VU7

- Molecule 43 is a protein called mt-SAF31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Fb	129	1091	701	198	184	8	0	0

- Molecule 44 is a protein called mt-SAF32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Fc	84	669	427	106	135	1	0	0

- Molecule 45 is a protein called mt-SAF33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Fd	96	758	481	147	122	8	0	0

- Molecule 46 is a protein called UNK-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	UA	21	126	84	21	21	0	0

- Molecule 47 is a protein called UNK-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	UB	27	162	108	27	27	0	0

- Molecule 48 is a protein called UNK-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	UC	10	Total	C	N	O	0	0
			60	40	10	10		

- Molecule 49 is a protein called UNK-D, UNK-M, UNK-Q.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	UD	9	Total	C	N	O	0	0
			54	36	9	9		
49	UM	9	Total	C	N	O	0	0
			54	36	9	9		
49	UQ	9	Total	C	N	O	0	0
			54	36	9	9		

- Molecule 50 is a protein called UNK-E, UNK-P.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	UE	45	Total	C	N	O	0	0
			270	180	45	45		
50	UP	45	Total	C	N	O	0	0
			270	180	45	45		

- Molecule 51 is a protein called UNK-F.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	UF	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 52 is a protein called UNK-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	UG	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 53 is a protein called UNK-H.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	UH	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 54 is a protein called UNK-I, UNK-M.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UI	8	Total	C	N	O	0	0
			48	32	8	8		
54	UN	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 55 is a protein called UNK-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	UJ	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 56 is a protein called UNK-L.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	UL	22	Total	C	N	O	0	0
			132	88	22	22		

- Molecule 57 is a protein called UNK-O.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	UO	30	Total	C	N	O	0	0
			180	120	30	30		

- Molecule 58 is a protein called UNK-U.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UU	24	Total	C	N	O	0	0
			144	96	24	24		

- Molecule 59 is a protein called UNK-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UY	468	Total	C	N	O	0	0
			2808	1872	468	468		

- Molecule 60 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CA	463	Total	C	N	O	P	0	0
			8851	3940	1294	3153	464		

- Molecule 61 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	F1	56	465	281	107	76	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	707	SER	GLY	conflict	UNP Q385R2
F1	973	THR	MET	conflict	UNP Q385R2

- Molecule 62 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	FF	16	141	89	30	20	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	70	ALA	PRO	conflict	UNP Q57W60
FF	179	PHE	LEU	conflict	UNP Q57W60

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

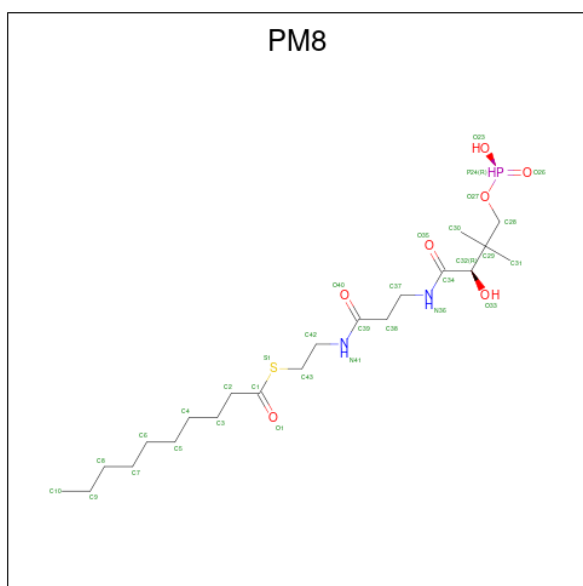
Mol	Chain	Residues	Atoms		AltConf
63	FPA	1	Total 1	Mg 1	0
63	FWB	1	Total 1	Mg 1	0
63	CAA	1	Total 1	Mg 1	0
63	CAB	1	Total 1	Mg 1	0

- Molecule 64 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
64	FWA	1	Total	O	P	0
			5	4	1	

- Molecule 65 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: C₂₁H₄₁N₂O₇PS).



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

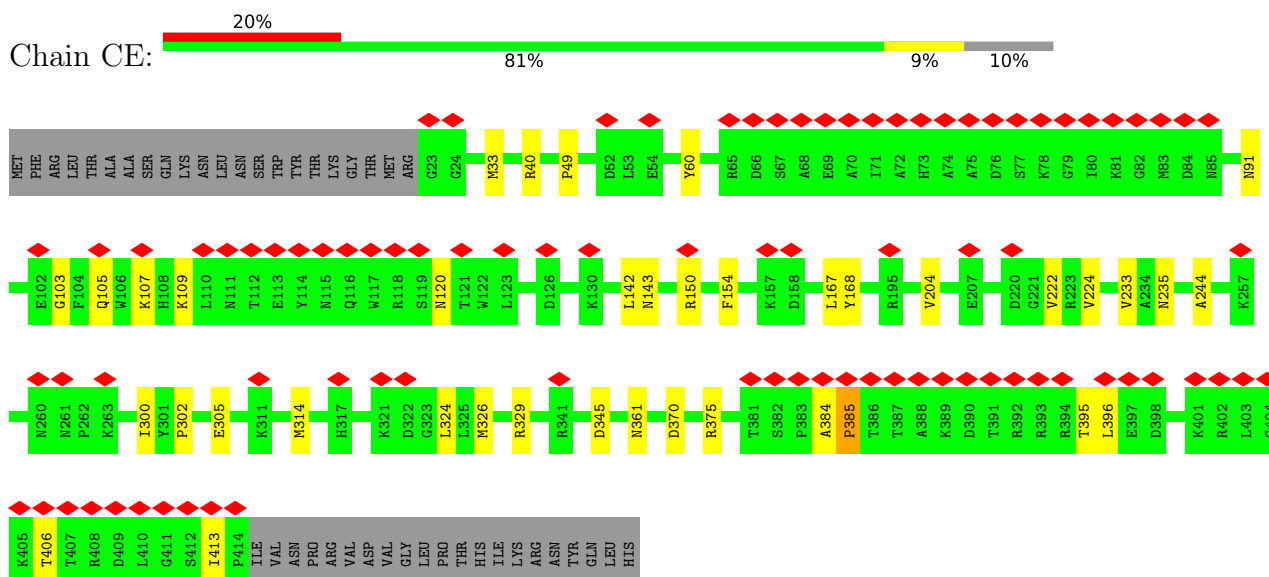
- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	FdA	1	Total 1	Zn 1	0

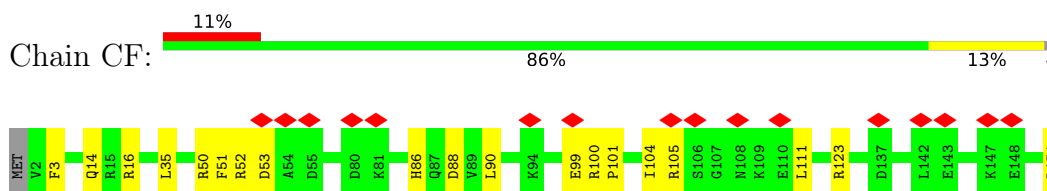
3 Residue-property plots [i](#)

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

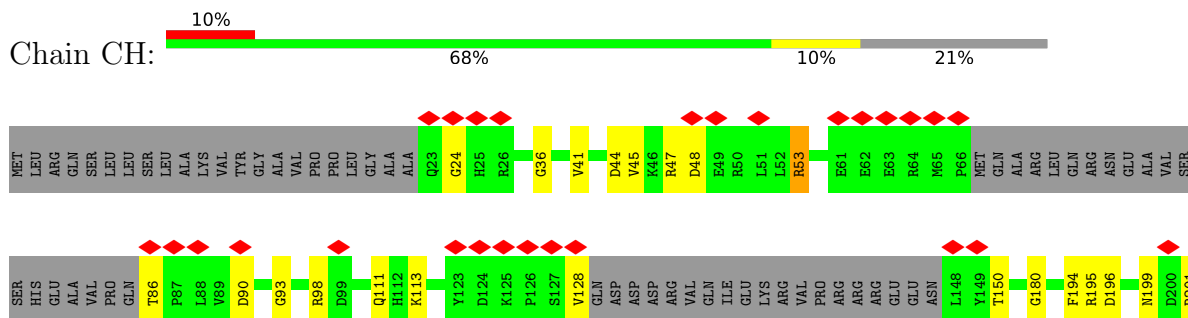
- Molecule 1: uS5m



- Molecule 2: bS6m

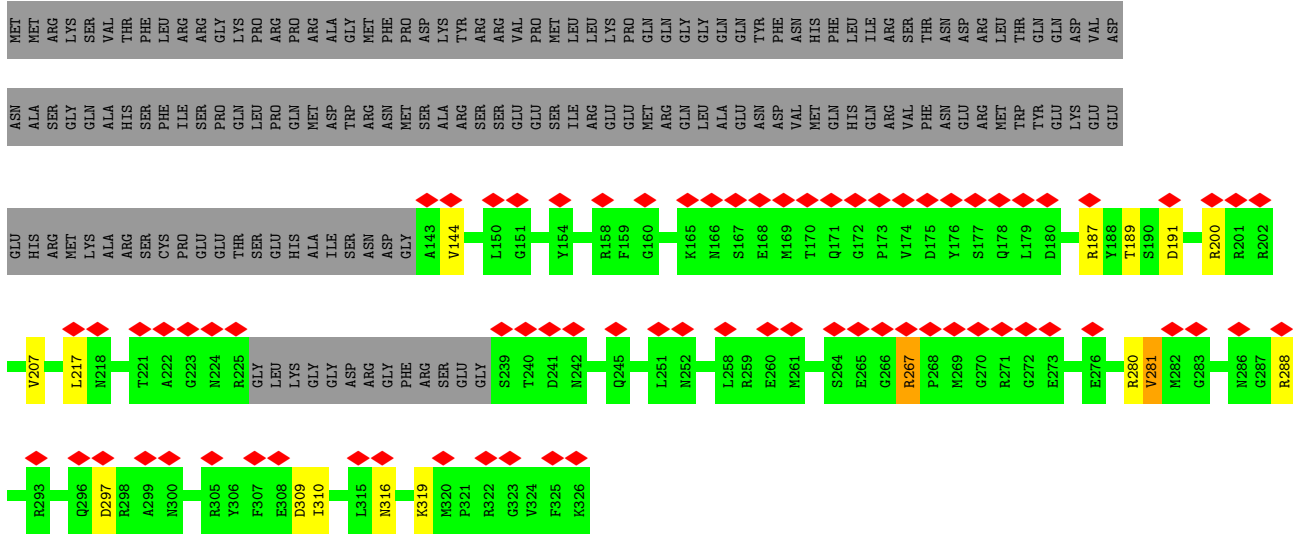


- Molecule 3: uS8m

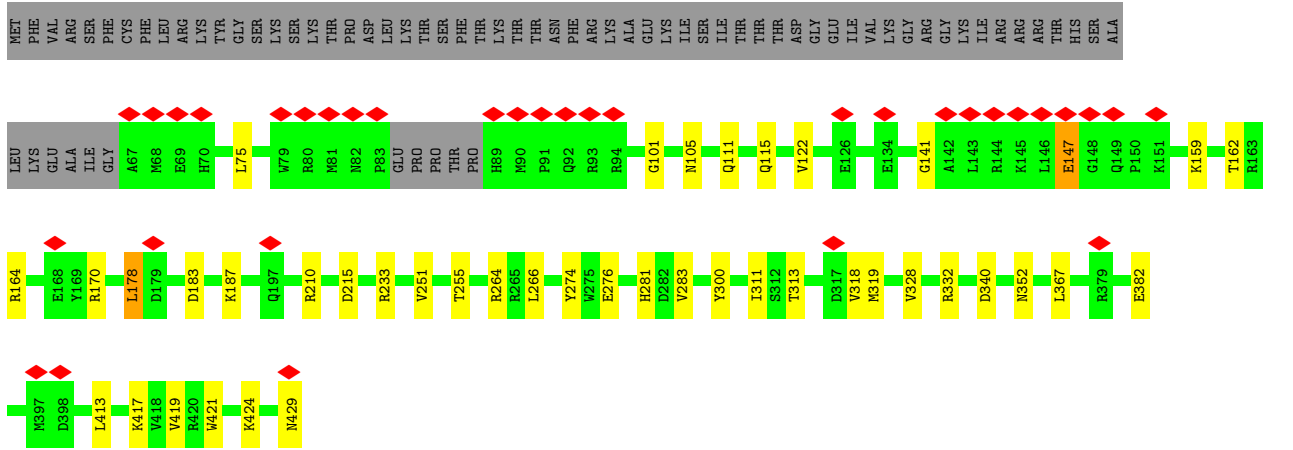
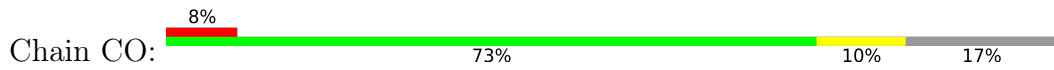




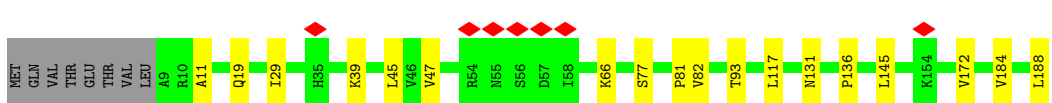
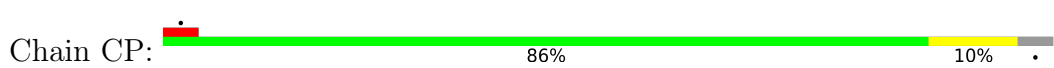
• Molecule 4: uS11m



