



wwPDB EM Validation Summary Report ⓘ

Jul 21, 2025 – 08:14 PM EDT

PDB ID : 8VVV / pdb_00008vvv
EMDB ID : EMD-43570
Title : Mammalian ribosomes bound to Anisomycin in the nonrotated conformation
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.
Deposited on : 2024-01-31
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

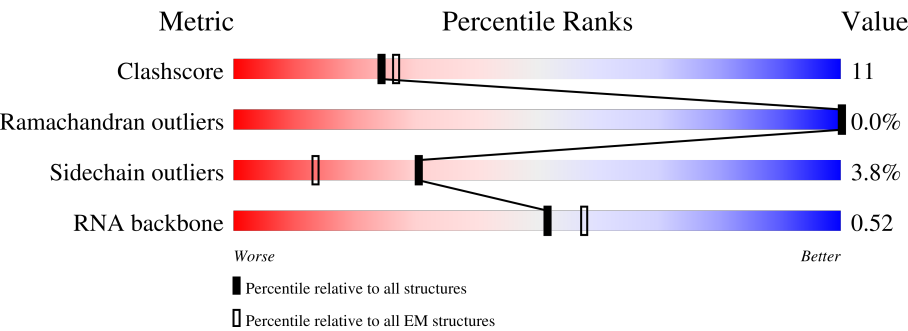
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	<div><div>6%</div><div>70%</div><div>26%</div><div>..</div></div>
2	B	403	<div><div>9%</div><div>73%</div><div>24%</div><div>..</div></div>
3	C	413	<div><div>11%</div><div>68%</div><div>18%</div><div>• 12%</div></div>
4	D	297	<div><div>8%</div><div>79%</div><div>18%</div><div>..</div></div>
5	E	291	<div><div>12%</div><div>59%</div><div>15%</div><div>26%</div></div>
6	F	249	<div><div>8%</div><div>66%</div><div>24%</div><div>10%</div></div>
7	G	319	<div><div>12%</div><div>57%</div><div>15%</div><div>• 27%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	213	
16	Q	188	
17	R	212	
18	S	224	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	AA	295	
27	BB	264	
28	CC	293	
29	5	3635	
30	7	120	
31	8	156	
32	a	147	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	b	245	
34	c	98	
35	d	107	
36	e	128	
37	f	109	
38	g	114	
39	h	122	
40	i	102	
41	j	86	
42	k	69	
43	l	50	
44	m	52	
45	n	25	
46	o	103	
47	p	91	
48	r	124	
49	s	196	
50	t	153	
51	v	839	
52	w	26	
53	9	1698	
54	DD	228	
55	EE	262	
56	FF	204	
57	GG	237	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	HH	194	
59	II	206	
60	JJ	185	
61	KK	96	
62	LL	158	
63	MM	117	
64	NN	149	
65	OO	136	
66	PP	120	
67	QQ	142	
68	RR	132	
69	SS	144	
70	TT	141	
71	UU	100	
72	VV	83	
73	WW	129	
74	XX	141	
75	YY	124	
76	ZZ	75	
77	aa	101	
78	bb	83	
79	cc	62	
80	dd	55	
81	ee	55	
82	ff	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	gg	313	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	B8H	5	3768	-	-	X	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 218932 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 uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1813	577	480	14		

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 5 is a protein called L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	43	SER	ALA	conflict	UNP G1TVT6

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	4	ASP	ASN	conflict	UNP G1TFE0
Q	14	ARG	TRP	conflict	UNP G1TFE0
Q	53	MET	LEU	conflict	UNP G1TFE0
Q	58	ARG	TRP	conflict	UNP G1TFE0
Q	75	ARG	GLN	conflict	UNP G1TFE0
Q	80	ALA	PRO	conflict	UNP G1TFE0
Q	86	VAL	ILE	conflict	UNP G1TFE0
Q	104	ARG	HIS	conflict	UNP G1TFE0
Q	110	ARG	CYS	conflict	UNP G1TFE0
Q	137	VAL	GLY	conflict	UNP G1TFE0
Q	157	GLY	ARG	conflict	UNP G1TFE0
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	LEU	VAL	conflict	UNP G1TSG1
U	32	GLY	ARG	conflict	UNP G1TSG1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	62	SER	THR	conflict	UNP G1TSG1
U	63	LEU	ILE	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1
U	106	THR	SER	conflict	UNP G1TSG1
U	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 21 is a protein called L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	78	SER	PHE	conflict	UNP G1SE28

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 27 is a protein called S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 28 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 29 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	3529	Total	C	N	O	P	0	0
			75791	33817	13856	24589	3529		

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 31 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 32 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 33 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 34 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 35 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 36 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 37 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 38 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 39 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 41 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 42 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 43 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 44 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 45 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 46 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 48 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 49 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 50 is a protein called eL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 51 is a protein called eukaryotic elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	839	Total	C	N	O	S	0	0
			6544	4162	1122	1216	44		

- Molecule 52 is a protein called Serpine mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	w	26	Total	C	N	O	0	0
			216	129	43	44		

- Molecule 53 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	9	1697	Total	C	N	O	P	0	0
			36243	16181	6506	11860	1696		

- Molecule 54 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 55 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 56 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 57 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 58 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 60 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 61 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 63 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 64 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 65 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 67 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 68 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 69 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 70 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 71 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 72 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 73 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 74 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 75 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 76 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	28	ARG	CYS	conflict	UNP G1TFE8
aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 78 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 80 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 82 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	A	1	Total	Mg	0
			1	1	
84	P	1	Total	Mg	0
			1	1	
84	V	1	Total	Mg	0
			1	1	
84	5	197	Total	Mg	0
			197	197	
84	7	6	Total	Mg	0
			6	6	
84	8	6	Total	Mg	0
			6	6	
84	a	1	Total	Mg	0
			1	1	
84	g	1	Total	Mg	0
			1	1	
84	j	1	Total	Mg	0
			1	1	
84	v	1	Total	Mg	0
			1	1	
84	9	75	Total	Mg	0
			75	75	
84	SS	1	Total	Mg	0
			1	1	

Continued on next page...

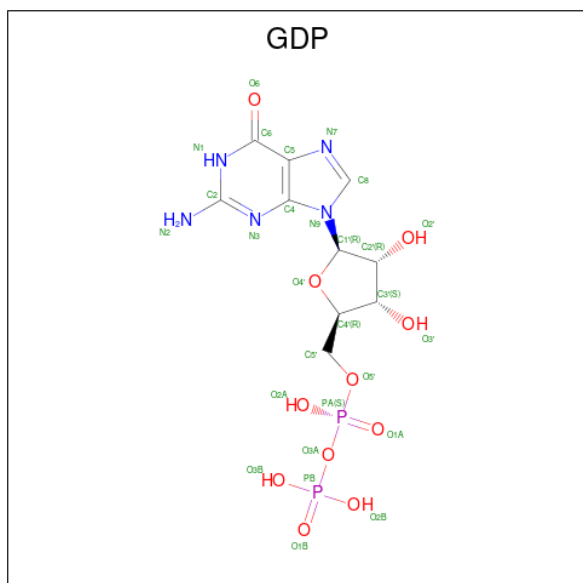
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
84	TT	1	Total	Mg	0
			1	1	
84	dd	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	
85	dd	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	

- Molecule 86 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

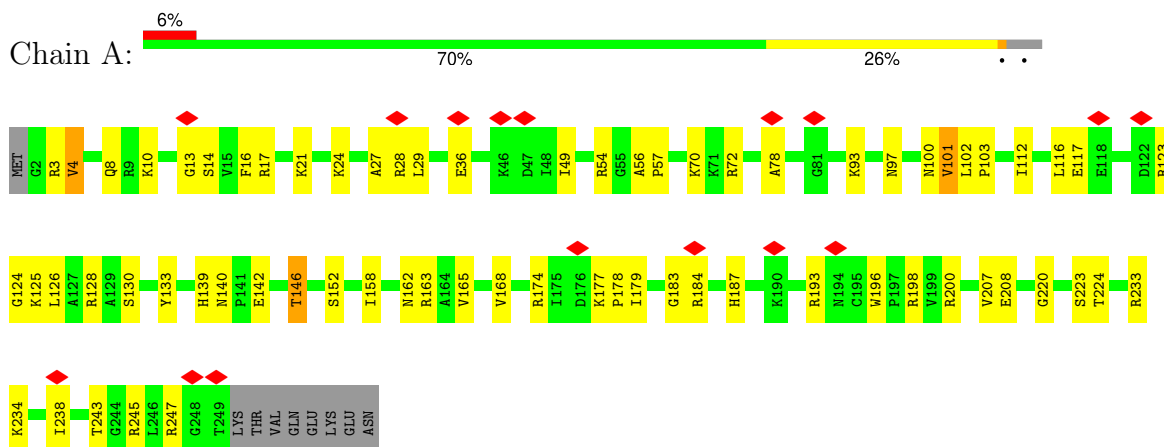


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	v	1	28	10	5	11	2	0

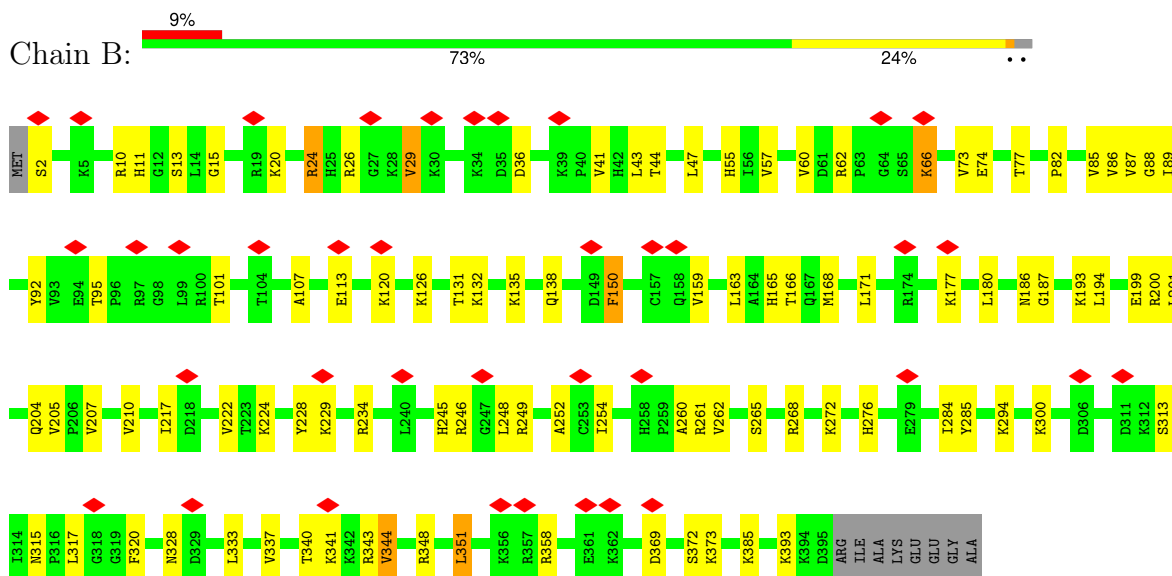
3 Residue-property plots

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: uL2

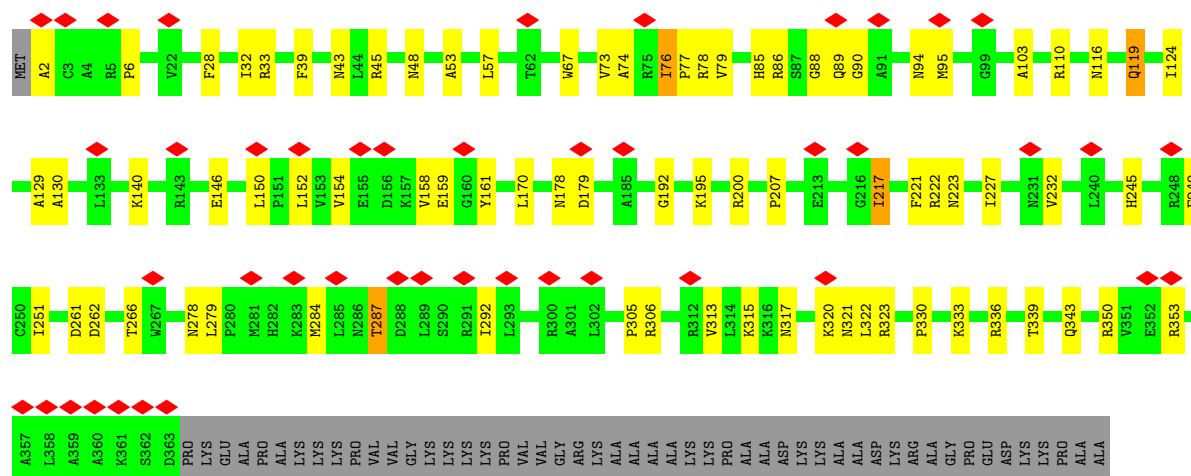


• Molecule 2: uL3

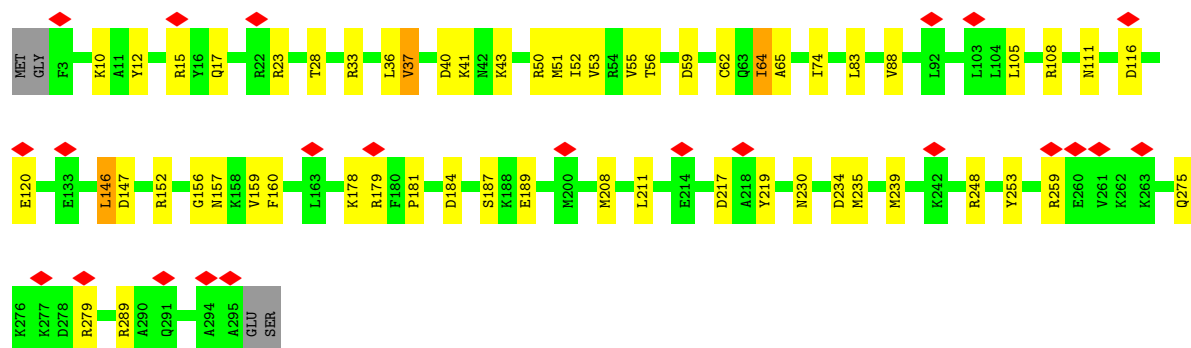
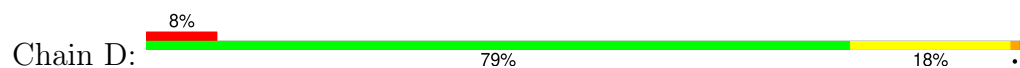


