wwPDB EM Validation Summary Report (i)

Mar 20, 2026 – 06:36 AM UTC

PDB ID	:	6SG9 / pdb_00006sg9
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 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 (i) 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 (i)) were used in the production of this report:

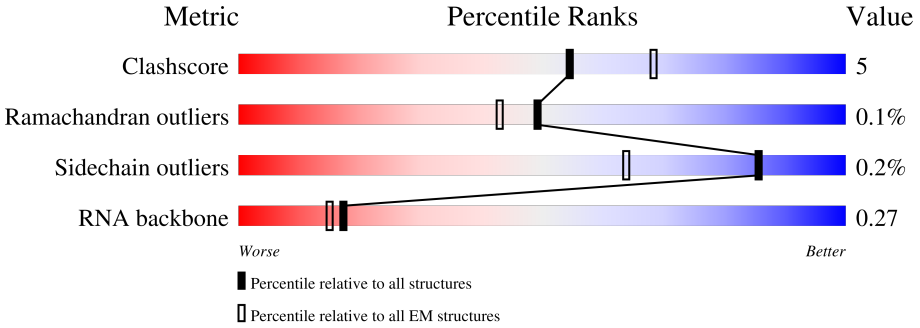
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

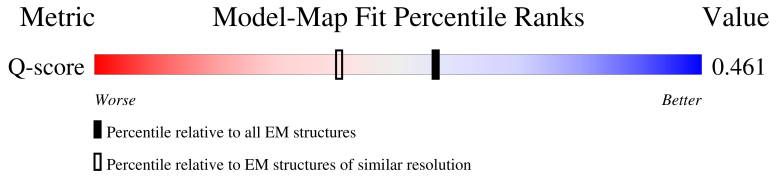
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 <=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	5% 95%
2	CK	326	11% 88%
3	Cn	250	5% 7% 93%

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Mol	Chain	Length	Quality of chain
4	FJ	362	9% 89%
5	FY	188	21% 47% 51%
6	Fa	171	13% 19% 77%
7	CA	802	12% 9% 8% 82%
8	CC	74	31% 72% 26%
9	CI	443	29% 83% 12% 5%
10	CJ	817	17% 72% 14% 14%
11	CN	166	64% 78% 14% 8%
12	CS	244	35% 29% 6% 65%
13	Cg	498	9% 84% 13%
14	Ci	181	31% 72% 9% 19%
15	Ck	874	19% 61% 12% 27%
16	DB	1181	24% 48% 10% 43%
17	DC	1165	17% 81% 8% 12%
18	DE	747	38% 69% 9% 21%
19	DF	666	14% 65% 9% 26%
20	DG	631	13% 76% 14% 10%
21	DH	581	17% 69% 12% 19%
22	DJ	396	11% 70% 7% 22%
23	DK	324	12% 67% 8% 24%
24	DT	247	8% 77% 12% 11%
25	DV	183	27% 76% 10% 14%
26	DW	179	25% 61% 12% 26%
27	DX	169	44% 60% 8% 32%
28	DY	163	36% 79% 16% 6%

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Mol	Chain	Length	Quality of chain
29	F1	1041	28% 69% 11% 20%
30	F4	811	27% 56% 11% 33%
31	FD	579	8% 59% 9% 32%
32	FF	474	32% 75% 11% 14%
33	FG	463	32% 5% 63%
34	FH	457	10% 60% 9% 31%
35	FI	445	12% 66% 12% 22%
36	FK	372	12% 48% 8% 44%
37	FL	353	16% 76% 15% 9%
38	FV	264	9% 72% 8% 20%
39	Fe	123	21% 83% 15%
40	Ua	70	26% 53% 14% 33%
41	Ub	42	71% 83% 17%
42	Uc	12	75% 75% 25%
43	Ud	59	19% 75% 25%
44	Ue	29	76% 97%
45	Uf	9	33% 67% 33%
46	Ug	167	43% 87% 13%
47	Uh	255	99% 81% 19%
48	Ui	32	22% 75% 25%
49	Uj	19	53% 89% 11%
50	Uk	27	26% 78% 22%
51	Ul	14	86% 100%
52	Um	11	36% 36% 64%
53	Ux	108	100% 81% 19%

2 Entry composition (i)

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.

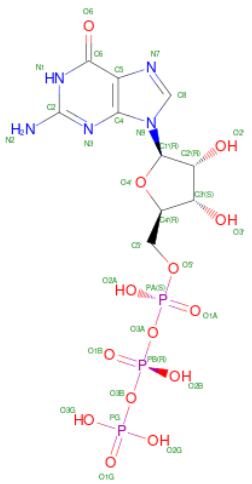
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	Um	11	66	44	11	11	0	0

- 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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



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

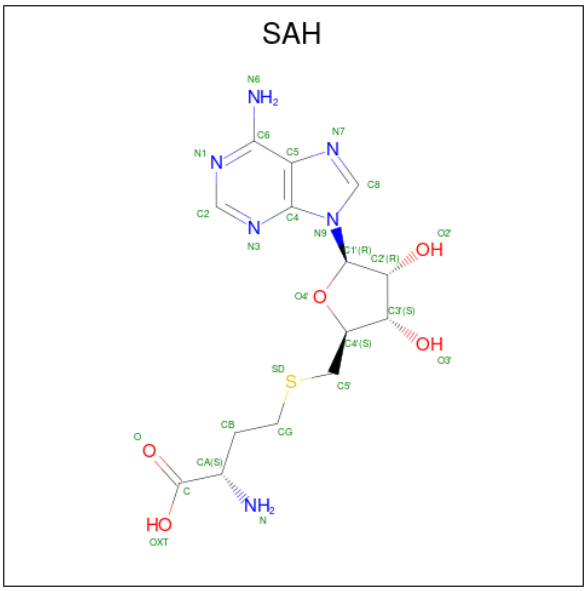
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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.

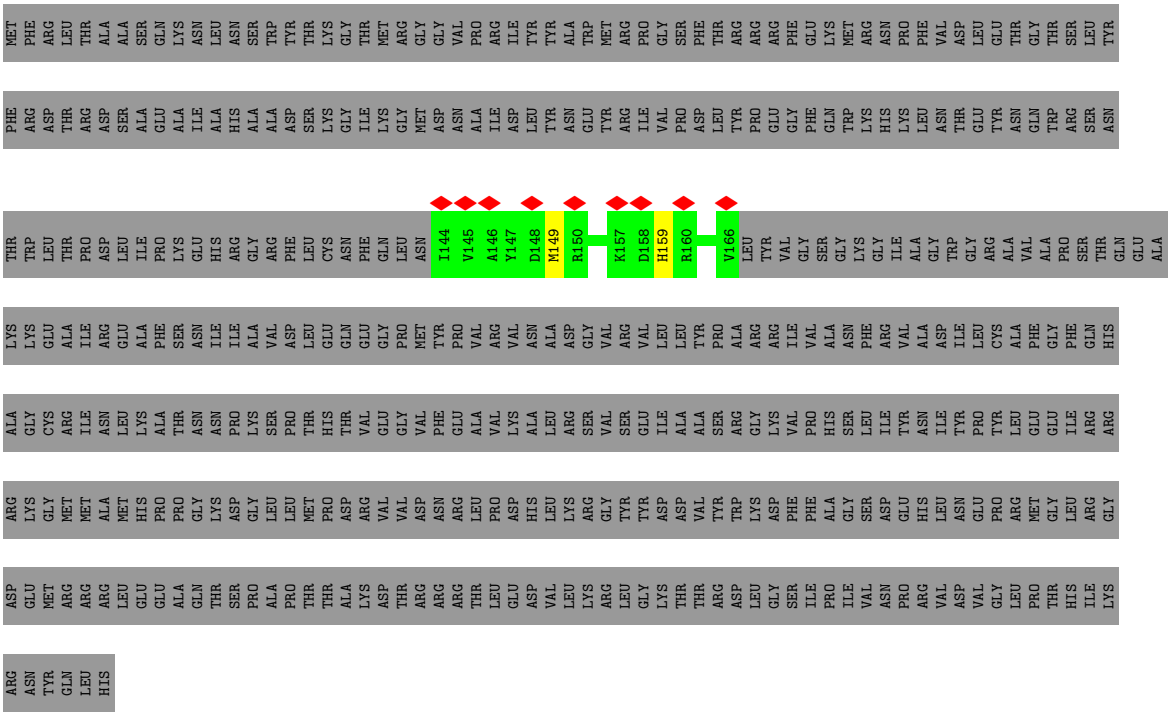
Mol	Chain	Residues	Atoms		AltConf
58	CgC	3	Total	O	0
			3	3	

3 Residue-property plots (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.

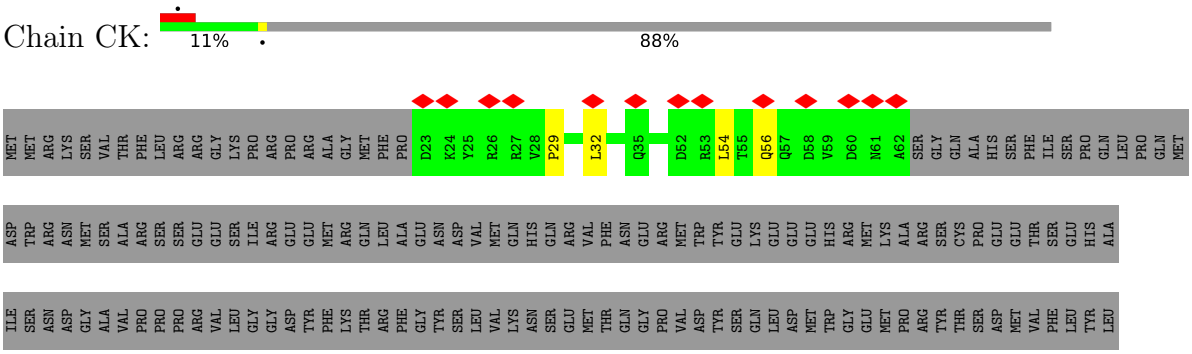
- Molecule 1: uS5m

Chain CE: 5% 95%



- Molecule 2: uS11m

Chain CK: 11% 88%



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

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

PRO LYS MET PRO ARG GLY VAL PHE LYS

- Molecule 3: mS38

Chain Cn: 5% 7% 93%

MET ARG ALA GLY CYS VAL ALA CYS SER ARG ILE PRO LYS LEU GLY ILE ALA ALA LEU GLY SER THR THR THR SER MET GLN ALA THR CYS GLN GLU THR GLN GLU LEU ARG CYS ALA THR THR GLN MET ALA PRO ALA VAL ILE PHE PRO LEU PRO PRO PRO LEU ARG GLY SER TYR ILE

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

GLN THR ASN VAL GLU VAL ASP SER VAL ALA TYR GLY ASP GLN LEU ASP GLU LEU SER ALA R141 W142 A143 A144 K145 F146 Y147 G148 P154 R155 N156 Y157 P158 TYR PRO SER SER ARG TRP LEU ALA ARG ARG PHE GLN MET LYS LYS HIS ARG ILE ILE LYS ARG PHE ARG PHE ARG ARG

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

LYS SER LYS TYR GLN VAL

- Molecule 4: mt-SAF18

Chain FJ: 9% 89%

MET LEU CYS HIS ASN ARG LEU LEU LEU VAL ASN LYS GLN THR GLN LYS TYR ARG THR LYS LEU ARG TYR ARG PHE ARG GLN PRO SER VAL VAL PRO LEU ARG GLN THR LEU GLN GLN ARG HIS ASN THR ILE LEU GLU VAL LEU ARG ARG ARG ILE ASN SER GLY ASP GLN SER PRO

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

LYS TYR MET GLU PRO PRO ILE PRO TYR SER SER LEU ALA ALA ARG LYS LEU ALA ALA GLY ALA LEU TRP PRO ALA ALA PRO ASP PRO GLU GLY MET ILE SER LYS GLU VAL ARG LEU LEU ARG HIS GLU SER SER MET SER PRO SER ALA ARG ALA PHE SER GLU ARG VAL ALA TYR HIS

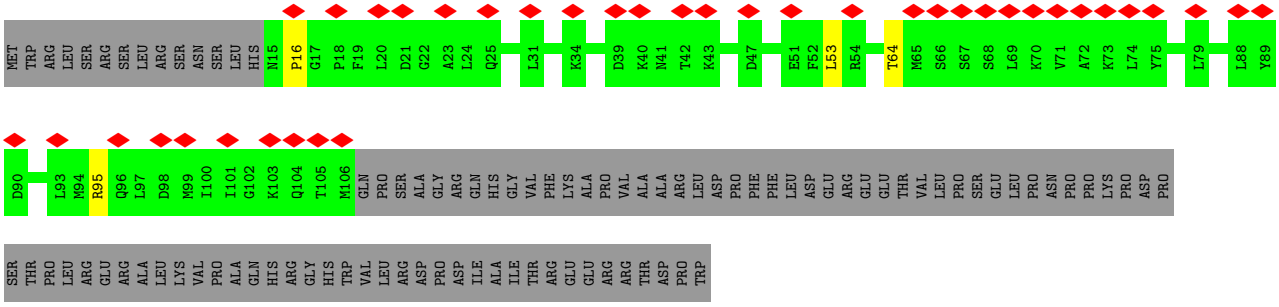
LEU ARG ARG SER LEU LYS ALA CYS PRO GLY HIS ILE ALA GLU HIS ILE ASP PHE THR GLN LEU ILE ILE GLN GLU VAL LEU GLY SER ARG ARG SER LYS GLU ILE TYR ILE VAL TRP PHE THR VAL ASP PRO GLY ALA ARG PHE GLU LEU GLU ARG LEU ASN HIS TRP

VAL GLN GLN LEU ILE ILE LYS ARG VAL LYS ARG ARG PRO HIS ILE PRO ARG VAL THR TRP ILE TYR ASP GLY GLY ARG LEU GLU R269 E270 L271 D274 Q277 E278 L279 Q280 S281 D285 T289 L290 E291 S292 R293 V294 K295 Y296 L297 K298 D301 Q305 R306 M307 K308 D309

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

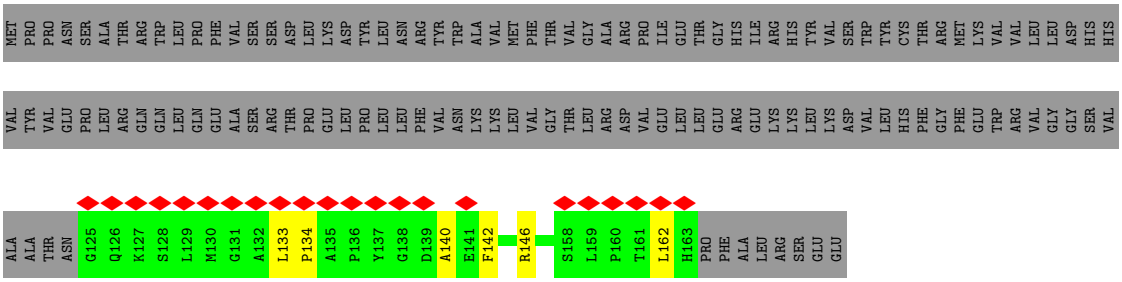
- Molecule 5: mt-SAF28

Chain FY: 21% 47% 51%



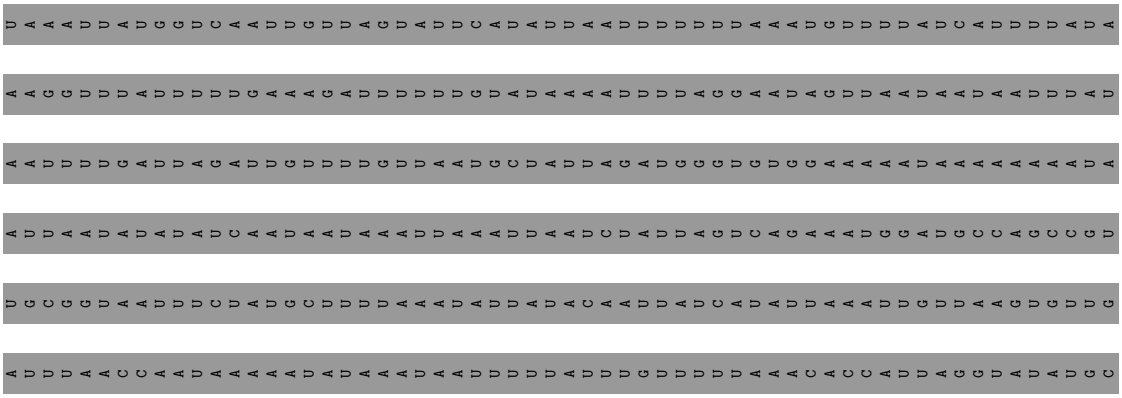
- Molecule 6: mt-SAF30

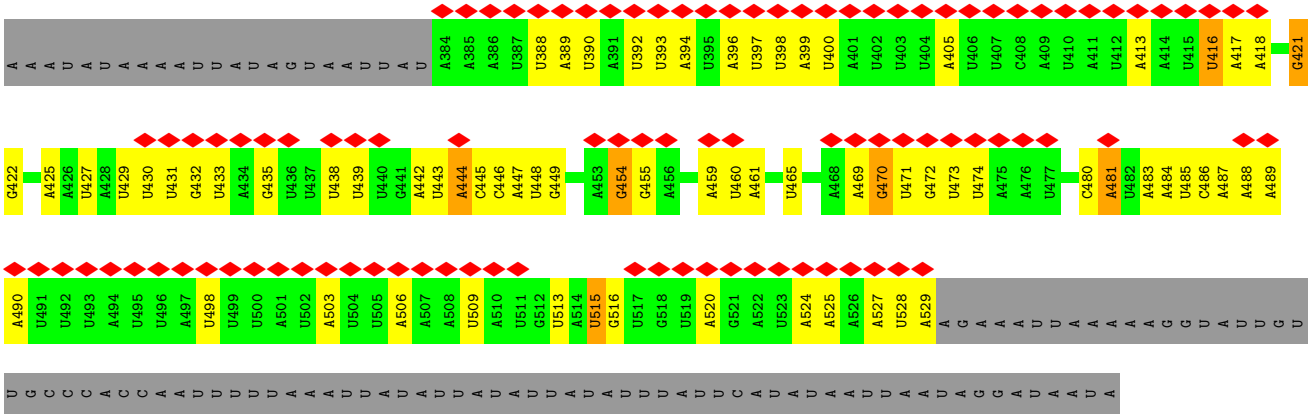
Chain Fa:

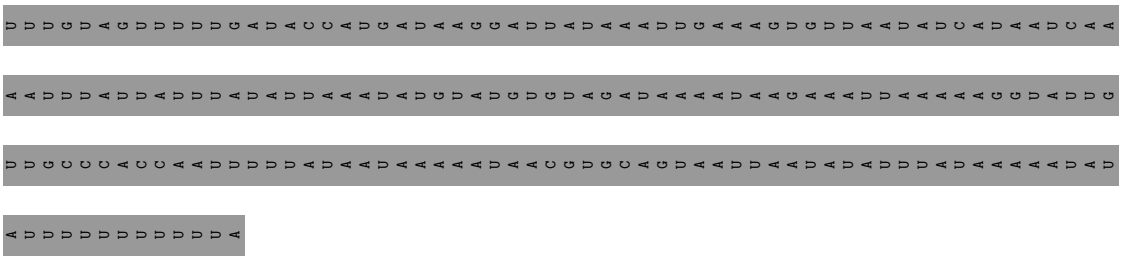


- Molecule 7: 9S rRNA

Chain CA:

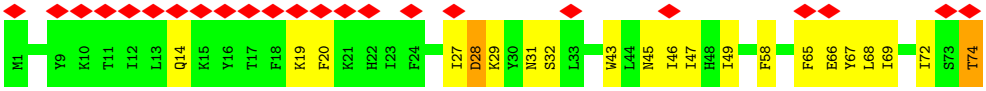






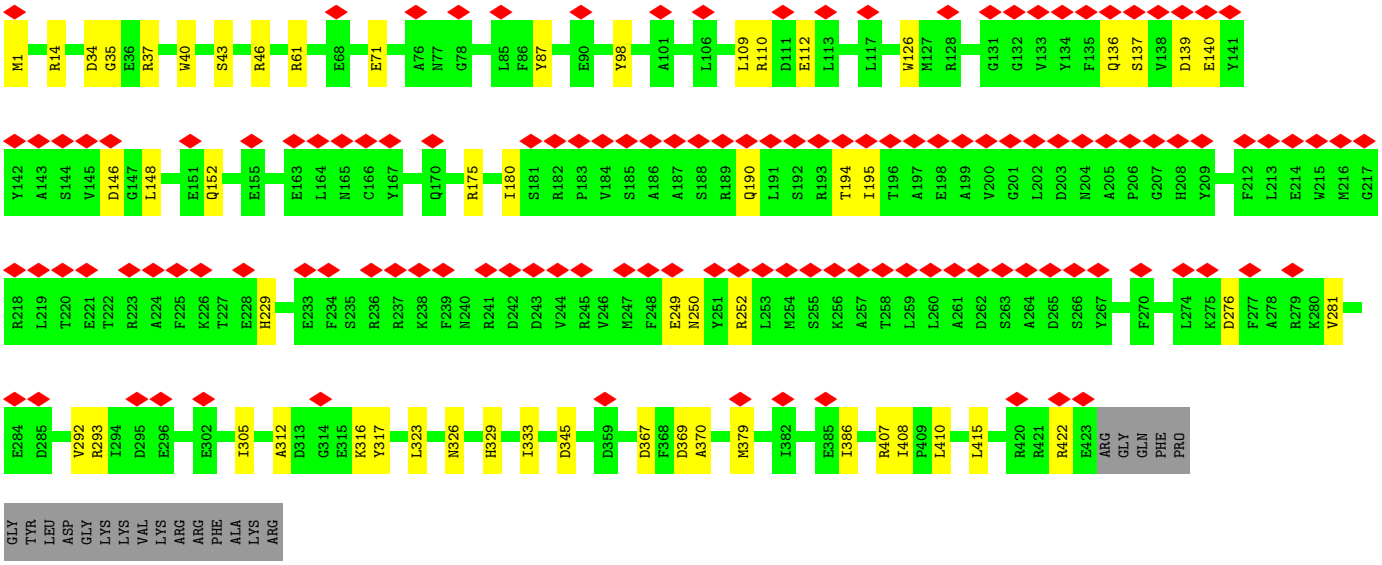
- Molecule 8: uS3m

Chain CC:



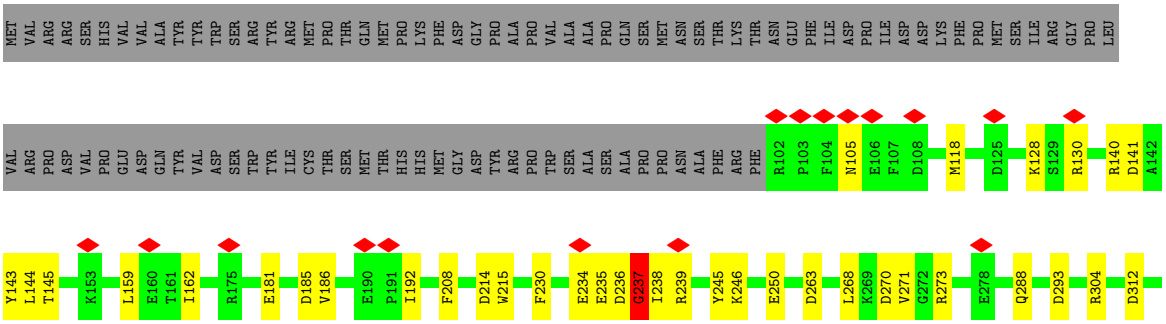
- Molecule 9: uS9m

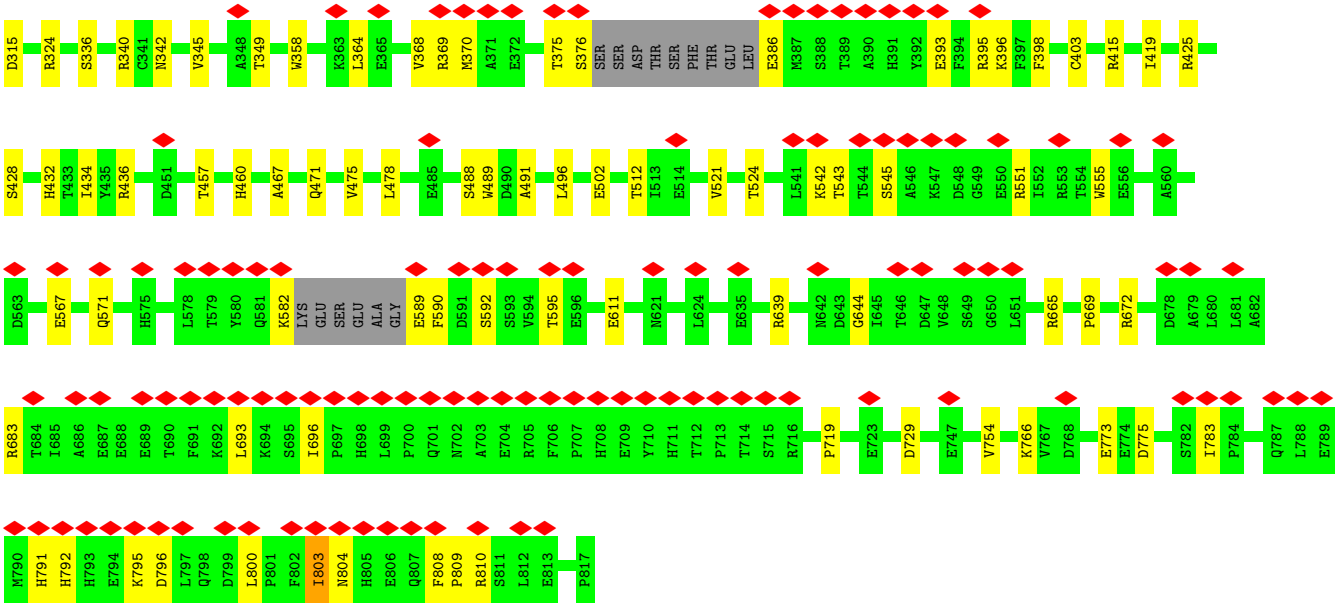
Chain CI:



- Molecule 10: uS10m

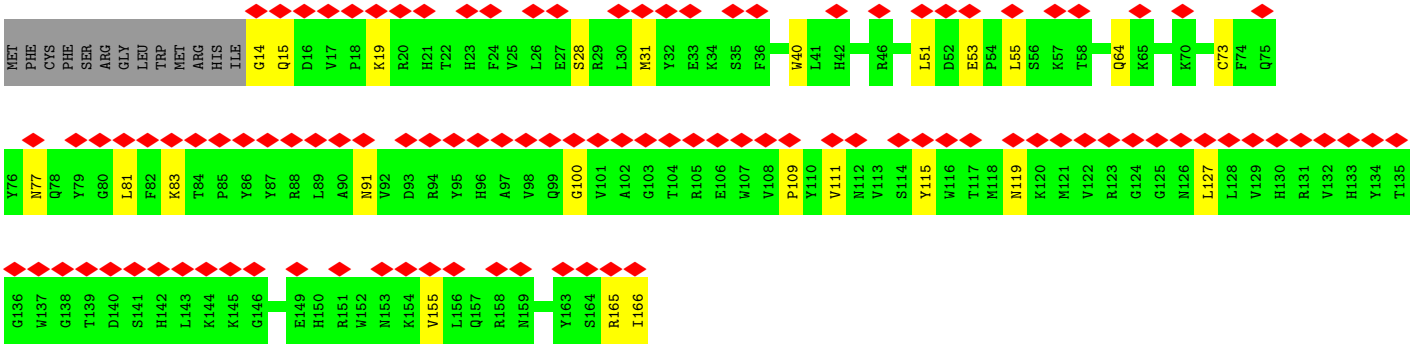
Chain CJ:





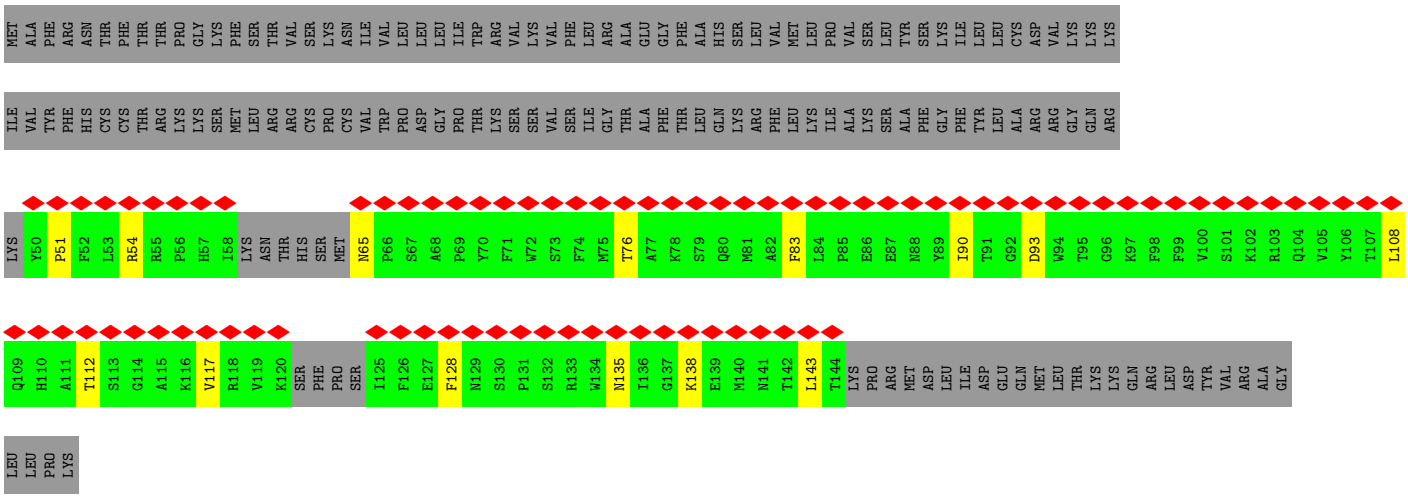
- Molecule 11: uS14m

Chain CN:



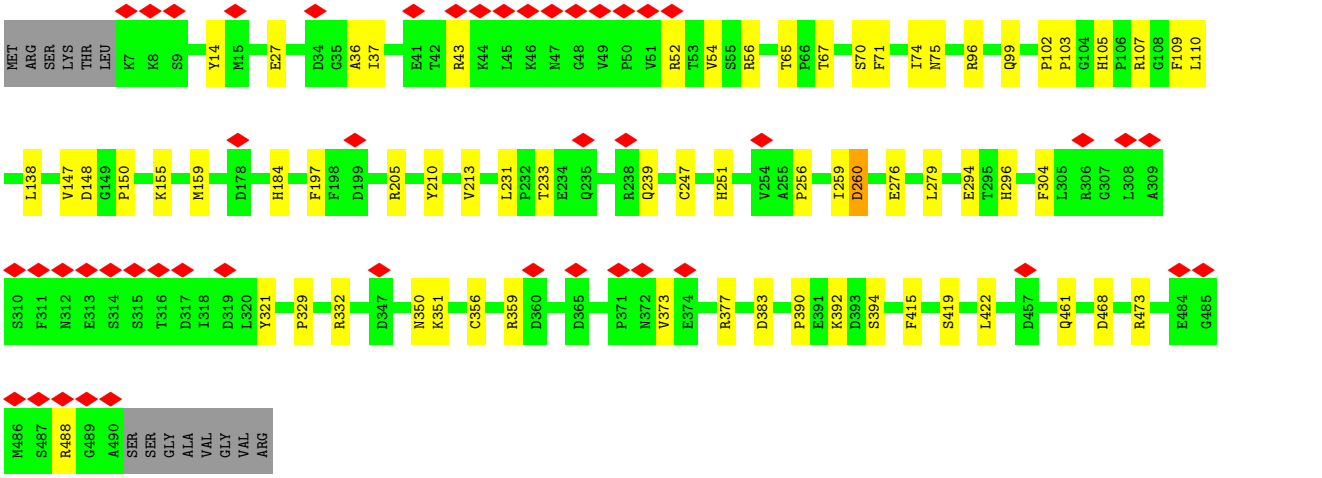
- Molecule 12: uS19m

Chain CS:



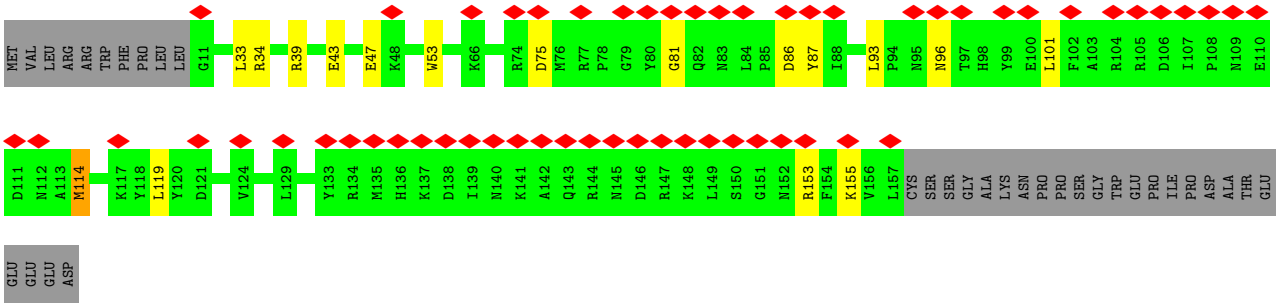
- Molecule 13: mS29

Chain Cg: 9% 84% 13%



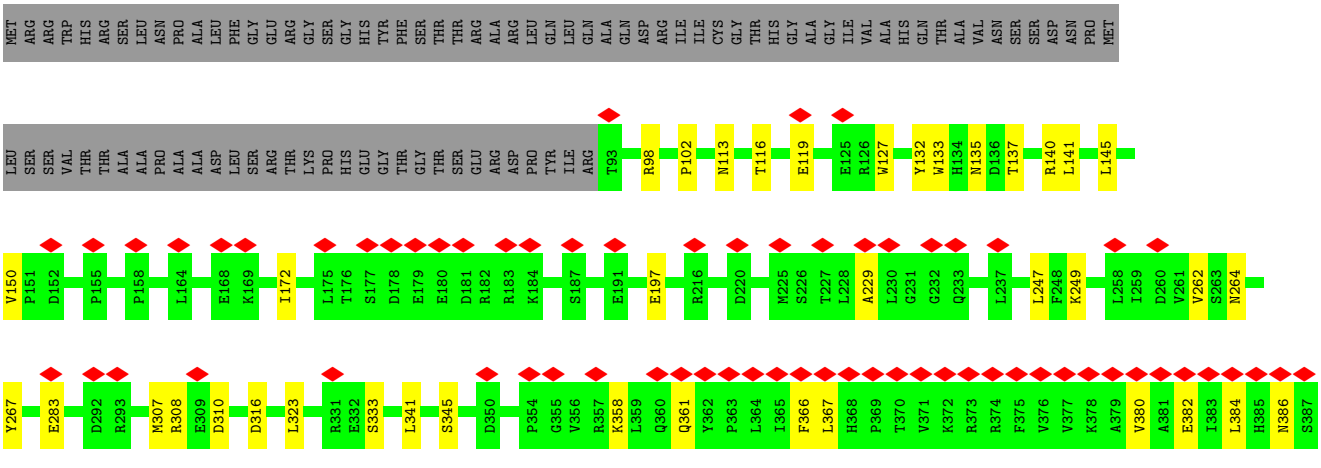
- Molecule 14: mS33

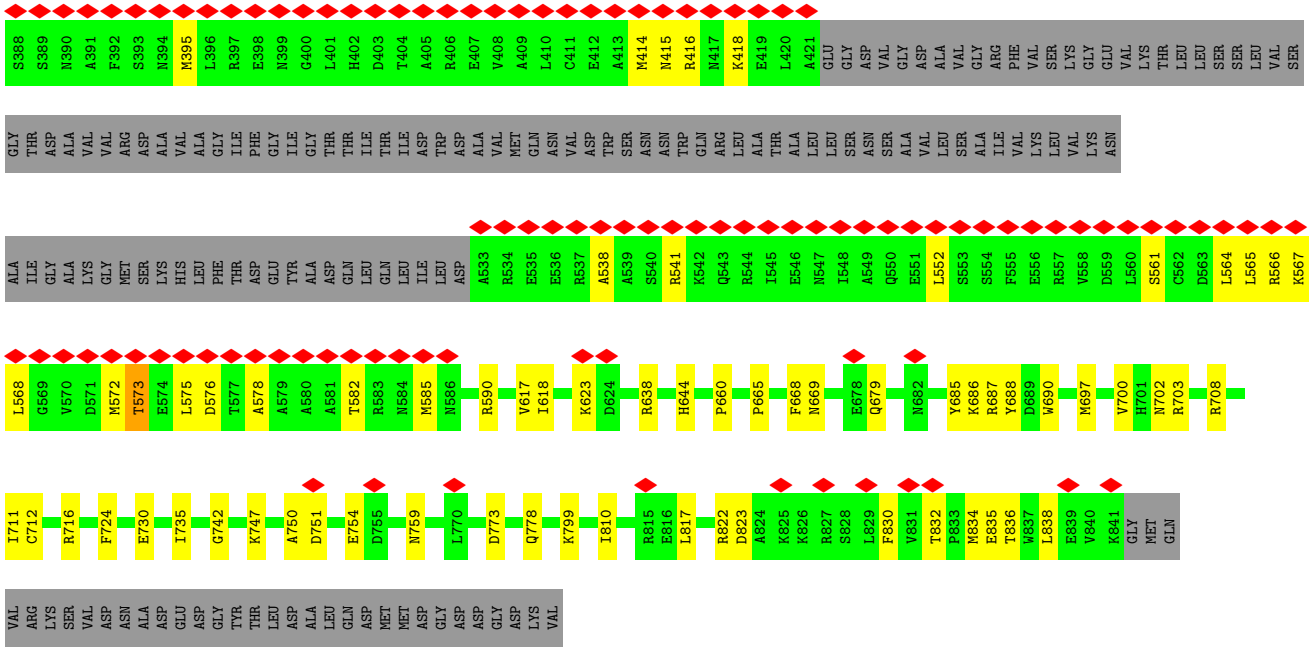
Chain Ci: 31% 72% 9% 19%



- Molecule 15: mS35

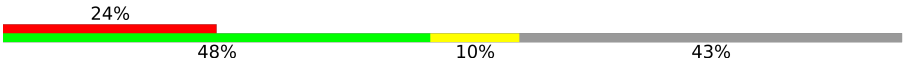
Chain Ck: 19% 61% 12% 27%

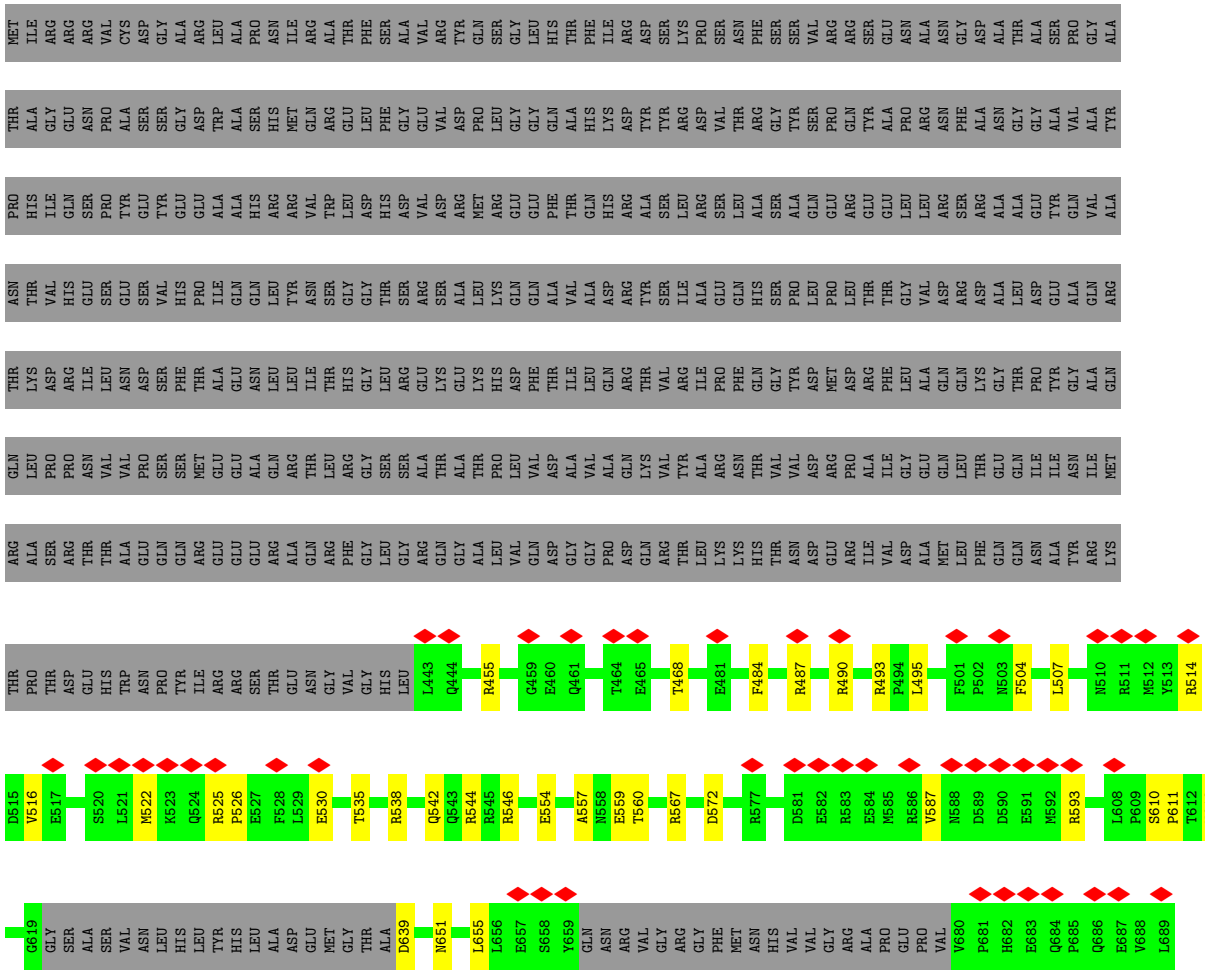


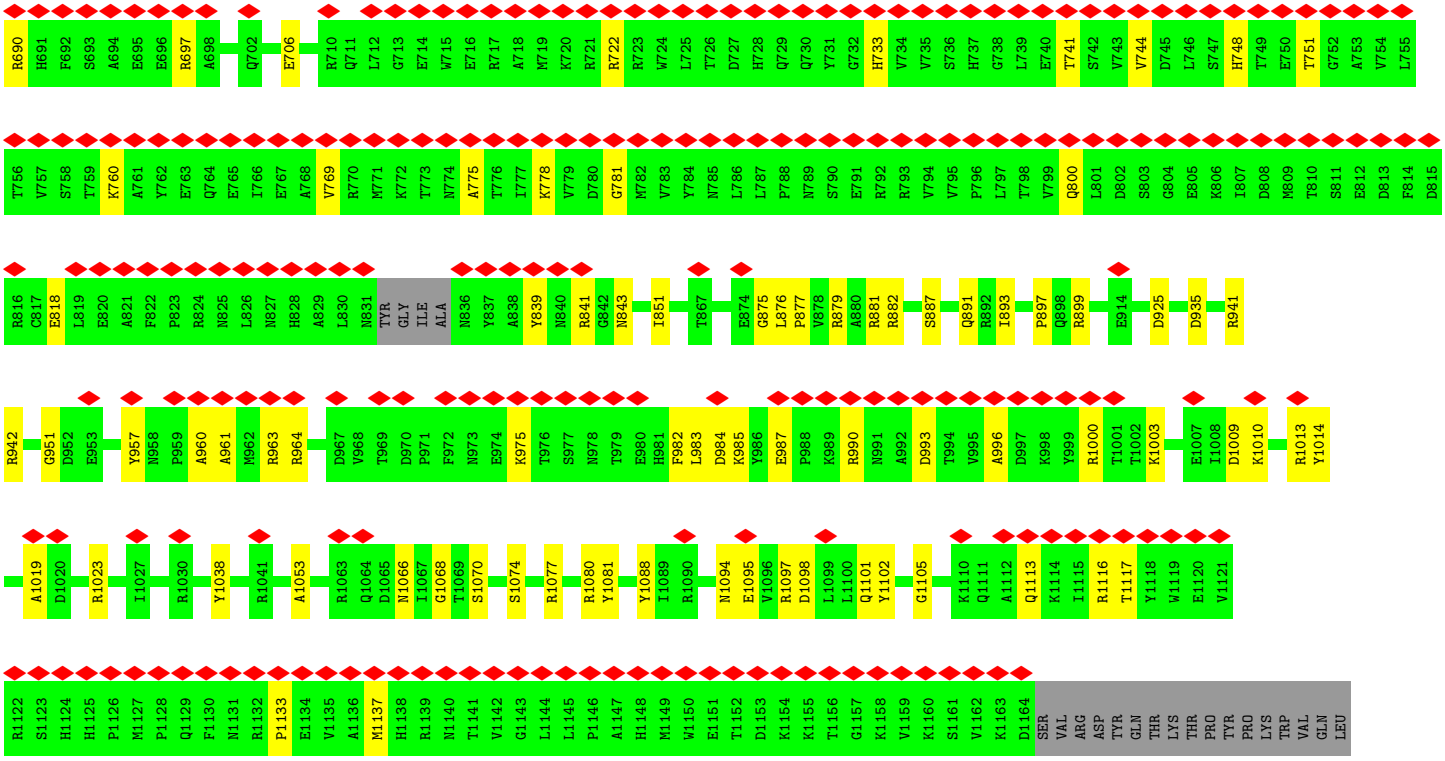


- Molecule 16: mS49

Chain DB:

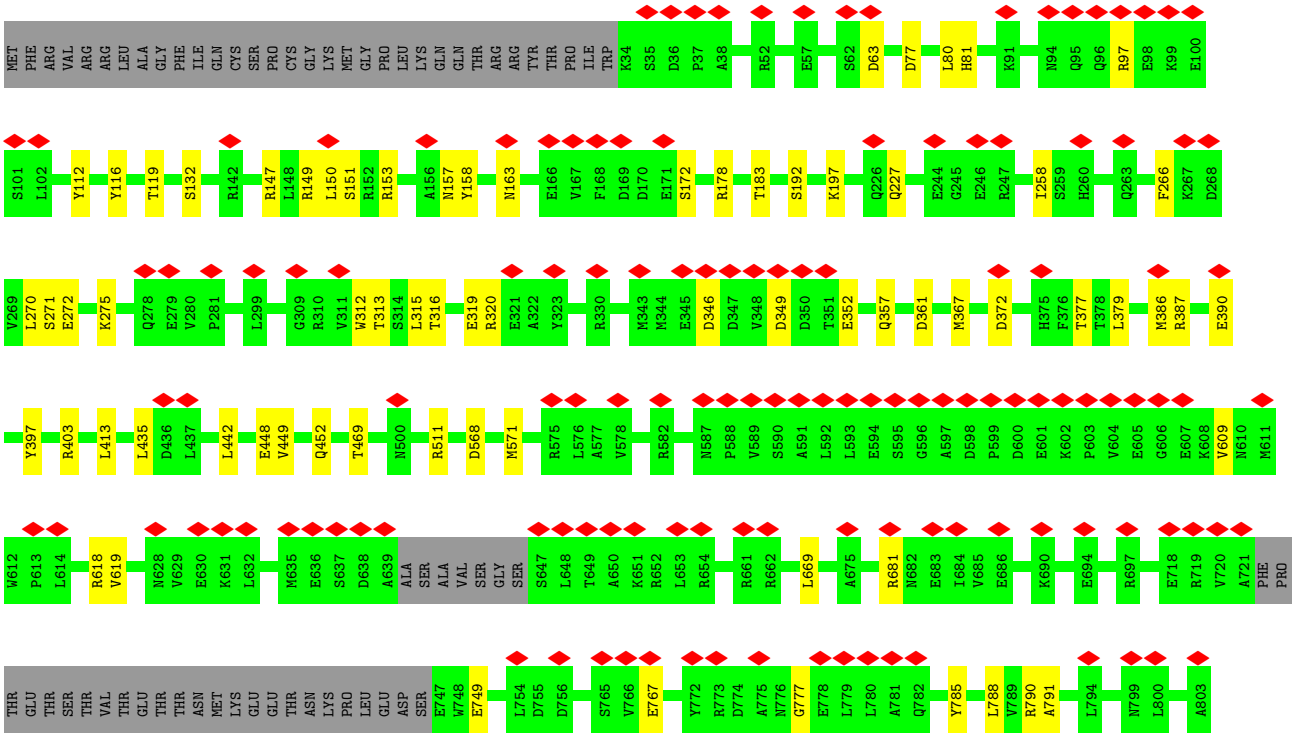


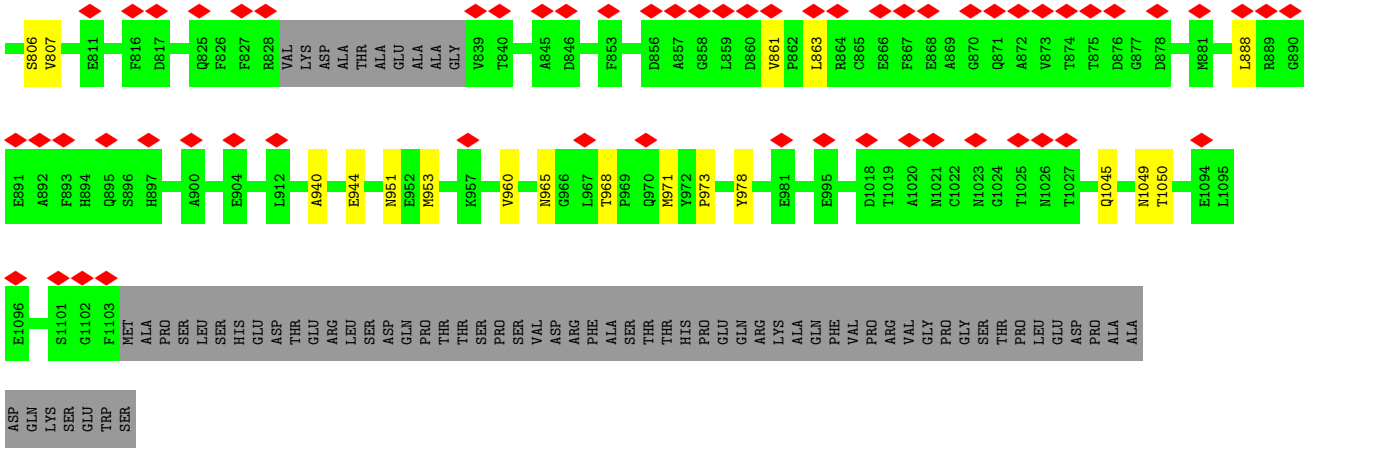




- Molecule 17: mS50

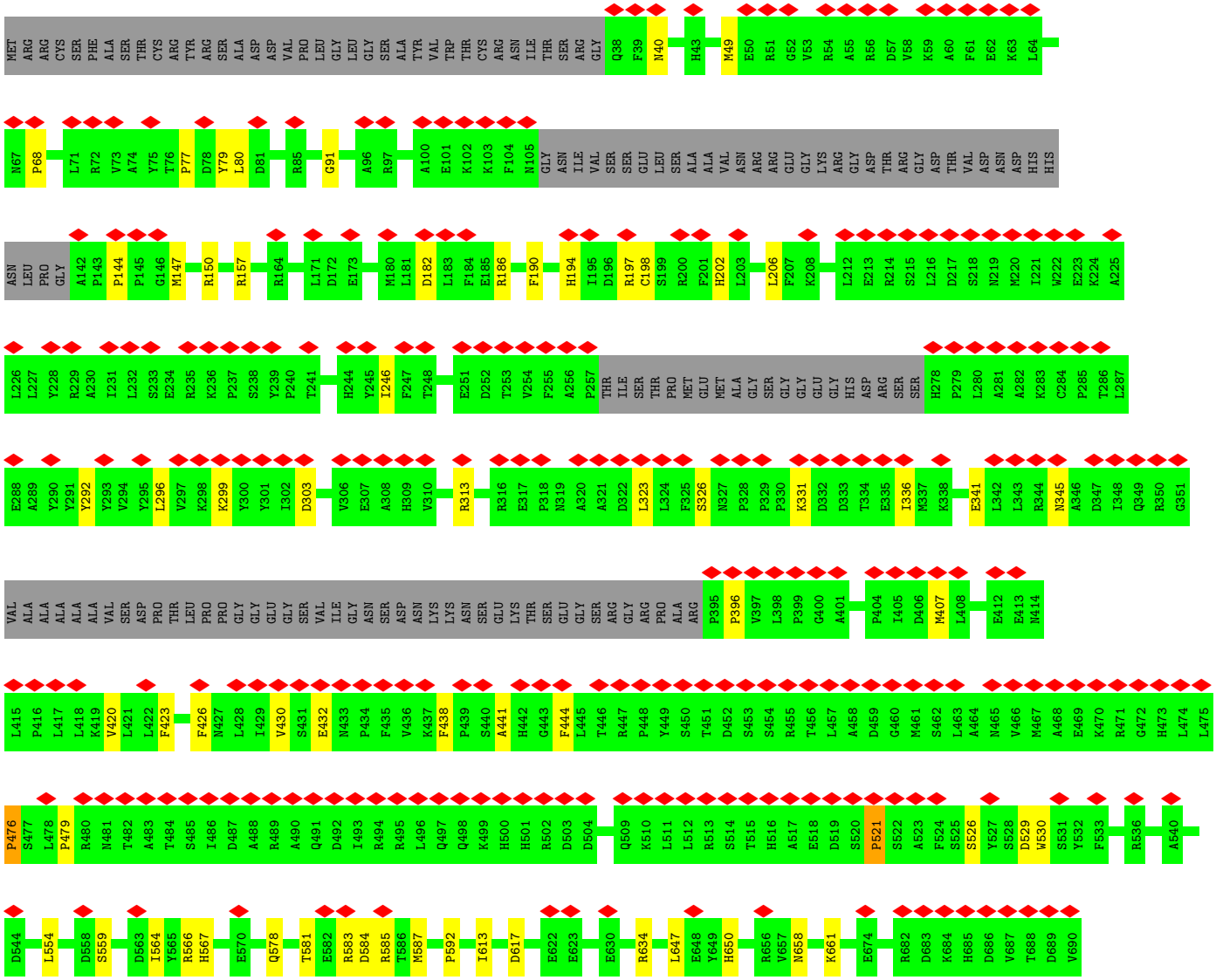
Chain DC:





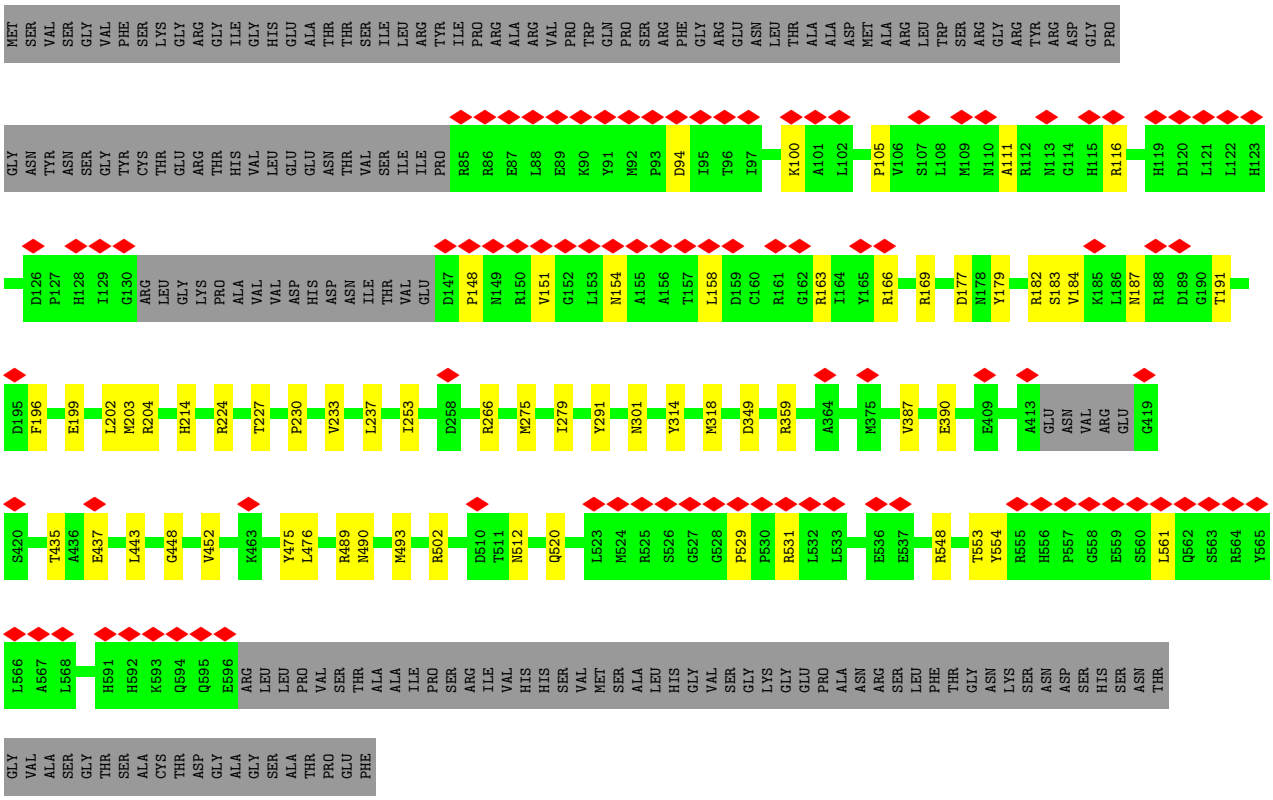
- Molecule 18: mS52

Chain DE:



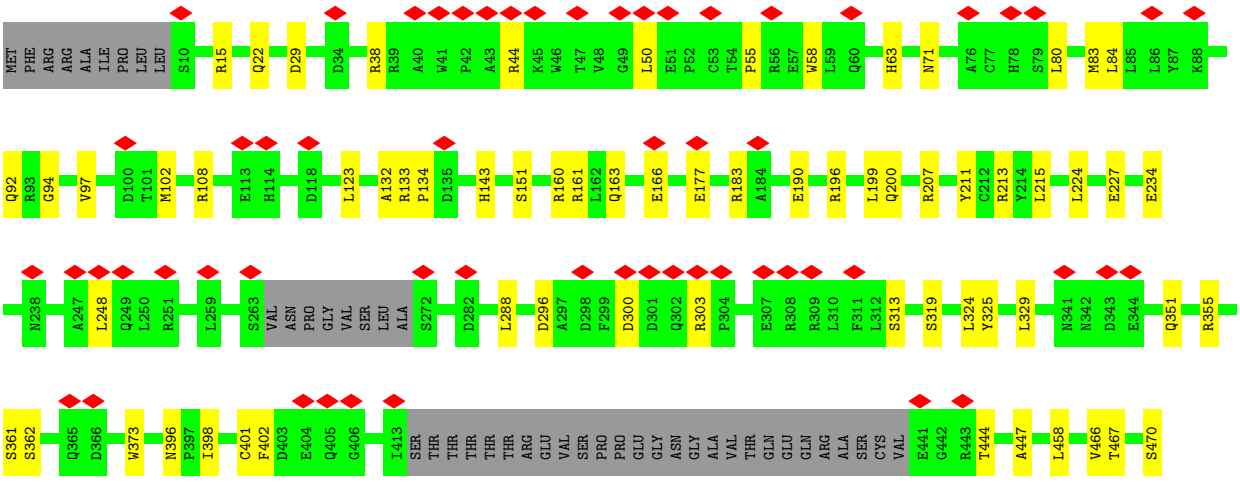
• Molecule 19: mS53

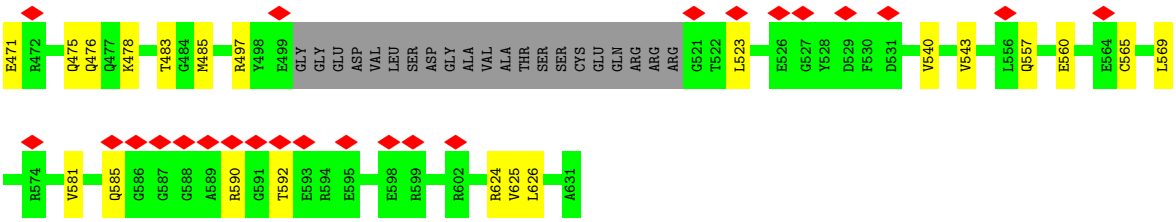
Chain DF:



• Molecule 20: mS54

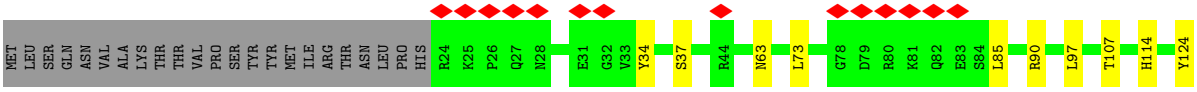
Chain DG:

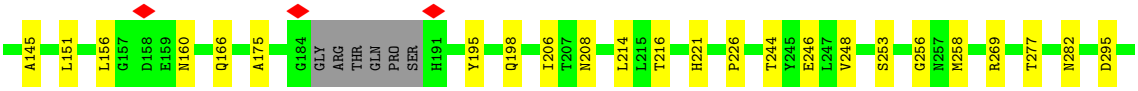


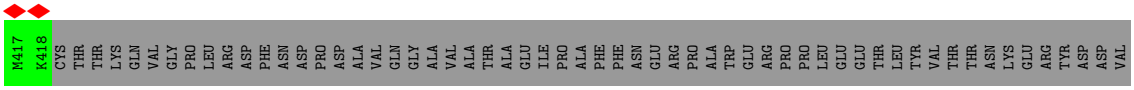


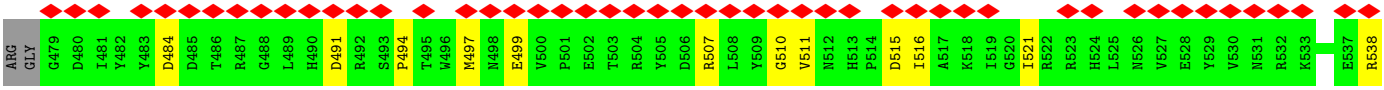
• Molecule 21: mS55 (KRIPP8)

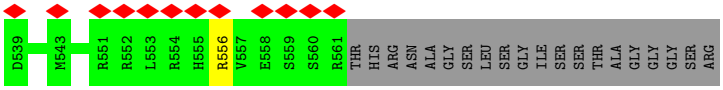
Chain DH:





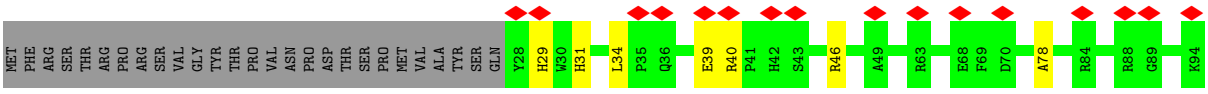


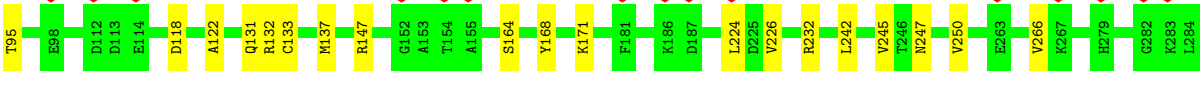


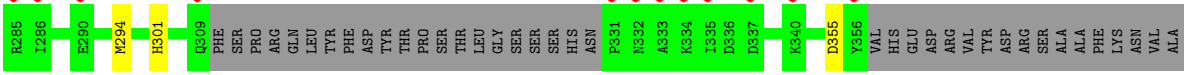


• Molecule 22: mS57

Chain DJ:

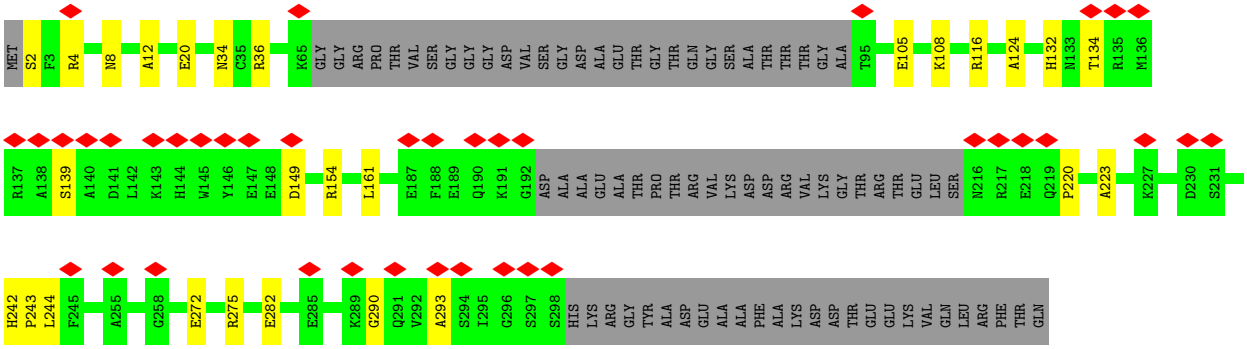






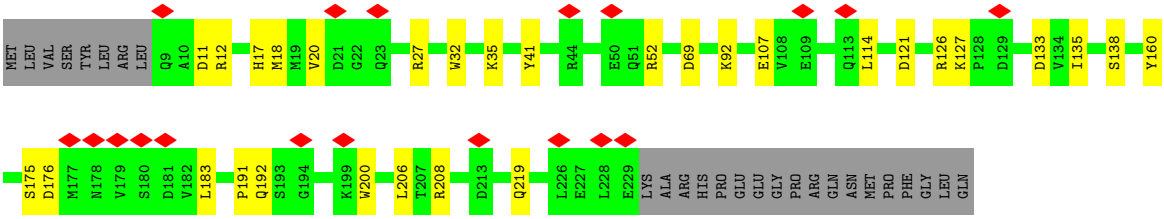
- Molecule 23: mS58

Chain DK:



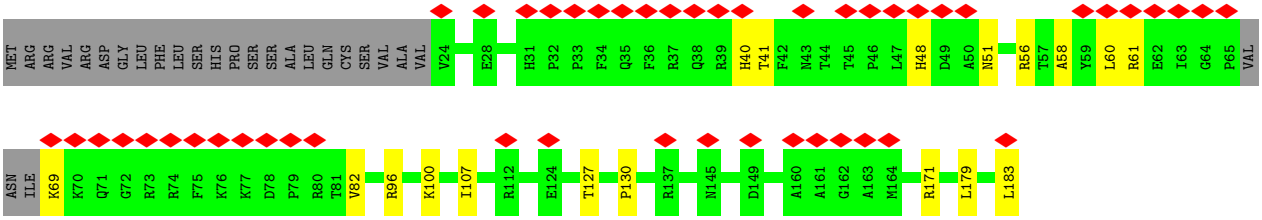
- Molecule 24: mS67

Chain DT:



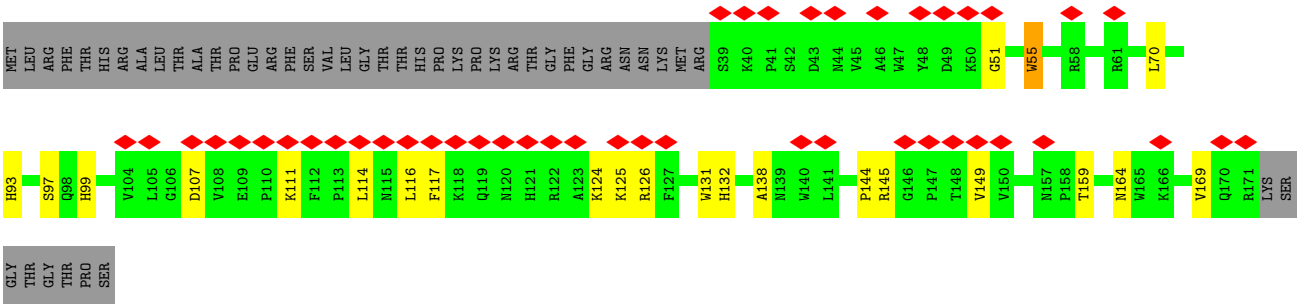
- Molecule 25: mS69

Chain DV:



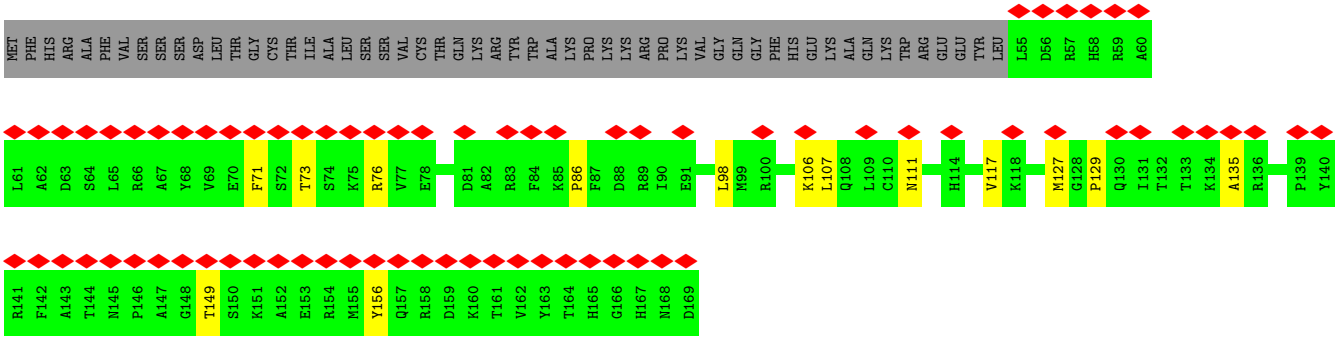
- Molecule 26: mS70

Chain DW:



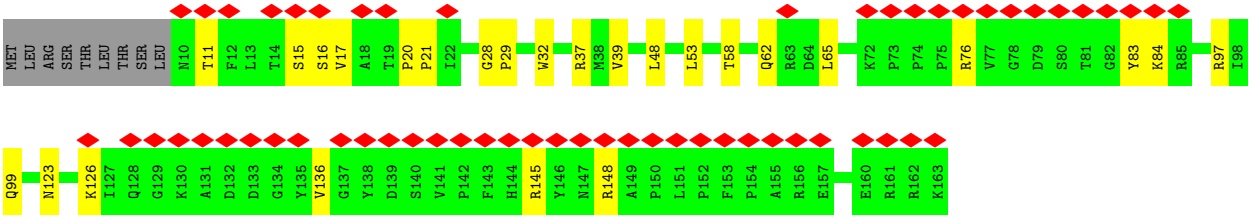
- Molecule 27: mS71

Chain DX:



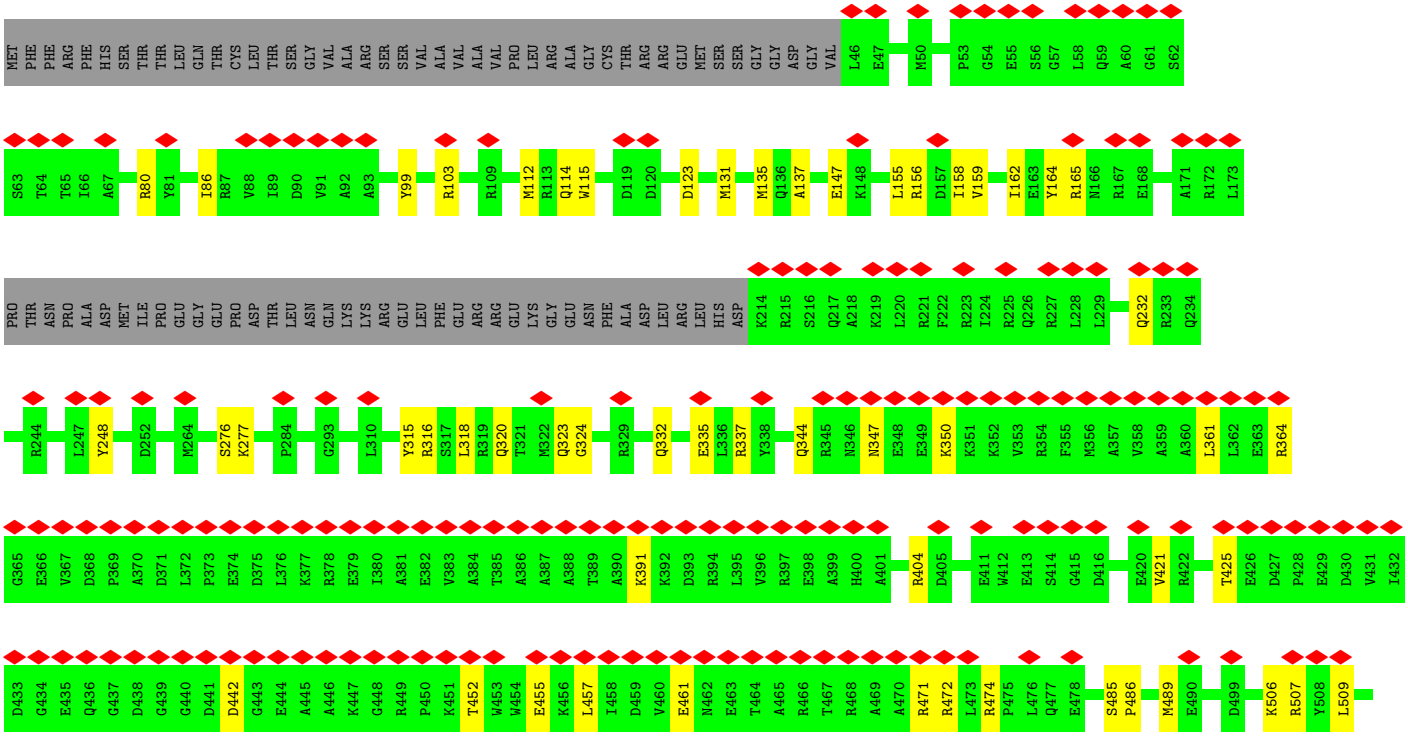
- Molecule 28: mS72

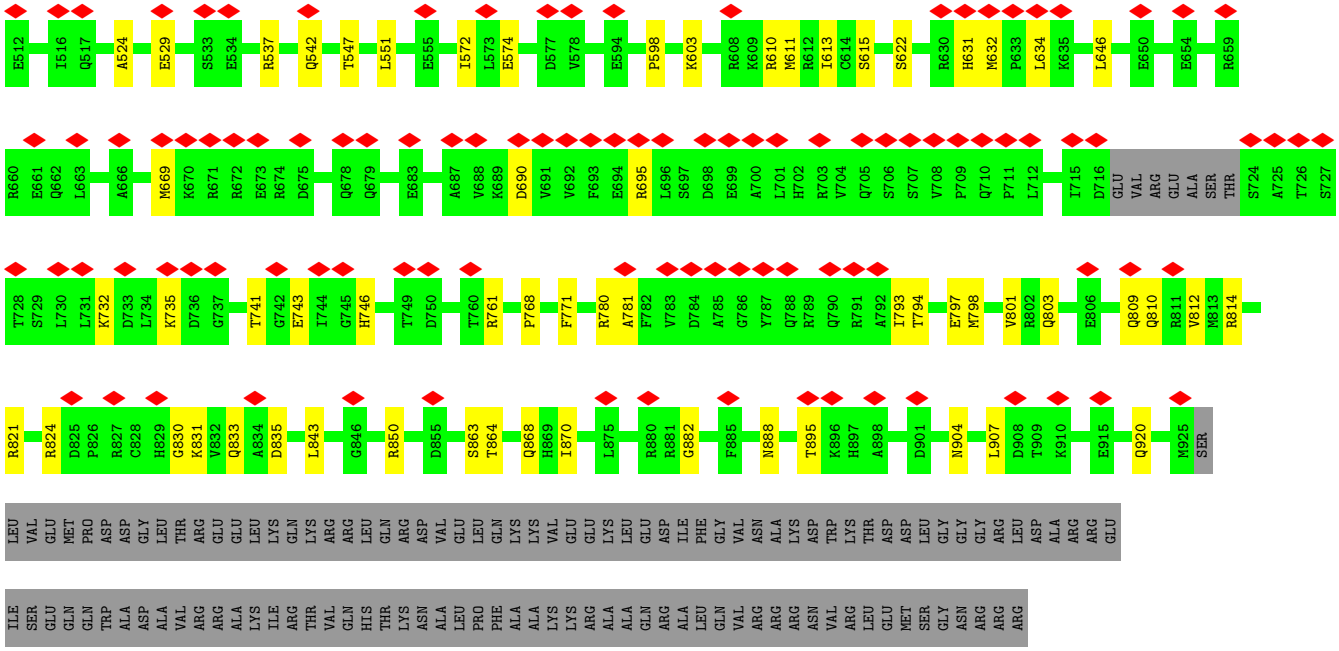
Chain DY:



- Molecule 29: mt-SAF1 (RSM22)

