



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 10:48 am GMT

PDB ID : 6SG9  
EMDB ID : EMD-10175  
Title : Head 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 Full wwPDB EM Validation 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.

The types of validation reports are described at

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

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

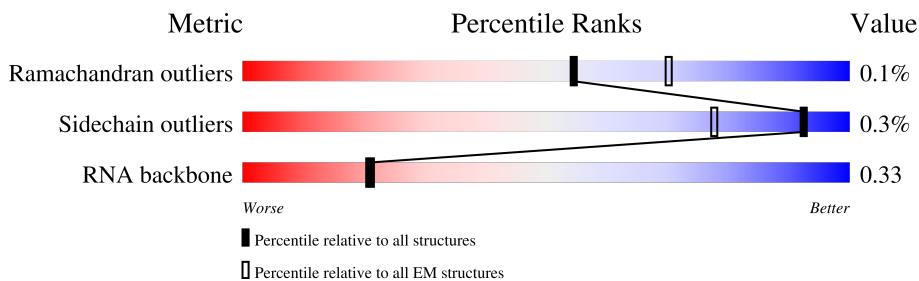
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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



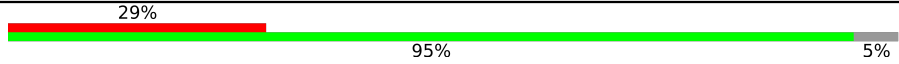
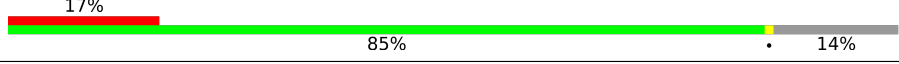
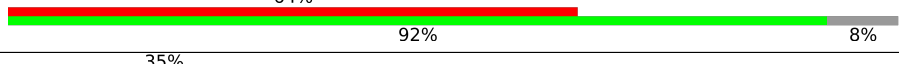

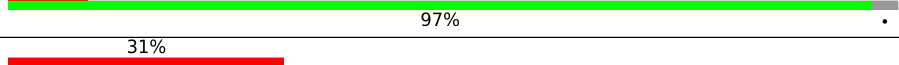
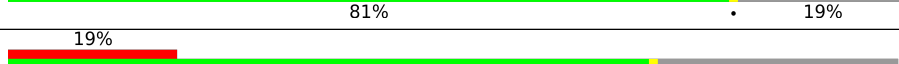
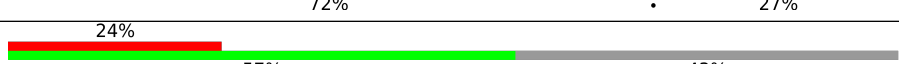
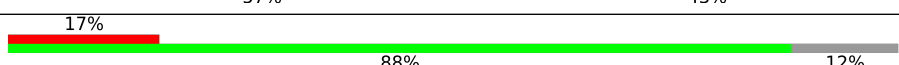
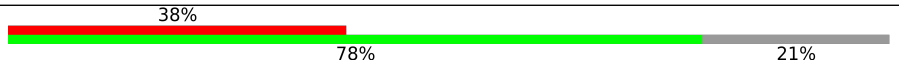

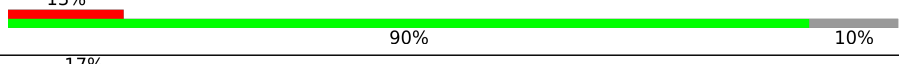
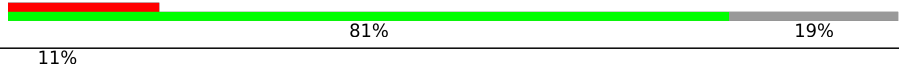
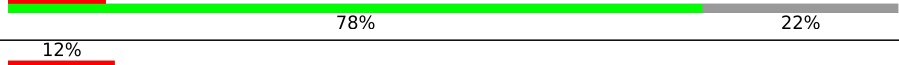

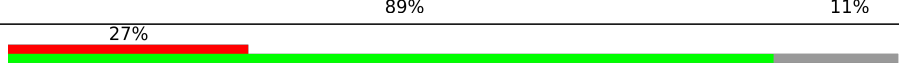


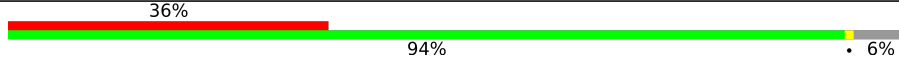







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	CE	435	
2	CK	326	
3	Cn	250	
4	FJ	362	
5	FY	188	
6	Fa	171	
7	CA	802	
8	CC	74	

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Mol	Chain	Length	Quality of chain
9	CI	443	
10	CJ	817	
11	CN	166	
12	CS	244	
13	Cg	498	
14	Ci	181	
15	Ck	874	
16	DB	1181	
17	DC	1165	
18	DE	747	
19	DF	666	
20	DG	631	
21	DH	581	
22	DJ	396	
23	DK	324	
24	DT	247	
25	DV	183	
26	DW	179	
27	DX	169	
28	DY	163	
29	F1	1041	
30	F4	811	
31	FD	579	
32	FF	474	
33	FG	463	

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Mol	Chain	Length	Quality of chain
34	FH	457	10% 69% 31%
35	FI	445	12% 78% 22%
36	FK	372	12% 56% 44%
37	FL	353	16% 90% 9%
38	FV	264	9% 80% 20%
39	Fe	123	21% 98% ..
40	Ua	70	26% 67% 33%
41	Ub	42	71% 100%
42	Uc	12	75% 100%
43	Ud	59	19% 100%
44	Ue	29	76% 100%
45	Uf	9	33% 100%
46	Ug	167	43% 100%
47	Uh	255	99% 100%
48	Ui	32	22% 100%
49	Uj	19	53% 100%
50	Uk	27	26% 100%
51	Ul	14	86% 100%
52	Um	11	36% 100%
53	Ux	108	100%

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 104694 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	23	200	132	35	31	2	0	0

- Molecule 2 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CK	40	337	209	65	62	1	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 3 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Cn	18	154	103	28	23	0	0

- Molecule 4 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	FJ	41	338	208	61	67	2	0	0

- Molecule 5 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	FY	92	723	463	123	131	6	0	0

- Molecule 6 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Fa	39	297	192	55	49	1	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 7 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	CA	146	2501	1098	308	949	146	0	0

- Molecule 8 is a protein called uS3m.

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

- Molecule 9 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CI	423	3357	2108	601	631	17	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CJ	701	5709	3605	1017	1064	23	0	0

- Molecule 11 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	CN	153	1285	820	242	216	7	0	0

- Molecule 12 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CS	85	708	463	121	121	3	0	0

- Molecule 13 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Cg	484	3922	2511	688	703	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 14 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Ci	147	1222	770	226	218	8	0	0

- Molecule 15 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Ck	638	5123	3220	927	953	23	0	0

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	DB	679	5688	3558	1062	1047	21	0	0

- Molecule 17 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	DC	1028	8223	5194	1453	1546	30	0	0

- Molecule 18 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DE	590	4639	2957	832	834	16	0	0

- Molecule 19 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	DF	491	3967	2496	745	703	23	0	0

- Molecule 20 is a protein called mS54.

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

- Molecule 21 is a protein called mS55 (KRIPP8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DH	472	3849	2417	720	693	19	0	0

- Molecule 22 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	DJ	308	2521	1612	446	450	13	0	0

- Molecule 23 is a protein called mS58.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	DK	245	1929	1213	349	362	5	0	0

- Molecule 24 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	DT	221	1912	1231	334	337	10	0	0

- Molecule 25 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	DV	157	1323	840	248	231	4	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	DW	133	1140	730	216	190	4	0	0

- Molecule 27 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	DX	115	967	612	182	166	7	0	0

- Molecule 28 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	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	conflict	UNP Q57YD4

- Molecule 29 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	F1	833	6729	4212	1265	1213	39	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 30 is a protein called mt-SAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	F4	541	4382	2783	775	802	22	0	0

- Molecule 31 is a protein called mt-SAF12 (KRIPP18).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	FD	394	3135	2004	546	566	19	0	0

- Molecule 32 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	FF	408	3265	2052	586	603	24	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 33 is a protein called mt-SAF15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	FG	169	1359	852	260	240	7	0	0

- Molecule 34 is a protein called mt-SAF16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	FH	317	2486	1555	440	471	20	0	0

- Molecule 35 is a protein called mt-SAF17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	FI	348	2786	1726	510	537	13	0	0

- Molecule 36 is a protein called mt-SAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	FK	208	1699	1084	284	325	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FK	38	HIS	ARG	conflict	UNP Q57XS8

- Molecule 37 is a protein called mt-SAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	FL	320	2555	1609	470	459	17	0	0

- Molecule 38 is a protein called mt-SAF25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	FV	210	1636	1039	283	303	11	0	0

- Molecule 39 is a protein called mt-SAF34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Fe	122	1033	642	200	184	7	0	0

- Molecule 40 is a protein called UNK-a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	Ua	47	282	188	47	47	0	0

- Molecule 41 is a protein called UNK-b.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	Ub	42	252	168	42	42	0	0

- Molecule 42 is a protein called UNK-c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	Uc	12	72	48	12	12	0	0

- Molecule 43 is a protein called UNK-d.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	Ud	59	354	236	59	59	0	0

- Molecule 44 is a protein called UNK-e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	Ue	29	174	116	29	29	0	0

- Molecule 45 is a protein called UNK-f.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	Uf	9	54	36	9	9	0	0

- Molecule 46 is a protein called UNK-g.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	Ug	167	1002	668	167	167	0	0

- Molecule 47 is a protein called UNK-h.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	Uh	255	1530	1020	255	255	0	0

- Molecule 48 is a protein called UNK-i.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	Ui	32	192	128	32	32	0	0

- Molecule 49 is a protein called UNK-j.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	Uj	19	114	76	19	19	0	0

- Molecule 50 is a protein called UNK-k.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	Uk	27	162	108	27	27	0	0

- Molecule 51 is a protein called UNK-l.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	Ul	14	84	56	14	14	0	0

- Molecule 52 is a protein called UNK-m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	Um	11	66	44	11	11	0	0

- Molecule 53 is a protein called UNK-x.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	Ux	108	648	432	108	108	0	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

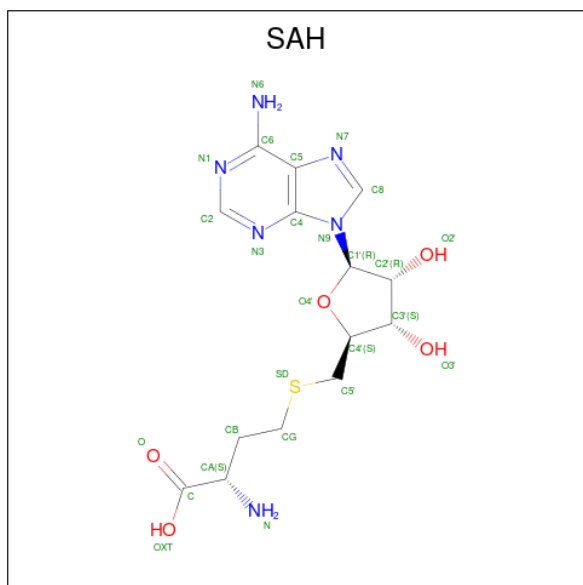
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	CgB	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	F1A	1	Total	Zn	0
			1	1	
56	FGA	1	Total	Zn	0
			1	1	
56	FLA	1	Total	Zn	0
			1	1	
56	FLB	1	Total	Zn	0
			1	1	
56	FeA	1	Total	Zn	0
			1	1	

- Molecule 57 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					AltConf
57	F1B	1	Total	C	N	O	S	0
			26	14	6	5	1	
57	FFA	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 58 is water.

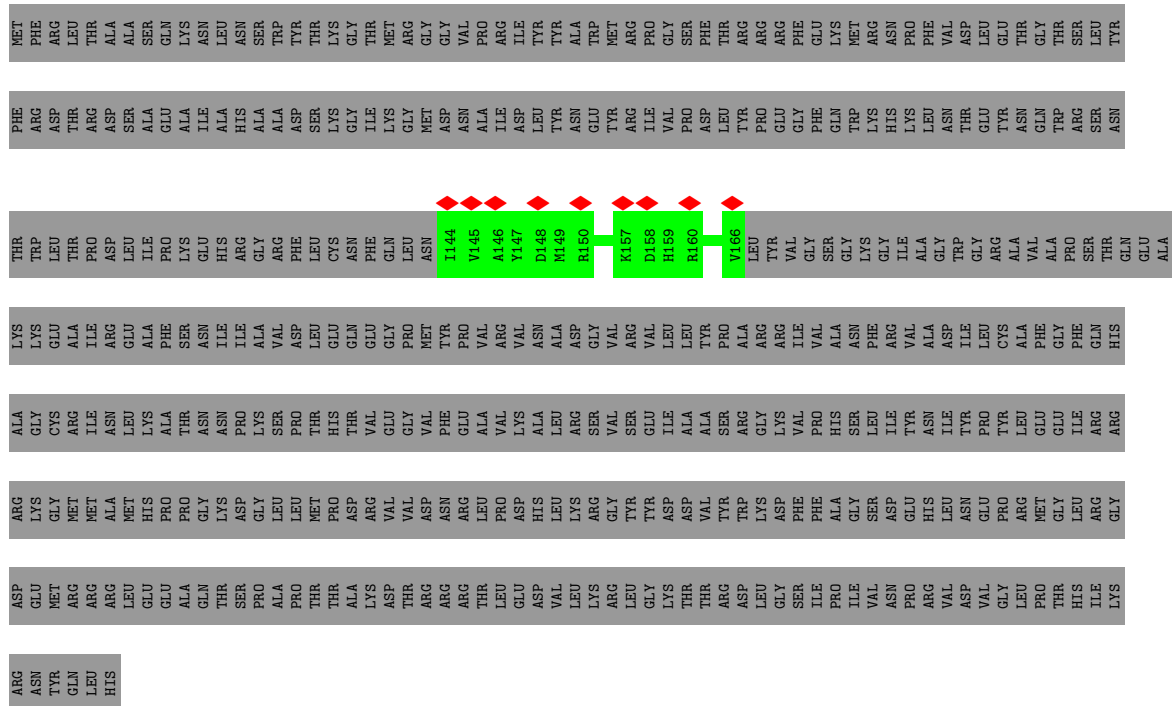
Mol	Chain	Residues	Atoms		AltConf
58	CgC	3	Total	O	0
			3	3	