• Molecule 3: uL4

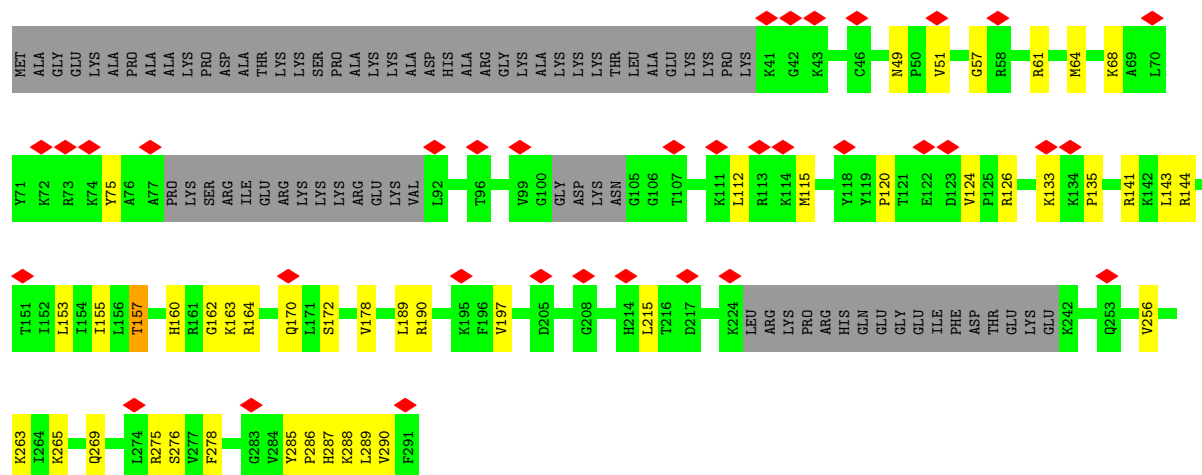




• Molecule 4: uL18

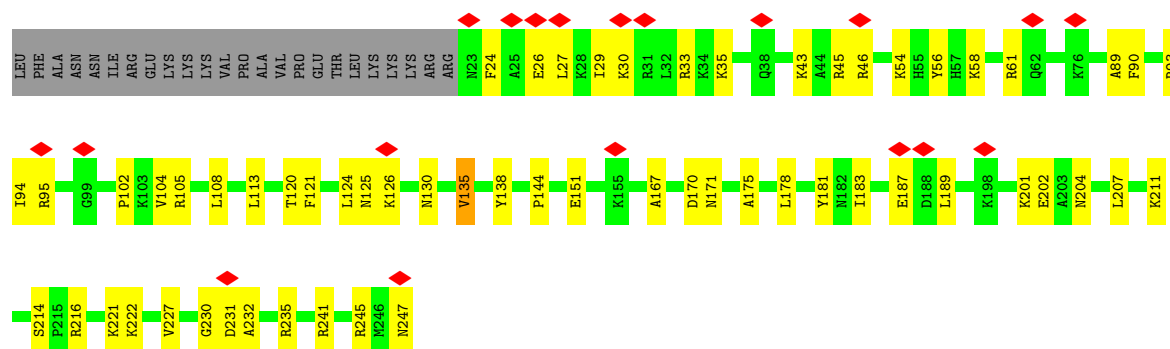


• Molecule 5: L6

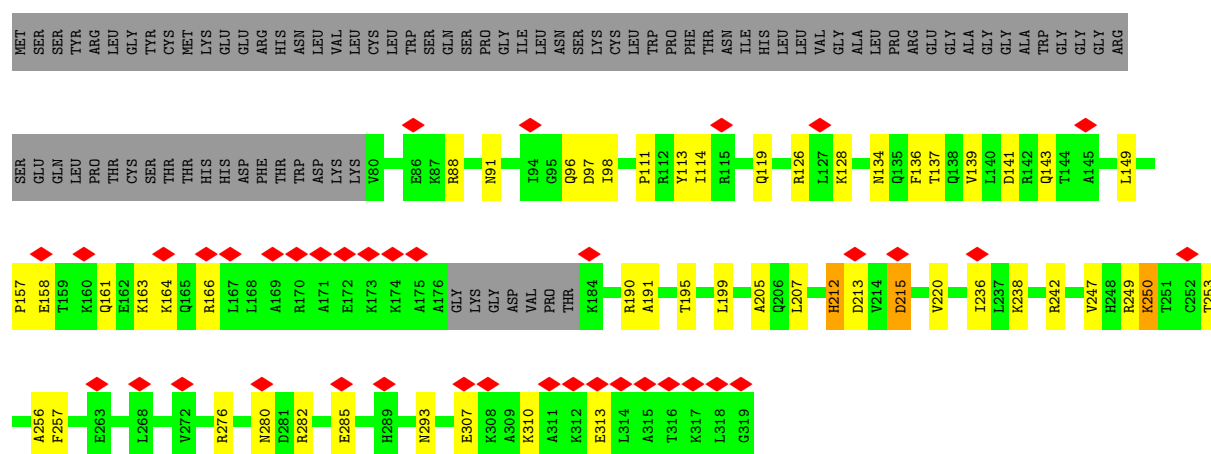


• Molecule 6: uL30

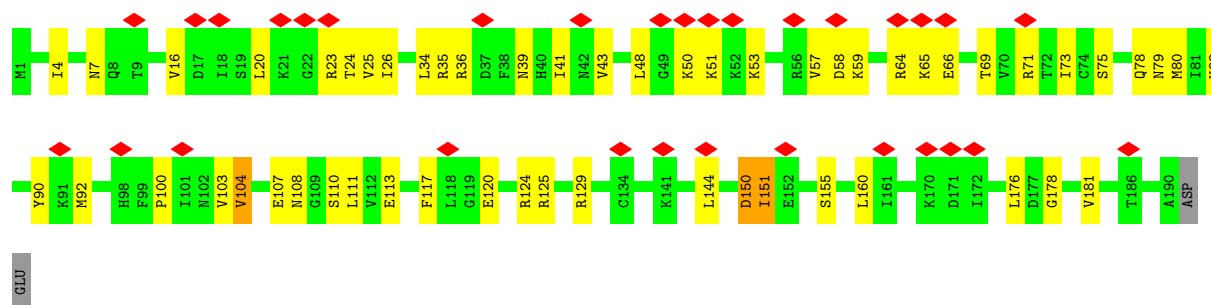




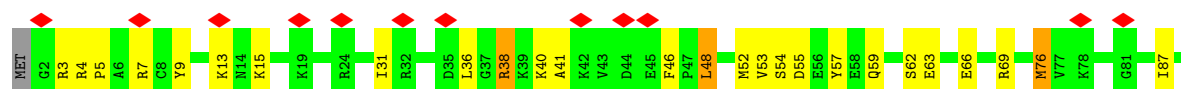
• Molecule 7: eL8

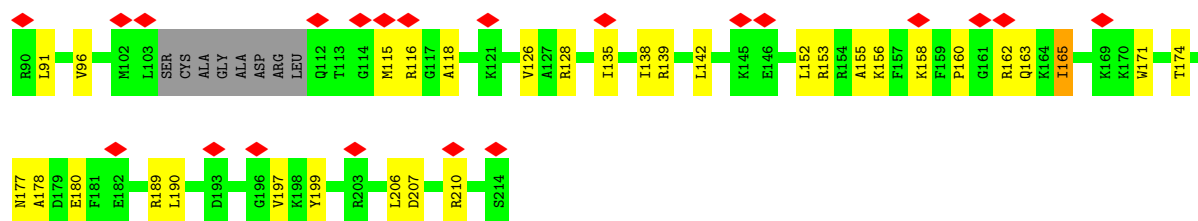


• Molecule 8: uL6

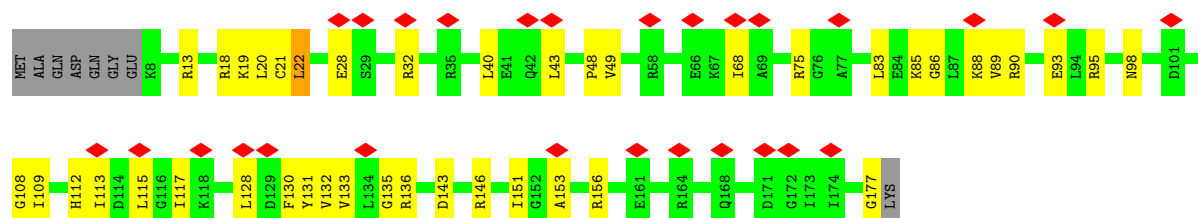


• Molecule 9: L10

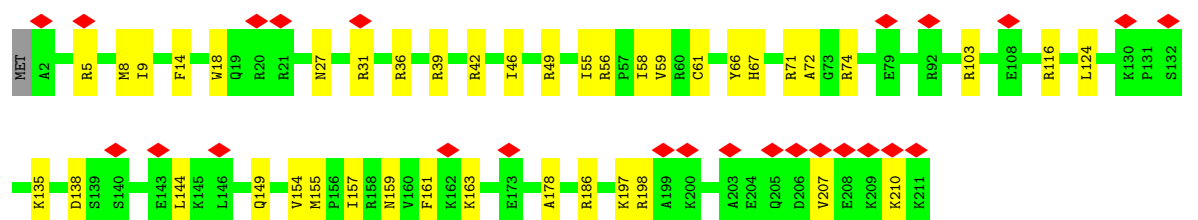
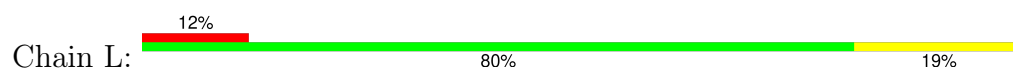




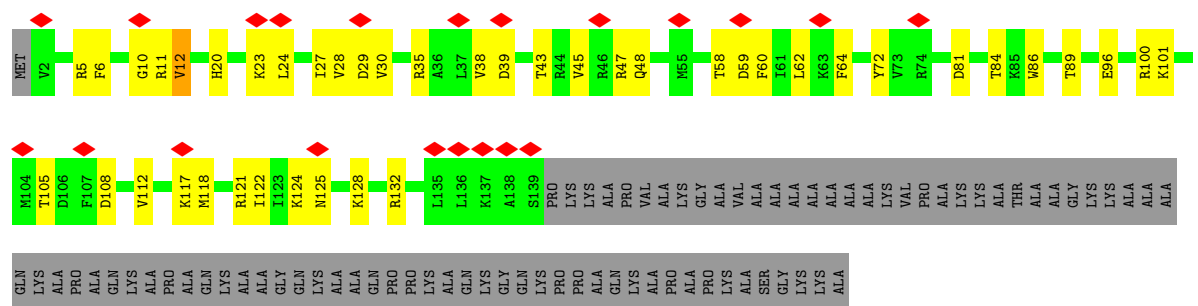
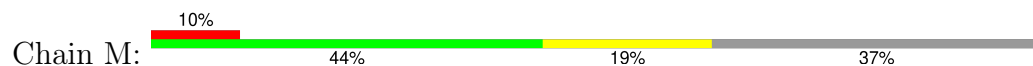
• Molecule 10: uL5



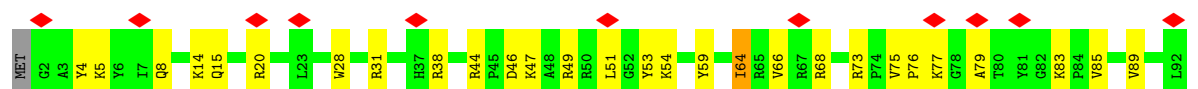
• Molecule 11: eL13

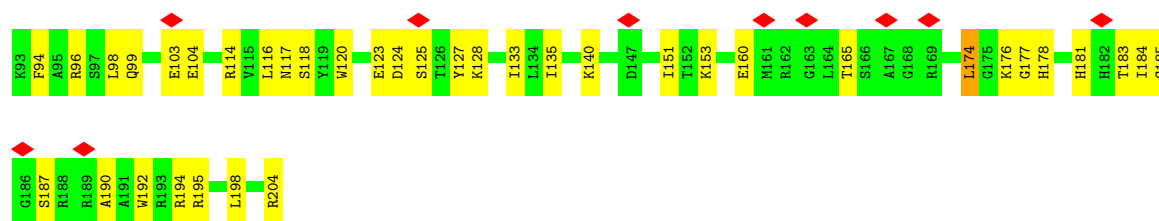


• Molecule 12: eL14

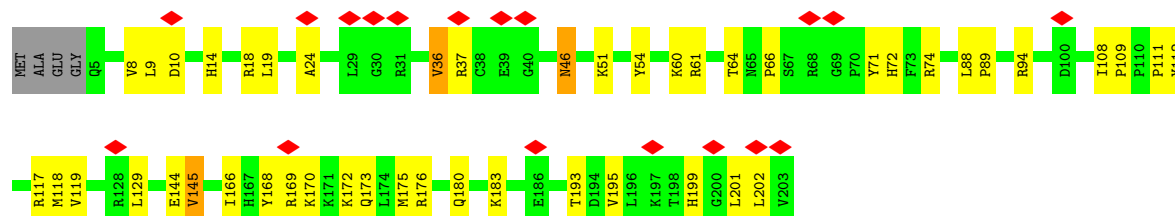
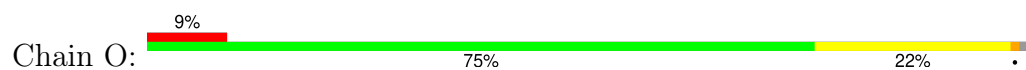


• Molecule 13: eL15

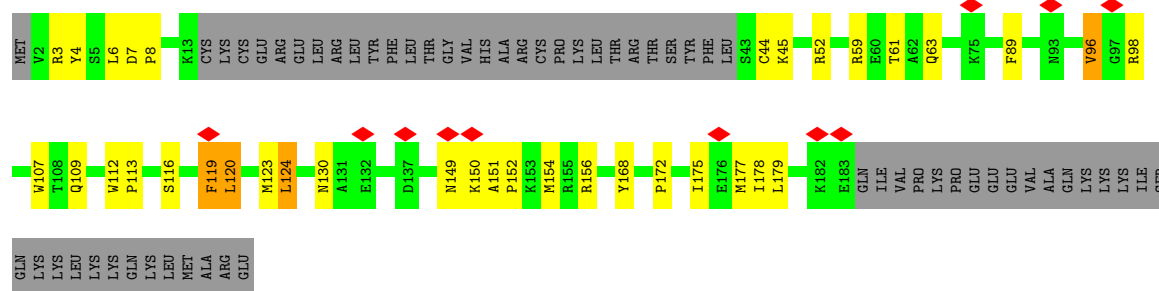




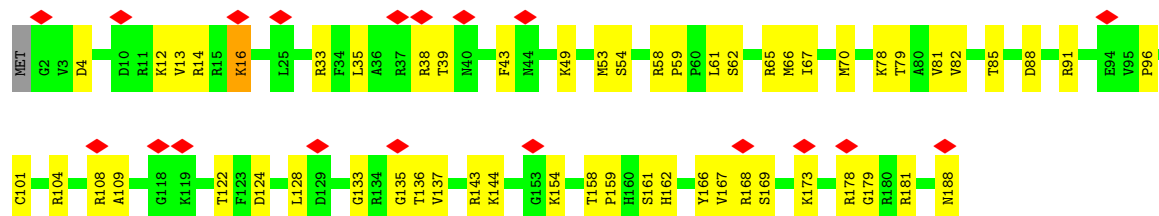
• Molecule 14: uL13



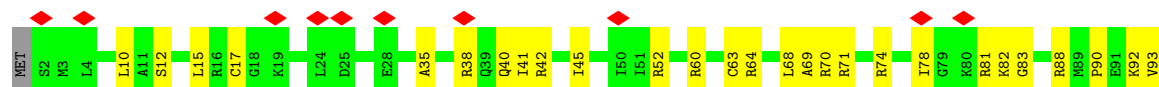
• Molecule 15: uL22



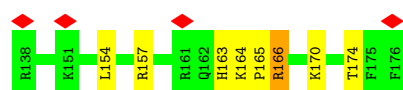
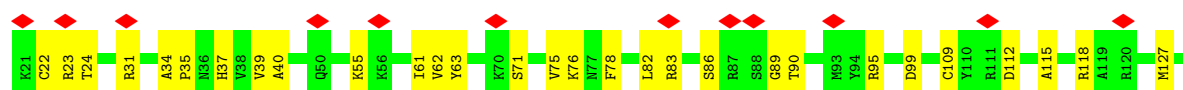
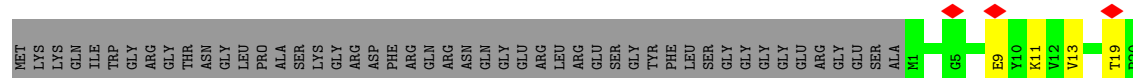
• Molecule 16: eL18