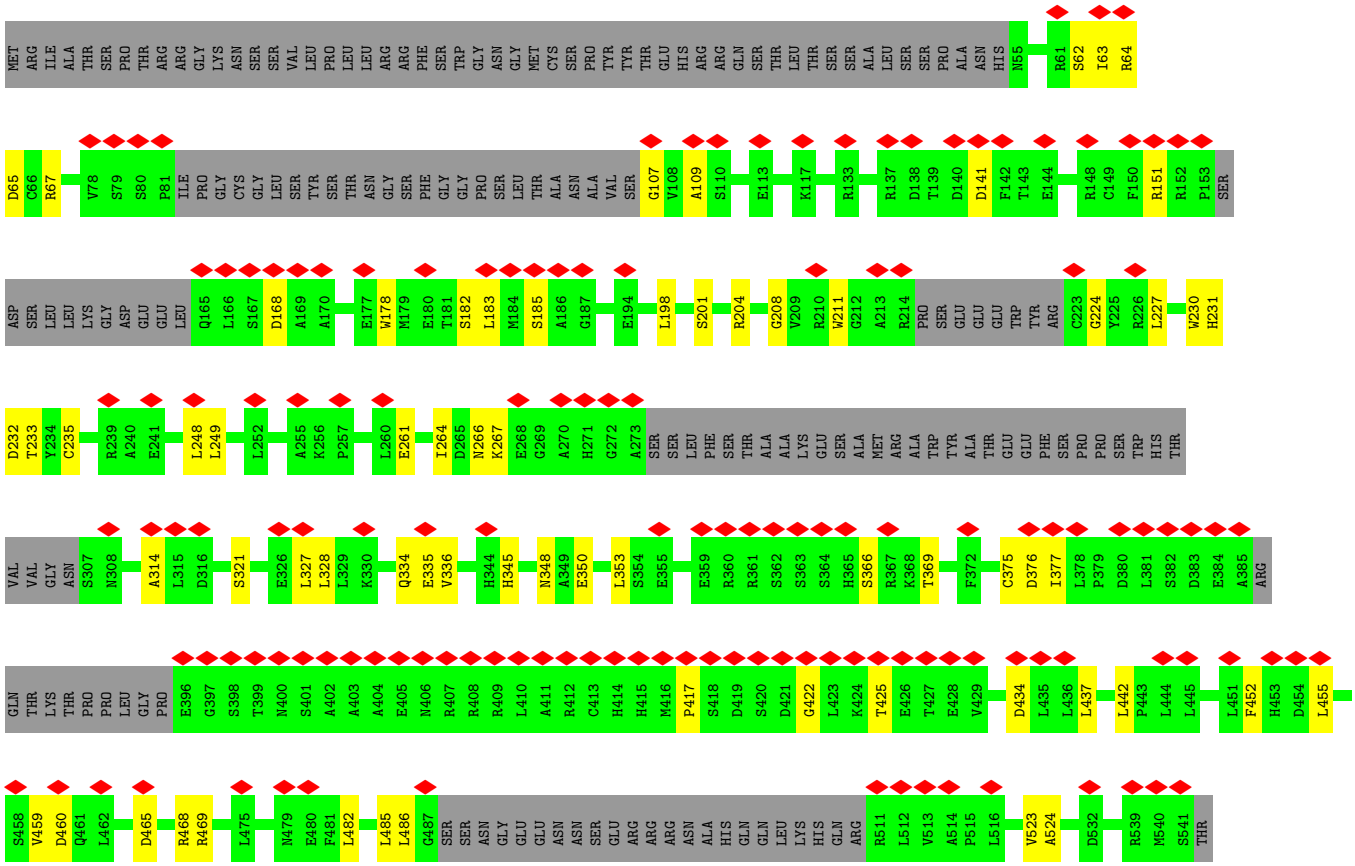
Chain F1:

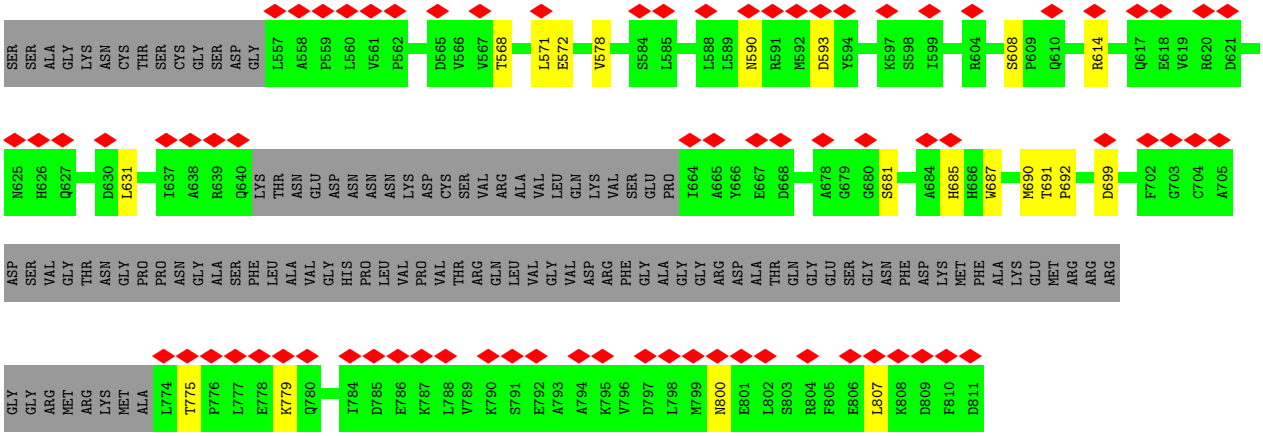




- Molecule 30: mt-SAF4

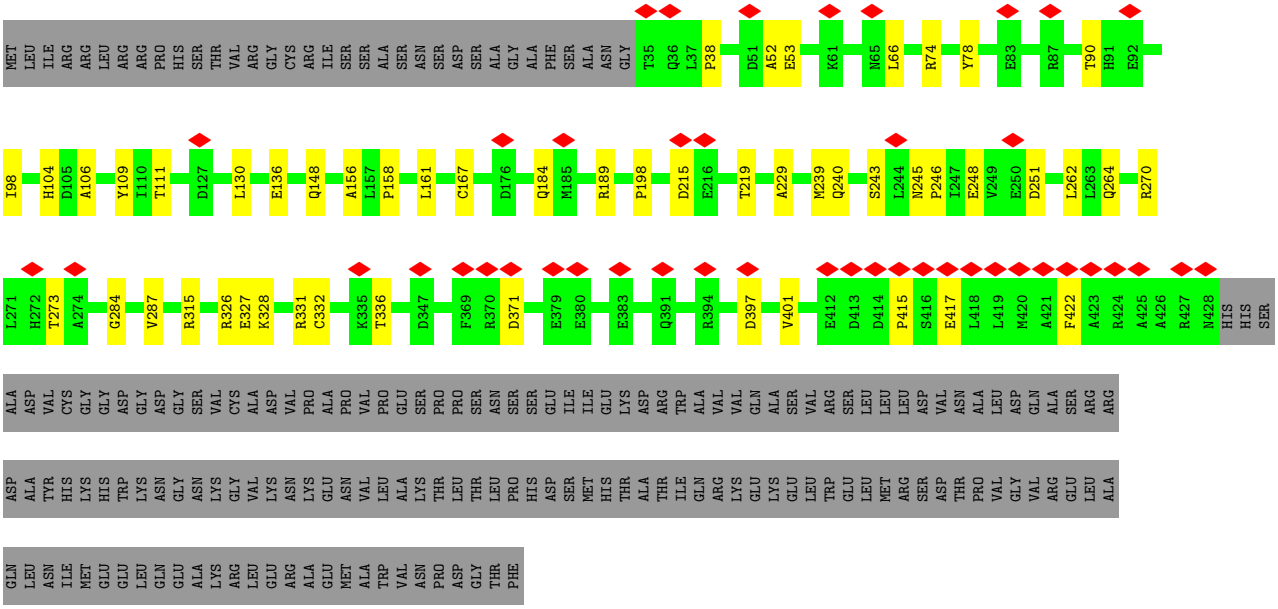
Chain F4:





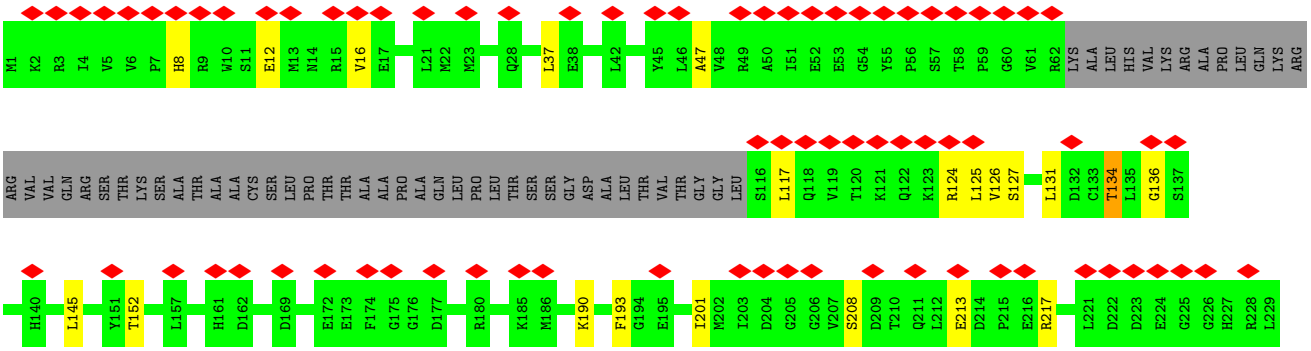
- Molecule 31: mt-SAF12 (KRIPP18)

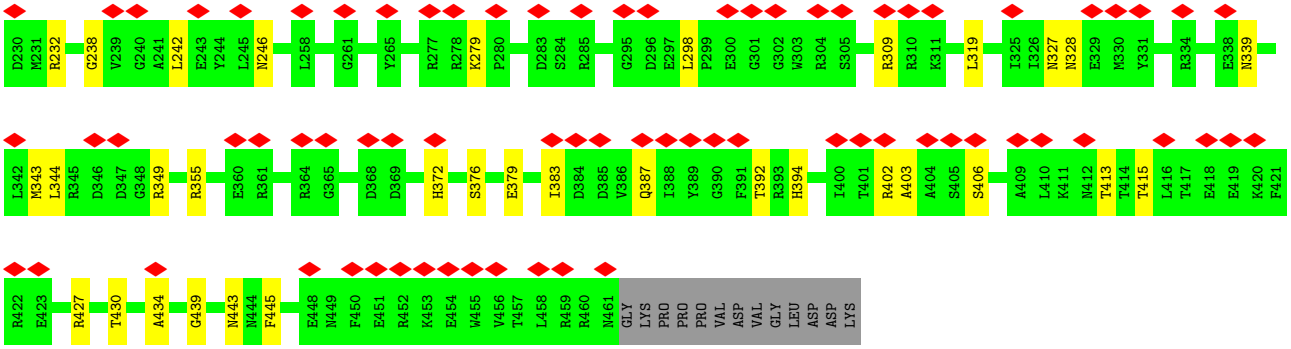
Chain FD:



- Molecule 32: mt-SAF14

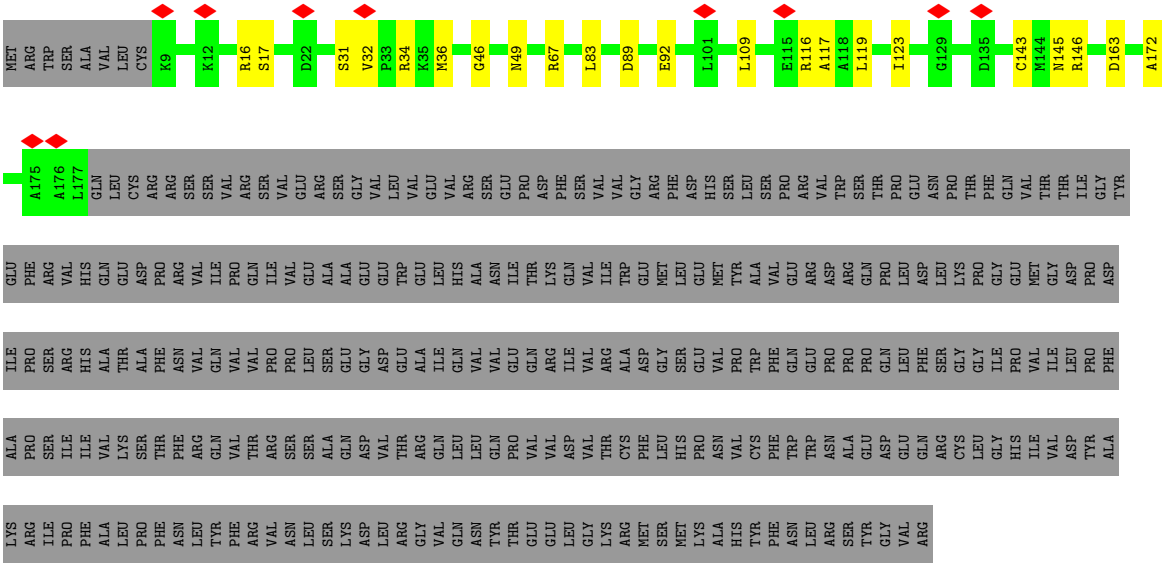
Chain FF:





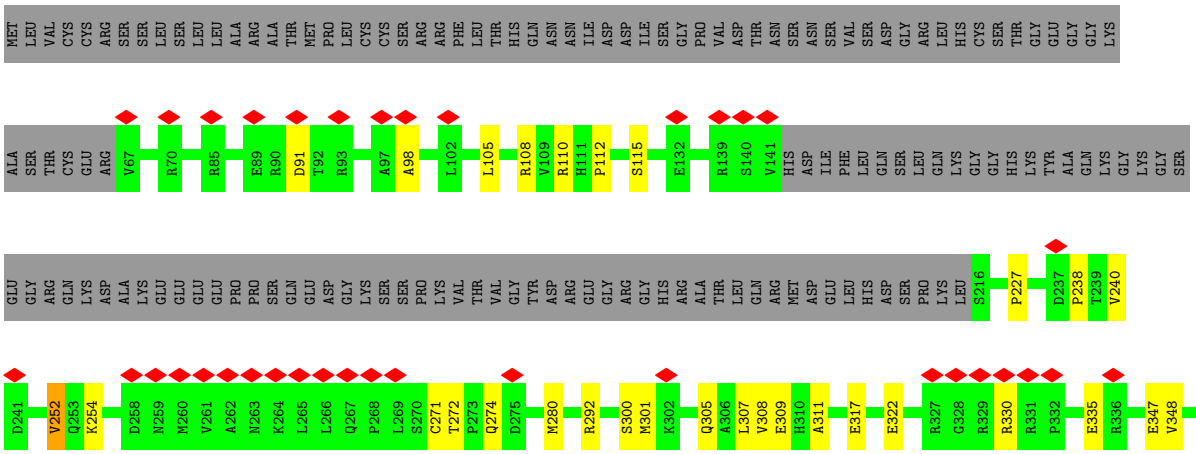
- Molecule 33: mt-SAF15

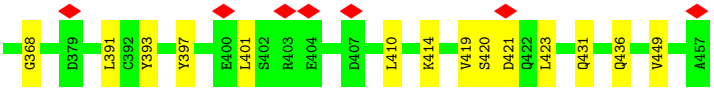
Chain FG:



- Molecule 34: mt-SAF16

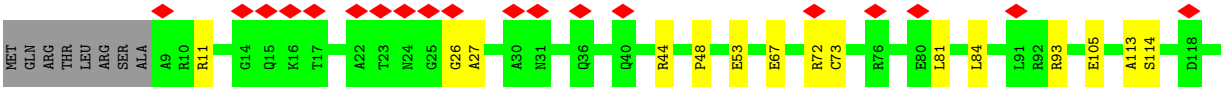
Chain FH:

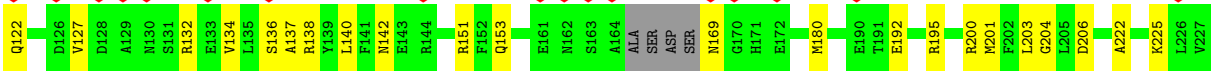


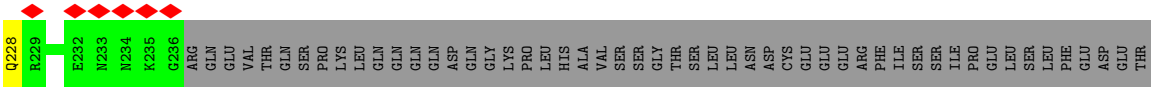


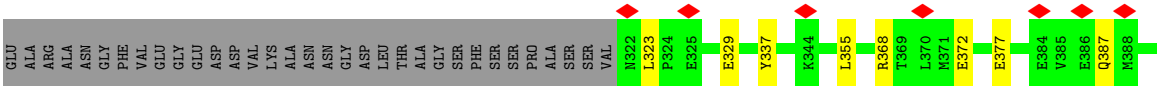
- Molecule 35: mt-SAF17

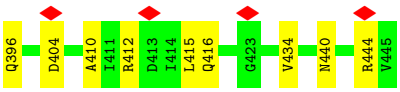
Chain FI:





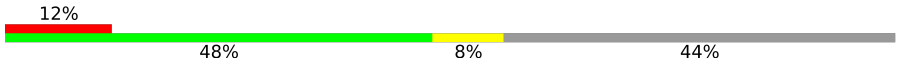


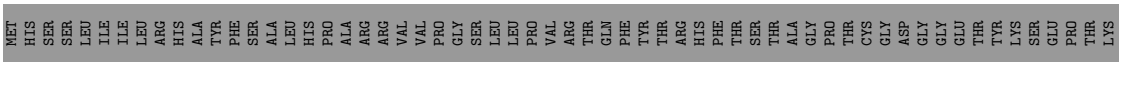


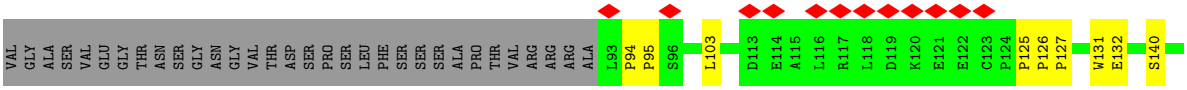


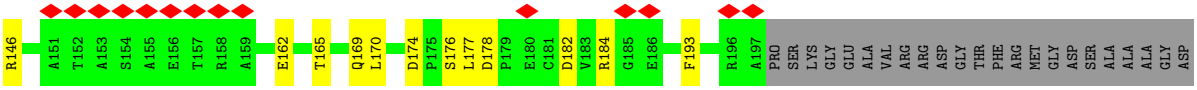
- Molecule 36: mt-SAF19

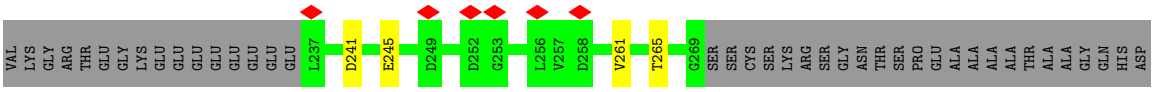
Chain FK:

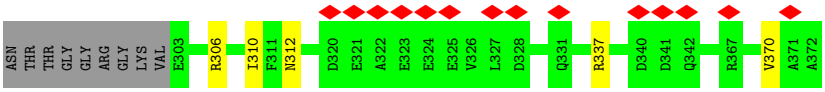






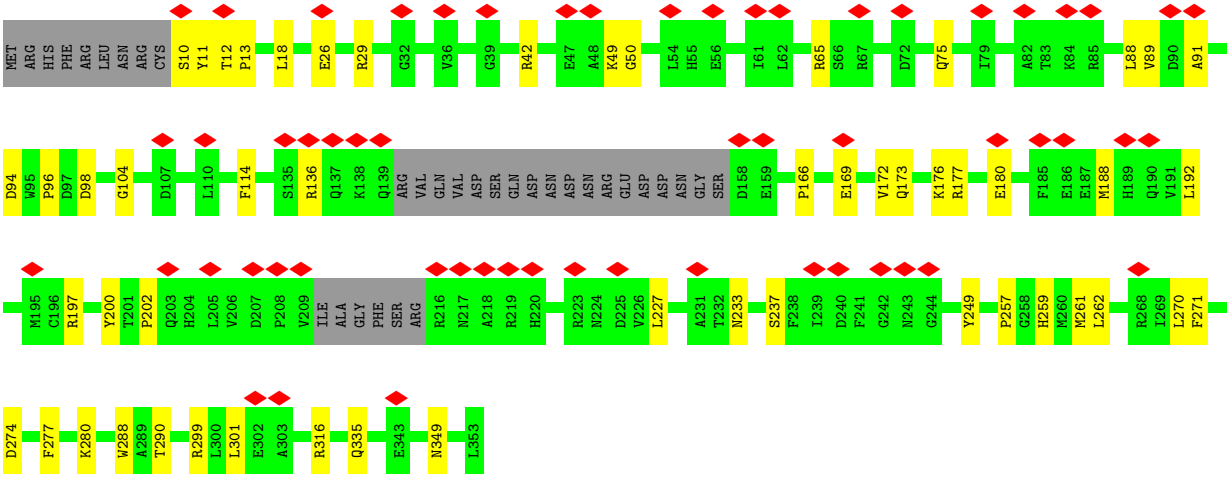






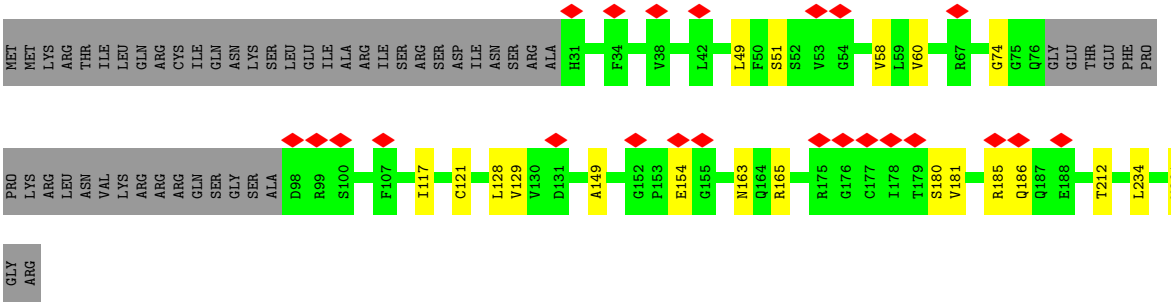
- Molecule 37: mt-SAF20

Chain FL:



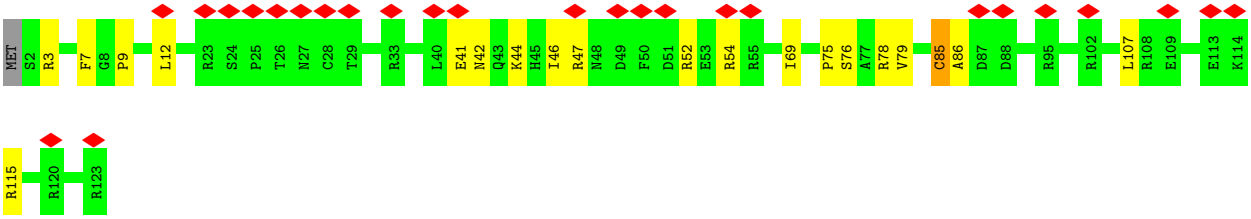
- Molecule 38: mt-SAF25

Chain FV:



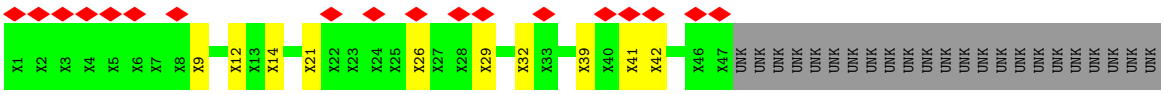
- Molecule 39: mt-SAF34

Chain Fe:



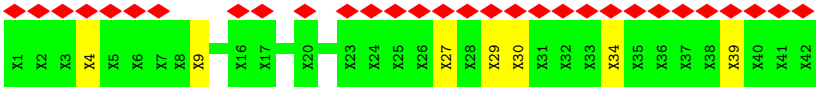
- Molecule 40: UNK-a

Chain Ua:



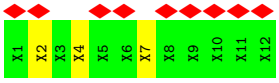
- Molecule 41: UNK-b

Chain Ub:



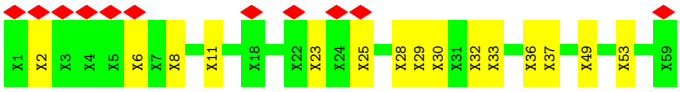
- Molecule 42: UNK-c

Chain Uc:



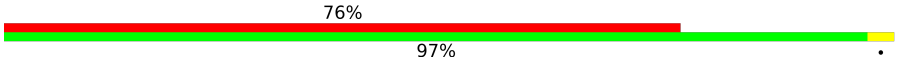
- Molecule 43: UNK-d

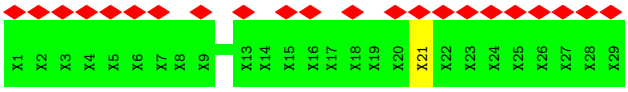
Chain Ud:



- Molecule 44: UNK-e

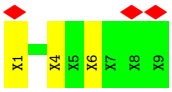
Chain Ue:





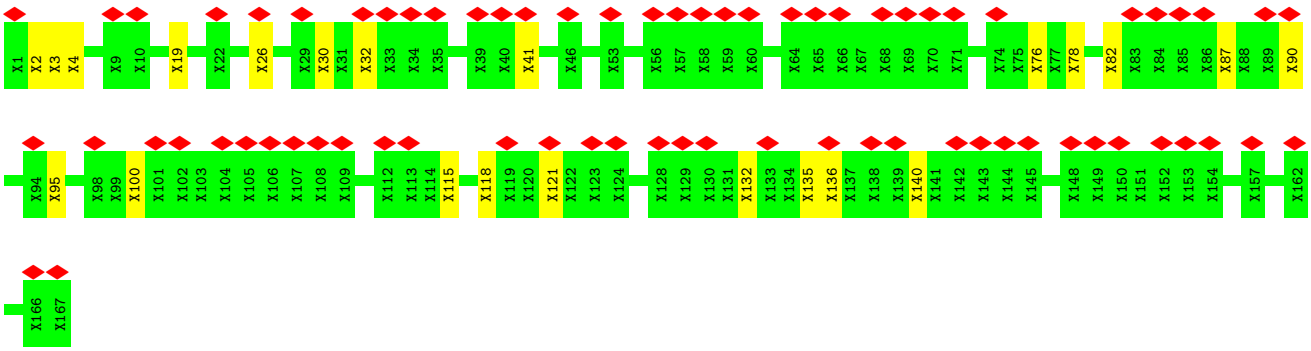
- Molecule 45: UNK-f

Chain Uf:



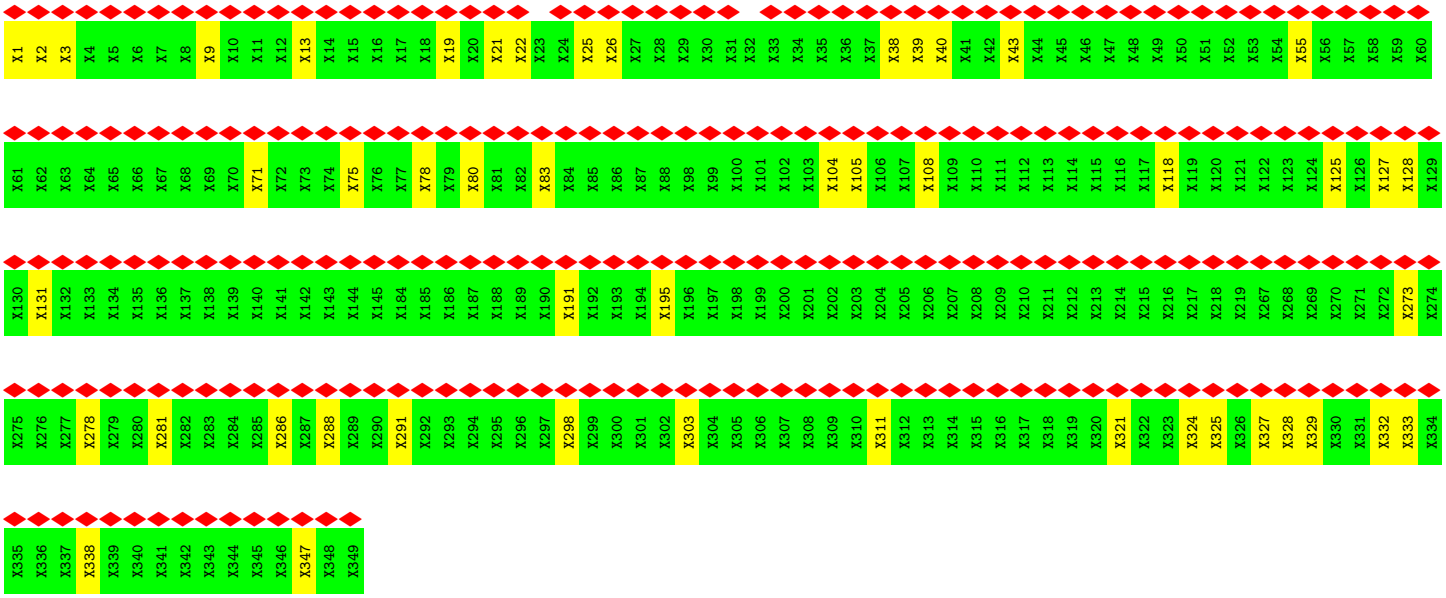
- Molecule 46: UNK-g

Chain Ug:



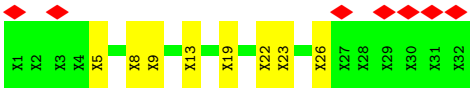
- Molecule 47: UNK-h

Chain Uh: 99% 81% 19%



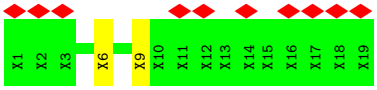
- Molecule 48: UNK-i

Chain Ui: 22% 75% 25%



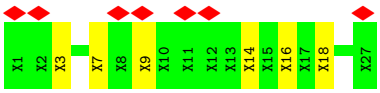
- Molecule 49: UNK-j

Chain Uj: 53% 89% 11%



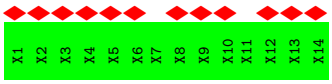
- Molecule 50: UNK-k

Chain Uk: 26% 78% 22%



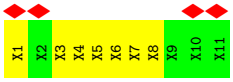
- Molecule 51: UNK-l

Chain Ul: 86% 100%



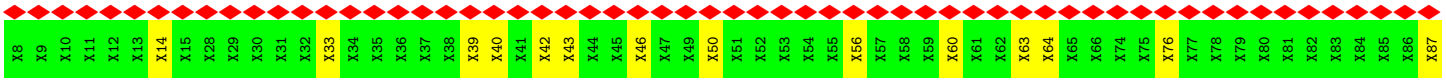
- Molecule 52: UNK-m

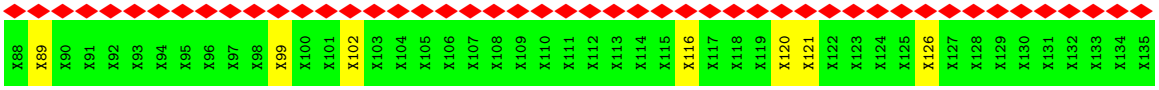
Chain Um:



- Molecule 53: UNK-x

Chain Ux:





4 Experimental information (i)

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 ($e^-/Å^2$)	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: GTP, ZN, MG, SAH

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	0.14	0/206	0.37	0/278
2	CK	0.20	0/343	0.43	0/461
3	Cn	0.19	0/161	0.50	0/218
4	FJ	0.18	0/340	0.43	0/454
5	FY	0.20	0/736	0.49	0/987
6	Fa	0.16	0/307	0.39	0/417
7	CA	0.14	0/2774	0.34	0/4302
8	CC	0.40	0/666	0.55	0/900
9	CI	0.18	0/3424	0.43	0/4626
10	CJ	0.18	0/5865	0.44	0/7974
11	CN	0.17	0/1323	0.42	0/1790
12	CS	0.16	0/731	0.40	0/987
13	Cg	0.18	0/4043	0.41	0/5489
14	Ci	0.18	0/1256	0.43	0/1695
15	Ck	0.19	0/5215	0.47	0/7050
16	DB	0.17	0/5830	0.44	0/7889
17	DC	0.16	0/8409	0.40	0/11399
18	DE	0.15	0/4756	0.42	3/6462 (0.0%)
19	DF	0.18	0/4056	0.45	2/5493 (0.0%)
20	DG	0.17	0/4674	0.43	0/6333
21	DH	0.20	0/3935	0.47	0/5321
22	DJ	0.16	0/2591	0.40	0/3508
23	DK	0.17	0/1965	0.41	0/2652
24	DT	0.19	0/1982	0.42	0/2686
25	DV	0.17	0/1358	0.46	0/1836
26	DW	0.18	0/1182	0.46	0/1613
27	DX	0.18	0/993	0.45	0/1336
28	DY	0.16	0/1337	0.40	0/1814
29	F1	0.19	0/6865	0.47	2/9259 (0.0%)
30	F4	0.17	0/4483	0.46	0/6061
31	FD	0.20	0/3216	0.46	1/4380 (0.0%)
32	FF	0.15	0/3335	0.44	0/4498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	FG	0.17	0/1386	0.43	0/1869
34	FH	0.19	0/2537	0.42	0/3442
35	FI	0.17	0/2834	0.43	0/3821
36	FK	0.15	0/1748	0.35	0/2378
37	FL	0.20	0/2613	0.45	0/3538
38	FV	0.16	0/1680	0.41	0/2281
39	Fe	0.19	0/1057	0.51	0/1421
All	All	0.18	0/102212	0.43	8/138918 (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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	DE	479	PRO	N-CA-CB	7.08	110.68	103.25
18	DE	476	PRO	N-CA-CB	6.67	110.26	103.25
18	DE	521	PRO	N-CA-CB	6.39	109.96	103.25
29	F1	158	ILE	CA-C-N	6.32	124.22	120.24
29	F1	158	ILE	C-N-CA	6.32	124.22	120.24

There are no chirality outliers.

5 of 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

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Mol	Chain	Res	Type	Group
32	FF	279	LYS	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	200	0	200	2	0
2	CK	337	0	328	3	0
3	Cn	154	0	144	1	0
4	FJ	338	0	344	7	0
5	FY	723	0	738	4	0
6	Fa	297	0	299	5	0
7	CA	2501	0	1249	22	0
8	CC	646	0	682	35	0
9	CI	3357	0	3310	39	0
10	CJ	5709	0	5508	76	0
11	CN	1285	0	1264	16	0
12	CS	708	0	688	11	0
13	Cg	3922	0	3811	49	0
14	Ci	1222	0	1192	16	0
15	Ck	5123	0	5154	76	0
16	DB	5688	0	5497	82	0
17	DC	8223	0	8043	57	0
18	DE	4639	0	4417	47	0
19	DF	3967	0	3957	46	0
20	DG	4575	0	4490	57	0
21	DH	3849	0	3811	44	0
22	DJ	2521	0	2464	25	0
23	DK	1929	0	1928	22	0
24	DT	1912	0	1787	26	0
25	DV	1323	0	1308	17	0
26	DW	1140	0	1117	15	0
27	DX	967	0	956	8	0
28	DY	1295	0	1290	17	0
29	F1	6729	0	6773	77	0
30	F4	4382	0	4291	53	0
31	FD	3135	0	3117	39	0
32	FF	3265	0	3204	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	FG	1359	0	1376	16	0
34	FH	2486	0	2430	34	0
35	FI	2786	0	2712	49	0
36	FK	1699	0	1589	24	0
37	FL	2555	0	2530	45	0
38	FV	1636	0	1567	17	0
39	Fe	1033	0	1004	17	0
40	Ua	282	0	285	11	0
41	Ub	252	0	256	13	0
42	Uc	72	0	76	3	0
43	Ud	354	0	356	12	0
44	Ue	174	0	176	2	0
45	Uf	54	0	56	3	0
46	Ug	1002	0	1026	13	0
47	Uh	1530	0	1557	38	0
48	Ui	192	0	194	9	0
49	Uj	114	0	118	1	0
50	Uk	162	0	164	4	0
51	Ul	84	0	86	0	0
52	Um	66	0	68	7	0
53	Ux	648	0	657	13	0
54	CgA	32	0	12	4	0
55	CgB	1	0	0	0	0
56	F1A	1	0	0	0	0
56	FGA	1	0	0	0	0
56	FLA	1	0	0	0	0
56	FLB	1	0	0	0	0
56	FeA	1	0	0	0	0
57	F1B	26	0	19	2	0
57	FFA	26	0	19	4	0
58	CgC	3	0	0	0	0
All	All	104694	0	101694	1056	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 5.

The worst 5 of 1056 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)
8:CC:66:GLU:HG2	39:Fe:12:LEU:HD11	1.35	1.08
18:DE:725:PRO:HG2	43:Ud:28:UNK:HG1	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FI:44:ARG:HH22	52:Um:7:UNK:HG1	1.30	0.95
30:F4:211:TRP:O	30:F4:224:GLY:HA2	1.75	0.86
8:CC:65:PHE:CD1	37:FL:257:PRO:HB3	2.12	0.83

There are no symmetry-related clashes.