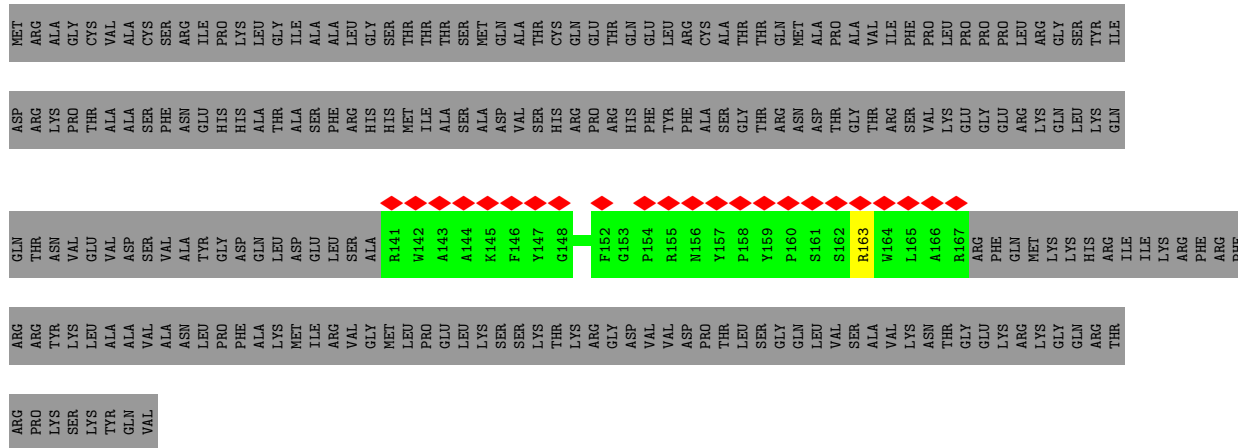
• Molecule 5: uS15m



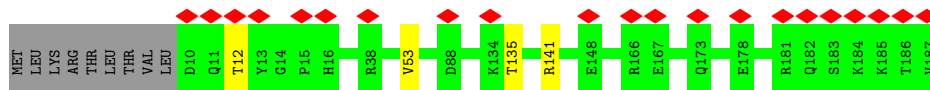
• Molecule 6: bS16m



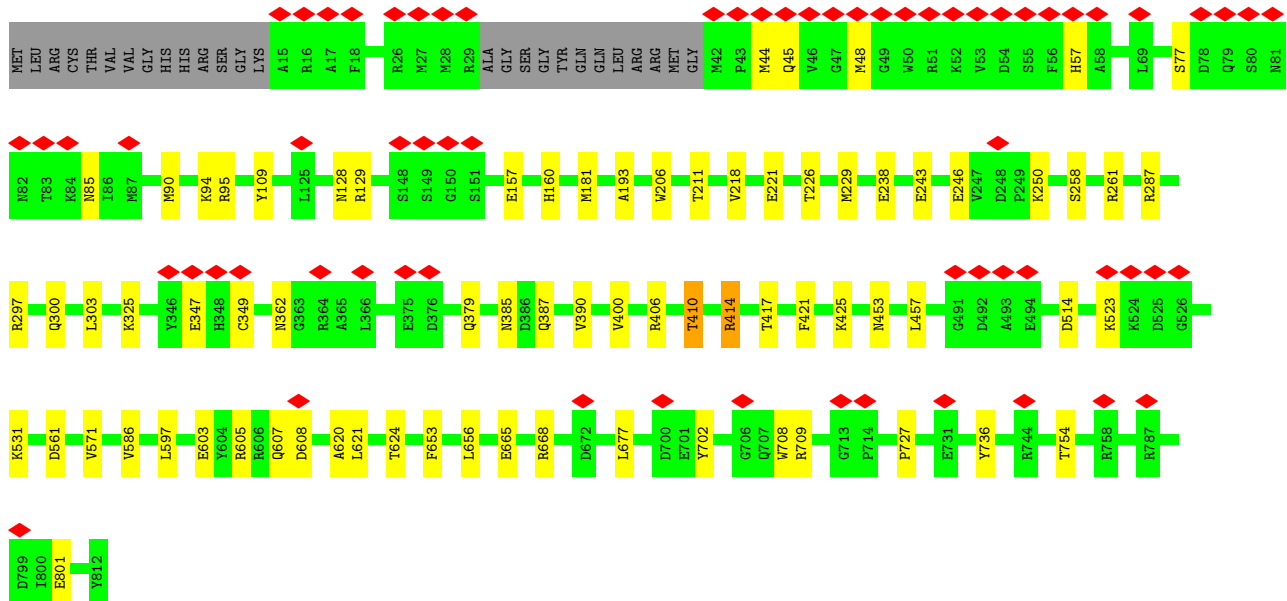
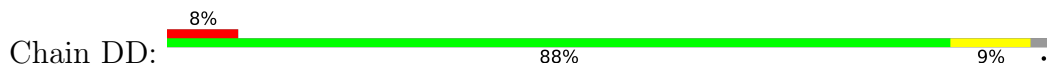
• Molecule 7: uS17m



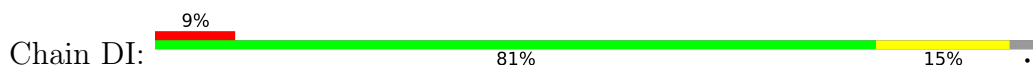
• Molecule 14: mS41

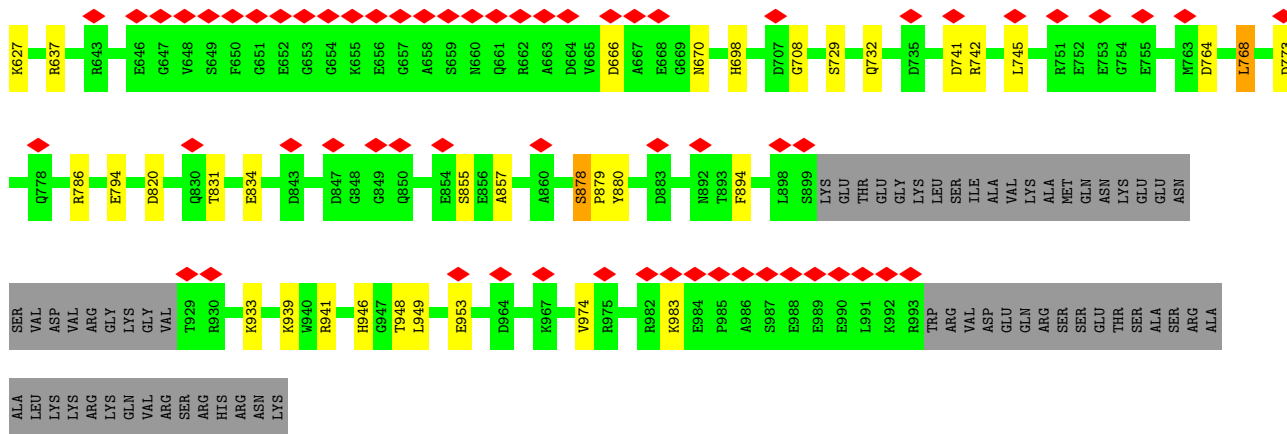


• Molecule 15: mS51 (KRIPP1)

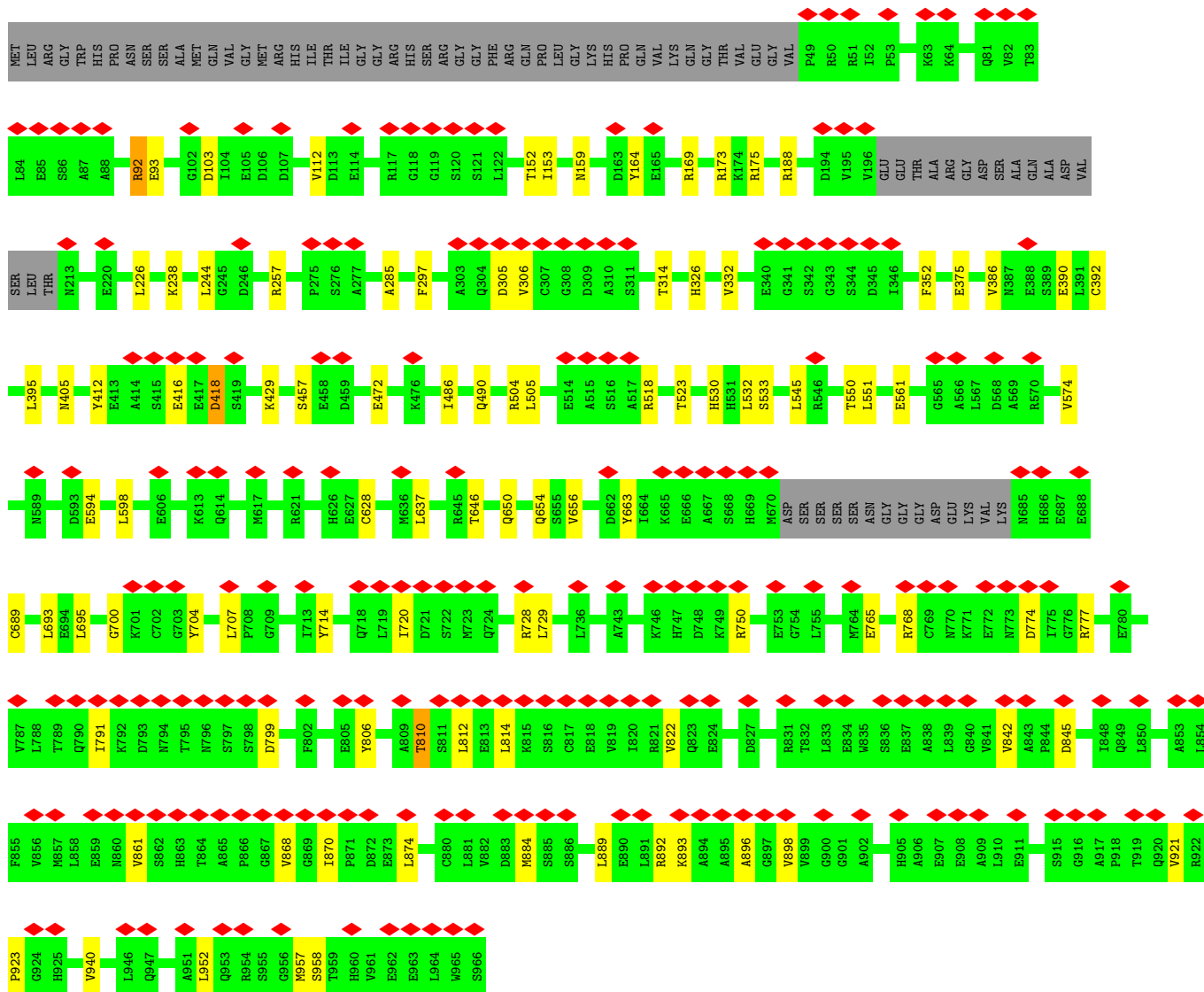
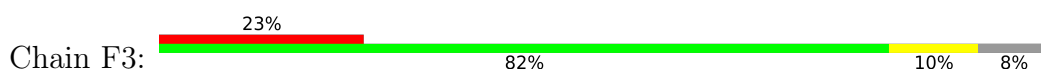