### 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.

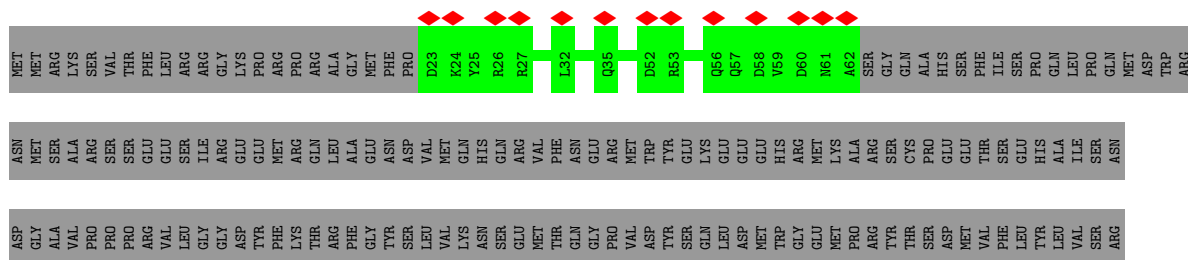
- Molecule 1: uS5m

Chain CE:  5% 95%



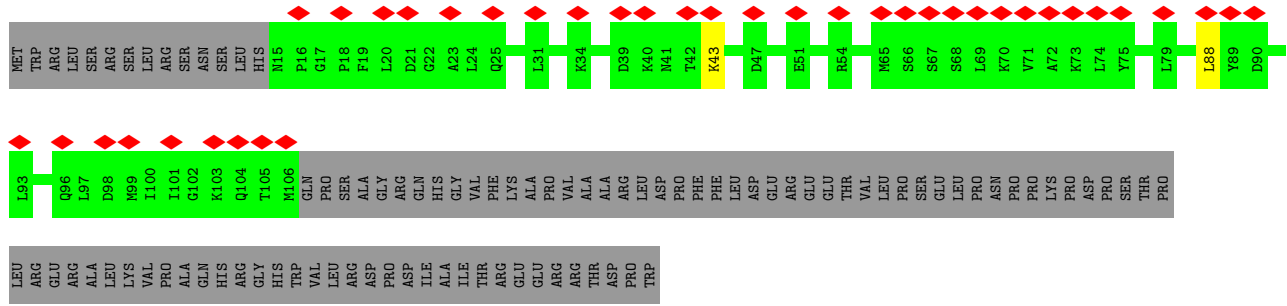
- Molecule 2: uS11m

Chain CK:  12% 88%

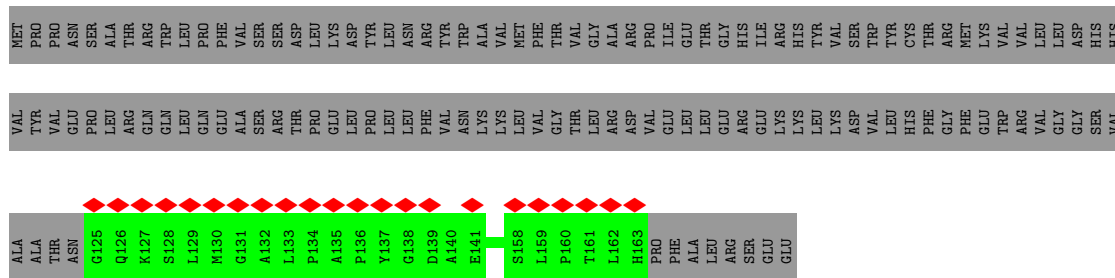




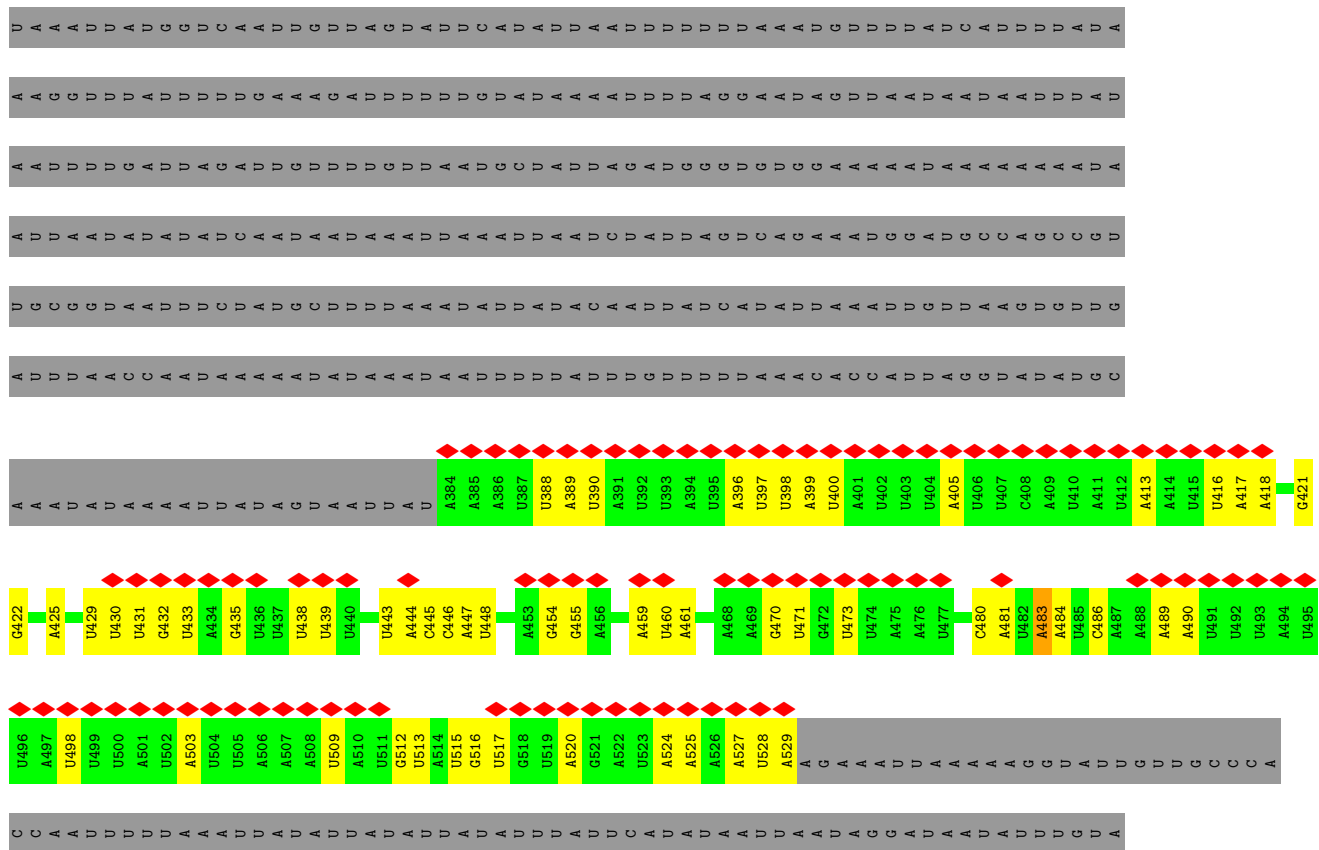




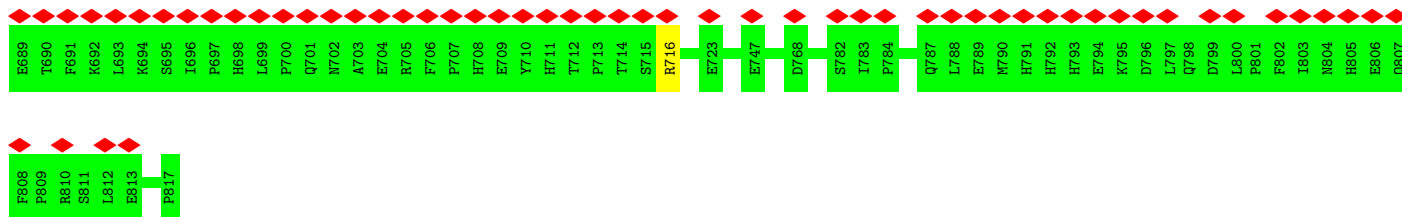
• Molecule 6: mt-SAF30



• Molecule 7: 9S rRNA

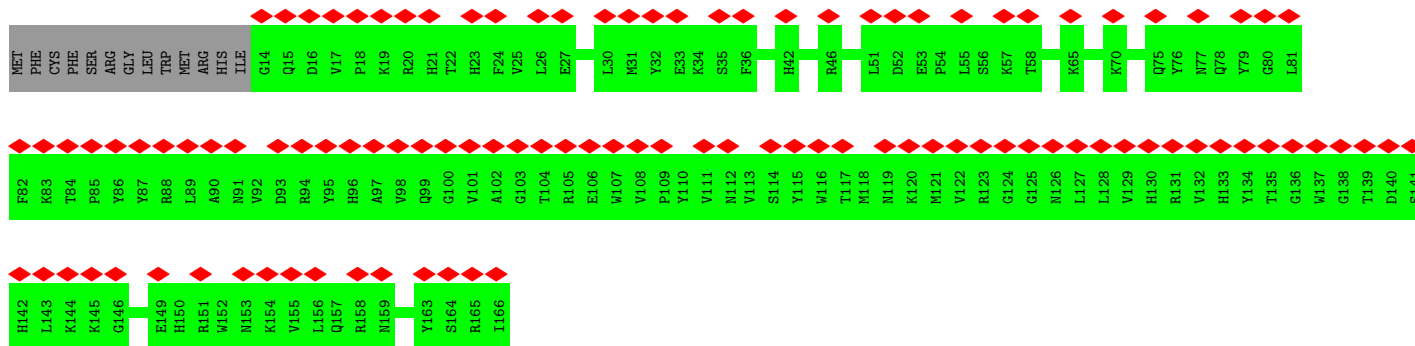






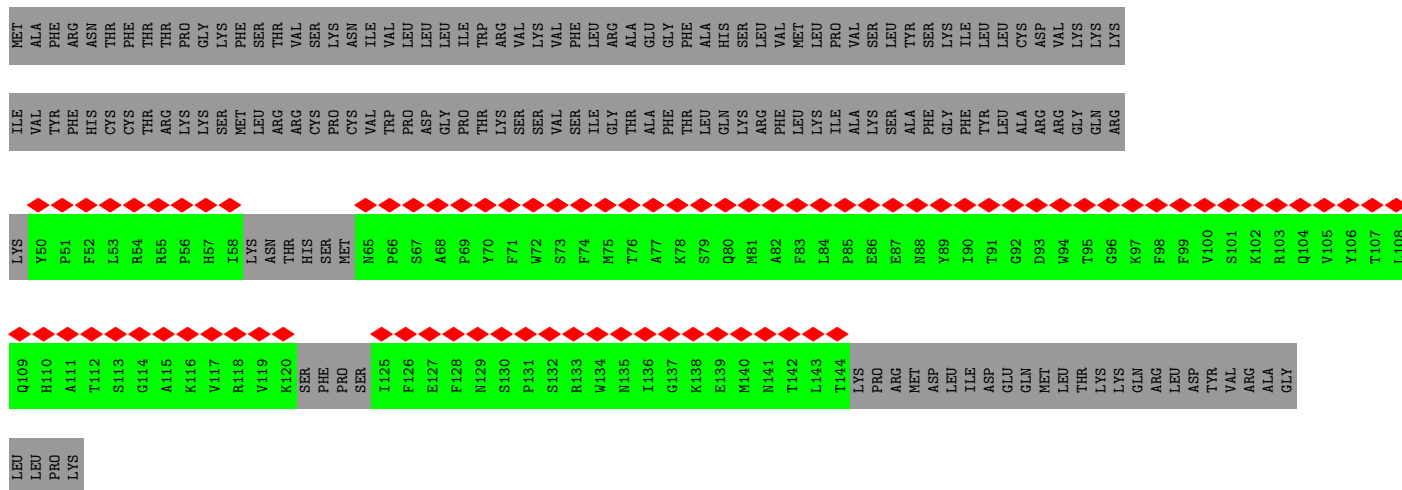
## ● Molecule 11: uS14m

Chain CN: 64% 92% 8%



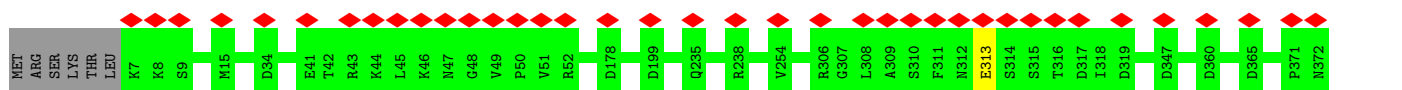
## ● Molecule 12: uS19m

Chain CS: 35% 35% 65%

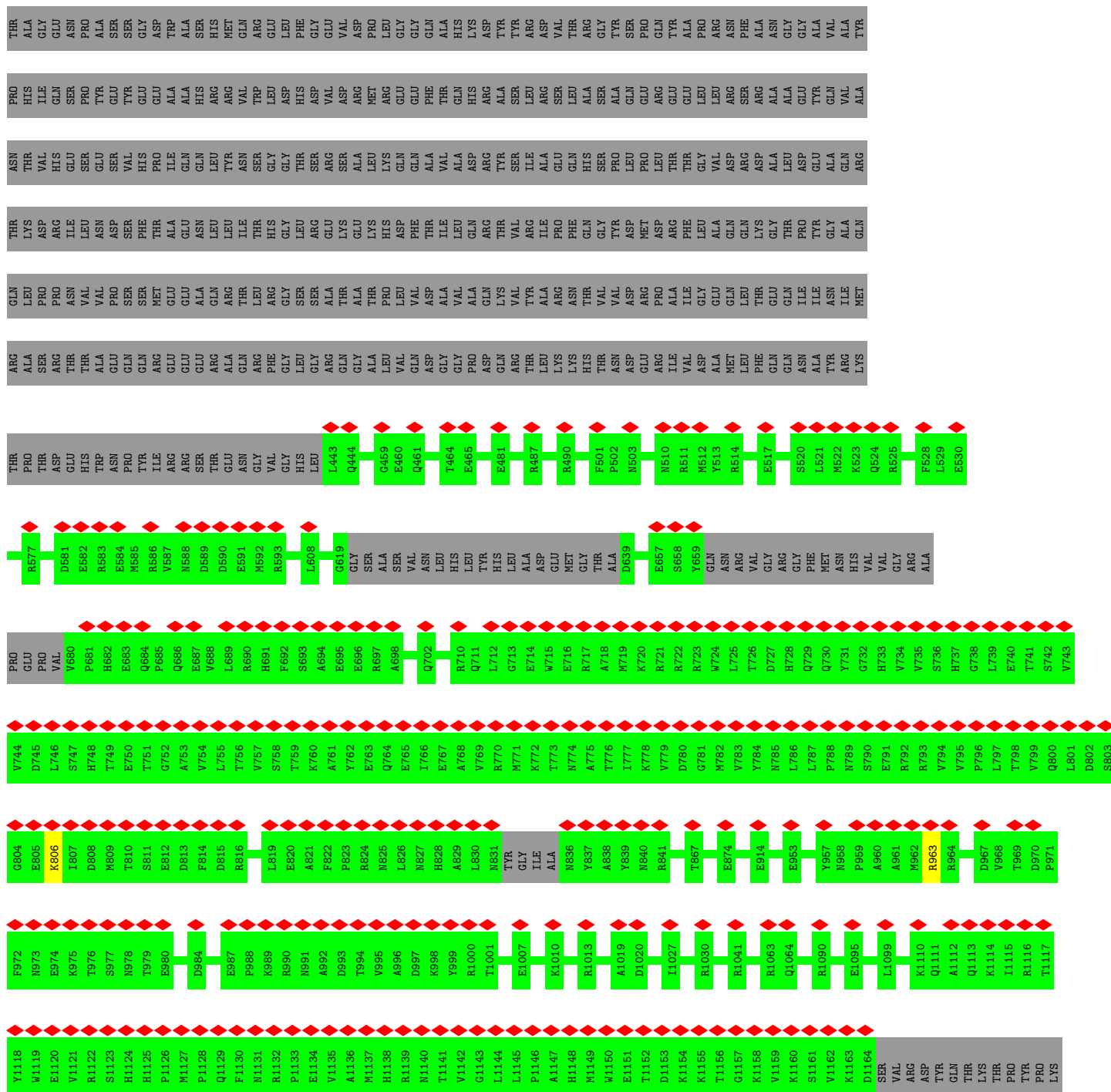


## ● Molecule 13: mS29

Chain Cg: 9% 97%



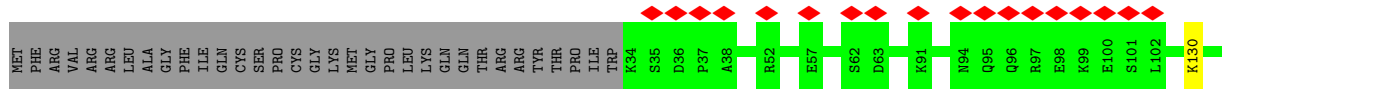
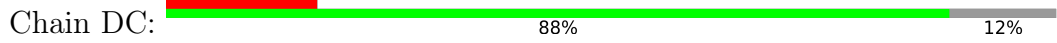