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
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%)	21	52
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%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	73
31	FD	392/579 (68%)	386 (98%)	6 (2%)	0	100	100
32	FF	404/474 (85%)	389 (96%)	13 (3%)	2 (0%)	24	57
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
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%)	49	78

5 of 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

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%)	77 (100%)	0	100	100
6	Fa	30/149 (20%)	30 (100%)	0	100	100
8	CC	73/73 (100%)	71 (97%)	2 (3%)	39	67
9	CI	355/371 (96%)	354 (100%)	1 (0%)	86	87
10	CJ	619/723 (86%)	617 (100%)	2 (0%)	86	87
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%)	424 (100%)	2 (0%)	81	85
14	Ci	130/160 (81%)	129 (99%)	1 (1%)	73	81
15	Ck	557/747 (75%)	555 (100%)	2 (0%)	84	86
16	DB	613/1030 (60%)	612 (100%)	1 (0%)	87	89
17	DC	867/985 (88%)	866 (100%)	1 (0%)	88	90
18	DE	464/644 (72%)	464 (100%)	0	100	100
19	DF	417/560 (74%)	417 (100%)	0	100	100
20	DG	490/543 (90%)	489 (100%)	1 (0%)	87	89
21	DH	413/504 (82%)	412 (100%)	1 (0%)	87	89
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%)	205 (100%)	0	100	100
25	DV	142/165 (86%)	142 (100%)	0	100	100
26	DW	124/163 (76%)	123 (99%)	1 (1%)	73	81
27	DX	102/149 (68%)	101 (99%)	1 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DY	137/146 (94%)	136 (99%)	1 (1%)	76	82
29	F1	718/895 (80%)	718 (100%)	0	100	100
30	F4	479/703 (68%)	476 (99%)	3 (1%)	78	83
31	FD	338/494 (68%)	338 (100%)	0	100	100
32	FF	348/400 (87%)	346 (99%)	2 (1%)	78	83
33	FG	147/414 (36%)	147 (100%)	0	100	100
34	FH	270/390 (69%)	269 (100%)	1 (0%)	84	86
35	FI	297/380 (78%)	297 (100%)	0	100	100
36	FK	181/308 (59%)	181 (100%)	0	100	100
37	FL	279/309 (90%)	279 (100%)	0	100	100
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%)	10368 (100%)	23 (0%)	85	89

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	DW	169	VAL
30	F4	459	VAL
28	DY	136	VAL
30	F4	523	VAL
13	Cg	260	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

Mol	Chain	Res	Type
20	DG	26	ASN
38	FV	194	HIS
23	DK	163	HIS
37	FL	349	ASN
34	FH	134	ASN

5.3.3 RNA (i)

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

5 of 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

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 oligosaccharides 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	F1B	1	-	27,28,28	1.08	4 (14%)	36,40,40	2.07	10 (27%)
54	GTP	CgA	1	-	33,34,34	0.91	0	50,54,54	1.72	9 (18%)
57	SAH	FFA	1	-	27,28,28	1.11	4 (14%)	36,40,40	2.09	10 (27%)

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	F1B	1	-	-	4/15/31/31	0/3/3/3
54	GTP	CgA	1	-	-	5/22/38/38	0/3/3/3
57	SAH	FFA	1	-	-	1/15/31/31	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FFA	1	SAH	C2-N3	2.59	1.38	1.33
57	FFA	1	SAH	C2-N1	2.55	1.38	1.33
57	F1B	1	SAH	C2-N1	2.48	1.38	1.33
57	F1B	1	SAH	C2-N3	2.45	1.38	1.33
57	F1B	1	SAH	OXT-C	-2.25	1.23	1.30

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	CgA	1	GTP	C5-C4-N3	-5.82	119.12	128.39
57	F1B	1	SAH	N3-C2-N1	-5.53	120.21	128.58
57	FFA	1	SAH	N3-C2-N1	-5.47	120.30	128.58
54	CgA	1	GTP	C2-N3-C4	5.22	121.30	112.30
57	FFA	1	SAH	C5-C4-N3	-4.84	120.05	126.72

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

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

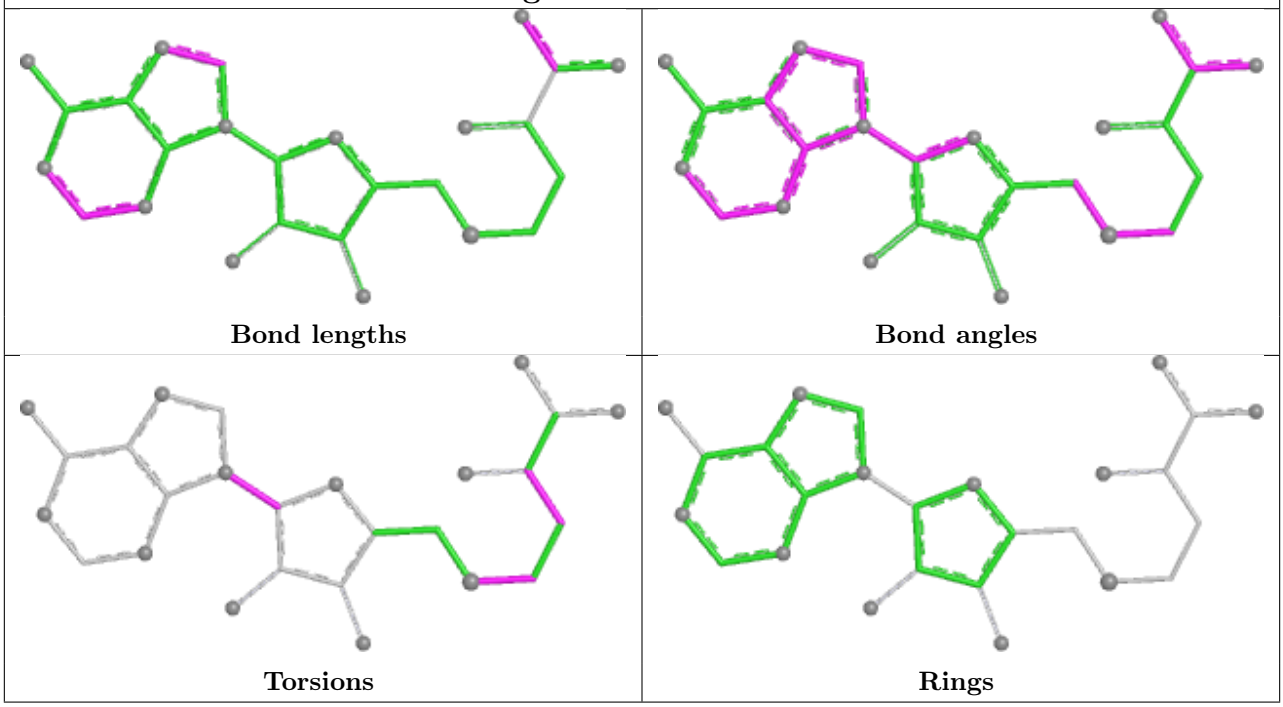
There are no ring outliers.

3 monomers are involved in 10 short contacts:

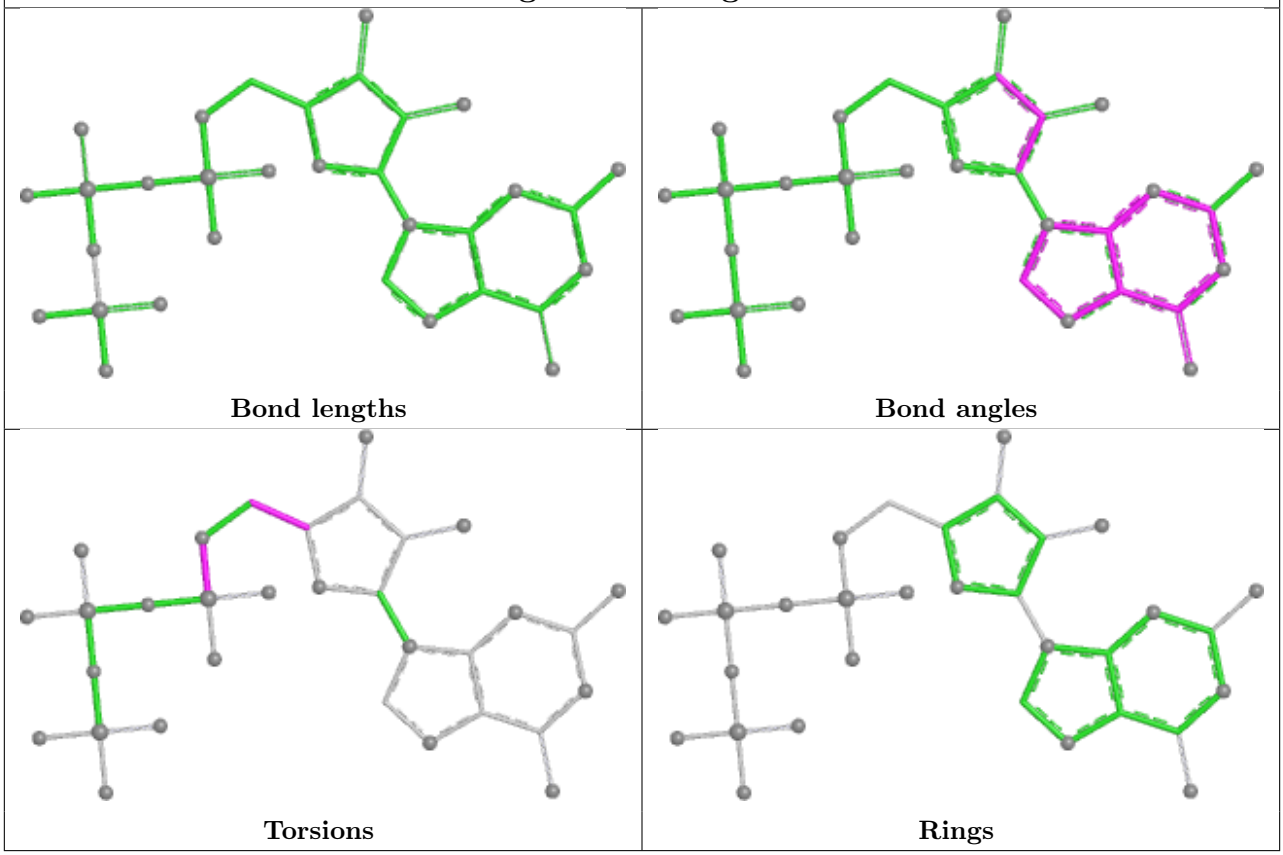
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	F1B	1	SAH	2	0
54	CgA	1	GTP	4	0
57	FFA	1	SAH	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

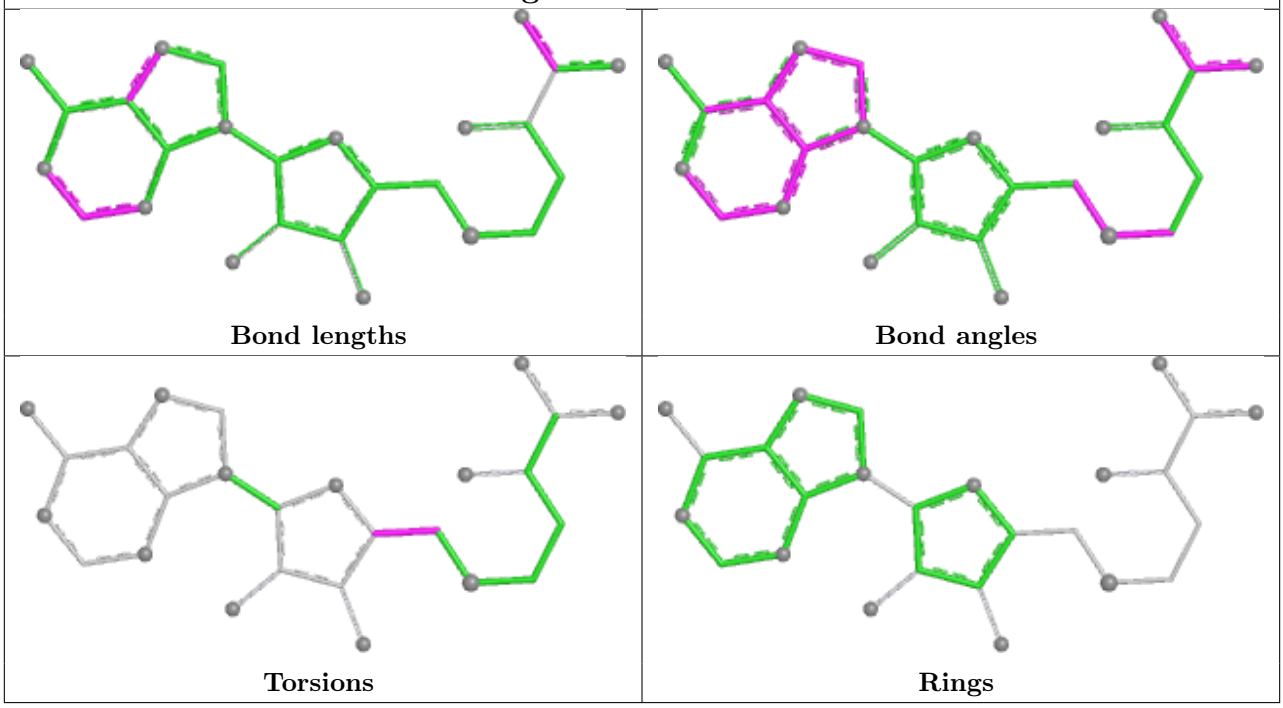
Ligand SAH F1B 1



Ligand GTP CgA 1



Ligand SAH FFA 1



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

The worst 5 of 24 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

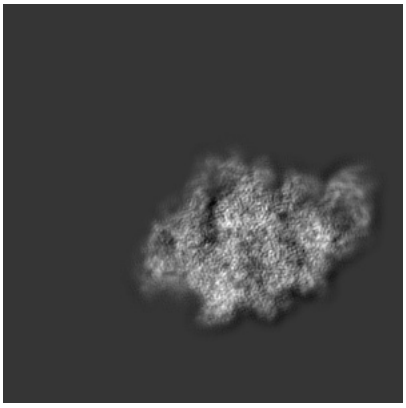
6 Map visualisation (i)

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.

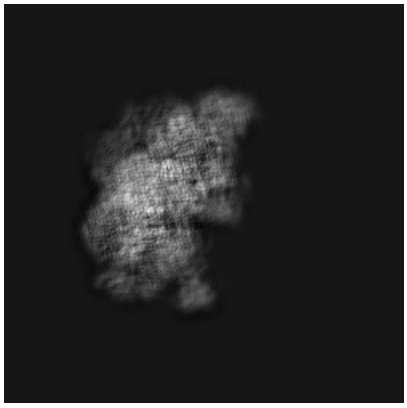
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

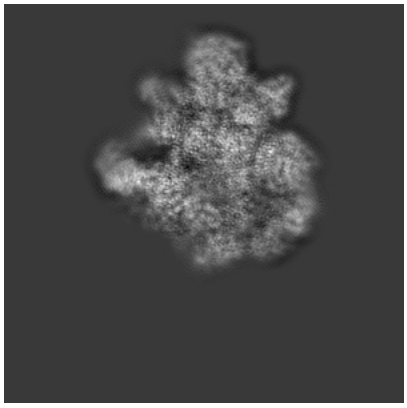
6.1.1 Primary map



X



Y

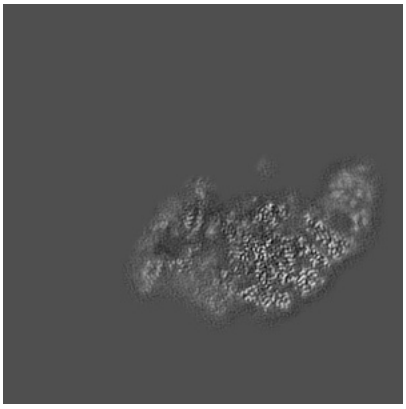


Z

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

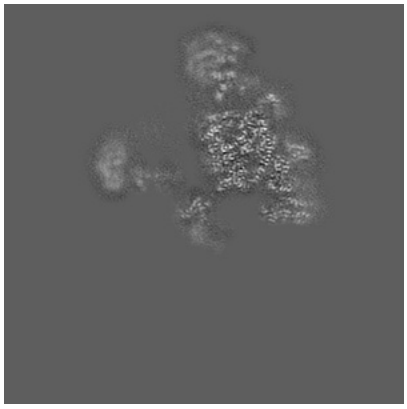
6.2 Central slices (i)

6.2.1 Primary map



X Index: 160

Y Index: 160

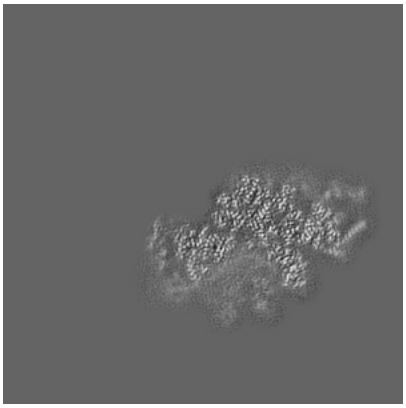


Z Index: 160

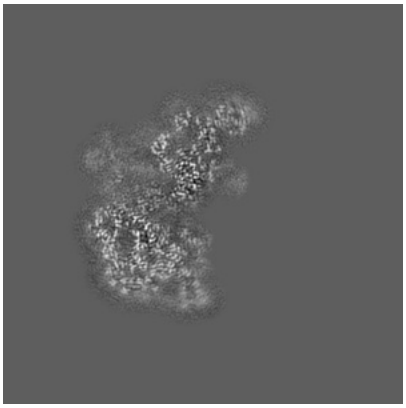
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

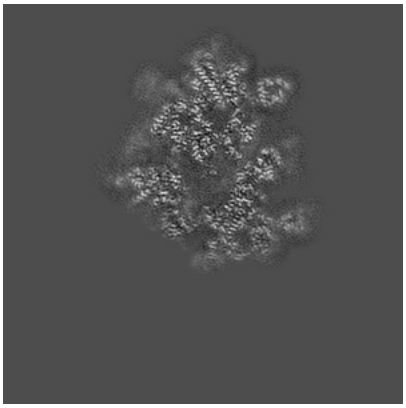
6.3.1 Primary map



X Index: 190



Y Index: 183

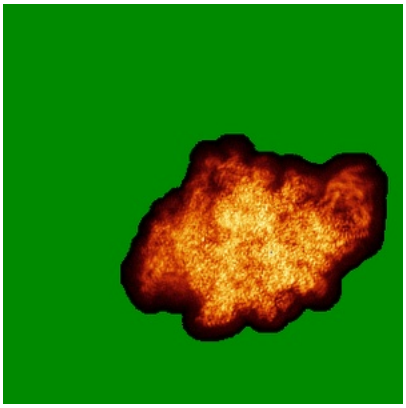


Z Index: 126

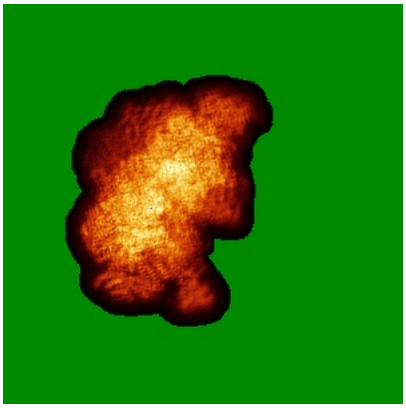
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

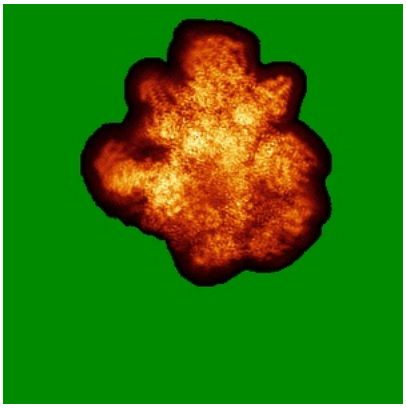
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

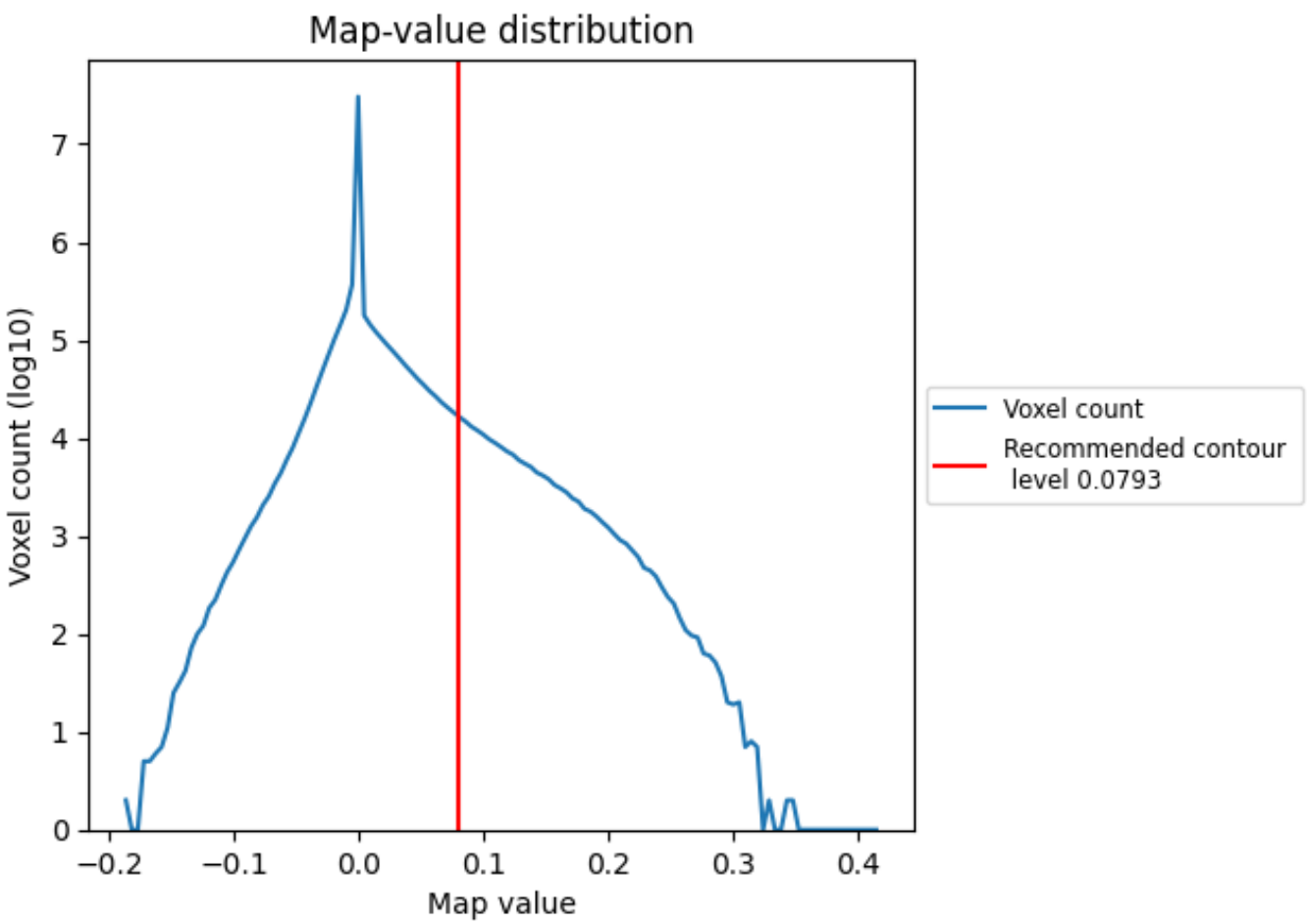
6.6 Mask visualisation (i)