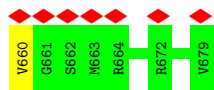
• Molecule 16: mS56



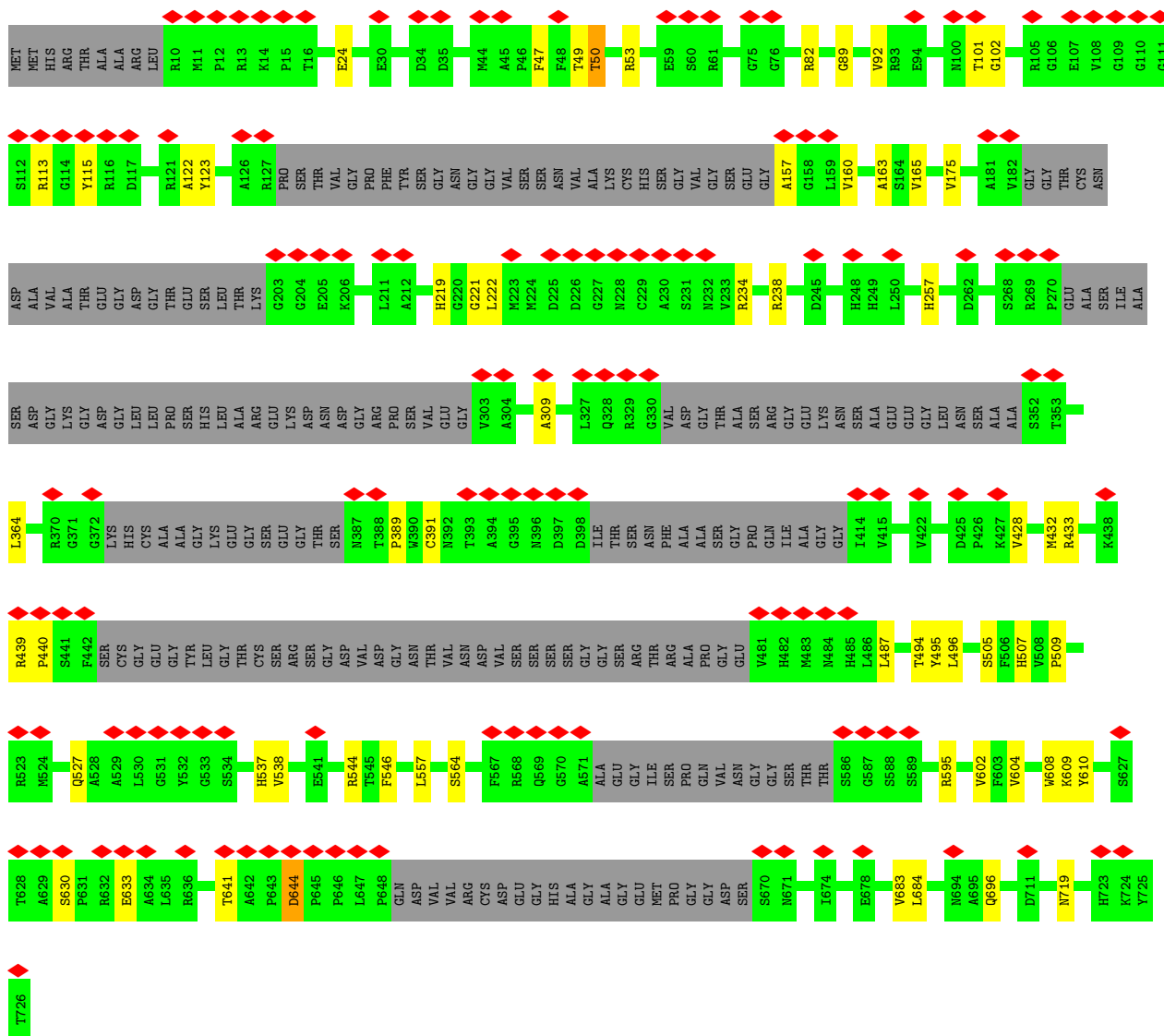


• Molecule 24: mt-SAF3

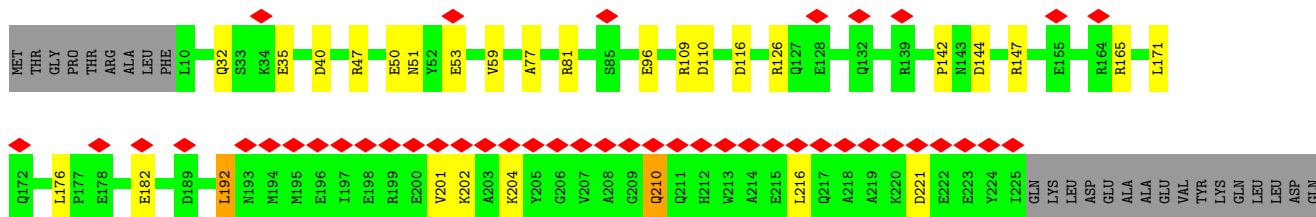


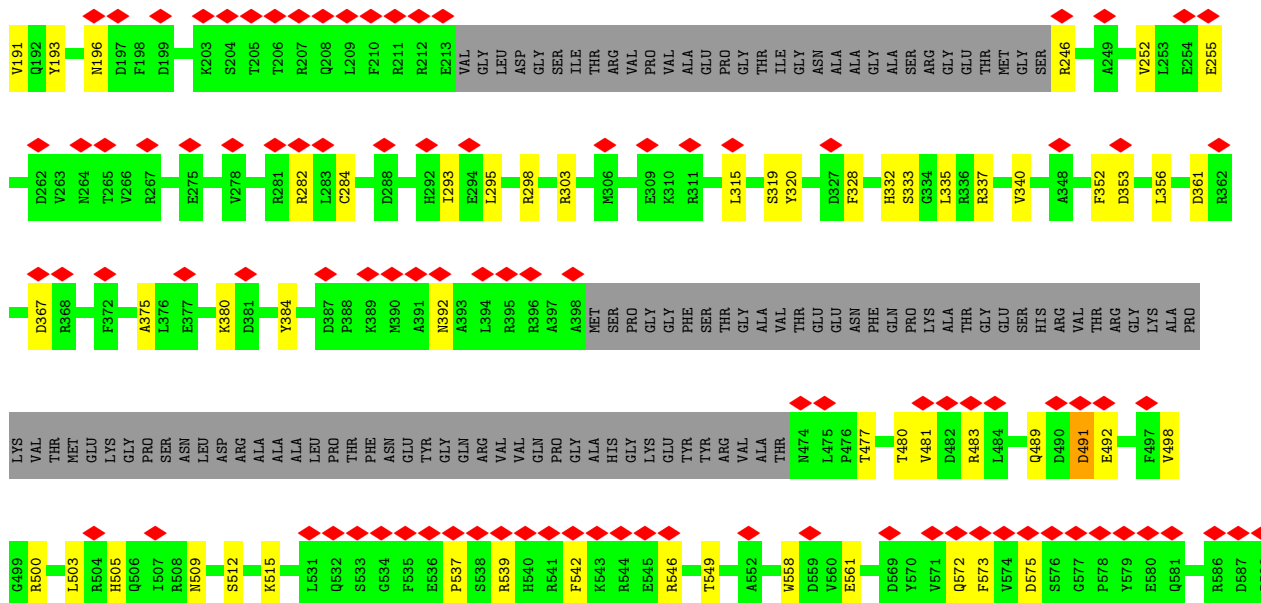


• Molecule 28: mt-SAF8

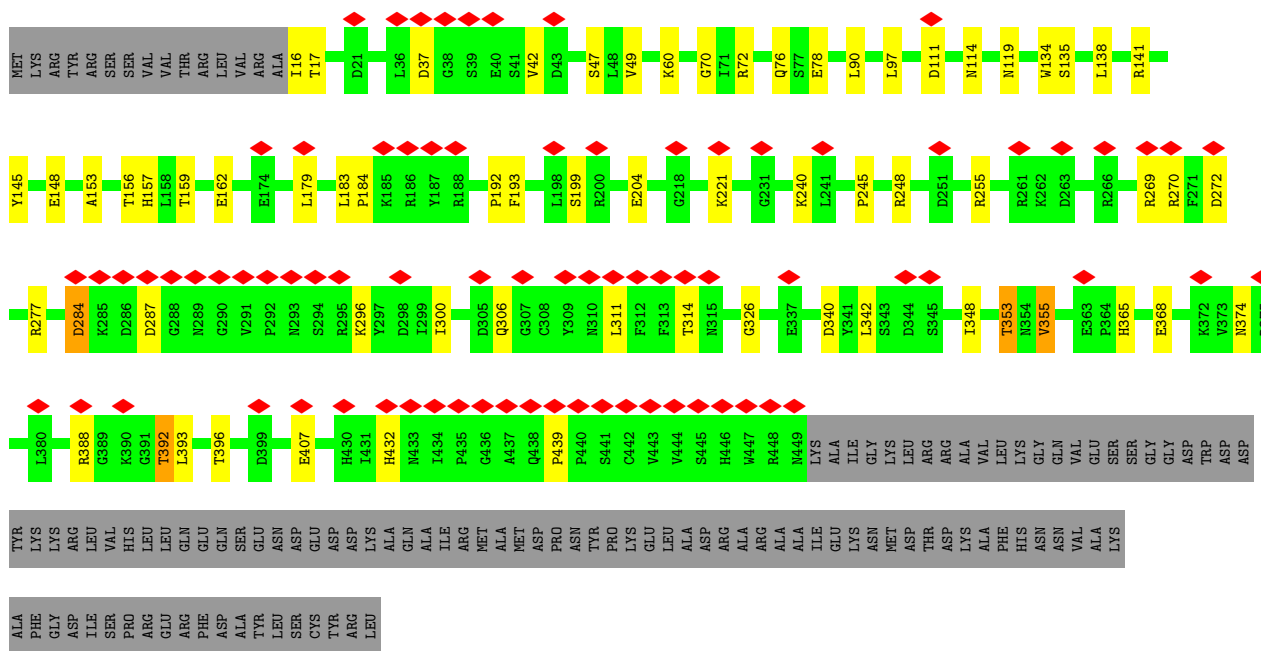


• Molecule 29: mt-SAF9

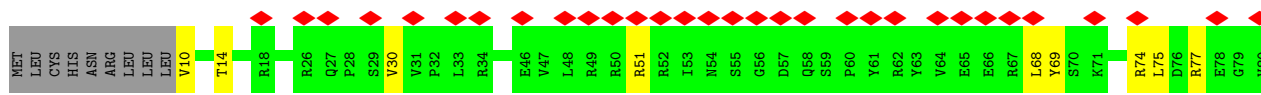
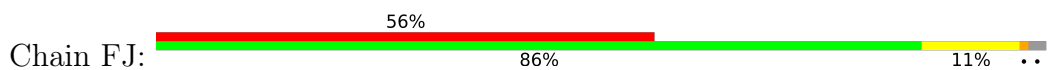


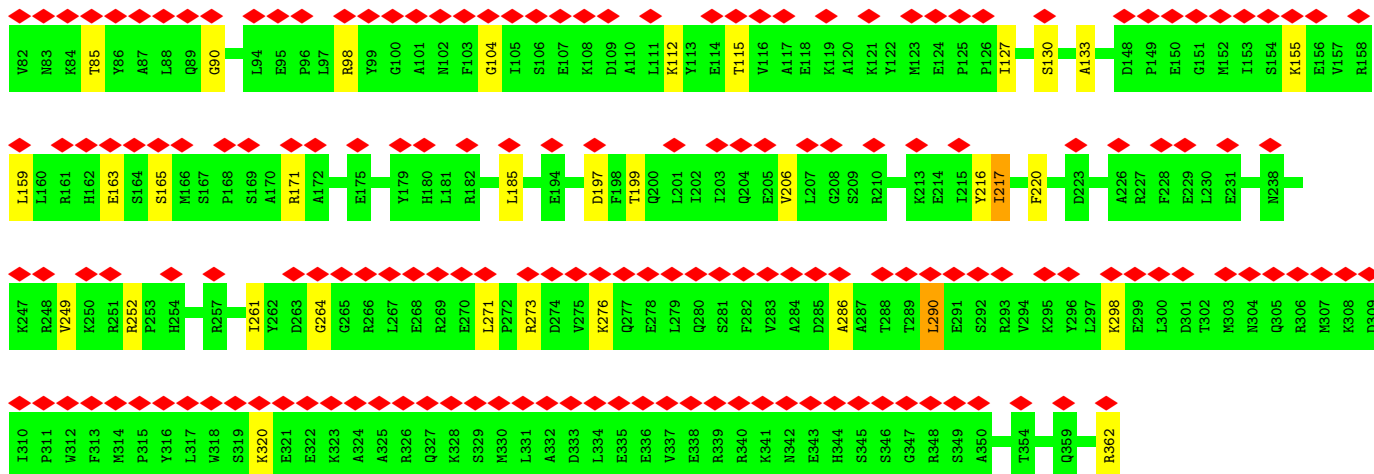


• Molecule 32: mt-SAF13

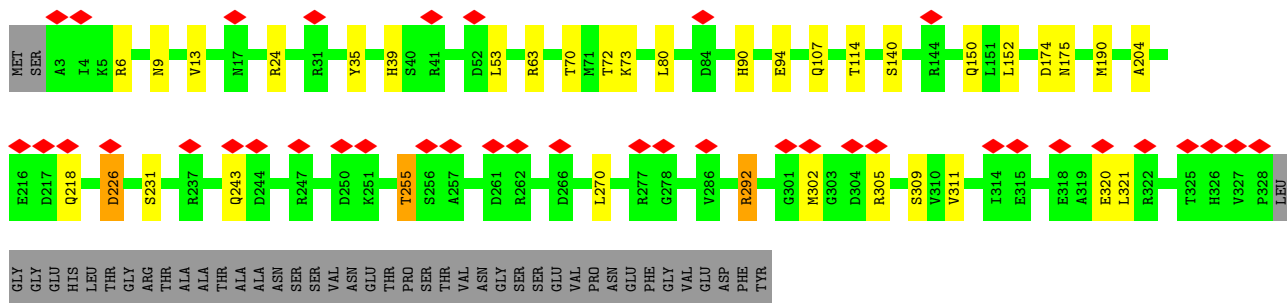
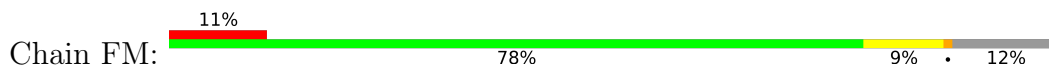


• Molecule 33: mt-SAF18

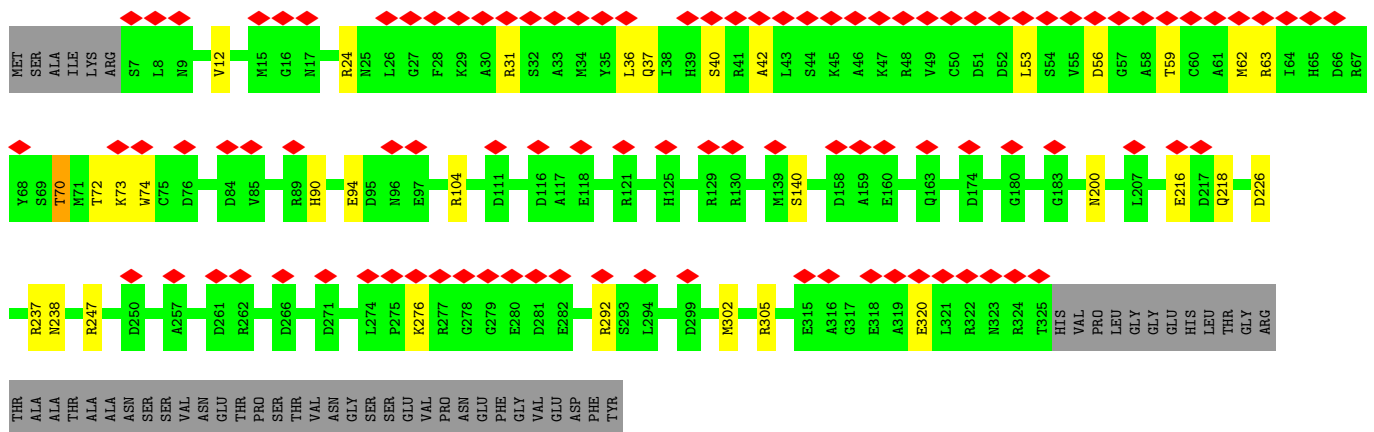
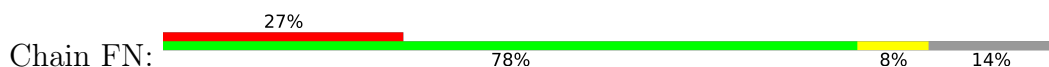




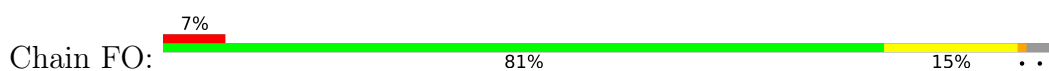
• Molecule 34: mt-SAF21

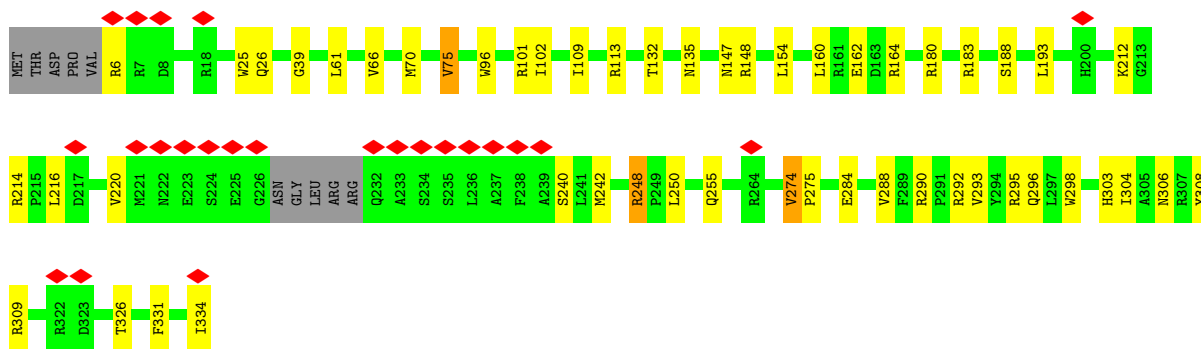


• Molecule 34: mt-SAF21

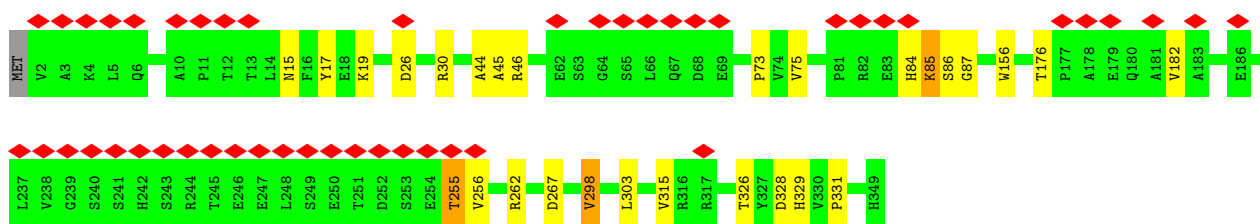
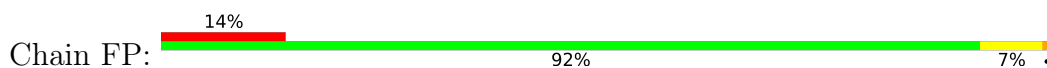


• Molecule 35: mt-SAF22 (KRIPP17)

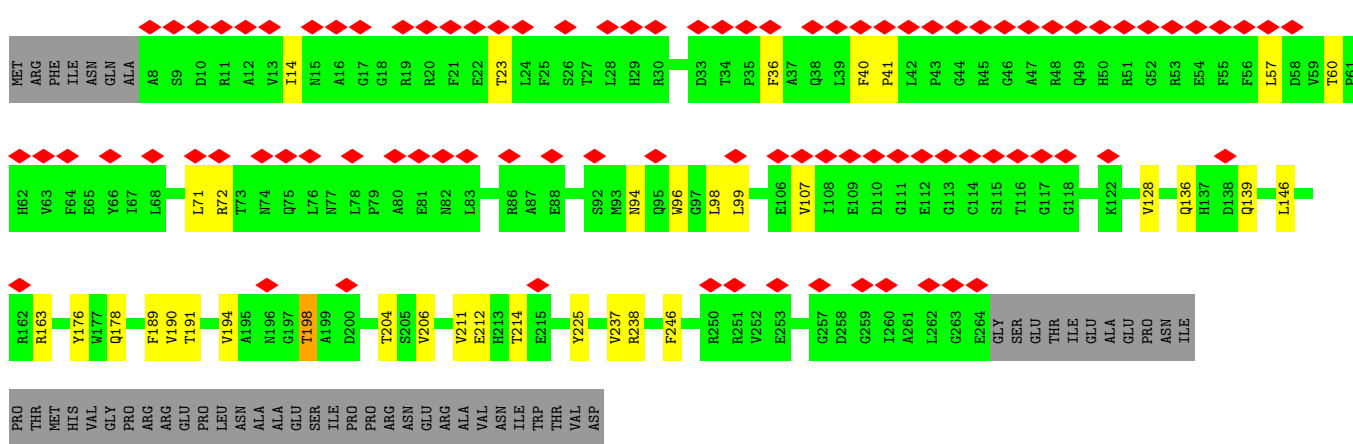
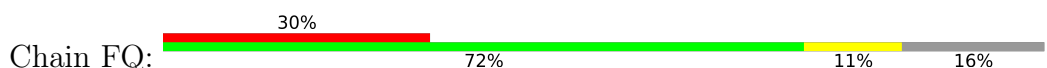




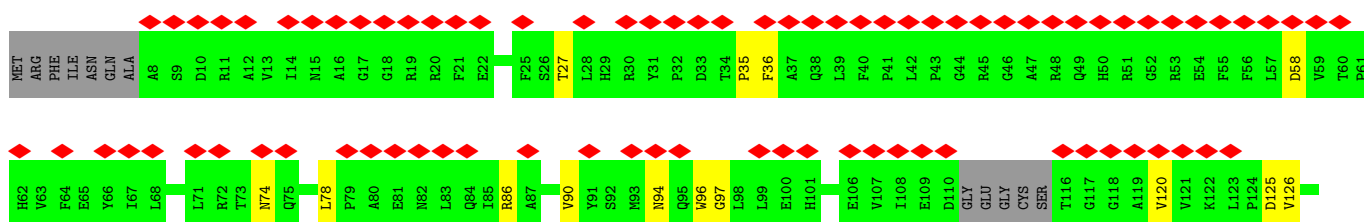
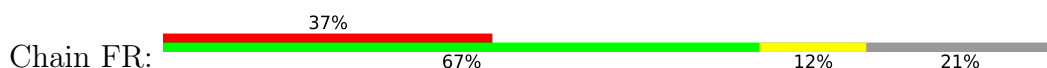
• Molecule 36: mt-SAF23