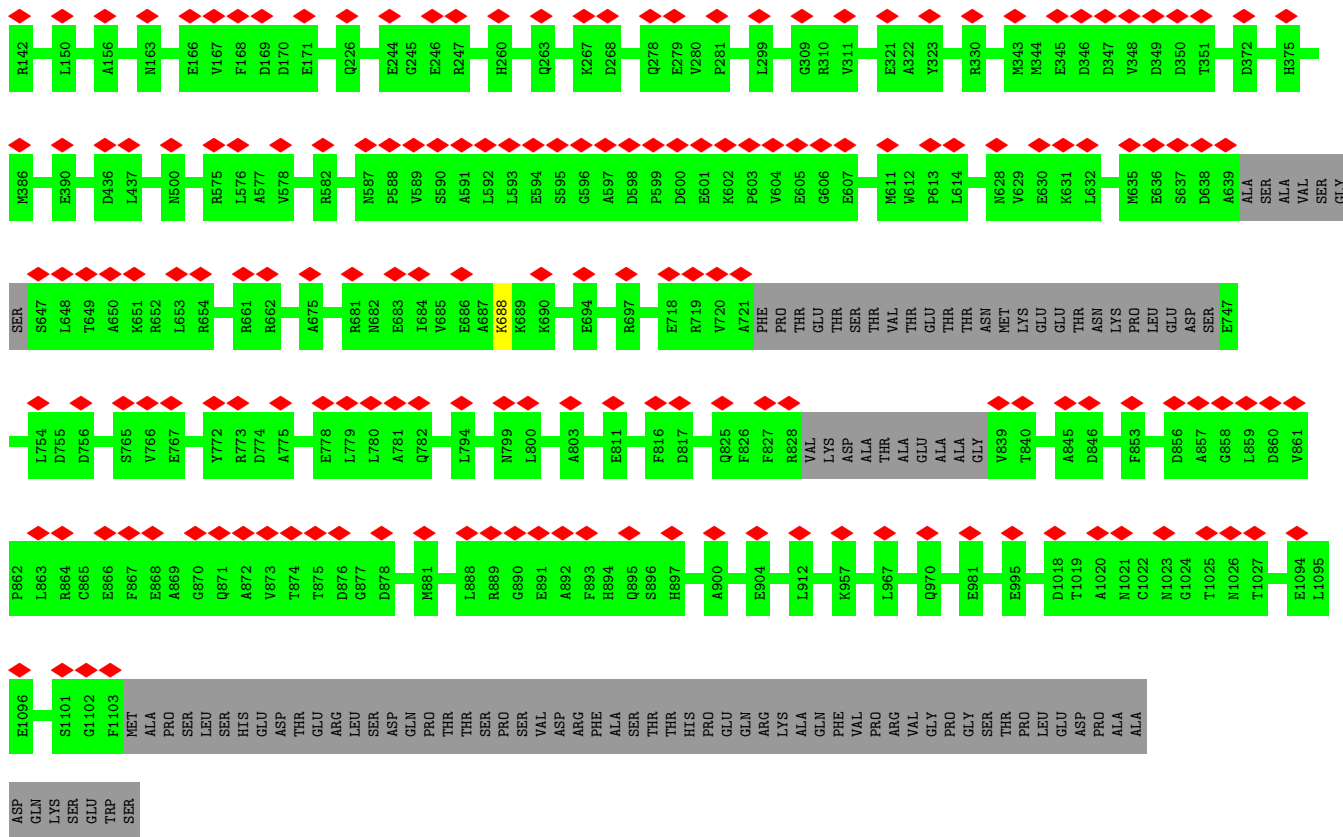


TRP  
VAL  
GLN  
LEU

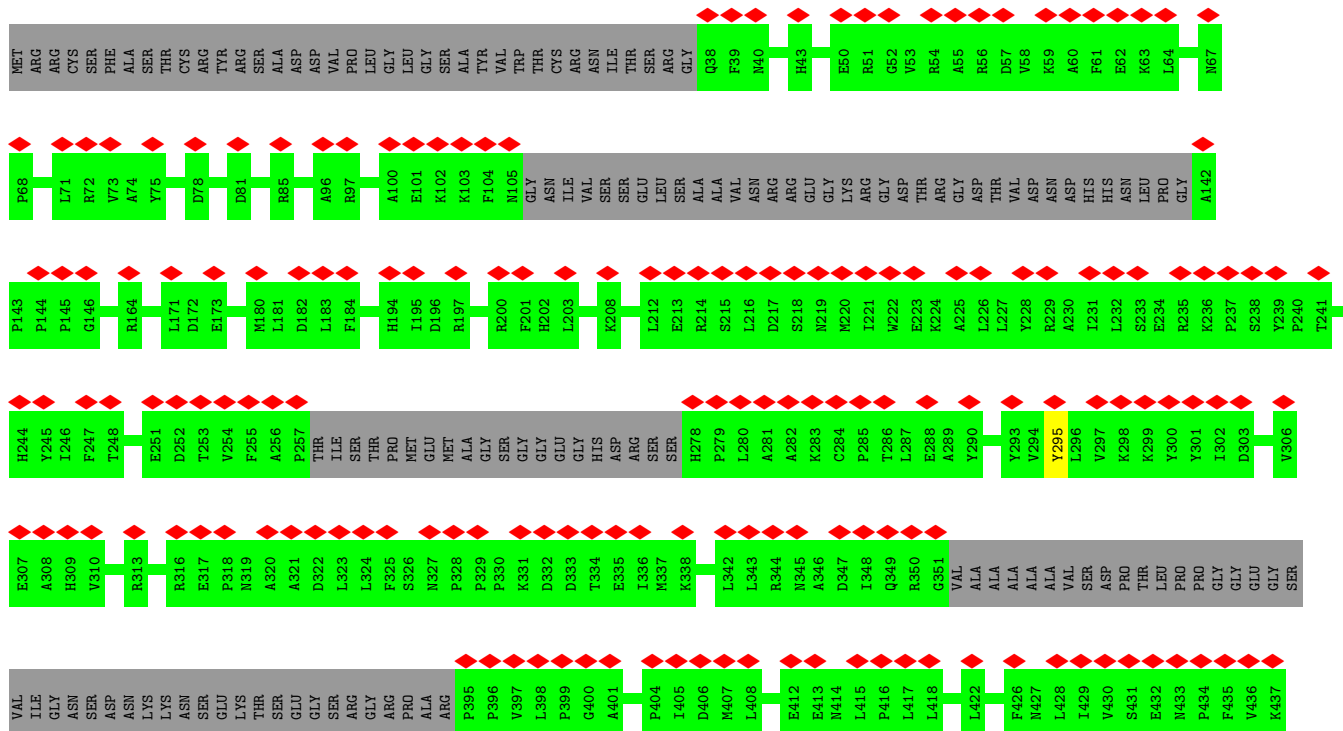
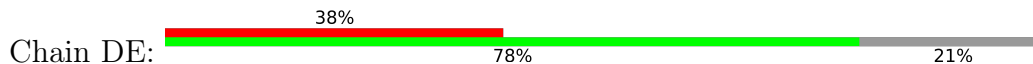
• Molecule 17: mS50

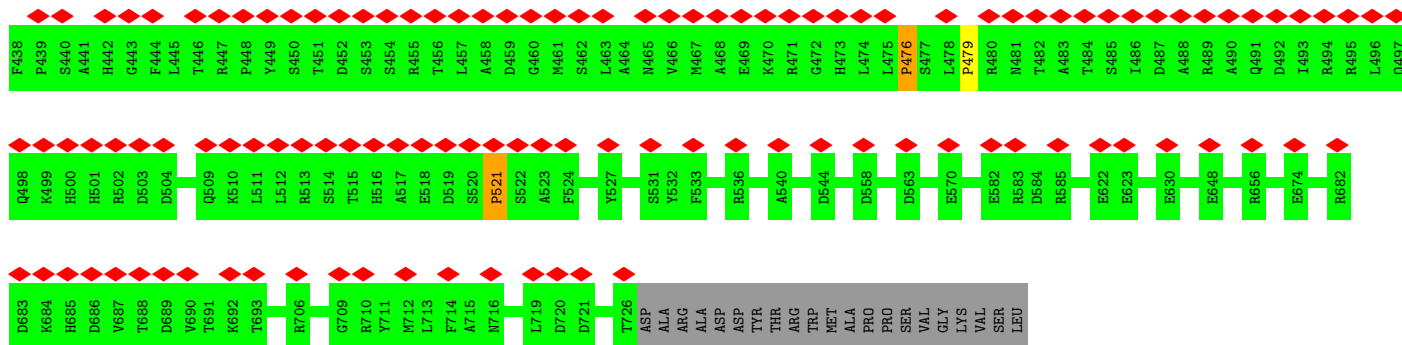
17%



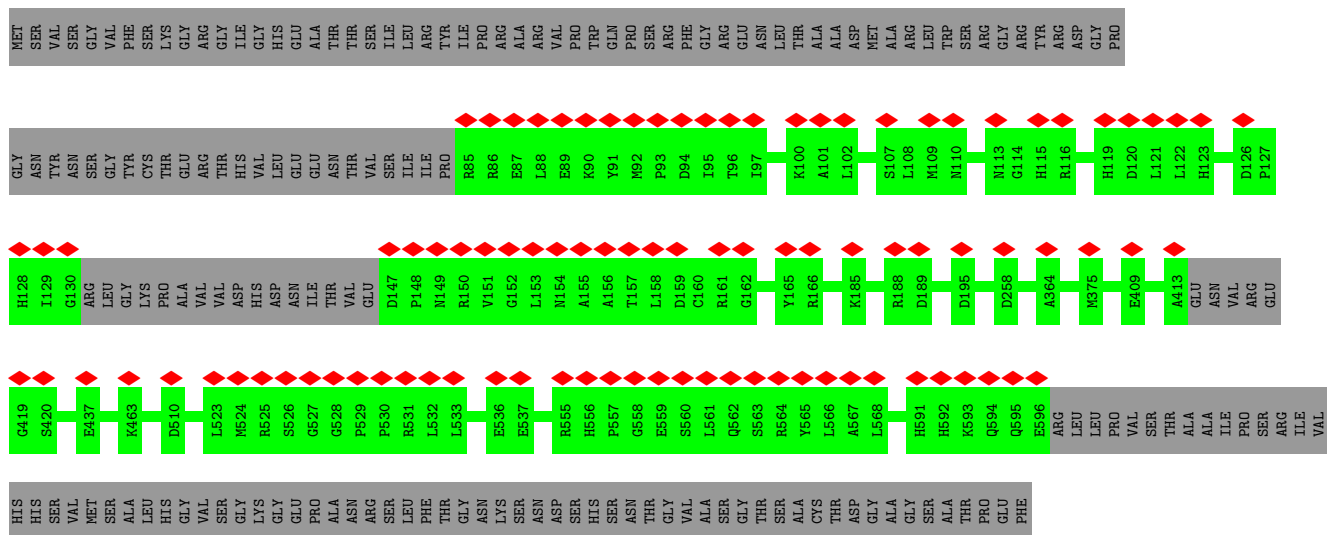
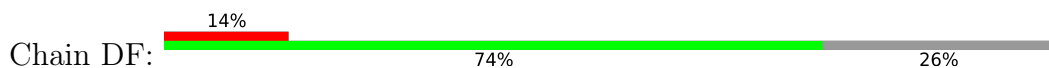


• Molecule 18: mS52

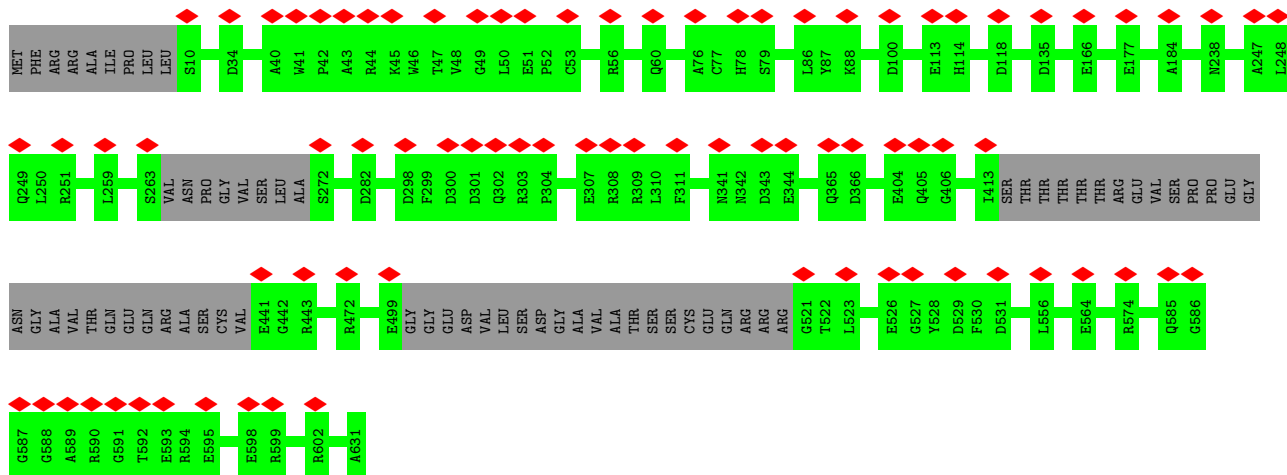




• Molecule 19: mS53



• Molecule 20: mS54



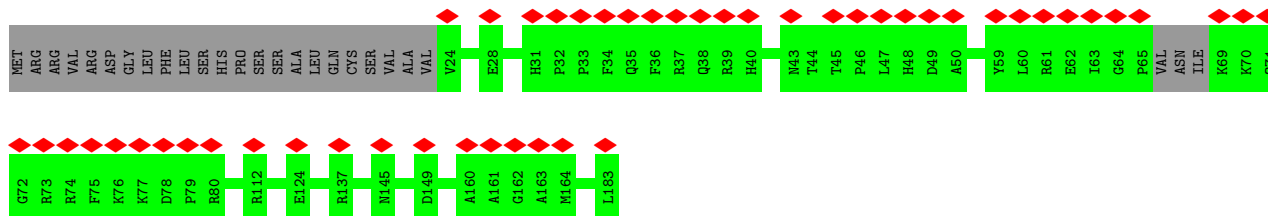
• Molecule 21: mS55 (KRIPP8)





