Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:03 pm GMT

PDB ID	:	7AOR
EMDB ID	:	EMD-11846
Title	:	mt-SSU from Trypanosoma cruzi in complex with mt-IF-3.
Authors	:	Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y.
Deposited on	:	2020-10-15
Resolution	:	3.50 Å(reported)

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

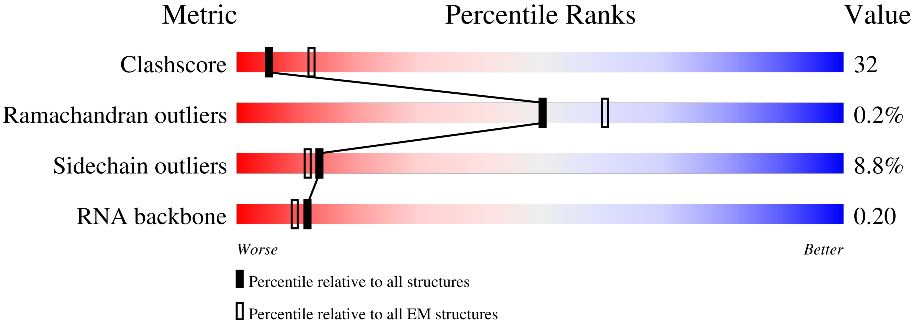
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

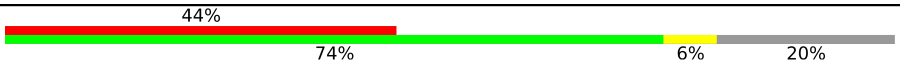
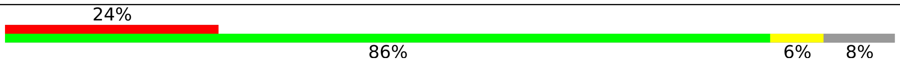
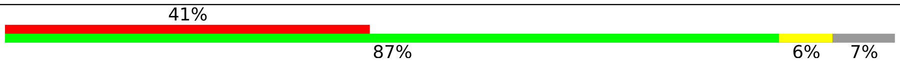
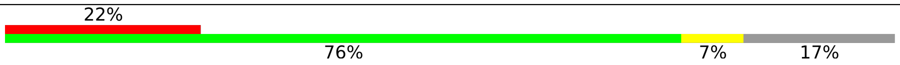
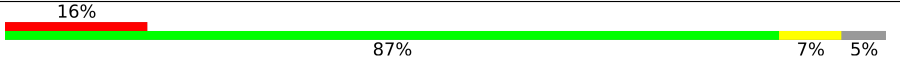
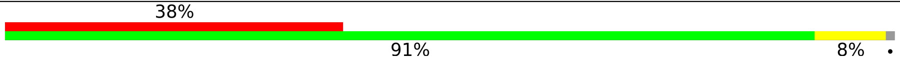
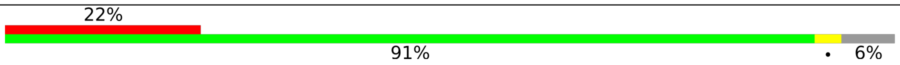
The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	u	874	
2	s	180	
3	r	500	
4	n	172	
5	h	166	
6	e	818	
7	az	163	

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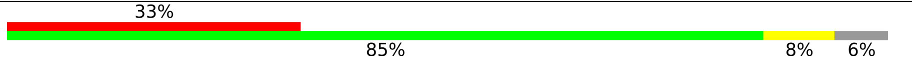
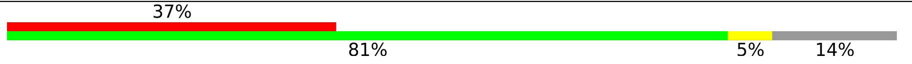
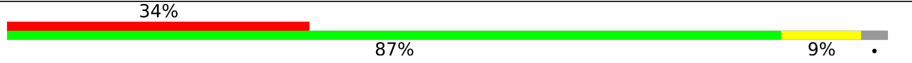
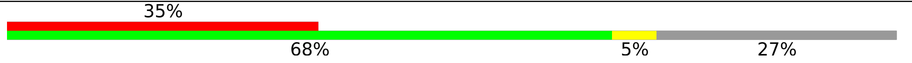
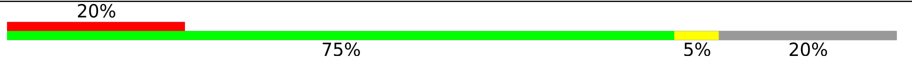
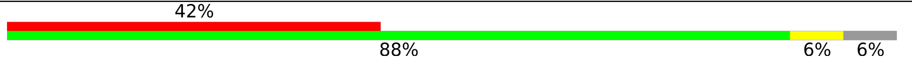
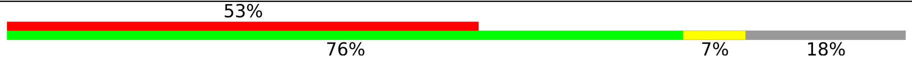
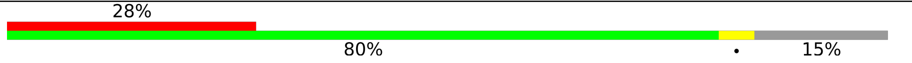
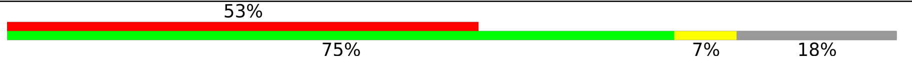
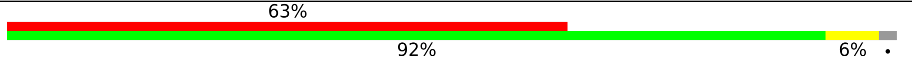
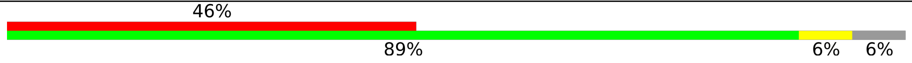
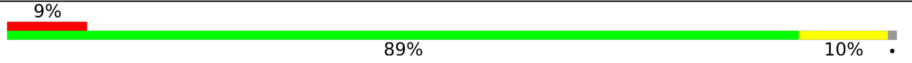
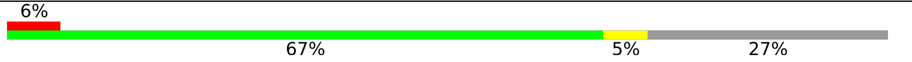
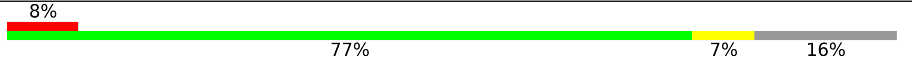
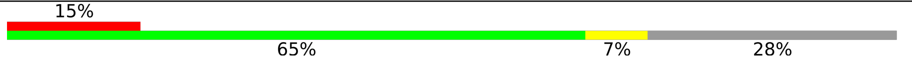
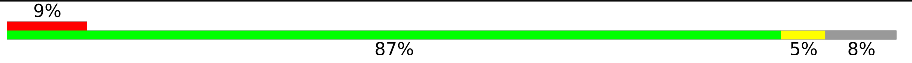
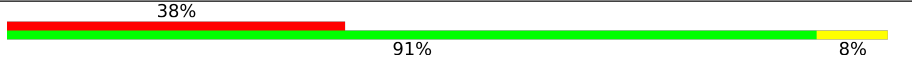
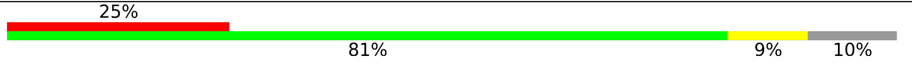
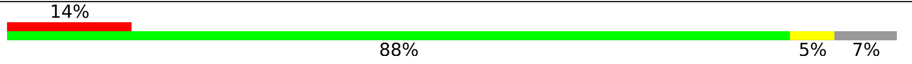
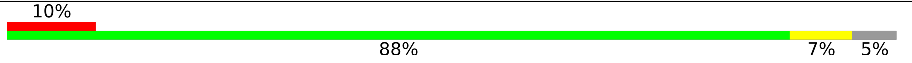
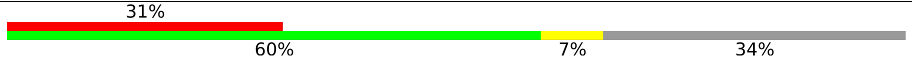
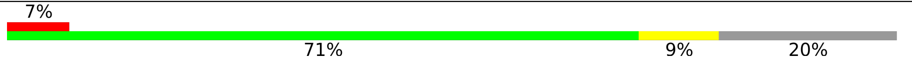
Mol	Chain	Length	Quality of chain
8	ay	218	
9	ax	172	
10	aw	186	
11	au	247	
12	ak	314	
13	aj	396	
14	ag	581	
15	af	677	
16	ae	678	
17	l	714	
18	ac	1152	
19	ab	1175	
20	ad	810	
21	m	319	
22	i	429	
23	f	325	
24	c	285	
25	d	445	
26	ba	217	
27	av	237	
28	at	259	
29	ar	268	
30	aq	299	
31	ap	277	
32	ao	283	

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Mol	Chain	Length	Quality of chain
33	ai	410	8% 89% 6% 5%
34	an	293	5% 88% 12%
35	z	1181	8% 83% 7% 9%
36	y	449	15% 51% 5% 44%
37	x	345	14% 67% 6% 27%
38	w	186	20% 88% 6% 6%
39	v	215	20% 83% 8% 9%
40	bb	238	13% 42% • 54%
41	t	256	24% 80% 8% 12%
42	al	308	20% 89% 6% 5%
43	q	442	6% 46% • 52%
44	p	308	15% 75% • 21%
45	Ca	603	8% 89% 10% •
46	g	193	16% 85% 10% 5%
47	j	189	• 85% 10% • 5%
48	b	160	6% 86% 8% 6%
49	bd	90	23% 40% 16% 44%
50	a	434	8% 89% 8% •
51	bc	376	28% 38% • 60%
52	aa	1827	14% 77% 8% 15%
53	k	309	• 52% 9% • 39%
54	be	82	17% 83% 12% • •
55	as	261	19% 88% 8% •
56	2	8129	• • • • 94%
56	A	8129	•• 98%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 173743 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 mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	u	697	5597	3524	1014	1035	24	0	0

- Molecule 2 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	s	165	1351	851	249	242	9	0	0

- Molecule 3 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	r	465	3806	2451	655	681	19	0	0

- Molecule 4 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	n	142	1169	760	203	201	5	0	0

- Molecule 5 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	h	157	1324	842	252	222	8	0	0

- Molecule 6 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	810	6577	4157	1153	1237	30	0	0

- Molecule 7 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	az	154	1292	828	243	217	4	0	0

- Molecule 8 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	ay	141	1200	765	229	202	4	0	0

- Molecule 9 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	ax	161	1366	868	263	228	7	0	0

- Molecule 10 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	aw	160	1338	851	251	232	4	0	0

- Molecule 11 is a protein called Rhodanese domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	au	239	2069	1331	371	357	10	0	0

- Molecule 12 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	ak	230	1865	1174	345	338	8	0	0

- Molecule 13 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	aj	315	2590	1667	450	459	14	0	0

- Molecule 14 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	ag	548	Total	C	N	O	S	0	0
			4472	2804	838	806	24		

- Molecule 15 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	af	558	Total	C	N	O	S	0	0
			4590	2897	829	838	26		

- Molecule 16 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ae	574	Total	C	N	O	S	0	0
			4634	2918	862	833	21		

- Molecule 17 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	l	588	Total	C	N	O	S	0	0
			4821	3070	855	880	16		

- Molecule 18 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	ac	1125	Total	C	N	O	S	0	0
			8864	5568	1581	1682	33		

- Molecule 19 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	ab	1110	Total	C	N	O	S	0	0
			9094	5669	1697	1697	31		

- Molecule 20 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ad	801	Total	C	N	O	S	0	0
			6610	4182	1197	1186	45		

- Molecule 21 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	m	232	1940	1234	356	344	6	0	0

- Molecule 22 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	i	360	2970	1890	543	522	15	0	0

- Molecule 23 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	f	233	1917	1195	358	354	10	0	0

- Molecule 24 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	c	263	2169	1358	417	384	10	0	0

- Molecule 25 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	d	445	3538	2229	635	657	17	0	0

- Molecule 26 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	ba	83	706	460	115	127	4	0	0

- Molecule 27 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	av	213	1752	1102	310	333	7	0	0

- Molecule 28 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	at	242	Total 1946	C 1216	N 364	O 352	S 14	0	0

- Molecule 29 is a protein called AKAP7_NLS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	ar	255	Total 2061	C 1303	N 382	O 368	S 8	0	0

- Molecule 30 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	aq	198	Total 1701	C 1092	N 304	O 297	S 8	0	0

- Molecule 31 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	ap	222	Total 1796	C 1109	N 329	O 344	S 14	0	0

- Molecule 32 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	ao	252	Total 2062	C 1305	N 383	O 362	S 12	0	0

- Molecule 33 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ai	390	Total 3205	C 2046	N 554	O 592	S 13	0	0

- Molecule 34 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	an	293	Total 2422	C 1533	N 458	O 419	S 12	0	0

- Molecule 35 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	z	1071	8630	5428	1553	1612	37	0	0

- Molecule 36 is a protein called Sod_Fe_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	y	253	1983	1260	360	350	13	0	0

- Molecule 37 is a protein called Superoxide dismutase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	x	252	2016	1294	353	364	5	0	0

- Molecule 38 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	w	175	1479	945	261	267	6	0	0

- Molecule 39 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	v	196	1567	964	306	288	9	0	0

- Molecule 40 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	bb	110	905	580	182	141	2	0	0

- Molecule 41 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	t	226	1797	1138	317	336	6	0	0

- Molecule 42 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	al	292	2372	1500	444	415	13	0	0

- Molecule 43 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	q	214	1840	1169	335	330	6	0	0

- Molecule 44 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	242	1998	1264	362	364	8	0	0

- Molecule 45 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Ca	592	5070	3247	913	890	20	0	0

- Molecule 46 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	g	184	1544	975	300	258	11	0	0

- Molecule 47 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	j	180	1501	963	280	251	7	0	0

- Molecule 48 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	b	150	1271	810	228	227	6	0	0

- Molecule 49 is a protein called MURF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	bd	50	430	296	65	68	1	0	0

- Molecule 50 is a protein called Ribosomal_S5_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	a	425	3436	2177	633	610	16	0	0

- Molecule 51 is a protein called mt-iF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	bc	151	1247	792	229	220	6	0	0

- Molecule 52 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	aa	1558	12549	7926	2247	2337	39	0	0

- Molecule 53 is a protein called 30S Ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	k	190	1577	1009	301	258	9	0	0

- Molecule 54 is a protein called Ribosome protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	be	79	665	459	101	97	8	0	0

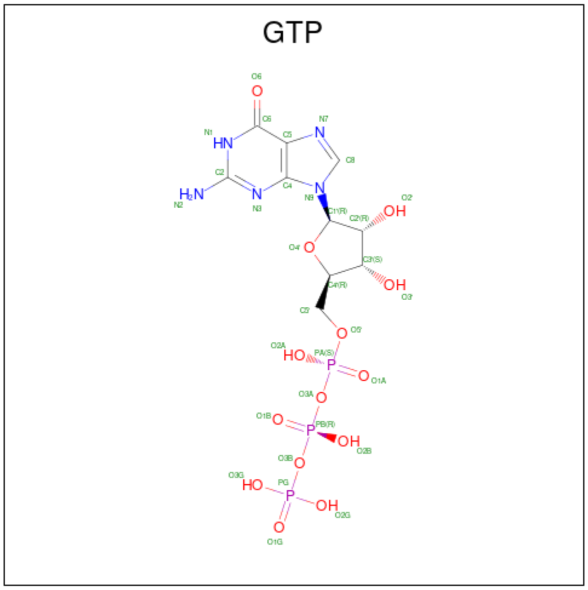
- Molecule 55 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	as	252	2024	1305	356	353	10	0	0

- Molecule 56 is a RNA chain called RNA (478-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	A	143	3030	1364	522	1001	143	0	0
56	2	470	9932	4470	1690	3302	470	0	0

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

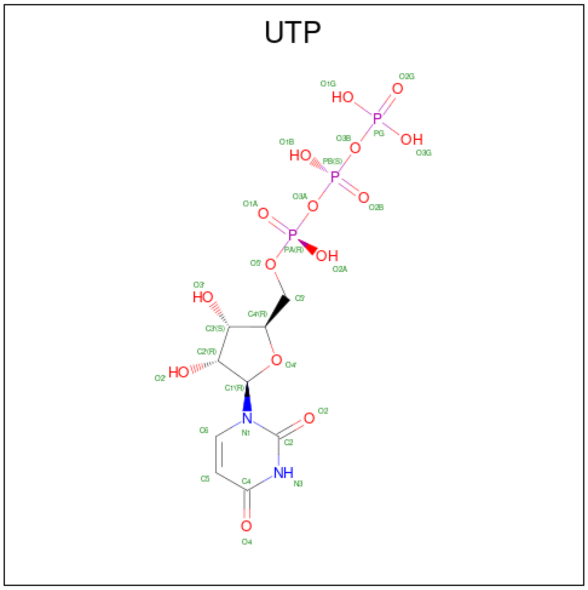


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	r	1	32	10	5	14	3	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	r	1	1	1	0

- Molecule 59 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



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

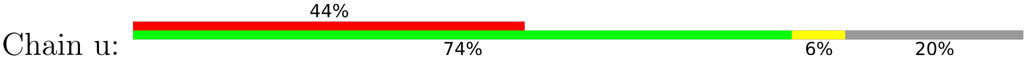
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

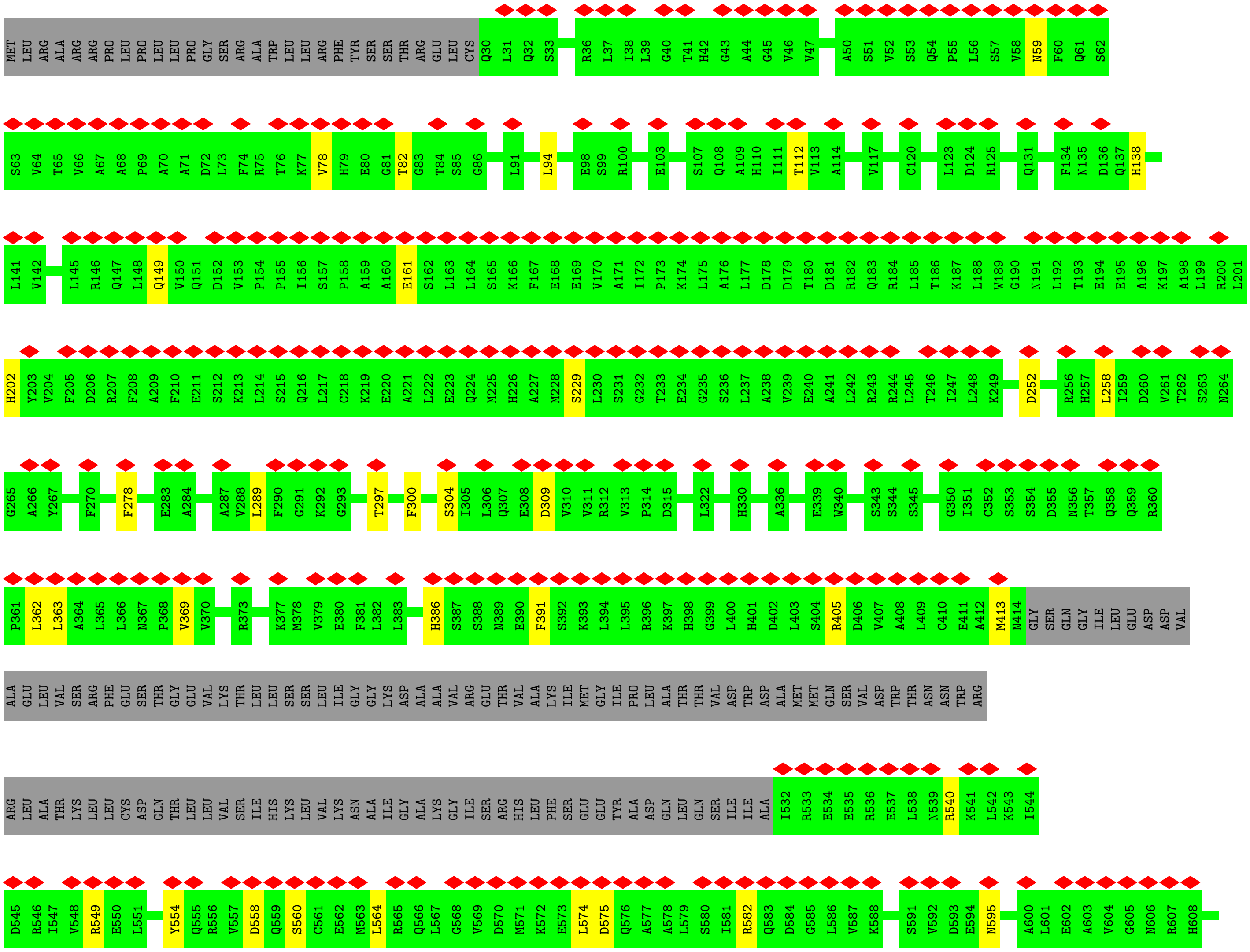
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	at	2	2	2	0
60	y	1	1	1	0
60	aa	1	1	1	0

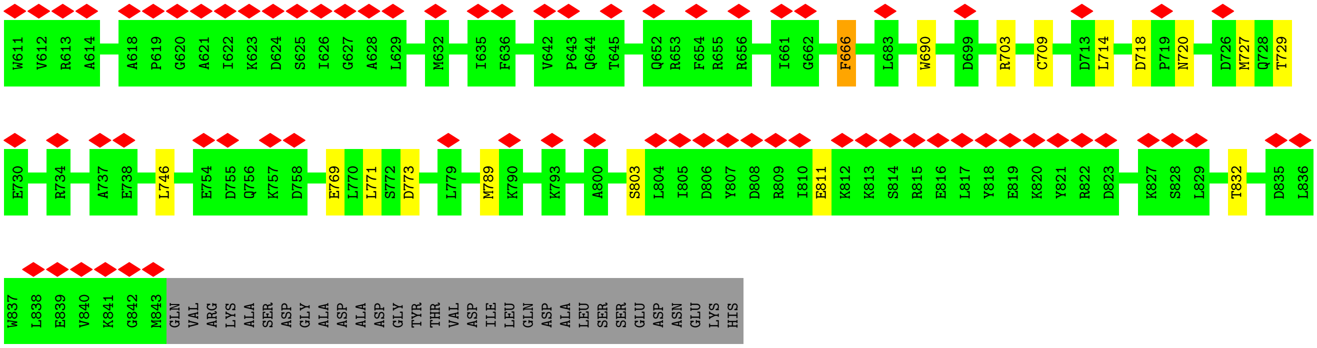
3 Residue-property plots ⓘ

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: mS35

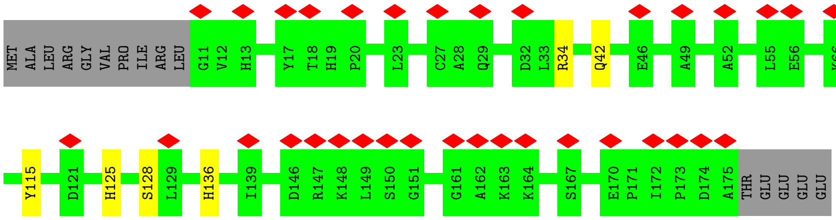






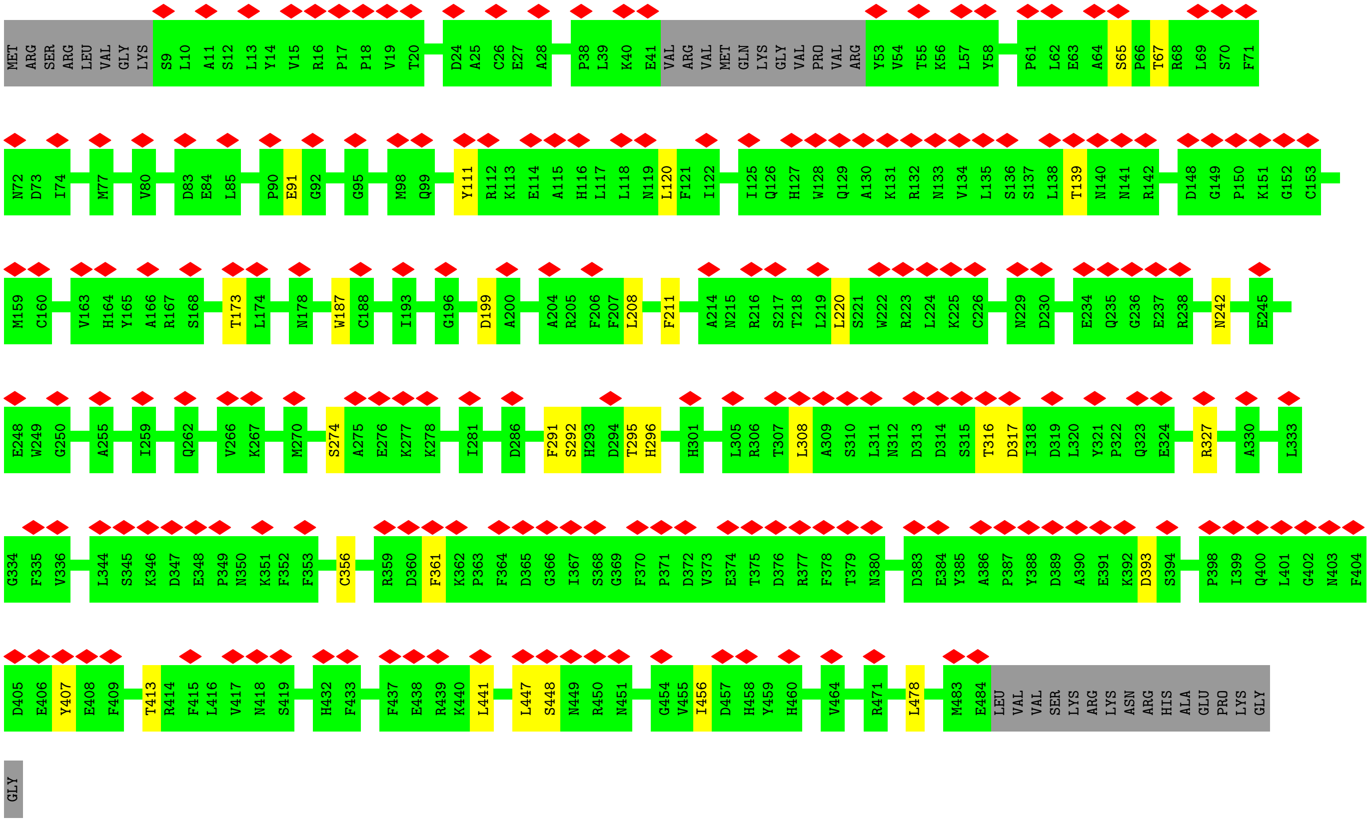
- Molecule 2: mS33

Chain s:



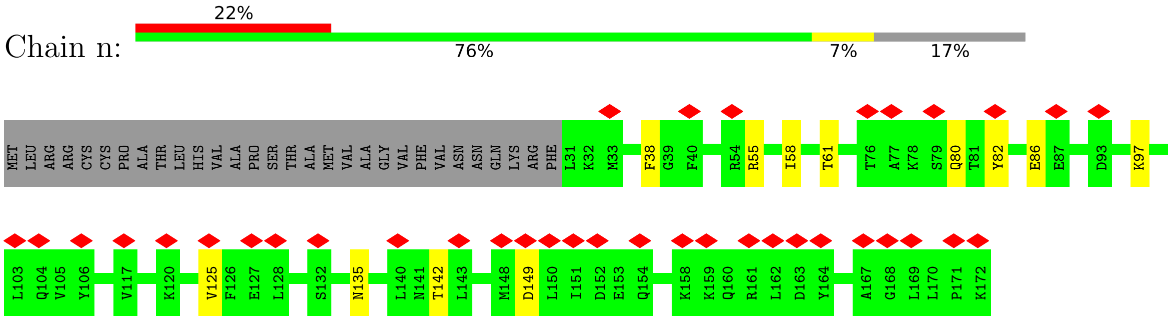
- Molecule 3: mS29

Chain r:



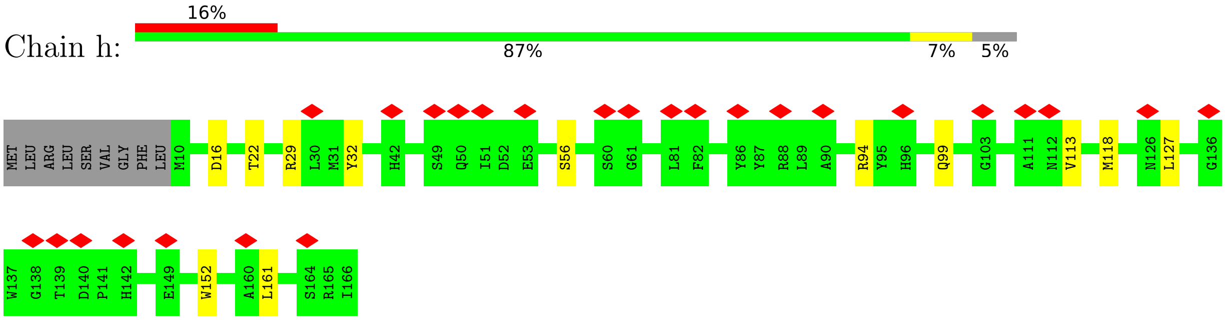
- Molecule 4: uS19

Chain n:



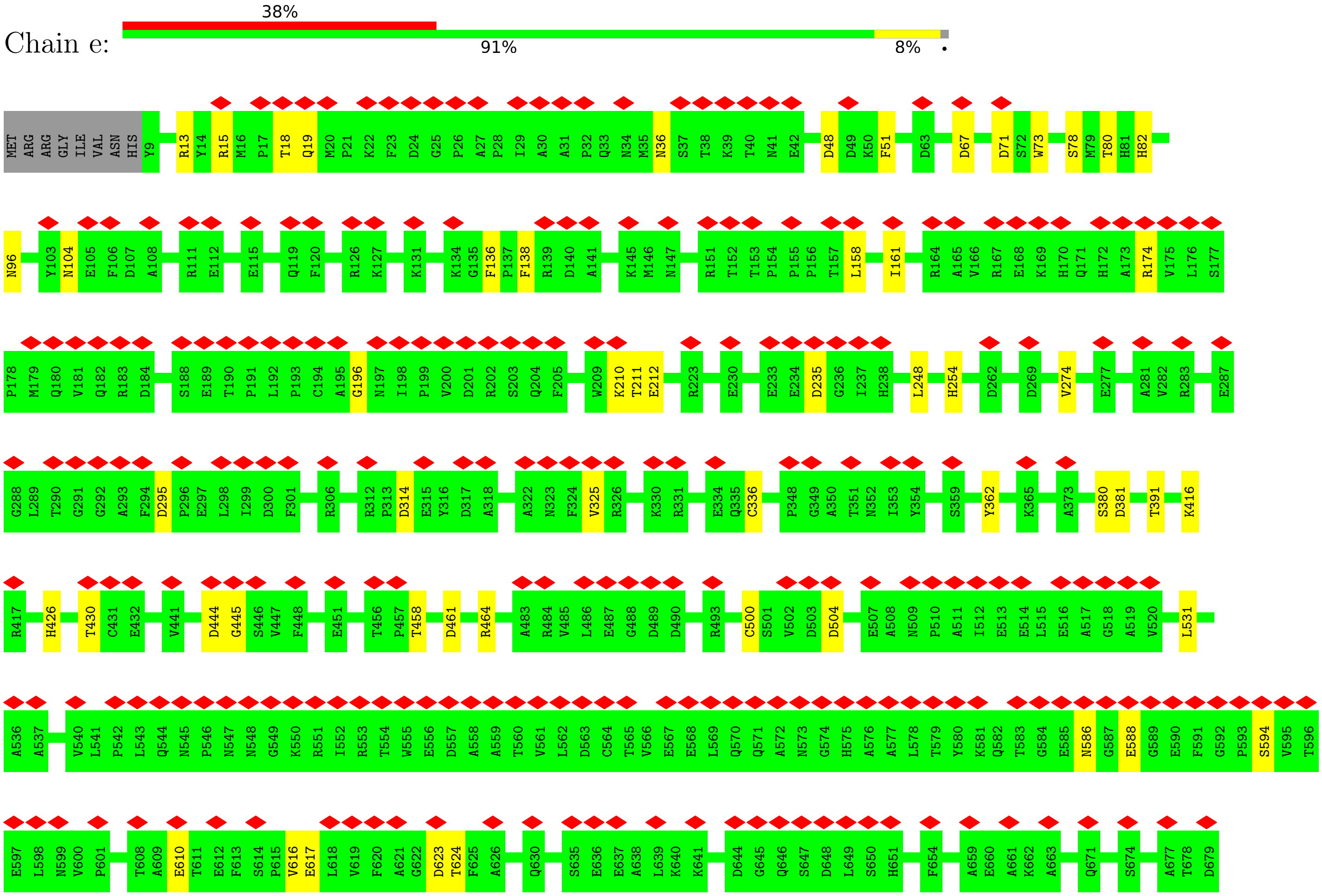
- Molecule 5: uS14m

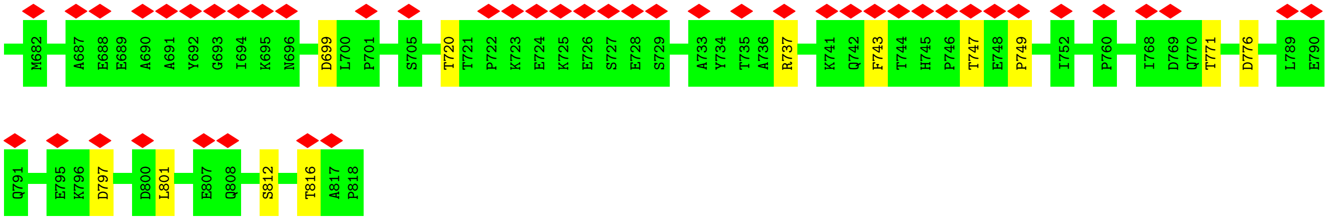
Chain h:



- Molecule 6: uS10m

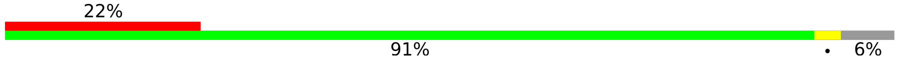
Chain e:

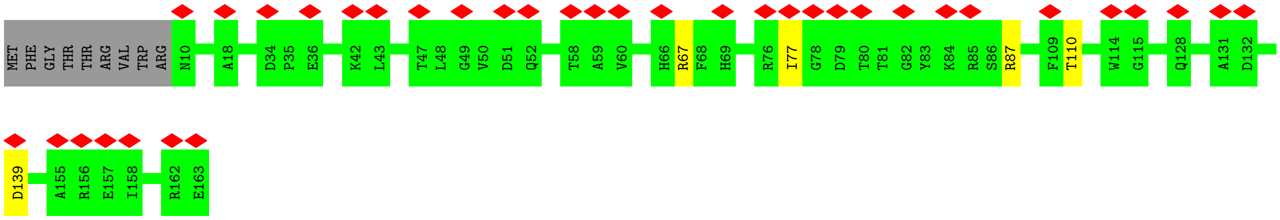




- Molecule 7: mS72

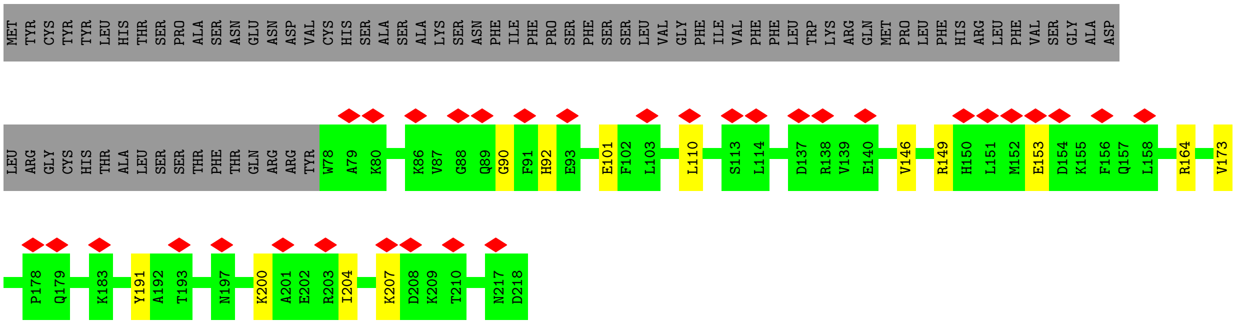
Chain az:





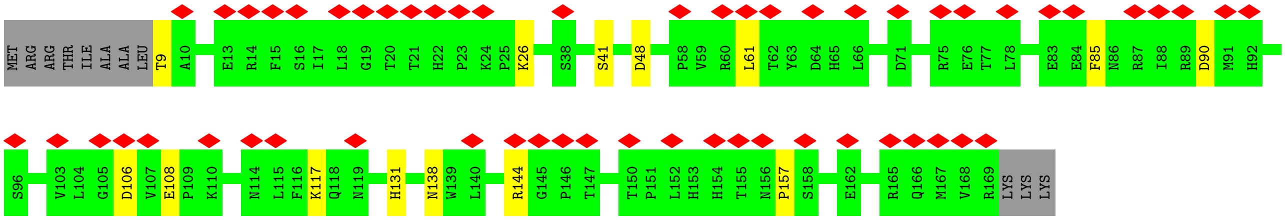
- Molecule 8: mS71

Chain ay:



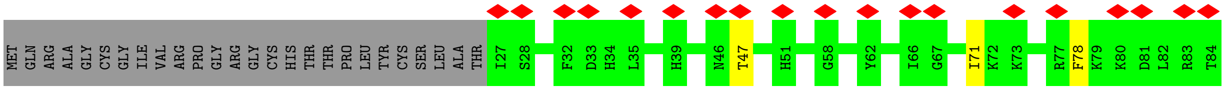
- Molecule 9: mS70

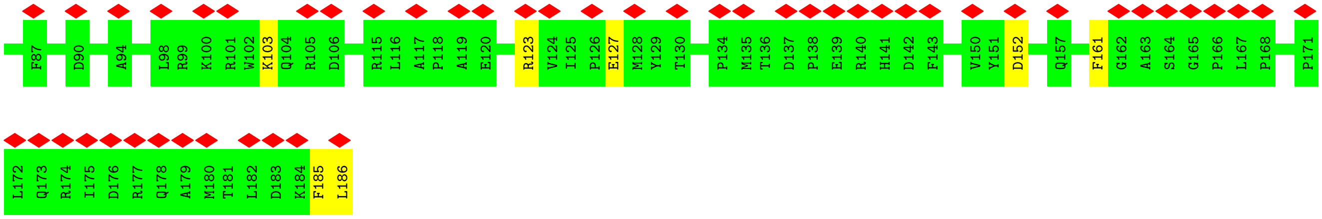
Chain ax:



- Molecule 10: mS69

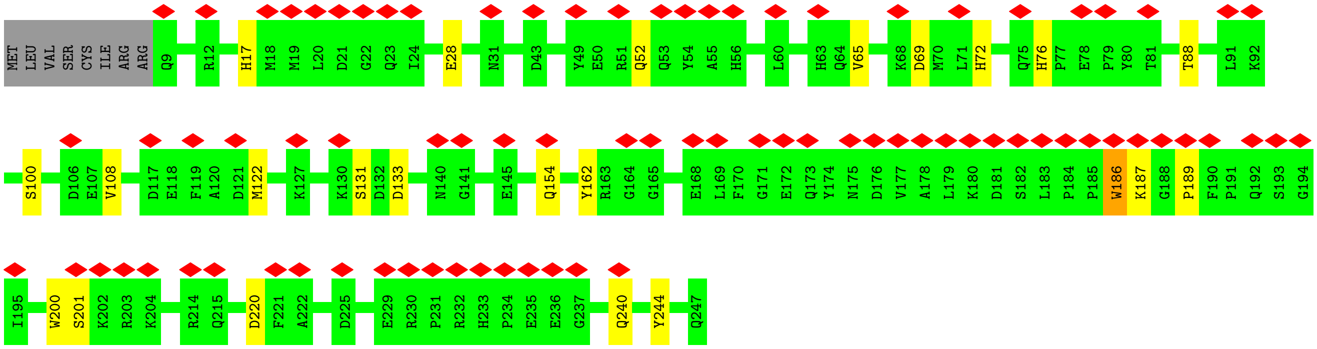
Chain aw:





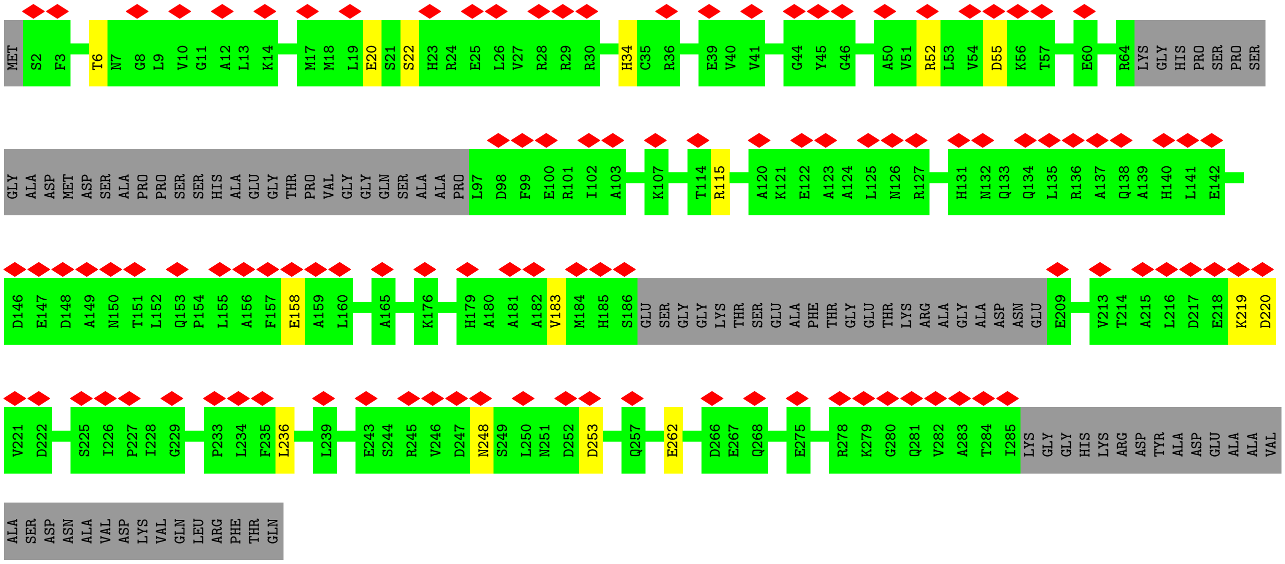
- Molecule 11: Rhodanese domain-containing protein

Chain au:



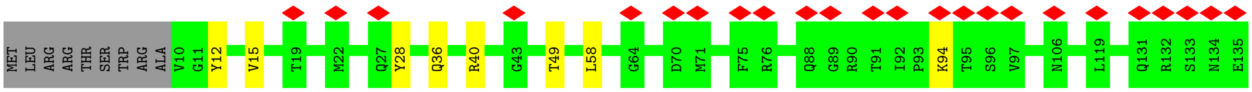
- Molecule 12: mS58

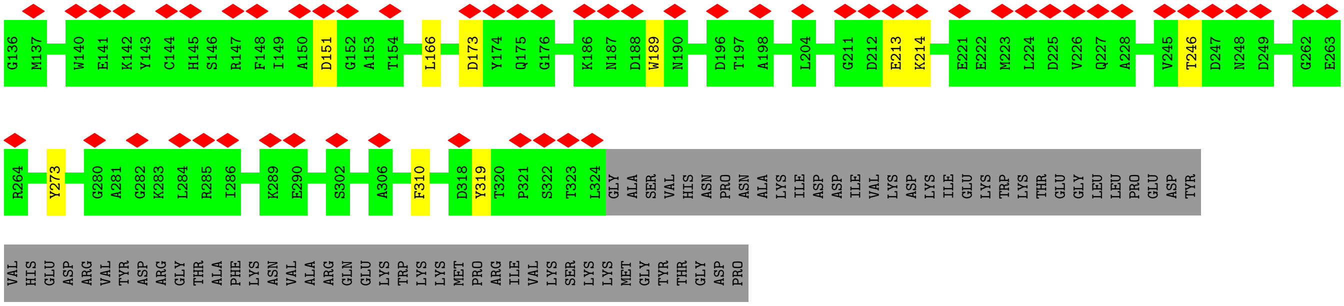
Chain ak:



- Molecule 13: mS57

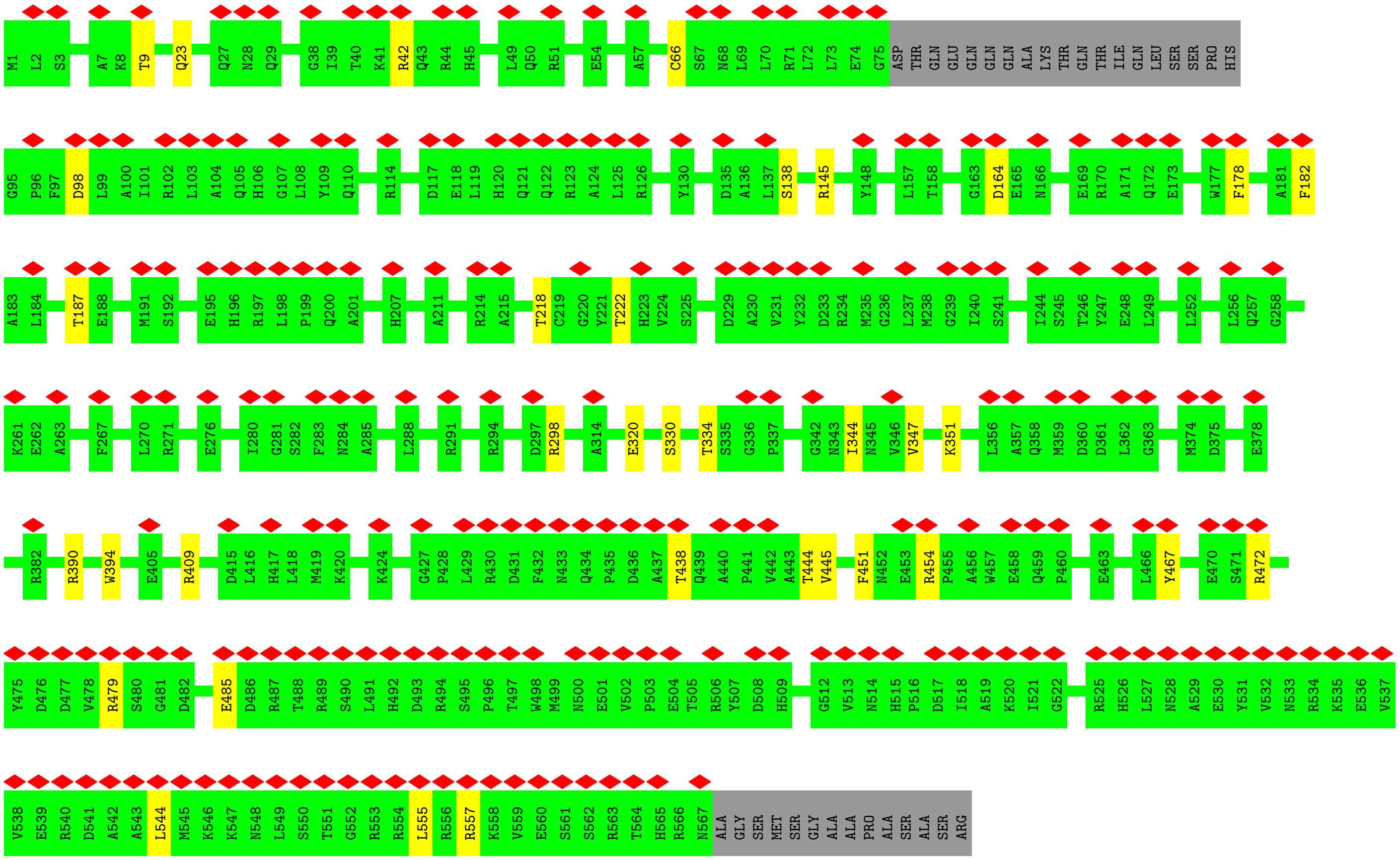
Chain aj:





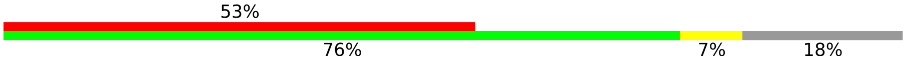
- Molecule 14: mS55

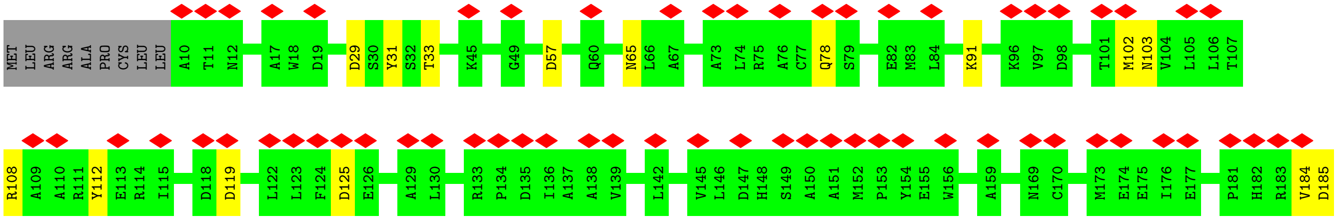
Chain ag:

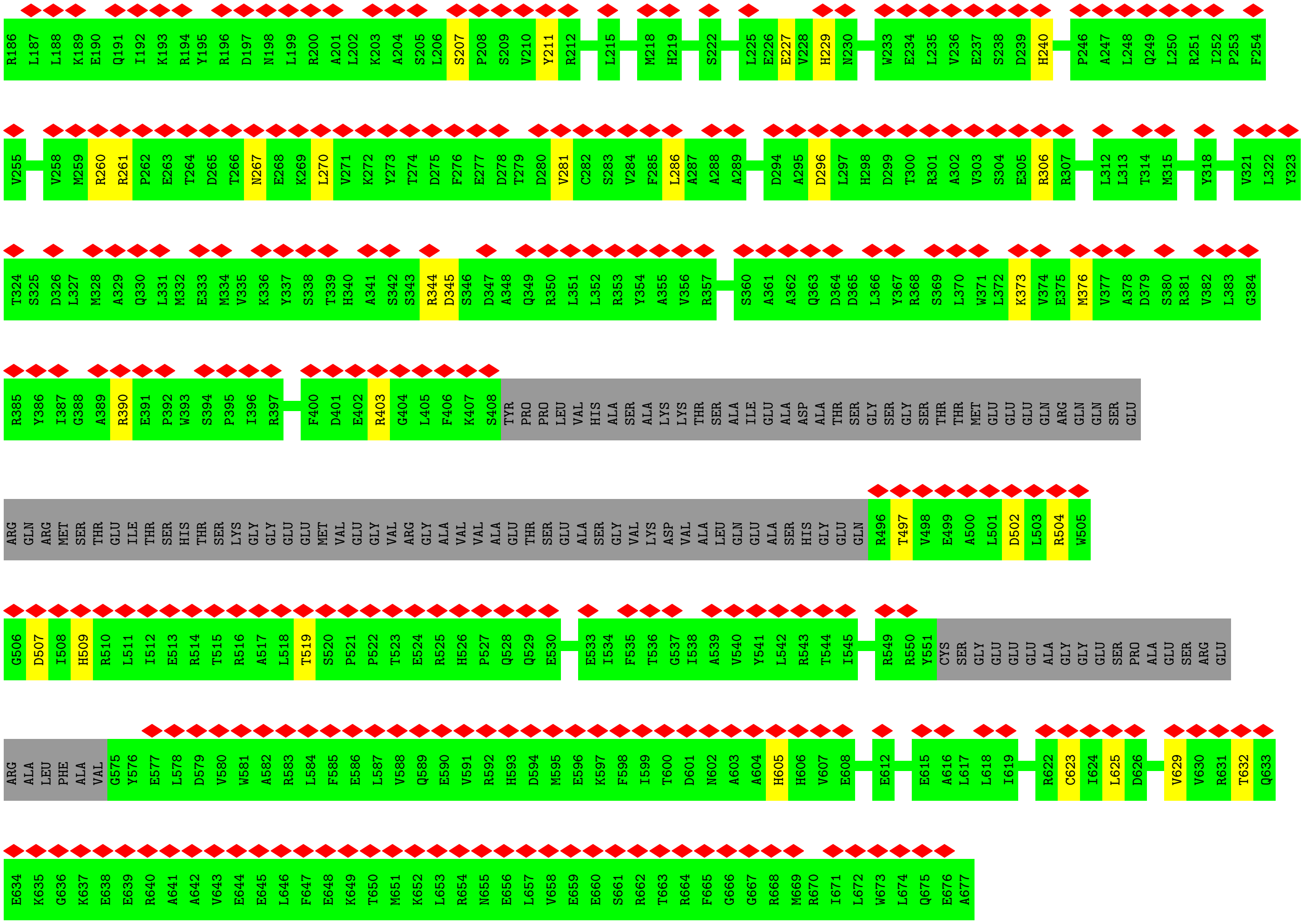


- Molecule 15: mS54

Chain af:

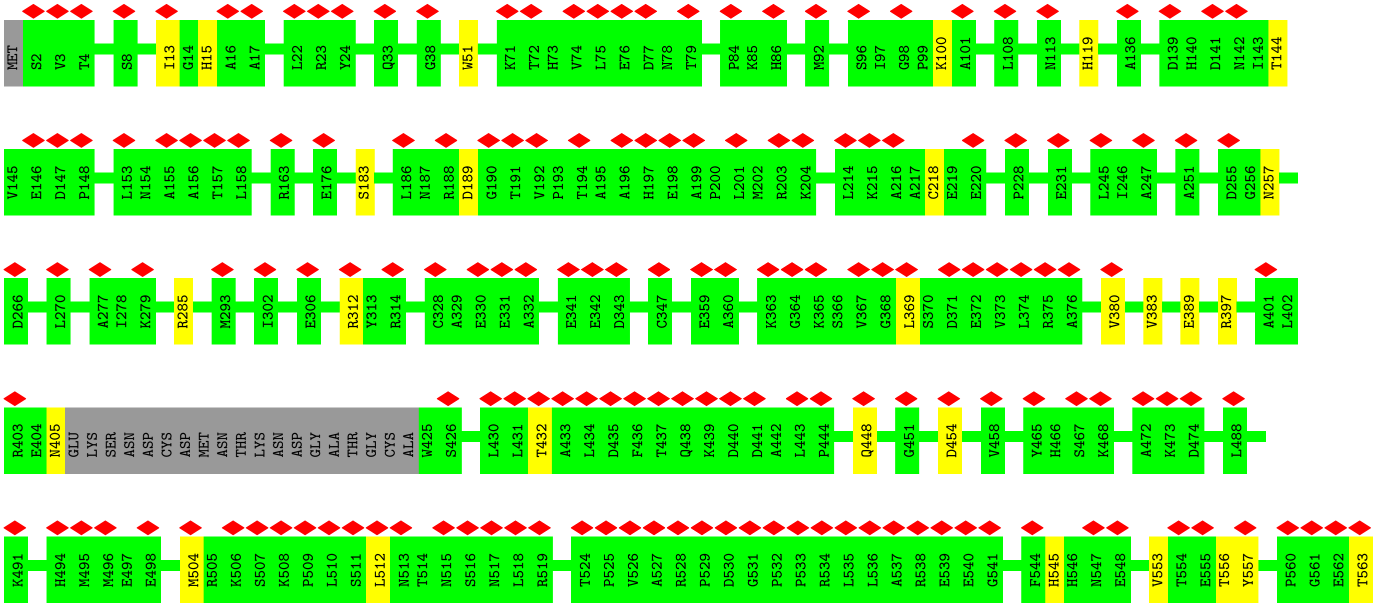


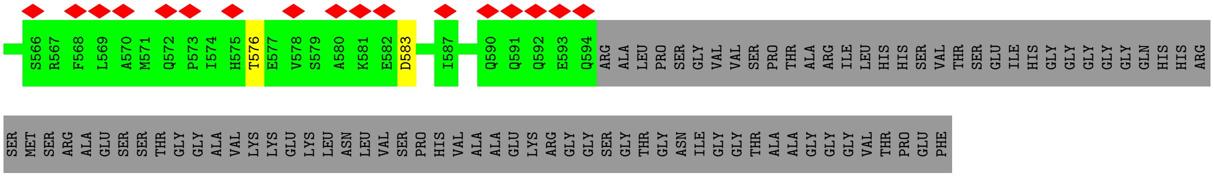




- Molecule 16: mS53

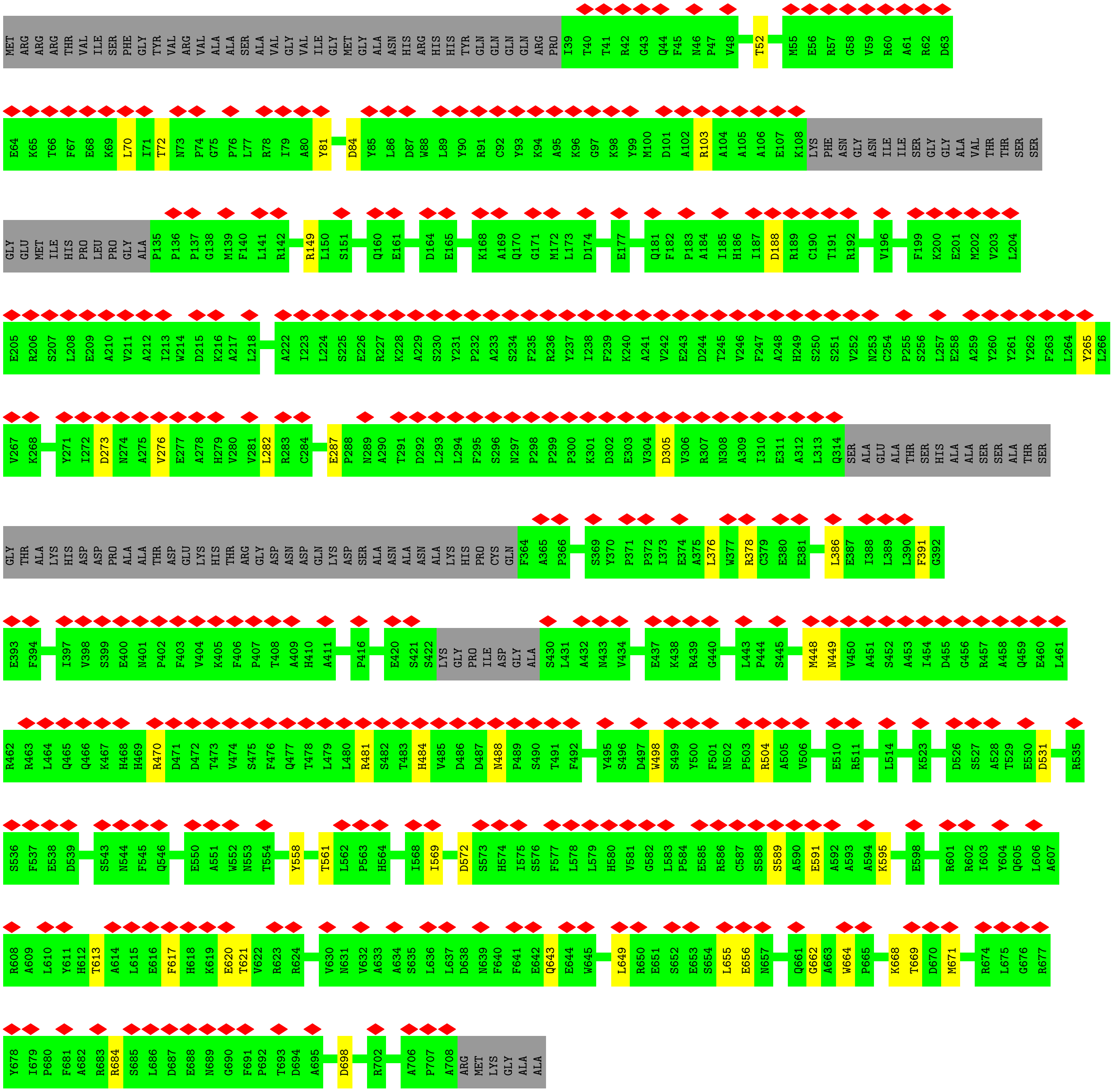
Chain ae:



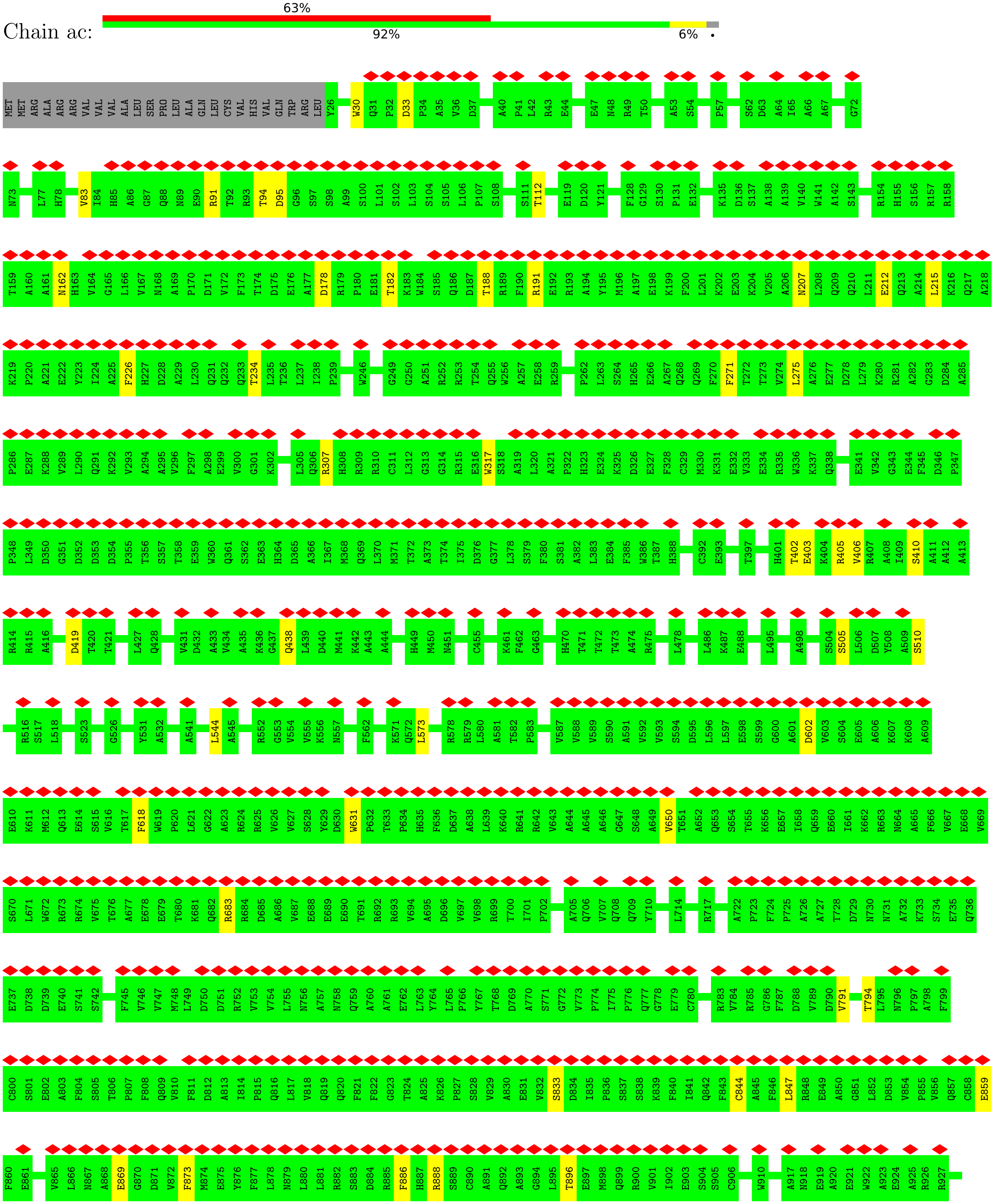


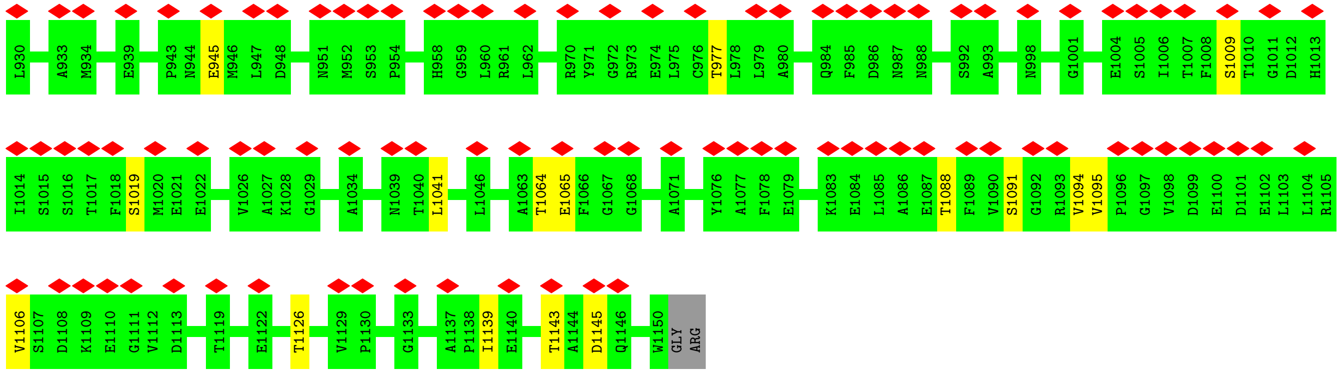
- Molecule 17: mS52

Chain l:



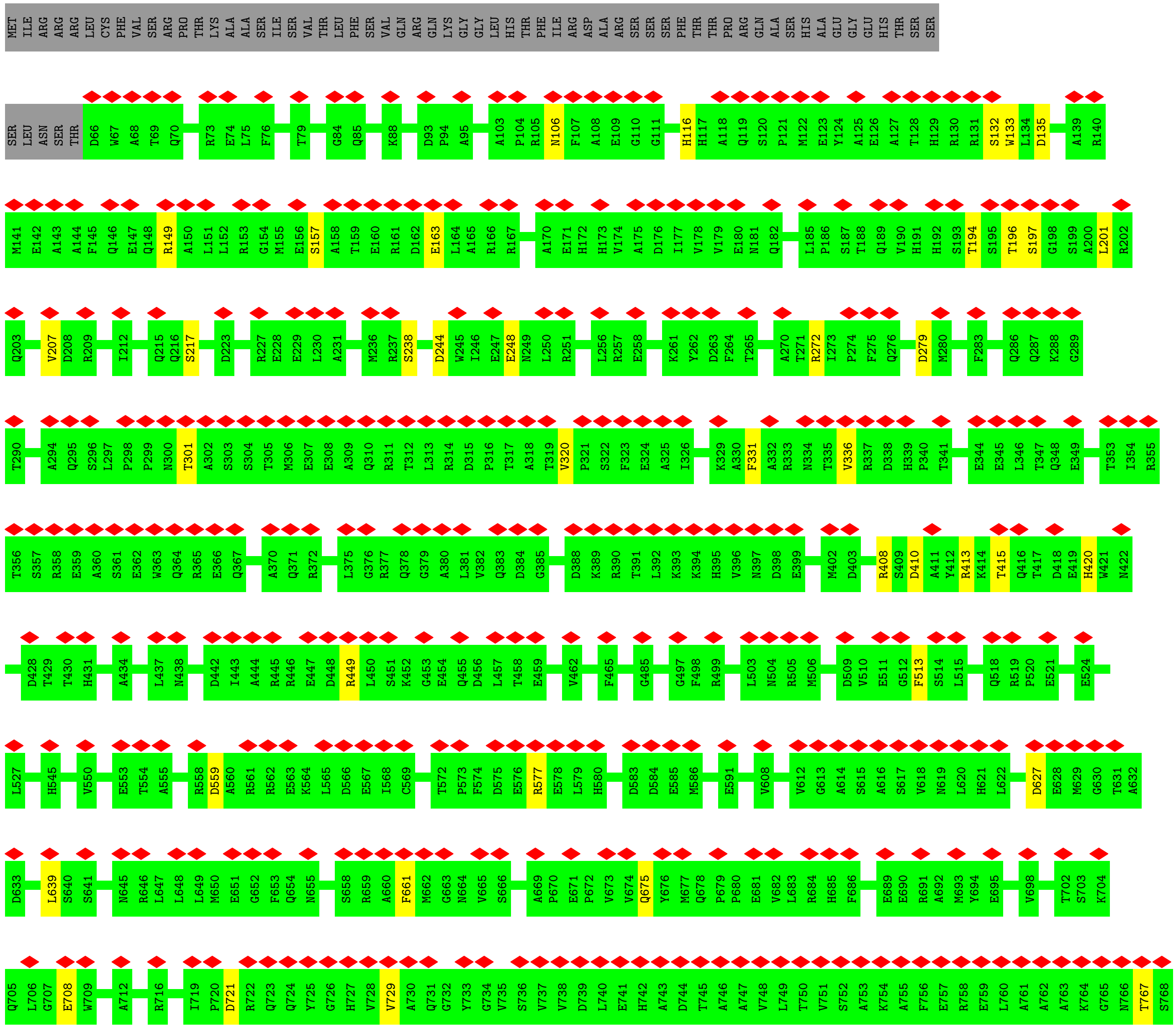
- Molecule 18: mS50

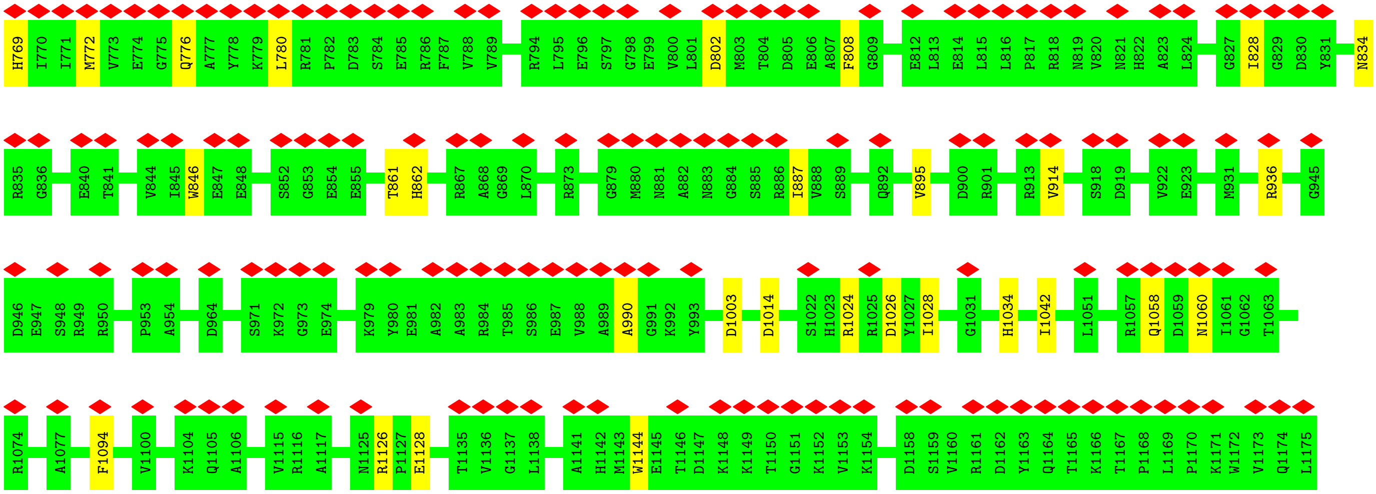




- Molecule 19: mS49

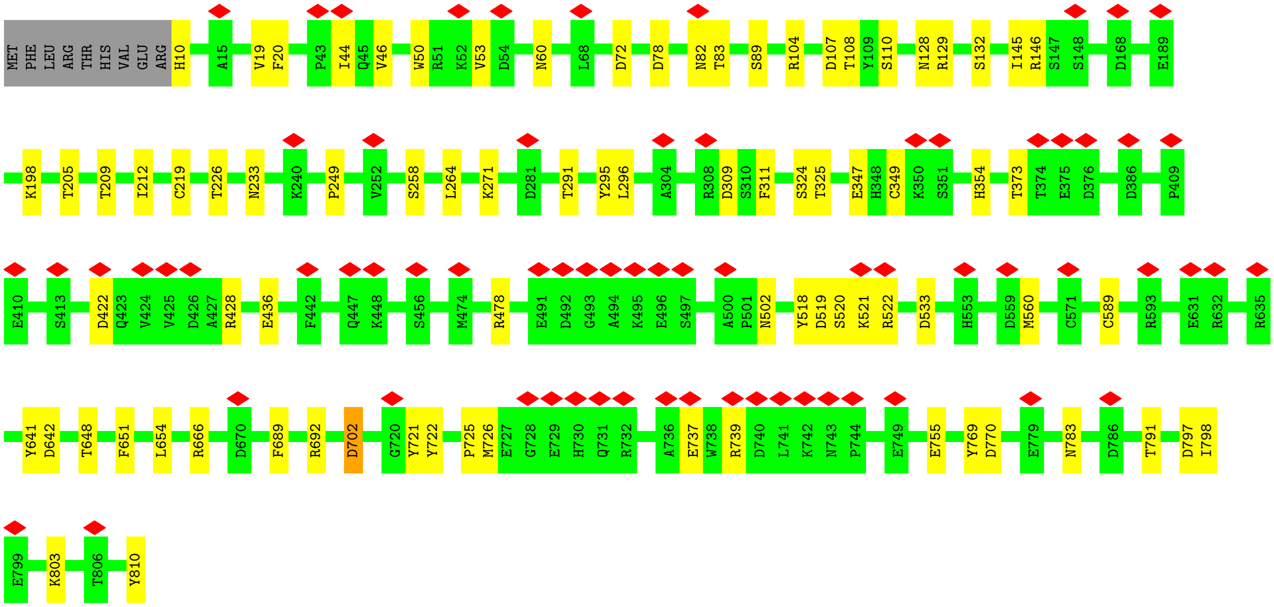
Chain ab:





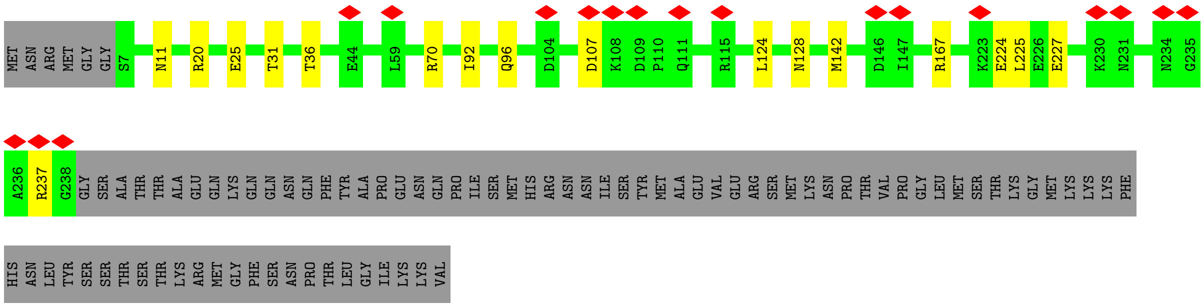
- Molecule 20: mS51

Chain ad:

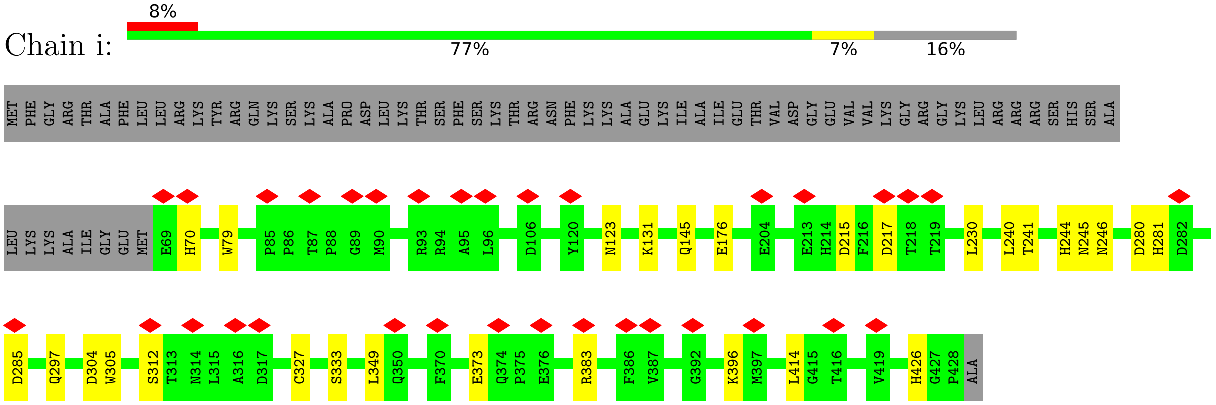


- Molecule 21: bS18m

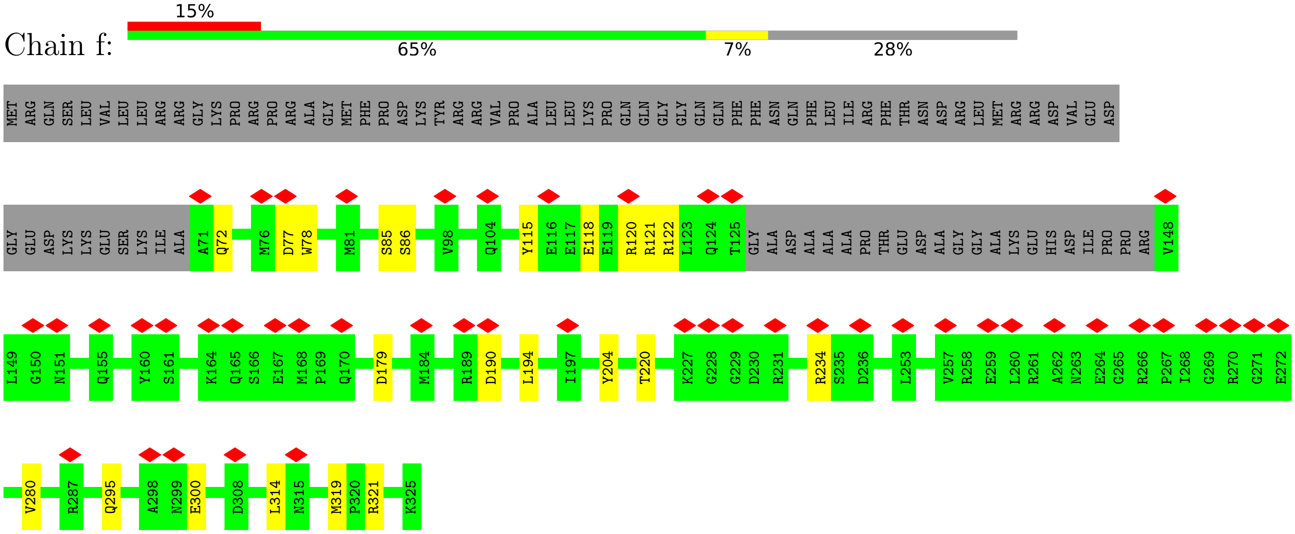
Chain m:



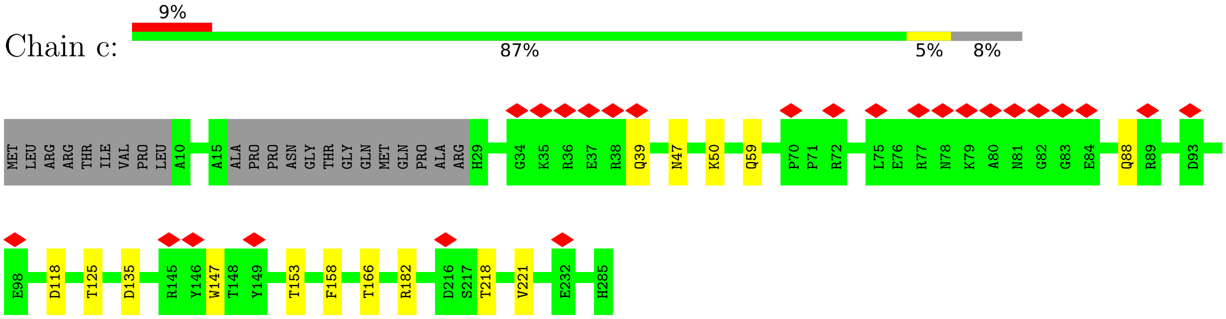
- Molecule 22: uS15m



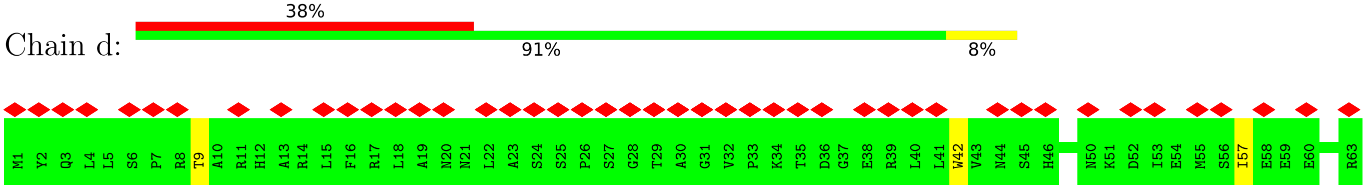
- Molecule 23: uS11m

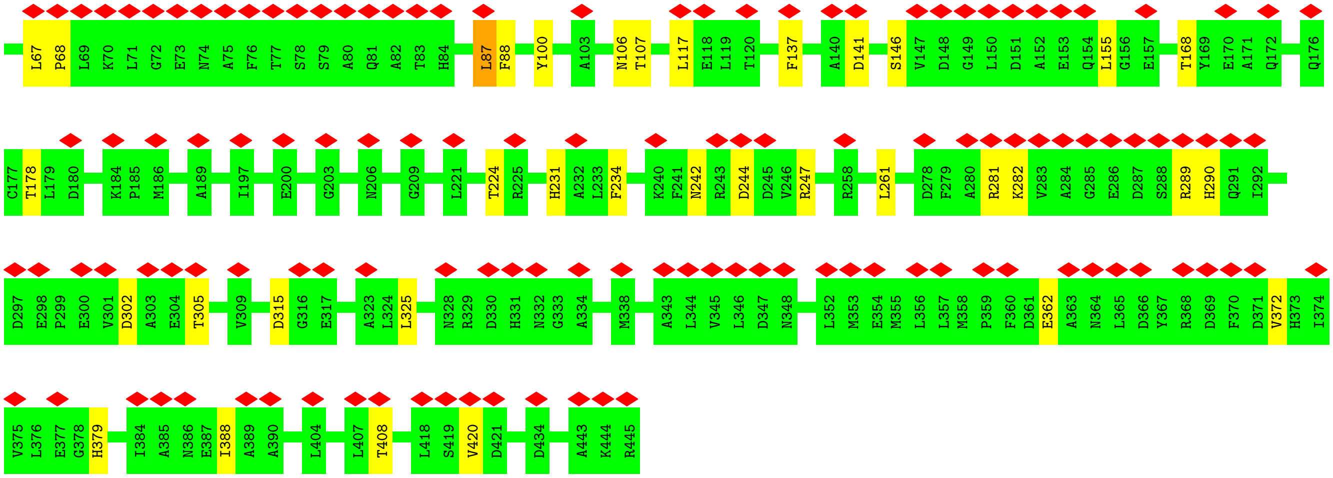


- Molecule 24: uS8m

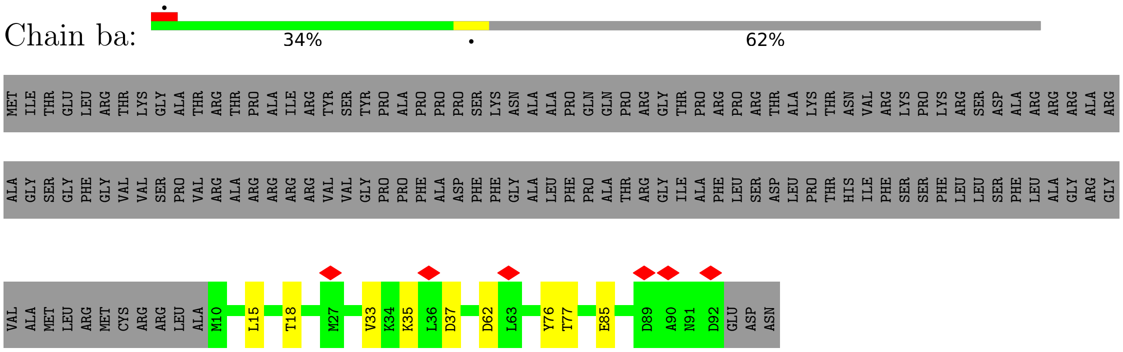


- Molecule 25: uS9m

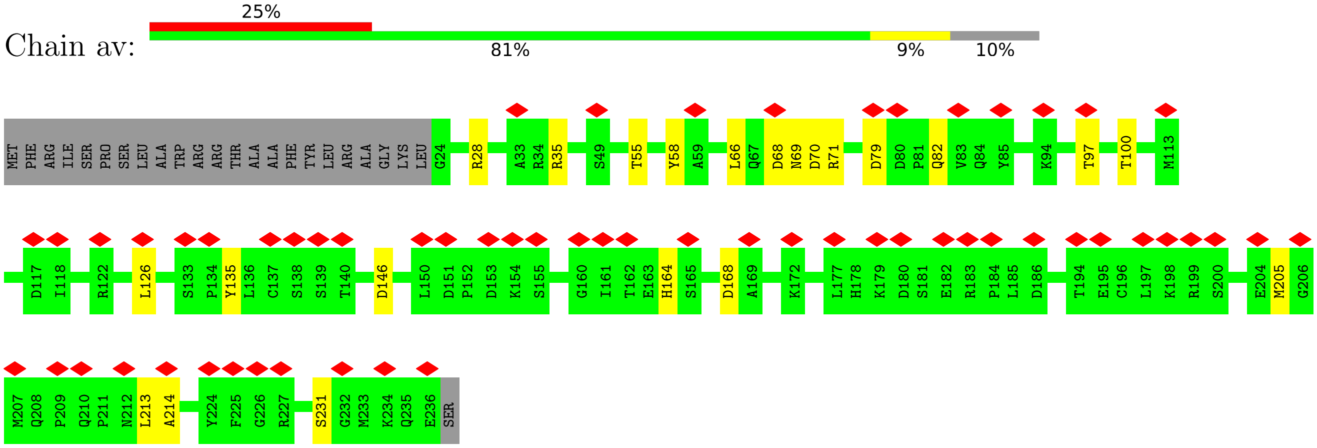




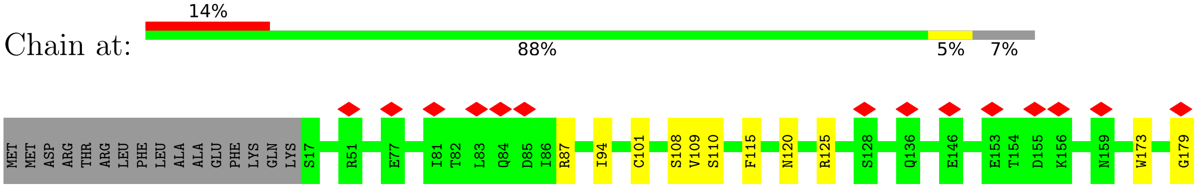
- Molecule 26: mS73

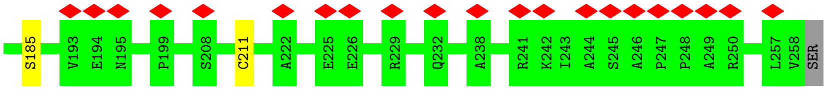


- Molecule 27: mS68



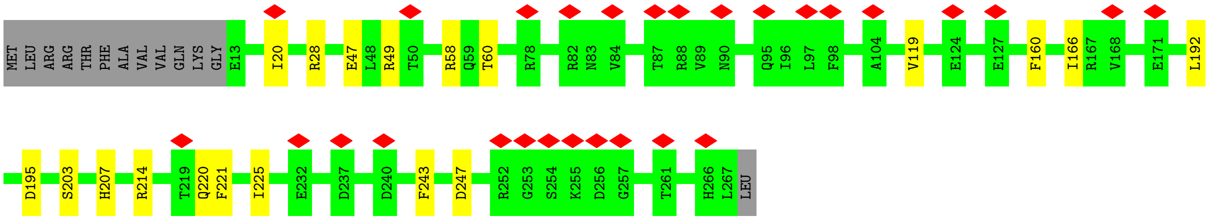
- Molecule 28: mS66





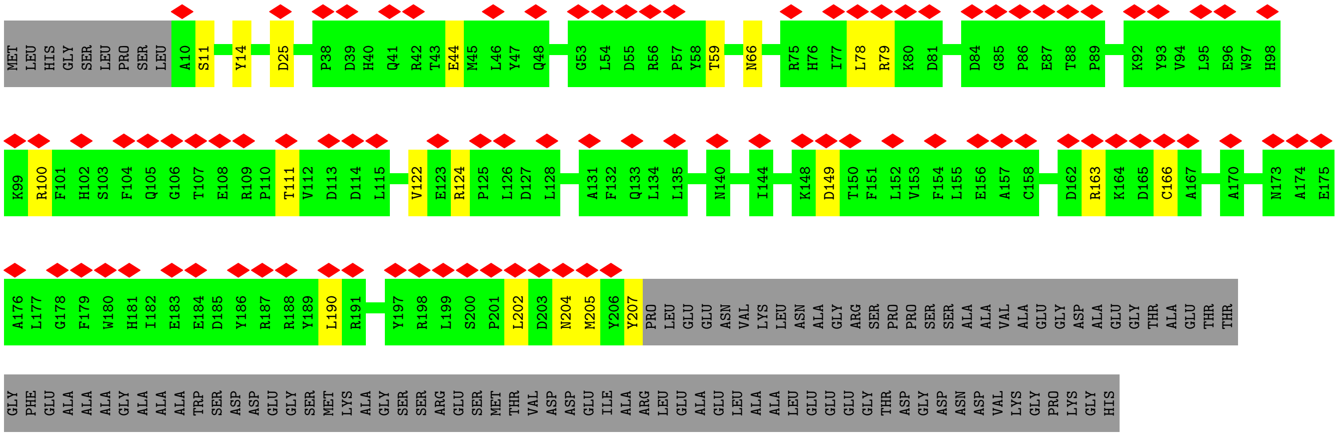
- Molecule 29: AKAP7_NLS domain-containing protein

Chain ar:



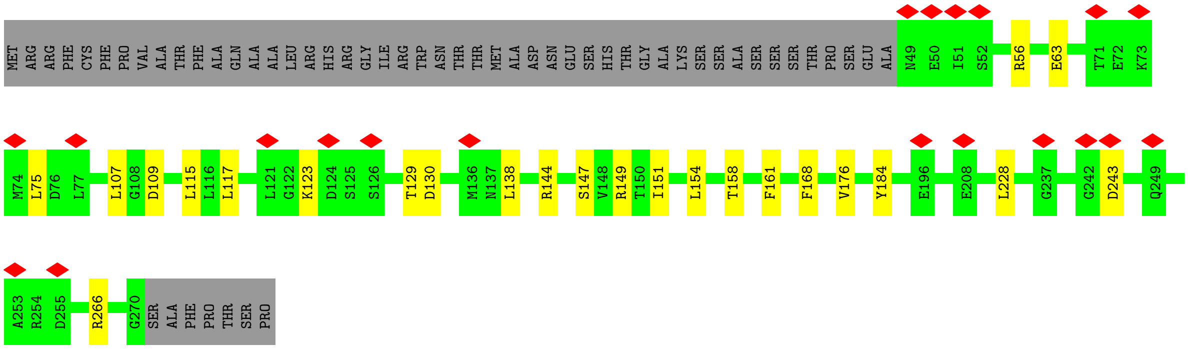
- Molecule 30: mS63

Chain aq:



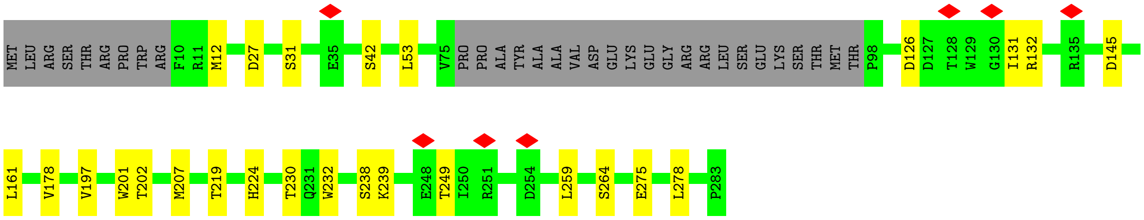
- Molecule 31: mS62

Chain ap:



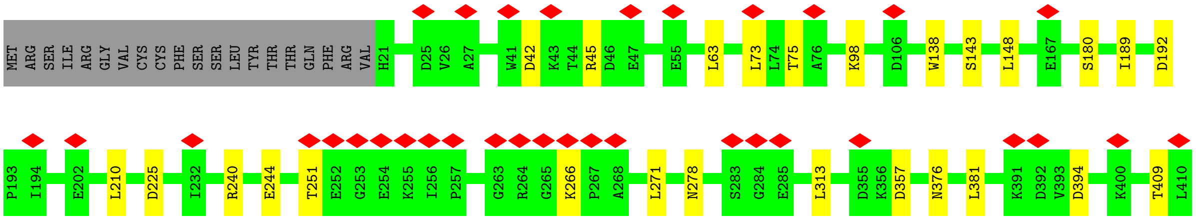
- Molecule 32: mS61

Chain ao:



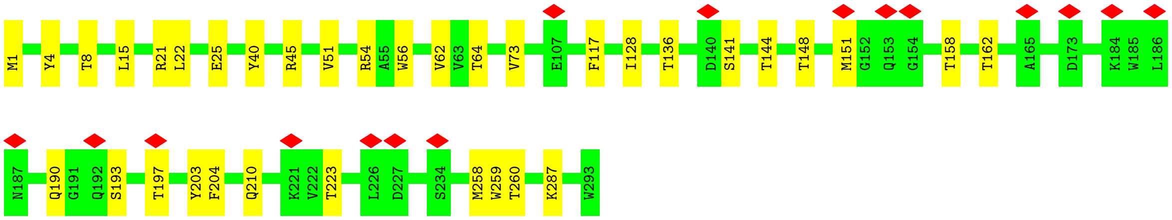
- Molecule 33: mS56

Chain ai:



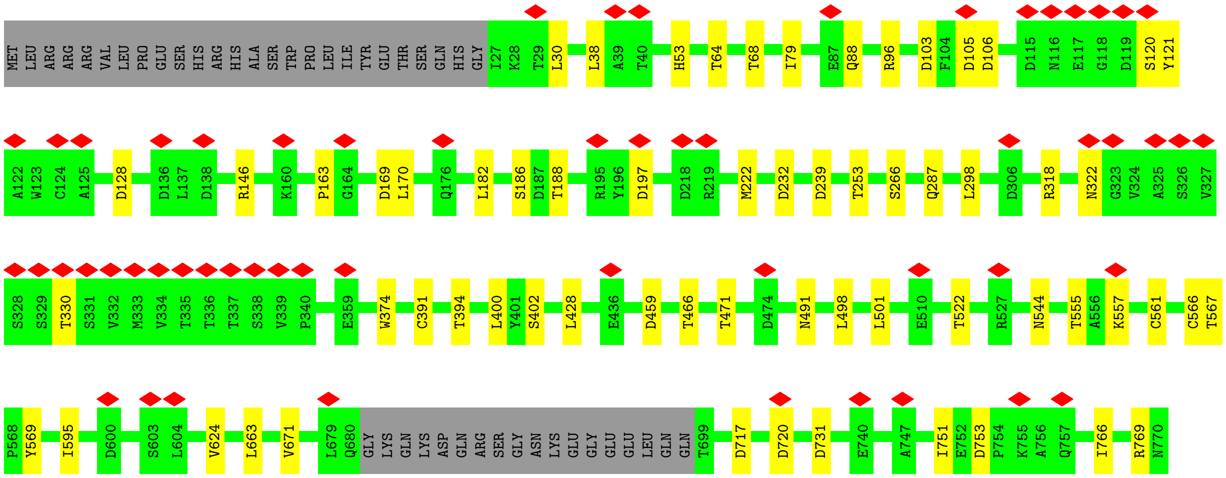
- Molecule 34: mS60

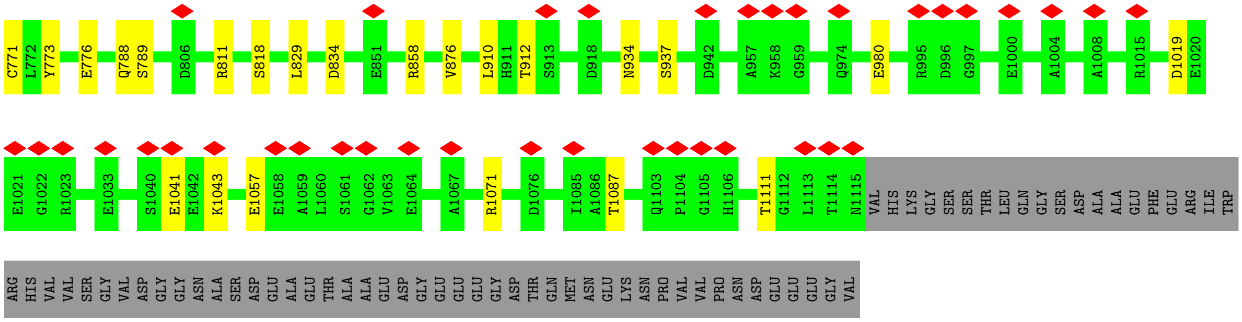
Chain an:



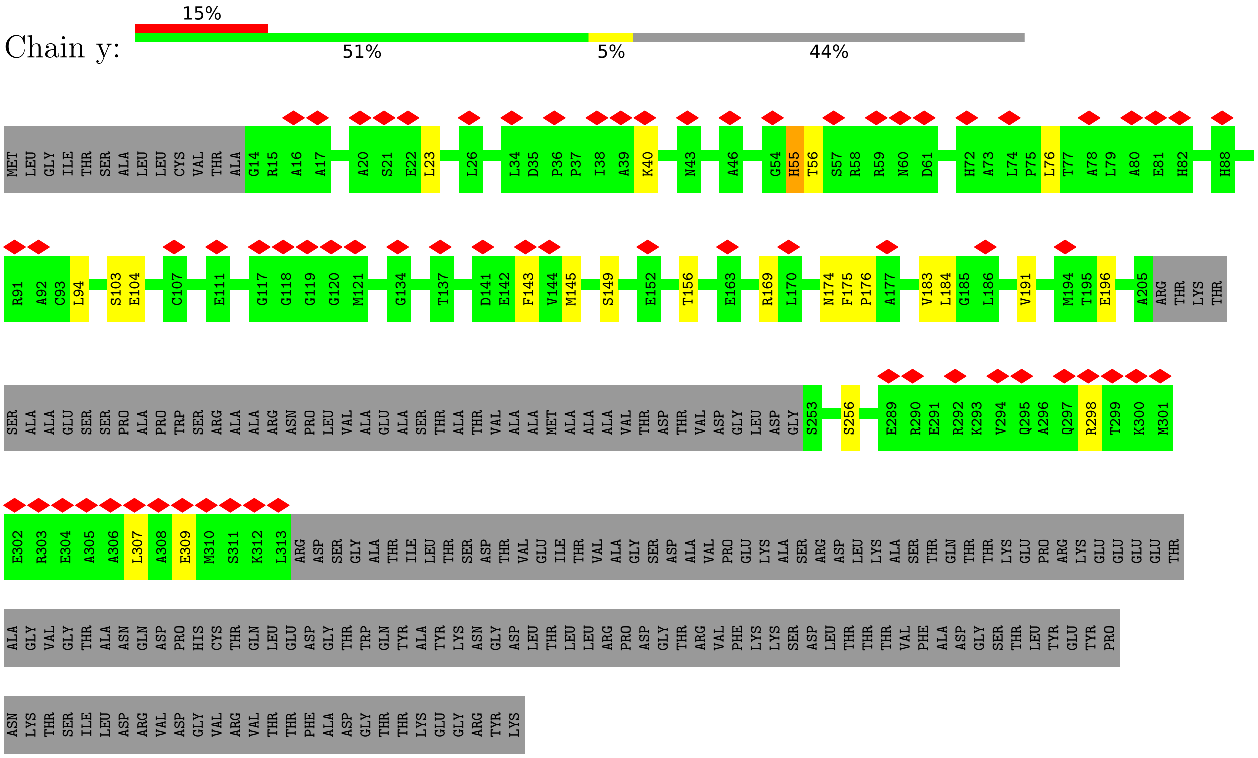
- Molecule 35: mS47

Chain z:

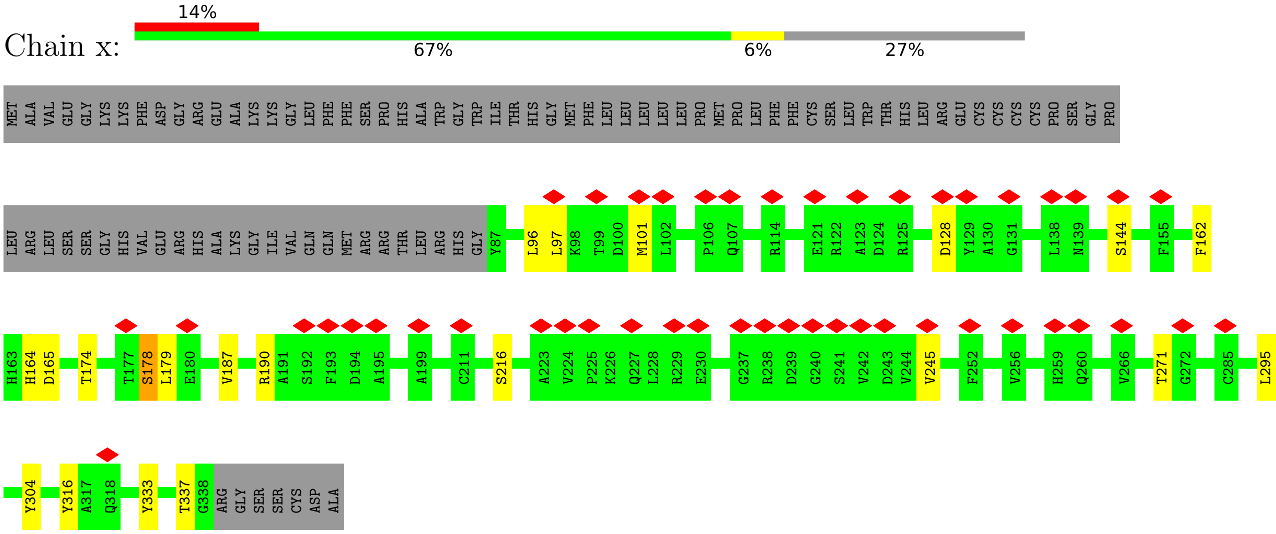




- Molecule 36: Sod_Fe_C domain-containing protein

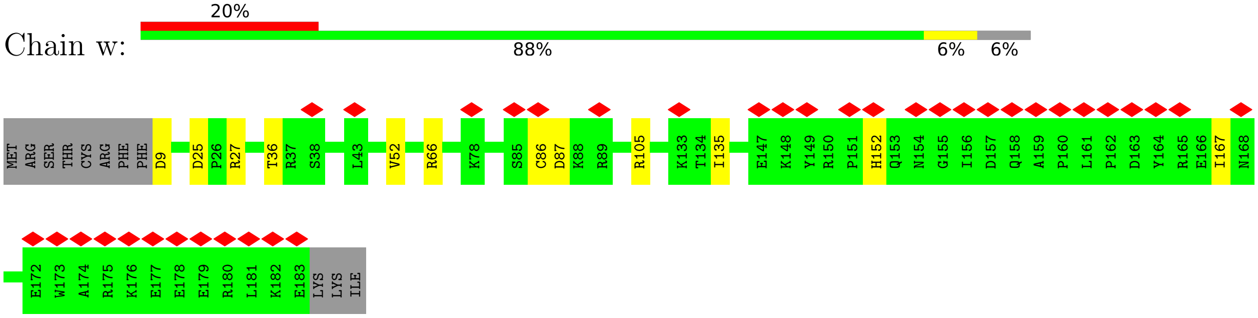


- Molecule 37: Superoxide dismutase, putative



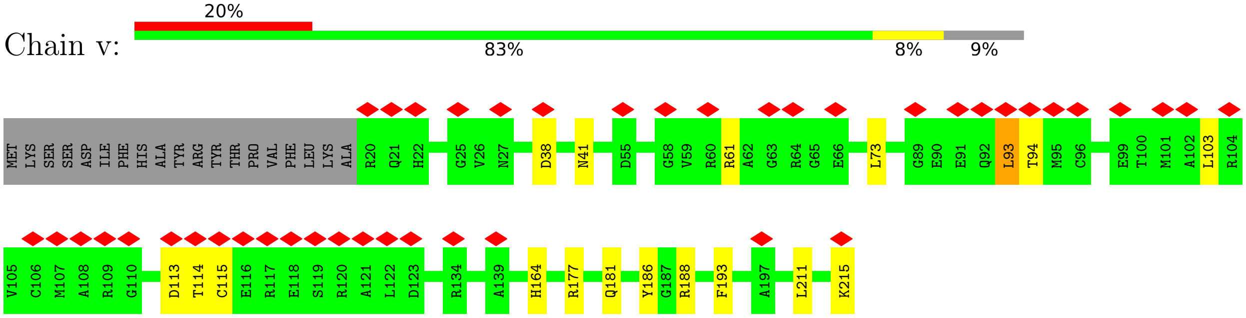
- Molecule 38: Protein FYV4, mitochondrial

Chain w:



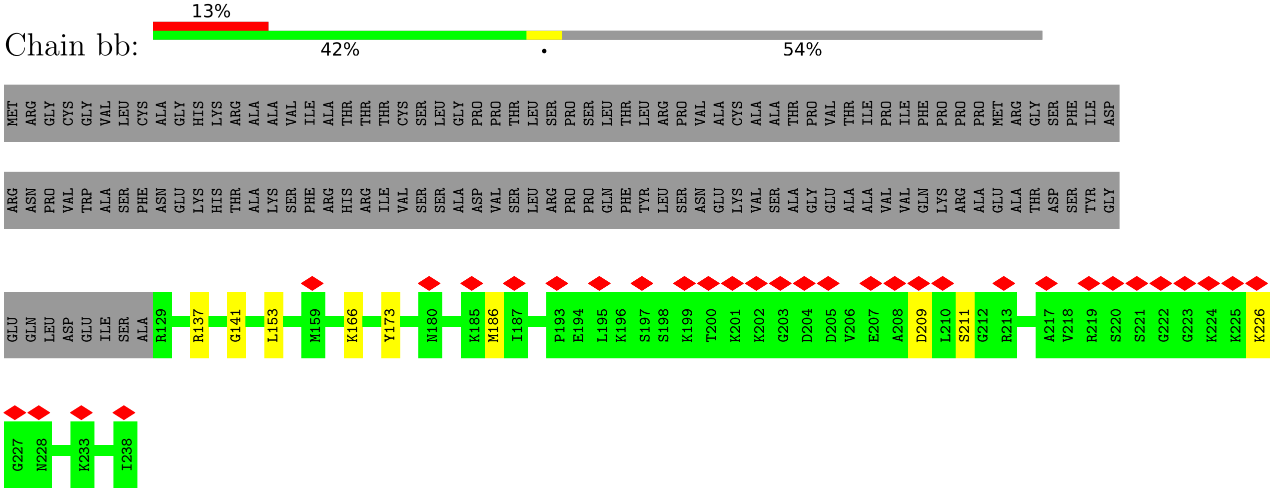
- Molecule 39: mS37

Chain v:



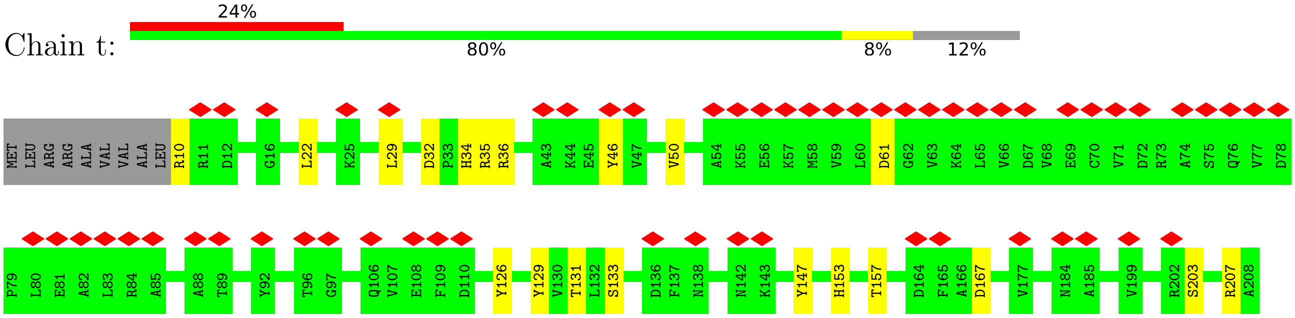
- Molecule 40: mS38

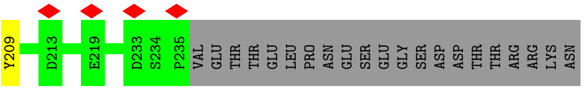
Chain bb:



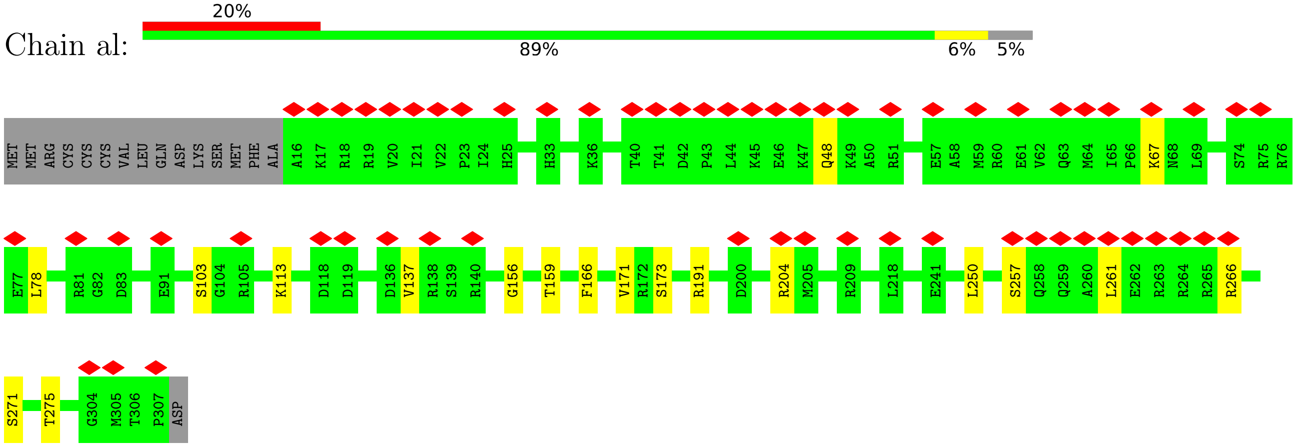
- Molecule 41: Trafficking protein particle complex subunit

Chain t:

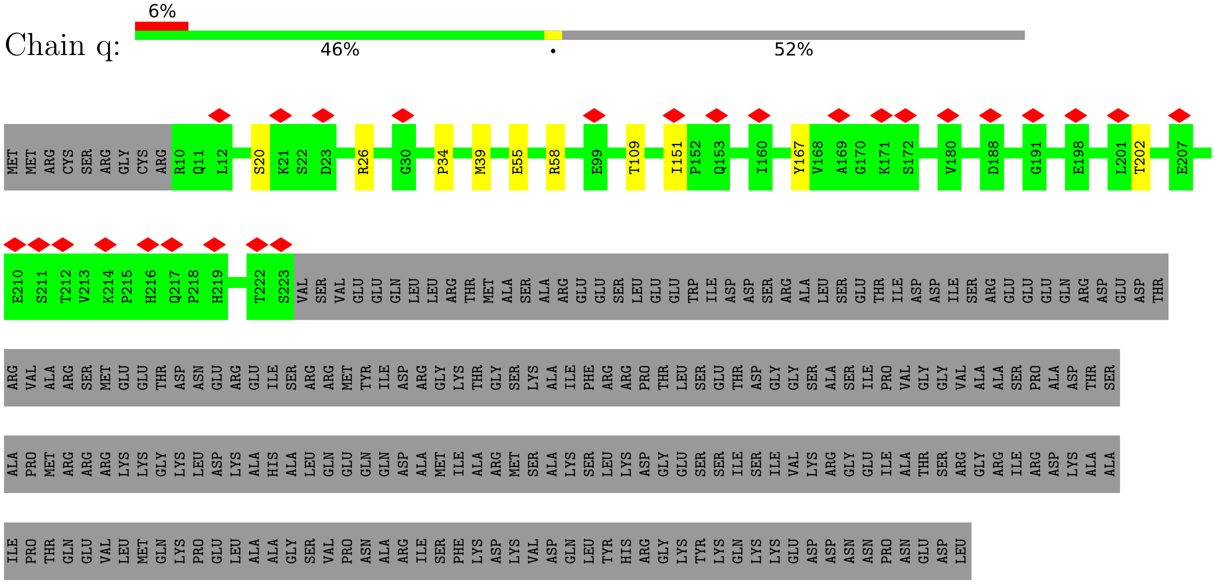




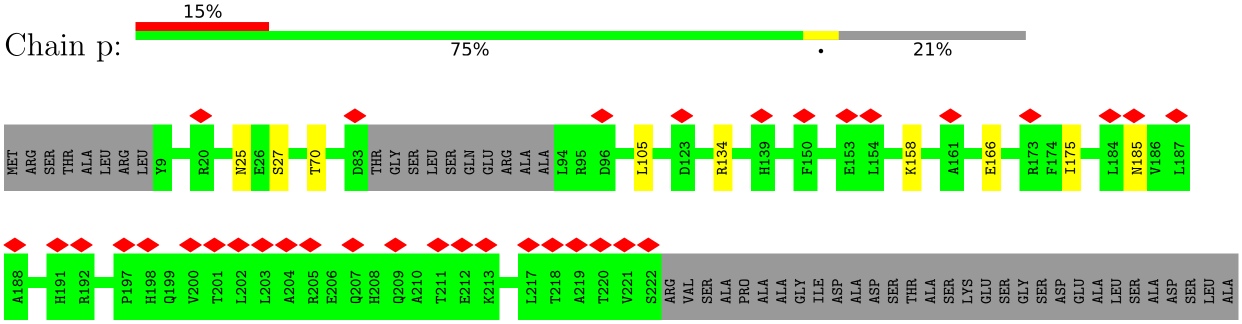
- Molecule 42: mS59

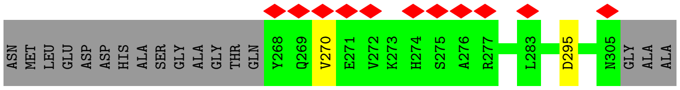


- Molecule 43: mS26



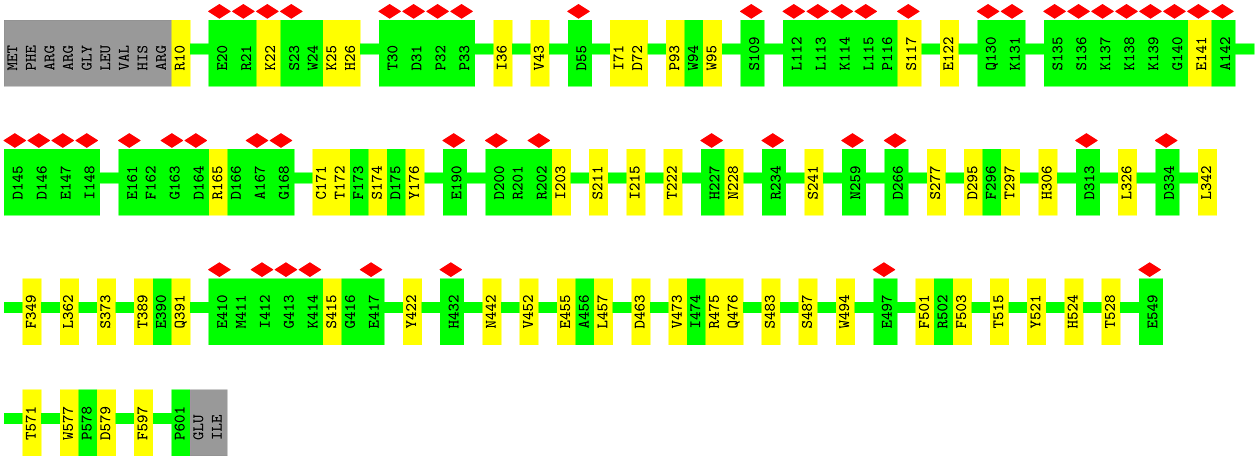
- Molecule 44: mS23





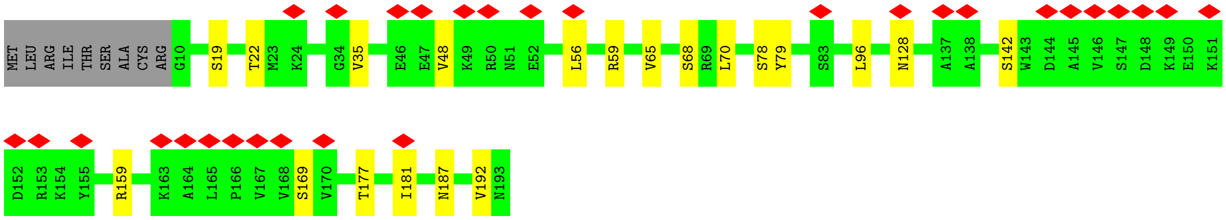
- Molecule 45: mS22

Chain Ca:



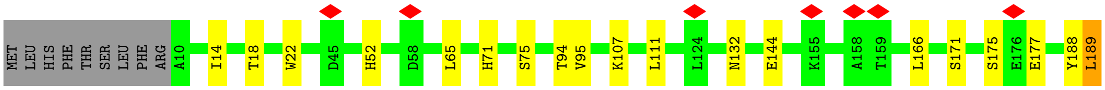
- Molecule 46: bS21m

Chain g:



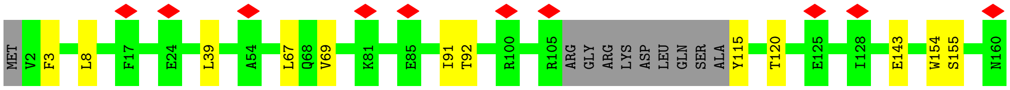
- Molecule 47: bS16m

Chain j:

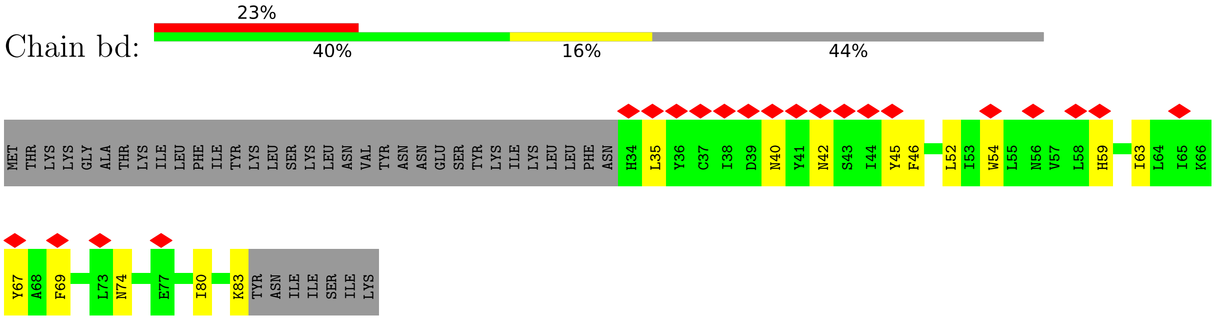


- Molecule 48: bS6m

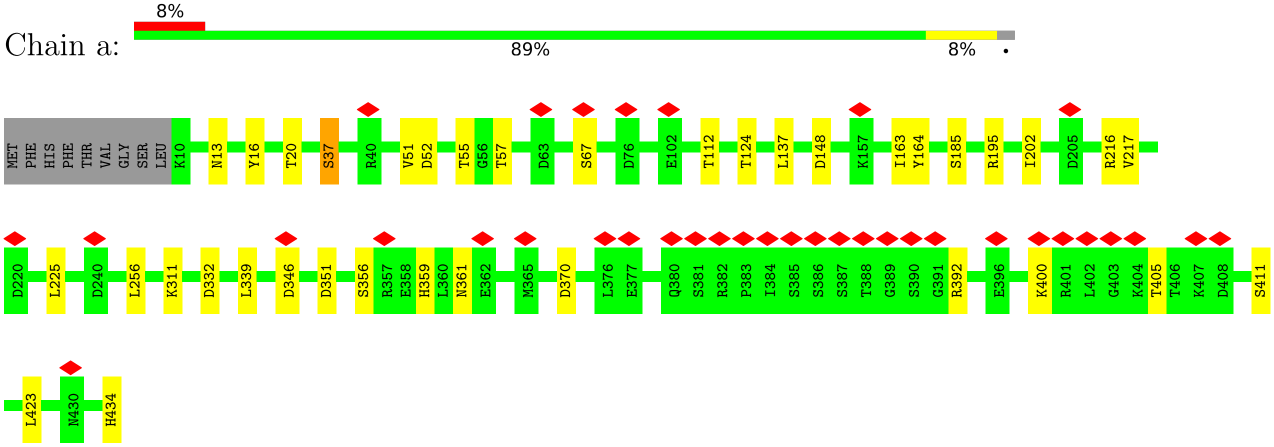
Chain b:



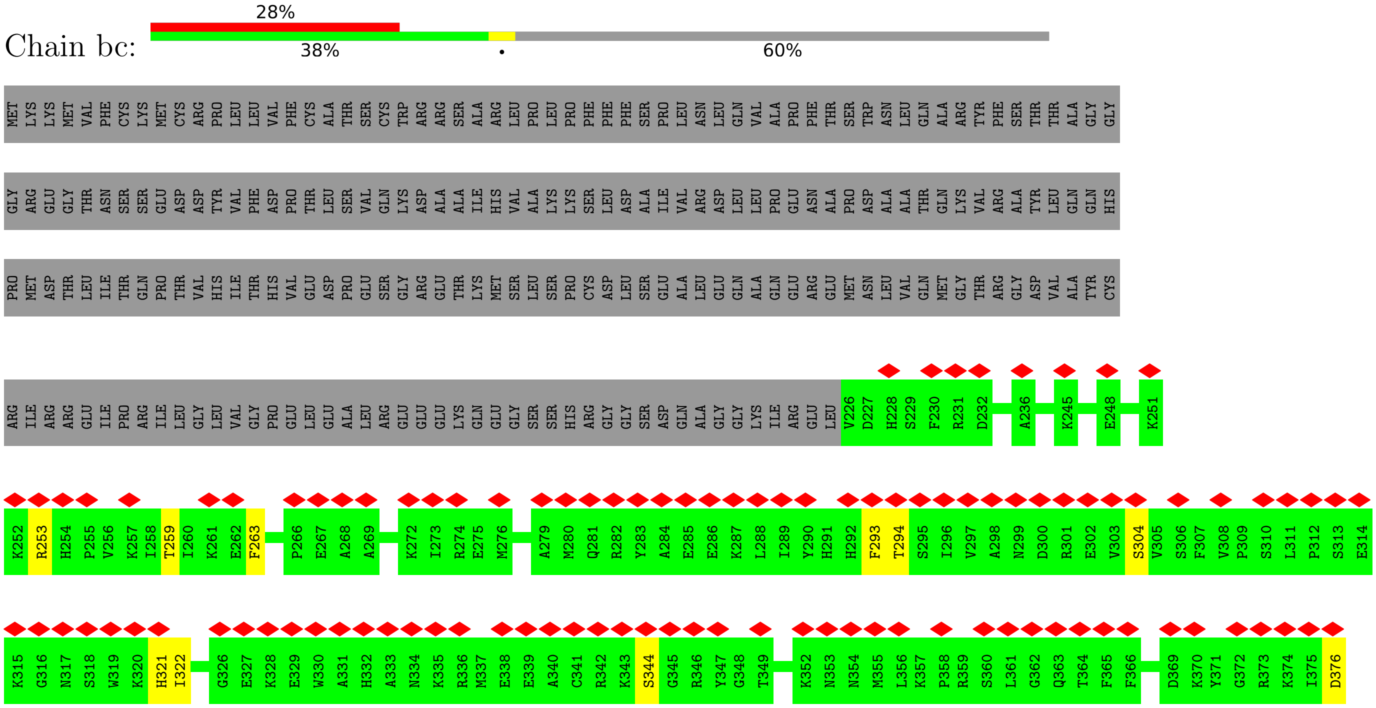
- Molecule 49: MURF5



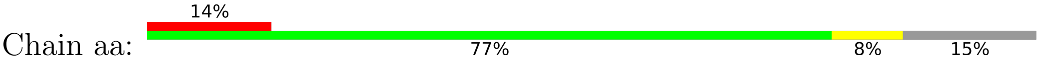
• Molecule 50: Ribosomal_S5_C domain-containing protein

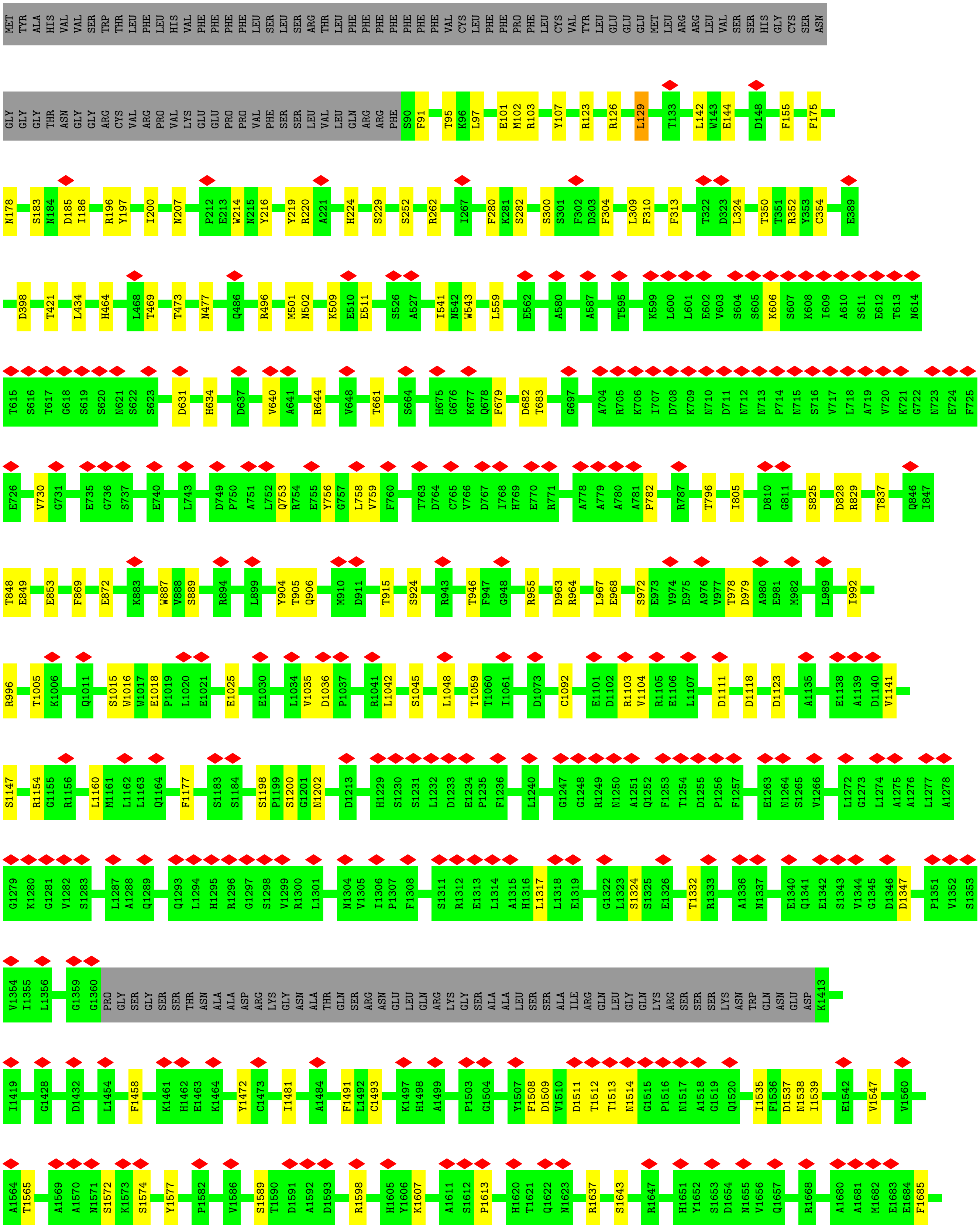


• Molecule 51: mt-iF3



• Molecule 52: mS48

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GLY GLY GLY THR ASN GLY GLY ARG TRP CYS VAL ARG PRO VAL LYS GLU GLU PRO PRO VAL PHE SER SER LEU VAL LEU GLN ARG ARG PHE S90 F91 T95 K96 L97 E101 M102 R103 Y107 R123 R126 L129 T133 L142 W143 E144 D148 F155 F175
N178 S183 N184 D185 I186 R196 Y197 I200 N207 P212 E213 W214 N215 Y216 Y219 R220 A221 H224 S229 S252 R262 I267 F280 K281 S282 S300 S301 F302 D303 F304 L309 F310 F313 T322 D323 L324 T350 T351 R352 Y353 C354 E389
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R996 T1005 K1006 Q1011 S1015 W1016 W1017 E1018 P1019 L1020 E1021 E1025 E1030 L1034 V1035 D1036 P1037 R1041 L1042 S1045 L1048 T1059 T1060 I1061 D1073 C1092 E1101 D1102 R1103 V1104 R1105 E1106 L1107 D1111 D1118 D1123 A1135 E1138 A1139 D1140 V1141
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V1354 I1355 L1356 G1359 G1360 PRO GLY SER GLY SER SER THR ASN ALA ALA ASP ARG LYS GLY ASN ALA THR GLN SER ARG ASN GLU LEU GLN ARG LYS GLY SER ALA ALA LEU SER SER ALA ILE ARG GLN LEU GLY GLN LYS ARG SER SER LYS ASN TRP GLN ASN GLU ASP K1413
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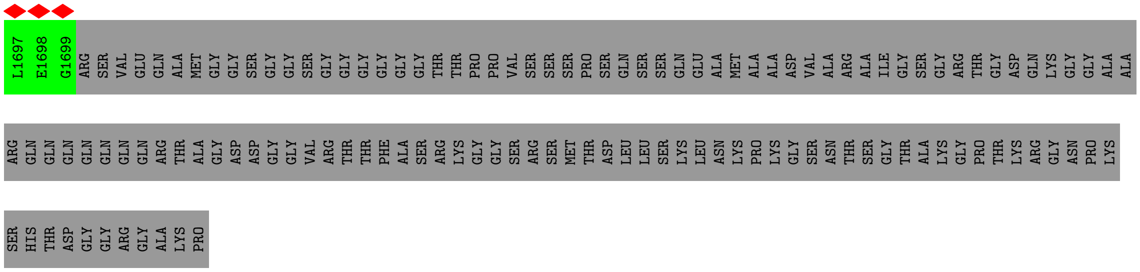
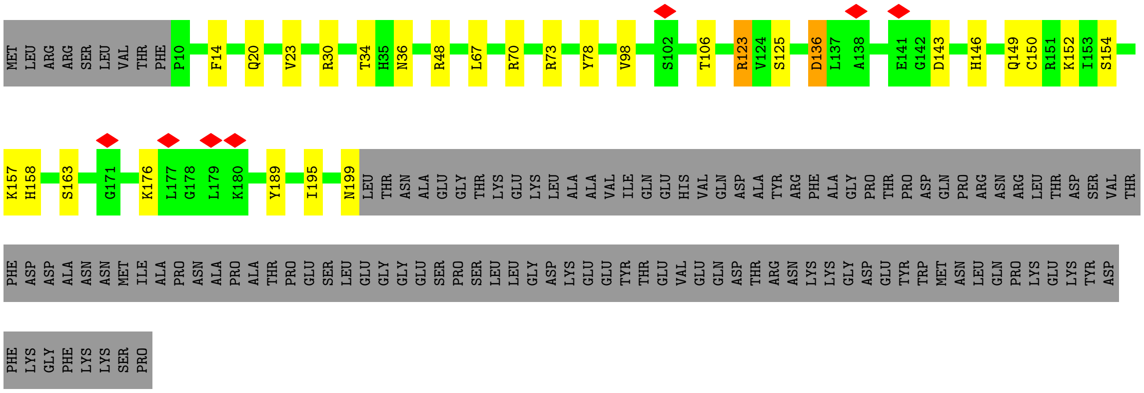


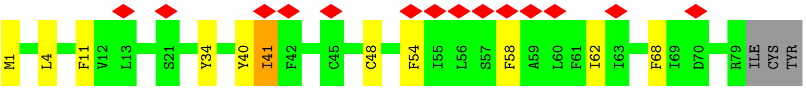
- Molecule 53: 30S Ribosomal protein S17-like protein

Chain k:



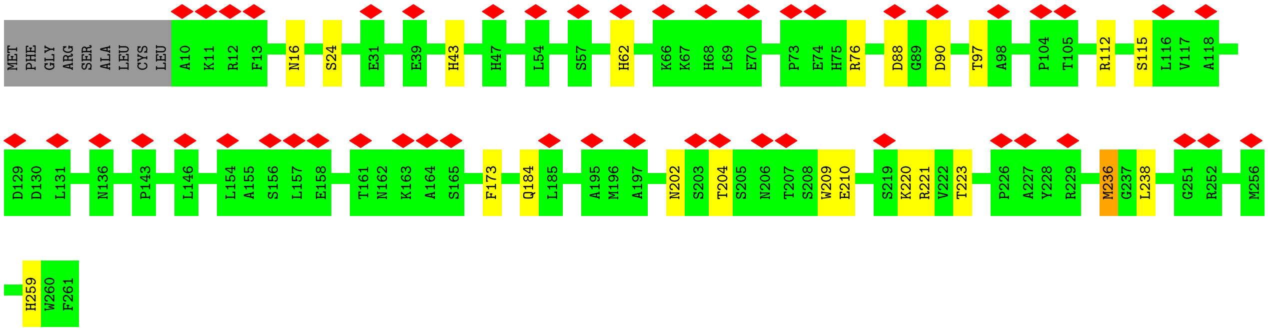
- Molecule 54: Ribosome protein S12

Chain be:



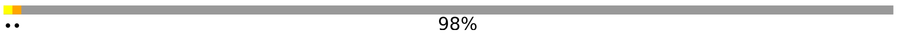
- Molecule 55: mS65

Chain as:



- Molecule 56: RNA (478-MER)

Chain A:



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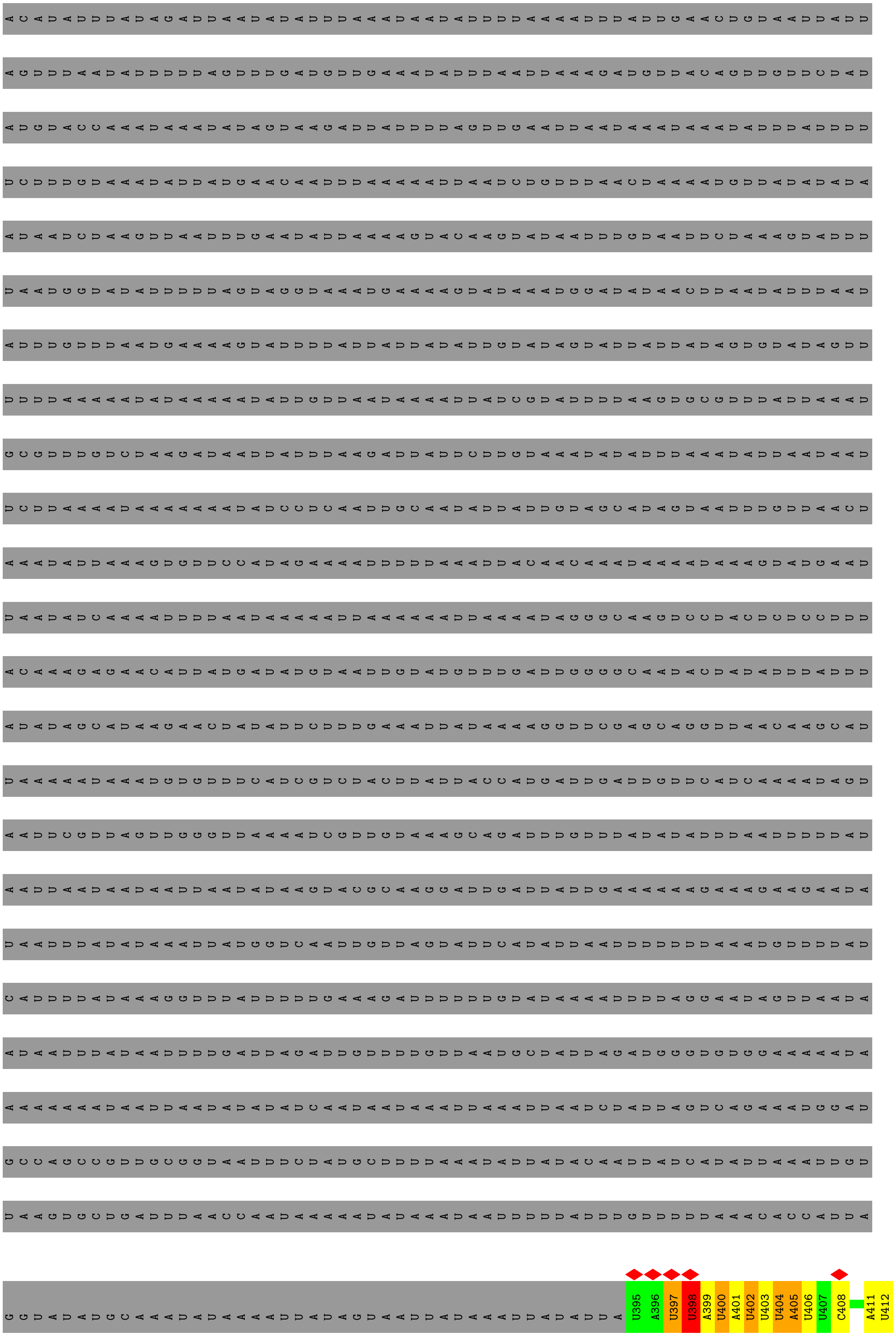
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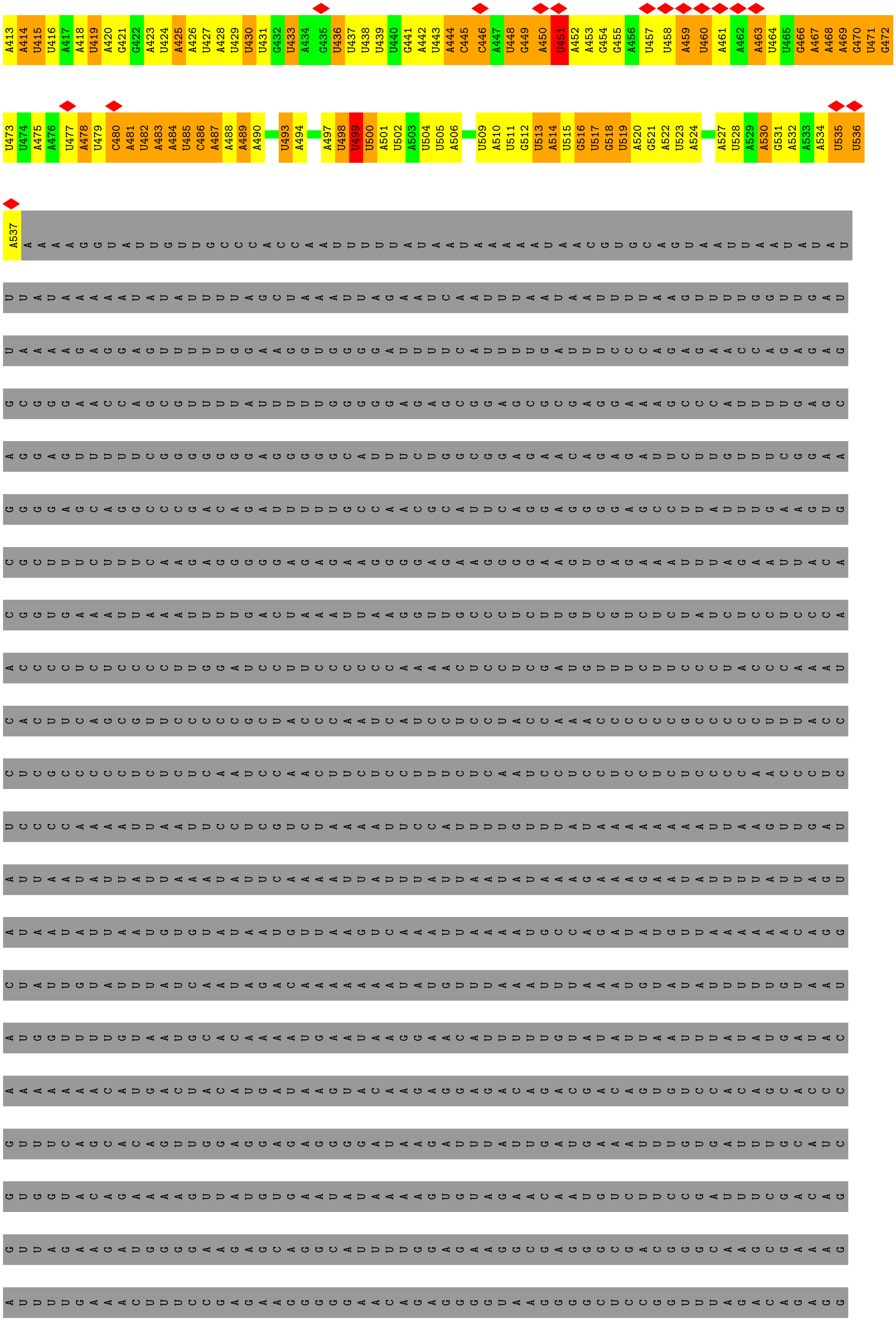

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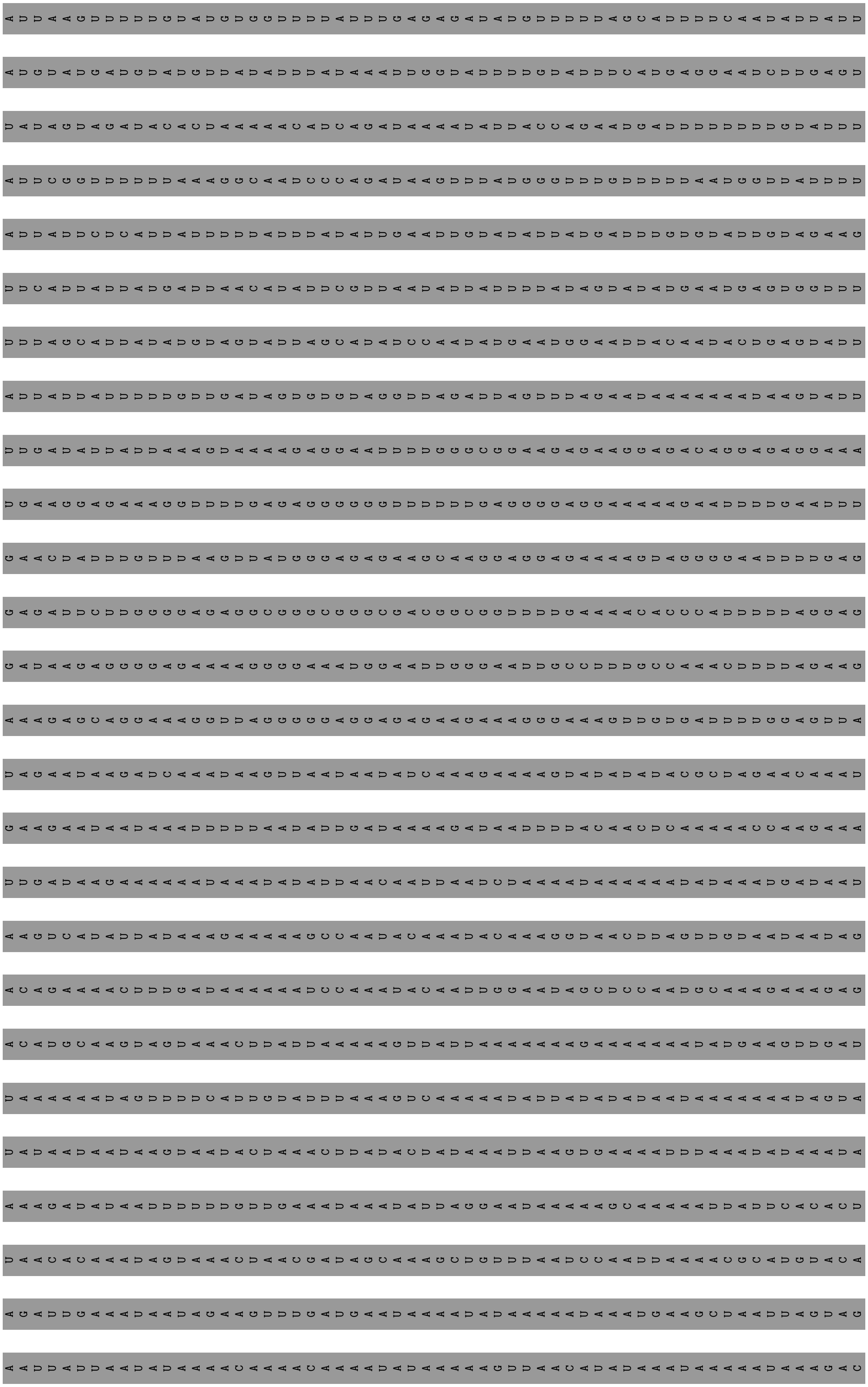
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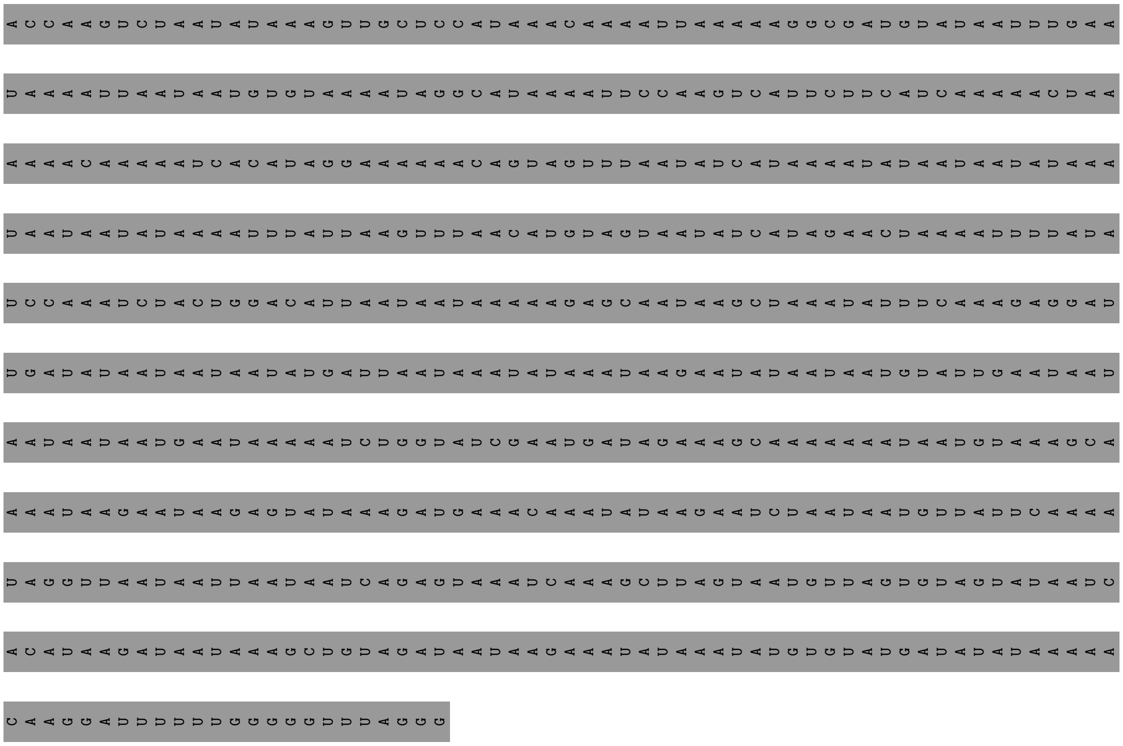

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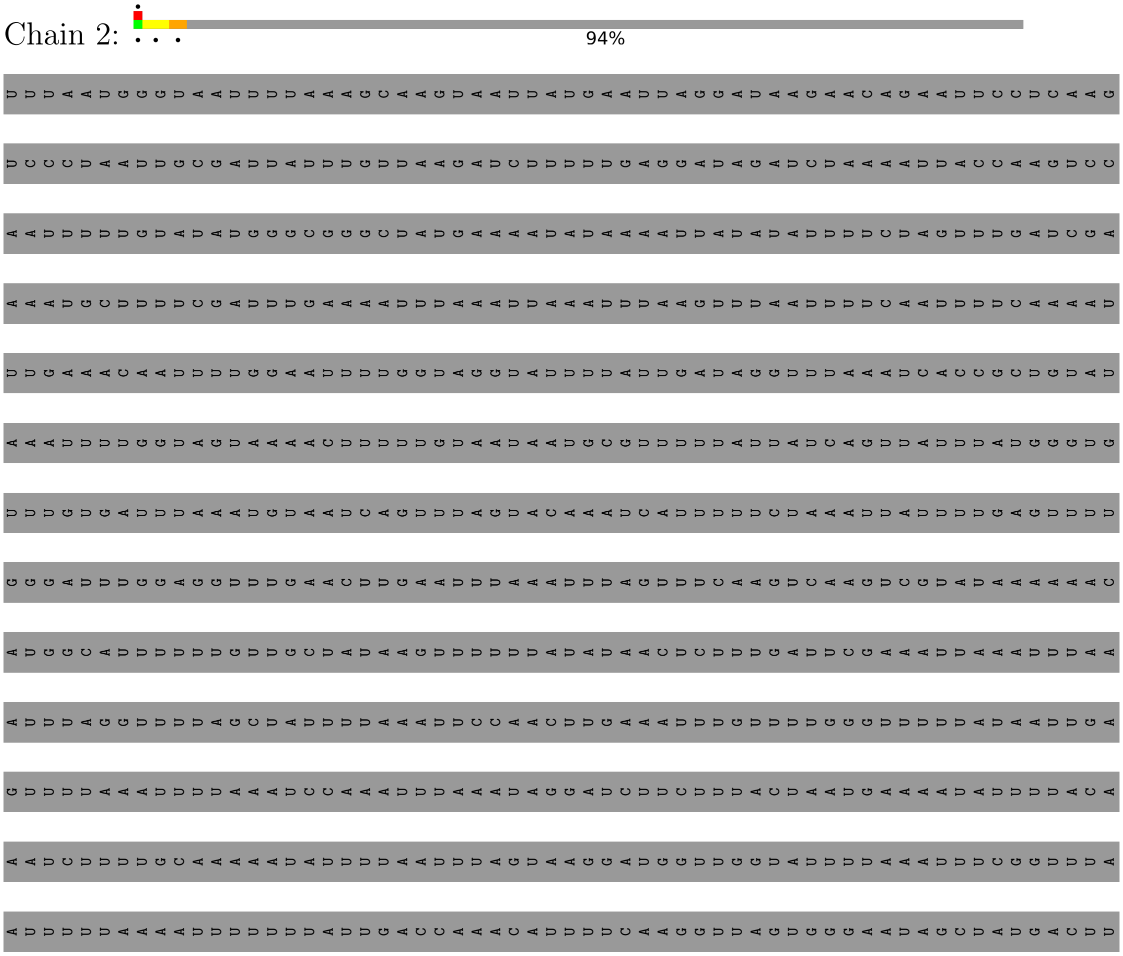