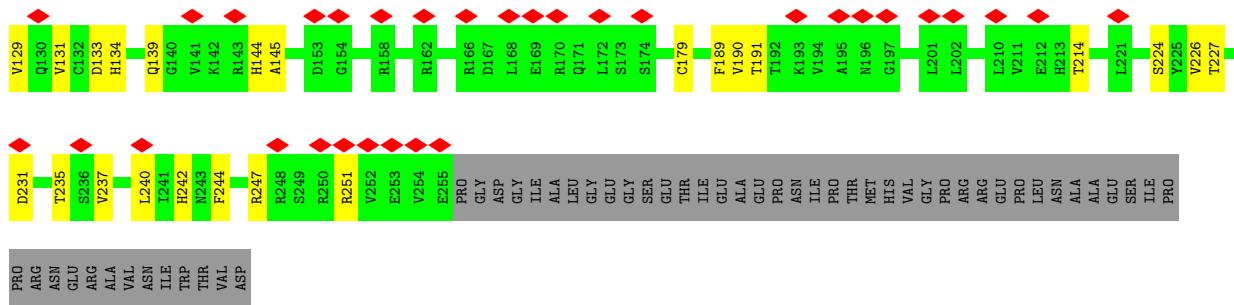


• Molecule 37: mt-SAF24

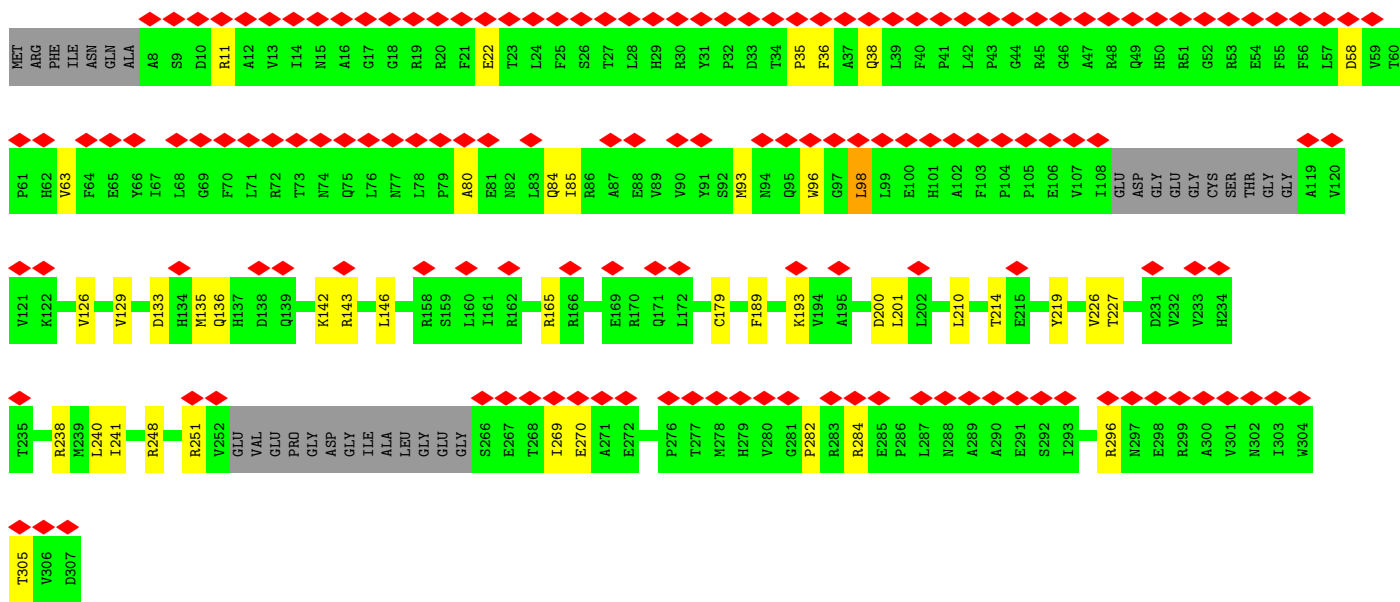
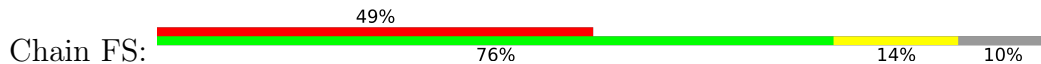