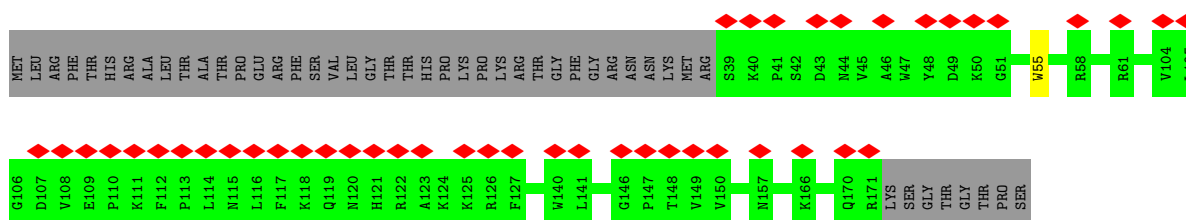
- Molecule 25: mS69

Chain DV: 27% 86% 14%



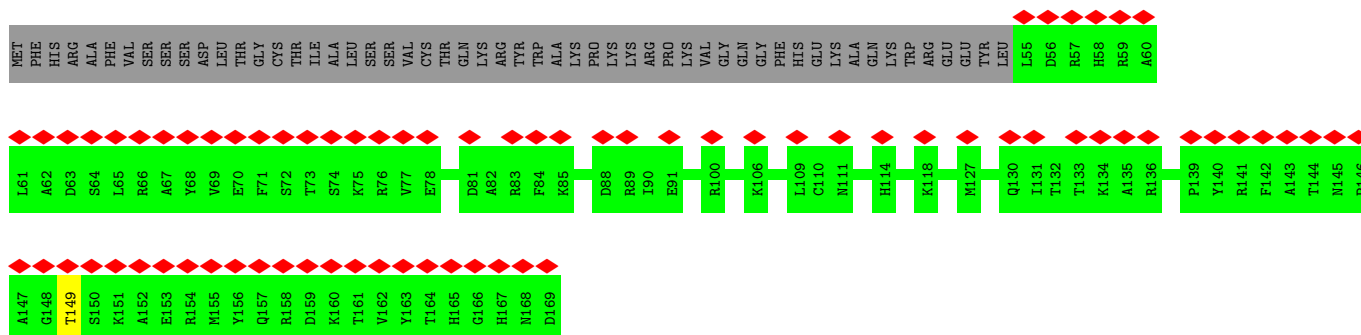
- Molecule 26: mS70

Chain DW: 25% 74% 26%



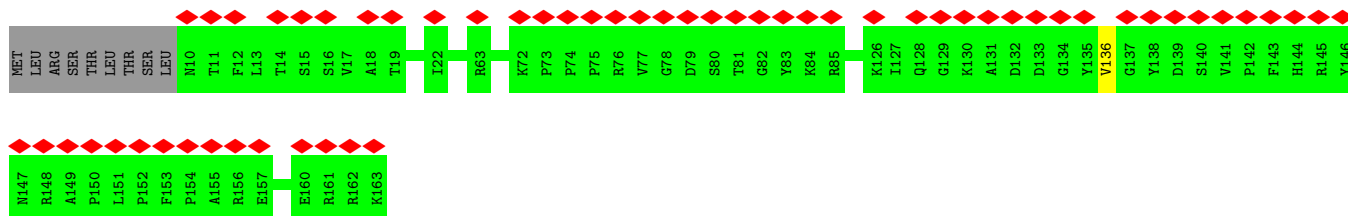
- Molecule 27: mS71

Chain DX: 44% 67% 32%



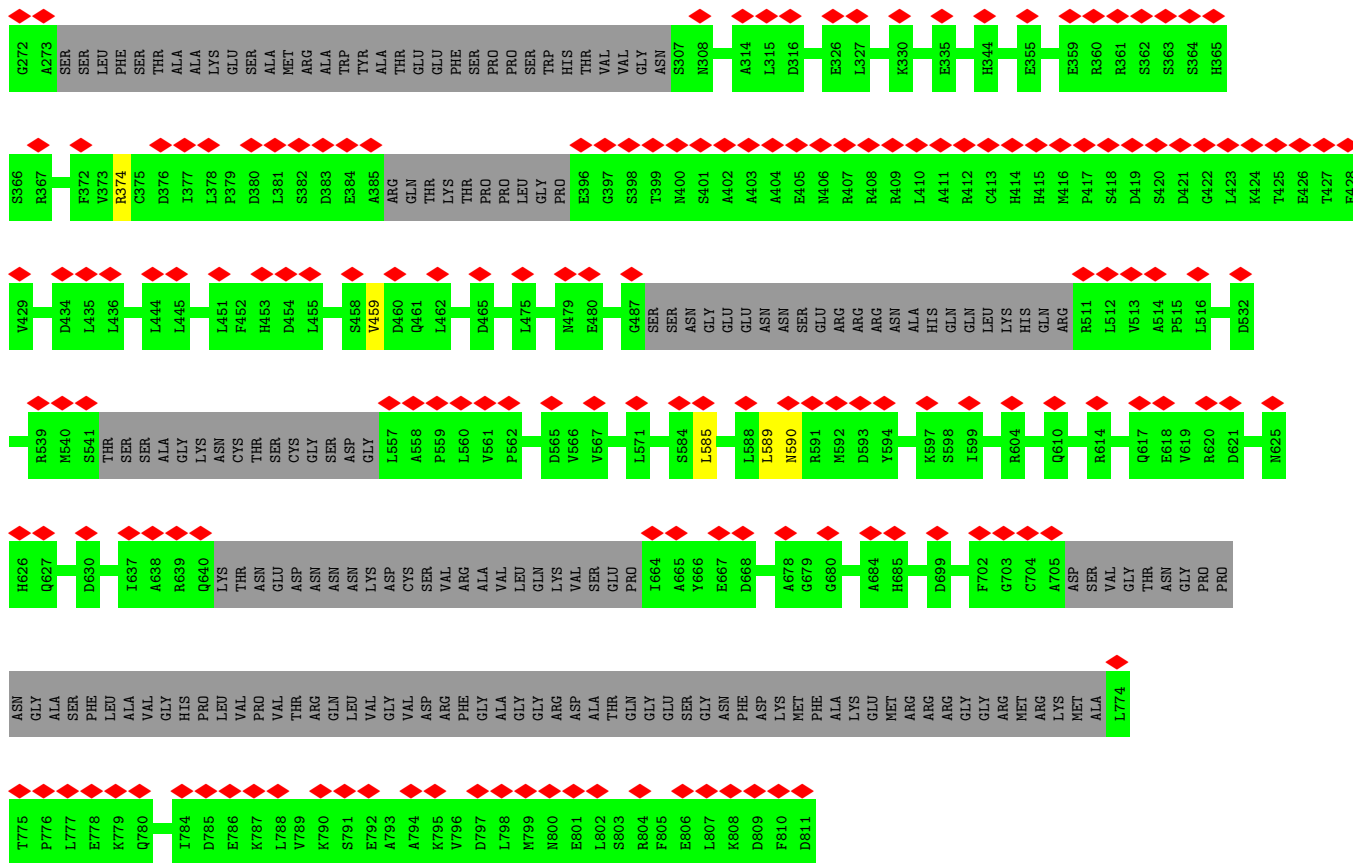
- Molecule 28: mS72

Chain DY: 36% 94% 6%

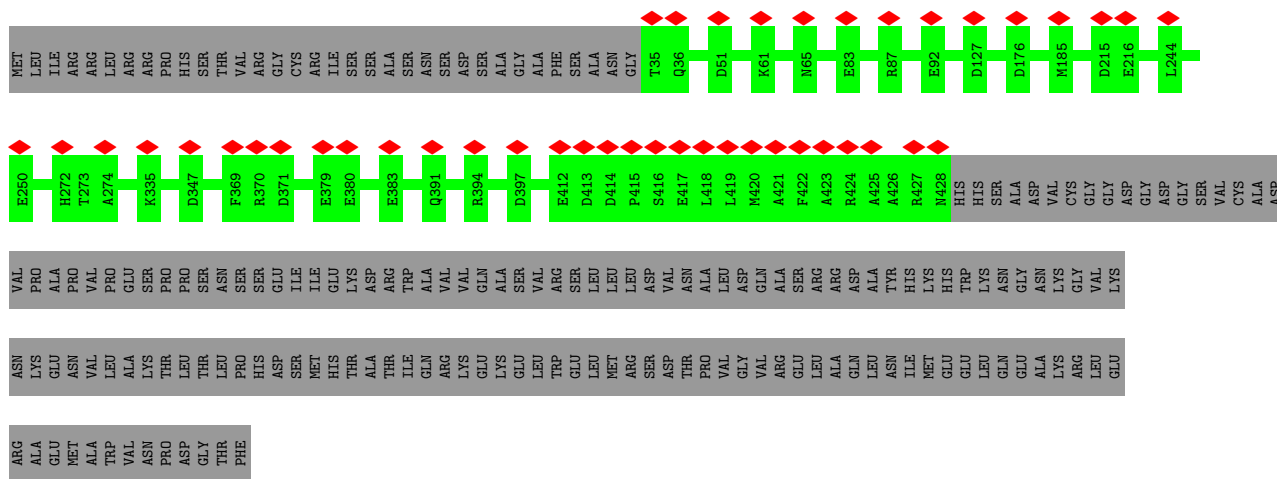


- Molecule 29: mt-SAF1 (RSM22)

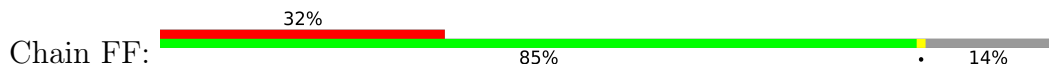


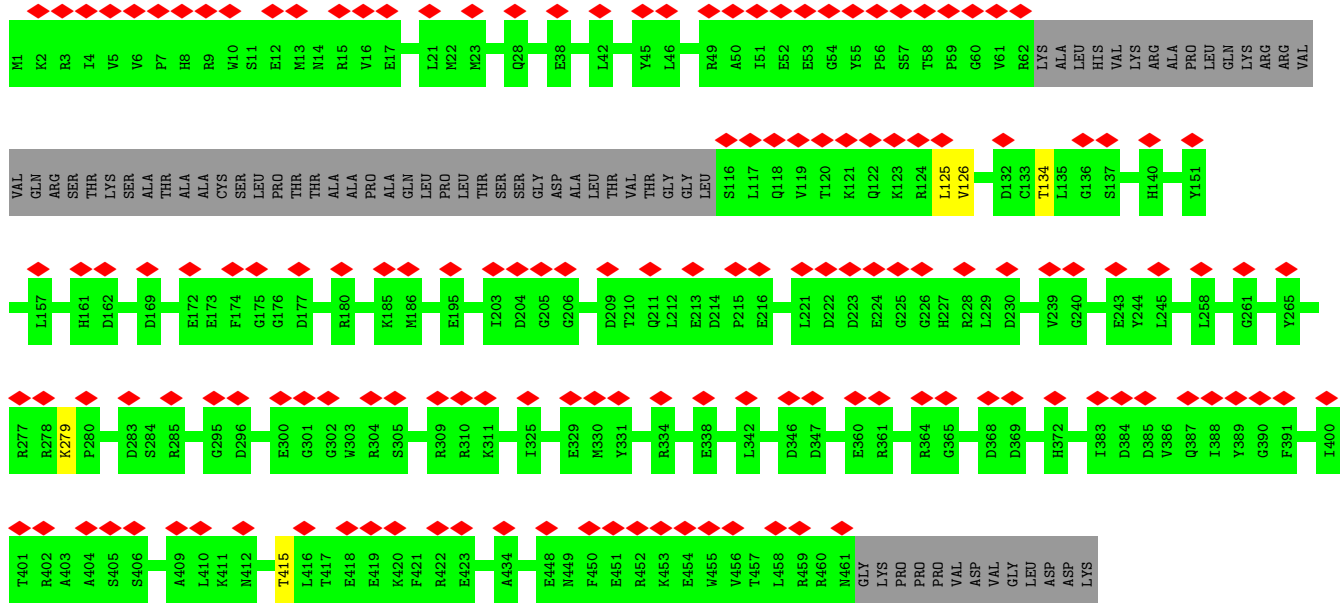


• Molecule 31: mt-SAF12 (KRIPP18)

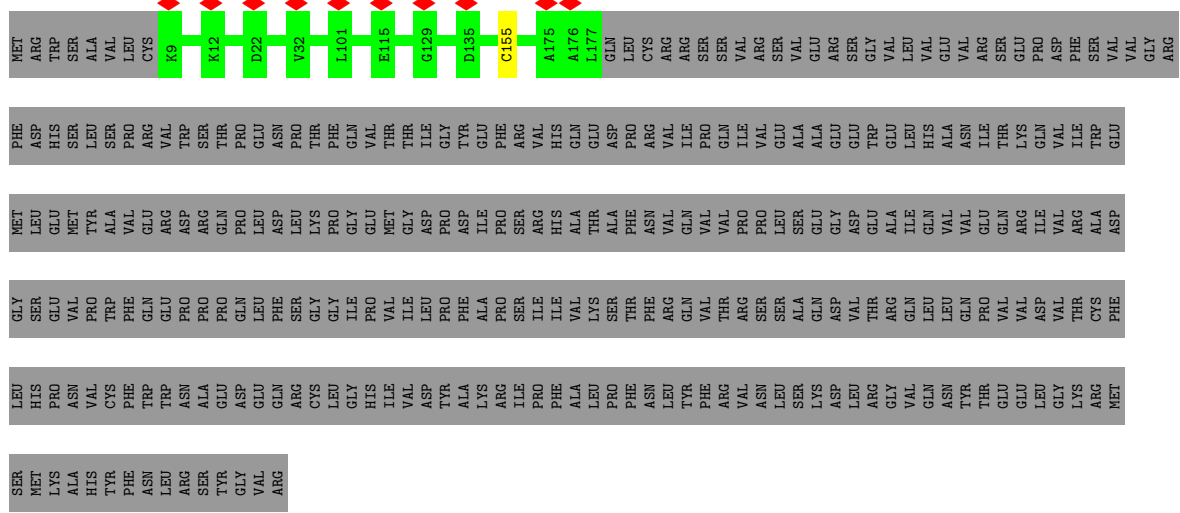


• Molecule 32: mt-SAF14

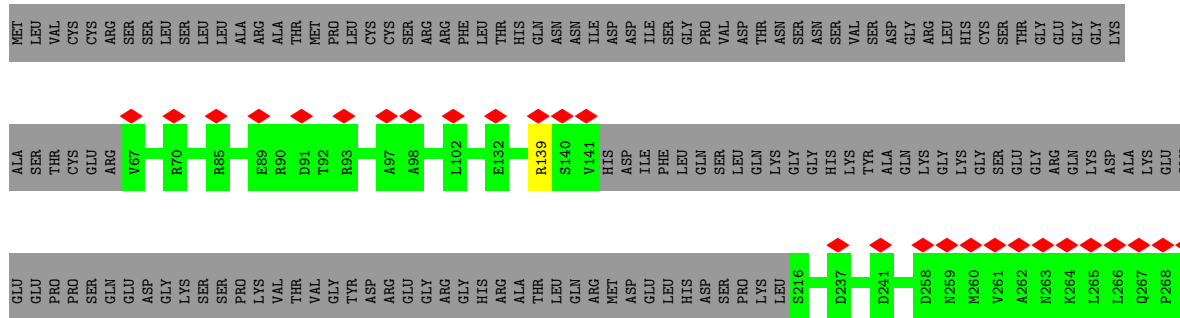




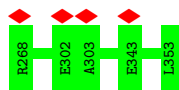
• Molecule 33: mt-SAF15



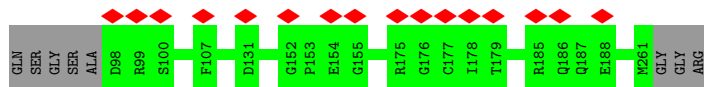
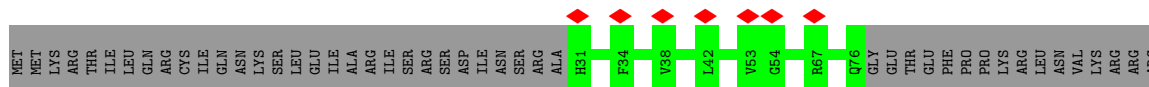
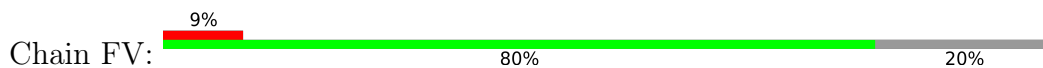
• Molecule 34: mt-SAF16



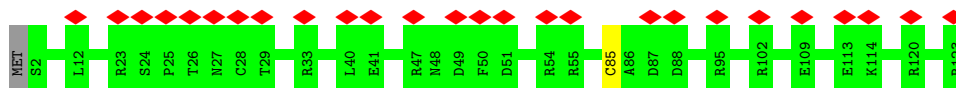




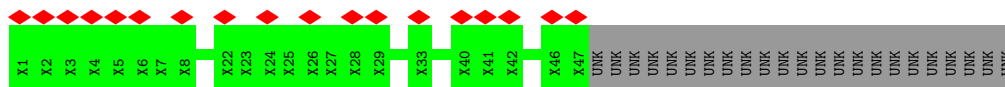
• Molecule 38: mt-SAF25



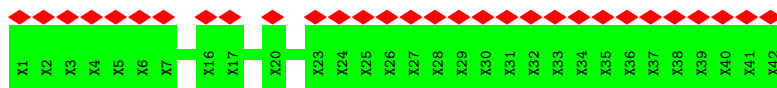
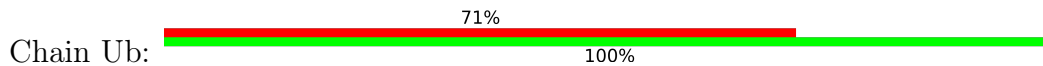
• Molecule 39: mt-SAF34



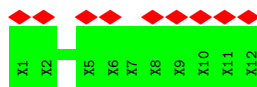
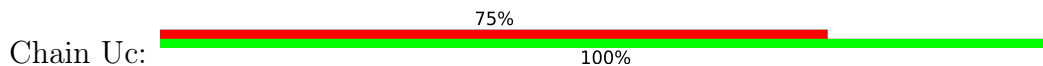
• Molecule 40: UNK-a



• Molecule 41: UNK-b

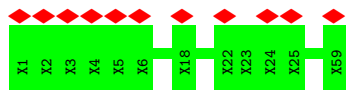


• Molecule 42: UNK-c

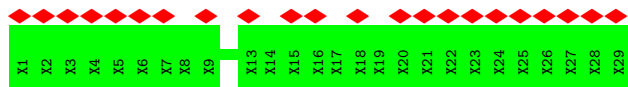
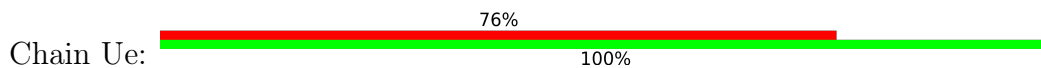