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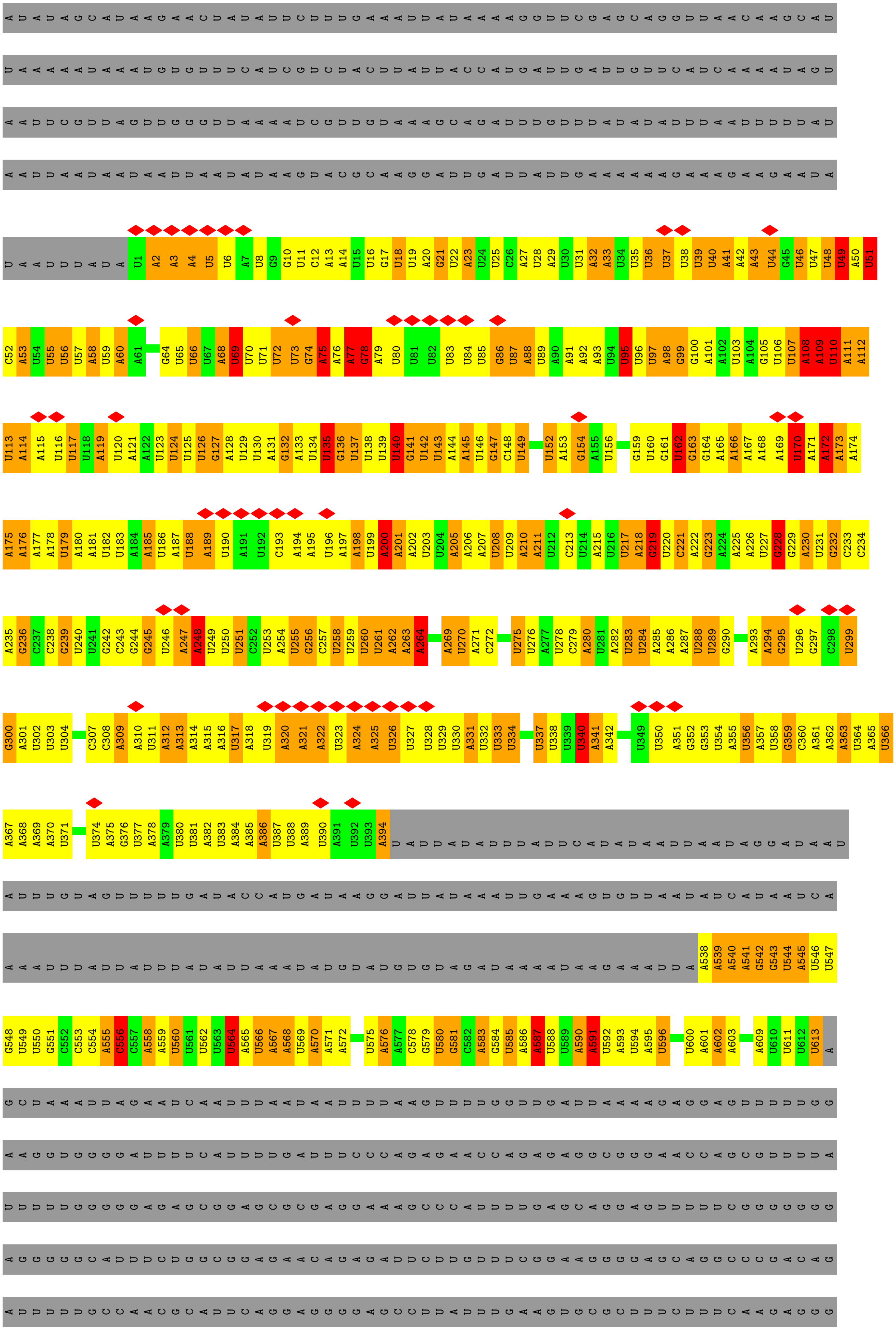
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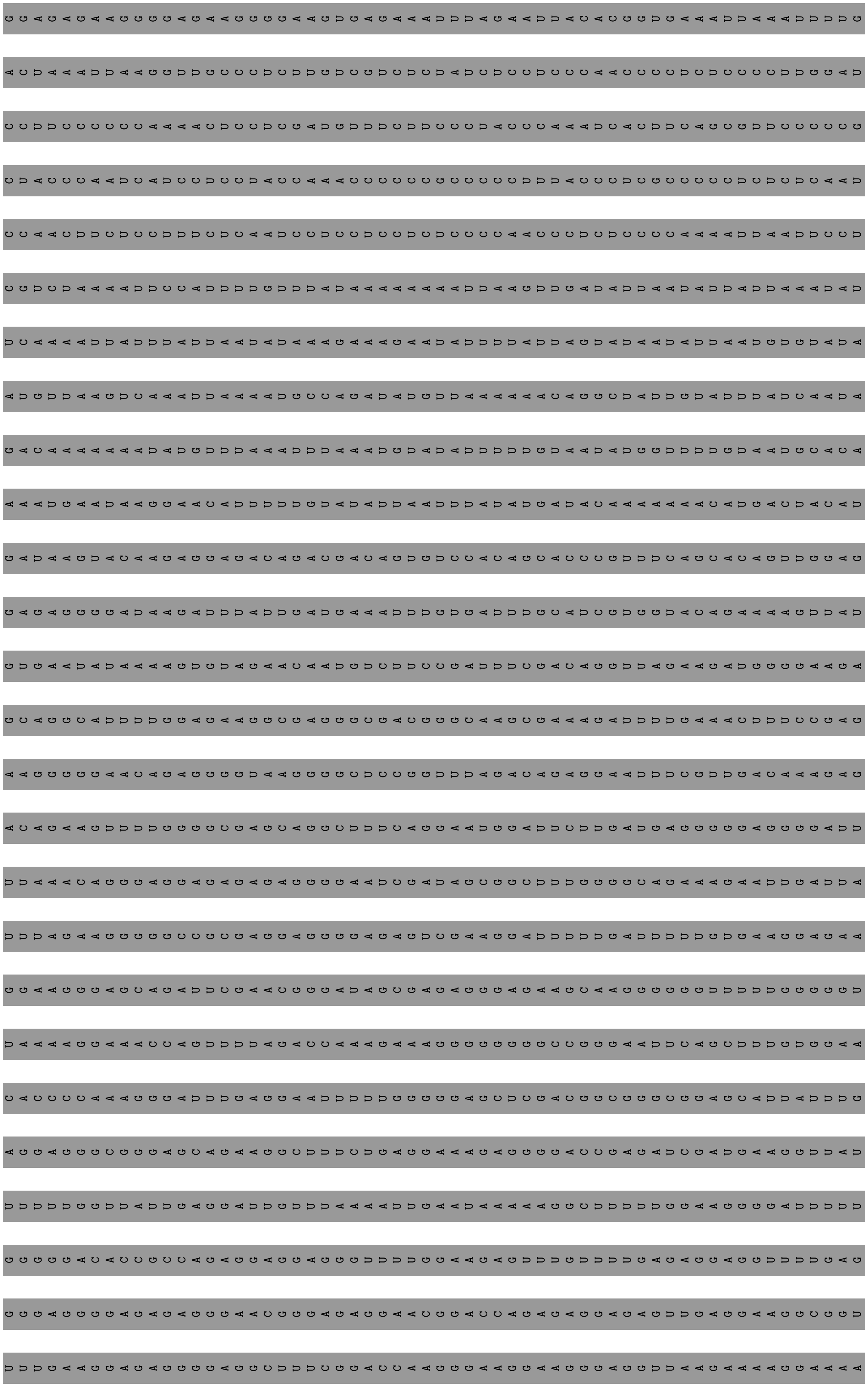
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4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.176	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	428.40002, 428.40002, 428.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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, MG, UTP, ZN

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	u	1.21	6/5704 (0.1%)	0.55	2/7702 (0.0%)
2	s	0.48	0/1391	0.54	0/1880
3	r	0.41	0/3925	0.52	0/5331
4	n	0.43	0/1202	0.54	0/1618
5	h	0.52	0/1364	0.51	0/1842
6	e	0.60	2/6771 (0.0%)	0.59	2/9218 (0.0%)
7	az	0.43	0/1334	0.58	0/1811
8	ay	0.40	0/1236	0.50	0/1663
9	ax	0.35	0/1415	0.51	0/1923
10	aw	0.44	0/1376	0.53	0/1862
11	au	0.48	0/2151	0.54	0/2920
12	ak	0.38	0/1905	0.52	0/2572
13	aj	0.42	0/2665	0.52	1/3618 (0.0%)
14	ag	0.43	0/4572	0.54	0/6180
15	af	0.38	0/4689	0.54	0/6342
16	ae	0.41	0/4746	0.53	0/6439
17	l	0.37	0/4950	0.52	0/6705
18	ac	0.35	0/9073	0.51	0/12323
19	ab	0.41	0/9319	0.53	0/12610
20	ad	0.63	1/6805 (0.0%)	0.60	1/9217 (0.0%)
21	m	0.69	1/1998 (0.1%)	0.59	0/2707
22	i	0.56	0/3048	0.59	0/4110
23	f	0.48	0/1958	0.59	0/2631
24	c	0.79	1/2216 (0.0%)	0.63	0/2984
25	d	0.50	0/3611	0.57	1/4871 (0.0%)
26	ba	0.78	0/734	0.60	0/996
27	av	0.51	0/1795	0.61	0/2432
28	at	0.51	1/1992 (0.1%)	0.56	0/2686
29	ar	0.49	0/2109	0.56	0/2852
30	aq	0.42	0/1751	0.55	0/2374
31	ap	0.51	0/1826	0.56	0/2453
32	ao	0.65	1/2119 (0.0%)	0.61	0/2871

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	ai	0.59	0/3273	0.58	0/4412
34	an	0.64	0/2484	0.60	0/3357
35	z	0.73	3/8856 (0.0%)	0.66	5/12020 (0.0%)
36	y	0.44	0/2030	0.58	0/2751
37	x	0.60	0/2075	0.62	0/2825
38	w	0.50	0/1524	0.55	0/2066
39	v	0.66	0/1603	0.65	1/2154 (0.0%)
40	bb	0.53	0/926	0.59	0/1230
41	t	2.02	6/1846 (0.3%)	0.58	0/2511
42	al	0.62	0/2430	0.60	0/3275
43	q	0.65	0/1892	0.59	0/2551
44	p	0.66	0/2047	0.58	0/2762
45	Ca	1.33	9/5233 (0.2%)	0.61	1/7083 (0.0%)
46	g	0.57	0/1580	0.57	1/2113 (0.0%)
47	j	0.61	0/1546	0.67	1/2090 (0.0%)
48	b	0.58	0/1299	0.59	0/1751
49	bd	0.46	0/441	0.66	0/601
50	a	0.75	0/3523	0.61	0/4759
51	bc	0.36	0/1278	0.53	0/1711
52	aa	0.52	0/12863	0.56	0/17416
53	k	0.76	1/1624 (0.1%)	0.66	0/2192
54	be	0.56	0/690	0.65	0/934
55	as	0.66	1/2088 (0.0%)	0.67	1/2844 (0.0%)
56	2	0.98	2/11110 (0.0%)	1.28	84/17276 (0.5%)
56	A	0.69	0/3392	1.11	19/5275 (0.4%)
All	All	0.67	35/179403 (0.0%)	0.66	120/245702 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	u	0	1
6	e	0	2
11	au	0	3
15	af	0	1
17	l	0	2
20	ad	0	3
25	d	0	2
27	av	0	1
29	ar	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	ao	0	2
33	ai	0	1
39	v	0	2
45	Ca	0	2
49	bd	0	2
52	aa	0	1
53	k	0	3
54	be	0	1
All	All	0	30

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Ca	95	TRP	CE3-CZ3	56.27	2.34	1.38
1	u	666	PHE	CE2-CZ	45.16	2.23	1.37
41	t	46	TYR	CD1-CE1	44.28	2.05	1.39
41	t	46	TYR	CD2-CE2	43.84	2.05	1.39
1	u	666	PHE	CD2-CE2	37.86	2.15	1.39
1	u	666	PHE	CE1-CZ	37.63	2.08	1.37
1	u	666	PHE	CD1-CE1	36.40	2.12	1.39
45	Ca	95	TRP	CZ3-CH2	36.20	1.98	1.40
41	t	46	TYR	CE1-CZ	33.09	1.81	1.38
41	t	46	TYR	CE2-CZ	30.77	1.78	1.38
35	z	1071	ARG	CD-NE	29.21	1.96	1.46
45	Ca	95	TRP	CE2-CZ2	29.06	1.89	1.39
45	Ca	95	TRP	CD2-CE2	25.98	1.72	1.41
1	u	666	PHE	CG-CD1	25.09	1.76	1.38
1	u	666	PHE	CG-CD2	24.97	1.76	1.38
41	t	46	TYR	CG-CD1	24.39	1.70	1.39
41	t	46	TYR	CG-CD2	24.24	1.70	1.39
55	as	236	MET	SD-CE	21.16	2.96	1.77
6	e	444	ASP	C-N	18.84	1.67	1.33
6	e	445	GLY	N-CA	18.63	1.74	1.46
45	Ca	95	TRP	CD2-CE3	17.79	1.67	1.40
45	Ca	95	TRP	CZ2-CH2	17.69	1.71	1.37
35	z	1071	ARG	NE-CZ	13.69	1.50	1.33
21	m	70	ARG	C-N	-7.26	1.17	1.34
45	Ca	494	TRP	CB-CG	-6.46	1.38	1.50
35	z	374	TRP	CB-CG	-6.31	1.38	1.50
20	ad	769	TYR	CA-CB	-5.95	1.40	1.53
56	2	77	A	N9-C4	-5.74	1.34	1.37
53	k	98	VAL	CB-CG2	-5.44	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2	140	U	C2-N3	-5.35	1.34	1.37
28	at	125	ARG	C-N	-5.23	1.22	1.34
24	c	147	TRP	CB-CG	5.21	1.59	1.50
32	ao	232	TRP	CB-CG	-5.17	1.41	1.50
45	Ca	501	PHE	CA-C	-5.09	1.39	1.52
45	Ca	577	TRP	CB-CG	-5.02	1.41	1.50

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	z	1071	ARG	CD-NE-CZ	21.92	154.28	123.60
6	e	444	ASP	C-N-CA	20.46	165.26	122.30
55	as	236	MET	CG-SD-CE	17.31	127.90	100.20
35	z	1071	ARG	NE-CZ-NH1	17.25	128.93	120.30
56	2	556	C	C5-C6-N1	8.72	125.36	121.00
56	2	109	A	C8-N9-C4	-8.70	102.32	105.80
6	e	749	PRO	C-N-CA	8.48	142.89	121.70
56	A	493	U	N3-C2-O2	-8.36	116.35	122.20
45	Ca	95	TRP	CE3-CZ3-CH2	-7.98	112.43	121.20
56	A	451	U	N1-C2-O2	7.70	128.19	122.80
56	2	143	U	C5-C6-N1	7.70	126.55	122.70
56	A	499	U	C2-N1-C1’	7.53	126.73	117.70
56	A	493	U	N1-C2-O2	7.48	128.03	122.80
56	2	196	U	C2-N1-C1’	7.46	126.65	117.70
56	2	172	A	C8-N9-C4	-7.33	102.87	105.80
1	u	666	PHE	CB-CG-CD1	-7.31	115.68	120.80
56	2	196	U	N1-C2-O2	7.27	127.89	122.80
56	A	451	U	C2-N1-C1’	7.24	126.38	117.70
35	z	1071	ARG	NE-CZ-NH2	-7.15	116.72	120.30
56	2	69	U	C2-N1-C1’	7.10	126.22	117.70
56	2	147	G	C8-N9-C4	-7.01	103.59	106.40
56	2	188	U	C2-N1-C1’	7.01	126.11	117.70
56	2	172	A	O4’-C1’-N9	7.00	113.80	108.20
56	2	556	C	C2-N1-C1’	6.98	126.48	118.80
56	2	188	U	N1-C2-O2	6.96	127.67	122.80
56	2	162	U	C2-N1-C1’	6.87	125.94	117.70
35	z	1071	ARG	CG-CD-NE	6.81	126.09	111.80
56	A	493	U	C2-N1-C1’	6.79	125.85	117.70
56	2	142	U	C5-C6-N1	6.78	126.09	122.70
56	2	109	A	N7-C8-N9	6.76	117.18	113.80
56	2	170	U	N3-C2-O2	-6.74	117.48	122.20
56	A	467	A	C8-N9-C4	6.59	108.44	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	ad	354	HIS	C-N-CA	-6.58	105.25	121.70
56	2	56	U	C5-C6-N1	6.53	125.97	122.70
56	2	132	G	C8-N9-C4	-6.39	103.84	106.40
56	2	543	G	C4-N9-C1'	6.39	134.80	126.50
56	2	162	U	C6-N1-C1'	-6.29	112.40	121.20
56	A	518	G	N3-C4-N9	6.27	129.76	126.00
56	2	146	U	O4'-C1'-N1	6.26	113.21	108.20
56	2	564	U	C2-N1-C1'	6.23	125.18	117.70
56	2	228	G	C4-N9-C1'	6.22	134.58	126.50
56	2	170	U	C2-N1-C1'	6.20	125.14	117.70
56	2	135	U	N1-C2-O2	6.16	127.11	122.80
56	2	196	U	N3-C2-O2	-6.13	117.91	122.20
56	2	258	U	N1-C2-O2	-6.08	118.54	122.80
56	2	248	A	N1-C6-N6	-6.05	114.97	118.60
56	2	127	G	C4-C5-N7	6.04	113.22	110.80
1	u	666	PHE	CD1-CG-CD2	5.92	126.00	118.30
56	2	75	A	N1-C6-N6	-5.89	115.06	118.60
56	2	228	G	C8-N9-C1'	-5.88	119.36	127.00
56	2	219	G	N3-C4-N9	5.87	129.52	126.00
56	2	162	U	N1-C2-O2	5.84	126.89	122.80
56	2	95	U	C2-N1-C1'	5.81	124.67	117.70
56	2	49	U	C6-N1-C2	5.78	124.47	121.00
56	2	564	U	N1-C2-O2	5.75	126.82	122.80
56	2	543	G	C8-N9-C1'	-5.75	119.53	127.00
56	2	257	C	N3-C2-O2	-5.69	117.92	121.90
56	2	591	A	N7-C8-N9	5.69	116.65	113.80
56	A	451	U	N3-C2-O2	-5.69	118.22	122.20
56	2	340	U	N3-C4-O4	5.69	123.38	119.40
39	v	93	LEU	CA-CB-CG	5.68	128.35	115.30
56	2	23	A	C8-N9-C4	-5.66	103.54	105.80
56	2	596	U	C5-C6-N1	5.66	125.53	122.70
56	2	289	U	C5-C6-N1	5.65	125.53	122.70
56	2	219	G	C8-N9-C1'	-5.61	119.71	127.00
56	2	126	U	C5-C6-N1	5.57	125.48	122.70
56	2	170	U	C6-N1-C2	-5.56	117.67	121.00
47	j	189	LEU	CA-CB-CG	5.53	128.02	115.30
56	2	108	A	N7-C8-N9	5.48	116.54	113.80
56	A	499	U	N1-C2-O2	5.46	126.62	122.80
56	2	219	G	C4-N9-C1'	5.45	133.59	126.50
56	A	467	A	N7-C8-N9	-5.45	111.08	113.80
56	2	587	A	N9-C4-C5	-5.45	103.62	105.80
56	2	163	G	C8-N9-C4	-5.44	104.23	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2	269	A	C4-C5-N7	5.42	113.41	110.70
46	g	96	LEU	CA-CB-CG	-5.42	102.84	115.30
56	2	251	U	C5-C6-N1	5.42	125.41	122.70
56	A	499	U	C6-N1-C1'	-5.40	113.64	121.20
56	2	78	G	C4-N9-C1'	-5.39	119.49	126.50
56	2	66	U	N3-C2-O2	-5.39	118.43	122.20
56	2	264	A	N7-C8-N9	5.36	116.48	113.80
56	2	109	A	N3-C4-C5	-5.35	123.06	126.80
56	2	110	U	C2-N1-C1'	5.34	124.11	117.70
56	A	493	U	C6-N1-C2	-5.33	117.81	121.00
56	2	288	U	C2-N1-C1'	5.32	124.08	117.70
56	A	518	G	C8-N9-C1'	-5.32	120.09	127.00
56	A	500	U	C2-N1-C1'	-5.32	111.32	117.70
56	2	66	U	C2-N1-C1'	5.29	124.05	117.70
56	2	196	U	C6-N1-C1'	-5.29	113.80	121.20
56	2	154	G	N3-C4-C5	-5.28	125.96	128.60
13	aj	15	VAL	C-N-CA	-5.27	108.52	121.70
56	2	556	C	N1-C2-O2	5.27	122.06	118.90
56	2	369	A	C5-C6-N1	5.26	120.33	117.70
56	2	170	U	N1-C2-O2	5.25	126.47	122.80
56	2	119	A	O4'-C1'-N9	5.23	112.39	108.20
25	d	87	LEU	CA-CB-CG	-5.22	103.28	115.30
56	2	269	A	N9-C4-C5	-5.22	103.71	105.80
56	A	451	U	C6-N1-C1'	-5.19	113.94	121.20
56	2	12	C	N3-C4-C5	5.19	123.97	121.90
56	A	518	G	N9-C4-C5	-5.18	103.33	105.40
56	2	219	G	N3-C4-C5	-5.18	126.01	128.60
56	A	500	U	C5-C6-N1	-5.15	120.12	122.70
56	2	51	U	N3-C2-O2	-5.14	118.60	122.20
35	z	400	LEU	CA-CB-CG	-5.14	103.48	115.30
56	2	147	G	N9-C4-C5	5.13	107.45	105.40
56	2	135	U	N3-C2-O2	-5.12	118.62	122.20
56	2	69	U	N3-C2-O2	-5.11	118.62	122.20
56	2	548	G	C6-C5-N7	-5.11	127.33	130.40
56	2	172	A	N7-C8-N9	5.11	116.35	113.80
56	2	141	G	N3-C4-N9	5.10	129.06	126.00
56	2	188	U	C6-N1-C1'	-5.09	114.08	121.20
56	2	69	U	C6-N1-C1'	-5.08	114.08	121.20
56	2	127	G	C5-N7-C8	-5.06	101.77	104.30
56	2	545	A	C6-N1-C2	-5.06	115.56	118.60
56	A	398	U	O4'-C1'-N1	5.05	112.24	108.20
56	2	200	A	C8-N9-C4	5.02	107.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2	137	U	O4'-C1'-N1	5.01	112.21	108.20
56	2	145	A	C8-N9-C4	5.01	107.80	105.80
56	2	591	A	C5-N7-C8	-5.01	101.40	103.90
56	2	12	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	Ca	422	TYR	Peptide
45	Ca	93	PRO	Peptide
52	aa	129	LEU	Peptide
20	ad	520	SER	Peptide
20	ad	725	PRO	Peptide
20	ad	82	ASN	Peptide
15	af	184	VAL	Peptide
33	ai	266	LYS	Peptide
32	ao	132	ARG	Peptide
32	ao	201	TRP	Peptide
29	ar	195	ASP	Peptide
11	au	154	GLN	Peptide
11	au	186	TRP	Peptide
11	au	187	LYS	Peptide
27	av	213	LEU	Peptide
49	bd	42	ASN	Peptide
49	bd	63	ILE	Peptide
54	be	40	TYR	Peptide
25	d	290	HIS	Peptide
25	d	67	LEU	Peptide
6	e	15	ARG	Peptide
6	e	18	THR	Peptide
53	k	123	ARG	Peptide
53	k	136	ASP	Peptide
53	k	150	CYS	Peptide
17	l	448	MET	Peptide
17	l	662	GLY	Peptide
1	u	229	SER	Peptide
39	v	113	ASP	Peptide
39	v	114	THR	Peptide

5.2 Too-close contacts ⓘ

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	u	5597	0	5628	0	0
2	s	1351	0	1315	0	0
3	r	3806	0	3680	0	0
4	n	1169	0	1188	0	0
5	h	1324	0	1304	0	0
6	e	6577	0	6289	0	0
7	az	1292	0	1287	0	0
8	ay	1200	0	1190	0	0
9	ax	1366	0	1342	0	0
10	aw	1338	0	1322	0	0
11	au	2069	0	1936	0	0
12	ak	1865	0	1836	0	0
13	aj	2590	0	2552	0	0
14	ag	4472	0	4434	0	0
15	af	4590	0	4545	0	0
16	ae	4634	0	4582	0	0
17	l	4821	0	4706	0	0
18	ac	8864	0	8621	0	0
19	ab	9094	0	8739	0	0
20	ad	6610	0	6371	0	0
21	m	1940	0	1881	0	0
22	i	2970	0	2976	0	0
23	f	1917	0	1854	0	0
24	c	2169	0	2146	0	0
25	d	3538	0	3515	0	0
26	ba	706	0	645	0	0
27	av	1752	0	1705	0	0
28	at	1946	0	1927	0	0
29	ar	2061	0	2058	0	0
30	aq	1701	0	1658	0	0
31	ap	1796	0	1747	0	0
32	ao	2062	0	2042	0	0
33	ai	3205	0	3206	0	0
34	an	2422	0	2434	0	0
35	z	8630	0	8339	0	0
36	y	1983	0	1989	0	0
37	x	2016	0	1932	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	w	1479	0	1458	0	0
39	v	1567	0	1500	0	0
40	bb	905	0	968	0	0
41	t	1797	0	1752	0	0
42	al	2372	0	2374	0	0
43	q	1840	0	1783	0	0
44	p	1998	0	1965	0	0
45	Ca	5070	0	4897	0	0
46	g	1544	0	1564	0	0
47	j	1501	0	1517	0	0
48	b	1271	0	1263	0	0
49	bd	430	0	448	0	0
50	a	3436	0	3427	0	0
51	bc	1247	0	1249	0	0
52	aa	12549	0	12207	0	0
53	k	1577	0	1587	0	0
54	be	665	0	668	0	0
55	as	2024	0	2025	0	0
56	2	9932	0	4972	313	0
56	A	3030	0	1513	72	0
57	r	32	0	11	0	0
58	r	1	0	0	0	0
59	aj	29	0	10	0	0
60	aa	1	0	0	0	0
60	at	2	0	0	0	0
60	y	1	0	0	0	0
All	All	173743	0	164079	383	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 32.