• Molecule 37: mt-SAF24

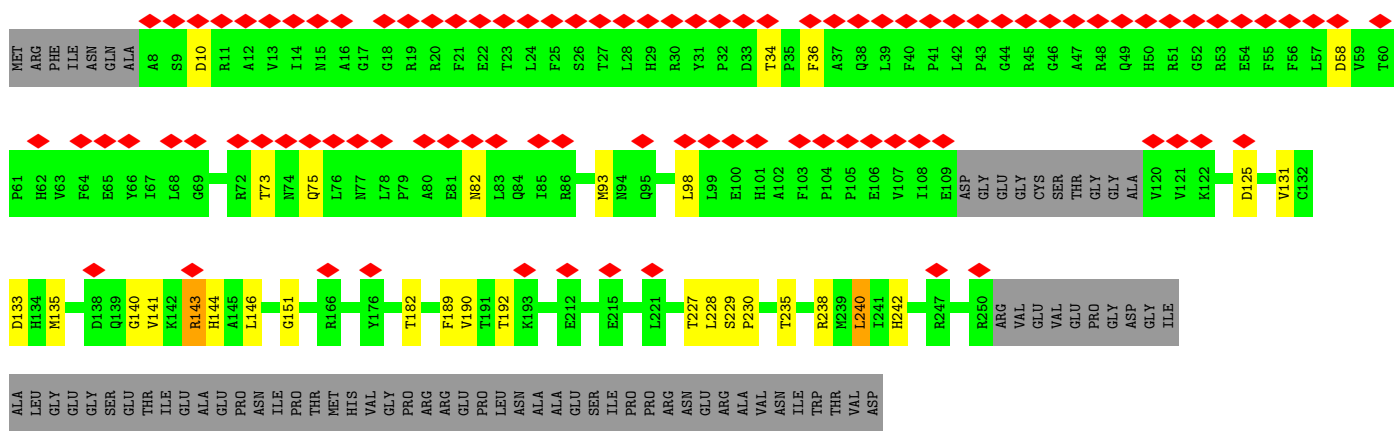




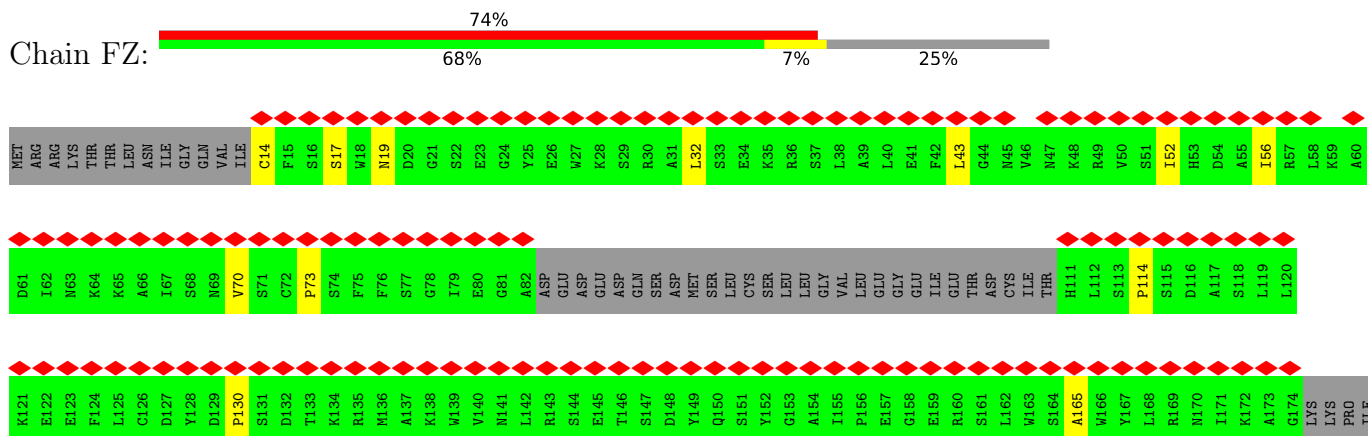
• Molecule 37: mt-SAF24



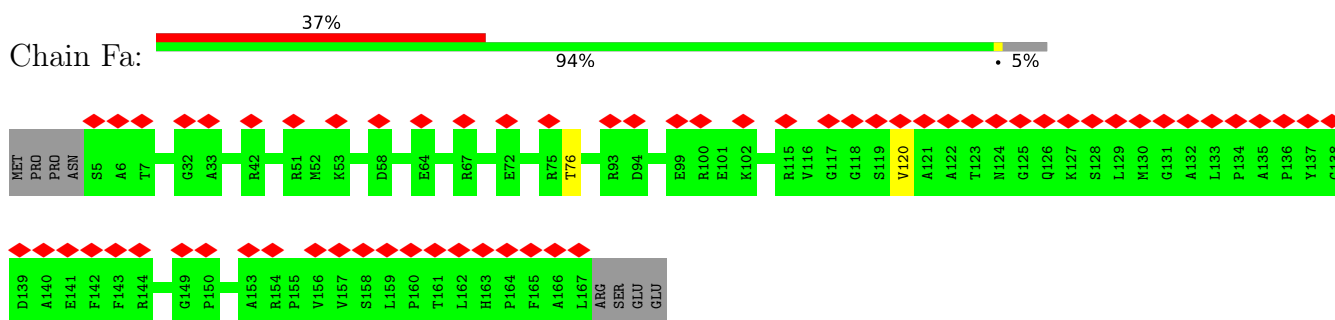
• Molecule 37: mt-SAF24



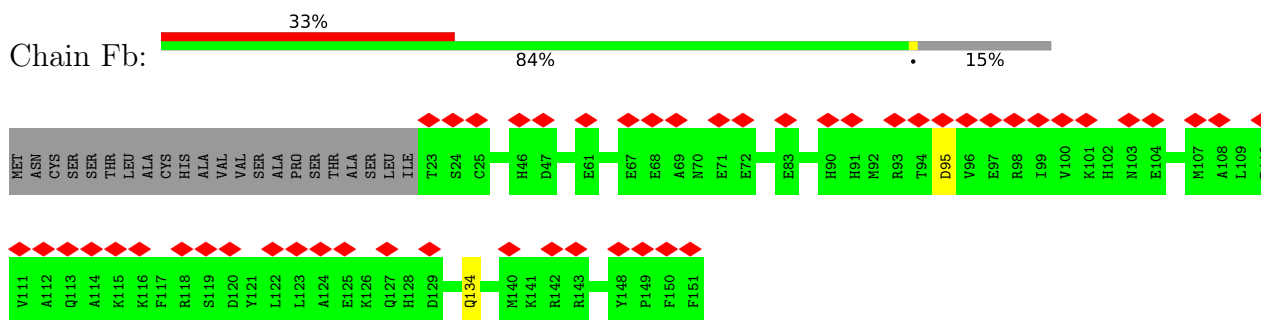
• Molecule 37: mt-SAF24



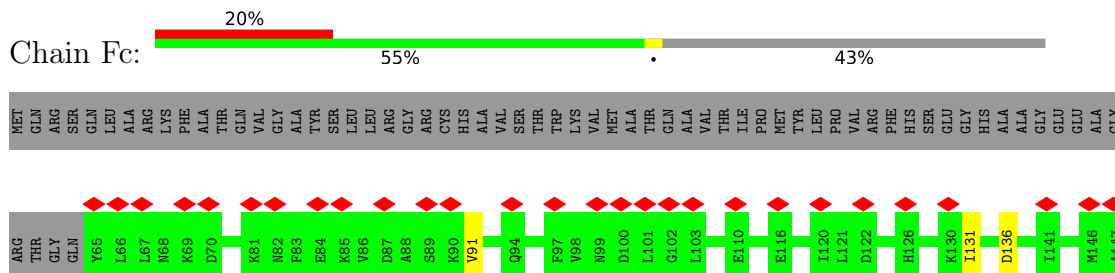
• Molecule 42: mt-SAF30



• Molecule 43: mt-SAF31

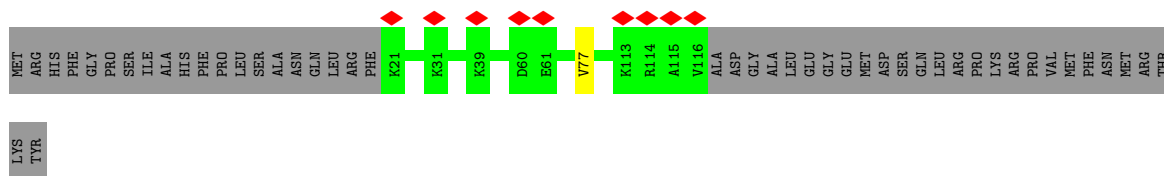


• Molecule 44: mt-SAF32

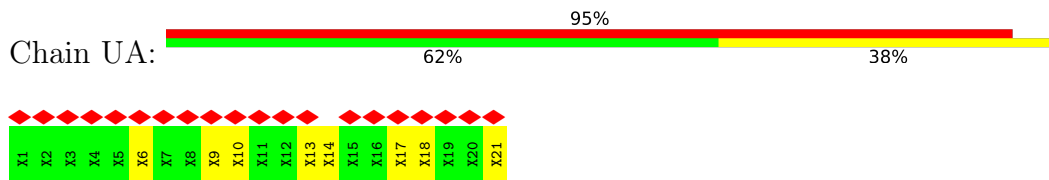


• Molecule 45: mt-SAF33

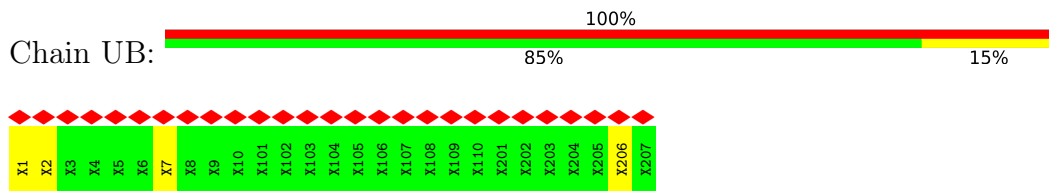




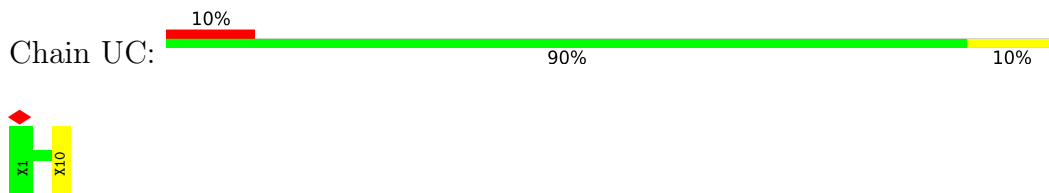
• Molecule 46: UNK-A



• Molecule 47: UNK-B



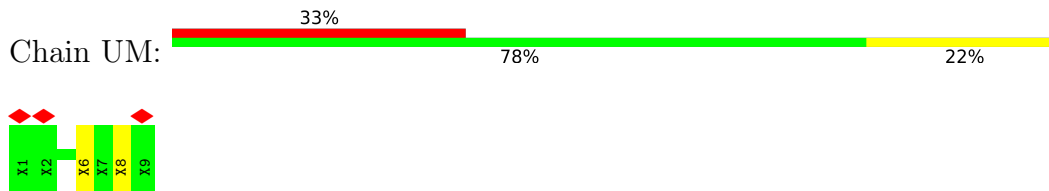
• Molecule 48: UNK-C



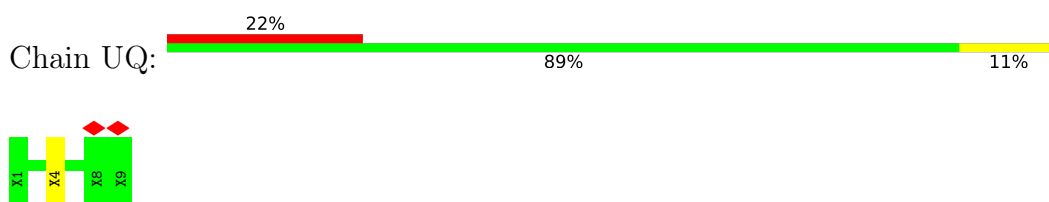
• Molecule 49: UNK-D, UNK-M, UNK-Q



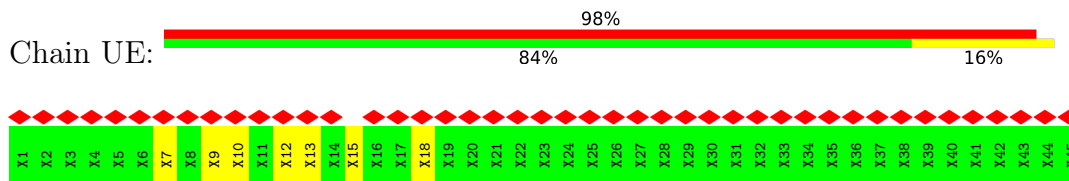
• Molecule 49: UNK-D, UNK-M, UNK-Q



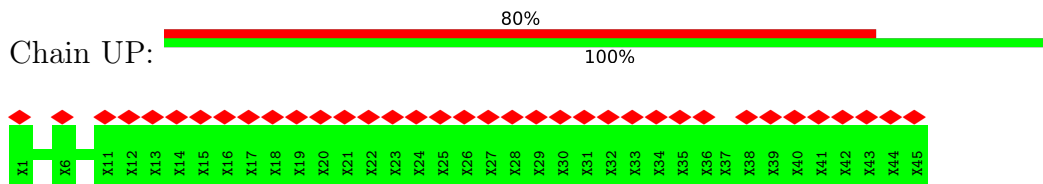
• Molecule 49: UNK-D, UNK-M, UNK-Q



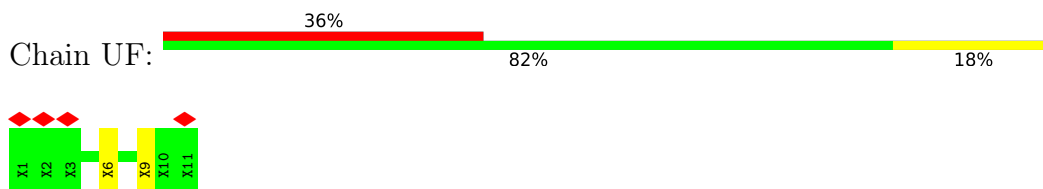
- Molecule 50: UNK-E, UNK-P



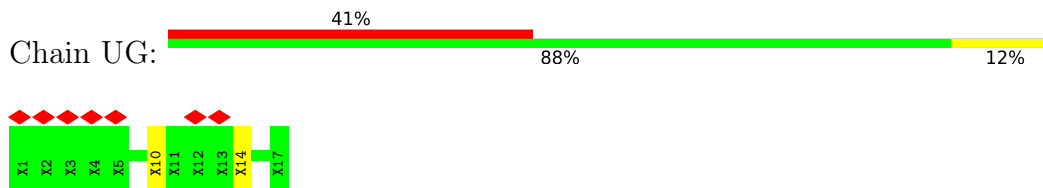
- Molecule 50: UNK-E, UNK-P



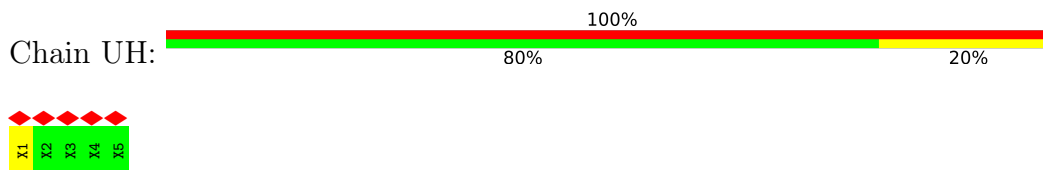
- Molecule 51: UNK-F



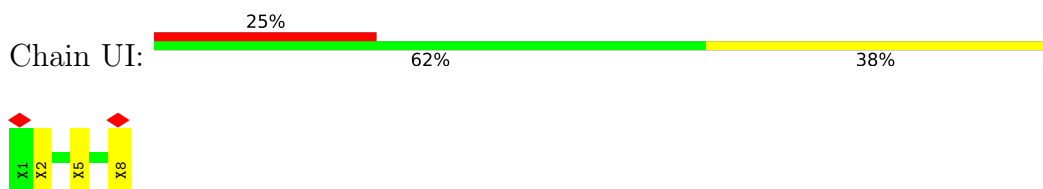
- Molecule 52: UNK-G



- Molecule 53: UNK-H

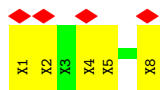


- Molecule 54: UNK-I, UNK-M

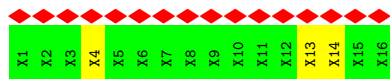
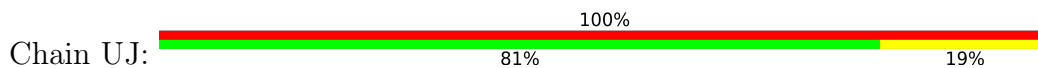


- Molecule 54: UNK-I, UNK-M

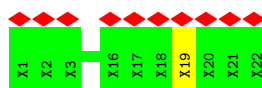




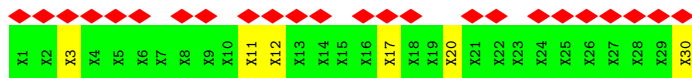
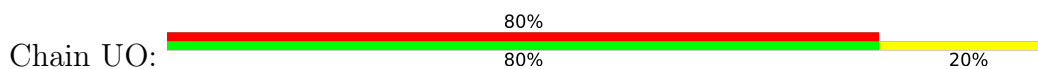
• Molecule 55: UNK-J



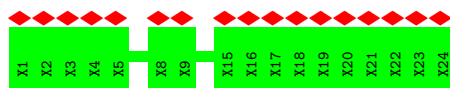
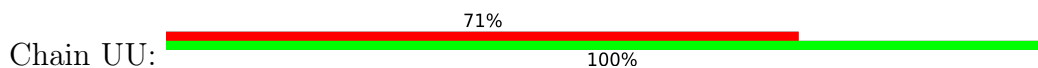
• Molecule 56: UNK-L



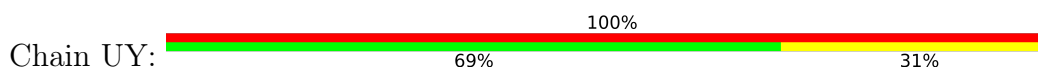
• Molecule 57: UNK-O

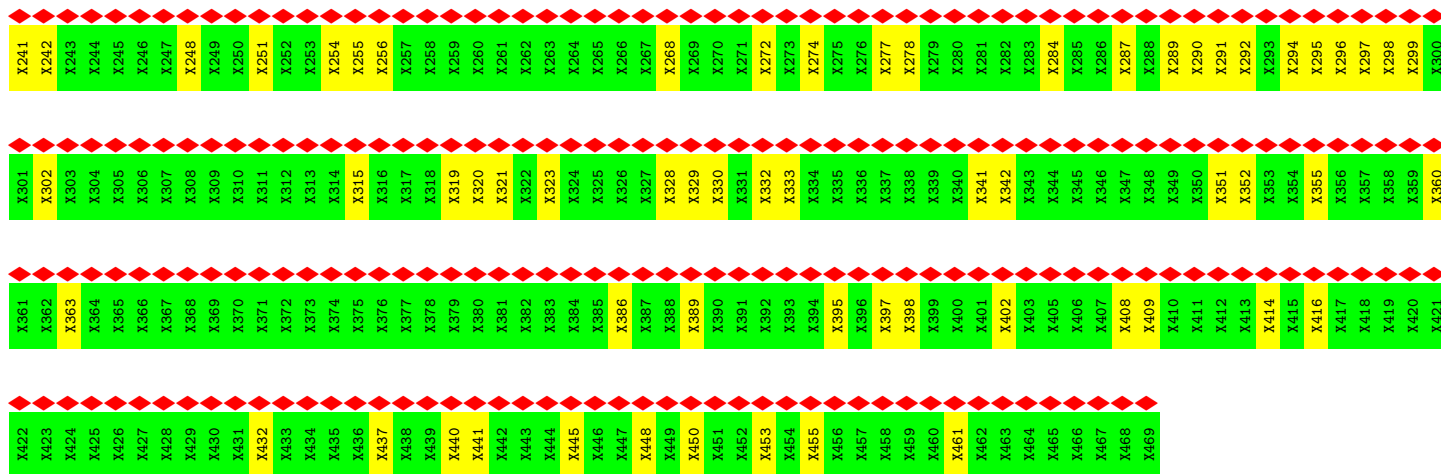


• Molecule 58: UNK-U

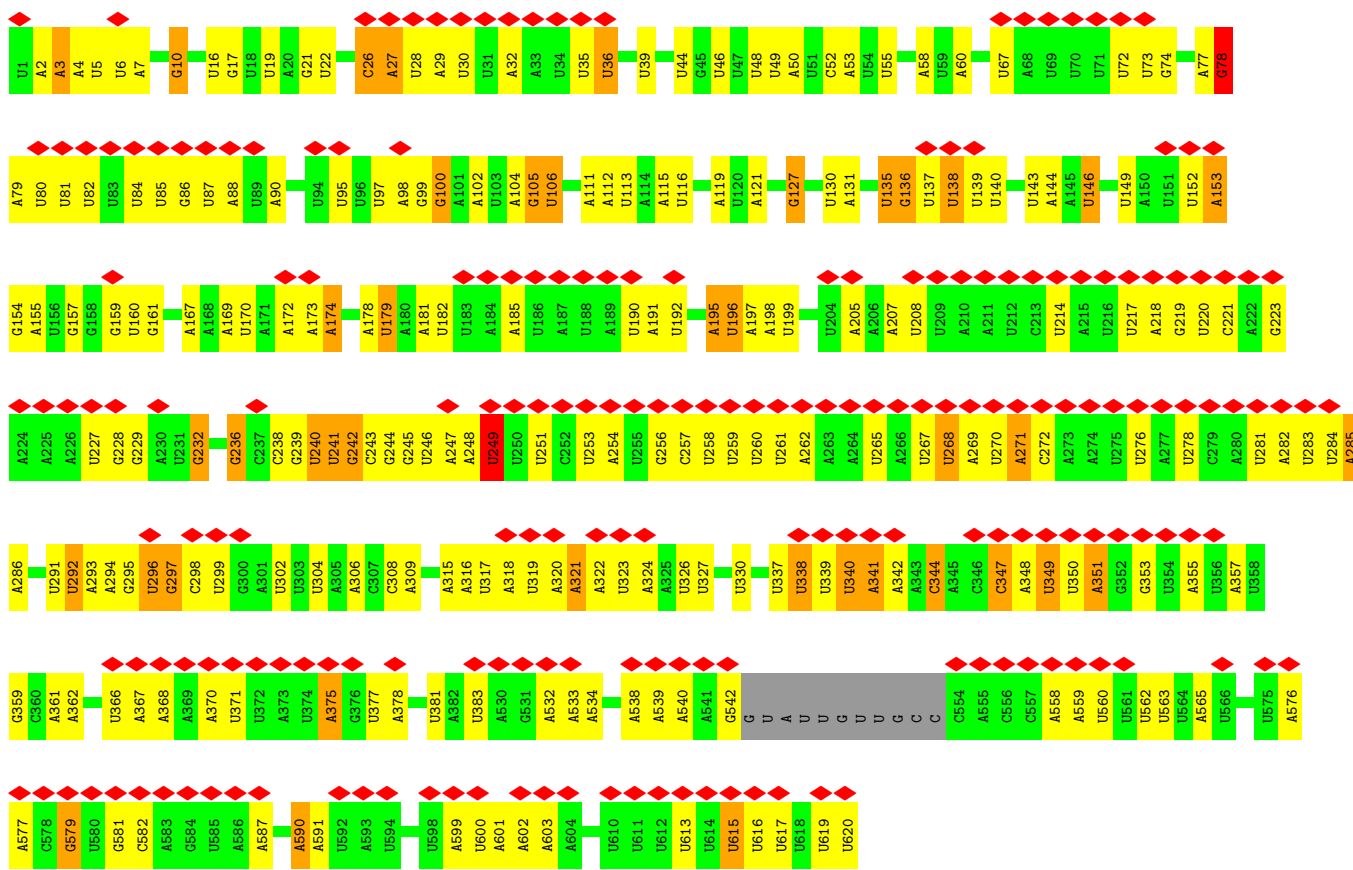
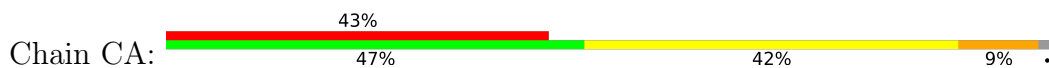


• Molecule 59: UNK-I





• Molecule 60: 9S rRNA



• Molecule 61: mt-SAF1 (RSM22)



MET	PHE	PHE	ARG	PHE	HIS	SER	THR	THR	THR	GLN	THR	CYS	LEU	THR	SER	GLY	VAL	ALA	ALA	ARG	SER	SER	VAL	ALA	VAL	ALA	VAL	PRO	VAL	ARG	ARG	GLY	GLY	ASP	GLY	VAL	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On the fly in RELION	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	100719	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.455	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0902	Depositor
Map size (Å)	333.6, 333.6, 333.6	wwPDB
Map dimensions	240, 240, 240	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: PO4, UBD, MG, ZN, PM8