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

7 Map analysis (i)

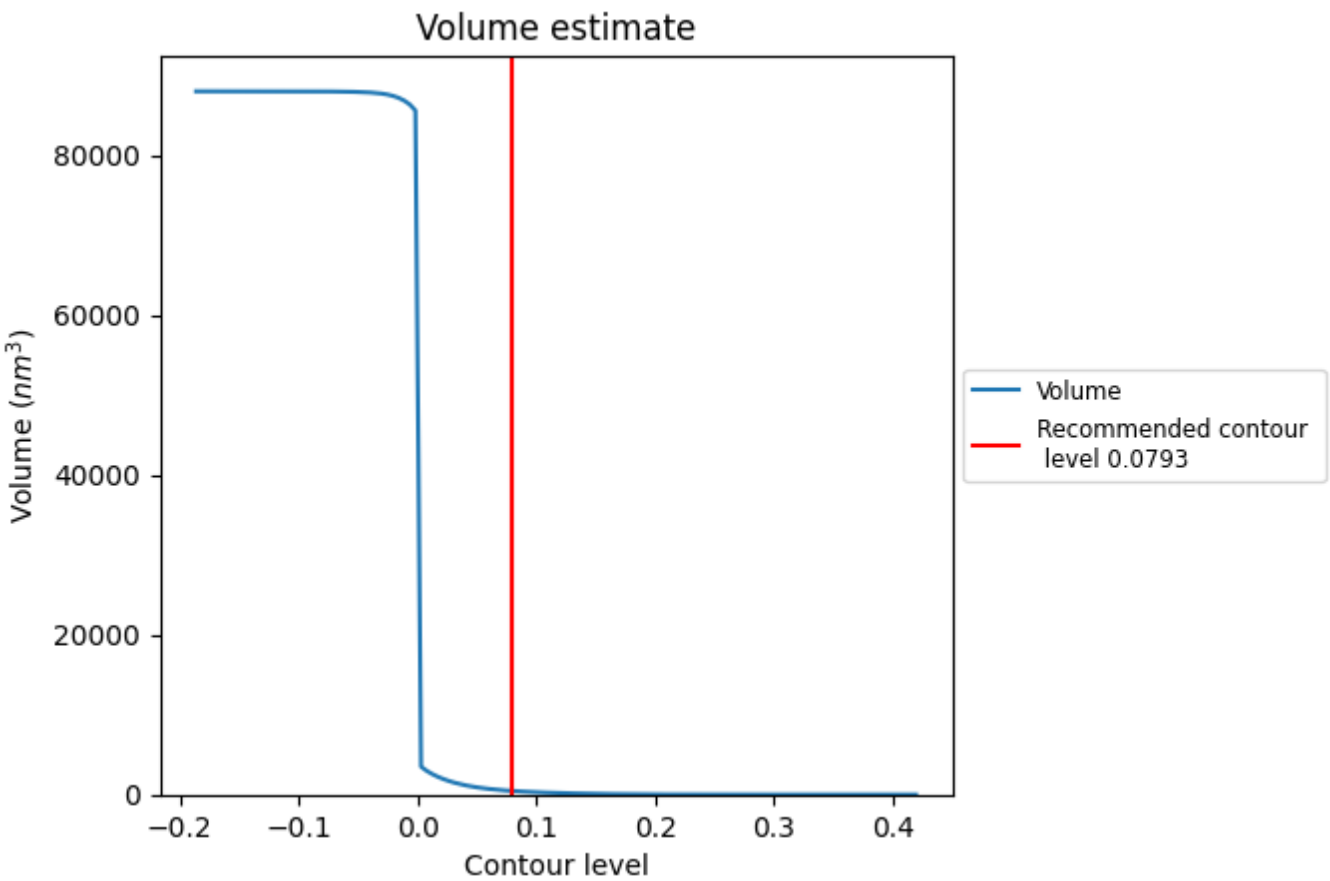
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

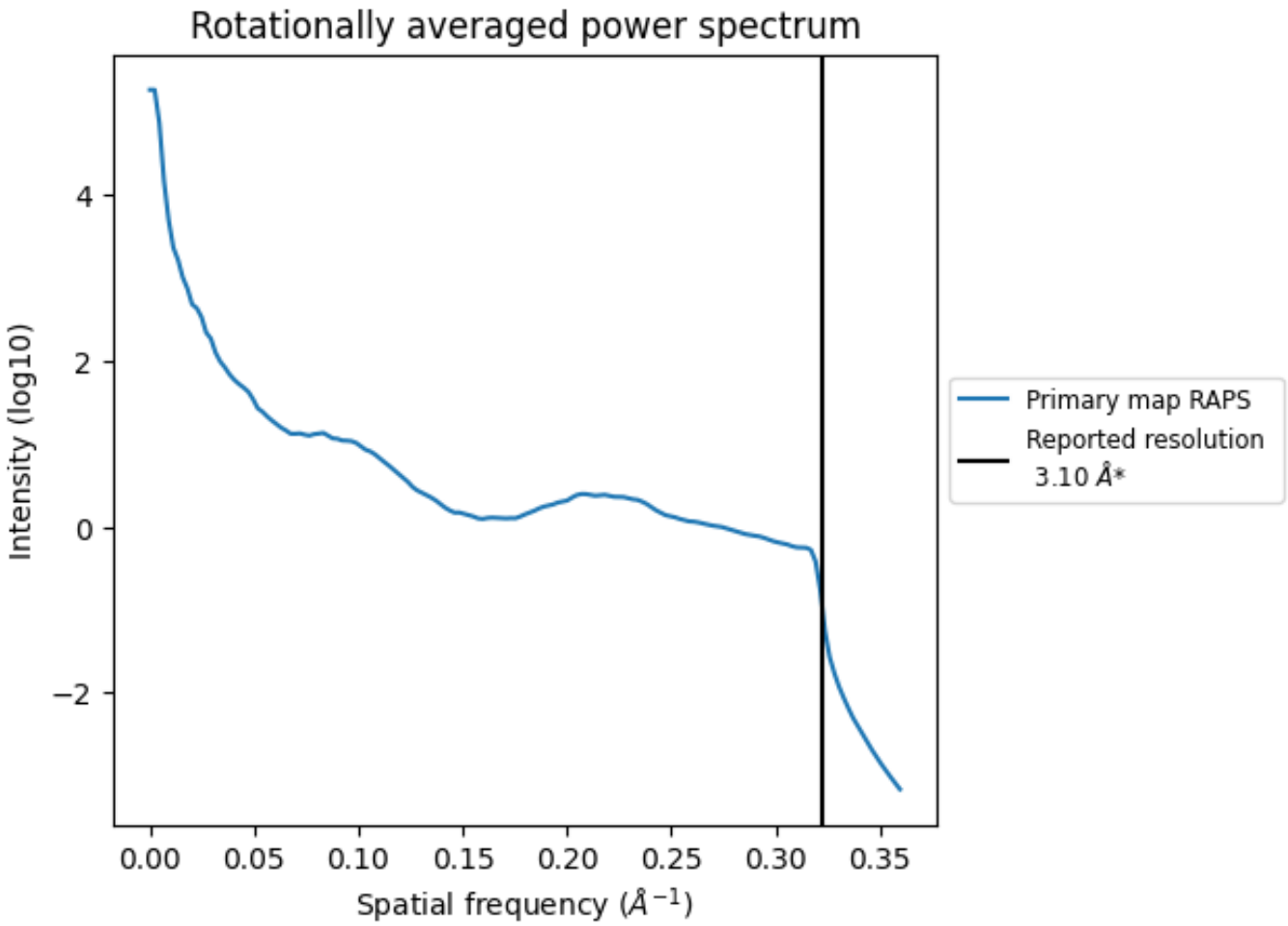
7.2 Volume estimate (i)



The volume at the recommended contour level is 459 nm^3; 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^{-1}

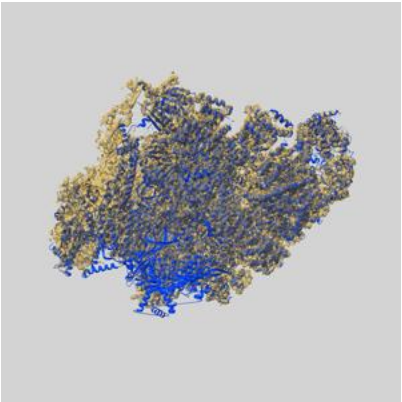
8 Fourier-Shell correlation (i)

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

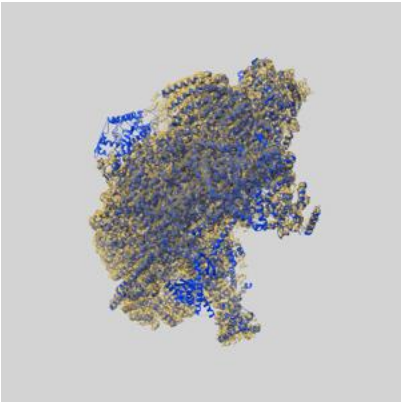
9 Map-model fit (i)

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.

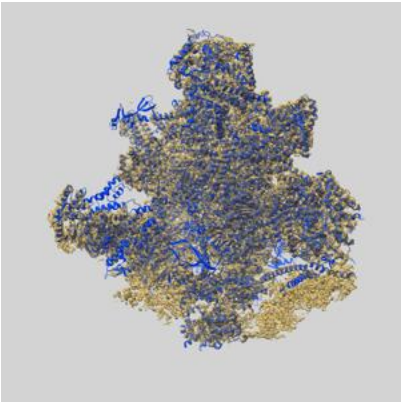
9.1 Map-model overlay (i)



X



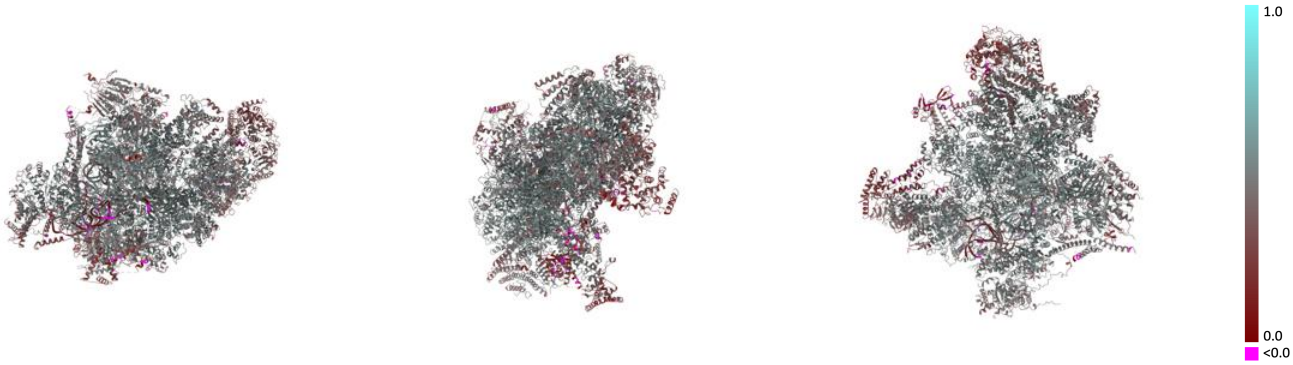
Y



Z

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.

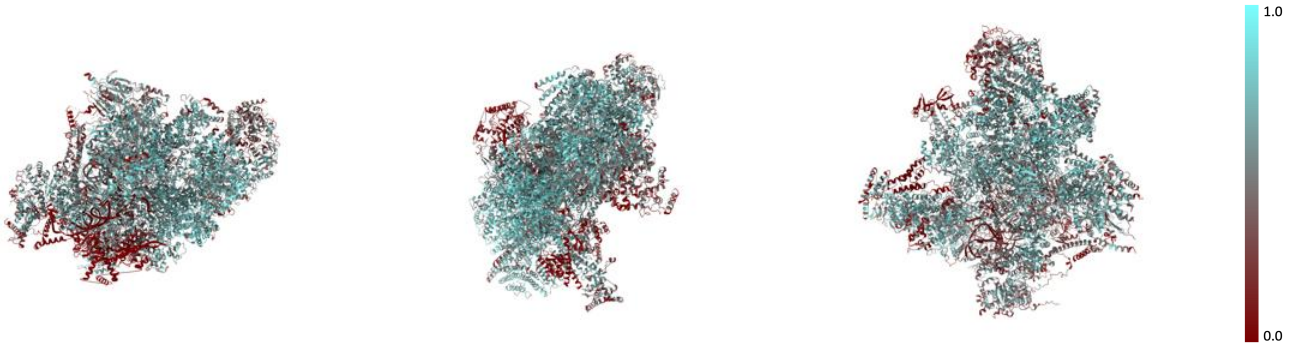
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

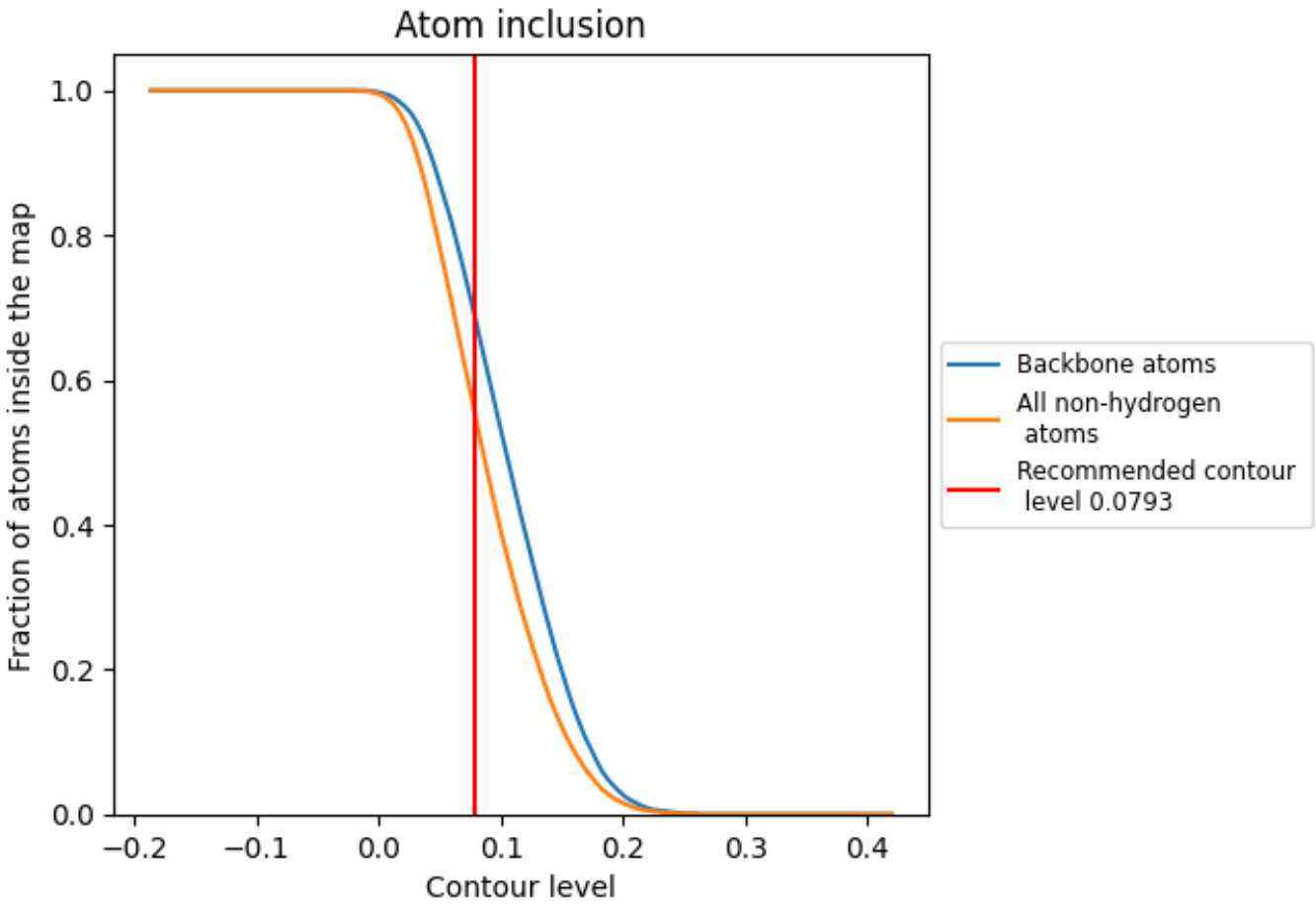
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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	0.5480	0.4610
CA	0.3180	0.3180
CC	0.5390	0.5120
CE	0.4510	0.4920
CI	0.5420	0.4770
CJ	0.6350	0.5040
CK	0.5930	0.4770
CN	0.3020	0.4910
CS	0.0160	0.4150
Cg	0.7400	0.5020
CgA	0.9380	0.4720
CgB	1.0000	0.5320
Ci	0.5200	0.5180
Ck	0.5750	0.4440
Cn	0.3130	0.5000
DB	0.4570	0.4230
DC	0.6000	0.4420
DE	0.4310	0.3500
DF	0.6410	0.4960
DG	0.6500	0.4450
DH	0.6180	0.5060
DJ	0.6700	0.4990
DK	0.6350	0.4890
DT	0.7200	0.5410
DV	0.5620	0.4940
DW	0.5450	0.4600
DX	0.2540	0.4300
DY	0.5320	0.4670
F1	0.5000	0.4740
F1A	1.0000	0.6220
F1B	0.3080	0.5250
F4	0.4670	0.4220
FD	0.6730	0.4940
FF	0.4800	0.4620
FFA	0.3080	0.4450

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Chain	Atom inclusion	Q-score
FG	0.7210	0.5170
FGA	1.0000	0.7780
FH	0.6410	0.5000
FI	0.6270	0.5200
FJ	0.4410	0.4760
FK	0.5910	0.5040
FL	0.6140	0.5310
FLA	1.0000	0.7440
FLB	1.0000	0.6060
FV	0.6500	0.5030
FY	0.4310	0.3760
Fa	0.4350	0.4890
Fe	0.6330	0.5030
FeA	1.0000	0.4100
Ua	0.4180	0.4280
Ub	0.2660	0.4360
Uc	0.2220	0.4390
Ud	0.5710	0.4040
Ue	0.1950	0.3470
Uf	0.4810	0.5200
Ug	0.4620	0.2980
Uh	0.0330	0.3480
Ui	0.5570	0.3940
Uj	0.4210	0.4160
Uk	0.5310	0.4780
Ul	0.2020	0.2770
Um	0.4550	0.4370
Ux	0.0050	0.3290