• Molecule 43: UNK-d





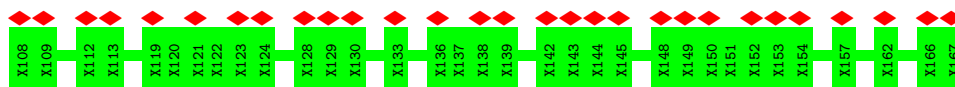
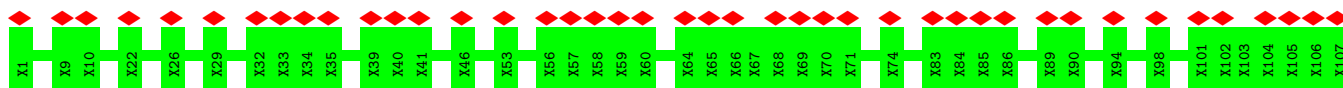
• Molecule 44: UNK-e



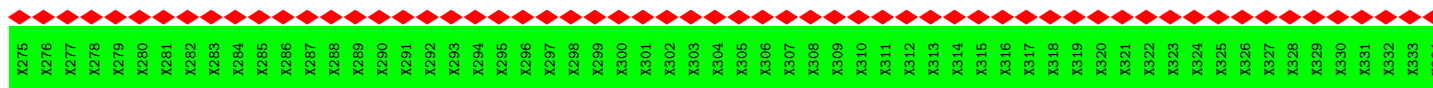
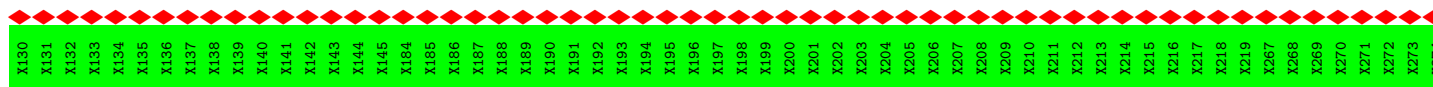
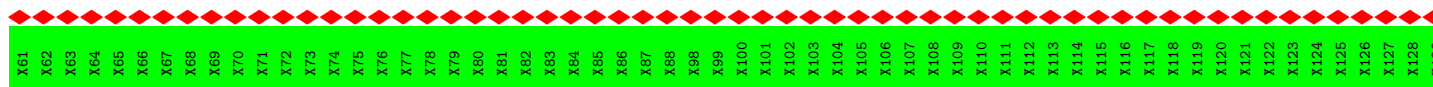
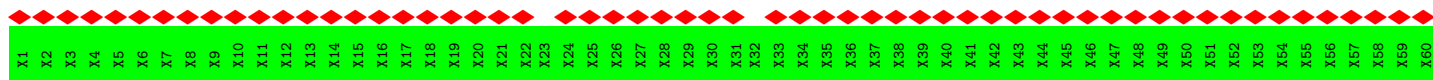
• Molecule 45: UNK-f



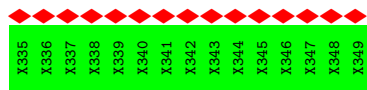
• Molecule 46: UNK-g



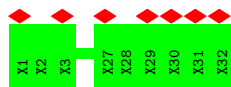
• Molecule 47: UNK-h



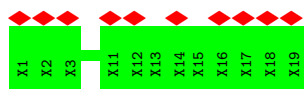




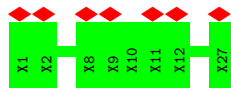
• Molecule 48: UNK-i



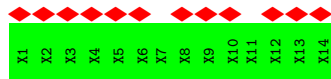
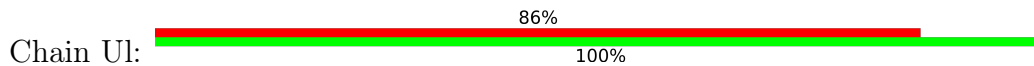
• Molecule 49: UNK-j



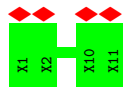
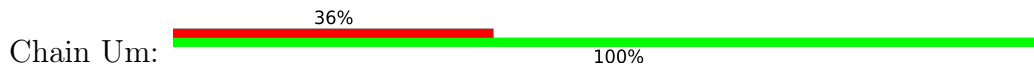
• Molecule 50: UNK-k



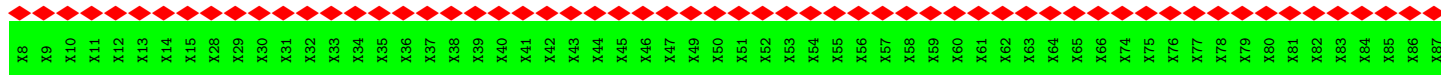
• Molecule 51: UNK-l



• Molecule 52: UNK-m



• Molecule 53: UNK-x



X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X98	X99	X100	X101	X102	X103	X104	X105	X106	X107	X108	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135
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## 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	0.420	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0793	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, GTP, ZN, 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	CE	0.26	0/206	0.42	0/278
2	CK	0.27	0/343	0.46	0/461
3	Cn	0.28	0/161	0.52	0/218
4	FJ	0.27	0/340	0.47	0/454
5	FY	0.29	0/736	0.52	1/987 (0.1%)
6	Fa	0.28	0/307	0.49	0/417
7	CA	0.25	0/2774	0.95	9/4302 (0.2%)
8	CC	0.36	0/666	0.54	0/900
9	CI	0.27	0/3424	0.48	0/4626
10	CJ	0.27	0/5865	0.47	0/7974
11	CN	0.26	0/1323	0.46	0/1790
12	CS	0.28	0/731	0.47	0/987
13	Cg	0.30	1/4043 (0.0%)	0.45	0/5489
14	Ci	0.27	0/1256	0.47	0/1695
15	Ck	0.27	0/5215	0.50	2/7050 (0.0%)
16	DB	0.27	0/5830	0.47	0/7889
17	DC	0.26	0/8409	0.45	0/11399
18	DE	0.25	0/4756	0.47	3/6462 (0.0%)
19	DF	0.27	0/4056	0.46	0/5493
20	DG	0.26	0/4674	0.46	0/6333
21	DH	0.27	0/3935	0.47	0/5321
22	DJ	0.26	0/2591	0.45	0/3508
23	DK	0.26	0/1965	0.44	0/2652
24	DT	0.28	0/1982	0.47	0/2686
25	DV	0.27	0/1358	0.46	0/1836
26	DW	0.27	0/1182	0.47	0/1613
27	DX	0.25	0/993	0.45	0/1336
28	DY	0.26	0/1337	0.43	0/1814
29	F1	0.27	0/6865	0.49	1/9259 (0.0%)
30	F4	0.26	0/4483	0.51	2/6061 (0.0%)
31	FD	0.28	0/3216	0.47	0/4380
32	FF	0.25	0/3335	0.47	0/4498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	FG	0.26	0/1386	0.47	0/1869
34	FH	0.29	0/2537	0.47	0/3442
35	FI	0.28	0/2834	0.49	1/3821 (0.0%)
36	FK	0.27	0/1748	0.44	0/2378
37	FL	0.28	0/2613	0.49	0/3538
38	FV	0.27	0/1680	0.47	0/2281
39	Fe	0.27	0/1057	0.51	0/1421
All	All	0.27	1/102212 (0.0%)	0.49	19/138918 (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
10	CJ	0	1
15	Ck	0	1
21	DH	0	1
26	DW	0	1
32	FF	0	1
39	Fe	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Cg	313	GLU	CA-CB	6.81	1.69	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Ck	228	LEU	CA-CB-CG	7.11	131.65	115.30
30	F4	589	LEU	CA-CB-CG	6.58	130.42	115.30
15	Ck	568	LEU	CA-CB-CG	6.36	129.92	115.30
7	CA	512	G	C4-N9-C1'	6.25	134.63	126.50
18	DE	479	PRO	N-CA-CB	6.15	110.68	103.30
7	CA	512	G	N3-C4-C5	-5.92	125.64	128.60
7	CA	517	U	C2-N1-C1'	5.91	124.80	117.70
18	DE	476	PRO	N-CA-CB	5.80	110.26	103.30
7	CA	486	C	C2-N1-C1'	5.69	125.06	118.80
7	CA	512	G	N3-C4-N9	5.61	129.36	126.00
18	DE	521	PRO	N-CA-CB	5.55	109.96	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	CA	517	U	N3-C2-O2	-5.51	118.34	122.20
35	FI	417	LEU	CA-CB-CG	5.36	127.63	115.30
7	CA	517	U	N1-C2-O2	5.27	126.49	122.80
7	CA	512	G	C8-N9-C1'	-5.19	120.25	127.00
30	F4	585	LEU	CA-CB-CG	5.18	127.20	115.30
7	CA	483	A	P-O3'-C3'	5.14	125.87	119.70
29	F1	173	LEU	CA-CB-CG	5.03	126.88	115.30
5	FY	88	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	CJ	237	GLY	Peptide
15	Ck	229	ALA	Peptide
21	DH	484	ASP	Peptide
26	DW	55	TRP	Peptide
32	FF	279	LYS	Peptide
39	Fe	85	CYS	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	21/435 (5%)	21 (100%)	0	0	100	100
2	CK	38/326 (12%)	36 (95%)	2 (5%)	0	100	100
3	Cn	16/250 (6%)	14 (88%)	2 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	FJ	39/362 (11%)	39 (100%)	0	0	100	100
5	FY	90/188 (48%)	85 (94%)	5 (6%)	0	100	100
6	Fa	37/171 (22%)	35 (95%)	2 (5%)	0	100	100
8	CC	72/74 (97%)	72 (100%)	0	0	100	100
9	CI	421/443 (95%)	405 (96%)	16 (4%)	0	100	100
10	CJ	695/817 (85%)	655 (94%)	36 (5%)	4 (1%)	25	59
11	CN	151/166 (91%)	149 (99%)	2 (1%)	0	100	100
12	CS	79/244 (32%)	74 (94%)	5 (6%)	0	100	100
13	Cg	482/498 (97%)	463 (96%)	19 (4%)	0	100	100
14	Ci	145/181 (80%)	138 (95%)	7 (5%)	0	100	100
15	Ck	634/874 (72%)	600 (95%)	34 (5%)	0	100	100
16	DB	671/1181 (57%)	648 (97%)	23 (3%)	0	100	100
17	DC	1020/1165 (88%)	998 (98%)	22 (2%)	0	100	100
18	DE	582/747 (78%)	564 (97%)	16 (3%)	2 (0%)	41	73
19	DF	485/666 (73%)	466 (96%)	19 (4%)	0	100	100
20	DG	558/631 (88%)	545 (98%)	13 (2%)	0	100	100
21	DH	466/581 (80%)	445 (96%)	21 (4%)	0	100	100
22	DJ	304/396 (77%)	296 (97%)	8 (3%)	0	100	100
23	DK	239/324 (74%)	228 (95%)	11 (5%)	0	100	100
24	DT	219/247 (89%)	208 (95%)	11 (5%)	0	100	100
25	DV	153/183 (84%)	147 (96%)	6 (4%)	0	100	100
26	DW	131/179 (73%)	121 (92%)	10 (8%)	0	100	100
27	DX	113/169 (67%)	109 (96%)	4 (4%)	0	100	100
28	DY	152/163 (93%)	147 (97%)	5 (3%)	0	100	100
29	F1	827/1041 (79%)	792 (96%)	35 (4%)	0	100	100
30	F4	521/811 (64%)	490 (94%)	30 (6%)	1 (0%)	47	79
31	FD	392/579 (68%)	386 (98%)	6 (2%)	0	100	100
32	FF	404/474 (85%)	389 (96%)	13 (3%)	2 (0%)	29	64
33	FG	167/463 (36%)	162 (97%)	5 (3%)	0	100	100
34	FH	313/457 (68%)	303 (97%)	10 (3%)	0	100	100
35	FI	342/445 (77%)	333 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	FK	202/372 (54%)	200 (99%)	2 (1%)	0	100	100
37	FL	314/353 (89%)	298 (95%)	16 (5%)	0	100	100
38	FV	206/264 (78%)	199 (97%)	7 (3%)	0	100	100
39	Fe	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
All	All	11821/17043 (69%)	11373 (96%)	439 (4%)	9 (0%)	54	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	DE	521	PRO
10	CJ	592	SER
10	CJ	238	ILE
30	F4	590	ASN
10	CJ	236	ASP
10	CJ	237	GLY
32	FF	125	LEU
32	FF	126	VAL
18	DE	476	PRO

### 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	22/372 (6%)	22 (100%)	0	100	100
2	CK	37/284 (13%)	37 (100%)	0	100	100
3	Cn	14/210 (7%)	14 (100%)	0	100	100
4	FJ	38/323 (12%)	38 (100%)	0	100	100
5	FY	77/163 (47%)	76 (99%)	1 (1%)	69	87
6	Fa	30/149 (20%)	30 (100%)	0	100	100
8	CC	73/73 (100%)	71 (97%)	2 (3%)	44	74
9	CI	355/371 (96%)	354 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	CJ	619/723 (86%)	616 (100%)	3 (0%)	88	94
11	CN	138/150 (92%)	138 (100%)	0	100	100
12	CS	76/220 (34%)	76 (100%)	0	100	100
13	Cg	426/437 (98%)	426 (100%)	0	100	100
14	Ci	130/160 (81%)	129 (99%)	1 (1%)	81	92
15	Ck	557/747 (75%)	553 (99%)	4 (1%)	84	93
16	DB	613/1030 (60%)	611 (100%)	2 (0%)	92	96
17	DC	867/985 (88%)	865 (100%)	2 (0%)	93	97
18	DE	464/644 (72%)	463 (100%)	1 (0%)	93	97
19	DF	417/560 (74%)	417 (100%)	0	100	100
20	DG	490/543 (90%)	490 (100%)	0	100	100
21	DH	413/504 (82%)	412 (100%)	1 (0%)	93	97
22	DJ	267/347 (77%)	267 (100%)	0	100	100
23	DK	203/261 (78%)	203 (100%)	0	100	100
24	DT	205/228 (90%)	204 (100%)	1 (0%)	88	94
25	DV	142/165 (86%)	142 (100%)	0	100	100
26	DW	124/163 (76%)	124 (100%)	0	100	100
27	DX	102/149 (68%)	101 (99%)	1 (1%)	76	90
28	DY	137/146 (94%)	136 (99%)	1 (1%)	84	93
29	F1	718/895 (80%)	717 (100%)	1 (0%)	93	98
30	F4	479/703 (68%)	477 (100%)	2 (0%)	91	96
31	FD	338/494 (68%)	338 (100%)	0	100	100
32	FF	348/400 (87%)	346 (99%)	2 (1%)	86	94
33	FG	147/414 (36%)	146 (99%)	1 (1%)	84	93
34	FH	270/390 (69%)	268 (99%)	2 (1%)	84	93
35	FI	297/380 (78%)	297 (100%)	0	100	100
36	FK	181/308 (59%)	180 (99%)	1 (1%)	86	94
37	FL	279/309 (90%)	278 (100%)	1 (0%)	91	96
38	FV	184/231 (80%)	184 (100%)	0	100	100
39	Fe	114/115 (99%)	114 (100%)	0	100	100
All	All	10391/14746 (70%)	10360 (100%)	31 (0%)	92	96