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	CE	0.26	0/3226	0.47	2/4364 (0.0%)
2	CF	0.25	0/1344	0.43	0/1813
3	CH	0.25	0/1864	0.44	0/2511
4	CK	0.26	0/1417	0.45	0/1911
5	CO	0.25	0/3057	0.44	1/4121 (0.0%)
6	CP	0.25	0/1533	0.47	0/2074
7	CQ	0.26	0/1856	0.45	0/2509
8	CR	0.25	0/1315	0.45	0/1785
9	Ca	0.25	0/4474	0.43	1/6052 (0.0%)
10	Cb	0.25	0/1304	0.43	0/1751
11	Cd	0.29	0/1662	0.40	0/2234
12	Cj	0.26	0/1842	0.45	0/2511
13	Cn	0.27	0/245	0.49	0/333
14	Cp	0.24	0/1551	0.41	0/2103
15	DD	0.26	0/6678	0.43	0/9051
16	DI	0.25	0/3248	0.42	0/4401
17	DL	0.26	0/1699	0.42	0/2293
18	DO	0.23	0/1680	0.39	0/2265
19	DP	0.24	0/1854	0.42	0/2511
20	DR	0.26	0/2107	0.46	0/2871
21	DU	0.26	0/1780	0.50	2/2416 (0.1%)
22	DZ	0.24	0/263	0.45	0/355
23	F2	0.25	0/7432	0.43	1/10042 (0.0%)
24	F3	0.25	0/6999	0.43	0/9472
25	F5	0.25	0/3533	0.42	3/4798 (0.1%)
26	F6	0.25	0/3728	0.45	1/5060 (0.0%)
27	F7	0.26	0/5342	0.44	0/7236
28	F8	0.26	0/4025	0.44	0/5450
29	F9	0.24	0/1785	0.38	0/2399
30	FA	0.25	0/4507	0.45	0/6139
31	FB	0.25	0/3132	0.44	0/4248
31	FC	0.24	0/2635	0.44	0/3572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	FE	0.25	0/3629	0.44	0/4935
33	FJ	0.25	0/2986	0.44	0/4030
34	FM	0.26	0/2489	0.44	0/3365
34	FN	0.25	0/2430	0.45	0/3285
35	FO	0.25	0/2733	0.44	0/3692
36	FP	0.25	0/2710	0.44	0/3709
37	FQ	0.25	0/2048	0.45	0/2786
37	FR	0.25	0/1966	0.44	0/2673
37	FS	0.25	0/2249	0.45	0/3063
37	FT	0.25	0/1897	0.44	0/2580
37	FU	0.25	0/2154	0.44	0/2933
38	FW	0.24	0/2077	0.42	0/2805
39	FX	0.24	0/1783	0.41	0/2410
40	FY	0.24	0/562	0.46	0/769
41	FZ	0.23	0/989	0.49	3/1336 (0.2%)
42	Fa	0.25	0/1363	0.44	0/1853
43	Fb	0.24	0/1123	0.40	0/1513
44	Fc	0.24	0/679	0.40	0/923
45	Fd	0.24	0/779	0.43	0/1054
60	CA	0.29	0/9830	1.00	38/15261 (0.2%)
61	F1	0.22	0/469	0.41	0/624
62	FF	0.21	0/144	0.35	0/192
All	All	0.25	0/136206	0.51	52/186442 (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
15	DD	0	1
24	F3	0	1
27	F7	0	2
28	F8	0	1
36	FP	0	1
38	FW	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CA	146	U	N3-C2-O2	-8.99	115.90	122.20
60	CA	146	U	N1-C2-O2	8.89	129.02	122.80
60	CA	99	G	C4-N9-C1'	8.00	136.90	126.50
60	CA	302	U	C2-N1-C1'	7.73	126.98	117.70
60	CA	146	U	C2-N1-C1'	7.67	126.90	117.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	DD	414	ARG	Peptide
24	F3	490	GLN	Peptide
27	F7	381	LEU	Peptide
27	F7	566	LYS	Peptide
28	F8	644	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CE	3147	0	3091	22	0
2	CF	1317	0	1309	14	0
3	CH	1824	0	1800	18	0
4	CK	1384	0	1361	11	0
5	CO	2979	0	2974	29	0
6	CP	1489	0	1510	12	0
7	CQ	1805	0	1811	34	0
8	CR	1274	0	1223	13	0
9	Ca	4340	0	4127	0	0
10	Cb	1274	0	1287	0	0
11	Cd	1616	0	1568	0	0
12	Cj	1792	0	1744	0	0
13	Cn	234	0	222	0	0
14	Cp	1506	0	1467	0	0
15	DD	6488	0	6251	50	0
16	DI	3182	0	3153	43	0
17	DL	1656	0	1632	11	0
18	DO	1648	0	1615	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	DP	1800	0	1765	12	0
20	DR	2042	0	2043	20	0
21	DU	1738	0	1640	15	0
22	DZ	254	0	230	5	0
23	F2	7274	0	7113	47	0
24	F3	6879	0	6854	52	0
25	F5	3474	0	3070	25	0
26	F6	3646	0	3608	35	0
27	F7	5225	0	5177	55	0
28	F8	3934	0	3908	33	0
29	F9	1755	0	1709	19	0
30	FA	4421	0	4534	44	0
31	FB	3055	0	3011	32	0
31	FC	2572	0	2544	32	0
32	FE	3523	0	3460	41	0
33	FJ	2917	0	2966	25	0
34	FM	2449	0	2440	18	0
34	FN	2392	0	2375	16	0
35	FO	2671	0	2636	40	0
36	FP	2643	0	2554	14	0
37	FQ	2003	0	1928	19	0
37	FR	1923	0	1862	19	0
37	FS	2198	0	2142	25	0
37	FT	1854	0	1802	20	0
37	FU	2105	0	2031	19	0
38	FW	2034	0	2035	18	0
39	FX	1741	0	1693	13	0
40	FY	544	0	533	13	0
41	FZ	973	0	869	6	0
42	Fa	1323	0	1336	0	0
43	Fb	1091	0	1085	0	0
44	Fc	669	0	663	0	0
45	Fd	758	0	764	0	0
46	UA	126	0	128	7	0
47	UB	162	0	169	4	0
48	UC	60	0	63	1	0
49	UD	54	0	57	6	0
49	UM	54	0	57	3	0
49	UQ	54	0	56	1	0
50	UE	270	0	272	5	0
50	UP	270	0	272	0	0
51	UF	66	0	69	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	UG	102	0	104	2	0
53	UH	30	0	33	1	0
54	UI	48	0	50	3	0
54	UN	48	0	50	4	0
55	UJ	96	0	99	2	0
56	UL	132	0	134	1	0
57	UO	180	0	183	8	0
58	UU	144	0	147	0	0
59	UY	2808	0	2852	102	0
60	CA	8851	0	4424	70	0
61	F1	465	0	492	3	0
62	FF	141	0	151	2	0
63	CAA	1	0	0	0	0
63	CAB	1	0	0	0	0
63	FPA	1	0	0	0	0
63	FWB	1	0	0	0	0
64	FWA	5	0	0	1	0
65	FcA	32	0	39	0	0
66	FdA	1	0	0	0	0
All	All	137038	0	130426	978	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 978 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:UY:355:UNK:HG1	60:CA:579:G:H5'	1.61	0.82
27:F7:206:PRO:HB3	59:UY:193:UNK:HB1	1.62	0.81
59:UY:9:UNK:HG1	59:UY:461:UNK:HB2	1.63	0.81
41:FZ:14:CYS:N	41:FZ:17:SER:HG	1.82	0.77
59:UY:351:UNK:HB1	60:CA:542:G:H5'	1.68	0.76

There are no symmetry-related clashes.

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	CE	390/435 (90%)	379 (97%)	9 (2%)	2 (0%)	29	64
2	CF	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
3	CH	216/282 (77%)	210 (97%)	6 (3%)	0	100	100
4	CK	167/326 (51%)	150 (90%)	17 (10%)	0	100	100
5	CO	354/429 (82%)	347 (98%)	7 (2%)	0	100	100
6	CP	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
7	CQ	217/336 (65%)	209 (96%)	8 (4%)	0	100	100
8	CR	149/320 (47%)	143 (96%)	6 (4%)	0	100	100
9	Ca	508/602 (84%)	493 (97%)	15 (3%)	0	100	100
10	Cb	149/311 (48%)	146 (98%)	3 (2%)	0	100	100
11	Cd	183/440 (42%)	182 (100%)	1 (0%)	0	100	100
12	Cj	224/257 (87%)	218 (97%)	6 (3%)	0	100	100
13	Cn	25/250 (10%)	19 (76%)	6 (24%)	0	100	100
14	Cp	176/187 (94%)	172 (98%)	4 (2%)	0	100	100
15	DD	782/812 (96%)	760 (97%)	22 (3%)	0	100	100
16	DI	388/407 (95%)	379 (98%)	9 (2%)	0	100	100
17	DL	199/307 (65%)	193 (97%)	6 (3%)	0	100	100
18	DO	202/282 (72%)	199 (98%)	3 (2%)	0	100	100
19	DP	210/274 (77%)	206 (98%)	4 (2%)	0	100	100
20	DR	250/270 (93%)	240 (96%)	10 (4%)	0	100	100
21	DU	217/228 (95%)	204 (94%)	13 (6%)	0	100	100
22	DZ	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
23	F2	909/1024 (89%)	890 (98%)	19 (2%)	0	100	100
24	F3	882/966 (91%)	856 (97%)	26 (3%)	0	100	100
25	F5	474/754 (63%)	459 (97%)	14 (3%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	F6	450/676 (67%)	435 (97%)	15 (3%)	0	100	100
27	F7	658/679 (97%)	615 (94%)	41 (6%)	2 (0%)	41	73
28	F8	493/726 (68%)	476 (97%)	17 (3%)	0	100	100
29	F9	214/608 (35%)	212 (99%)	2 (1%)	0	100	100
30	FA	573/642 (89%)	555 (97%)	18 (3%)	0	100	100
31	FB	373/579 (64%)	365 (98%)	8 (2%)	0	100	100
31	FC	305/579 (53%)	293 (96%)	12 (4%)	0	100	100
32	FE	432/553 (78%)	414 (96%)	18 (4%)	0	100	100
33	FJ	351/362 (97%)	335 (95%)	16 (5%)	0	100	100
34	FM	324/370 (88%)	320 (99%)	4 (1%)	0	100	100
34	FN	317/370 (86%)	310 (98%)	7 (2%)	0	100	100
35	FO	320/334 (96%)	308 (96%)	12 (4%)	0	100	100
36	FP	346/349 (99%)	332 (96%)	13 (4%)	1 (0%)	41	73
37	FQ	255/307 (83%)	250 (98%)	5 (2%)	0	100	100
37	FR	239/307 (78%)	232 (97%)	7 (3%)	0	100	100
37	FS	271/307 (88%)	265 (98%)	6 (2%)	0	100	100
37	FT	229/307 (75%)	224 (98%)	5 (2%)	0	100	100
37	FU	266/307 (87%)	259 (97%)	7 (3%)	0	100	100
38	FW	243/263 (92%)	237 (98%)	6 (2%)	0	100	100
39	FX	218/239 (91%)	212 (97%)	6 (3%)	0	100	100
40	FY	63/188 (34%)	59 (94%)	4 (6%)	0	100	100
41	FZ	129/178 (72%)	123 (95%)	6 (5%)	0	100	100
42	Fa	161/171 (94%)	160 (99%)	1 (1%)	0	100	100
43	Fb	127/151 (84%)	124 (98%)	3 (2%)	0	100	100
44	Fc	82/148 (55%)	81 (99%)	1 (1%)	0	100	100
45	Fd	94/143 (66%)	93 (99%)	1 (1%)	0	100	100
61	F1	54/1041 (5%)	52 (96%)	2 (4%)	0	100	100
62	FF	14/474 (3%)	13 (93%)	1 (7%)	0	100	100
All	All	15235/21299 (72%)	14757 (97%)	472 (3%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CE	385	PRO
36	FP	85	LYS
1	CE	384	ALA
25	F5	495	MET
27	F7	565	LEU

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	CE	325/372 (87%)	320 (98%)	5 (2%)	65	85
2	CF	143/144 (99%)	140 (98%)	3 (2%)	53	79
3	CH	195/246 (79%)	189 (97%)	6 (3%)	40	70
4	CK	147/284 (52%)	141 (96%)	6 (4%)	30	64
5	CO	314/377 (83%)	306 (98%)	8 (2%)	47	75
6	CP	160/168 (95%)	156 (98%)	4 (2%)	47	75
7	CQ	194/297 (65%)	191 (98%)	3 (2%)	65	85
8	CR	130/279 (47%)	126 (97%)	4 (3%)	40	70
9	Ca	449/543 (83%)	437 (97%)	12 (3%)	44	74
10	Cb	132/267 (49%)	127 (96%)	5 (4%)	33	66
11	Cd	168/381 (44%)	167 (99%)	1 (1%)	86	94
12	Cj	193/219 (88%)	191 (99%)	2 (1%)	76	90
13	Cn	22/210 (10%)	21 (96%)	1 (4%)	27	60
14	Cp	166/175 (95%)	162 (98%)	4 (2%)	49	76
15	DD	691/711 (97%)	681 (99%)	10 (1%)	67	86
16	DI	350/365 (96%)	348 (99%)	2 (1%)	86	94
17	DL	173/263 (66%)	168 (97%)	5 (3%)	42	72
18	DO	170/229 (74%)	167 (98%)	3 (2%)	59	82
19	DP	191/239 (80%)	189 (99%)	2 (1%)	76	90
20	DR	221/235 (94%)	215 (97%)	6 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	DU	179/201 (89%)	173 (97%)	6 (3%)	37	69
22	DZ	25/84 (30%)	25 (100%)	0	100	100
23	F2	763/867 (88%)	754 (99%)	9 (1%)	71	88
24	F3	748/809 (92%)	729 (98%)	19 (2%)	47	75
25	F5	293/642 (46%)	283 (97%)	10 (3%)	37	69
26	F6	401/590 (68%)	393 (98%)	8 (2%)	55	80
27	F7	554/577 (96%)	538 (97%)	16 (3%)	42	72
28	F8	410/561 (73%)	404 (98%)	6 (2%)	65	85
29	F9	175/504 (35%)	170 (97%)	5 (3%)	42	72
30	FA	477/526 (91%)	460 (96%)	17 (4%)	35	67
31	FB	322/483 (67%)	316 (98%)	6 (2%)	57	81
31	FC	272/483 (56%)	265 (97%)	7 (3%)	46	74
32	FE	386/486 (79%)	379 (98%)	7 (2%)	59	82
33	FJ	314/323 (97%)	308 (98%)	6 (2%)	57	81
34	FM	257/292 (88%)	250 (97%)	7 (3%)	44	74
34	FN	251/292 (86%)	246 (98%)	5 (2%)	55	80
35	FO	281/290 (97%)	274 (98%)	7 (2%)	47	75
36	FP	270/286 (94%)	262 (97%)	8 (3%)	41	71
37	FQ	211/264 (80%)	203 (96%)	8 (4%)	33	66
37	FR	206/264 (78%)	199 (97%)	7 (3%)	37	69
37	FS	238/264 (90%)	232 (98%)	6 (2%)	47	75
37	FT	200/264 (76%)	194 (97%)	6 (3%)	41	71
37	FU	222/264 (84%)	218 (98%)	4 (2%)	59	82
38	FW	223/234 (95%)	222 (100%)	1 (0%)	91	96
39	FX	178/195 (91%)	176 (99%)	2 (1%)	73	89
40	FY	61/163 (37%)	59 (97%)	2 (3%)	38	69
41	FZ	86/156 (55%)	84 (98%)	2 (2%)	50	77
42	Fa	141/149 (95%)	139 (99%)	2 (1%)	67	86
43	Fb	117/135 (87%)	115 (98%)	2 (2%)	60	83
44	Fc	78/127 (61%)	75 (96%)	3 (4%)	33	66
45	Fd	79/119 (66%)	78 (99%)	1 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	F1	46/895 (5%)	45 (98%)	1 (2%)	52	78
62	FF	16/400 (4%)	16 (100%)	0	100	100
All	All	13014/18193 (72%)	12726 (98%)	288 (2%)	54	78

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	FO	304	ILE
45	Fd	77	VAL
36	FP	303	LEU
37	FS	296	ARG
21	DU	172	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
35	FO	303	HIS
36	FP	212	ASN
38	FW	178	HIS
16	DI	285	GLN
16	DI	175	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
60	CA	459/474 (96%)	190 (41%)	6 (1%)

5 of 190 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
60	CA	3	A
60	CA	4	A
60	CA	5	U
60	CA	6	U
60	CA	7	A

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
60	CA	285	A
60	CA	296	U
60	CA	349	U
60	CA	160	U
60	CA	78	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	UBD	CA	620	60	23,25,26	0.63	0	31,37,40	0.60	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	UBD	CA	620	60	-	3/12/30/31	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CA	620	UBD	O6P-P2-O5P	2.23	119.41	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CA	620	UBD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
60	CA	620	UBD	C3'-O3'-P2-O5P
60	CA	620	UBD	C3'-O3'-P2-O6P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	PO4	FWA	1	-	4,4,4	0.98	0	6,6,6	0.44	0
65	PM8	FcA	1	44	25,31,31	0.73	1 (4%)	30,38,38	0.91	1 (3%)