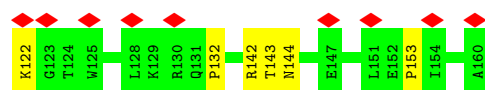
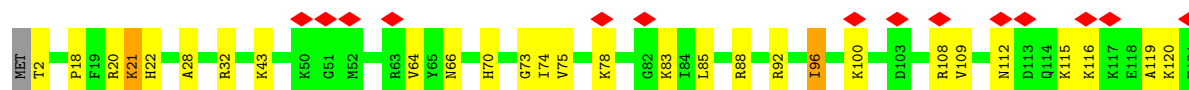
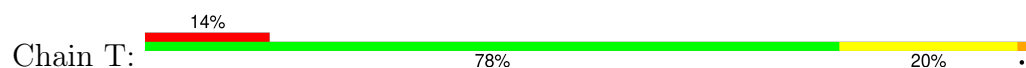
• Molecule 17: eL19



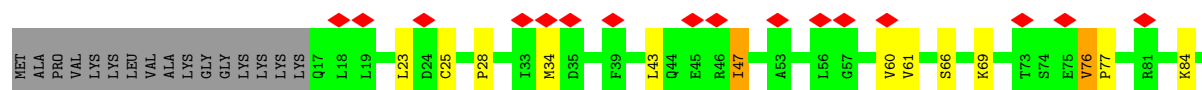
- Molecule 18: eL20



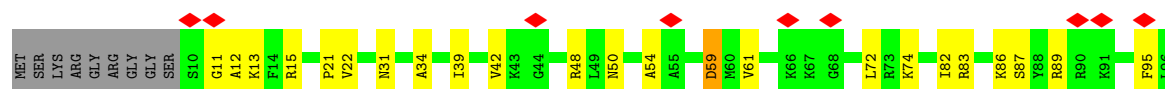
- Molecule 19: eL21



- Molecule 20: eL22

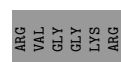
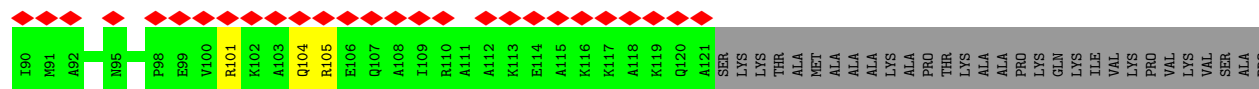
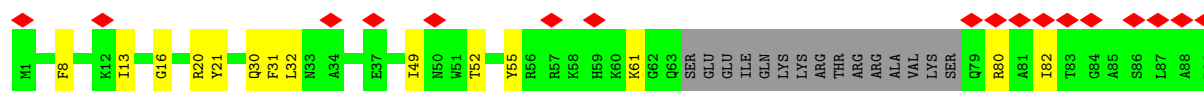


- Molecule 21: L23

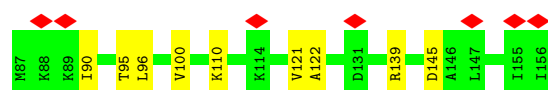
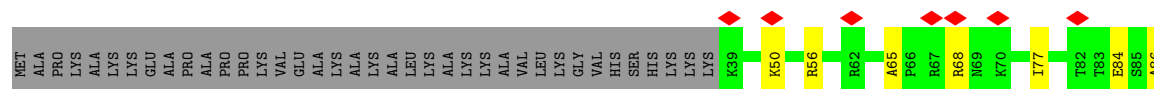




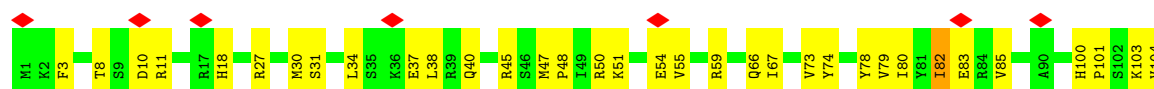
• Molecule 22: uL24



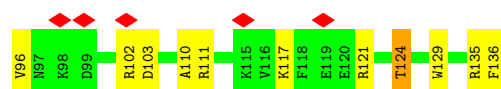
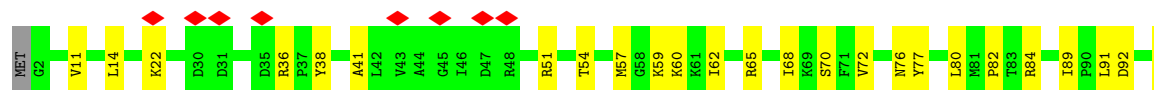
• Molecule 23: uL23

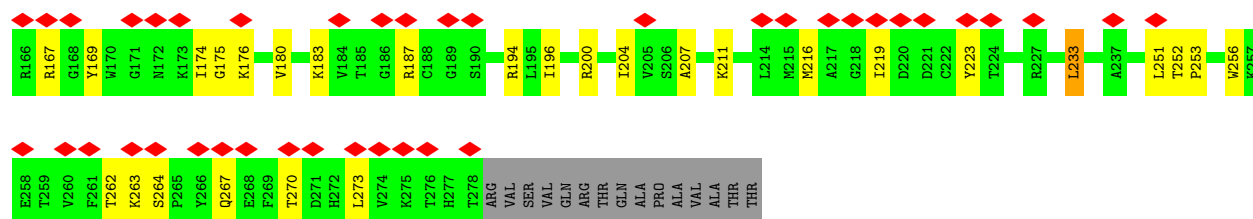


• Molecule 24: L26

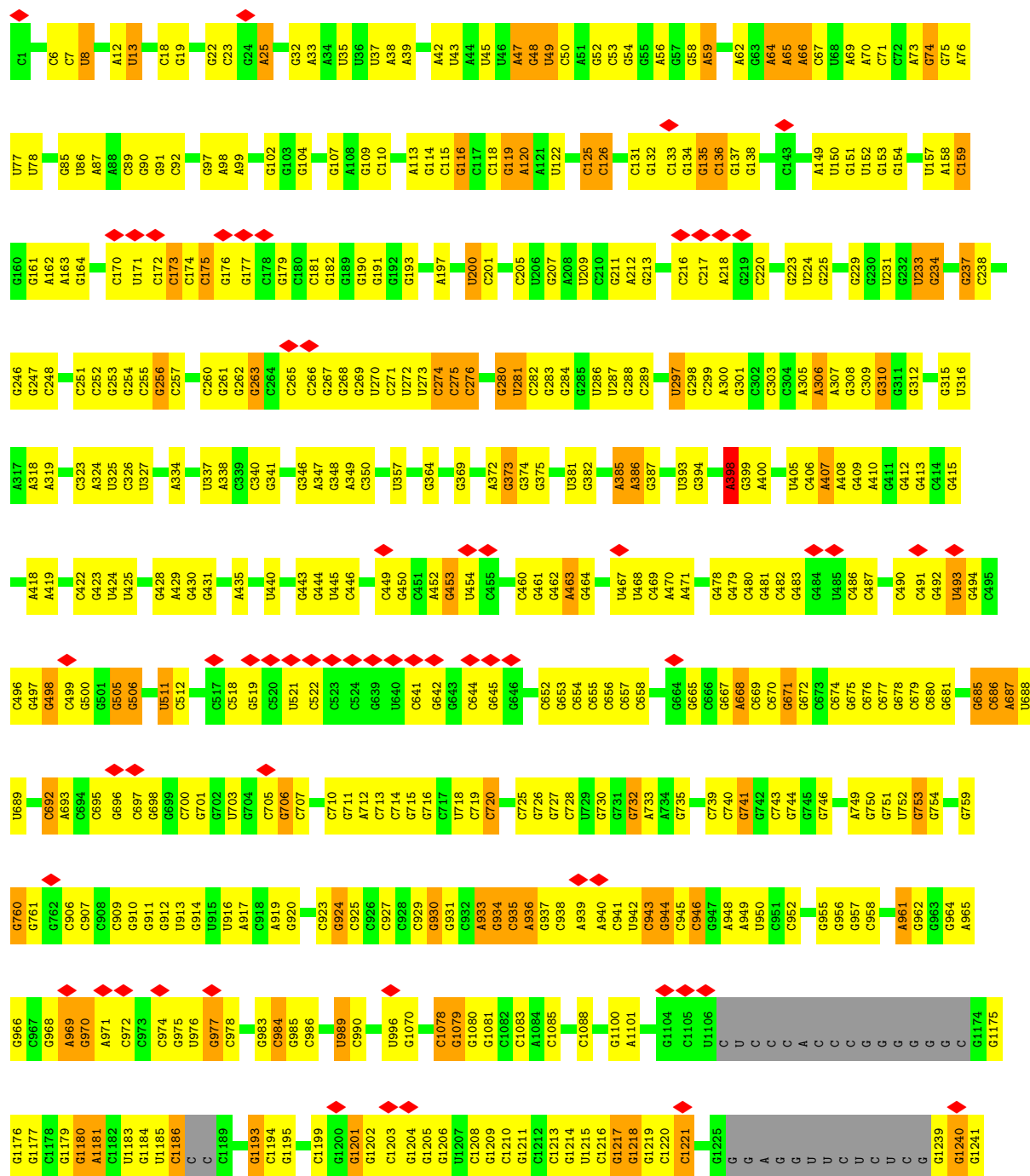
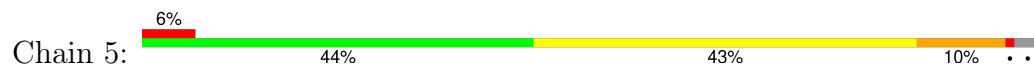


• Molecule 25: L27





• Molecule 29: 28S rRNA



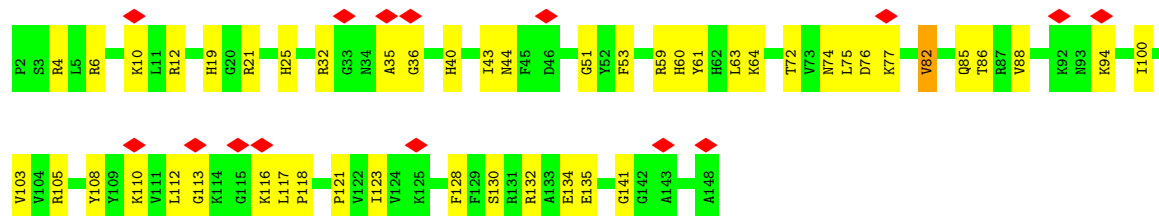
C2447	C2448	C2449	C2454	A2455	A2459	C2463	C2464	C2465	A2466	C2467	C2468	C2469	C2470	C2471	C2472	U2473	U2474	U2477	G2480	G2481	A2482	A2483	C2484	C2485	C2486	C2487	C2488	C2489	A2490	U2491	G2492	G2493	C2494	C2495	U2496	C2497	C2498	C2499	A2508	C2509	C2510	C2511	C2512	A2513	U2514	A2519	C2520	G2521	G2522								
C2343	C2344	C2345	C2346	A2347	G2351	C2354	C2357	A2366	C2367	U2368	C2369	A2370	C2371	A2376	A2380	A2381	C2382	C2383	C2386	U2390	U2391	C2396	A2395	C2396	A2401	A2402	G2405	G2406	A2407	G2408	A2409	A2410	G2411	G2412	C2416	C2417	A2418	U2419	G2420	A2423	C2428	A2429	C2430	G2431	U2431	G2439											
G2270	G2271	C2272	U2273	A2274	G2279	C2280	A2282	C2283	G2284	G2289	C2290	A2291	C2292	G2293	C2294	C2295	C2298	A2381	C2382	C2383	G2386	U2390	U2391	C2396	A2395	C2396	A2401	A2402	G2405	G2406	A2407	G2408	A2409	A2410	G2411	G2412	C2416	C2417	A2418	U2419	G2420	A2423	C2428	A2429	C2430	G2431	U2431	G2439									
G2055	G2056	C2057	G2058	C2059	U2060	G2061	A2062	G2063	G2066	U2067	C2068	G2069	G2070	A2075	C2079	G2081	C2082	C2083	G2084	U2085	U2086	C2087	C2088	C2089	U2090	G2095	U2096	G2099	C2100	A2101	G2102	A2103	G2104	C2105	G2106	A2107	G2108	A2109	A2110	A2111	G2112	A2113	A2115	G2116	U2117	C2264	G2265	G2266	G2267	A2269							
G1978	G1979	U1980	G1981	G1982	C1983	C1984	U1985	U1986	G1987	C1988	G1989	A1990	G1991	U1992	C1993	G1994	G1995	A1996	U1997	U1998	C2000	G2001	C2002	U2003	G2006	G2007	A2008	G2009	U2010	G2013	U2014	A2015	A2016	C2017	A2018	U2021	C2022	G2027	A2031	A2032	A2035	A2036	U2044	G2045	A2046	A2047	G2051	G2052	A2053	U2054							
A1897	G1901	A1902	A1903	G1910	U1911	U1912	A1913	A1914	G1915	C1920	U1924	G1925	C1926	C1927	G1928	U1933	C1934	A1935	U1936	C1937	A1938	G1939	A1940	C1944	A1945	U1946	A1947	A1948	A1949	A1950	G1951	G1954	U1955	U1956	G1957	U1960	G1961	A1962	U1963	A1964	U1965	A1966	G1967	A1970	A1973	G1974	G1975	A1976	U1977								
A1748	A1749	A1752	G1756	G1759	U1760	C1761	U1762	U1763	G1764	G1765	G1766	C1768	C1769	G1770	A1771	A1772	A1773	C1774	G1775	A1776	U1777	C1778	U1779	C1780	A1781	A1782	U1785	A1786	U1787	A1792	A1793	A1794	C1795	U1798	A1799	A1800	A1801	U1802	G1803	A1808	G1809	A1810	A1811	G1812	C1813	C1814	G1821	C1822	U1823	G1824							
G1825	U1826	G1830	A1831	C1832	C1833	C1834	G1836	G1837	C1838	G1841	A1842	A1843	G1846	C1847	G1848	C1853	C1854	U1855	A1856	C1857	U1858	C1859	G1861	U1866	U1867	G1870	U1871	U1872	A1873	A1874	G1875	C1876	A1877	G1878	A1879	A1880	C1881	U1882	G1883	C1884	C1885	G1886	C1887	U1888	G1889	C1890	G1891	G1892	G1893	A1894							
A1553	A1559	A1560	G1561	C1562	C1563	A1564	G1565	A1566	A1569	A1570	A1571	C1572	U1575	G1576	G1579	G1580	G1583	U1584	C1585	C1586	C1587	U1588	U1597	C1598	A1599	C1600	C1601	U1602	A1607	U1608	C1609	G1610	G1611	U1612	G1618	A1619	C1620	U1621	U1622	G1623	A1627	U1628	A1629	G1630	C1631	C1632	G1633	G1634	G1635								
U1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	G1496	A1497	G1498	G1499	U1500	G1501	G1502	A1503	U1504	C1505	A1506	C1507	U1508	A1509	G1510	C1511	G1512	C1513	A1514	C1515	U1516	U1517	U1518	C1519	A1520	A1521	G1522	G1523	A1524	G1528	A1529	A1530	A1531	G1536	U1537	U1538	A1539	A1540	C1541	U1542	C1547	U1477	C1478
G1406	C1407	C1408	G1409	G1410	C1411	G	C	C	C	C	C	C	G1418	C1419	C1420	G1421	G1425	A1426	G1427	C1436	A1439	C1440	G1441	C1442	C1443	U1444	U1446	C1447	C1448	C1449	U1450	U1451	C1452	C1453	G1454	C1455	C1456	G1457	G1461	C1462	G1463	C1464	A1465	C1466	C1467	A1468	C1469	C1470	G1471	C1474	U1477	C1478					
A1332	A1333	A1334	G1335	A1336	C1337	C1338	A1339	A1340	G1344	U1345	C1346	U1347	A1348	C1349	C1350	A1351	C1352	G1353	U1354	A1355	C1356	G1357	A1360	G1364	G1365	C1366	G1367	C1368	G1376	A1377	A1378	G1383	G1386	G1387	G1388	G1389	C1390	C1391	C1392	C1393	G1396	A1397	A1398	A1399	A1403	A1404	G1405										