All (383) 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)
56:2:590:A:H2’	56:2:591:A:C8	2.07	0.90
56:2:125:U:O2	56:2:127:G:N2	2.06	0.89
56:A:517:U:OP1	56:A:519:U:N3	2.04	0.89
56:2:337:U:H5’	56:2:356:U:H4’	1.54	0.89
56:2:236:G:HO2’	56:2:251:U:HO2’	1.20	0.87
56:A:469:A:N3	56:A:470:G:N2	2.21	0.87
56:2:233:C:N4	56:2:245:G:OP2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:551:G:H1	56:2:585:U:H3	1.17	0.86
56:2:2:A:H1’	56:2:3:A:H5”	1.57	0.86
56:2:49:U:O2	56:2:53:A:N6	2.09	0.85
56:2:60:A:O2’	56:2:154:G:OP1	1.95	0.85
56:2:324:A:O2’	56:2:325:A:O5’	1.96	0.84
56:A:443:U:O4	56:A:446:C:N4	2.10	0.83
56:2:107:U:H2’	56:2:108:A:C8	2.12	0.83
56:2:108:A:H2’	56:2:109:A:H8	1.44	0.81
56:2:108:A:H2’	56:2:109:A:C8	2.17	0.80
56:2:28:U:O2	56:2:239:G:N2	2.16	0.79
56:2:289:U:H3’	56:2:290:G:H21	1.46	0.78
56:2:319:U:H2’	56:2:320:A:H8	1.47	0.78
56:2:143:U:O2	56:2:271:A:N6	2.13	0.78
56:2:340:U:H4’	56:2:341:A:H2’	1.64	0.77
56:2:132:G:H2’	56:2:133:A:H8	1.49	0.77
56:2:96:U:O2	56:2:132:G:N2	2.17	0.76
56:2:394:A:N7	56:2:539:A:N6	2.32	0.76
56:2:134:U:O2’	56:2:136:G:OP1	2.04	0.76
56:2:107:U:H2’	56:2:108:A:H8	1.48	0.75
56:2:583:A:H1’	56:2:602:A:H2’	1.68	0.75
56:2:359:G:OP1	56:2:360:C:N4	2.20	0.75
56:2:564:U:H3	56:2:570:A:N6	1.84	0.75
56:2:3:A:H3’	56:2:4:A:H8	1.50	0.75
56:2:87:U:O2’	56:2:88:A:OP1	2.03	0.74
56:2:200:A:O2’	56:2:201:A:OP1	2.05	0.73
56:2:172:A:H3’	56:2:173:A:N3	2.05	0.72
56:2:232:G:N1	56:2:248:A:OP1	2.14	0.72
56:2:590:A:H2’	56:2:591:A:H8	1.55	0.71
56:2:320:A:H3’	56:2:321:A:C8	2.25	0.71
56:2:107:U:O2’	56:2:108:A:H5’	1.89	0.71
56:2:132:G:H2’	56:2:133:A:C8	2.25	0.70
56:2:194:A:H2’	56:2:195:A:H2’	1.72	0.70
56:A:445:C:H5’	56:A:480:C:H41	1.57	0.70
56:2:263:A:O2’	56:2:264:A:O4’	2.09	0.70
56:2:3:A:H3’	56:2:4:A:C8	2.29	0.67
56:2:73:U:H1’	56:2:74:G:H3’	1.75	0.67
56:2:185:A:OP1	56:2:186:U:O2’	2.08	0.67
56:2:320:A:OP2	56:2:321:A:N6	2.27	0.67
56:2:132:G:C2	56:2:133:A:C5	2.83	0.67
56:2:48:U:H2’	56:2:49:U:H5’	1.76	0.66
56:2:96:U:H3	56:2:132:G:H1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:287:A:N7	56:2:322:A:N6	2.44	0.66
56:2:148:C:O2'	56:2:270:U:OP1	2.15	0.65
56:2:260:U:H4'	56:2:261:U:H5'	1.79	0.65
56:A:522:A:H2'	56:A:523:U:O4'	1.97	0.65
56:2:286:A:H1'	56:2:287:A:C8	2.32	0.65
56:2:121:A:H8	56:2:121:A:OP2	1.78	0.64
56:2:17:G:O2'	56:2:18:U:OP2	2.16	0.64
56:2:253:U:C2	56:2:254:A:C8	2.87	0.63
56:2:222:A:H2'	56:2:223:G:C8	2.33	0.63
56:2:2:A:O2'	56:2:3:A:OP2	2.14	0.63
56:2:210:A:N3	56:2:211:A:N6	2.46	0.63
56:2:142:U:O2	56:2:147:G:O6	2.17	0.62
56:2:554:C:H1'	56:2:583:A:C2	2.34	0.62
56:2:75:A:C6	56:2:76:A:C5	2.86	0.62
56:2:293:A:H2'	56:2:294:A:C8	2.35	0.62
56:2:319:U:H2'	56:2:320:A:C8	2.33	0.62
56:2:41:A:H2'	56:2:42:A:O4'	2.00	0.61
56:2:73:U:N3	56:2:75:A:N7	2.47	0.61
56:A:402:U:H2'	56:A:403:U:C6	2.35	0.61
56:A:468:A:N3	56:A:470:G:N1	2.41	0.61
56:2:35:U:H3'	56:2:36:U:H5"	1.83	0.61
56:2:219:G:C2	56:2:258:U:O2	2.54	0.60
56:A:405:A:C5	56:A:524:A:C6	2.89	0.60
56:2:66:U:H4'	56:2:68:A:N7	2.16	0.60
56:2:163:G:O2'	56:2:165:A:N6	2.35	0.60
56:A:451:U:H3'	56:A:470:G:N7	2.17	0.59
56:A:466:G:O2'	56:A:467:A:OP2	2.19	0.59
56:2:48:U:N3	56:2:55:U:O4	2.17	0.59
56:2:235:A:N1	56:2:251:U:H1'	2.18	0.59
56:2:235:A:C2	56:2:251:U:H1'	2.38	0.59
56:A:400:U:O2'	56:A:527:A:N6	2.36	0.59
56:2:68:A:H2'	56:2:136:G:O6	2.03	0.59
56:A:534:A:O2'	56:A:535:U:OP2	2.15	0.59
56:A:537:A:H2'	56:2:538:A:P	2.43	0.59
56:2:125:U:O5'	56:2:127:G:H5'	2.03	0.58
56:2:179:U:O2'	56:2:180:A:H5"	2.03	0.58
56:2:4:A:H4'	56:2:5:U:C5	2.39	0.58
56:2:293:A:H1'	56:2:315:A:H5"	1.86	0.58
56:2:87:U:HO2'	56:2:88:A:P	2.25	0.58
56:2:140:U:O2'	56:2:141:G:H5'	2.04	0.58
56:2:21:G:O6	56:2:383:U:O4	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:543:G:C8	56:2:587:A:N6	2.72	0.57
56:2:232:G:H22	56:2:248:A:P	2.27	0.57
56:2:362:A:H2'	56:2:363:A:O4'	2.03	0.57
56:2:75:A:C5	56:2:164:G:C2	2.93	0.57
56:2:75:A:C6	56:2:164:G:N2	2.73	0.57
56:2:123:U:H2'	56:2:124:U:O4'	2.04	0.57
56:2:217:U:H3'	56:2:218:A:H8	1.70	0.57
56:2:234:C:N4	56:2:244:G:O2'	2.34	0.56
56:2:189:A:O2'	56:2:190:U:O4'	2.22	0.56
56:2:555:A:O2'	56:2:601:A:O2'	2.19	0.56
56:A:444:A:O2'	56:A:481:A:N7	2.28	0.56
56:2:76:A:H2'	56:2:77:A:C8	2.41	0.56
56:2:263:A:O2'	56:2:264:A:H8	1.87	0.56
56:2:293:A:O2'	56:2:294:A:O5'	2.24	0.56
56:2:590:A:C2	56:2:613:U:C2	2.94	0.56
56:A:530:A:H2'	56:A:531:G:C8	2.41	0.56
56:2:141:G:H2'	56:2:142:U:C6	2.41	0.56
56:2:332:U:O2'	56:2:333:U:H5'	2.06	0.56
56:2:555:A:HO2'	56:2:601:A:HO2'	1.54	0.56
56:2:50:A:O2'	56:2:51:U:O5'	2.22	0.56
56:2:540:A:H2'	56:2:541:A:C8	2.41	0.56
56:2:575:U:HO2'	56:2:576:A:H8	1.53	0.56
56:A:461:A:C2	56:A:463:A:H2'	2.41	0.55
56:A:472:G:H2'	56:A:473:U:H6	1.70	0.55
56:2:142:U:C2	56:2:147:G:O6	2.58	0.55
56:2:263:A:HO2'	56:2:264:A:H8	1.55	0.55
56:2:287:A:C4	56:2:288:U:C5	2.94	0.55
56:2:200:A:HO2'	56:2:201:A:P	2.30	0.55
56:2:381:U:H2'	56:2:382:A:C8	2.42	0.55
56:A:397:U:OP2	56:A:398:U:H5'	2.07	0.54
56:A:436:U:H2'	56:A:437:U:C6	2.42	0.54
56:2:228:G:H3'	56:2:229:G:H8	1.71	0.54
56:A:444:A:H8	56:A:483:A:OP2	1.89	0.54
56:2:299:U:O2'	56:2:300:G:O4'	2.24	0.54
56:2:332:U:H2'	56:2:333:U:C6	2.43	0.54
56:2:21:G:O6	56:2:383:U:C4	2.60	0.54
56:2:594:U:C2	56:2:595:A:C8	2.96	0.54
56:2:68:A:C2	56:2:136:G:N7	2.75	0.53
56:2:218:A:H3'	56:2:219:G:H8	1.74	0.53
56:2:75:A:N6	56:2:76:A:C6	2.76	0.53
56:2:186:U:H5'	56:2:187:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A:461:A:N6	56:A:463:A:N7	2.56	0.53
56:2:130:U:C2	56:2:131:A:C8	2.96	0.53
56:2:554:C:H2’	56:2:555:A:C8	2.43	0.53
56:A:419:U:H2’	56:A:420:A:O4’	2.08	0.53
56:2:32:A:H2’	56:2:33:A:O4’	2.09	0.53
56:2:103:U:O2’	56:2:129:U:O2’	2.24	0.53
56:2:231:U:H3’	56:2:232:G:C8	2.43	0.53
56:2:568:A:H2’	56:2:569:U:C5	2.43	0.53
56:A:536:U:O2’	56:A:537:A:N7	2.41	0.52
56:2:43:A:C8	56:2:44:U:H5	2.28	0.52
56:2:77:A:OP2	56:2:78:G:O2’	2.16	0.52
56:2:580:U:C4	56:2:581:G:N7	2.77	0.52
56:2:135:U:C2	56:2:154:G:O6	2.62	0.52
56:2:353:G:H2’	56:2:354:U:O4’	2.10	0.52
56:2:564:U:H3	56:2:570:A:H61	1.55	0.52
56:2:13:A:HO2’	56:2:144:A:HO2’	1.54	0.52
56:2:125:U:O2	56:2:127:G:C2	2.63	0.52
56:2:111:A:N1	56:2:114:A:N6	2.58	0.52
56:2:254:A:H2’	56:2:255:U:O4’	2.09	0.52
56:2:164:G:C2	56:2:165:A:C2	2.98	0.52
56:2:302:U:H2’	56:2:303:U:C6	2.45	0.52
56:2:567:A:H3’	56:2:570:A:O2’	2.10	0.52
56:2:596:U:O5’	56:2:596:U:H6	1.93	0.52
56:2:551:G:O6	56:2:585:U:O4	2.28	0.51
56:A:453:A:H2’	56:A:454:G:O4’	2.09	0.51
56:2:46:U:C4	56:2:47:U:C4	2.98	0.51
56:2:337:U:C5’	56:2:356:U:H4’	2.34	0.51
56:2:355:A:H5”	56:2:356:U:H5’	1.93	0.51
56:2:243:C:H1’	56:2:250:U:C2	2.46	0.51
56:A:522:A:H8	56:A:522:A:O5’	1.94	0.51
56:2:559:A:H3’	56:2:560:U:H5”	1.91	0.51
56:A:403:U:H2’	56:A:404:U:C6	2.46	0.51
56:2:175:A:N1	56:2:180:A:N6	2.59	0.51
56:2:333:U:O2’	56:2:334:U:H5’	2.10	0.51
56:A:530:A:C6	56:A:531:G:C6	2.99	0.51
56:2:320:A:O2’	56:2:321:A:H5’	2.11	0.51
56:2:227:U:C2	56:2:228:G:C8	2.99	0.51
56:A:460:U:C2	56:A:461:A:N6	2.78	0.50
56:A:402:U:H2’	56:A:403:U:H6	1.77	0.50
56:2:284:U:H4’	56:2:285:A:O5’	2.11	0.50
56:2:594:U:N3	56:2:595:A:N7	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A:405:A:O2'	56:A:406:U:H5'	2.11	0.50
56:2:356:U:H2'	56:2:356:U:OP2	2.10	0.50
56:2:226:A:O2'	56:2:227:U:O4'	2.27	0.50
56:2:98:A:H2'	56:2:99:G:C8	2.47	0.49
56:2:141:G:C2	56:2:149:U:H1'	2.47	0.49
56:A:516:G:H8	56:A:516:G:OP2	1.95	0.49
56:A:453:A:N6	56:A:469:A:OP1	2.45	0.49
56:2:13:A:H2'	56:2:14:A:O4'	2.12	0.49
56:2:186:U:C2	56:2:187:A:N1	2.79	0.49
56:2:226:A:O2'	56:2:227:U:O5'	2.31	0.49
56:2:263:A:C4	56:2:264:A:C8	3.01	0.49
56:A:445:C:H5'	56:A:480:C:N4	2.27	0.49
56:A:461:A:C6	56:A:463:A:C5	3.01	0.49
56:2:42:A:H61	56:2:173:A:H2'	1.77	0.49
56:2:114:A:C6	56:2:117:U:C4	3.01	0.49
56:2:75:A:C5	56:2:76:A:C5	3.01	0.49
56:2:287:A:H62	56:2:322:A:H61	1.61	0.49
56:2:303:U:H2'	56:2:304:U:C6	2.48	0.49
56:A:441:G:N2	56:A:478:A:O4'	2.46	0.48
56:2:74:G:HO2'	56:2:75:A:P	2.36	0.48
56:2:230:A:H5'	56:2:231:U:OP2	2.12	0.48
56:2:283:U:C4	56:2:328:U:O4	2.66	0.48
56:2:73:U:H6	56:2:74:G:H21	1.60	0.48
56:2:583:A:N6	56:2:584:G:O6	2.46	0.48
56:2:110:U:H5'	56:2:111:A:OP2	2.13	0.48
56:2:42:A:H5'	56:2:43:A:OP2	2.14	0.48
56:2:313:A:H8	56:2:313:A:OP2	1.95	0.48
56:2:161:G:H4'	56:2:162:U:H5	1.79	0.48
56:2:228:G:C4	56:2:229:G:C8	3.02	0.48
56:A:424:U:OP1	56:A:425:A:H5"	2.14	0.48
56:2:129:U:H2'	56:2:130:U:H5'	1.95	0.48
56:A:448:U:H3'	56:A:449:G:N3	2.29	0.48
56:2:161:G:H5'	56:2:162:U:OP1	2.14	0.48
56:2:542:G:O2'	56:2:543:G:H5'	2.14	0.48
56:A:460:U:O2	56:A:461:A:N6	2.46	0.47
56:2:131:A:C2	56:2:132:G:C8	3.03	0.47
56:2:290:G:N7	56:2:318:A:N6	2.62	0.47
56:2:558:A:H2'	56:2:559:A:O4'	2.13	0.47
56:2:75:A:C6	56:2:76:A:C4	3.02	0.47
56:2:320:A:H2'	56:2:321:A:O4'	2.14	0.47
56:2:145:A:H61	56:2:271:A:C2'	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:294:A:O2'	56:2:313:A:N3	2.39	0.47
56:2:111:A:N3	56:2:113:U:H2'	2.29	0.47
56:2:219:G:N2	56:2:258:U:O2	2.48	0.47
56:2:233:C:H4'	56:2:234:C:C5'	2.45	0.47
56:A:397:U:H3'	56:A:398:U:H5'	1.95	0.47
56:2:166:A:C6	56:2:168:A:C2	3.03	0.47
56:2:288:U:C2	56:2:289:U:C5	3.02	0.47
56:2:365:A:H4'	56:2:366:U:C2	2.49	0.47
56:2:386:A:H2'	56:2:387:U:O4'	2.15	0.47
56:2:60:A:H4'	56:2:154:G:H5"	1.97	0.47
56:2:217:U:H3'	56:2:218:A:C8	2.50	0.47
56:2:294:A:OP2	56:2:294:A:H8	1.98	0.47
56:2:28:U:H1'	56:2:239:G:N3	2.30	0.47
56:2:31:U:O2	56:2:142:U:H4'	2.15	0.47
56:2:76:A:C6	56:2:77:A:C6	3.03	0.47
56:2:135:U:H5	56:2:153:A:N7	2.13	0.47
56:2:253:U:N3	56:2:254:A:N7	2.63	0.47
56:2:229:G:C4	56:2:230:A:C8	3.03	0.47
56:2:555:A:H2'	56:2:556:C:C6	2.50	0.47
56:A:453:A:H8	56:A:453:A:O5'	1.98	0.47
56:2:331:A:H2'	56:2:332:U:C6	2.50	0.46
56:A:430:U:H5'	56:A:433:U:H5"	1.97	0.46
56:A:433:U:OP1	56:A:433:U:H3'	2.14	0.46
56:2:40:U:H4'	56:2:41:A:OP1	2.14	0.46
56:2:107:U:HO2'	56:2:108:A:H5'	1.78	0.46
56:2:219:G:C2	56:2:220:U:C2	3.03	0.46
56:2:320:A:C2'	56:2:321:A:H5'	2.45	0.46
56:A:485:U:H3'	56:A:486:C:C5	2.51	0.46
56:2:198:A:H8	56:2:198:A:OP1	1.99	0.46
56:2:594:U:H2'	56:2:595:A:H8	1.79	0.46
56:A:414:A:O2'	56:A:484:A:OP1	2.33	0.46
56:2:324:A:HO2'	56:2:325:A:P	2.36	0.46
56:2:594:U:H2'	56:2:595:A:C8	2.51	0.46
56:2:75:A:C4	56:2:76:A:C8	3.04	0.46
56:2:95:U:H6	56:2:95:U:H2'	1.54	0.46
56:2:97:U:O2'	56:2:98:A:H5'	2.15	0.46
56:2:325:A:H2'	56:2:326:U:C2	2.51	0.46
56:2:40:U:H1'	56:2:41:A:O4'	2.16	0.46
56:2:152:U:H3'	56:2:153:A:H8	1.81	0.46
56:2:168:A:C8	56:2:168:A:H3'	2.51	0.46
56:2:220:U:H2'	56:2:226:A:N7	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:299:U:HO2'	56:2:300:G:C1'	2.29	0.46
56:2:566:U:H4'	56:2:567:A:OP1	2.16	0.46
56:2:186:U:H4'	56:2:187:A:O4'	2.16	0.46
56:2:285:A:H2'	56:2:285:A:N3	2.30	0.46
56:2:38:U:H4'	56:2:39:U:OP1	2.14	0.46
56:2:222:A:H3'	56:2:223:G:H2'	1.98	0.46
56:2:275:U:H6	56:2:275:U:H5'	1.81	0.46
56:2:107:U:O2	56:2:121:A:O2'	2.18	0.45
56:2:294:A:H4'	56:2:313:A:O2'	2.16	0.45
56:2:313:A:H2'	56:2:314:A:O4'	2.16	0.45
56:2:324:A:H2'	56:2:325:A:C8	2.52	0.45
56:A:498:U:H1'	56:A:499:U:C4	2.52	0.45
56:2:162:U:H5"	56:2:163:G:OP2	2.17	0.45
56:2:228:G:C5	56:2:229:G:C8	3.03	0.45
56:2:263:A:N3	56:2:264:A:C8	2.84	0.45
56:2:230:A:H2'	56:2:230:A:N3	2.32	0.45
56:A:444:A:C6	56:A:483:A:C2	3.05	0.45
56:2:46:U:H2'	56:2:47:U:O4'	2.17	0.45
56:2:161:G:H4'	56:2:162:U:C5	2.51	0.45
56:A:460:U:O2'	56:A:461:A:OP2	2.28	0.45
56:A:486:C:OP1	56:A:487:A:O2'	2.27	0.45
56:A:518:G:H4'	56:A:519:U:H5"	1.98	0.45
56:2:141:G:N2	56:2:149:U:H1'	2.31	0.45
56:2:189:A:H2'	56:2:190:U:C6	2.52	0.45
56:A:460:U:C2	56:A:461:A:C6	3.05	0.44
56:A:467:A:HO2'	56:A:468:A:P	2.41	0.44
56:2:208:U:O2'	56:2:209:U:H2'	2.17	0.44
56:2:239:G:H8	56:2:239:G:O5'	2.00	0.44
56:2:377:U:O4	56:2:572:A:H1'	2.18	0.44
56:2:170:U:H3'	56:2:170:U:O2	2.17	0.44
56:2:275:U:H5'	56:2:275:U:C6	2.52	0.44
56:2:359:G:H5"	56:2:360:C:C4	2.53	0.44
56:A:424:U:OP1	56:A:425:A:H2'	2.18	0.44
56:2:205:A:HO2'	56:2:206:A:P	2.40	0.44
56:2:312:A:O2'	56:2:313:A:N7	2.50	0.44
56:A:461:A:N6	56:A:463:A:C5	2.86	0.44
56:2:544:U:C2	56:2:585:U:H1'	2.52	0.44
56:2:553:C:O2'	56:2:554:C:H5'	2.17	0.44
56:A:472:G:H2'	56:A:473:U:C6	2.52	0.44
56:2:58:A:H62	56:2:165:A:H62	1.66	0.44
56:2:65:U:O4	56:2:135:U:H5"	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:108:A:C6	56:2:119:A:C2	3.06	0.44
56:2:354:U:O5’	56:2:354:U:H6	2.00	0.44
56:2:186:U:O4’	56:2:187:A:C4	2.71	0.44
56:2:262:A:O5’	56:2:263:A:H5”	2.18	0.44
56:A:451:U:O2’	56:A:471:U:O4	2.35	0.43
56:2:578:C:H2’	56:2:579:G:O4’	2.17	0.43
56:2:592:U:H2’	56:2:593:A:H8	1.83	0.43
56:2:130:U:H2’	56:2:131:A:O4’	2.18	0.43
56:2:152:U:H2’	56:2:153:A:C1’	2.48	0.43
56:2:229:G:H2’	56:2:230:A:C8	2.51	0.43
56:A:446:C:N4	56:A:478:A:C2	2.86	0.43
56:2:205:A:O2’	56:2:206:A:OP2	2.31	0.43
56:A:521:G:H2’	56:A:522:A:O4’	2.19	0.43
56:2:51:U:OP2	56:2:51:U:C2	2.72	0.43
56:2:318:A:H2’	56:2:318:A:N3	2.33	0.43
56:2:46:U:O2	56:2:176:A:H2	2.01	0.43
56:A:450:A:H2	56:A:475:A:N7	2.17	0.43
56:A:459:A:H4’	56:A:460:U:OP1	2.18	0.43
56:A:493:U:O2	56:A:493:U:H2’	2.19	0.43
56:2:591:A:H2’	56:2:592:U:H6	1.84	0.43
56:2:36:U:H1’	56:2:37:U:C2	2.54	0.43
56:2:125:U:O5’	56:2:126:U:H3’	2.18	0.43
56:2:228:G:C6	56:2:229:G:C5	3.06	0.43
56:2:294:A:H2’	56:2:295:G:C4	2.54	0.43
56:2:359:G:O2’	56:2:360:C:H5’	2.18	0.43
56:2:180:A:H8	56:2:180:A:O5’	2.01	0.43
56:2:227:U:N3	56:2:228:G:N7	2.67	0.43
56:2:29:A:H2’	56:2:29:A:N3	2.34	0.42
56:2:75:A:C5	56:2:76:A:N7	2.86	0.42
56:A:403:U:H2’	56:A:404:U:H6	1.81	0.42
56:2:132:G:N1	56:2:133:A:N6	2.68	0.42
56:2:247:A:H2’	56:2:247:A:N3	2.35	0.42
56:2:226:A:C2	56:2:256:G:N1	2.87	0.42
56:2:319:U:C5	56:2:321:A:N1	2.88	0.42
56:2:388:U:C4	56:2:543:G:N2	2.87	0.42
56:A:537:A:H2’	56:2:538:A:OP2	2.19	0.42
56:2:200:A:O2’	56:2:201:A:P	2.75	0.42
56:2:269:A:H2’	56:2:270:U:O4’	2.19	0.42
56:A:488:A:HO2’	56:A:489:A:P	2.42	0.42
56:2:128:A:H2’	56:2:129:U:H6	1.84	0.42
56:2:185:A:C8	56:2:185:A:H3’	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2:310:A:N3	56:2:310:A:H2’	2.35	0.42
56:2:171:A:H5’	56:2:172:A:OP2	2.20	0.42
56:2:321:A:H2’	56:2:322:A:C8	2.55	0.42
56:2:382:A:H8	56:2:382:A:O5’	2.02	0.42
56:A:461:A:N1	56:A:463:A:H2’	2.35	0.42
56:A:513:U:O2’	56:A:514:A:H2’	2.20	0.42
56:A:405:A:C6	56:A:524:A:C6	3.08	0.41
56:2:71:U:O2’	56:2:88:A:H1’	2.20	0.41
56:2:130:U:H2’	56:2:131:A:H8	1.85	0.41
56:2:287:A:H3’	56:2:288:U:H5	1.85	0.41
56:2:68:A:H5”	56:2:69:U:OP2	2.20	0.41
56:2:86:G:N3	56:2:86:G:H2’	2.35	0.41
56:2:132:G:C2	56:2:133:A:C6	3.08	0.41
56:2:254:A:C2	56:2:255:U:C2	3.08	0.41
56:2:287:A:H2’	56:2:288:U:C6	2.55	0.41
56:2:39:U:OP2	56:2:39:U:H6	2.03	0.41
56:2:287:A:N6	56:2:322:A:H61	2.18	0.41
56:2:308:C:H2’	56:2:309:A:C8	2.55	0.41
56:2:544:U:C4	56:2:585:U:H4’	2.55	0.41
56:2:593:A:C6	56:2:594:U:C4	3.08	0.41
56:2:27:A:C2	56:2:28:U:C6	3.09	0.41
56:2:107:U:O5’	56:2:107:U:H6	2.03	0.41
56:2:112:A:N3	56:2:112:A:H2’	2.35	0.41
56:2:324:A:H2’	56:2:325:A:C5	2.55	0.41
56:A:518:G:N3	56:A:518:G:H2’	2.35	0.41
56:A:534:A:HO2’	56:A:535:U:P	2.40	0.41
56:2:317:U:H6	56:2:317:U:H2’	1.71	0.41
56:2:92:A:H2’	56:2:93:A:C8	2.56	0.41
56:2:238:C:O2’	56:2:240:U:OP2	2.24	0.41
56:2:321:A:H2’	56:2:322:A:N7	2.36	0.41
56:A:448:U:H5”	56:A:449:G:N2	2.36	0.41
56:2:149:U:H6	56:2:149:U:O5’	2.04	0.41
56:2:230:A:C4	56:2:231:U:C5	3.09	0.41
56:2:243:C:H4’	56:2:250:U:C4	2.55	0.41
56:2:555:A:H2	56:2:601:A:N3	2.19	0.41
56:2:22:U:H2’	56:2:23:A:C8	2.56	0.41
56:2:571:A:H2’	56:2:572:A:C8	2.57	0.41
56:2:280:A:N3	56:2:363:A:H2’	2.37	0.40
56:A:467:A:O2’	56:A:468:A:O5’	2.30	0.40
56:2:221:C:H5’	56:2:249:U:H2’	2.03	0.40
56:2:283:U:OP2	56:2:283:U:H2’	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A:423:A:O2'	56:A:424:U:H5'	2.21	0.40
56:2:42:A:N6	56:2:173:A:C4	2.89	0.40
56:2:570:A:H5"	56:2:571:A:OP2	2.21	0.40
56:2:302:U:H2'	56:2:303:U:H6	1.87	0.40
56:A:415:U:C2	56:A:482:U:O4	2.75	0.40
56:2:72:U:H5'	56:2:88:A:O4'	2.21	0.40
56:2:321:A:OP2	56:2:321:A:H8	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	693/874 (79%)	638 (92%)	55 (8%)	0	100	100
2	s	163/180 (91%)	138 (85%)	23 (14%)	2 (1%)	13	50
3	r	461/500 (92%)	408 (88%)	53 (12%)	0	100	100
4	n	140/172 (81%)	122 (87%)	18 (13%)	0	100	100
5	h	155/166 (93%)	143 (92%)	12 (8%)	0	100	100
6	e	808/818 (99%)	712 (88%)	94 (12%)	2 (0%)	47	81
7	az	152/163 (93%)	138 (91%)	14 (9%)	0	100	100
8	ay	139/218 (64%)	127 (91%)	11 (8%)	1 (1%)	22	61
9	ax	159/172 (92%)	148 (93%)	10 (6%)	1 (1%)	25	64
10	aw	158/186 (85%)	135 (85%)	23 (15%)	0	100	100
11	au	237/247 (96%)	205 (86%)	31 (13%)	1 (0%)	34	72
12	ak	224/314 (71%)	205 (92%)	19 (8%)	0	100	100
13	aj	313/396 (79%)	274 (88%)	38 (12%)	1 (0%)	41	75
14	ag	544/581 (94%)	500 (92%)	43 (8%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	af	552/677 (82%)	505 (92%)	46 (8%)	1 (0%)	47	81
16	ae	570/678 (84%)	518 (91%)	52 (9%)	0	100	100
17	l	580/714 (81%)	520 (90%)	60 (10%)	0	100	100
18	ac	1123/1152 (98%)	1022 (91%)	101 (9%)	0	100	100
19	ab	1108/1175 (94%)	994 (90%)	113 (10%)	1 (0%)	51	84
20	ad	799/810 (99%)	692 (87%)	102 (13%)	5 (1%)	25	64
21	m	230/319 (72%)	201 (87%)	29 (13%)	0	100	100
22	i	358/429 (83%)	306 (86%)	51 (14%)	1 (0%)	41	75
23	f	229/325 (70%)	196 (86%)	33 (14%)	0	100	100
24	c	259/285 (91%)	228 (88%)	31 (12%)	0	100	100
25	d	443/445 (100%)	398 (90%)	44 (10%)	1 (0%)	47	81
26	ba	81/217 (37%)	68 (84%)	13 (16%)	0	100	100
27	av	211/237 (89%)	174 (82%)	35 (17%)	2 (1%)	17	56
28	at	240/259 (93%)	201 (84%)	38 (16%)	1 (0%)	34	72
29	ar	253/268 (94%)	220 (87%)	33 (13%)	0	100	100
30	aq	196/299 (66%)	177 (90%)	19 (10%)	0	100	100
31	ap	220/277 (79%)	196 (89%)	24 (11%)	0	100	100
32	ao	248/283 (88%)	209 (84%)	39 (16%)	0	100	100
33	ai	388/410 (95%)	333 (86%)	55 (14%)	0	100	100
34	an	291/293 (99%)	248 (85%)	41 (14%)	2 (1%)	22	61
35	z	1067/1181 (90%)	901 (84%)	163 (15%)	3 (0%)	41	75
36	y	249/449 (56%)	196 (79%)	51 (20%)	2 (1%)	19	58
37	x	250/345 (72%)	213 (85%)	36 (14%)	1 (0%)	34	72
38	w	173/186 (93%)	150 (87%)	22 (13%)	1 (1%)	25	64
39	v	194/215 (90%)	153 (79%)	37 (19%)	4 (2%)	7	38
40	bb	108/238 (45%)	95 (88%)	12 (11%)	1 (1%)	17	56
41	t	224/256 (88%)	193 (86%)	30 (13%)	1 (0%)	34	72
42	al	290/308 (94%)	257 (89%)	32 (11%)	1 (0%)	41	75
43	q	212/442 (48%)	185 (87%)	26 (12%)	1 (0%)	29	68
44	p	236/308 (77%)	206 (87%)	30 (13%)	0	100	100
45	Ca	590/603 (98%)	509 (86%)	80 (14%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	g	182/193 (94%)	163 (90%)	19 (10%)	0	100	100
47	j	178/189 (94%)	140 (79%)	38 (21%)	0	100	100
48	b	146/160 (91%)	123 (84%)	23 (16%)	0	100	100
49	bd	48/90 (53%)	41 (85%)	7 (15%)	0	100	100
50	a	423/434 (98%)	363 (86%)	59 (14%)	1 (0%)	47	81
51	bc	149/376 (40%)	138 (93%)	11 (7%)	0	100	100
52	aa	1554/1827 (85%)	1363 (88%)	186 (12%)	5 (0%)	41	75
53	k	188/309 (61%)	156 (83%)	32 (17%)	0	100	100
54	be	77/82 (94%)	67 (87%)	9 (12%)	1 (1%)	12	48
55	as	250/261 (96%)	211 (84%)	39 (16%)	0	100	100
All	All	19513/22991 (85%)	17122 (88%)	2345 (12%)	46 (0%)	50	81

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	be	41	ILE
13	aj	36	GLN
37	x	178	SER
39	v	94	THR
2	s	42	GLN
6	e	104	ASN
8	ay	90	GLY
34	an	15	LEU
35	z	569	TYR
45	Ca	349	PHE
20	ad	347	GLU
22	i	240	LEU
36	y	55	HIS
39	v	93	LEU
52	aa	123	ARG
14	ag	138	SER
15	af	185	ASP
19	ab	990	ALA
20	ad	521	LYS
20	ad	702	ASP
34	an	210	GLN
39	v	115	CYS
41	t	153	HIS

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Mol	Chain	Res	Type
43	q	34	PRO
50	a	37	SER
52	aa	220	ARG
2	s	73	MET
9	ax	157	PRO
20	ad	249	PRO
25	d	68	PRO
27	av	146	ASP
35	z	910	LEU
52	aa	107	TYR
11	au	189	PRO
52	aa	782	PRO
52	aa	1613	PRO
6	e	196	GLY
39	v	211	LEU
40	bb	141	GLY
27	av	214	ALA
28	at	179	GLY
42	al	156	GLY
20	ad	798	ILE
35	z	163	PRO
36	y	176	PRO
38	w	135	ILE

5.3.2 Protein sidechains ⓘ

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	u	613/762 (80%)	562 (92%)	51 (8%)	11	40
2	s	144/157 (92%)	136 (94%)	8 (6%)	21	54
3	r	413/443 (93%)	381 (92%)	32 (8%)	13	42
4	n	127/152 (84%)	115 (91%)	12 (9%)	8	35
5	h	142/150 (95%)	130 (92%)	12 (8%)	10	39
6	e	712/719 (99%)	652 (92%)	60 (8%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	az	136/144 (94%)	131 (96%)	5 (4%)	34	65
8	ay	126/195 (65%)	114 (90%)	12 (10%)	8	34
9	ax	149/158 (94%)	136 (91%)	13 (9%)	10	38
10	aw	144/164 (88%)	134 (93%)	10 (7%)	15	47
11	au	220/228 (96%)	200 (91%)	20 (9%)	9	36
12	ak	197/257 (77%)	182 (92%)	15 (8%)	13	43
13	aj	280/351 (80%)	264 (94%)	16 (6%)	20	53
14	ag	477/502 (95%)	443 (93%)	34 (7%)	14	46
15	af	490/583 (84%)	447 (91%)	43 (9%)	10	38
16	ae	492/567 (87%)	462 (94%)	30 (6%)	18	51
17	l	514/606 (85%)	467 (91%)	47 (9%)	9	36
18	ac	934/957 (98%)	870 (93%)	64 (7%)	15	47
19	ab	954/1011 (94%)	886 (93%)	68 (7%)	14	46
20	ad	703/712 (99%)	631 (90%)	72 (10%)	7	32
21	m	202/278 (73%)	186 (92%)	16 (8%)	12	41
22	i	314/371 (85%)	286 (91%)	28 (9%)	9	37
23	f	201/276 (73%)	179 (89%)	22 (11%)	6	29
24	c	228/246 (93%)	214 (94%)	14 (6%)	18	51
25	d	373/373 (100%)	338 (91%)	35 (9%)	8	35
26	ba	73/180 (41%)	64 (88%)	9 (12%)	4	23
27	av	191/210 (91%)	172 (90%)	19 (10%)	8	33
28	at	212/227 (93%)	201 (95%)	11 (5%)	23	56
29	ar	227/238 (95%)	209 (92%)	18 (8%)	12	41
30	aq	181/253 (72%)	161 (89%)	20 (11%)	6	29
31	ap	189/233 (81%)	165 (87%)	24 (13%)	4	22
32	ao	225/252 (89%)	202 (90%)	23 (10%)	7	32
33	ai	351/370 (95%)	326 (93%)	25 (7%)	14	46
34	an	250/250 (100%)	217 (87%)	33 (13%)	4	21
35	z	920/1011 (91%)	840 (91%)	80 (9%)	10	38
36	y	209/366 (57%)	186 (89%)	23 (11%)	6	29
37	x	206/284 (72%)	185 (90%)	21 (10%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	w	163/174 (94%)	152 (93%)	11 (7%)	16	48
39	v	164/181 (91%)	152 (93%)	12 (7%)	14	45
40	bb	92/197 (47%)	84 (91%)	8 (9%)	10	38
41	t	193/220 (88%)	174 (90%)	19 (10%)	8	33
42	al	247/262 (94%)	229 (93%)	18 (7%)	14	45
43	q	196/390 (50%)	187 (95%)	9 (5%)	27	61
44	p	213/258 (83%)	202 (95%)	11 (5%)	23	56
45	Ca	534/544 (98%)	483 (90%)	51 (10%)	8	34
46	g	163/171 (95%)	144 (88%)	19 (12%)	5	26
47	j	159/168 (95%)	140 (88%)	19 (12%)	5	25
48	b	138/146 (94%)	126 (91%)	12 (9%)	10	38
49	bd	48/86 (56%)	36 (75%)	12 (25%)	0	4
50	a	364/372 (98%)	327 (90%)	37 (10%)	7	32
51	bc	134/327 (41%)	124 (92%)	10 (8%)	13	43
52	aa	1340/1552 (86%)	1189 (89%)	151 (11%)	6	27
53	k	169/272 (62%)	142 (84%)	27 (16%)	2	14
54	be	70/73 (96%)	60 (86%)	10 (14%)	3	19
55	as	221/228 (97%)	199 (90%)	22 (10%)	7	32
All	All	17127/19857 (86%)	15624 (91%)	1503 (9%)	13	38

All (1503) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	u	59	ASN
1	u	78	VAL
1	u	82	THR
1	u	94	LEU
1	u	112	THR
1	u	138	HIS
1	u	149	GLN
1	u	161	GLU
1	u	202	HIS
1	u	252	ASP
1	u	258	LEU
1	u	278	PHE
1	u	289	LEU

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Mol	Chain	Res	Type
1	u	297	THR
1	u	300	PHE
1	u	304	SER
1	u	309	ASP
1	u	362	LEU
1	u	363	LEU
1	u	369	VAL
1	u	386	HIS
1	u	391	PHE
1	u	405	ARG
1	u	413	MET
1	u	540	ARG
1	u	549	ARG
1	u	554	TYR
1	u	558	ASP
1	u	560	SER
1	u	564	LEU
1	u	574	LEU
1	u	575	ASP
1	u	582	ARG
1	u	595	ASN
1	u	666	PHE
1	u	690	TRP
1	u	703	ARG
1	u	709	CYS
1	u	714	LEU
1	u	718	ASP
1	u	720	ASN
1	u	727	MET
1	u	729	THR
1	u	746	LEU
1	u	769	GLU
1	u	771	LEU
1	u	773	ASP
1	u	789	MET
1	u	803	SER
1	u	811	GLU
1	u	832	THR
2	s	34	ARG
2	s	80	TYR
2	s	82	GLN
2	s	111	ASP

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Mol	Chain	Res	Type
2	s	115	TYR
2	s	125	HIS
2	s	128	SER
2	s	136	HIS
3	r	65	SER
3	r	67	THR
3	r	91	GLU
3	r	111	TYR
3	r	120	LEU
3	r	139	THR
3	r	173	THR
3	r	187	TRP
3	r	199	ASP
3	r	208	LEU
3	r	211	PHE
3	r	220	LEU
3	r	242	ASN
3	r	274	SER
3	r	291	PHE
3	r	292	SER
3	r	295	THR
3	r	296	HIS
3	r	308	LEU
3	r	316	THR
3	r	317	ASP
3	r	327	ARG
3	r	356	CYS
3	r	361	PHE
3	r	393	ASP
3	r	407	TYR
3	r	413	THR
3	r	441	LEU
3	r	447	LEU
3	r	448	SER
3	r	456	ILE
3	r	478	LEU
4	n	38	PHE
4	n	55	ARG
4	n	58	ILE
4	n	61	THR
4	n	80	GLN
4	n	82	TYR

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Mol	Chain	Res	Type
4	n	86	GLU
4	n	97	LYS
4	n	125	VAL
4	n	135	ASN
4	n	142	THR
4	n	149	ASP
5	h	16	ASP
5	h	22	THR
5	h	29	ARG
5	h	32	TYR
5	h	56	SER
5	h	94	ARG
5	h	99	GLN
5	h	113	VAL
5	h	118	MET
5	h	127	LEU
5	h	152	TRP
5	h	161	LEU
6	e	13	ARG
6	e	19	GLN
6	e	36	ASN
6	e	48	ASP
6	e	51	PHE
6	e	67	ASP
6	e	71	ASP
6	e	73	TRP
6	e	78	SER
6	e	80	THR
6	e	82	HIS
6	e	96	ASN
6	e	136	PHE
6	e	138	PHE
6	e	158	LEU
6	e	161	ILE
6	e	174	ARG
6	e	210	LYS
6	e	211	THR
6	e	212	GLU
6	e	235	ASP
6	e	248	LEU
6	e	254	HIS
6	e	274	VAL

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Mol	Chain	Res	Type
6	e	295	ASP
6	e	314	ASP
6	e	325	VAL
6	e	336	CYS
6	e	362	TYR
6	e	380	SER
6	e	381	ASP
6	e	391	THR
6	e	416	LYS
6	e	426	HIS
6	e	430	THR
6	e	458	THR
6	e	461	ASP
6	e	464	ARG
6	e	500	CYS
6	e	504	ASP
6	e	531	LEU
6	e	586	ASN
6	e	588	GLU
6	e	594	SER
6	e	610	GLU
6	e	616	VAL
6	e	617	GLU
6	e	623	ASP
6	e	624	THR
6	e	699	ASP
6	e	720	THR
6	e	737	ARG
6	e	743	PHE
6	e	747	THR
6	e	771	THR
6	e	776	ASP
6	e	797	ASP
6	e	801	LEU
6	e	812	SER
6	e	816	THR
7	az	67	ARG
7	az	77	ILE
7	az	87	ARG
7	az	110	THR
7	az	139	ASP
8	ay	92	HIS

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Mol	Chain	Res	Type
8	ay	101	GLU
8	ay	110	LEU
8	ay	146	VAL
8	ay	149	ARG
8	ay	153	GLU
8	ay	164	ARG
8	ay	173	VAL
8	ay	191	TYR
8	ay	200	LYS
8	ay	204	ILE
8	ay	207	LYS
9	ax	9	THR
9	ax	26	LYS
9	ax	41	SER
9	ax	48	ASP
9	ax	61	LEU
9	ax	85	PHE
9	ax	90	ASP
9	ax	106	ASP
9	ax	108	GLU
9	ax	117	LYS
9	ax	131	HIS
9	ax	138	ASN
9	ax	144	ARG
10	aw	47	THR
10	aw	71	ILE
10	aw	78	PHE
10	aw	103	LYS
10	aw	123	ARG
10	aw	127	GLU
10	aw	152	ASP
10	aw	161	PHE
10	aw	185	PHE
10	aw	186	LEU
11	au	17	HIS
11	au	28	GLU
11	au	52	GLN
11	au	65	VAL
11	au	69	ASP
11	au	72	HIS
11	au	76	HIS
11	au	88	THR

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Mol	Chain	Res	Type
11	au	100	SER
11	au	108	VAL
11	au	122	MET
11	au	131	SER
11	au	133	ASP
11	au	162	TYR
11	au	186	TRP
11	au	200	TRP
11	au	201	SER
11	au	220	ASP
11	au	240	GLN
11	au	244	TYR
12	ak	6	THR
12	ak	20	GLU
12	ak	22	SER
12	ak	34	HIS
12	ak	52	ARG
12	ak	55	ASP
12	ak	115	ARG
12	ak	158	GLU
12	ak	183	VAL
12	ak	219	LYS
12	ak	220	ASP
12	ak	236	LEU
12	ak	248	ASN
12	ak	253	ASP
12	ak	262	GLU
13	aj	12	TYR
13	aj	28	TYR
13	aj	40	ARG
13	aj	49	THR
13	aj	58	LEU
13	aj	94	LYS
13	aj	151	ASP
13	aj	166	LEU
13	aj	173	ASP
13	aj	189	TRP
13	aj	213	GLU
13	aj	214	LYS
13	aj	246	THR
13	aj	273	TYR
13	aj	310	PHE

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Mol	Chain	Res	Type
13	aj	319	TYR
14	ag	9	THR
14	ag	23	GLN
14	ag	42	ARG
14	ag	66	CYS
14	ag	98	ASP
14	ag	145	ARG
14	ag	164	ASP
14	ag	178	PHE
14	ag	182	PHE
14	ag	187	THR
14	ag	218	THR
14	ag	222	THR
14	ag	298	ARG
14	ag	320	GLU
14	ag	330	SER
14	ag	334	THR
14	ag	344	ILE
14	ag	347	VAL
14	ag	351	LYS
14	ag	390	ARG
14	ag	394	TRP
14	ag	409	ARG
14	ag	438	THR
14	ag	444	THR
14	ag	445	VAL
14	ag	451	PHE
14	ag	454	ARG
14	ag	467	TYR
14	ag	472	ARG
14	ag	479	ARG
14	ag	485	GLU
14	ag	544	LEU
14	ag	555	LEU
14	ag	557	ARG
15	af	29	ASP
15	af	31	TYR
15	af	33	THR
15	af	57	ASP
15	af	65	ASN
15	af	78	GLN
15	af	91	LYS

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Mol	Chain	Res	Type
15	af	102	MET
15	af	103	ASN
15	af	108	ARG
15	af	112	TYR
15	af	119	ASP
15	af	125	ASP
15	af	207	SER
15	af	211	TYR
15	af	227	GLU
15	af	229	HIS
15	af	240	HIS
15	af	260	ARG
15	af	261	ARG
15	af	267	ASN
15	af	270	LEU
15	af	281	VAL
15	af	286	LEU
15	af	296	ASP
15	af	306	ARG
15	af	344	ARG
15	af	345	ASP
15	af	373	LYS
15	af	376	MET
15	af	390	ARG
15	af	403	ARG
15	af	497	THR
15	af	502	ASP
15	af	504	ARG
15	af	507	ASP
15	af	509	HIS
15	af	519	THR
15	af	605	HIS
15	af	623	CYS
15	af	625	LEU
15	af	629	VAL
15	af	632	THR
16	ae	13	ILE
16	ae	15	HIS
16	ae	51	TRP
16	ae	100	LYS
16	ae	119	HIS
16	ae	144	THR

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Mol	Chain	Res	Type
16	ae	183	SER
16	ae	189	ASP
16	ae	218	CYS
16	ae	257	ASN
16	ae	285	ARG
16	ae	312	ARG
16	ae	369	LEU
16	ae	380	VAL
16	ae	383	VAL
16	ae	389	GLU
16	ae	397	ARG
16	ae	405	ASN
16	ae	432	THR
16	ae	448	GLN
16	ae	454	ASP
16	ae	504	MET
16	ae	512	LEU
16	ae	545	HIS
16	ae	553	VAL
16	ae	556	THR
16	ae	557	TYR
16	ae	563	THR
16	ae	576	THR
16	ae	583	ASP
17	l	52	THR
17	l	70	LEU
17	l	72	THR
17	l	81	TYR
17	l	84	ASP
17	l	103	ARG
17	l	149	ARG
17	l	188	ASP
17	l	265	TYR
17	l	273	ASP
17	l	276	VAL
17	l	282	LEU
17	l	287	GLU
17	l	305	ASP
17	l	376	LEU
17	l	378	ARG
17	l	386	LEU
17	l	391	PHE

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Mol	Chain	Res	Type
17	l	449	ASN
17	l	470	ARG
17	l	481	ARG
17	l	484	HIS
17	l	488	ASN
17	l	498	TRP
17	l	504	ARG
17	l	531	ASP
17	l	558	TYR
17	l	561	THR
17	l	569	ILE
17	l	572	ASP
17	l	589	SER
17	l	591	GLU
17	l	595	LYS
17	l	613	THR
17	l	617	PHE
17	l	620	GLU
17	l	621	THR
17	l	643	GLN
17	l	649	LEU
17	l	655	LEU
17	l	656	GLU
17	l	664	TRP
17	l	668	LYS
17	l	669	THR
17	l	671	MET
17	l	684	ARG
17	l	698	ASP
18	ac	30	TRP
18	ac	33	ASP
18	ac	83	VAL
18	ac	91	ARG
18	ac	94	THR
18	ac	95	ASP
18	ac	112	THR
18	ac	162	ASN
18	ac	178	ASP
18	ac	182	THR
18	ac	188	THR
18	ac	191	ARG
18	ac	207	ASN

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Mol	Chain	Res	Type
18	ac	212	GLU
18	ac	215	LEU
18	ac	226	PHE
18	ac	234	THR
18	ac	271	PHE
18	ac	275	LEU
18	ac	307	ARG
18	ac	317	TRP
18	ac	402	THR
18	ac	403	GLU
18	ac	405	ARG
18	ac	406	VAL
18	ac	410	SER
18	ac	419	ASP
18	ac	438	GLN
18	ac	505	SER
18	ac	510	SER
18	ac	544	LEU
18	ac	573	LEU
18	ac	602	ASP
18	ac	618	PHE
18	ac	631	TRP
18	ac	650	VAL
18	ac	683	ARG
18	ac	791	VAL
18	ac	794	THR
18	ac	833	SER
18	ac	844	CYS
18	ac	847	LEU
18	ac	859	GLU
18	ac	869	GLU
18	ac	873	PHE
18	ac	886	PHE
18	ac	888	ARG
18	ac	896	THR
18	ac	945	GLU
18	ac	977	THR
18	ac	1009	SER
18	ac	1019	SER
18	ac	1041	LEU
18	ac	1064	THR
18	ac	1065	GLU

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Mol	Chain	Res	Type
18	ac	1088	THR
18	ac	1091	SER
18	ac	1094	VAL
18	ac	1095	VAL
18	ac	1106	VAL
18	ac	1126	THR
18	ac	1139	ILE
18	ac	1143	THR
18	ac	1145	ASP
19	ab	106	ASN
19	ab	116	HIS
19	ab	132	SER
19	ab	133	TRP
19	ab	135	ASP
19	ab	149	ARG
19	ab	157	SER
19	ab	163	GLU
19	ab	194	THR
19	ab	196	THR
19	ab	197	SER
19	ab	201	LEU
19	ab	207	VAL
19	ab	217	SER
19	ab	238	SER
19	ab	244	ASP
19	ab	248	GLU
19	ab	272	ARG
19	ab	279	ASP
19	ab	301	THR
19	ab	320	VAL
19	ab	331	PHE
19	ab	336	VAL
19	ab	408	ARG
19	ab	410	ASP
19	ab	413	ARG
19	ab	415	THR
19	ab	420	HIS
19	ab	449	ARG
19	ab	513	PHE
19	ab	559	ASP
19	ab	577	ARG
19	ab	627	ASP

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Mol	Chain	Res	Type
19	ab	639	LEU
19	ab	661	PHE
19	ab	675	GLN
19	ab	708	GLU
19	ab	721	ASP
19	ab	729	VAL
19	ab	767	THR
19	ab	769	HIS
19	ab	772	MET
19	ab	776	GLN
19	ab	780	LEU
19	ab	802	ASP
19	ab	808	PHE
19	ab	828	ILE
19	ab	834	ASN
19	ab	846	TRP
19	ab	861	THR
19	ab	862	HIS
19	ab	887	ILE
19	ab	895	VAL
19	ab	914	VAL
19	ab	936	ARG
19	ab	1003	ASP
19	ab	1014	ASP
19	ab	1024	ARG
19	ab	1026	ASP
19	ab	1028	ILE
19	ab	1034	HIS
19	ab	1042	ILE
19	ab	1058	GLN
19	ab	1060	ASN
19	ab	1094	PHE
19	ab	1126	ARG
19	ab	1128	GLU
19	ab	1144	TRP
20	ad	10	HIS
20	ad	19	VAL
20	ad	20	PHE
20	ad	44	ILE
20	ad	46	VAL
20	ad	50	TRP
20	ad	53	VAL

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Mol	Chain	Res	Type
20	ad	60	ASN
20	ad	72	ASP
20	ad	78	ASP
20	ad	83	THR
20	ad	89	SER
20	ad	104	ARG
20	ad	107	ASP
20	ad	108	THR
20	ad	110	SER
20	ad	128	ASN
20	ad	129	ARG
20	ad	132	SER
20	ad	145	ILE
20	ad	146	ARG
20	ad	198	LYS
20	ad	205	THR
20	ad	209	THR
20	ad	212	ILE
20	ad	219	CYS
20	ad	226	THR
20	ad	233	ASN
20	ad	258	SER
20	ad	264	LEU
20	ad	271	LYS
20	ad	291	THR
20	ad	295	TYR
20	ad	296	LEU
20	ad	309	ASP
20	ad	311	PHE
20	ad	324	SER
20	ad	325	THR
20	ad	349	CYS
20	ad	373	THR
20	ad	422	ASP
20	ad	428	ARG
20	ad	436	GLU
20	ad	478	ARG
20	ad	502	ASN
20	ad	518	TYR
20	ad	519	ASP
20	ad	522	ARG
20	ad	533	ASP

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Mol	Chain	Res	Type
20	ad	560	MET
20	ad	589	CYS
20	ad	641	TYR
20	ad	642	ASP
20	ad	648	THR
20	ad	651	PHE
20	ad	654	LEU
20	ad	666	ARG
20	ad	689	PHE
20	ad	692	ARG
20	ad	702	ASP
20	ad	721	TYR
20	ad	722	TYR
20	ad	726	MET
20	ad	737	GLU
20	ad	739	ARG
20	ad	755	GLU
20	ad	770	ASP
20	ad	783	ASN
20	ad	791	THR
20	ad	797	ASP
20	ad	803	LYS
20	ad	810	TYR
21	m	11	ASN
21	m	20	ARG
21	m	25	GLU
21	m	31	THR
21	m	36	THR
21	m	92	ILE
21	m	96	GLN
21	m	107	ASP
21	m	124	LEU
21	m	128	ASN
21	m	142	MET
21	m	167	ARG
21	m	224	GLU
21	m	225	LEU
21	m	227	GLU
21	m	237	ARG
22	i	70	HIS
22	i	79	TRP
22	i	123	ASN