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	FY	43	LYS
8	CC	18	PHE
8	CC	74	THR
9	CI	128	ARG
10	CJ	375	THR
10	CJ	547	LYS
10	CJ	716	ARG
14	Ci	114	MET
15	Ck	169	LYS
15	Ck	335	ARG
15	Ck	573	THR
15	Ck	687	ARG
16	DB	806	LYS
16	DB	963	ARG
17	DC	130	LYS
17	DC	688	LYS
18	DE	295	TYR
21	DH	107	THR
24	DT	105	ARG
27	DX	149	THR
28	DY	136	VAL
29	F1	84	ARG
30	F4	374	ARG
30	F4	459	VAL
32	FF	134	THR
32	FF	415	THR
33	FG	155	CYS
34	FH	139	ARG
34	FH	329	ARG
36	FK	120	LYS
37	FL	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
2	CK	56	GLN
5	FY	104	GLN
8	CC	31	ASN
8	CC	48	HIS
9	CI	84	ASN
9	CI	136	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	CI	229	HIS
10	CJ	170	HIS
10	CJ	450	HIS
10	CJ	460	HIS
10	CJ	476	ASN
10	CJ	761	GLN
10	CJ	791	HIS
10	CJ	804	ASN
11	CN	63	HIS
11	CN	96	HIS
11	CN	153	ASN
12	CS	88	ASN
12	CS	104	GLN
12	CS	110	HIS
13	Cg	75	ASN
13	Cg	87	GLN
13	Cg	99	GLN
13	Cg	184	HIS
13	Cg	239	GLN
13	Cg	301	HIS
13	Cg	323	GLN
13	Cg	453	GLN
13	Cg	460	HIS
13	Cg	474	GLN
14	Ci	19	HIS
14	Ci	145	ASN
15	Ck	97	GLN
15	Ck	361	GLN
15	Ck	399	ASN
15	Ck	644	HIS
15	Ck	679	GLN
15	Ck	728	GLN
16	DB	542	GLN
16	DB	643	HIS
16	DB	730	GLN
16	DB	958	ASN
16	DB	1113	GLN
17	DC	81	HIS
17	DC	227	GLN
17	DC	263	GLN
17	DC	303	HIS
17	DC	520	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	DC	682	ASN
17	DC	776	ASN
17	DC	841	HIS
17	DC	871	GLN
17	DC	951	ASN
18	DE	202	HIS
18	DE	345	ASN
18	DE	596	HIS
18	DE	658	ASN
18	DE	699	ASN
18	DE	703	GLN
19	DF	175	GLN
19	DF	187	ASN
19	DF	283	HIS
19	DF	396	GLN
19	DF	572	HIS
19	DF	592	HIS
20	DG	26	ASN
20	DG	71	ASN
20	DG	92	GLN
20	DG	143	HIS
20	DG	170	ASN
20	DG	191	GLN
20	DG	200	GLN
20	DG	351	GLN
20	DG	476	GLN
20	DG	477	GLN
21	DH	123	HIS
21	DH	160	ASN
21	DH	191	HIS
21	DH	255	GLN
21	DH	275	HIS
21	DH	343	ASN
22	DJ	31	HIS
22	DJ	82	GLN
22	DJ	174	ASN
22	DJ	247	ASN
22	DJ	301	HIS
23	DK	132	HIS
23	DK	163	HIS
23	DK	171	GLN
23	DK	242	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	DT	72	HIS
24	DT	178	ASN
24	DT	192	GLN
24	DT	219	GLN
25	DV	40	HIS
25	DV	51	ASN
26	DW	154	HIS
27	DX	111	ASN
28	DY	99	GLN
28	DY	106	GLN
29	F1	331	HIS
29	F1	332	GLN
29	F1	344	GLN
29	F1	477	GLN
29	F1	502	ASN
29	F1	518	HIS
29	F1	542	GLN
29	F1	631	HIS
29	F1	763	ASN
29	F1	776	HIS
29	F1	810	GLN
29	F1	862	HIS
30	F4	56	GLN
30	F4	266	ASN
30	F4	308	ASN
30	F4	320	HIS
30	F4	334	GLN
30	F4	348	ASN
30	F4	472	HIS
30	F4	479	ASN
30	F4	686	HIS
30	F4	800	ASN
31	FD	100	HIS
31	FD	240	GLN
32	FF	161	HIS
33	FG	145	ASN
33	FG	162	ASN
34	FH	111	HIS
34	FH	134	ASN
34	FH	436	GLN
34	FH	451	ASN
35	FI	97	HIS

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Mol	Chain	Res	Type
35	FI	120	GLN
35	FI	153	GLN
35	FI	228	GLN
35	FI	340	HIS
36	FK	169	GLN
36	FK	312	ASN
37	FL	23	ASN
37	FL	70	ASN
37	FL	127	ASN
37	FL	263	HIS
37	FL	335	GLN
38	FV	63	ASN
38	FV	76	GLN
38	FV	150	HIS
38	FV	194	HIS
38	FV	207	HIS
39	Fe	22	ASN
39	Fe	42	ASN
39	Fe	101	GLN
39	Fe	117	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	CA	145/802 (18%)	55 (37%)	1 (0%)

All (55) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	CA	388	U
7	CA	389	A
7	CA	390	U
7	CA	396	A
7	CA	397	U
7	CA	398	U
7	CA	399	A
7	CA	400	U
7	CA	405	A
7	CA	413	A
7	CA	416	U
7	CA	417	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	CA	418	A
7	CA	421	G
7	CA	422	G
7	CA	425	A
7	CA	429	U
7	CA	430	U
7	CA	431	U
7	CA	432	G
7	CA	433	U
7	CA	435	G
7	CA	438	U
7	CA	439	U
7	CA	443	U
7	CA	444	A
7	CA	445	C
7	CA	446	C
7	CA	447	A
7	CA	448	U
7	CA	454	G
7	CA	455	G
7	CA	459	A
7	CA	460	U
7	CA	461	A
7	CA	470	G
7	CA	471	U
7	CA	473	U
7	CA	480	C
7	CA	481	A
7	CA	484	A
7	CA	489	A
7	CA	490	A
7	CA	498	U
7	CA	503	A
7	CA	509	U
7	CA	513	U
7	CA	515	U
7	CA	516	G
7	CA	520	A
7	CA	524	A
7	CA	525	A
7	CA	527	A
7	CA	528	U

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Mol	Chain	Res	Type
7	CA	529	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	CA	483	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
57	SAH	FFA	1	-	24,28,28	1.22	3 (12%)	25,40,40	1.75	5 (20%)
57	SAH	F1B	1	-	24,28,28	1.19	3 (12%)	25,40,40	1.71	5 (20%)
54	GTP	CgA	1	-	26,34,34	1.13	1 (3%)	32,54,54	1.66	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
57	SAH	FFA	1	-	-	1/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SAH	F1B	1	-	-	3/11/31/31	0/3/3/3
54	GTP	CgA	1	-	-	5/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CgA	1	GTP	C5-C6	-4.04	1.39	1.47
57	FFA	1	SAH	C2-N3	4.00	1.38	1.32
57	F1B	1	SAH	C2-N3	3.84	1.38	1.32
57	FFA	1	SAH	C2-N1	2.45	1.38	1.33
57	F1B	1	SAH	C2-N1	2.38	1.38	1.33
57	F1B	1	SAH	OXT-C	-2.16	1.23	1.30
57	FFA	1	SAH	OXT-C	-2.16	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	F1B	1	SAH	N3-C2-N1	-5.42	120.21	128.68
57	FFA	1	SAH	N3-C2-N1	-5.36	120.30	128.68
57	FFA	1	SAH	C5'-SD-CG	-4.21	89.64	102.27
57	F1B	1	SAH	C5'-SD-CG	-3.94	90.45	102.27
54	CgA	1	GTP	C3'-C2'-C1'	3.67	106.50	100.98
54	CgA	1	GTP	PB-O3B-PG	-3.59	120.49	132.83
54	CgA	1	GTP	PA-O3A-PB	-3.43	121.07	132.83
54	CgA	1	GTP	C5-C6-N1	3.33	119.83	113.95
54	CgA	1	GTP	C2-N1-C6	-3.07	119.44	125.10
54	CgA	1	GTP	C8-N7-C5	2.93	108.57	102.99
57	FFA	1	SAH	C3'-C2'-C1'	2.82	105.23	100.98
57	FFA	1	SAH	OXT-C-O	-2.65	118.07	124.09
57	F1B	1	SAH	OXT-C-O	-2.64	118.09	124.09
57	F1B	1	SAH	C3'-C2'-C1'	2.57	104.84	100.98
57	FFA	1	SAH	OXT-C-CA	2.23	120.98	113.38
57	F1B	1	SAH	OXT-C-CA	2.21	120.92	113.38
54	CgA	1	GTP	O6-C6-C5	-2.18	120.12	124.37
54	CgA	1	GTP	N2-C2-N1	2.00	120.97	116.71

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	CgA	1	GTP	C5'-O5'-PA-O3A

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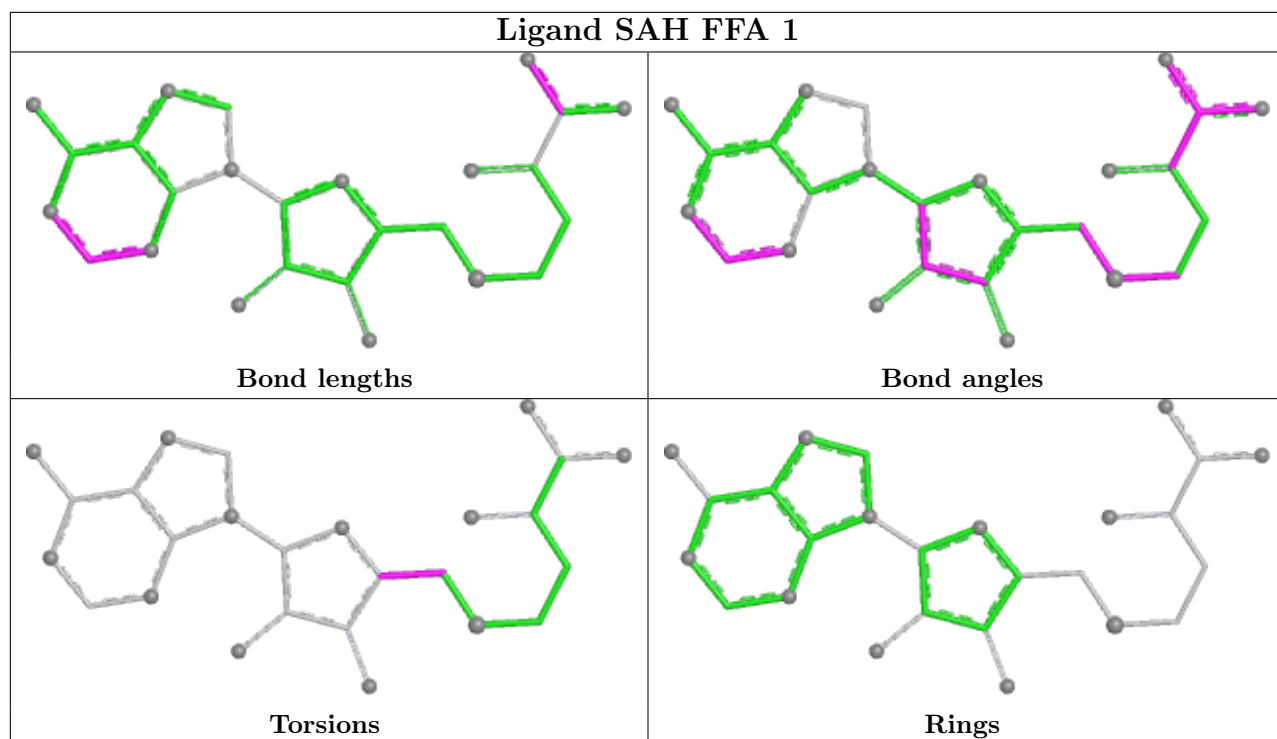
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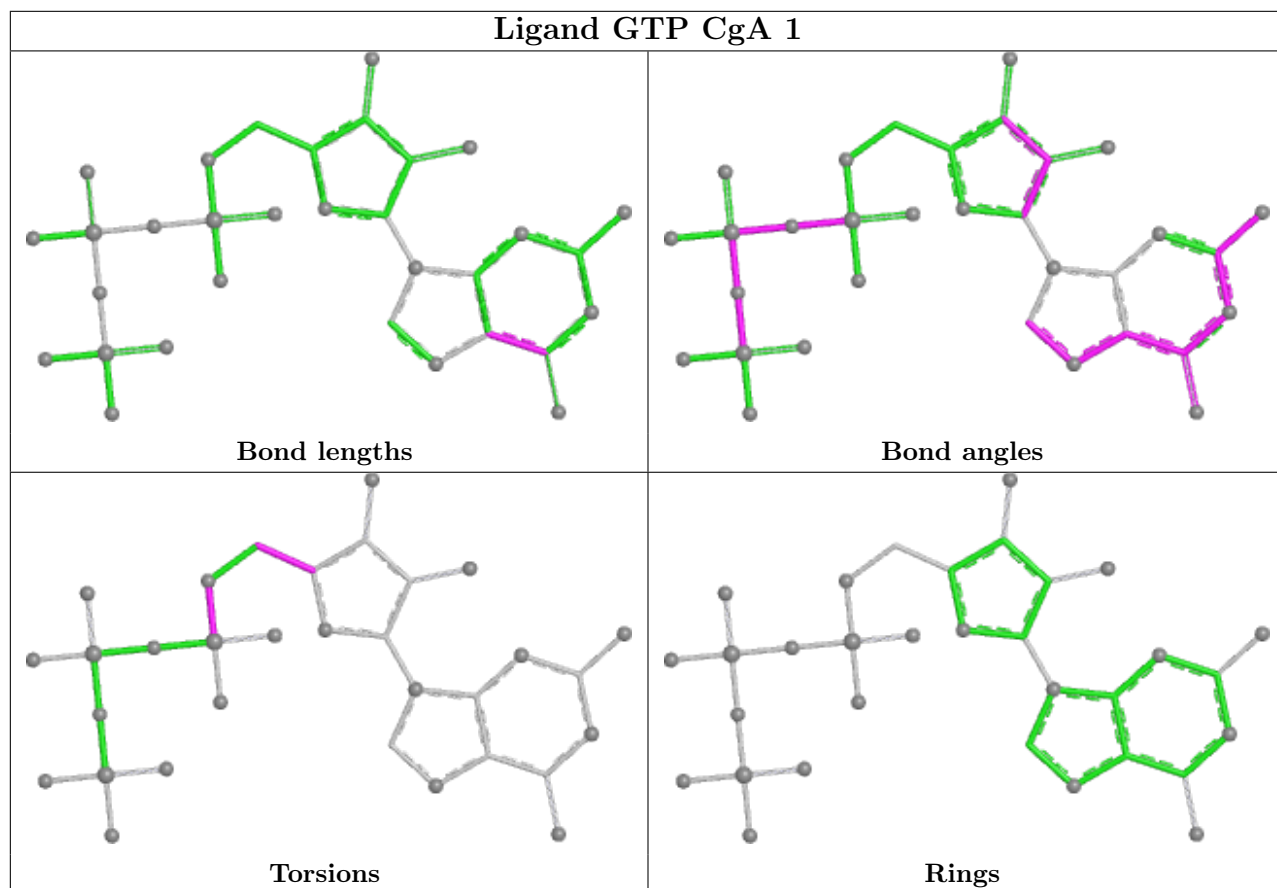
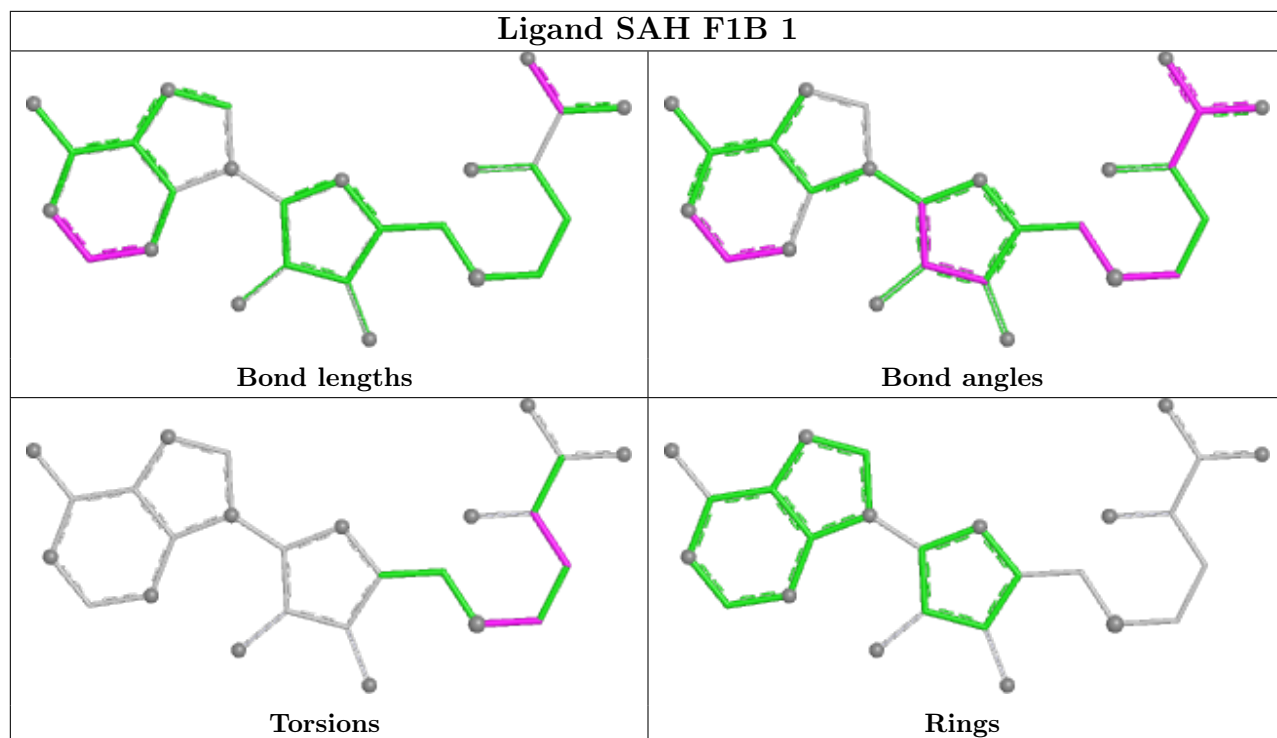
Mol	Chain	Res	Type	Atoms
54	CgA	1	GTP	C5'-O5'-PA-O1A
54	CgA	1	GTP	C5'-O5'-PA-O2A
57	F1B	1	SAH	N-CA-CB-CG
57	F1B	1	SAH	C-CA-CB-CG
54	CgA	1	GTP	C3'-C4'-C5'-O5'
54	CgA	1	GTP	O4'-C4'-C5'-O5'
57	F1B	1	SAH	CB-CG-SD-C5'
57	FFA	1	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	Uh	11
46	Ug	10
53	Ux	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	219:UNK	C	267:UNK	N	51.70
1	Uh	13:UNK	C	14:UNK	N	49.42
1	Uh	88:UNK	C	98:UNK	N	42.41
1	Uh	124:UNK	C	125:UNK	N	39.54
1	Uh	199:UNK	C	200:UNK	N	38.31
1	Ug	129:UNK	C	130:UNK	N	35.86
1	Uh	145:UNK	C	184:UNK	N	35.70
1	Ug	102:UNK	C	103:UNK	N	29.52
1	Uh	39:UNK	C	40:UNK	N	25.40
1	Ug	83:UNK	C	84:UNK	N	24.22
1	Uh	68:UNK	C	69:UNK	N	21.45
1	Uh	134:UNK	C	135:UNK	N	17.15
1	Uh	280:UNK	C	281:UNK	N	15.55
1	Ux	15:UNK	C	28:UNK	N	14.78
1	Ux	66:UNK	C	74:UNK	N	12.83
1	Ug	52:UNK	C	53:UNK	N	12.79
1	Ug	70:UNK	C	71:UNK	N	12.48
1	Ux	47:UNK	C	49:UNK	N	12.00
1	Ug	39:UNK	C	40:UNK	N	10.97
1	Ug	26:UNK	C	27:UNK	N	8.39
1	Uh	323:UNK	C	324:UNK	N	7.01
1	Ug	46:UNK	C	47:UNK	N	6.52
1	Ug	145:UNK	C	146:UNK	N	4.54
1	Ug	33:UNK	C	34:UNK	N	4.41