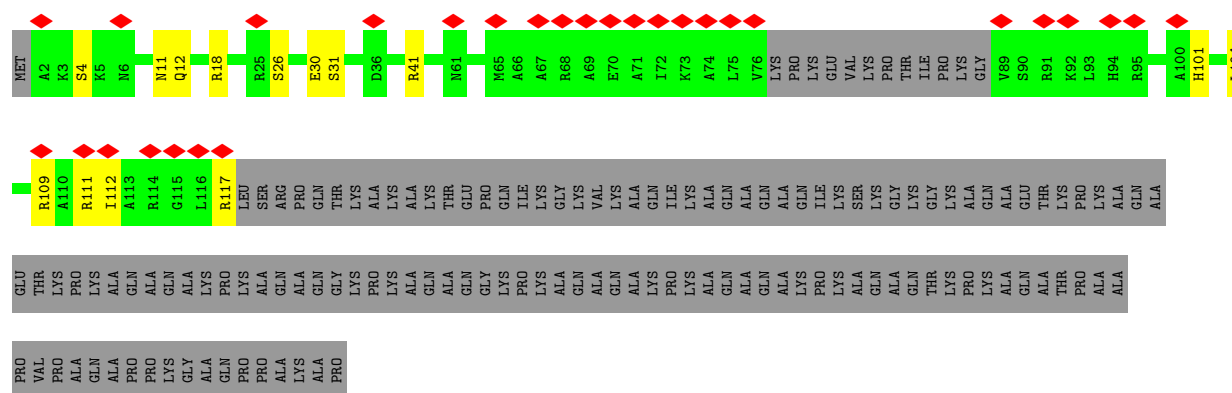
- Molecule 32: uL15

Chain a: 



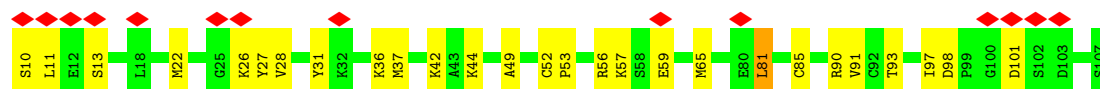
- Molecule 33: eL29

Chain b: 




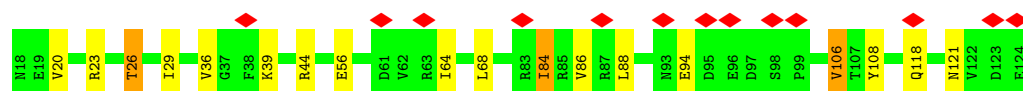
- Molecule 34: eL30

Chain c: 




- Molecule 35: eL31

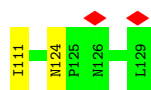
Chain d: 



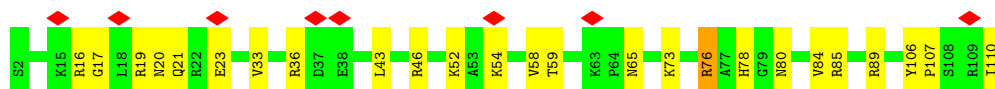
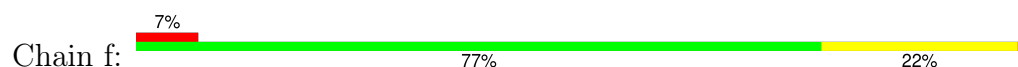
- Molecule 36: eL32

Chain e: 

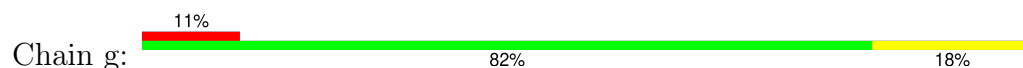




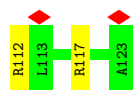
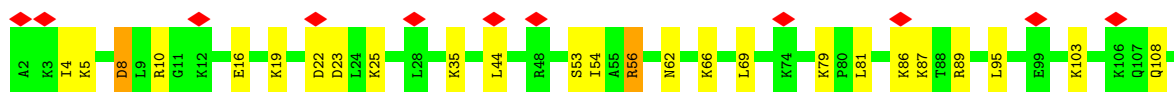
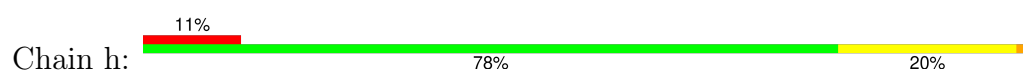
• Molecule 37: eL33



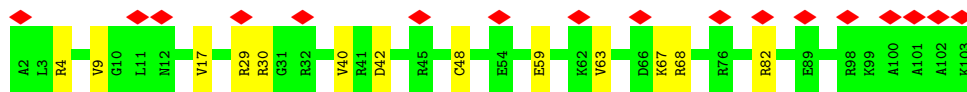
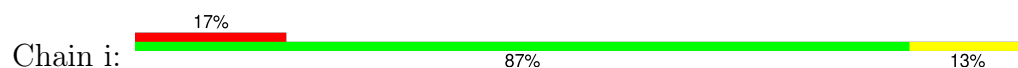
• Molecule 38: eL34



• Molecule 39: uL29



• Molecule 40: eL36



• Molecule 41: eL37

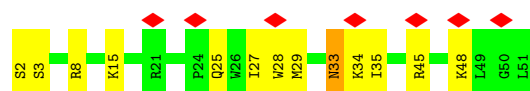
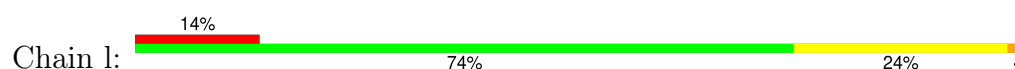


• Molecule 42: eL38

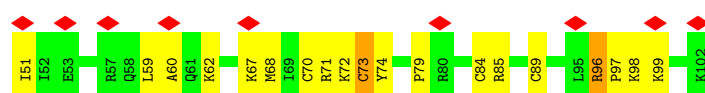




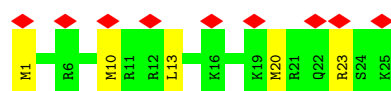
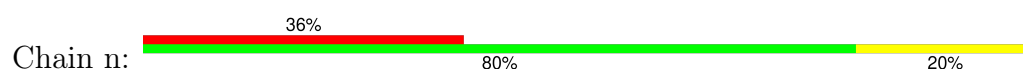
• Molecule 43: eL39



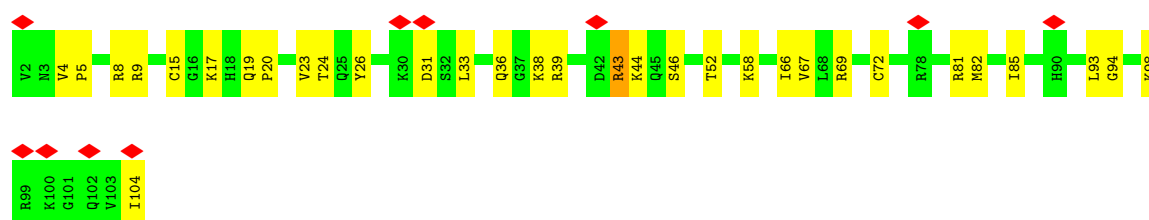
• Molecule 44: eL40



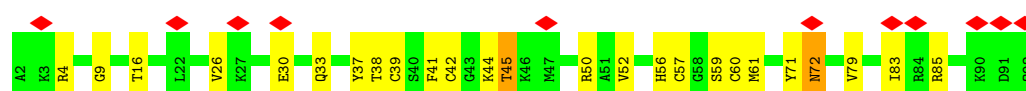
• Molecule 45: eL41



• Molecule 46: eL42

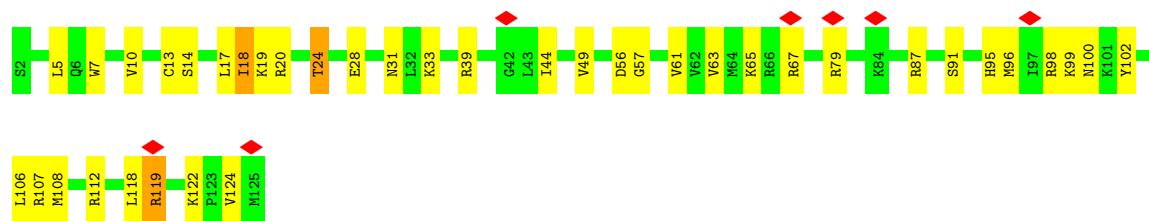


• Molecule 47: eL43

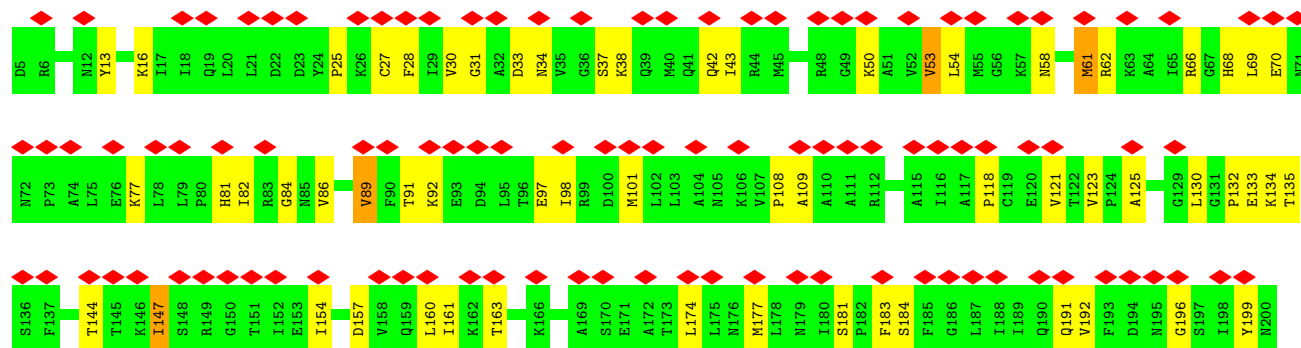


• Molecule 48: eL28

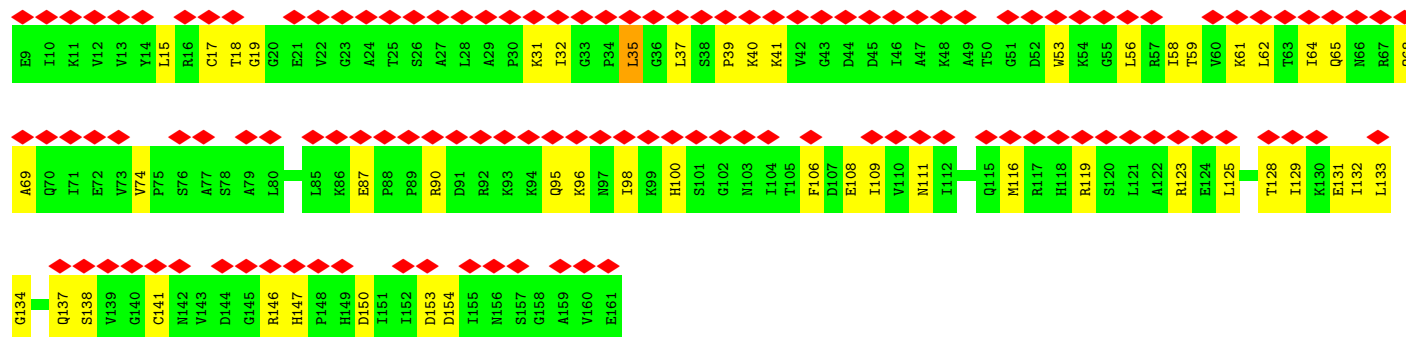
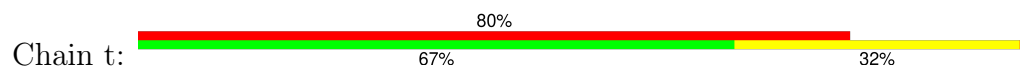