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
65	PM8	FcA	1	44	-	2/36/38/38	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	FcA	1	PM8	C2-C1	2.37	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	FcA	1	PM8	O1-C1-C2	-2.37	121.19	123.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

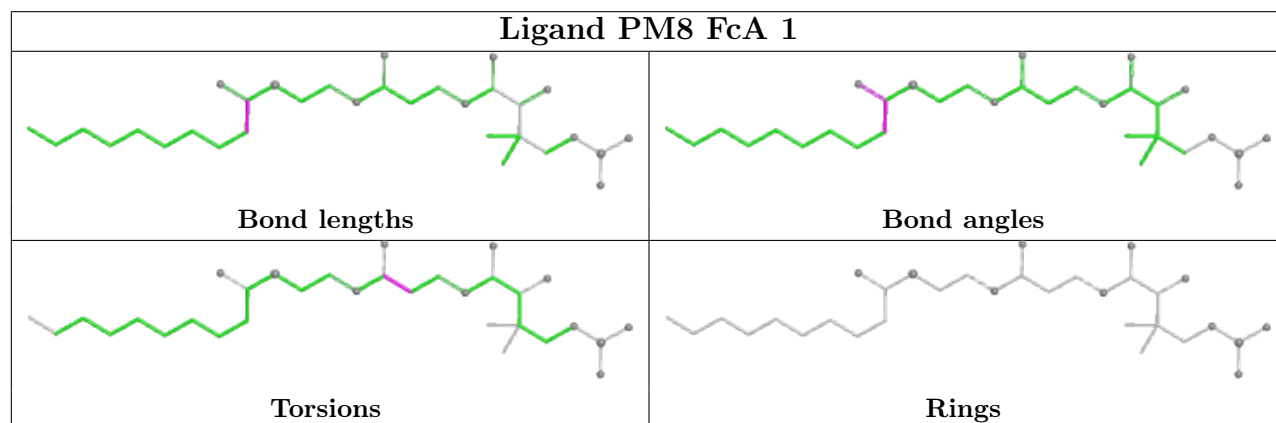
Mol	Chain	Res	Type	Atoms
65	FcA	1	PM8	C37-C38-C39-O40
65	FcA	1	PM8	C37-C38-C39-N41

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	FWA	1	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	UY	13
47	UB	2
60	CA	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UY	347:UNK	C	348:UNK	N	76.88
1	UY	439:UNK	C	440:UNK	N	65.92
1	UB	10:UNK	C	101:UNK	N	45.41
1	UY	338:UNK	C	339:UNK	N	40.51
1	UY	411:UNK	C	412:UNK	N	35.07

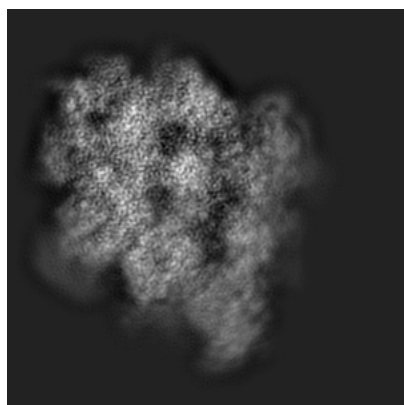
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10177. These allow visual inspection of the internal detail of the map and identification of artifacts.

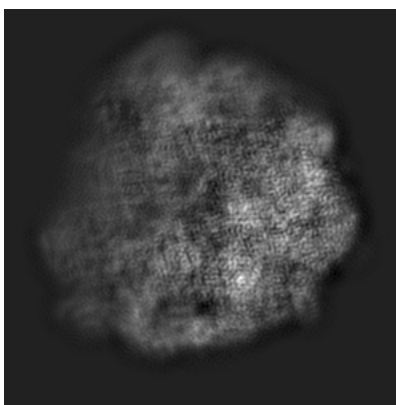
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

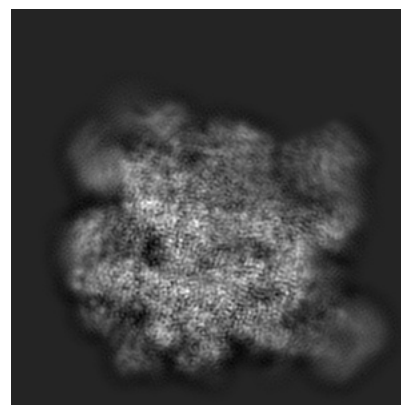
6.1.1 Primary map



X



Y

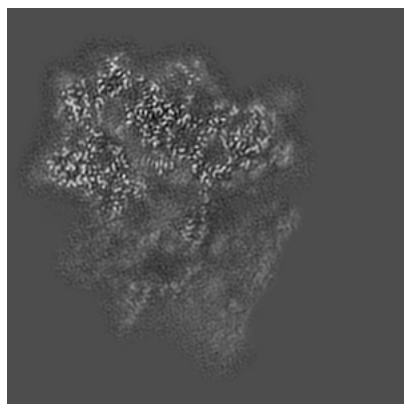


Z

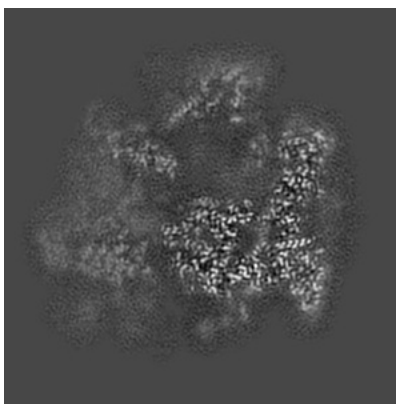
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

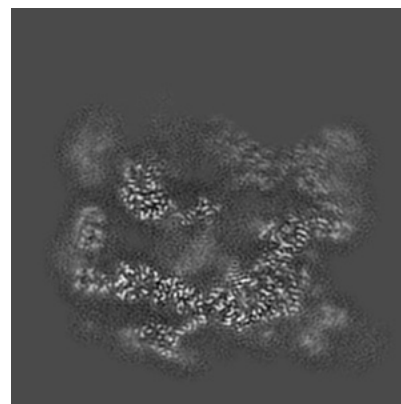
6.2.1 Primary map



X Index: 120



Y Index: 120

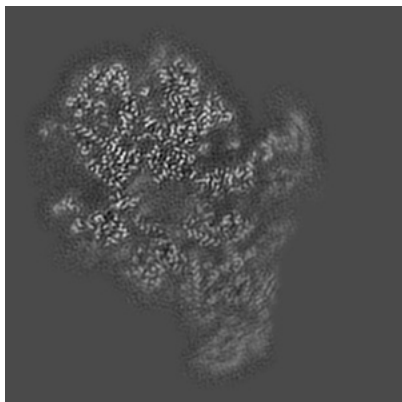


Z Index: 120

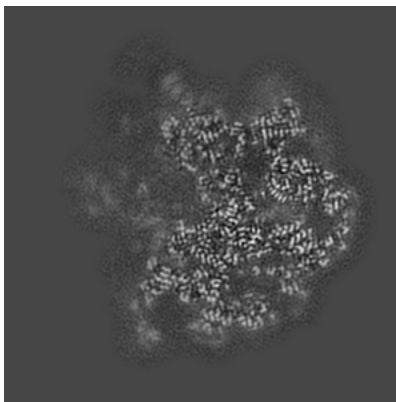
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

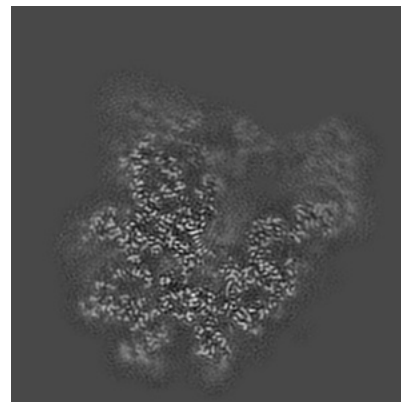
6.3.1 Primary map



X Index: 98



Y Index: 70



Z Index: 140

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 0.0902. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

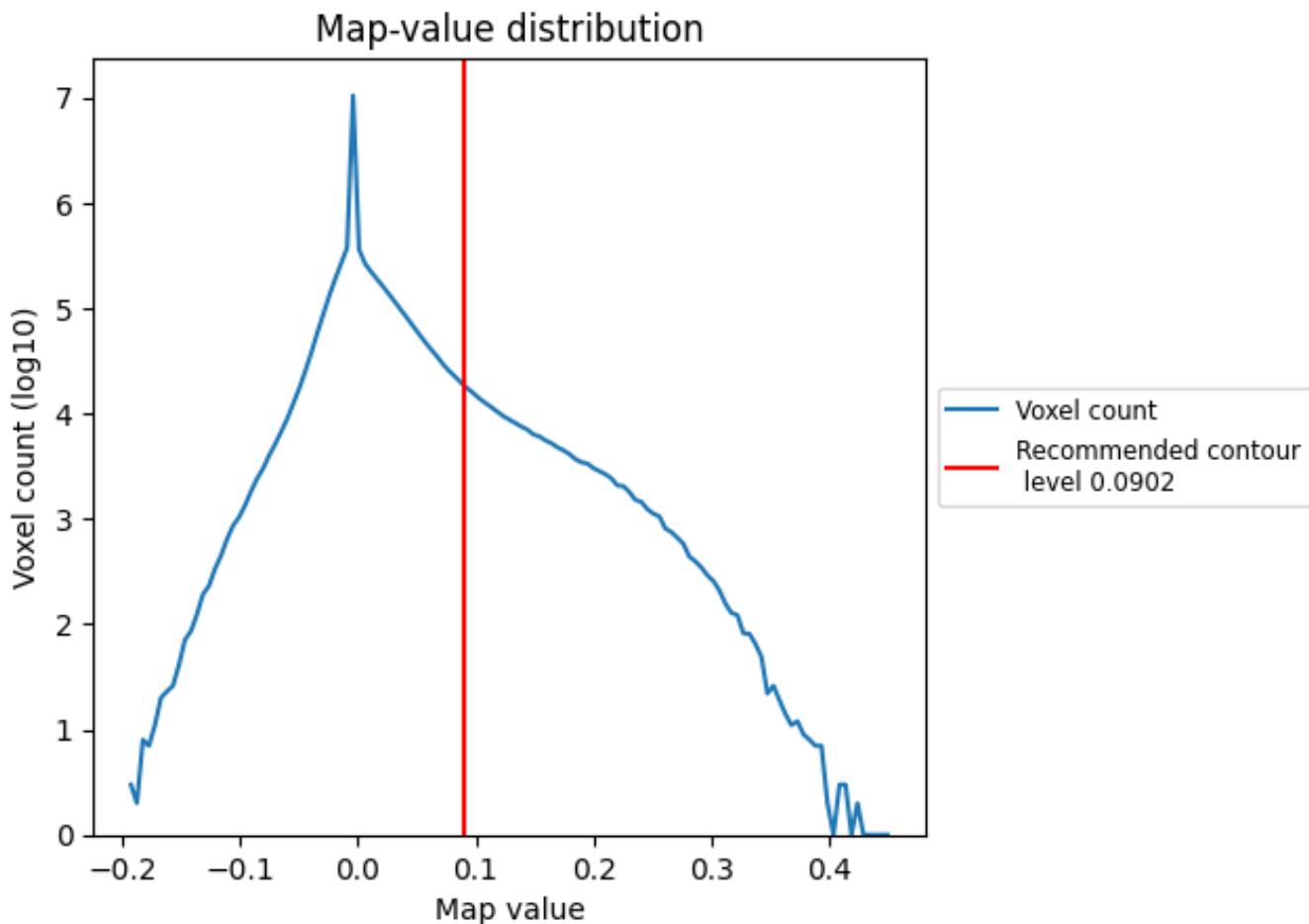
6.5 Mask visualisation

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

7 Map analysis [i](#)

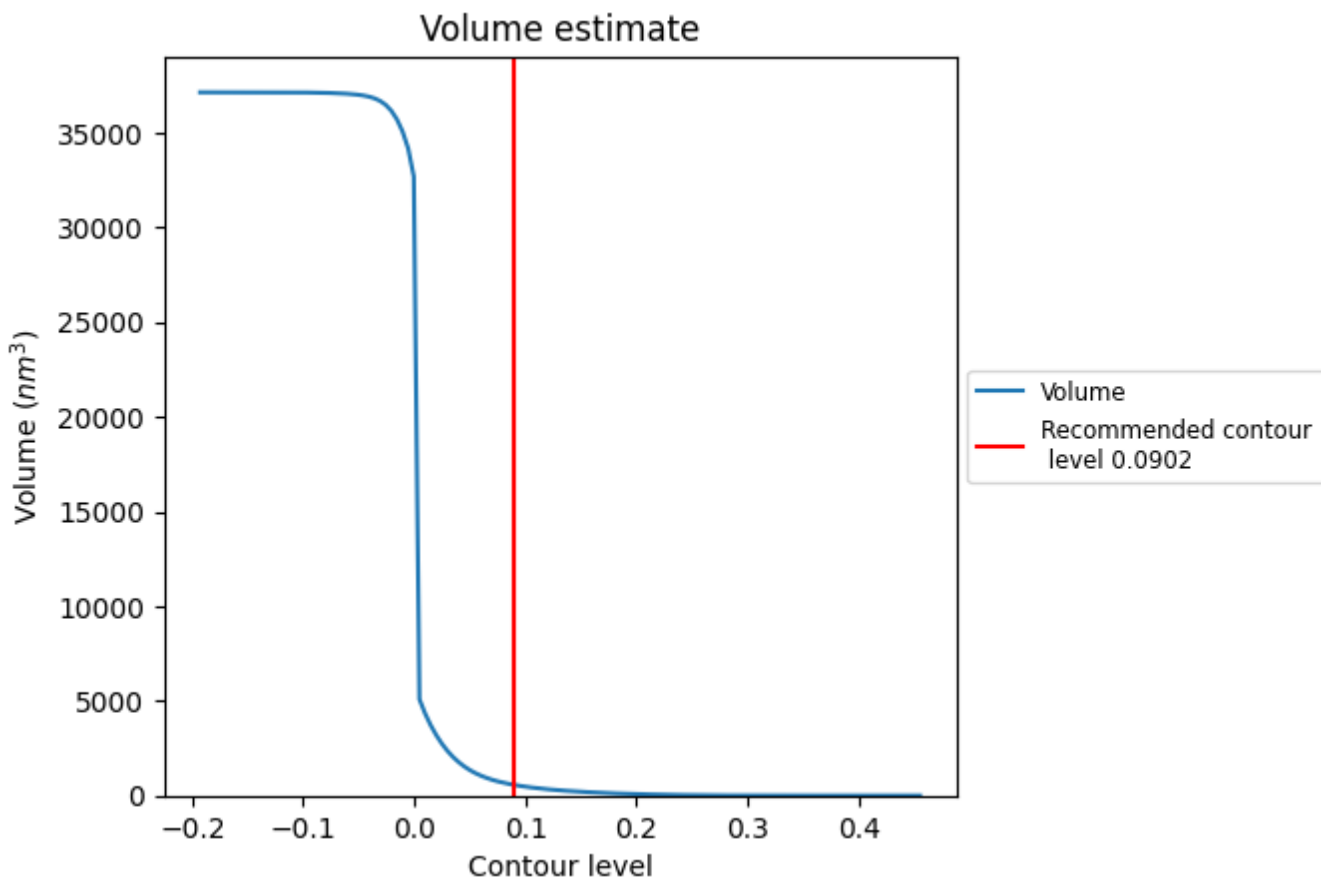
This section contains the results of statistical analysis of the map.

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.