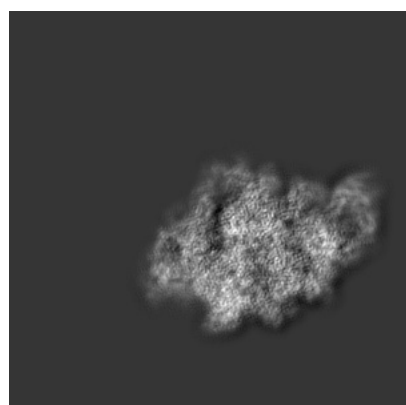
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10175. These allow visual inspection of the internal detail of the map and identification of artifacts.

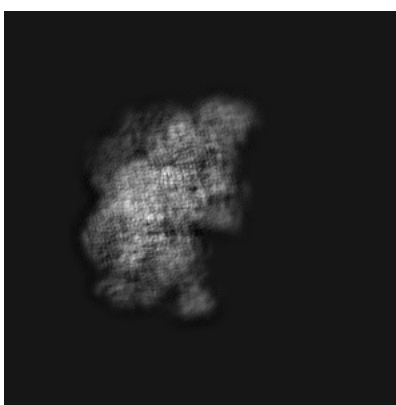
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

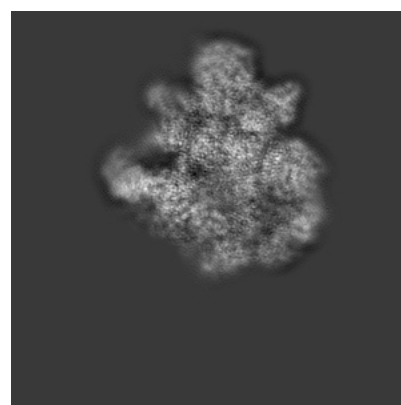
#### 6.1.1 Primary map



X



Y

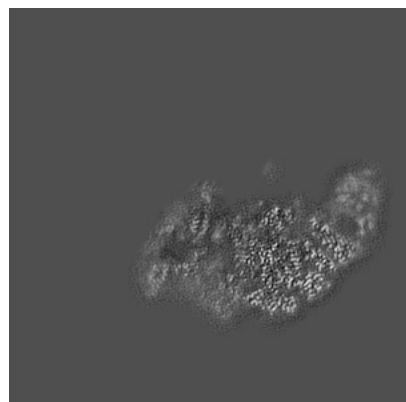


Z

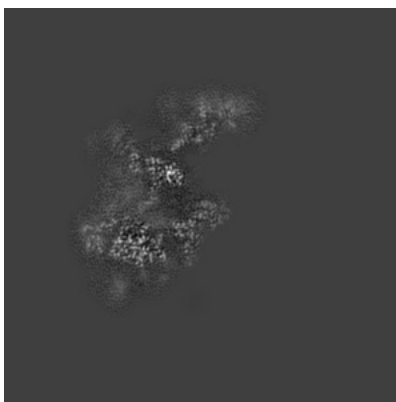
The images above show the map projected in three orthogonal directions.

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

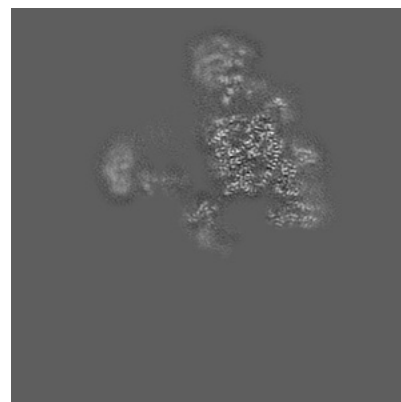
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

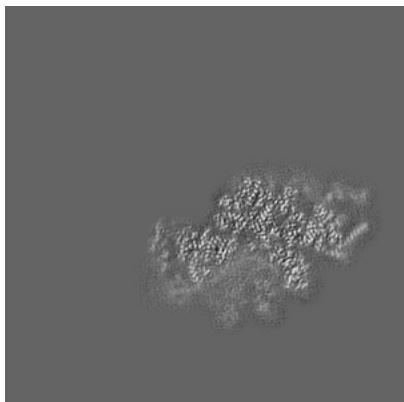


Z Index: 160

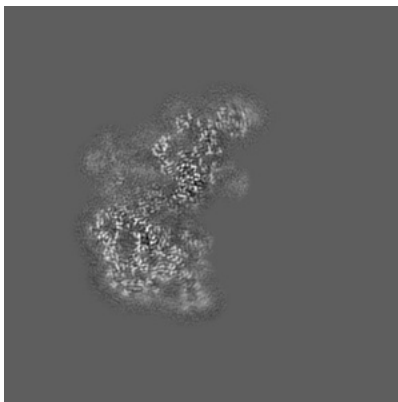
The images above show central slices of the map in three orthogonal directions.

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

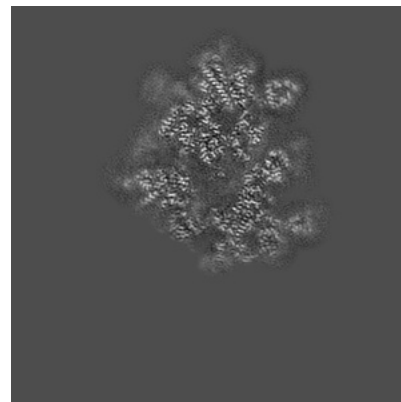
### 6.3.1 Primary map



X Index: 190



Y Index: 183

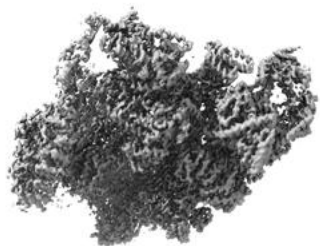


Z Index: 126

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 0.0793. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

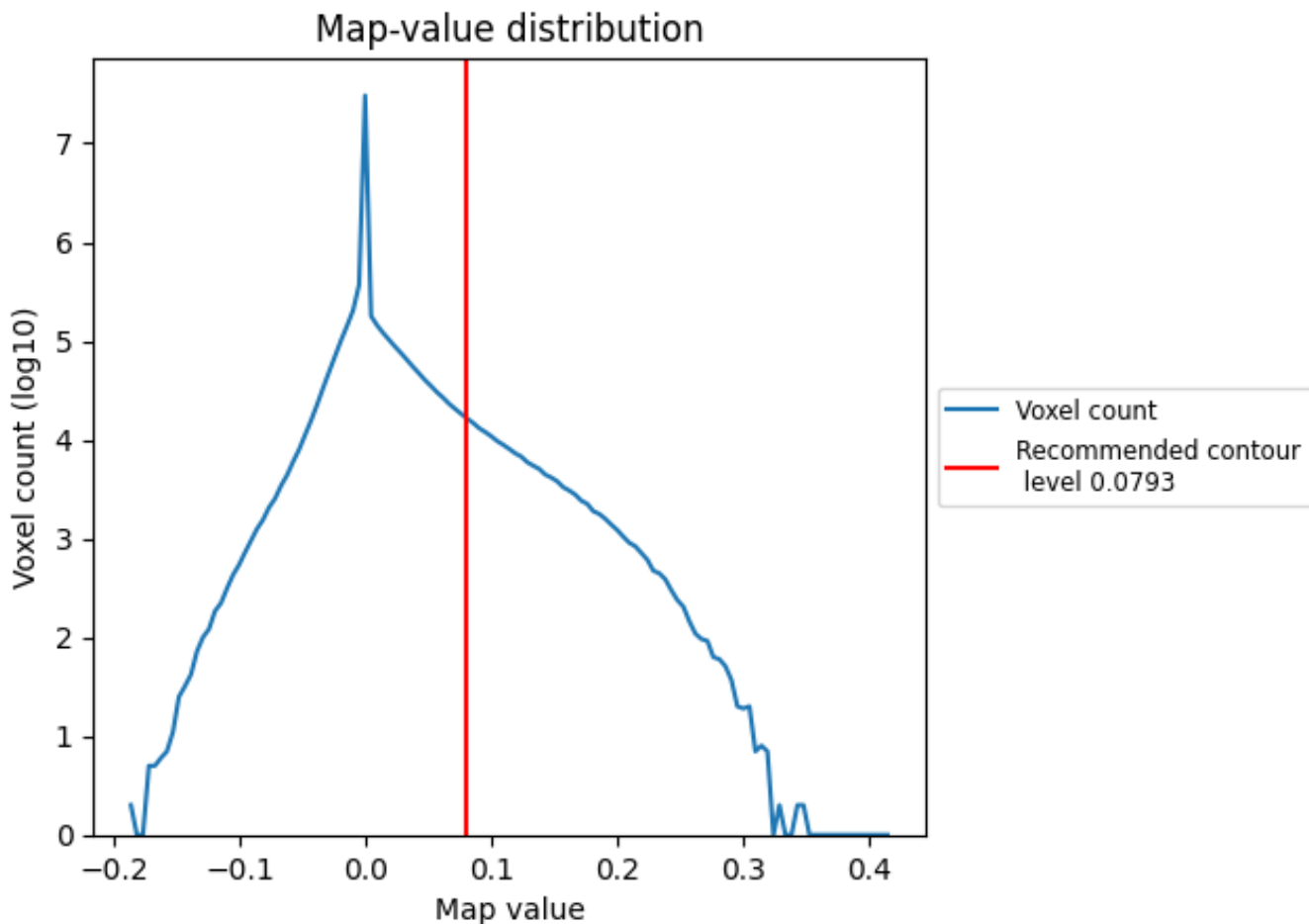
## 6.5 Mask visualisation

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.

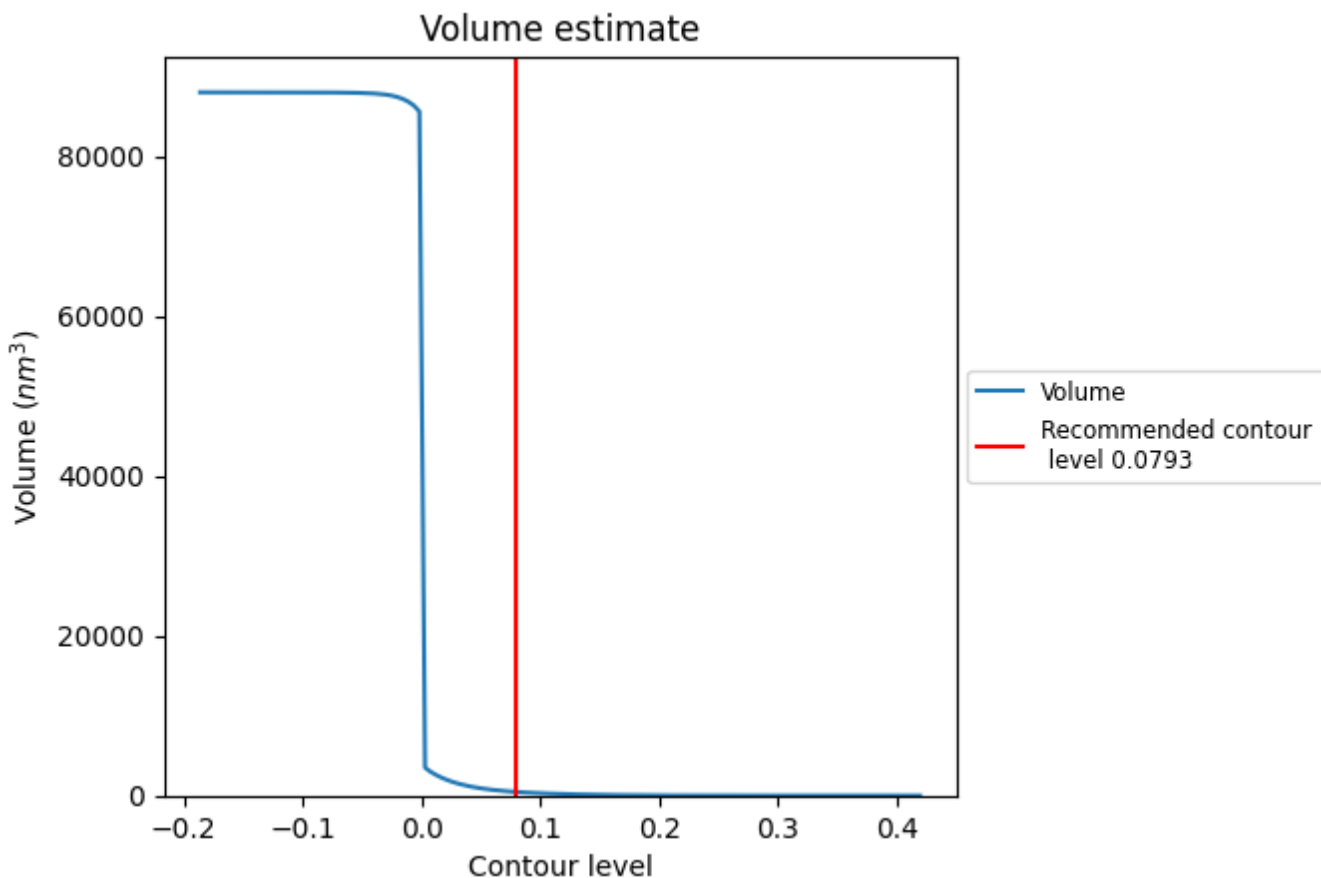
### 7.1 Map-value distribution [i](#)



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.