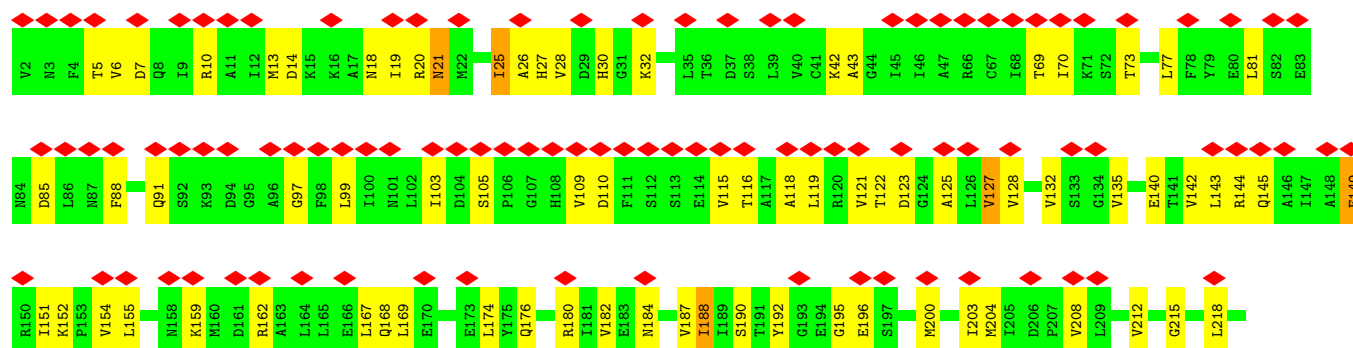
• Molecule 49: uL10

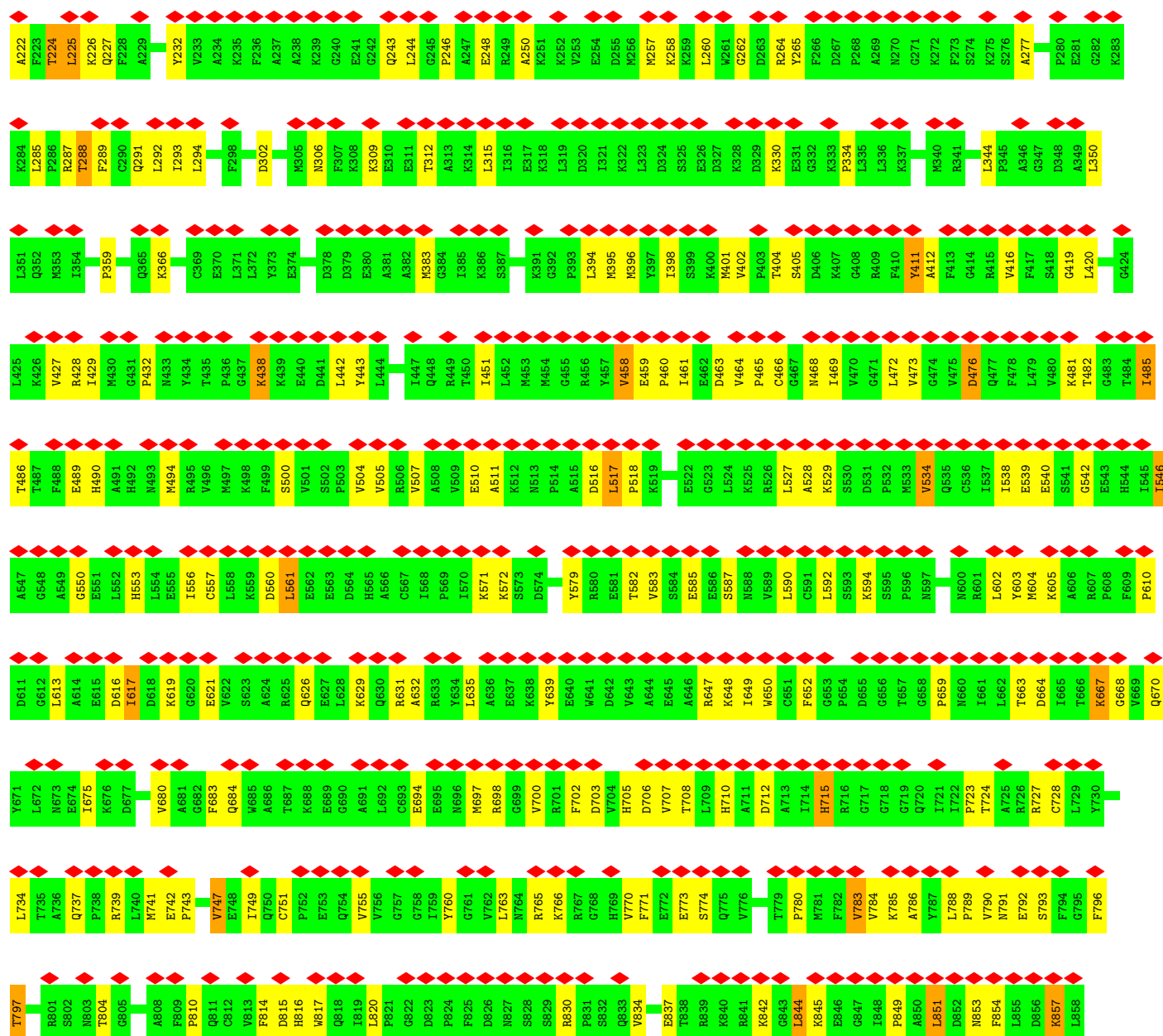


• Molecule 50: eL11

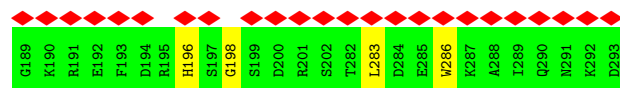
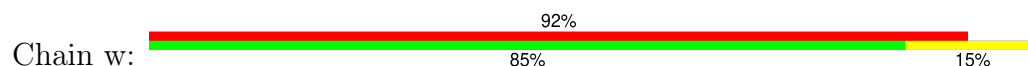


• Molecule 51: eukaryotic elongation factor 2

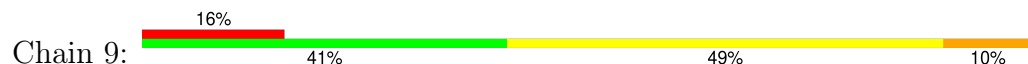




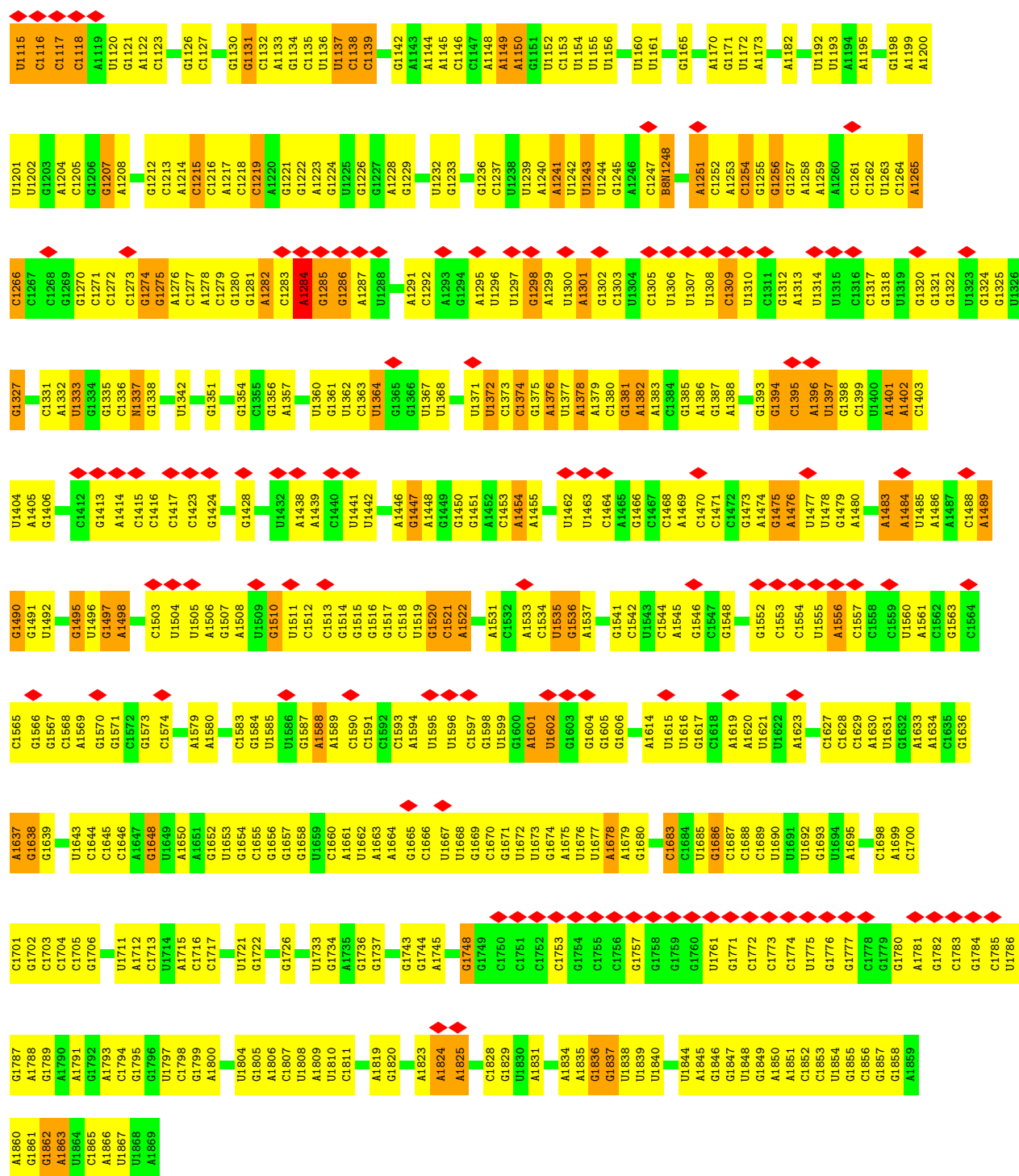
• Molecule 52: Serpine mRNA binding protein 1

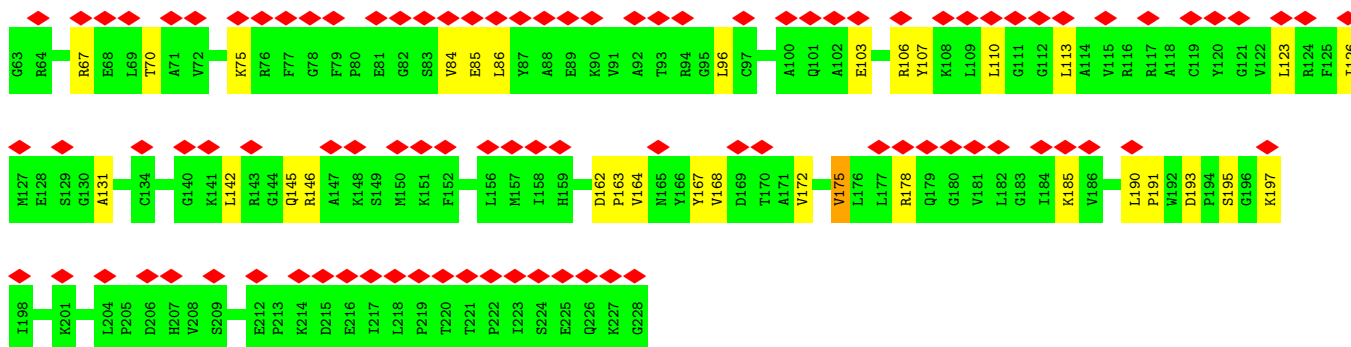


• Molecule 53: 18S rRNA

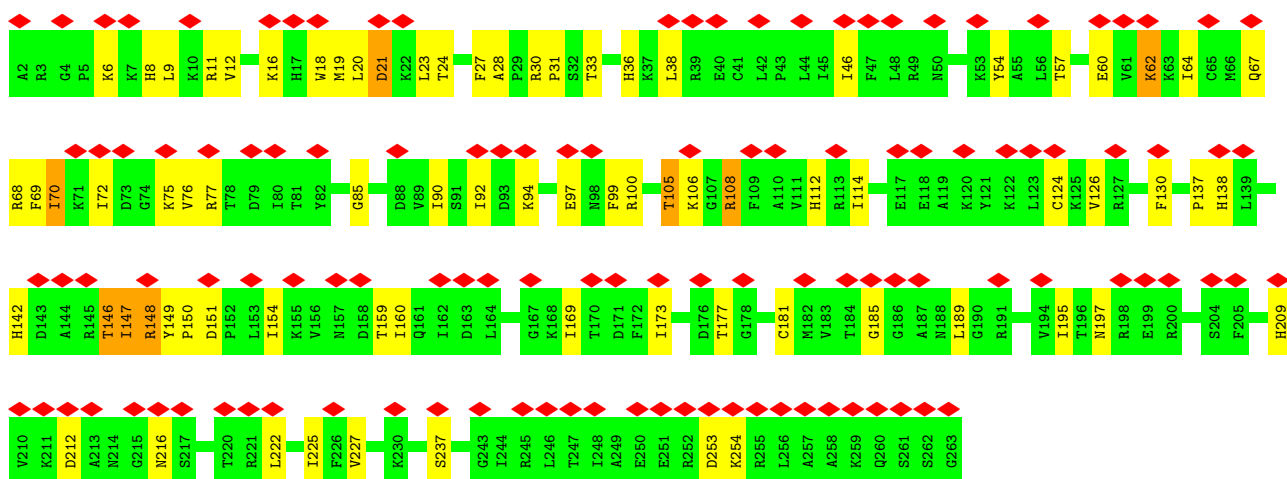
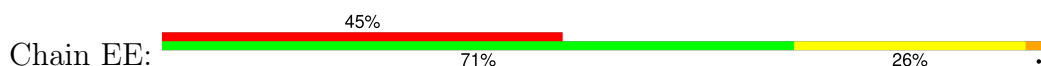