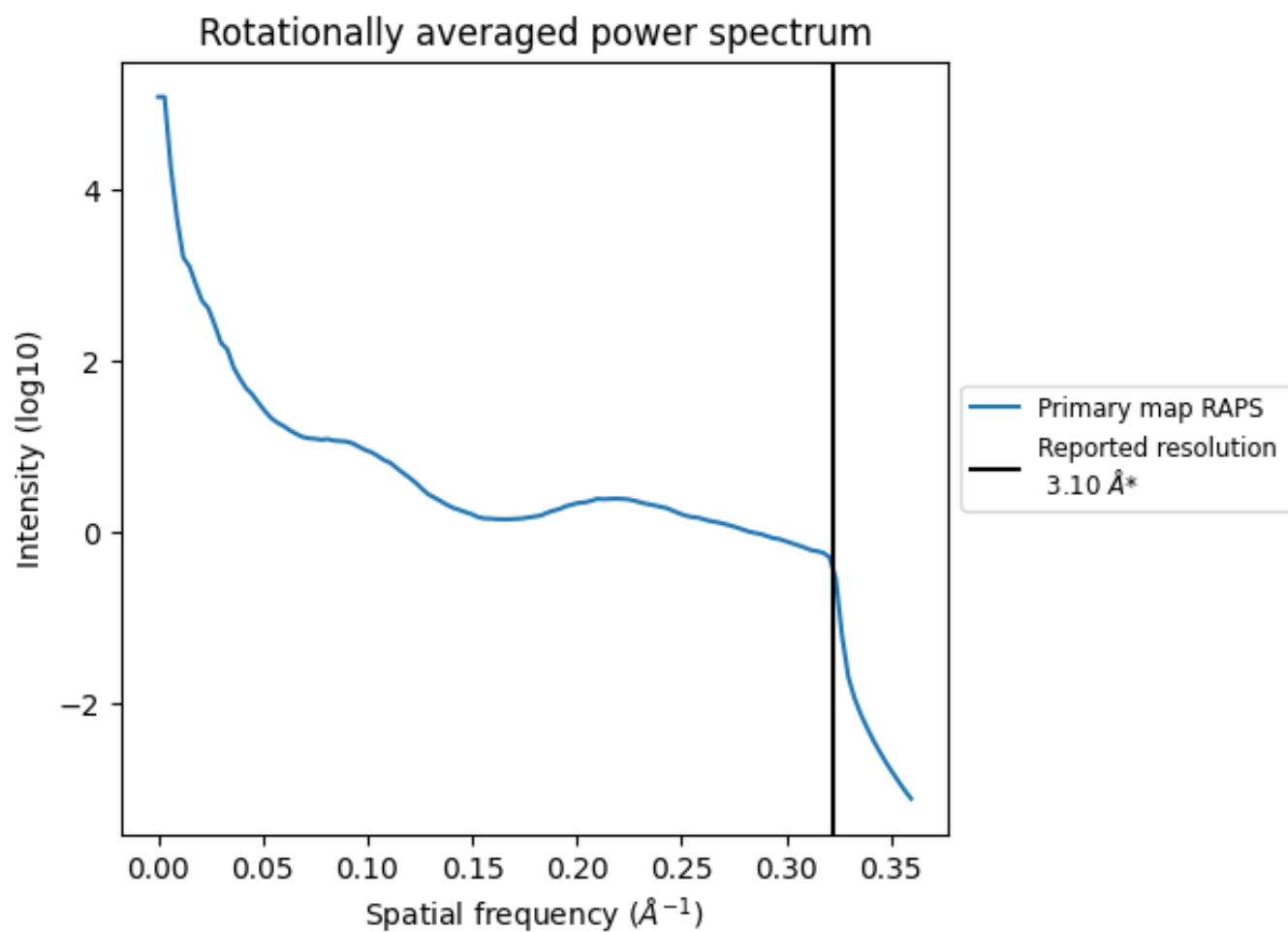
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 505 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 0.323 Å⁻¹

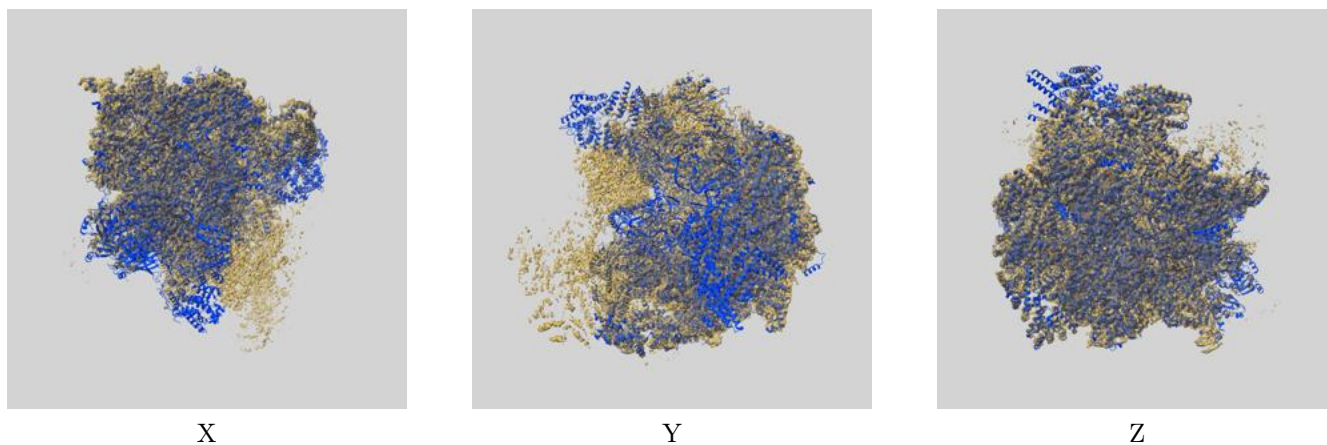
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

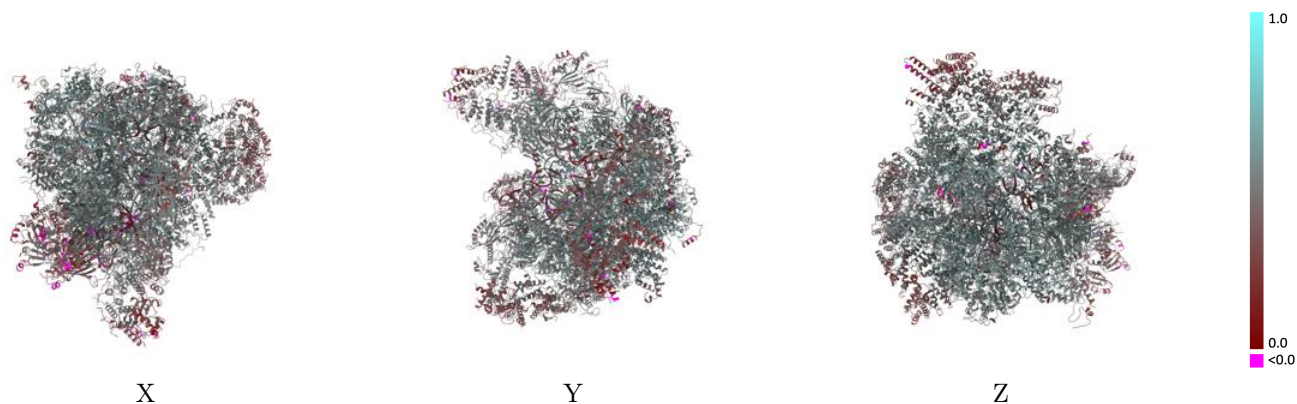
This section contains information regarding the fit between EMDB map EMD-10177 and PDB model 6SGA. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



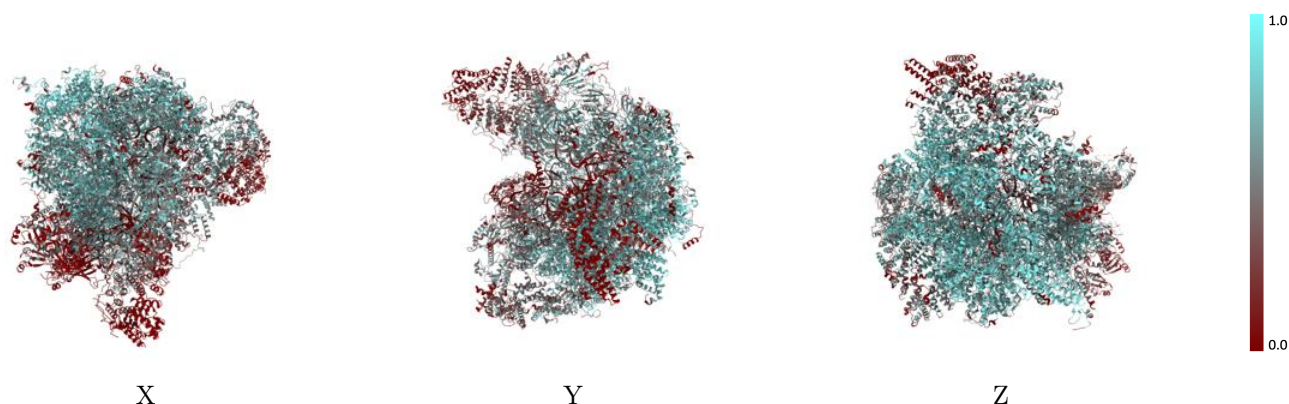
The images above show the 3D surface view of the map at the recommended contour level 0.0902 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



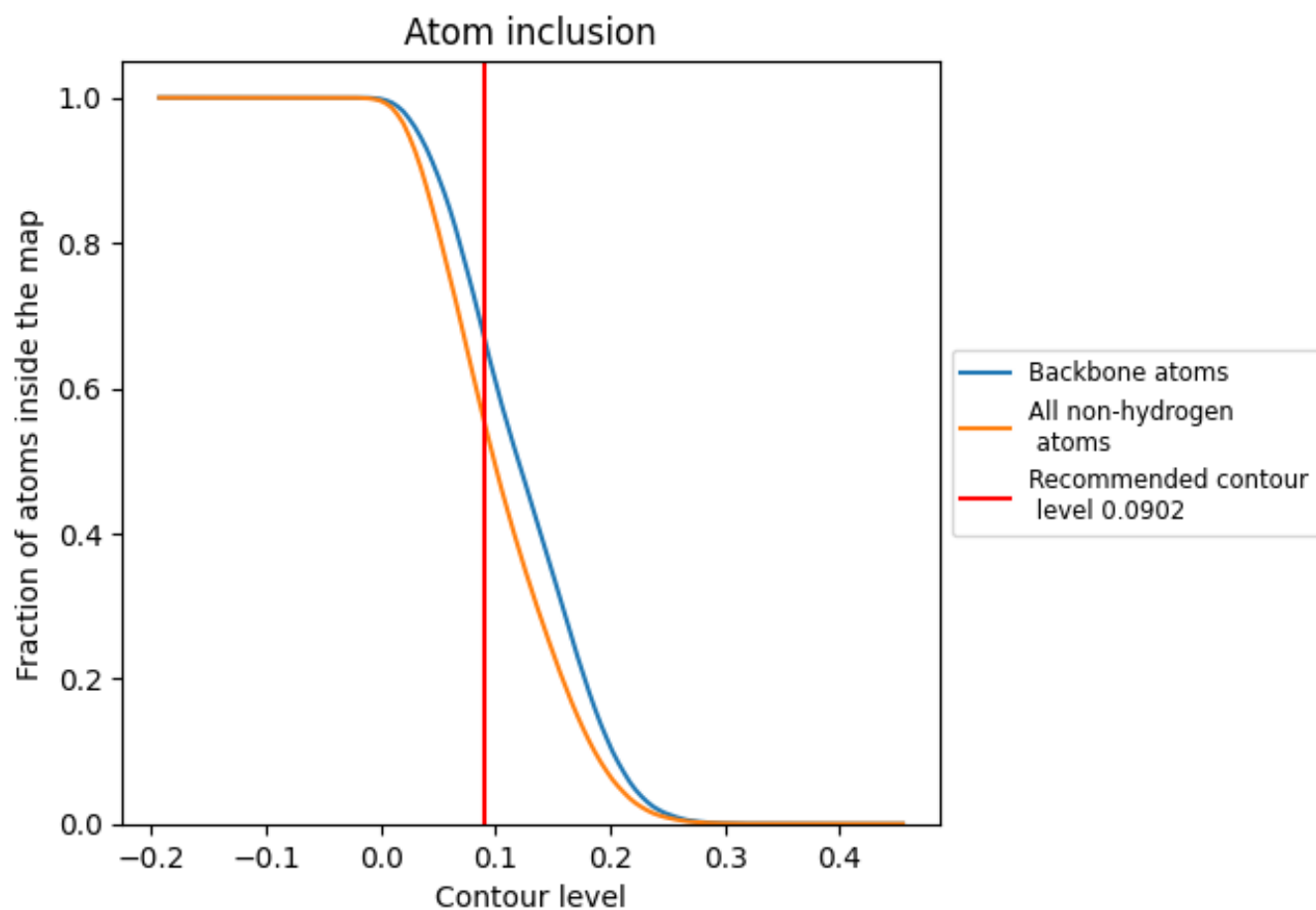
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0902).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 55% 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 (0.0902) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5541	 0.4790
CA	 0.5249	 0.4310
CAA	 1.0000	 0.7430
CAB	 1.0000	 0.7010
CE	 0.6106	 0.5220
CF	 0.6596	 0.5140
CH	 0.6875	 0.5500
CK	 0.4292	 0.4490
CO	 0.7077	 0.5420
CP	 0.7486	 0.5570
CQ	 0.6417	 0.5420
CR	 0.4789	 0.4400
Ca	 0.6410	 0.5160
Cb	 0.4680	 0.4420
Cd	 0.7572	 0.5370
Cj	 0.7928	 0.5500
Cn	 0.1086	 0.4470
Cp	 0.6909	 0.5300
DD	 0.7411	 0.5470
DI	 0.7131	 0.5250
DL	 0.5228	 0.5070
DO	 0.5441	 0.4470
DP	 0.7722	 0.5180
DR	 0.7677	 0.5400
DU	 0.6033	 0.5080
DZ	 0.4821	 0.5020
F1	 0.4227	 0.4860
F2	 0.6897	 0.5150
F3	 0.5808	 0.4640
F5	 0.2911	 0.3750
F6	 0.4466	 0.3890
F7	 0.6707	 0.5050
F8	 0.5692	 0.5030
F9	 0.5704	 0.5100
FA	 0.1772	 0.4120









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Chain	Atom inclusion	Q-score
FB	0.5496	0.5160
FC	0.4655	0.4440
FE	0.6086	0.5240
FF	0.3731	0.4860
FJ	0.3568	0.4750
FM	0.6418	0.5140
FN	0.4921	0.4310
FO	0.7284	0.5410
FP	0.7212	0.5160
FPA	1.0000	0.6700
FQ	0.4885	0.4600
FR	0.4112	0.4420
FS	0.3410	0.4240
FT	0.4497	0.4330
FU	0.3639	0.4180
FW	0.6993	0.5360
FWA	1.0000	0.5460
FWB	1.0000	0.6970
FX	0.7689	0.5160
FY	0.4198	0.4330
FZ	0.0475	0.4030
Fa	0.4439	0.5050
Fb	0.4774	0.3940
Fc	0.4902	0.3850
FcA	0.2812	0.4790
Fd	0.6825	0.5140
FdA	1.0000	0.6870
UA	0.1111	0.2570
UB	0.0062	0.2460
UC	0.6500	0.4240
UD	0.7963	0.4990
UE	0.0815	0.2610
UF	0.4697	0.4310
UG	0.4706	0.4580
UH	0.2333	0.4530
UI	0.5000	0.4280
UJ	0.0521	0.3050
UL	0.3712	0.4080
UM	0.5370	0.4520
UN	0.4167	0.3840
UO	0.2222	0.3200
UP	0.1630	0.3500

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Chain	Atom inclusion	Q-score
UQ	 0.4815	 0.3800
UU	 0.2431	 0.4200
UY	 0.0011	 0.2780