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Mol	Chain	Res	Type
22	i	131	LYS
22	i	145	GLN
22	i	176	GLU
22	i	215	ASP
22	i	217	ASP
22	i	230	LEU
22	i	241	THR
22	i	244	HIS
22	i	245	ASN
22	i	246	ASN
22	i	280	ASP
22	i	281	HIS
22	i	285	ASP
22	i	297	GLN
22	i	304	ASP
22	i	305	TRP
22	i	312	SER
22	i	327	CYS
22	i	333	SER
22	i	349	LEU
22	i	373	GLU
22	i	383	ARG
22	i	396	LYS
22	i	414	LEU
22	i	426	HIS
23	f	72	GLN
23	f	77	ASP
23	f	78	TRP
23	f	85	SER
23	f	86	SER
23	f	115	TYR
23	f	118	GLU
23	f	120	ARG
23	f	121	ARG
23	f	122	ARG
23	f	179	ASP
23	f	190	ASP
23	f	194	LEU
23	f	204	TYR
23	f	220	THR
23	f	234	ARG
23	f	280	VAL

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Mol	Chain	Res	Type
23	f	295	GLN
23	f	300	GLU
23	f	314	LEU
23	f	319	MET
23	f	321	ARG
24	c	39	GLN
24	c	47	ASN
24	c	50	LYS
24	c	59	GLN
24	c	88	GLN
24	c	118	ASP
24	c	125	THR
24	c	135	ASP
24	c	153	THR
24	c	158	PHE
24	c	166	THR
24	c	182	ARG
24	c	218	THR
24	c	221	VAL
25	d	9	THR
25	d	42	TRP
25	d	57	ILE
25	d	87	LEU
25	d	88	PHE
25	d	100	TYR
25	d	106	ASN
25	d	107	THR
25	d	117	LEU
25	d	137	PHE
25	d	141	ASP
25	d	146	SER
25	d	155	LEU
25	d	168	THR
25	d	178	THR
25	d	224	THR
25	d	231	HIS
25	d	234	PHE
25	d	242	ASN
25	d	244	ASP
25	d	247	ARG
25	d	261	LEU
25	d	281	ARG

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Mol	Chain	Res	Type
25	d	282	LYS
25	d	289	ARG
25	d	302	ASP
25	d	305	THR
25	d	315	ASP
25	d	325	LEU
25	d	362	GLU
25	d	372	VAL
25	d	379	HIS
25	d	388	ILE
25	d	408	THR
25	d	420	VAL
26	ba	15	LEU
26	ba	18	THR
26	ba	33	VAL
26	ba	35	LYS
26	ba	37	ASP
26	ba	62	ASP
26	ba	76	TYR
26	ba	77	THR
26	ba	85	GLU
27	av	28	ARG
27	av	35	ARG
27	av	55	THR
27	av	58	TYR
27	av	66	LEU
27	av	68	ASP
27	av	69	ASN
27	av	70	ASP
27	av	71	ARG
27	av	79	ASP
27	av	82	GLN
27	av	97	THR
27	av	100	THR
27	av	126	LEU
27	av	135	TYR
27	av	164	HIS
27	av	168	ASP
27	av	205	MET
27	av	231	SER
28	at	87	ARG
28	at	94	ILE

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Mol	Chain	Res	Type
28	at	101	CYS
28	at	108	SER
28	at	109	VAL
28	at	110	SER
28	at	115	PHE
28	at	120	ASN
28	at	173	TRP
28	at	185	SER
28	at	211	CYS
29	ar	20	ILE
29	ar	28	ARG
29	ar	47	GLU
29	ar	49	ARG
29	ar	58	ARG
29	ar	60	THR
29	ar	119	VAL
29	ar	160	PHE
29	ar	166	ILE
29	ar	192	LEU
29	ar	203	SER
29	ar	207	HIS
29	ar	214	ARG
29	ar	220	GLN
29	ar	221	PHE
29	ar	225	ILE
29	ar	243	PHE
29	ar	247	ASP
30	aq	11	SER
30	aq	14	TYR
30	aq	25	ASP
30	aq	44	GLU
30	aq	59	THR
30	aq	66	ASN
30	aq	78	LEU
30	aq	79	ARG
30	aq	100	ARG
30	aq	111	THR
30	aq	122	VAL
30	aq	124	ARG
30	aq	149	ASP
30	aq	163	ARG
30	aq	166	CYS

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Mol	Chain	Res	Type
30	aq	190	LEU
30	aq	202	LEU
30	aq	204	ASN
30	aq	205	MET
30	aq	207	TYR
31	ap	56	ARG
31	ap	63	GLU
31	ap	75	LEU
31	ap	107	LEU
31	ap	109	ASP
31	ap	115	LEU
31	ap	117	LEU
31	ap	123	LYS
31	ap	129	THR
31	ap	130	ASP
31	ap	138	LEU
31	ap	144	ARG
31	ap	147	SER
31	ap	149	ARG
31	ap	151	ILE
31	ap	154	LEU
31	ap	158	THR
31	ap	161	PHE
31	ap	168	PHE
31	ap	176	VAL
31	ap	184	TYR
31	ap	228	LEU
31	ap	243	ASP
31	ap	266	ARG
32	ao	12	MET
32	ao	27	ASP
32	ao	31	SER
32	ao	42	SER
32	ao	53	LEU
32	ao	126	ASP
32	ao	131	ILE
32	ao	145	ASP
32	ao	161	LEU
32	ao	178	VAL
32	ao	197	VAL
32	ao	202	THR
32	ao	207	MET

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Mol	Chain	Res	Type
32	ao	219	THR
32	ao	224	HIS
32	ao	230	THR
32	ao	238	SER
32	ao	239	LYS
32	ao	249	THR
32	ao	259	LEU
32	ao	264	SER
32	ao	275	GLU
32	ao	278	LEU
33	ai	42	ASP
33	ai	45	ARG
33	ai	63	LEU
33	ai	73	LEU
33	ai	75	THR
33	ai	98	LYS
33	ai	138	TRP
33	ai	143	SER
33	ai	148	LEU
33	ai	180	SER
33	ai	189	ILE
33	ai	192	ASP
33	ai	210	LEU
33	ai	225	ASP
33	ai	240	ARG
33	ai	244	GLU
33	ai	251	THR
33	ai	271	LEU
33	ai	278	ASN
33	ai	313	LEU
33	ai	357	ASP
33	ai	376	ASN
33	ai	381	LEU
33	ai	394	ASP
33	ai	409	THR
34	an	1	MET
34	an	4	TYR
34	an	8	THR
34	an	21	ARG
34	an	22	LEU
34	an	25	GLU
34	an	40	TYR

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Mol	Chain	Res	Type
34	an	45	ARG
34	an	51	VAL
34	an	54	ARG
34	an	56	TRP
34	an	62	VAL
34	an	64	THR
34	an	73	VAL
34	an	117	PHE
34	an	128	ILE
34	an	136	THR
34	an	141	SER
34	an	144	THR
34	an	148	THR
34	an	151	MET
34	an	158	THR
34	an	162	THR
34	an	190	GLN
34	an	193	SER
34	an	197	THR
34	an	203	TYR
34	an	204	PHE
34	an	223	THR
34	an	258	MET
34	an	259	TRP
34	an	260	THR
34	an	287	LYS
35	z	30	LEU
35	z	38	LEU
35	z	53	HIS
35	z	64	THR
35	z	68	THR
35	z	79	ILE
35	z	88	GLN
35	z	96	ARG
35	z	103	ASP
35	z	105	ASP
35	z	106	ASP
35	z	120	SER
35	z	121	TYR
35	z	128	ASP
35	z	146	ARG
35	z	169	ASP

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Mol	Chain	Res	Type
35	z	170	LEU
35	z	182	LEU
35	z	186	SER
35	z	188	THR
35	z	197	ASP
35	z	222	MET
35	z	232	ASP
35	z	239	ASP
35	z	253	THR
35	z	266	SER
35	z	287	GLN
35	z	298	LEU
35	z	318	ARG
35	z	322	ASN
35	z	330	THR
35	z	391	CYS
35	z	394	THR
35	z	402	SER
35	z	428	LEU
35	z	459	ASP
35	z	466	THR
35	z	471	THR
35	z	491	ASN
35	z	498	LEU
35	z	501	LEU
35	z	522	THR
35	z	544	ASN
35	z	555	THR
35	z	557	LYS
35	z	561	CYS
35	z	566	CYS
35	z	567	THR
35	z	595	ILE
35	z	624	VAL
35	z	663	LEU
35	z	671	VAL
35	z	717	ASP
35	z	720	ASP
35	z	731	ASP
35	z	751	ILE
35	z	753	ASP
35	z	766	ILE

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Mol	Chain	Res	Type
35	z	769	ARG
35	z	771	CYS
35	z	773	TYR
35	z	776	GLU
35	z	788	GLN
35	z	789	SER
35	z	811	ARG
35	z	818	SER
35	z	829	LEU
35	z	834	ASP
35	z	858	ARG
35	z	876	VAL
35	z	912	THR
35	z	934	ASN
35	z	937	SER
35	z	980	GLU
35	z	1019	ASP
35	z	1041	GLU
35	z	1043	LYS
35	z	1057	GLU
35	z	1087	THR
35	z	1111	THR
36	y	23	LEU
36	y	40	LYS
36	y	55	HIS
36	y	56	THR
36	y	76	LEU
36	y	94	LEU
36	y	103	SER
36	y	104	GLU
36	y	143	PHE
36	y	145	MET
36	y	149	SER
36	y	156	THR
36	y	169	ARG
36	y	174	ASN
36	y	175	PHE
36	y	183	VAL
36	y	184	LEU
36	y	191	VAL
36	y	196	GLU
36	y	256	SER

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Mol	Chain	Res	Type
36	y	298	ARG
36	y	307	LEU
36	y	309	GLU
37	x	96	LEU
37	x	97	LEU
37	x	101	MET
37	x	128	ASP
37	x	144	SER
37	x	162	PHE
37	x	164	HIS
37	x	165	ASP
37	x	174	THR
37	x	178	SER
37	x	179	LEU
37	x	187	VAL
37	x	190	ARG
37	x	216	SER
37	x	245	VAL
37	x	271	THR
37	x	295	LEU
37	x	304	TYR
37	x	316	TYR
37	x	333	TYR
37	x	337	THR
38	w	9	ASP
38	w	25	ASP
38	w	27	ARG
38	w	36	THR
38	w	52	VAL
38	w	66	ARG
38	w	86	CYS
38	w	87	ASP
38	w	105	ARG
38	w	152	HIS
38	w	167	ILE
39	v	38	ASP
39	v	41	ASN
39	v	61	ARG
39	v	73	LEU
39	v	103	LEU
39	v	164	HIS
39	v	177	ARG

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Mol	Chain	Res	Type
39	v	181	GLN
39	v	186	TYR
39	v	188	ARG
39	v	193	PHE
39	v	215	LYS
40	bb	137	ARG
40	bb	153	LEU
40	bb	166	LYS
40	bb	173	TYR
40	bb	186	MET
40	bb	209	ASP
40	bb	211	SER
40	bb	226	LYS
41	t	10	ARG
41	t	22	LEU
41	t	29	LEU
41	t	32	ASP
41	t	34	HIS
41	t	35	ARG
41	t	36	ARG
41	t	50	VAL
41	t	61	ASP
41	t	126	TYR
41	t	129	TYR
41	t	131	THR
41	t	133	SER
41	t	147	TYR
41	t	157	THR
41	t	167	ASP
41	t	203	SER
41	t	207	ARG
41	t	209	TYR
42	al	48	GLN
42	al	67	LYS
42	al	78	LEU
42	al	103	SER
42	al	113	LYS
42	al	137	VAL
42	al	159	THR
42	al	166	PHE
42	al	171	VAL
42	al	173	SER

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Mol	Chain	Res	Type
42	al	191	ARG
42	al	204	ARG
42	al	250	LEU
42	al	257	SER
42	al	261	LEU
42	al	266	ARG
42	al	271	SER
42	al	275	THR
43	q	20	SER
43	q	26	ARG
43	q	39	MET
43	q	55	GLU
43	q	58	ARG
43	q	109	THR
43	q	151	ILE
43	q	167	TYR
43	q	202	THR
44	p	25	ASN
44	p	27	SER
44	p	70	THR
44	p	105	LEU
44	p	134	ARG
44	p	158	LYS
44	p	166	GLU
44	p	175	ILE
44	p	185	ASN
44	p	270	VAL
44	p	295	ASP
45	Ca	10	ARG
45	Ca	22	LYS
45	Ca	25	LYS
45	Ca	26	HIS
45	Ca	36	ILE
45	Ca	43	VAL
45	Ca	71	ILE
45	Ca	72	ASP
45	Ca	117	SER
45	Ca	122	GLU
45	Ca	141	GLU
45	Ca	165	ARG
45	Ca	171	CYS
45	Ca	172	THR

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Mol	Chain	Res	Type
45	Ca	174	SER
45	Ca	176	TYR
45	Ca	203	ILE
45	Ca	211	SER
45	Ca	215	ILE
45	Ca	222	THR
45	Ca	228	ASN
45	Ca	241	SER
45	Ca	277	SER
45	Ca	295	ASP
45	Ca	297	THR
45	Ca	306	HIS
45	Ca	326	LEU
45	Ca	342	LEU
45	Ca	362	LEU
45	Ca	373	SER
45	Ca	389	THR
45	Ca	391	GLN
45	Ca	415	SER
45	Ca	442	ASN
45	Ca	452	VAL
45	Ca	455	GLU
45	Ca	457	LEU
45	Ca	463	ASP
45	Ca	473	VAL
45	Ca	475	ARG
45	Ca	476	GLN
45	Ca	483	SER
45	Ca	487	SER
45	Ca	503	PHE
45	Ca	515	THR
45	Ca	521	TYR
45	Ca	524	HIS
45	Ca	528	THR
45	Ca	571	THR
45	Ca	579	ASP
45	Ca	597	PHE
46	g	19	SER
46	g	22	THR
46	g	35	VAL
46	g	48	VAL
46	g	56	LEU

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Mol	Chain	Res	Type
46	g	59	ARG
46	g	65	VAL
46	g	68	SER
46	g	70	LEU
46	g	78	SER
46	g	79	TYR
46	g	128	ASN
46	g	142	SER
46	g	159	ARG
46	g	169	SER
46	g	177	THR
46	g	181	ILE
46	g	187	ASN
46	g	192	VAL
47	j	14	ILE
47	j	18	THR
47	j	22	TRP
47	j	52	HIS
47	j	65	LEU
47	j	71	HIS
47	j	75	SER
47	j	94	THR
47	j	95	VAL
47	j	107	LYS
47	j	111	LEU
47	j	132	ASN
47	j	144	GLU
47	j	166	LEU
47	j	171	SER
47	j	175	SER
47	j	177	GLU
47	j	188	TYR
47	j	189	LEU
48	b	3	PHE
48	b	8	LEU
48	b	39	LEU
48	b	67	LEU
48	b	69	VAL
48	b	91	ILE
48	b	92	THR
48	b	115	TYR
48	b	120	THR

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Mol	Chain	Res	Type
48	b	143	GLU
48	b	154	TRP
48	b	155	SER
49	bd	35	LEU
49	bd	40	ASN
49	bd	45	TYR
49	bd	46	PHE
49	bd	52	LEU
49	bd	54	TRP
49	bd	59	HIS
49	bd	67	TYR
49	bd	69	PHE
49	bd	74	ASN
49	bd	80	ILE
49	bd	83	LYS
50	a	13	ASN
50	a	16	TYR
50	a	20	THR
50	a	37	SER
50	a	51	VAL
50	a	52	ASP
50	a	55	THR
50	a	57	THR
50	a	67	SER
50	a	112	THR
50	a	124	THR
50	a	137	LEU
50	a	148	ASP
50	a	163	ILE
50	a	164	TYR
50	a	185	SER
50	a	195	ARG
50	a	202	ILE
50	a	216	ARG
50	a	217	VAL
50	a	225	LEU
50	a	256	LEU
50	a	311	LYS
50	a	332	ASP
50	a	339	LEU
50	a	346	ASP
50	a	351	ASP

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Mol	Chain	Res	Type
50	a	356	SER
50	a	359	HIS
50	a	361	ASN
50	a	370	ASP
50	a	392	ARG
50	a	400	LYS
50	a	405	THR
50	a	411	SER
50	a	423	LEU
50	a	434	HIS
51	bc	253	ARG
51	bc	259	THR
51	bc	263	PHE
51	bc	293	PHE
51	bc	294	THR
51	bc	304	SER
51	bc	321	HIS
51	bc	322	ILE
51	bc	344	SER
51	bc	376	ASP
52	aa	91	PHE
52	aa	95	THR
52	aa	97	LEU
52	aa	101	GLU
52	aa	102	MET
52	aa	103	ARG
52	aa	126	ARG
52	aa	129	LEU
52	aa	142	LEU
52	aa	144	GLU
52	aa	155	PHE
52	aa	175	PHE
52	aa	178	ASN
52	aa	183	SER
52	aa	185	ASP
52	aa	186	ILE
52	aa	196	ARG
52	aa	197	TYR
52	aa	200	ILE
52	aa	207	ASN
52	aa	214	TRP
52	aa	216	TYR

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Mol	Chain	Res	Type
52	aa	219	TYR
52	aa	224	HIS
52	aa	229	SER
52	aa	252	SER
52	aa	262	ARG
52	aa	280	PHE
52	aa	282	SER
52	aa	300	SER
52	aa	304	PHE
52	aa	309	LEU
52	aa	310	PHE
52	aa	313	PHE
52	aa	324	LEU
52	aa	350	THR
52	aa	352	ARG
52	aa	354	CYS
52	aa	398	ASP
52	aa	421	THR
52	aa	434	LEU
52	aa	464	HIS
52	aa	469	THR
52	aa	473	THR
52	aa	477	ASN
52	aa	496	ARG
52	aa	501	MET
52	aa	502	ASN
52	aa	509	LYS
52	aa	511	GLU
52	aa	541	ILE
52	aa	543	TRP
52	aa	559	LEU
52	aa	606	LYS
52	aa	631	ASP
52	aa	634	HIS
52	aa	640	VAL
52	aa	644	ARG
52	aa	661	THR
52	aa	679	PHE
52	aa	682	ASP
52	aa	683	THR
52	aa	730	VAL
52	aa	753	GLN

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Mol	Chain	Res	Type
52	aa	756	TYR
52	aa	758	LEU
52	aa	759	VAL
52	aa	796	THR
52	aa	805	ILE
52	aa	825	SER
52	aa	828	ASP
52	aa	829	ARG
52	aa	837	THR
52	aa	848	THR
52	aa	849	GLU
52	aa	853	GLU
52	aa	869	PHE
52	aa	872	GLU
52	aa	887	TRP
52	aa	889	SER
52	aa	904	TYR
52	aa	905	THR
52	aa	906	GLN
52	aa	915	THR
52	aa	924	SER
52	aa	946	THR
52	aa	955	ARG
52	aa	963	ASP
52	aa	964	ARG
52	aa	967	LEU
52	aa	968	GLU
52	aa	972	SER
52	aa	978	THR
52	aa	979	ASP
52	aa	992	ILE
52	aa	996	ARG
52	aa	1005	THR
52	aa	1015	SER
52	aa	1016	TRP
52	aa	1018	GLU
52	aa	1025	GLU
52	aa	1035	VAL
52	aa	1036	ASP
52	aa	1042	LEU
52	aa	1045	SER
52	aa	1048	LEU

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Mol	Chain	Res	Type
52	aa	1059	THR
52	aa	1092	CYS
52	aa	1103	ARG
52	aa	1104	VAL
52	aa	1111	ASP
52	aa	1118	ASP
52	aa	1123	ASP
52	aa	1141	VAL
52	aa	1147	SER
52	aa	1154	ARG
52	aa	1160	LEU
52	aa	1177	PHE
52	aa	1198	SER
52	aa	1200	SER
52	aa	1202	ASN
52	aa	1317	LEU
52	aa	1324	SER
52	aa	1332	THR
52	aa	1347	ASP
52	aa	1458	PHE
52	aa	1472	TYR
52	aa	1481	ILE
52	aa	1491	PHE
52	aa	1493	CYS
52	aa	1508	PHE
52	aa	1509	ASP
52	aa	1511	ASP
52	aa	1512	THR
52	aa	1513	THR
52	aa	1514	ASN
52	aa	1535	ILE
52	aa	1537	ASP
52	aa	1538	ASN
52	aa	1539	ILE
52	aa	1547	VAL
52	aa	1565	THR
52	aa	1572	SER
52	aa	1574	SER
52	aa	1577	TYR
52	aa	1589	SER
52	aa	1598	ARG
52	aa	1607	LYS

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Mol	Chain	Res	Type
52	aa	1637	ARG
52	aa	1643	SER
52	aa	1685	PHE
53	k	14	PHE
53	k	20	GLN
53	k	23	VAL
53	k	30	ARG
53	k	34	THR
53	k	36	ASN
53	k	48	ARG
53	k	67	LEU
53	k	70	ARG
53	k	73	ARG
53	k	78	TYR
53	k	106	THR
53	k	123	ARG
53	k	125	SER
53	k	136	ASP
53	k	143	ASP
53	k	146	HIS
53	k	149	GLN
53	k	152	LYS
53	k	154	SER
53	k	157	LYS
53	k	158	HIS
53	k	163	SER
53	k	176	LYS
53	k	189	TYR
53	k	195	ILE
53	k	199	ASN
54	be	1	MET
54	be	4	LEU
54	be	11	PHE
54	be	34	TYR
54	be	41	ILE
54	be	48	CYS
54	be	54	PHE
54	be	58	PHE
54	be	62	ILE
54	be	68	PHE
55	as	16	ASN
55	as	24	SER

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Mol	Chain	Res	Type
55	as	43	HIS
55	as	62	HIS
55	as	76	ARG
55	as	88	ASP
55	as	90	ASP
55	as	97	THR
55	as	112	ARG
55	as	115	SER
55	as	173	PHE
55	as	184	GLN
55	as	202	ASN
55	as	204	THR
55	as	209	TRP
55	as	210	GLU
55	as	220	LYS
55	as	221	ARG
55	as	223	THR
55	as	236	MET
55	as	238	LEU
55	as	259	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (431) such sidechains are listed below:

Mol	Chain	Res	Type
1	u	30	GLN
1	u	97	GLN
1	u	135	ASN
1	u	137	GLN
1	u	147	GLN
1	u	307	GLN
1	u	333	ASN
1	u	358	GLN
1	u	359	GLN
1	u	401	HIS
1	u	539	ASN
1	u	559	GLN
1	u	566	GLN
1	u	576	GLN
1	u	608	HIS
1	u	695	GLN
1	u	728	GLN
2	s	13	HIS

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Mol	Chain	Res	Type
2	s	29	GLN
2	s	42	GLN
2	s	96	ASN
2	s	112	ASN
2	s	143	GLN
3	r	75	ASN
3	r	87	GLN
3	r	99	GLN
3	r	127	HIS
3	r	184	HIS
3	r	215	ASN
3	r	312	ASN
3	r	400	GLN
3	r	432	HIS
3	r	449	ASN
3	r	458	HIS
4	n	65	ASN
4	n	88	ASN
4	n	110	HIS
5	h	23	HIS
5	h	153	ASN
6	e	19	GLN
6	e	33	GLN
6	e	81	HIS
6	e	82	HIS
6	e	150	ASN
6	e	172	HIS
6	e	224	ASN
6	e	410	GLN
6	e	428	GLN
6	e	434	HIS
6	e	443	HIS
6	e	452	HIS
6	e	460	HIS
6	e	462	HIS
6	e	463	HIS
6	e	478	ASN
6	e	496	GLN
6	e	573	ASN
6	e	630	GLN
6	e	675	GLN
6	e	703	ASN

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Mol	Chain	Res	Type
6	e	709	HIS
6	e	712	HIS
6	e	745	HIS
6	e	787	GLN
6	e	792	HIS
7	az	10	ASN
7	az	90	GLN
7	az	104	HIS
7	az	144	HIS
7	az	147	ASN
8	ay	160	ASN
9	ax	98	HIS
9	ax	120	HIS
9	ax	153	HIS
9	ax	154	HIS
10	aw	39	HIS
10	aw	43	HIS
10	aw	51	HIS
10	aw	86	GLN
10	aw	96	GLN
11	au	45	HIS
11	au	56	HIS
11	au	63	HIS
11	au	82	HIS
11	au	139	HIS
11	au	158	HIS
11	au	247	GLN
12	ak	143	HIS
12	ak	150	ASN
12	ak	170	GLN
12	ak	179	HIS
12	ak	248	ASN
12	ak	257	GLN
12	ak	259	GLN
13	aj	16	ASN
13	aj	33	ASN
13	aj	45	ASN
13	aj	106	ASN
13	aj	314	GLN
14	ag	29	GLN
14	ag	152	GLN
14	ag	223	HIS

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Mol	Chain	Res	Type
14	ag	275	ASN
14	ag	385	HIS
14	ag	400	GLN
14	ag	410	ASN
14	ag	417	HIS
14	ag	434	GLN
14	ag	439	GLN
14	ag	500	ASN
14	ag	509	HIS
15	af	24	ASN
15	af	26	ASN
15	af	40	HIS
15	af	71	ASN
15	af	143	HIS
15	af	191	GLN
15	af	216	HIS
15	af	240	HIS
15	af	298	HIS
15	af	529	GLN
15	af	589	GLN
16	ae	41	ASN
16	ae	62	ASN
16	ae	78	ASN
16	ae	115	HIS
16	ae	123	HIS
16	ae	140	HIS
16	ae	213	HIS
16	ae	257	ASN
16	ae	271	HIS
16	ae	447	GLN
16	ae	449	ASN
16	ae	549	HIS
16	ae	572	GLN
16	ae	575	HIS
16	ae	594	GLN
17	l	49	HIS
17	l	194	HIS
17	l	279	HIS
17	l	459	GLN
17	l	465	GLN
17	l	468	HIS
17	l	477	GLN

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Mol	Chain	Res	Type
17	l	488	ASN
17	l	626	ASN
17	l	639	ASN
18	ac	78	HIS
18	ac	85	HIS
18	ac	155	HIS
18	ac	207	ASN
18	ac	210	GLN
18	ac	247	HIS
18	ac	268	GLN
18	ac	269	GLN
18	ac	308	HIS
18	ac	338	GLN
18	ac	369	GLN
18	ac	451	ASN
18	ac	456	GLN
18	ac	482	HIS
18	ac	534	GLN
18	ac	576	ASN
18	ac	577	HIS
18	ac	736	GLN
18	ac	819	GLN
18	ac	842	GLN
18	ac	879	ASN
18	ac	913	HIS
18	ac	958	HIS
18	ac	988	ASN
18	ac	1039	ASN
18	ac	1054	GLN
18	ac	1120	HIS
18	ac	1123	GLN
18	ac	1146	GLN
19	ab	87	HIS
19	ab	106	ASN
19	ab	172	HIS
19	ab	173	HIS
19	ab	181	ASN
19	ab	232	HIS
19	ab	249	ASN
19	ab	334	ASN
19	ab	348	GLN
19	ab	383	GLN

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Mol	Chain	Res	Type
19	ab	420	HIS
19	ab	435	HIS
19	ab	535	HIS
19	ab	545	HIS
19	ab	556	GLN
19	ab	645	ASN
19	ab	655	ASN
19	ab	664	ASN
19	ab	685	HIS
19	ab	701	GLN
19	ab	727	HIS
19	ab	731	GLN
19	ab	821	ASN
19	ab	834	ASN
19	ab	842	GLN
19	ab	849	GLN
19	ab	877	HIS
19	ab	902	GLN
19	ab	906	ASN
19	ab	1023	HIS
19	ab	1045	GLN
19	ab	1049	GLN
19	ab	1060	ASN
19	ab	1070	ASN
19	ab	1118	HIS
19	ab	1123	GLN
19	ab	1174	GLN
20	ad	59	ASN
20	ad	137	HIS
20	ad	160	HIS
20	ad	171	ASN
20	ad	176	HIS
20	ad	233	ASN
20	ad	300	GLN
20	ad	353	HIS
20	ad	354	HIS
20	ad	402	GLN
20	ad	450	HIS
20	ad	481	ASN
20	ad	502	ASN
20	ad	505	GLN
20	ad	561	HIS

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Mol	Chain	Res	Type
20	ad	658	GLN
20	ad	705	GLN
20	ad	801	GLN
21	m	28	ASN
21	m	39	HIS
21	m	65	GLN
21	m	128	ASN
21	m	151	ASN
21	m	211	ASN
22	i	100	HIS
22	i	237	ASN
22	i	284	GLN
22	i	356	GLN
22	i	359	HIS
23	f	72	GLN
23	f	106	GLN
23	f	124	GLN
23	f	155	GLN
23	f	223	ASN
23	f	241	ASN
23	f	288	GLN
23	f	299	ASN
23	f	315	ASN
24	c	59	GLN
24	c	61	ASN
24	c	128	ASN
24	c	160	HIS
24	c	245	ASN
24	c	270	GLN
25	d	21	ASN
25	d	44	ASN
25	d	84	HIS
25	d	89	HIS
25	d	106	ASN
25	d	172	GLN
25	d	176	GLN
26	ba	59	ASN
27	av	72	HIS
27	av	82	GLN
27	av	108	HIS
27	av	229	ASN
28	at	58	ASN

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Mol	Chain	Res	Type
28	at	91	HIS
28	at	116	HIS
28	at	201	HIS
29	ar	41	GLN
29	ar	103	HIS
30	aq	40	HIS
30	aq	48	GLN
30	aq	67	GLN
30	aq	116	HIS
30	aq	143	ASN
31	ap	200	GLN
32	ao	55	GLN
32	ao	224	HIS
32	ao	225	ASN
32	ao	228	ASN
32	ao	253	ASN
32	ao	262	HIS
33	ai	85	GLN
33	ai	86	GLN
33	ai	323	GLN
33	ai	374	GLN
33	ai	376	ASN
34	an	19	HIS
34	an	27	GLN
34	an	87	GLN
34	an	112	ASN
34	an	150	HIS
34	an	282	HIS
35	z	55	ASN
35	z	83	HIS
35	z	116	ASN
35	z	153	HIS
35	z	201	HIS
35	z	210	ASN
35	z	277	HIS
35	z	308	HIS
35	z	350	GLN
35	z	490	HIS
35	z	544	ASN
35	z	605	GLN
35	z	606	HIS
35	z	627	HIS

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Mol	Chain	Res	Type
35	z	639	GLN
35	z	645	HIS
35	z	743	GLN
35	z	770	ASN
35	z	784	GLN
35	z	841	HIS
35	z	880	ASN
35	z	917	GLN
35	z	925	HIS
35	z	971	HIS
35	z	974	GLN
35	z	975	ASN
35	z	984	HIS
35	z	1005	ASN
35	z	1009	GLN
36	y	60	ASN
36	y	263	GLN
37	x	88	HIS
37	x	139	ASN
37	x	171	ASN
37	x	173	HIS
37	x	201	HIS
37	x	209	ASN
37	x	235	GLN
37	x	260	GLN
37	x	274	GLN
38	w	81	ASN
38	w	152	HIS
39	v	47	ASN
39	v	155	HIS
39	v	181	GLN
39	v	214	ASN
42	al	48	GLN
42	al	117	ASN
42	al	126	HIS
42	al	268	HIS
43	q	72	ASN
43	q	113	GLN
43	q	119	HIS
43	q	143	GLN
43	q	178	ASN
43	q	208	HIS

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Mol	Chain	Res	Type
43	q	219	HIS
44	p	67	GLN
45	Ca	63	GLN
45	Ca	76	GLN
45	Ca	105	GLN
45	Ca	120	ASN
45	Ca	144	GLN
45	Ca	178	GLN
45	Ca	181	ASN
45	Ca	228	ASN
45	Ca	231	GLN
45	Ca	400	ASN
45	Ca	424	GLN
45	Ca	435	HIS
45	Ca	437	ASN
45	Ca	440	GLN
45	Ca	441	HIS
45	Ca	451	ASN
45	Ca	476	GLN
45	Ca	507	ASN
45	Ca	518	GLN
45	Ca	520	GLN
45	Ca	522	GLN
45	Ca	582	ASN
46	g	16	HIS
46	g	37	HIS
46	g	132	GLN
46	g	182	HIS
48	b	56	ASN
48	b	156	ASN
49	bd	56	ASN
50	a	108	HIS
50	a	132	HIS
50	a	141	GLN
50	a	218	ASN
50	a	248	GLN
50	a	430	ASN
51	bc	237	HIS
51	bc	334	ASN
51	bc	354	ASN
52	aa	99	HIS
52	aa	104	GLN

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Mol	Chain	Res	Type
52	aa	109	HIS
52	aa	118	ASN
52	aa	167	GLN
52	aa	284	HIS
52	aa	287	HIS
52	aa	296	HIS
52	aa	337	HIS
52	aa	423	GLN
52	aa	432	ASN
52	aa	464	HIS
52	aa	466	HIS
52	aa	508	GLN
52	aa	574	HIS
52	aa	666	HIS
52	aa	954	GLN
52	aa	957	HIS
52	aa	1083	HIS
52	aa	1095	ASN
52	aa	1164	GLN
52	aa	1316	HIS
52	aa	1417	HIS
52	aa	1494	ASN
52	aa	1514	ASN
52	aa	1543	HIS
52	aa	1553	HIS
52	aa	1605	HIS
52	aa	1632	ASN
52	aa	1655	ASN
52	aa	1657	GLN
52	aa	1661	GLN
53	k	121	ASN
53	k	149	GLN
55	as	43	HIS
55	as	108	GLN
55	as	184	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	2	468/8129 (5%)	249 (53%)	8 (1%)
56	A	142/8129 (1%)	90 (63%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	610/16258 (3%)	339 (55%)	10 (1%)

All (339) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
56	A	397	U
56	A	398	U
56	A	399	A
56	A	400	U
56	A	401	A
56	A	402	U
56	A	404	U
56	A	405	A
56	A	408	C
56	A	411	A
56	A	412	U
56	A	413	A
56	A	414	A
56	A	415	U
56	A	416	U
56	A	418	A
56	A	419	U
56	A	421	G
56	A	425	A
56	A	426	A
56	A	427	U
56	A	428	A
56	A	429	U
56	A	430	U
56	A	431	U
56	A	433	U
56	A	436	U
56	A	438	U
56	A	439	U
56	A	442	A
56	A	444	A
56	A	445	C
56	A	446	C
56	A	448	U
56	A	449	G
56	A	450	A
56	A	451	U

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Mol	Chain	Res	Type
56	A	452	A
56	A	455	G
56	A	457	U
56	A	458	U
56	A	459	A
56	A	460	U
56	A	463	A
56	A	464	U
56	A	466	G
56	A	468	A
56	A	469	A
56	A	470	G
56	A	471	U
56	A	472	G
56	A	477	U
56	A	478	A
56	A	479	U
56	A	480	C
56	A	481	A
56	A	482	U
56	A	483	A
56	A	484	A
56	A	485	U
56	A	486	C
56	A	487	A
56	A	489	A
56	A	490	A
56	A	494	A
56	A	497	A
56	A	498	U
56	A	499	U
56	A	500	U
56	A	501	A
56	A	502	U
56	A	504	U
56	A	505	U
56	A	506	A
56	A	509	U
56	A	510	A
56	A	511	U
56	A	512	G
56	A	513	U

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Mol	Chain	Res	Type
56	A	514	A
56	A	515	U
56	A	516	G
56	A	517	U
56	A	519	U
56	A	520	A
56	A	528	U
56	A	530	A
56	A	532	A
56	A	535	U
56	A	536	U
56	2	2	A
56	2	3	A
56	2	4	A
56	2	5	U
56	2	6	U
56	2	8	U
56	2	10	G
56	2	11	U
56	2	16	U
56	2	18	U
56	2	19	U
56	2	20	A
56	2	21	G
56	2	25	U
56	2	32	A
56	2	33	A
56	2	36	U
56	2	37	U
56	2	39	U
56	2	41	A
56	2	43	A
56	2	44	U
56	2	46	U
56	2	48	U
56	2	49	U
56	2	51	U
56	2	52	C
56	2	53	A
56	2	55	U
56	2	56	U
56	2	57	U

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Mol	Chain	Res	Type
56	2	58	A
56	2	59	U
56	2	60	A
56	2	64	G
56	2	68	A
56	2	69	U
56	2	70	U
56	2	72	U
56	2	73	U
56	2	74	G
56	2	75	A
56	2	77	A
56	2	78	G
56	2	79	A
56	2	80	U
56	2	83	U
56	2	84	U
56	2	85	U
56	2	86	G
56	2	87	U
56	2	88	A
56	2	89	U
56	2	91	A
56	2	95	U
56	2	97	U
56	2	98	A
56	2	99	G
56	2	100	G
56	2	101	A
56	2	105	G
56	2	106	U
56	2	107	U
56	2	108	A
56	2	109	A
56	2	110	U
56	2	111	A
56	2	112	A
56	2	113	U
56	2	114	A
56	2	115	A
56	2	116	U
56	2	117	U

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Mol	Chain	Res	Type
56	2	120	U
56	2	124	U
56	2	135	U
56	2	136	G
56	2	137	U
56	2	138	U
56	2	139	U
56	2	140	U
56	2	149	U
56	2	152	U
56	2	156	U
56	2	159	G
56	2	160	U
56	2	162	U
56	2	166	A
56	2	167	A
56	2	169	A
56	2	170	U
56	2	172	A
56	2	173	A
56	2	174	A
56	2	175	A
56	2	176	A
56	2	177	A
56	2	178	A
56	2	179	U
56	2	181	A
56	2	182	U
56	2	183	U
56	2	185	A
56	2	188	U
56	2	189	A
56	2	193	C
56	2	197	A
56	2	198	A
56	2	199	U
56	2	200	A
56	2	201	A
56	2	202	A
56	2	203	U
56	2	205	A
56	2	207	A

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Mol	Chain	Res	Type
56	2	208	U
56	2	210	A
56	2	211	A
56	2	213	C
56	2	215	A
56	2	217	U
56	2	218	A
56	2	219	G
56	2	221	C
56	2	223	G
56	2	225	A
56	2	228	G
56	2	230	A
56	2	232	G
56	2	236	G
56	2	239	G
56	2	242	G
56	2	245	G
56	2	246	U
56	2	247	A
56	2	248	A
56	2	255	U
56	2	256	G
56	2	259	U
56	2	260	U
56	2	261	U
56	2	262	A
56	2	263	A
56	2	264	A
56	2	270	U
56	2	272	C
56	2	275	U
56	2	276	U
56	2	278	U
56	2	279	C
56	2	280	A
56	2	282	A
56	2	283	U
56	2	284	U
56	2	294	A
56	2	295	G
56	2	296	U

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Mol	Chain	Res	Type
56	2	297	G
56	2	299	U
56	2	300	G
56	2	301	A
56	2	307	C
56	2	309	A
56	2	311	U
56	2	312	A
56	2	313	A
56	2	316	A
56	2	317	U
56	2	320	A
56	2	321	A
56	2	322	A
56	2	323	U
56	2	324	A
56	2	325	A
56	2	326	U
56	2	327	U
56	2	329	U
56	2	330	U
56	2	331	A
56	2	333	U
56	2	334	U
56	2	337	U
56	2	338	U
56	2	340	U
56	2	341	A
56	2	342	A
56	2	350	U
56	2	351	A
56	2	352	G
56	2	356	U
56	2	357	A
56	2	358	U
56	2	359	G
56	2	361	A
56	2	363	A
56	2	364	U
56	2	366	U
56	2	367	A
56	2	368	A