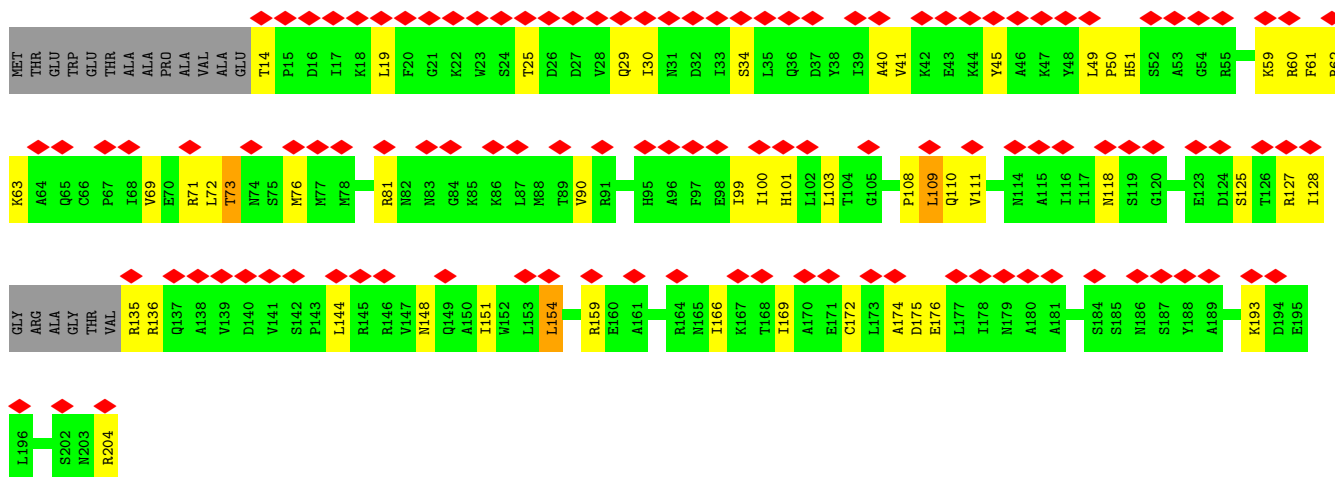




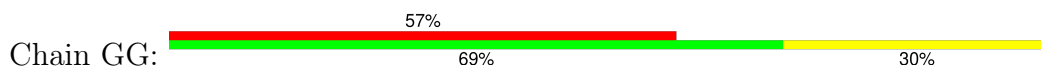
• Molecule 55: eS4

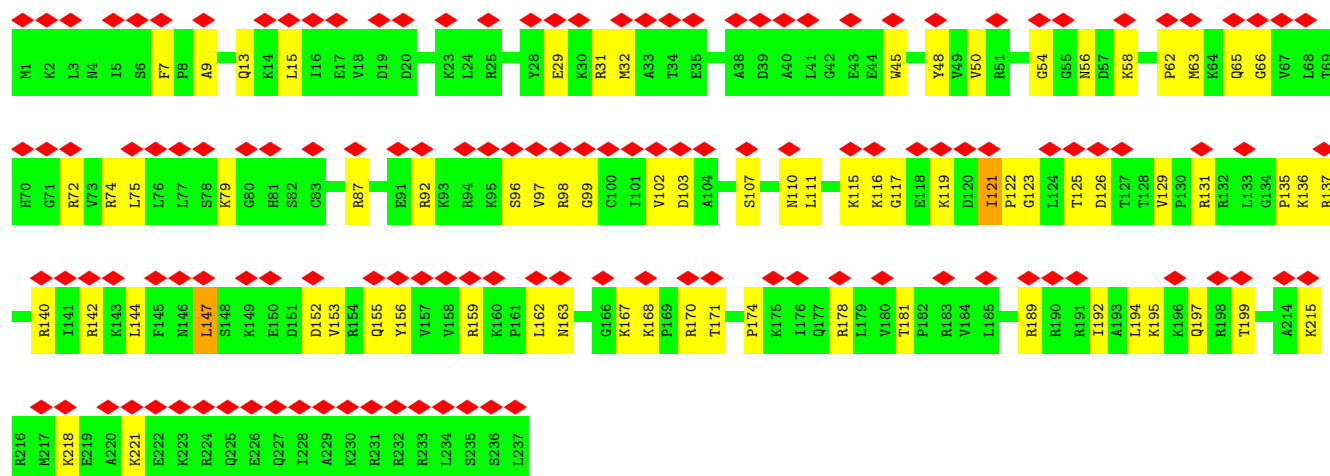


• Molecule 56: uS7

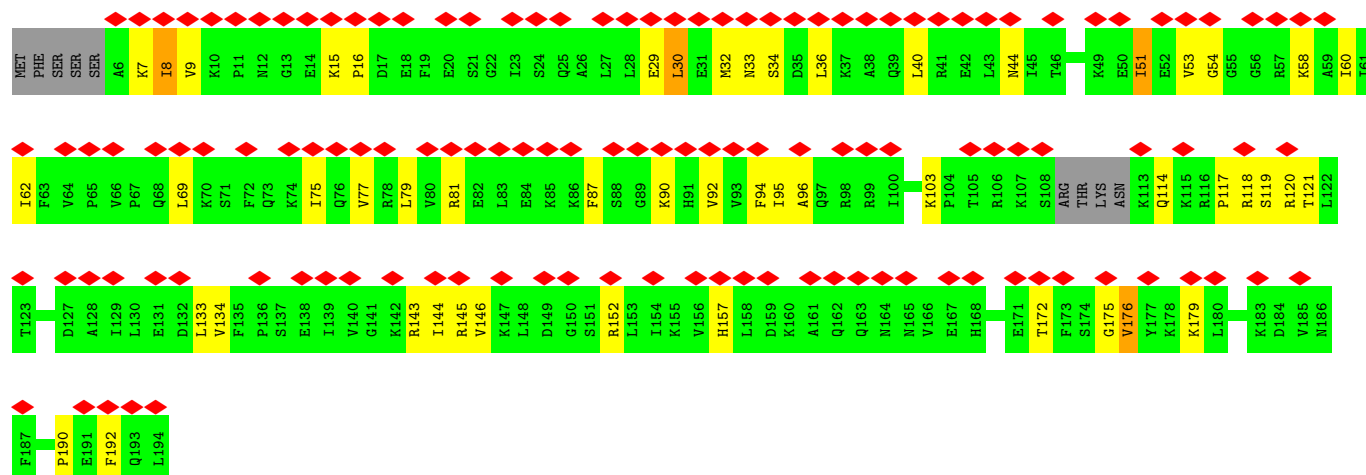


• Molecule 57: eS6

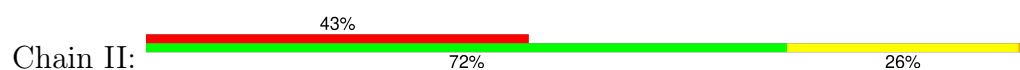




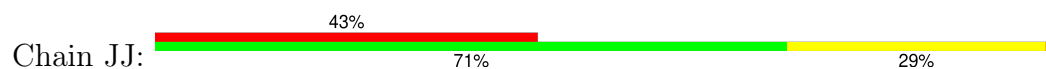
• Molecule 58: eS7

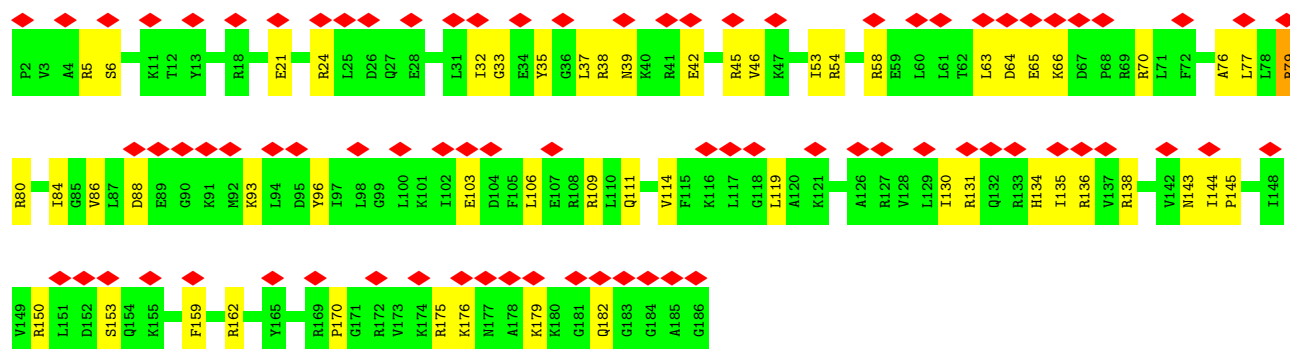


• Molecule 59: eS8

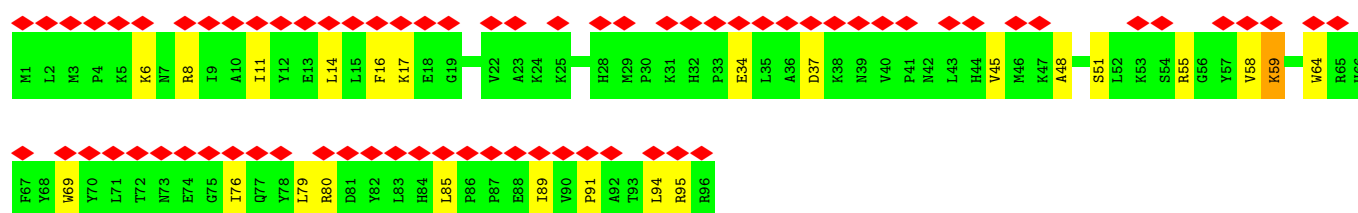
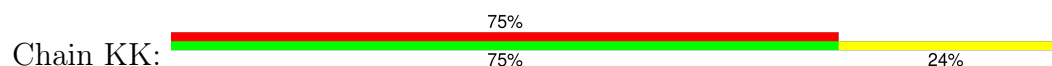


• Molecule 60: uS4

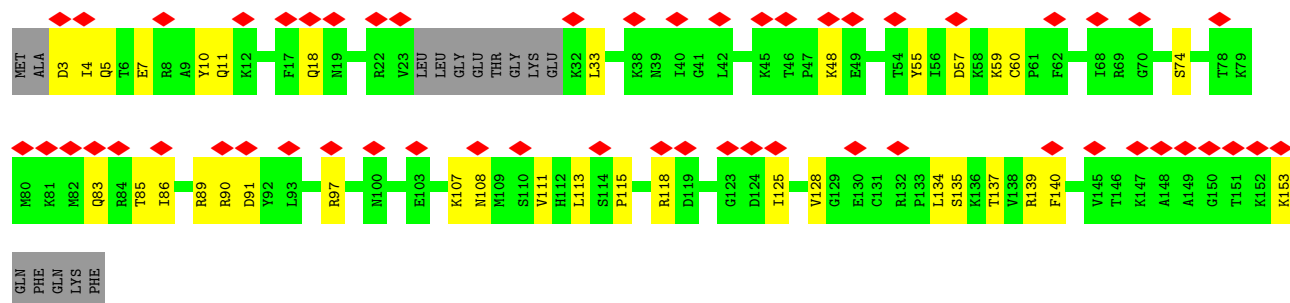




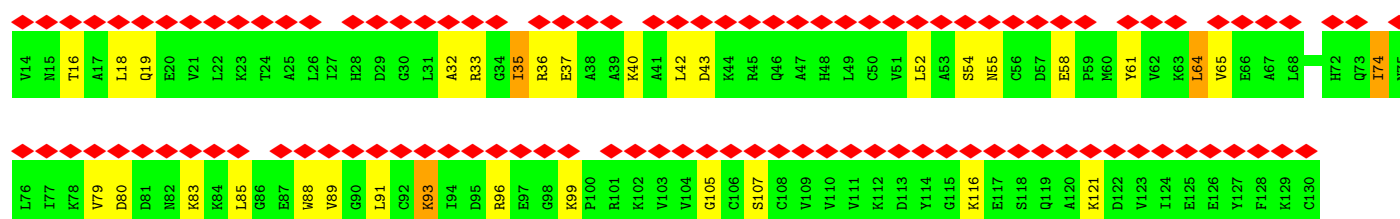
• Molecule 61: eS10



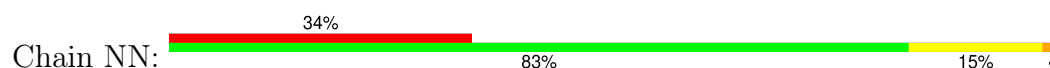
• Molecule 62: uS17

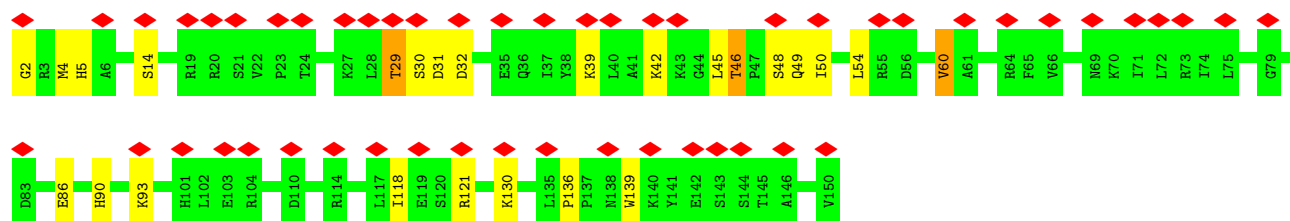


• Molecule 63: eS12

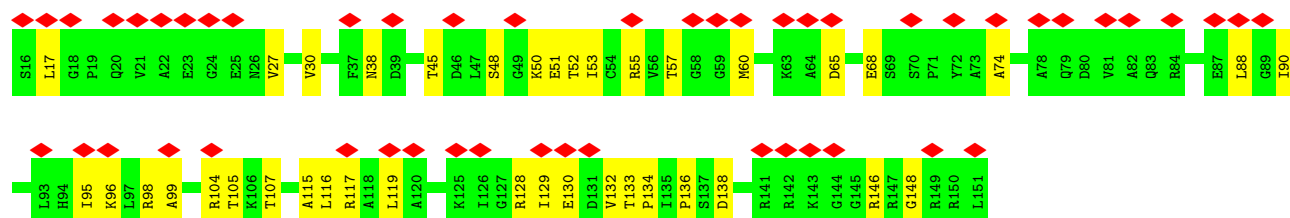
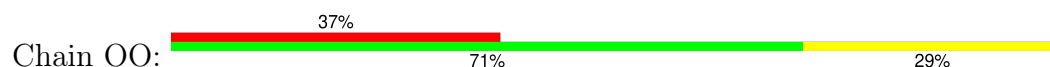


• Molecule 64: uS15

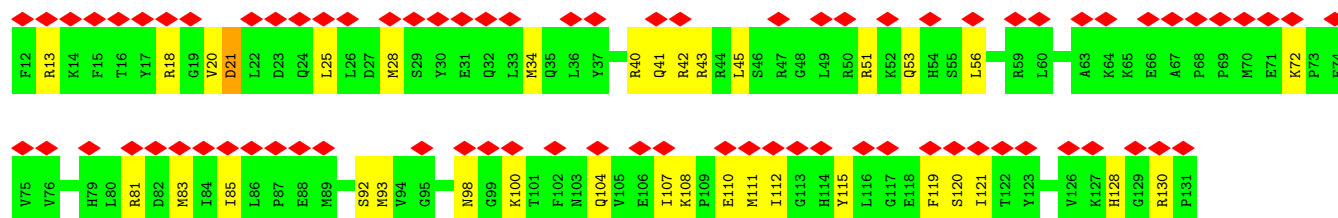
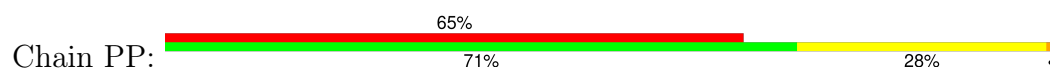




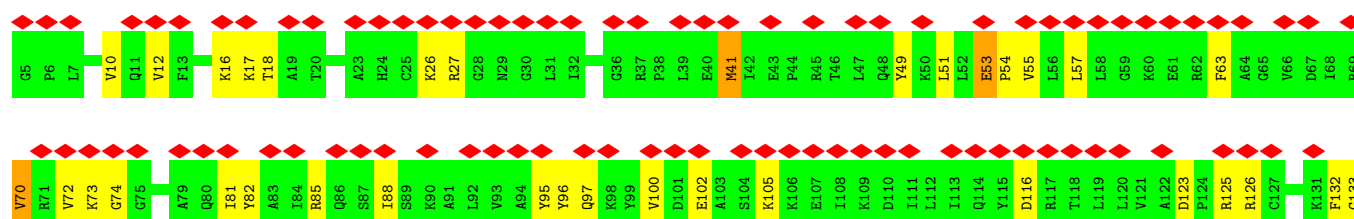
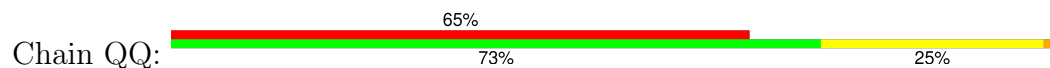
• Molecule 65: uS11