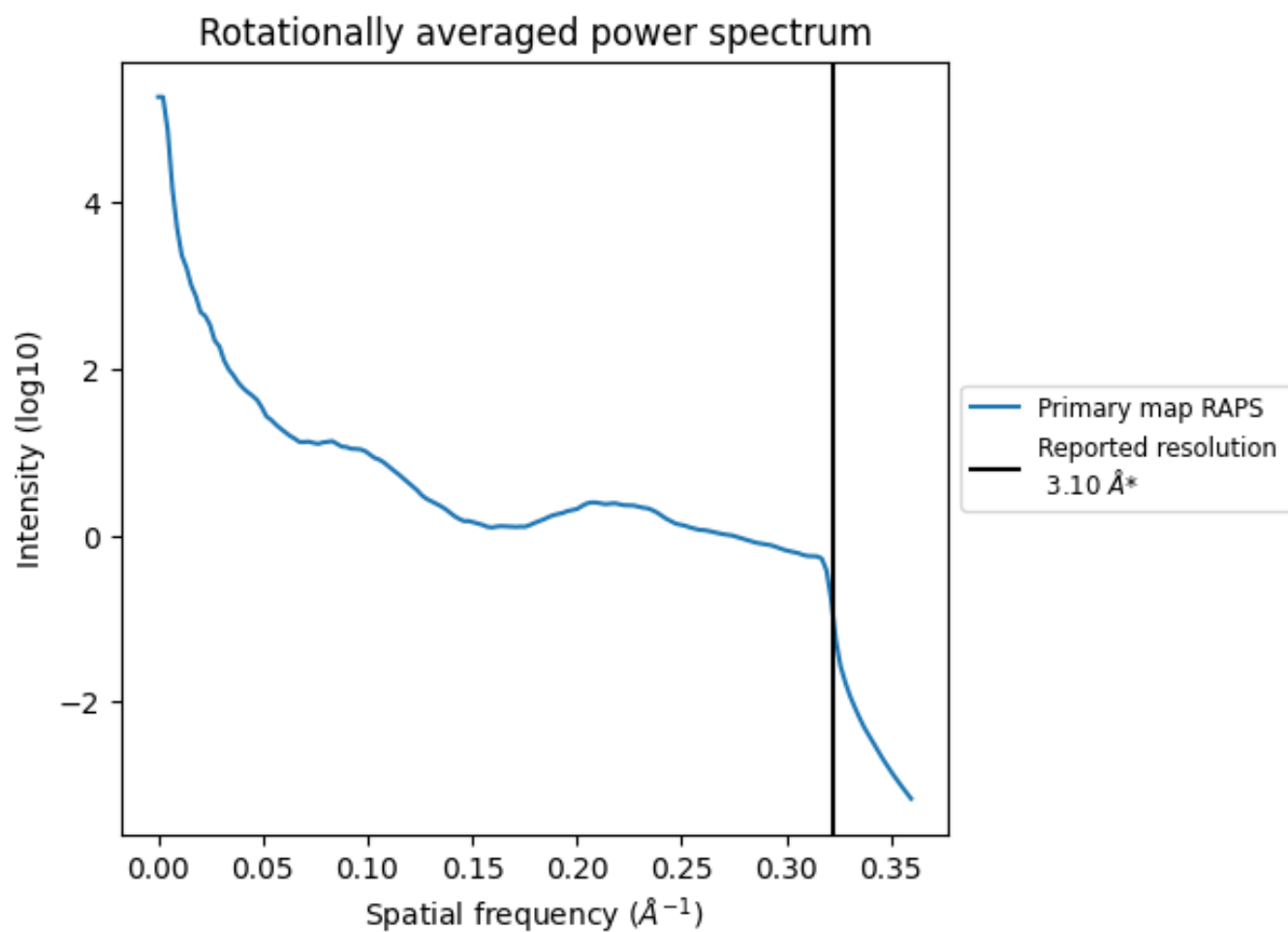
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 459 nm<sup>3</sup>; this corresponds to an approximate mass of 414 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<sup>-1</sup>

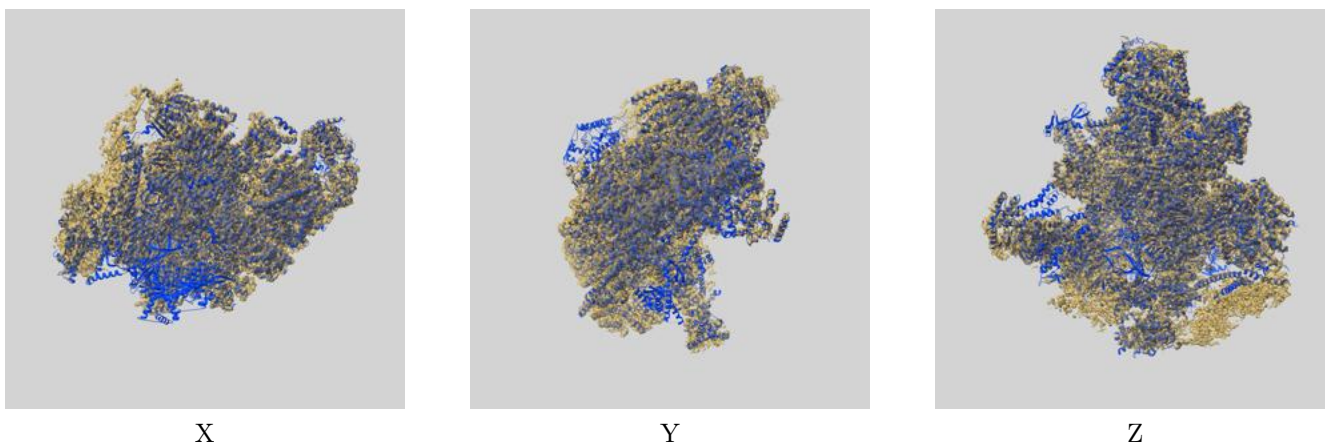
## 8 Fourier-Shell correlation

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

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

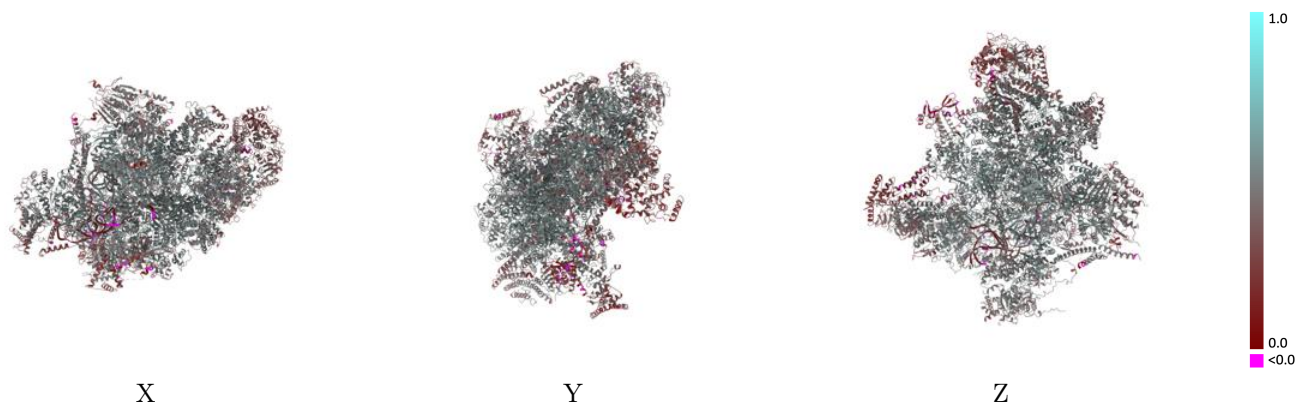
This section contains information regarding the fit between EMDB map EMD-10175 and PDB model 6SG9. Per-residue inclusion information can be found in section 3 on page 16.

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



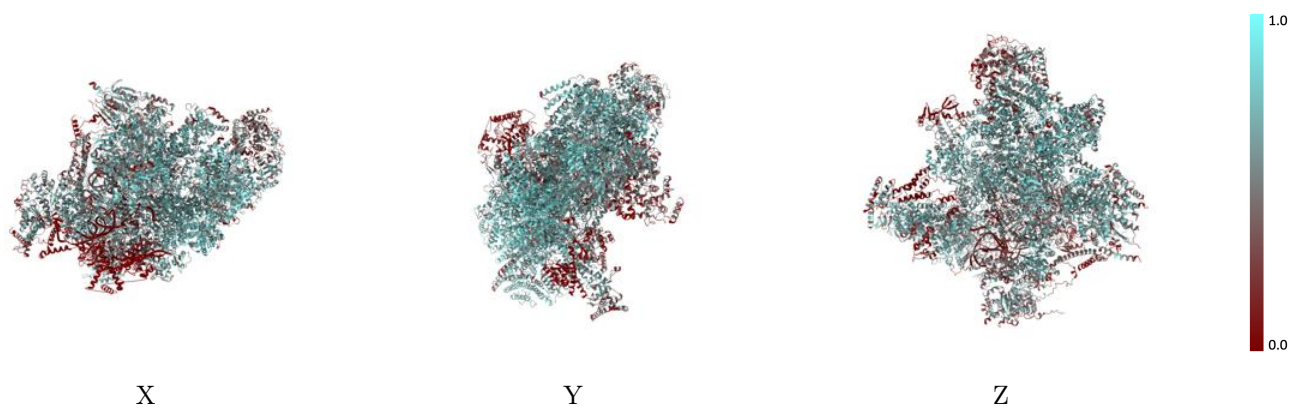
The images above show the 3D surface view of the map at the recommended contour level 0.0793 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



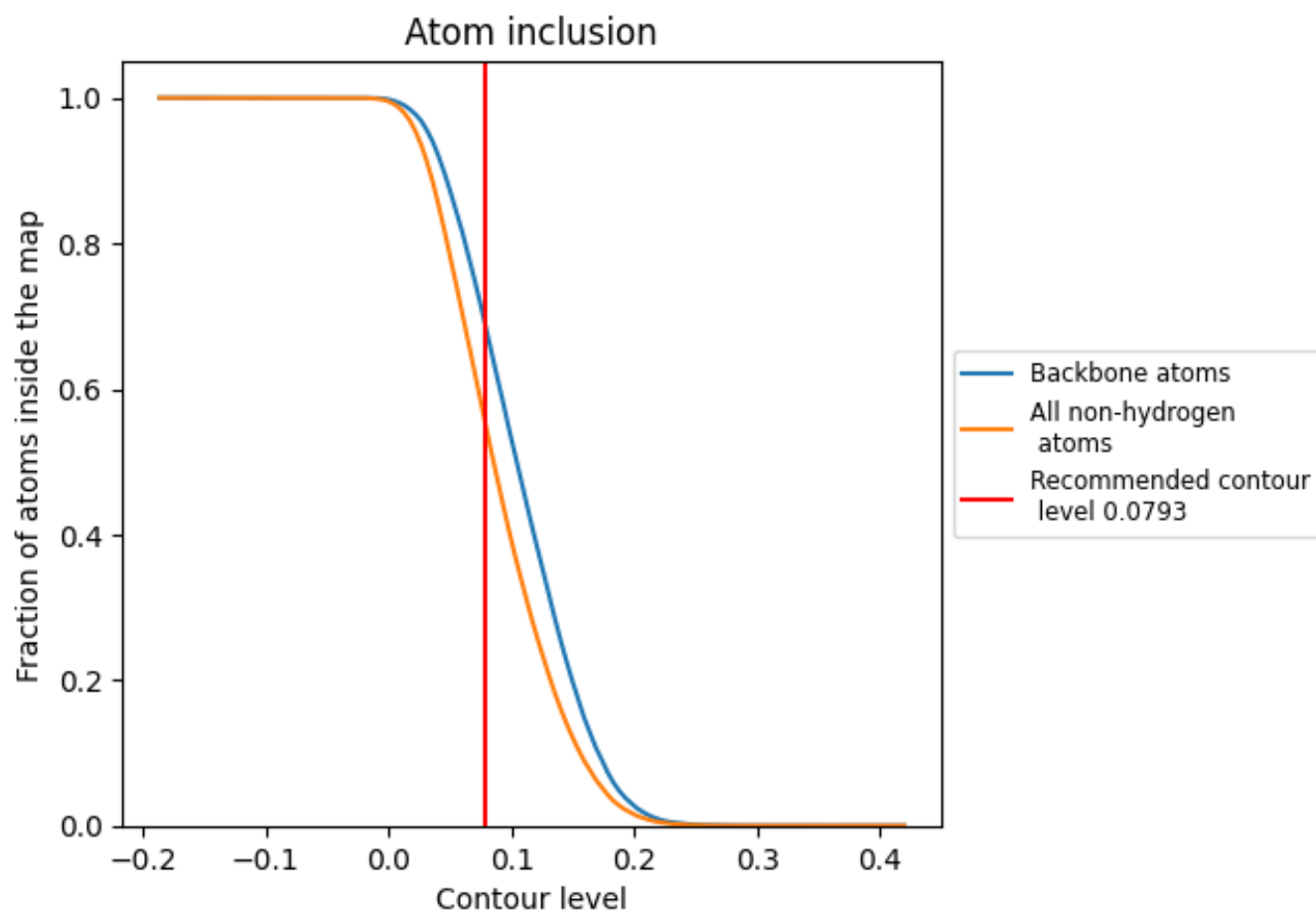
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0793).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% 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 (0.0793) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5481	 0.4610
CA	 0.3175	 0.3180
CC	 0.5391	 0.5120
CE	 0.4508	 0.4920
CI	 0.5418	 0.4770
CJ	 0.6346	 0.5040
CK	 0.5933	 0.4770
CN	 0.3025	 0.4910
CS	 0.0159	 0.4150
Cg	 0.7395	 0.5020
CgA	 0.9375	 0.4720
CgB	 1.0000	 0.5320
Ci	 0.5203	 0.5180
Ck	 0.5752	 0.4440
Cn	 0.3129	 0.5000
DB	 0.4569	 0.4230
DC	 0.6002	 0.4420
DE	 0.4313	 0.3500
DF	 0.6414	 0.4960
DG	 0.6501	 0.4450
DH	 0.6180	 0.5060
DJ	 0.6697	 0.4990
DK	 0.6348	 0.4890
DT	 0.7197	 0.5410
DV	 0.5622	 0.4940
DW	 0.5449	 0.4600
DX	 0.2543	 0.4300
DY	 0.5318	 0.4670
F1	 0.4997	 0.4740
F1A	 1.0000	 0.6220
F1B	 0.3077	 0.5250
F4	 0.4667	 0.4220
FD	 0.6734	 0.4940
FF	 0.4803	 0.4620
FFA	 0.3077	 0.4450



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Chain	Atom inclusion	Q-score
FG	 0.7212	 0.5170
FGA	 1.0000	 0.7780
FH	 0.6410	 0.5000
FI	 0.6273	 0.5200
FJ	 0.4407	 0.4760
FK	 0.5911	 0.5040
FL	 0.6140	 0.5310
FLA	 1.0000	 0.7440
FLB	 1.0000	 0.6060
FV	 0.6497	 0.5030
FY	 0.4314	 0.3760
Fa	 0.4355	 0.4890
Fe	 0.6327	 0.5030
FeA	 1.0000	 0.4100
Ua	 0.4184	 0.4270
Ub	 0.2659	 0.4360
Uc	 0.2222	 0.4390
Ud	 0.5706	 0.4040
Ue	 0.1954	 0.3470
Uf	 0.4815	 0.5200
Ug	 0.4621	 0.2980
Uh	 0.0333	 0.3480
Ui	 0.5573	 0.3940
Uj	 0.4211	 0.4160
Uk	 0.5309	 0.4780
Ul	 0.2024	 0.2770
Um	 0.4545	 0.4370
Ux	 0.0046	 0.3290