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Mol	Chain	Res	Type
56	2	370	A
56	2	371	U
56	2	374	U
56	2	375	A
56	2	376	G
56	2	378	A
56	2	380	U
56	2	384	A
56	2	385	A
56	2	386	A
56	2	389	A
56	2	390	U
56	2	394	A
56	2	539	A
56	2	540	A
56	2	541	A
56	2	542	G
56	2	544	U
56	2	545	A
56	2	546	U
56	2	547	U
56	2	549	U
56	2	550	U
56	2	555	A
56	2	556	C
56	2	558	A
56	2	560	U
56	2	562	U
56	2	564	U
56	2	565	A
56	2	566	U
56	2	567	A
56	2	568	A
56	2	570	A
56	2	576	A
56	2	580	U
56	2	581	G
56	2	583	A
56	2	585	U
56	2	586	A
56	2	587	A
56	2	588	U

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Mol	Chain	Res	Type
56	2	590	A
56	2	591	A
56	2	600	U
56	2	602	A
56	2	603	A
56	2	609	A
56	2	611	U
56	2	613	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	A	512	G
56	A	514	A
56	2	40	U
56	2	87	U
56	2	97	U
56	2	177	A
56	2	200	A
56	2	262	A
56	2	324	A
56	2	366	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	GTP	r	901	58	26,34,34	3.64	13 (50%)	32,54,54	1.90	12 (37%)
59	UTP	aj	401	-	22,30,30	4.42	6 (27%)	27,47,47	1.32	4 (14%)

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	GTP	r	901	58	-	5/18/38/38	0/3/3/3
59	UTP	aj	401	-	-	4/20/38/38	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	aj	401	UTP	O4'-C1'	14.35	1.61	1.41
59	aj	401	UTP	C2'-C1'	-12.42	1.34	1.53
57	r	901	GTP	C3'-C4'	-9.63	1.28	1.53
57	r	901	GTP	O4'-C4'	7.36	1.61	1.45
57	r	901	GTP	O4'-C1'	-7.19	1.31	1.41
59	aj	401	UTP	O4'-C4'	-5.75	1.32	1.45
57	r	901	GTP	C2-N3	5.45	1.46	1.33
57	r	901	GTP	C4-N3	4.85	1.49	1.37
57	r	901	GTP	C2-N2	4.79	1.45	1.34
57	r	901	GTP	C6-N1	3.88	1.43	1.37
57	r	901	GTP	O2'-C2'	-3.43	1.34	1.43
57	r	901	GTP	C5-C4	-3.04	1.35	1.43
57	r	901	GTP	C2-N1	2.89	1.44	1.37
59	aj	401	UTP	O3'-C3'	-2.86	1.36	1.43
59	aj	401	UTP	O2'-C2'	2.66	1.49	1.43
57	r	901	GTP	O6-C6	-2.64	1.17	1.23
57	r	901	GTP	O3'-C3'	2.45	1.48	1.43
57	r	901	GTP	C5-C6	2.26	1.52	1.47
59	aj	401	UTP	C6-N1	-2.03	1.33	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	r	901	GTP	C5-C6-N1	3.92	120.87	113.95
57	r	901	GTP	O6-C6-C5	-3.83	116.89	124.37
57	r	901	GTP	C3'-C2'-C1'	-3.57	95.60	100.98
59	aj	401	UTP	PB-O3B-PG	-3.43	121.04	132.83
57	r	901	GTP	C2-N1-C6	-3.21	119.19	125.10
59	aj	401	UTP	PB-O3A-PA	-2.91	122.86	132.83
57	r	901	GTP	O4'-C4'-C3'	-2.90	99.37	105.11
57	r	901	GTP	PB-O3B-PG	-2.51	124.20	132.83
57	r	901	GTP	O4'-C1'-C2'	-2.47	103.31	106.93
57	r	901	GTP	C5'-C4'-C3'	-2.43	106.09	115.18
57	r	901	GTP	C8-N7-C5	2.26	107.29	102.99
57	r	901	GTP	C2'-C3'-C4'	-2.20	98.37	102.64
59	aj	401	UTP	O2A-PA-O5'	2.15	117.73	107.75
59	aj	401	UTP	O4'-C1'-C2'	-2.02	103.97	106.93
57	r	901	GTP	N1-C2-N3	-2.02	119.54	123.32
57	r	901	GTP	O3'-C3'-C2'	2.00	118.30	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

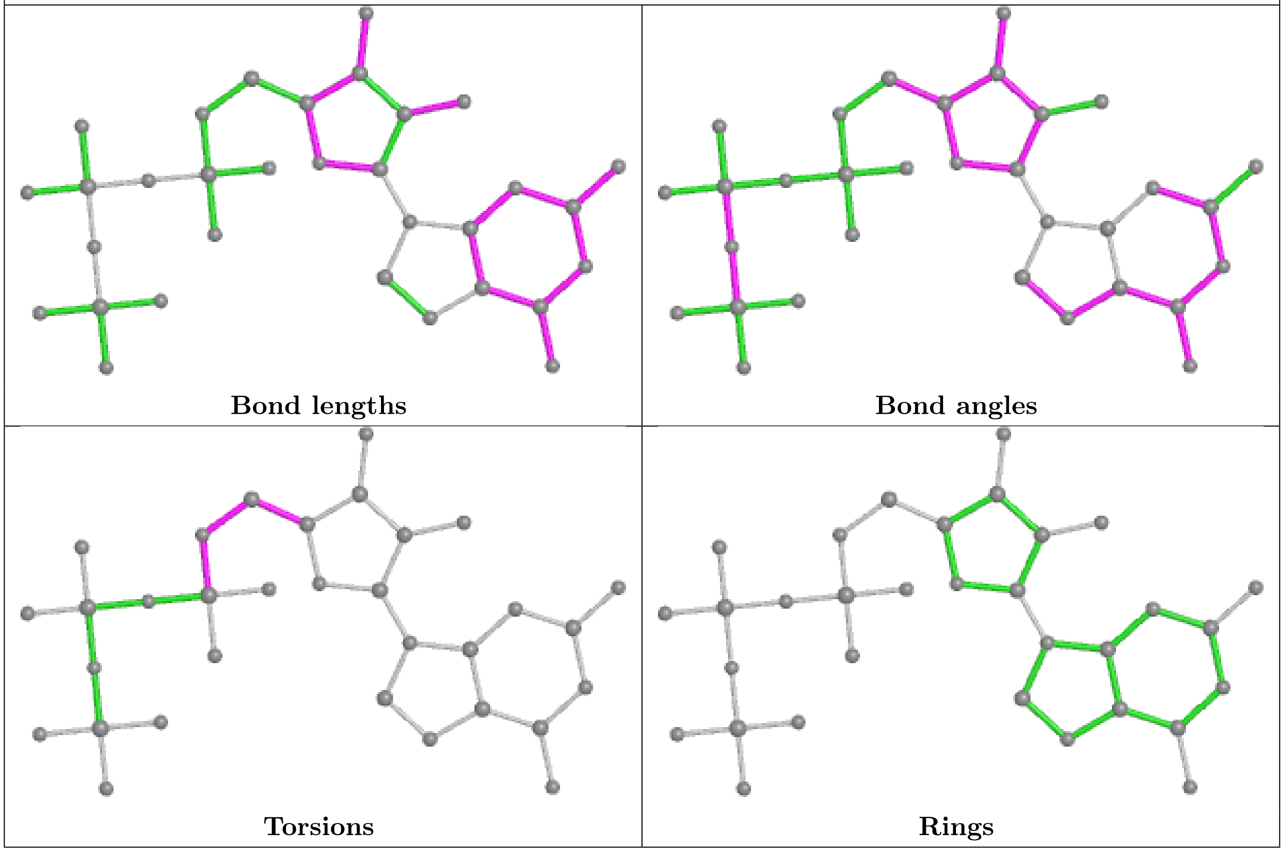
Mol	Chain	Res	Type	Atoms
57	r	901	GTP	C5'-O5'-PA-O3A
57	r	901	GTP	C5'-O5'-PA-O1A
57	r	901	GTP	C5'-O5'-PA-O2A
59	aj	401	UTP	O4'-C4'-C5'-O5'
59	aj	401	UTP	O4'-C1'-N1-C6
59	aj	401	UTP	C2'-C1'-N1-C6
59	aj	401	UTP	C3'-C4'-C5'-O5'
57	r	901	GTP	C3'-C4'-C5'-O5'
57	r	901	GTP	C4'-C5'-O5'-PA

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 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 GTP r 901



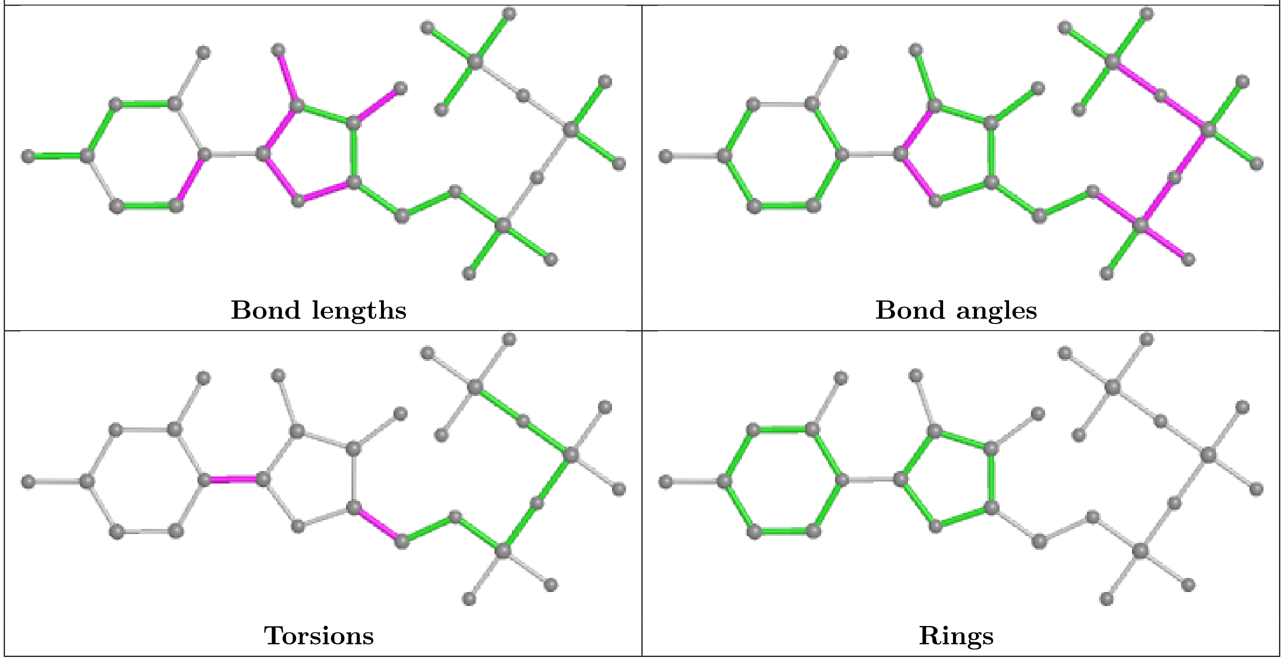
Bond lengths

Bond angles

Torsions

Rings

Ligand UTP aj 401



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	e	1
21	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	444:ASP	C	445:GLY	N	1.67
1	m	70:ARG	C	71:PHE	N	1.17

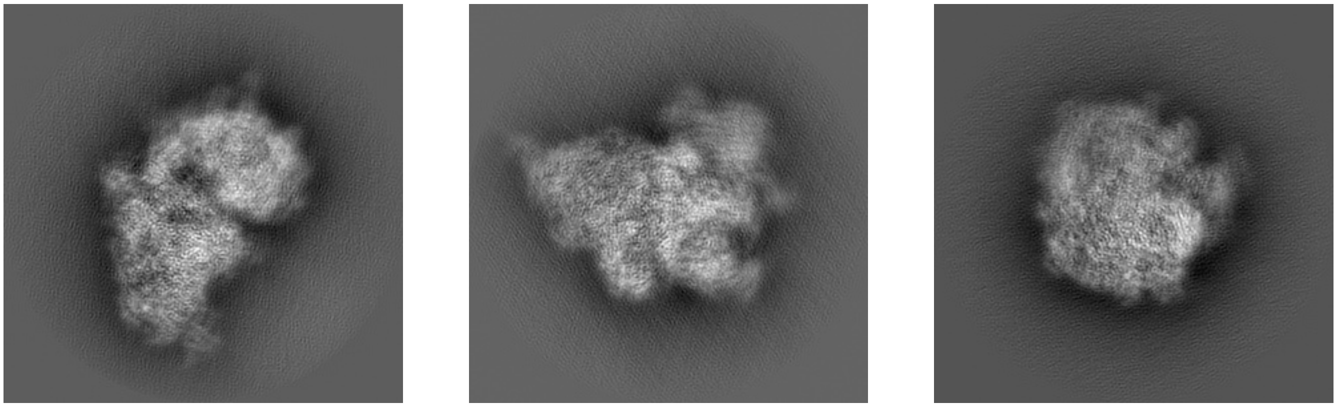
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11846. 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 ⓘ

6.1.1 Primary map

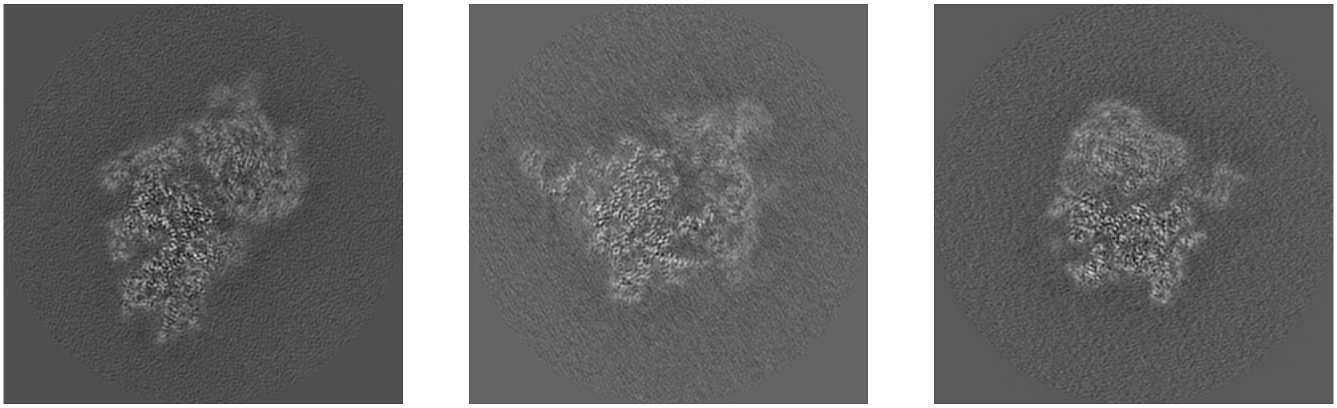


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

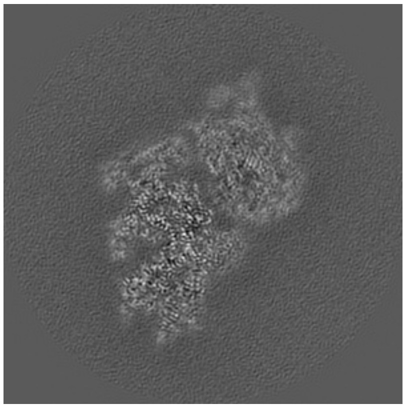


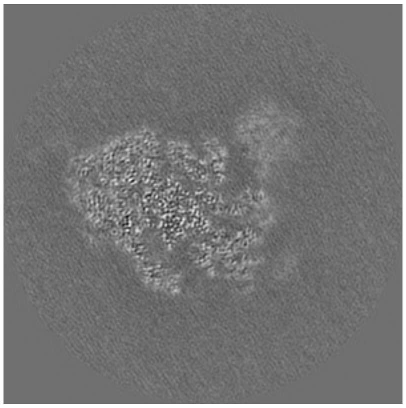
X Index: 180 Y Index: 180 Z Index: 180

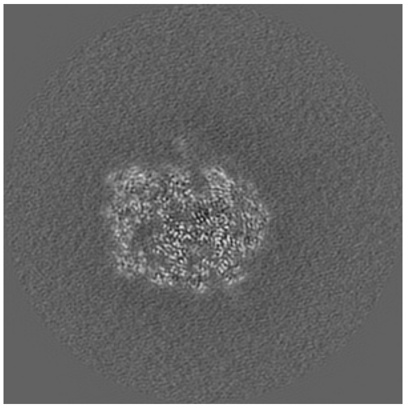
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map


X Index: 181

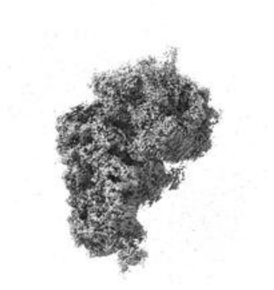

Y Index: 155

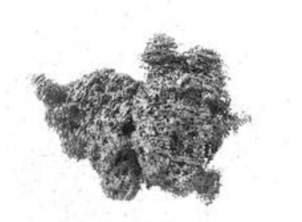

Z Index: 155

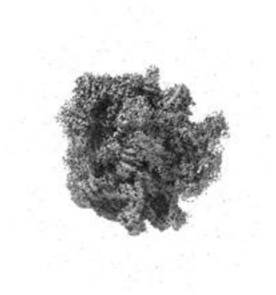
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map


X


Y


Z

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

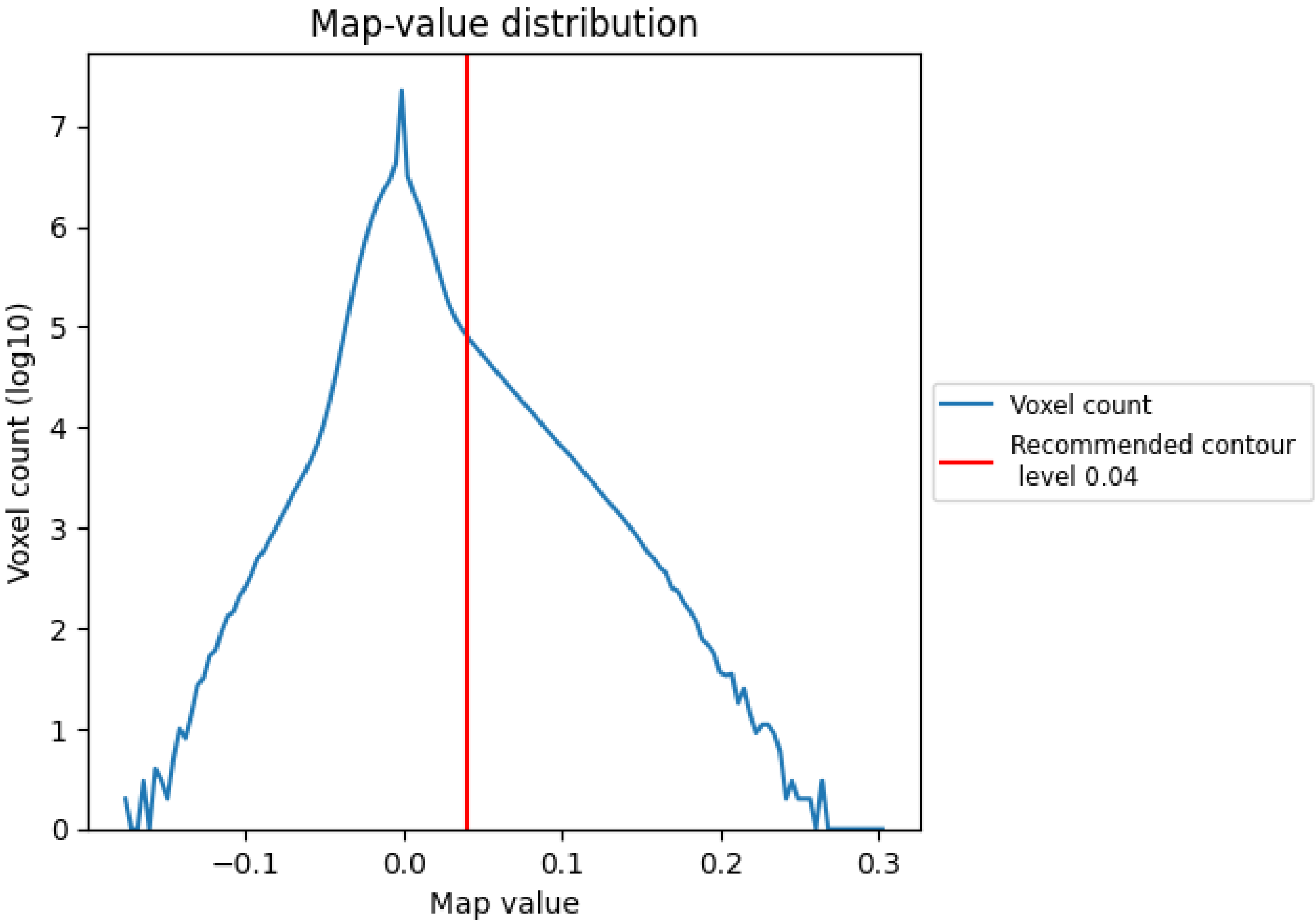
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

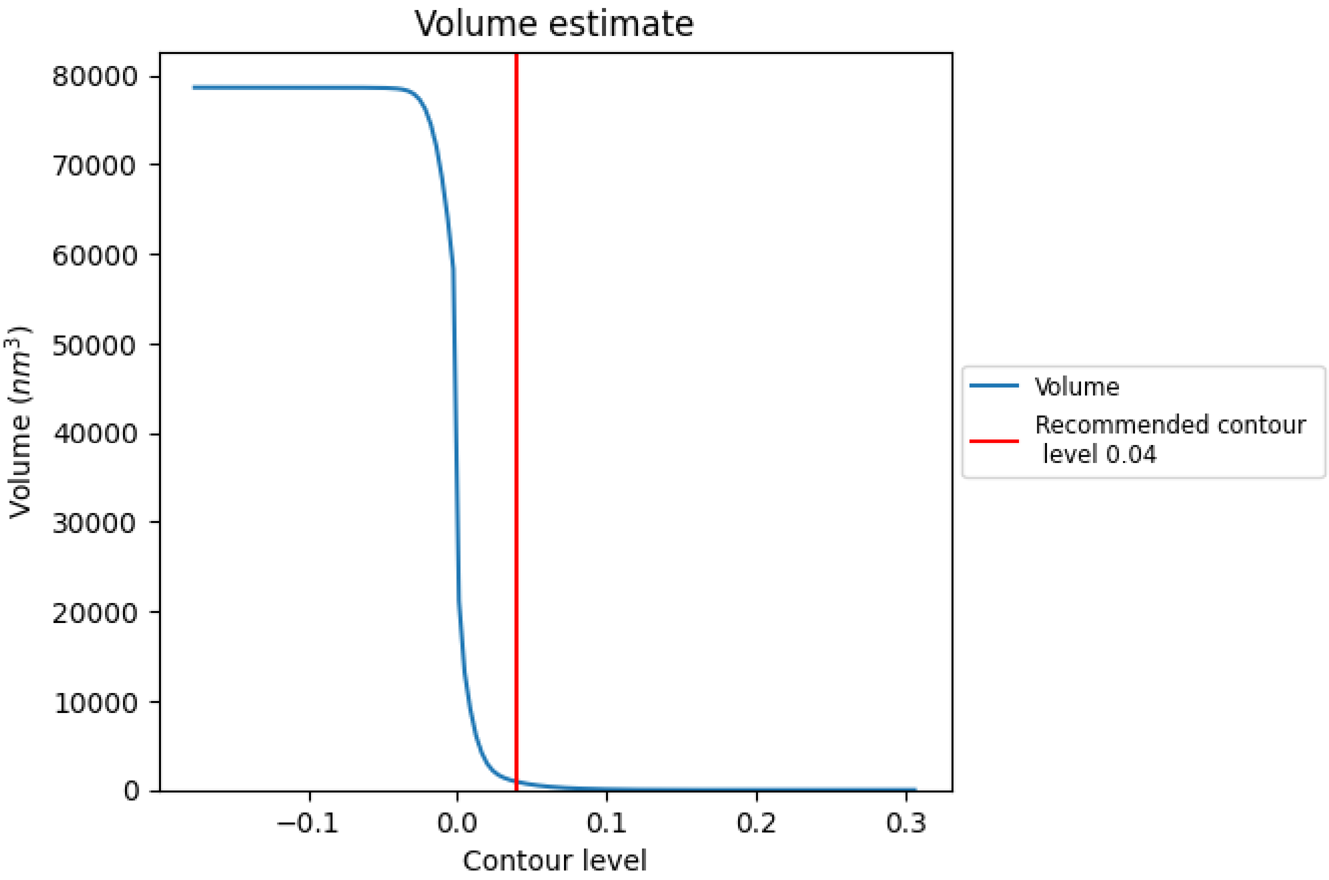
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

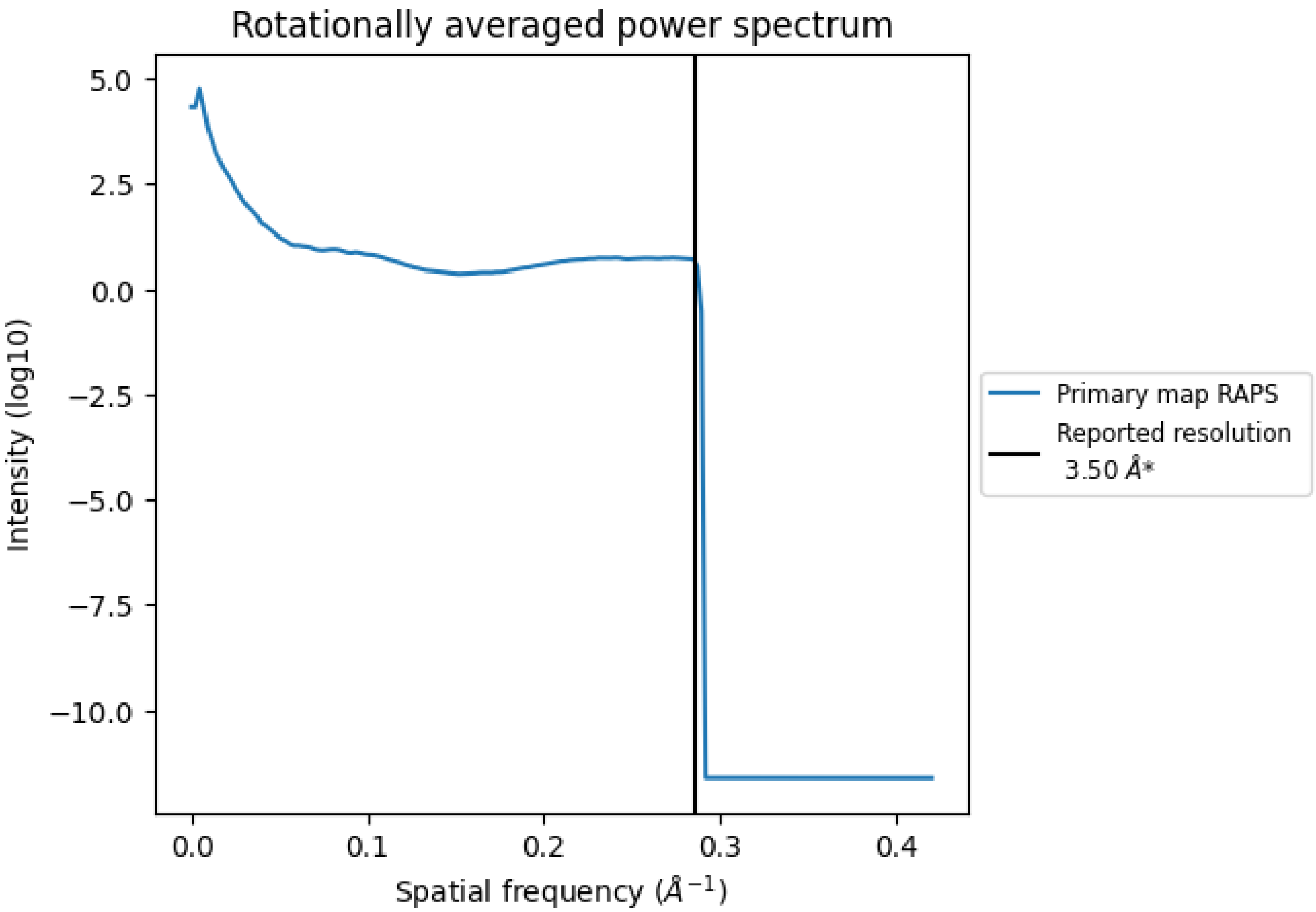
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 906 nm^3; this corresponds to an approximate mass of 819 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

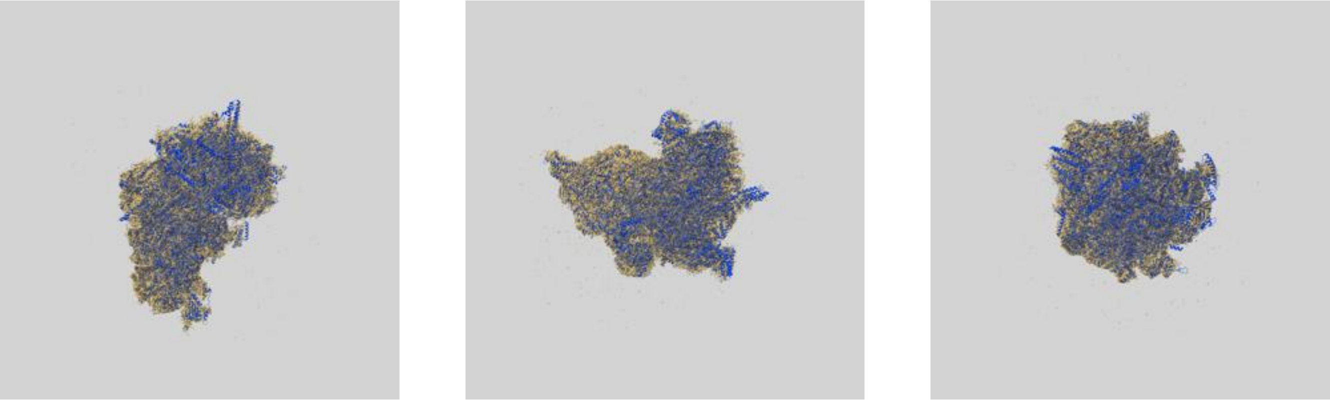
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11846 and PDB model 7AOR. Per-residue inclusion information can be found in section 3 on page 15.

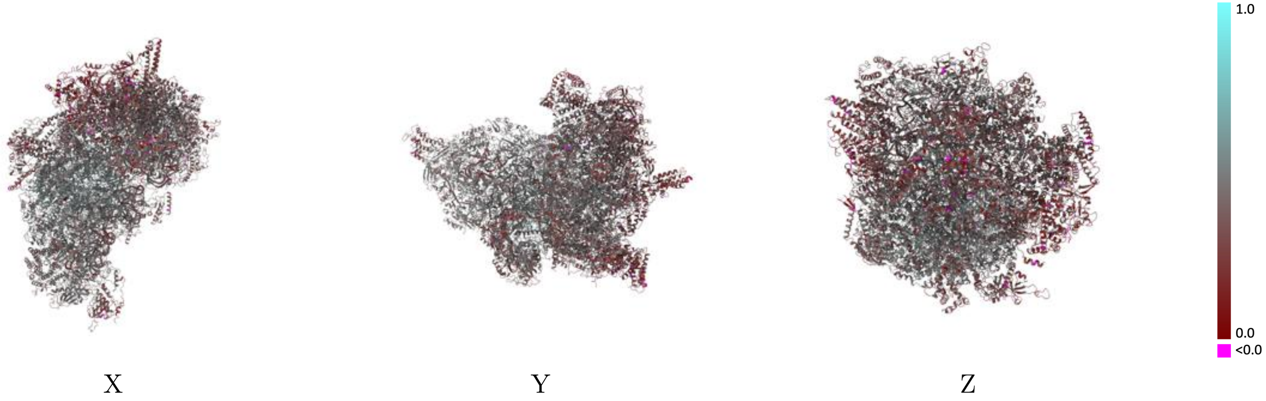
9.1 Map-model overlay ⓘ



X Y Z

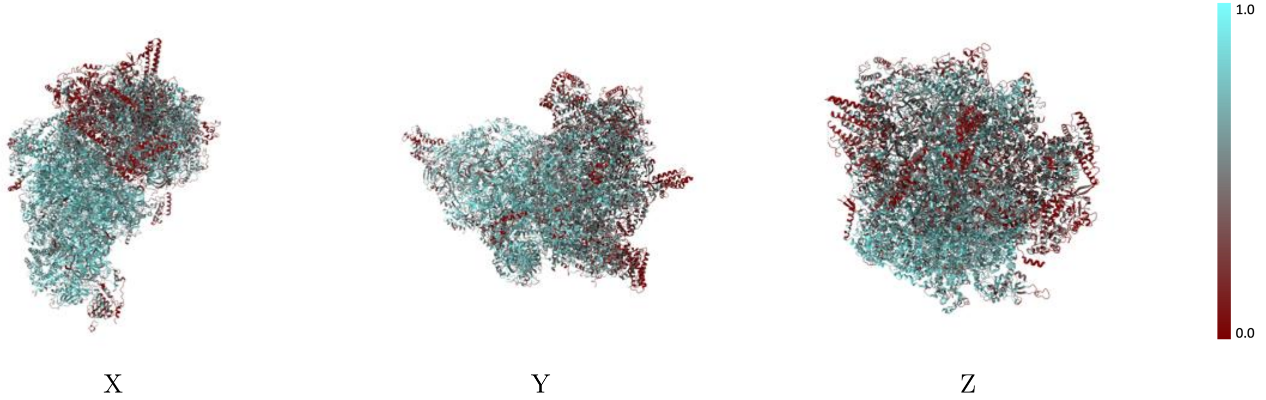
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



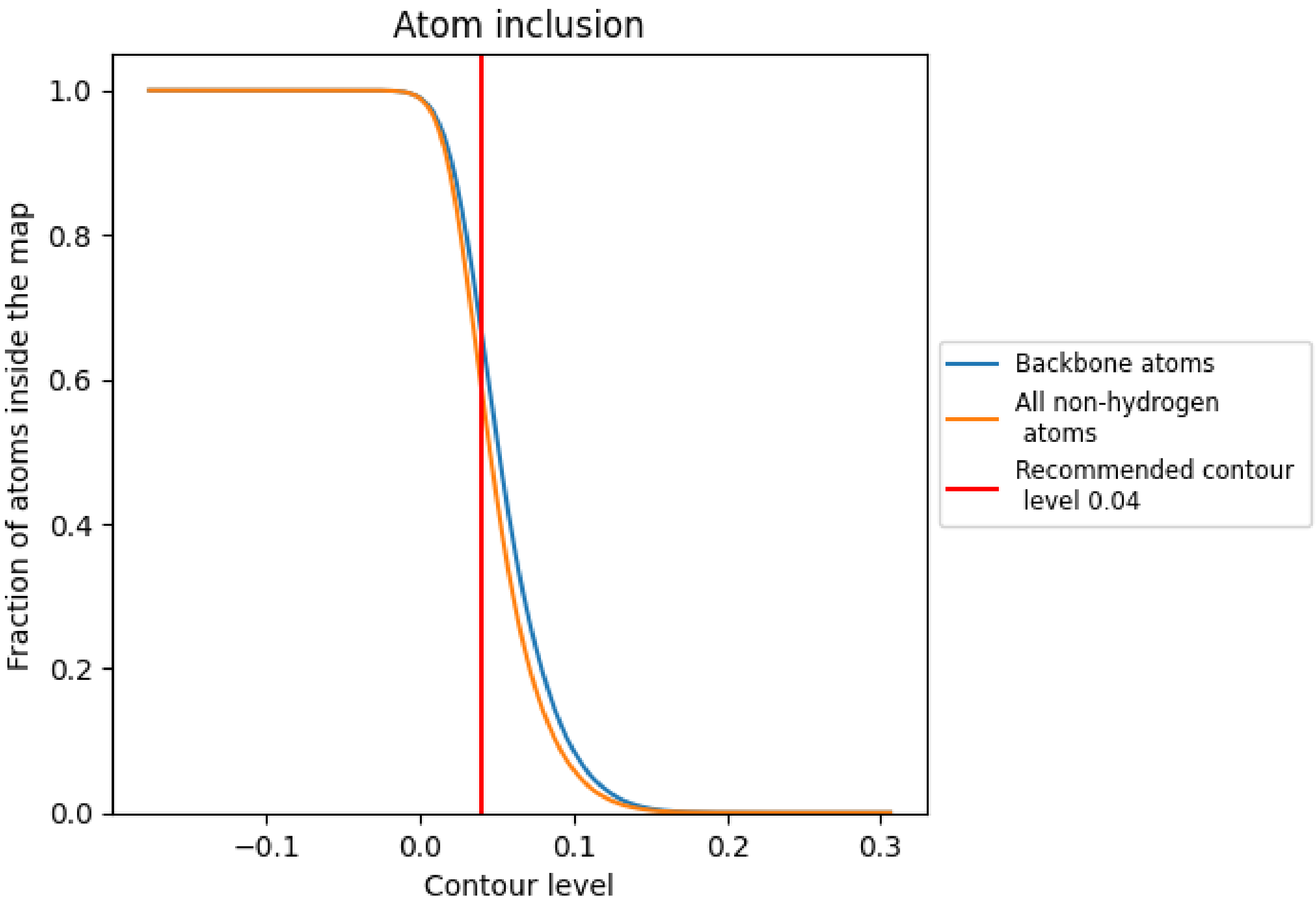
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 67% of all backbone atoms, 59% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5918	0.4160
2	0.7414	0.4140
A	0.6597	0.3980
Ca	0.7416	0.4910
a	0.7315	0.4960
aa	0.6642	0.4110
ab	0.4429	0.3700
ac	0.3202	0.3360
ad	0.7426	0.4560
ae	0.5338	0.3860
af	0.3257	0.3100
ag	0.4689	0.4070
ai	0.7244	0.4790
aj	0.5950	0.4130
ak	0.4275	0.3980
al	0.6325	0.4760
an	0.7687	0.4550
ao	0.7897	0.5040
ap	0.7141	0.4600
aq	0.4735	0.3900
ar	0.7103	0.4430
as	0.6550	0.4210
at	0.6873	0.4310
au	0.5236	0.4330
av	0.5845	0.4390
aw	0.4641	0.4270
ax	0.5110	0.3730
ay	0.5845	0.3680
az	0.5987	0.3830
b	0.7193	0.4210
ba	0.7384	0.5020
bb	0.5982	0.4280
bc	0.2977	0.3440
bd	0.3986	0.3240
be	0.6454	0.4130

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Chain	Atom inclusion	Q-score
c	0.7266	0.5110
d	0.4971	0.4040
e	0.5107	0.4220
f	0.6004	0.4110
g	0.6660	0.4350
h	0.6424	0.4530
i	0.7044	0.4490
j	0.7672	0.4550
k	0.7954	0.4860
l	0.3254	0.3050
m	0.7265	0.4820
n	0.5823	0.4020
p	0.6475	0.4570
q	0.7377	0.4480
r	0.4619	0.3730
s	0.5792	0.4350
t	0.6097	0.4240
u	0.3917	0.3530
v	0.6629	0.4600
w	0.6219	0.4190
x	0.6454	0.4280
y	0.5934	0.3770
z	0.7458	0.4810