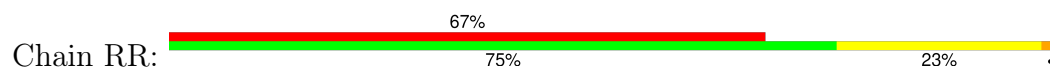
• Molecule 66: uS19

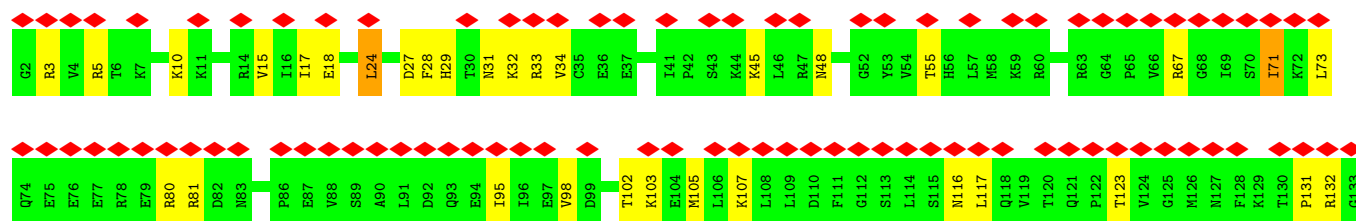


• Molecule 67: uS9

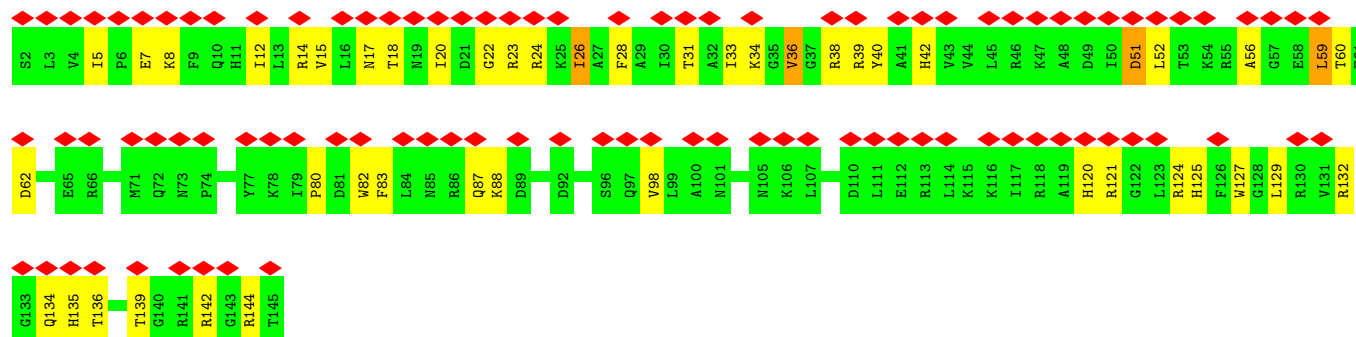


• Molecule 68: eS17

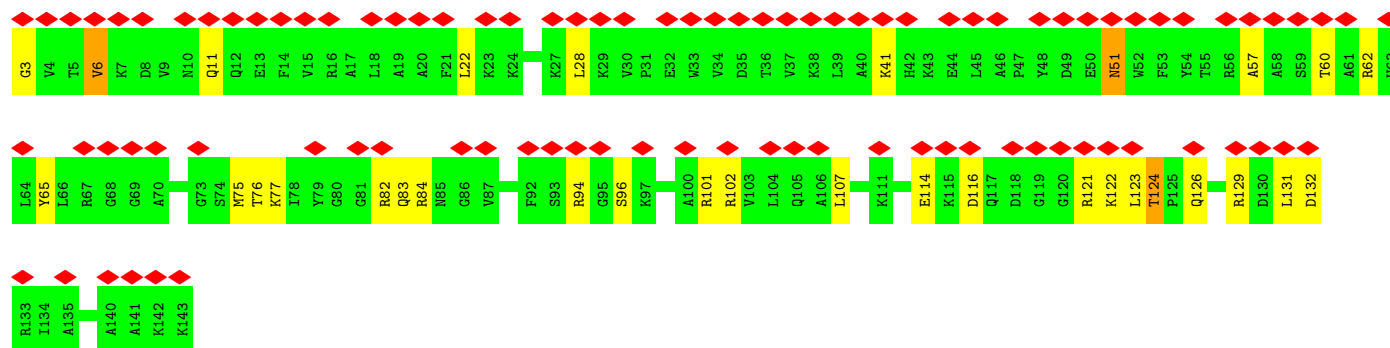
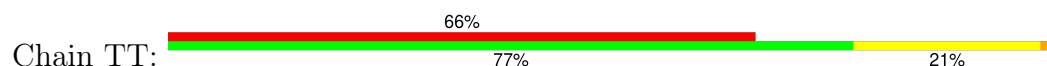




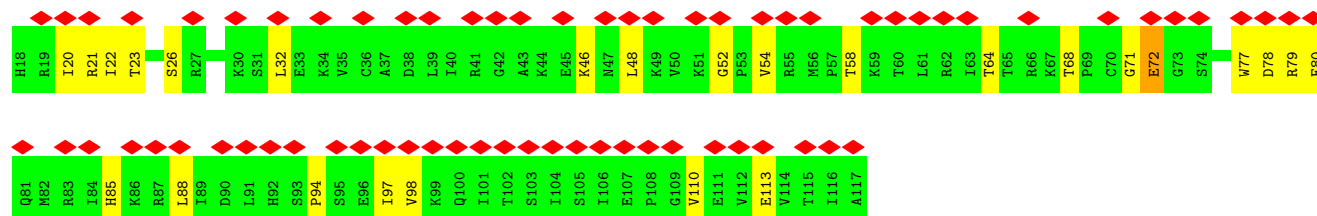
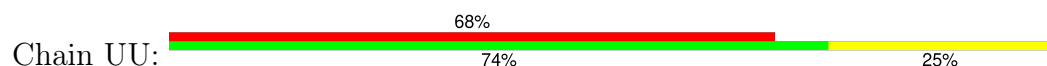
• Molecule 69: uS13



• Molecule 70: eS19

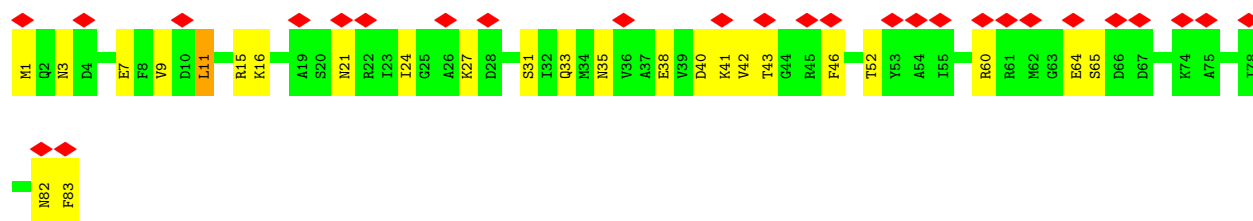


• Molecule 71: uS10

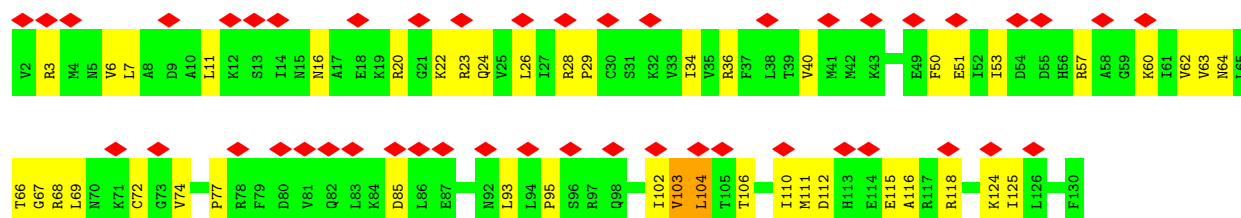
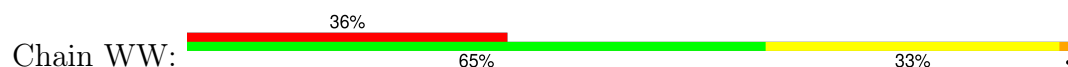


• Molecule 72: eS21

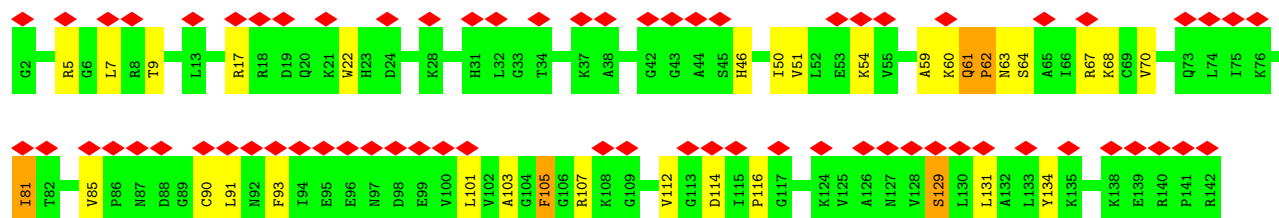
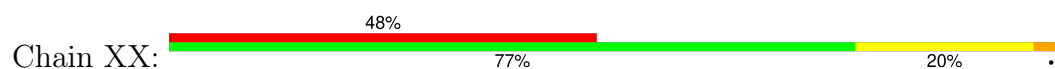




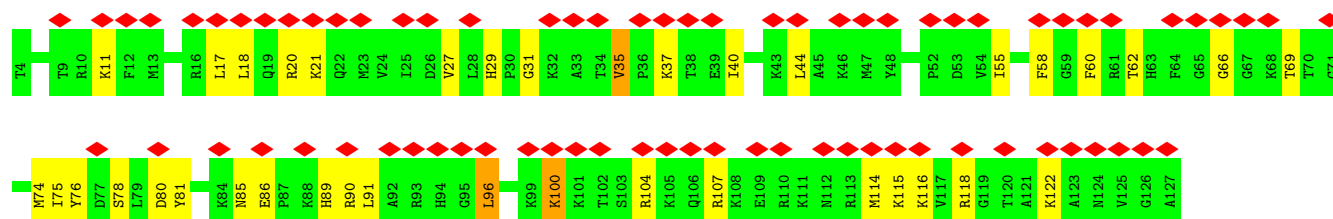
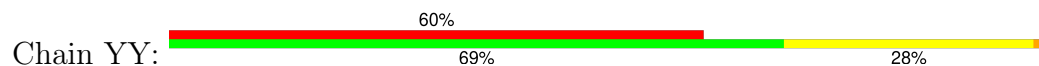
• Molecule 73: uS8



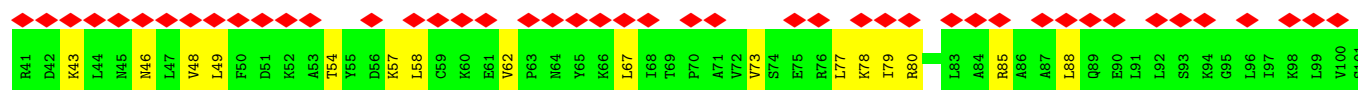
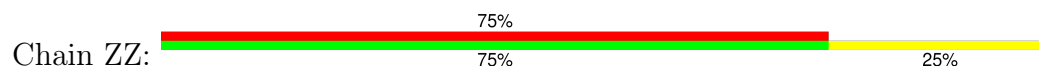
• Molecule 74: uS12

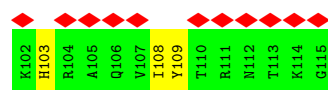


• Molecule 75: eS24

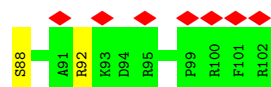
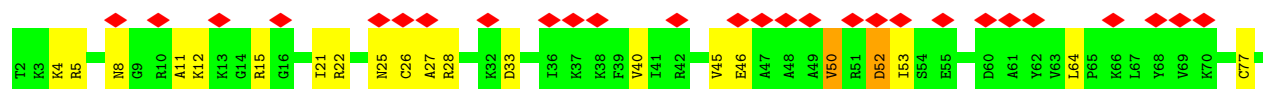
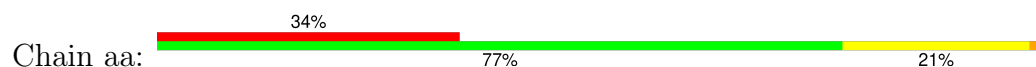


• Molecule 76: eS25

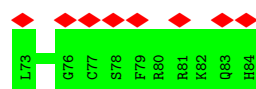
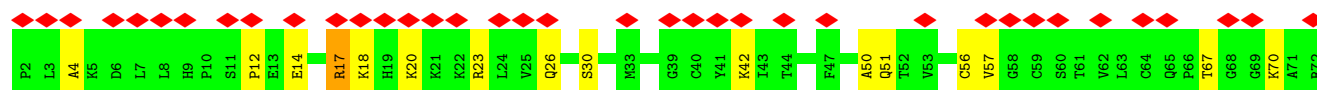
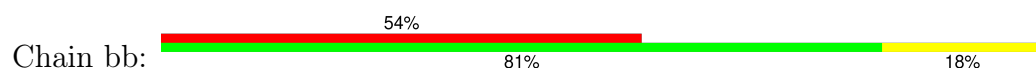




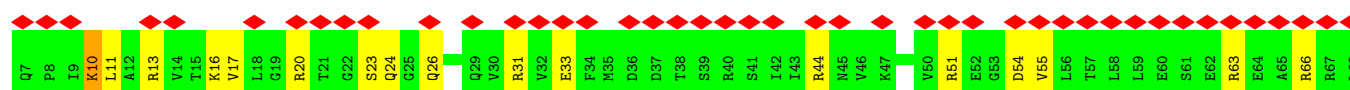
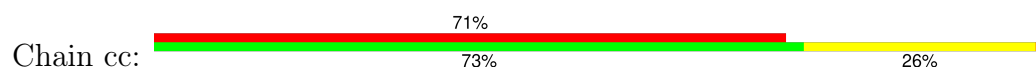
• Molecule 77: eS26



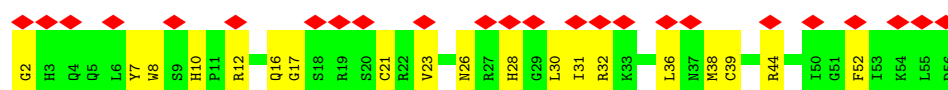
• Molecule 78: eS27



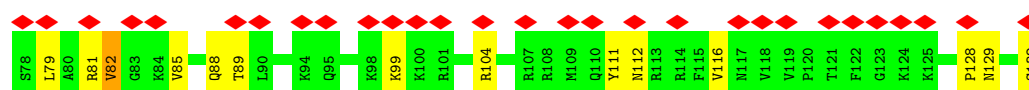
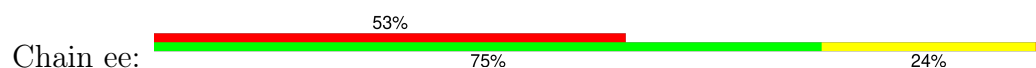
• Molecule 79: eS28



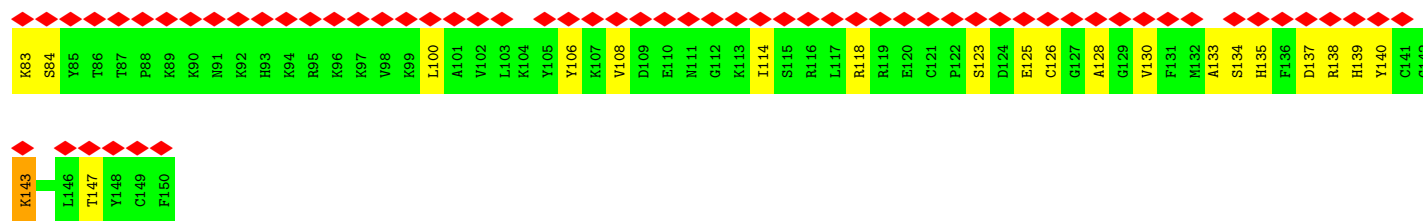
• Molecule 80: uS14



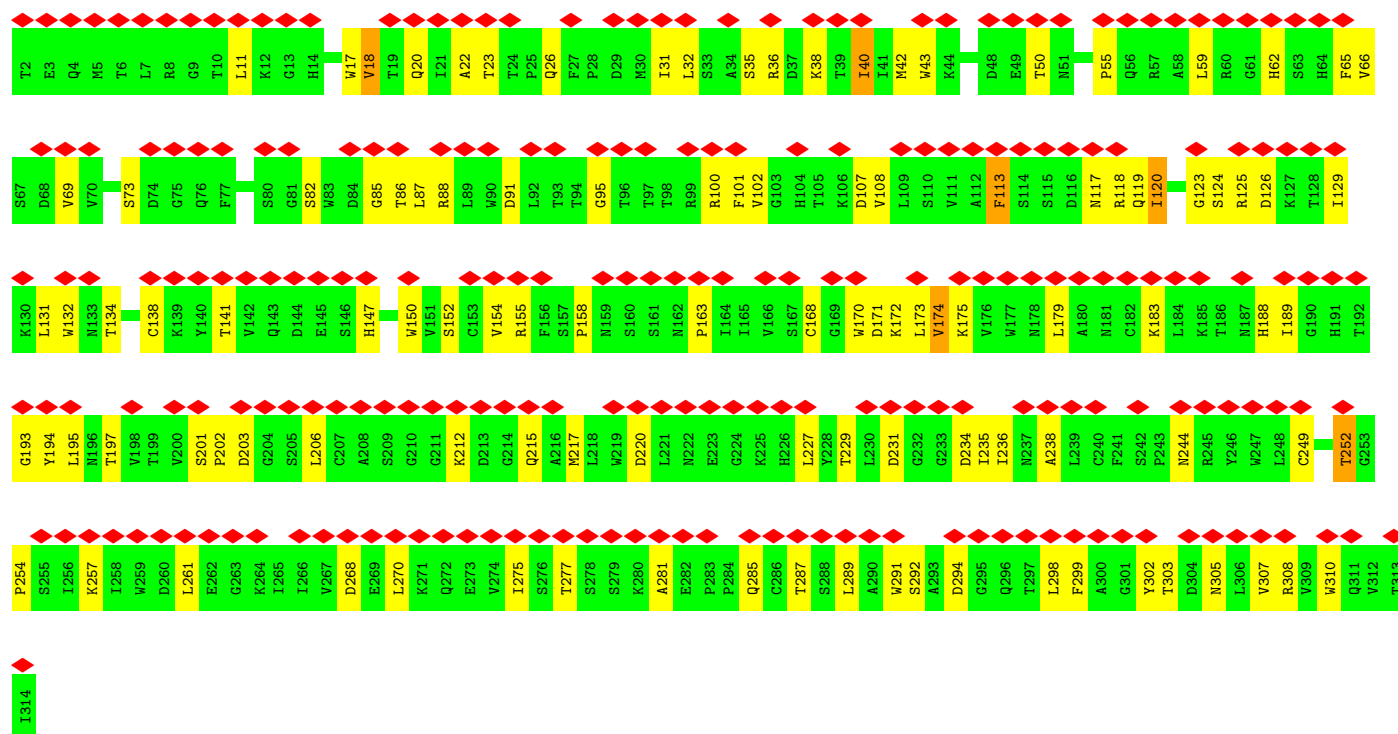
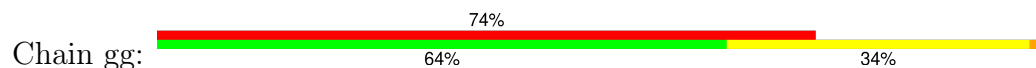
• Molecule 81: eS30



• Molecule 82: eS31



• Molecule 83: RACK1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3313	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.579	Depositor
Minimum map value	-19.958	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.653	Depositor
Recommended contour level	6.2	Depositor
Map size (Å)	686.87994, 686.87994, 686.87994	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E6G, OMC, A2M, 5MC, B8K, 6MZ, MG, P4U, OMU, 1MA, BGH, 5MU, I4U, GDP, B8T, JMH, UR3, PSU, 2MG, 7MG, B9B, DDE, P7G, E7G, B8H, 4AC, MLZ, B8W, M7A, B9H, ZN, MHG, B8N, OMG

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	A	0.10	0/1936	0.26	0/2596
2	B	0.10	0/3240	0.24	0/4339
3	C	0.09	0/2927	0.21	0/3932
4	D	0.08	0/2437	0.21	0/3264
5	E	0.08	0/1762	0.22	0/2362
6	F	0.09	0/1911	0.23	0/2549
7	G	0.09	0/1910	0.24	0/2569
8	H	0.10	0/1535	0.25	0/2063
9	I	0.09	0/1702	0.20	0/2272
10	J	0.09	0/1385	0.22	0/1852
11	L	0.08	0/1733	0.22	0/2316
12	M	0.13	0/1158	0.26	0/1547
13	N	0.10	0/1746	0.22	0/2338
14	O	0.09	0/1662	0.22	0/2222
15	P	0.09	0/1268	0.25	0/1700
16	Q	0.09	0/1539	0.24	0/2054
17	R	0.08	0/1524	0.22	0/2013
18	S	0.10	0/1501	0.25	0/2012
19	T	0.09	0/1326	0.22	0/1770
20	U	0.10	0/823	0.28	0/1104
21	V	0.09	0/993	0.23	0/1332
22	W	0.08	0/873	0.24	0/1158
23	X	0.08	0/984	0.22	0/1323
24	Y	0.09	0/1132	0.22	0/1504
25	Z	0.08	0/1130	0.23	0/1507
26	AA	0.08	0/1747	0.22	0/2374
27	BB	0.08	0/1756	0.23	0/2350
28	CC	0.09	0/1753	0.23	0/2369
29	5	0.13	0/82204	0.25	0/128128
30	7	0.10	0/2858	0.21	0/4455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	8	0.13	0/3559	0.23	0/5543
32	a	0.10	0/1191	0.22	0/1590
33	b	0.08	0/861	0.19	0/1138
34	c	0.09	0/771	0.20	0/1034
35	d	0.10	0/903	0.23	0/1216
36	e	0.08	0/1071	0.22	0/1429
37	f	0.09	0/895	0.24	0/1198
38	g	0.09	0/916	0.20	0/1220
39	h	0.07	0/1021	0.19	0/1348
40	i	0.08	0/841	0.22	0/1112
41	j	0.09	0/720	0.25	0/952
42	k	0.09	0/575	0.23	0/761
43	l	0.09	0/459	0.26	0/608
44	m	0.12	0/425	0.33	0/561
45	n	0.08	0/240	0.18	0/305
46	o	0.09	0/855	0.22	0/1128
47	p	0.09	0/718	0.21	0/953
48	r	0.09	0/1010	0.27	0/1354
49	s	0.09	0/1530	0.26	0/2064
50	t	0.10	0/1174	0.30	0/1582
51	v	0.10	0/6651	0.31	0/8982
52	w	0.06	0/218	0.15	0/287
53	9	0.15	4/40371 (0.0%)	0.34	14/62907 (0.0%)
54	DD	0.10	0/1796	0.25	0/2417
55	EE	0.08	0/2118	0.22	0/2849
56	FF	0.08	0/1492	0.26	0/2005
57	GG	0.07	0/1946	0.23	0/2590
58	HH	0.08	0/1510	0.22	0/2022
59	II	0.10	0/1715	0.25	0/2287
60	JJ	0.07	0/1550	0.20	0/2069
61	KK	0.09	0/834	0.31	0/1125
62	LL	0.07	0/1195	0.20	0/1597
63	MM	0.09	0/918	0.31	0/1233
64	NN	0.07	0/1226	0.21	0/1649
65	OO	0.08	0/1029	0.22	0/1380
66	PP	0.08	0/1017	0.26	0/1358
67	QQ	0.09	0/1146	0.25	0/1534
68	RR	0.08	0/1082	0.20	0/1452
69	SS	0.08	0/1208	0.24	0/1618
70	TT	0.08	0/1115	0.21	0/1493
71	UU	0.07	0/805	0.22	0/1081
72	VV	0.07	0/643	0.21	0/860
73	WW	0.09	0/1051	0.23	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XX	0.09	0/1116	0.25	0/1490
75	YY	0.07	0/1028	0.22	0/1366
76	ZZ	0.10	0/604	0.21	0/810
77	aa	0.09	0/828	0.25	0/1109
78	bb	0.07	0/665	0.21	0/891
79	cc	0.08	0/490	0.23	0/656
80	dd	0.08	0/470	0.22	0/623
81	ee	0.07	0/447	0.22	0/587
82	ff	0.07	0/567	0.21	0/753
83	gg	0.08	0/2493	0.25	0/3394
All	All	0.12	4/231534 (0.0%)	0.27	14/338350 (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
74	XX	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	9	1284	A	N9-C4	9.42	1.56	1.37
53	9	1286	G	N9-C8	-9.38	1.19	1.37
53	9	1286	G	N9-C4	9.35	1.56	1.38
53	9	1284	A	N9-C8	-9.35	1.19	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	9	1284	A	N7-C8-N9	-23.91	42.09	113.80
53	9	1286	G	N7-C8-N9	-23.71	41.97	113.10
53	9	1286	G	C4-C5-N7	-23.09	41.53	110.80
53	9	1284	A	C4-C5-N7	-22.92	41.94	110.70
53	9	1286	G	C8-N9-C4	-20.32	45.44	106.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
74	XX	61	GLN	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	A	1898	0	1993	59	0
2	B	3172	0	3310	80	0
3	C	2884	0	3054	61	0
4	D	2391	0	2424	43	0
5	E	1729	0	1887	30	0
6	F	1875	0	1995	43	0
7	G	1879	0	2027	36	0
8	H	1516	0	1595	40	0
9	I	1664	0	1712	39	0
10	J	1362	0	1399	24	0
11	L	1702	0	1820	32	0
12	M	1137	0	1208	31	0
13	N	1701	0	1749	51	0
14	O	1630	0	1778	38	0
15	P	1242	0	1274	30	0
16	Q	1515	0	1634	46	0
17	R	1508	0	1664	34	0
18	S	1462	0	1508	29	0
19	T	1298	0	1366	28	0
20	U	809	0	833	13	0
21	V	979	0	1039	21	0
22	W	860	0	903	14	0
23	X	967	0	1040	11	0
24	Y	1115	0	1205	34	0
25	Z	1107	0	1182	25	0
26	AA	1710	0	1708	39	0
27	BB	1729	0	1803	45	0
28	CC	1716	0	1806	33	0
29	5	75791	0	38047	1469	0
30	7	2558	0	1296	28	0
31	8	3209	0	1631	72	0
32	a	1162	0	1209	45	0
33	b	848	0	920	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	761	0	794	20	0
35	d	888	0	930	12	0
36	e	1053	0	1147	19	0
37	f	876	0	912	20	0
38	g	906	0	998	13	0
39	h	1013	0	1147	22	0
40	i	830	0	916	8	0
41	j	705	0	737	30	0
42	k	569	0	637	11	0
43	l	447	0	480	11	0
44	m	430	0	466	14	0
45	n	239	0	289	3	0
46	o	842	0	912	21	0
47	p	708	0	756	21	0
48	r	994	0	1051	31	0
49	s	1507	0	1564	34	0
50	t	1160	0	1218	33	0
51	v	6544	0	6638	179	0
52	w	216	0	199	6	0
53	9	36243	0	18277	779	0
54	DD	1768	0	1866	28	0
55	EE	2076	0	2177	55	0
56	FF	1471	0	1522	36	0
57	GG	1923	0	2089	58	0
58	HH	1488	0	1582	33	0
59	II	1686	0	1772	41	0
60	JJ	1525	0	1640	42	0
61	KK	810	0	836	18	0
62	LL	1175	0	1249	23	0
63	MM	908	0	939	23	0
64	NN	1202	0	1289	20	0
65	OO	1016	0	1039	28	0
66	PP	997	0	1045	28	0
67	QQ	1128	0	1195	27	0
68	RR	1068	0	1121	21	0
69	SS	1190	0	1248	33	0
70	TT	1097	0	1132	26	0
71	UU	795	0	862	19	0
72	VV	636	0	637	19	0
73	WW	1034	0	1080	34	0
74	XX	1098	0	1167	23	0
75	YY	1011	0	1083	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	ZZ	598	0	656	17	0
77	aa	814	0	864	17	0
78	bb	651	0	672	12	0
79	cc	488	0	514	14	0
80	dd	459	0	448	19	0
81	ee	443	0	492	16	0
82	ff	555	0	563	19	0
83	gg	2436	0	2393	68	0
84	5	197	0	0	0	0
84	7	6	0	0	0	0
84	8	6	0	0	0	0
84	9	75	0	0	0	0
84	A	1	0	0	0	0
84	P	1	0	0	0	0
84	SS	1	0	0	0	0
84	TT	1	0	0	0	0
84	V	1	0	0	0	0
84	a	1	0	0	0	0
84	dd	1	0	0	0	0
84	g	1	0	0	0	0
84	j	1	0	0	0	0
84	v	1	0	0	0	0
85	aa	1	0	0	0	0
85	dd	1	0	0	0	0
85	ff	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
86	v	28	0	12	3	0
All	All	218932	0	165271	3990	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 11.

The worst 5 of 3990 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)
29:5:4089:5MU:C4	29:5:4089:5MU:C5	1.83	1.63
29:5:1866:B8H:C4	29:5:1866:B8H:C5	1.83	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:3768:B8H:C4	29:5:3768:B8H:C5	1.83	1.56
29:5:4302:B8H:C4	29:5:4302:B8H:C5	1.83	1.56
29:5:1866:B8H:C6	29:5:1866:B8H:N1	1.67	1.56

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	233 (95%)	13 (5%)	0	100	100
2	B	392/403 (97%)	378 (96%)	14 (4%)	0	100	100
3	C	359/413 (87%)	349 (97%)	10 (3%)	0	100	100
4	D	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
5	E	208/291 (72%)	202 (97%)	6 (3%)	0	100	100
6	F	223/249 (90%)	216 (97%)	7 (3%)	0	100	100
7	G	229/319 (72%)	225 (98%)	4 (2%)	0	100	100
8	H	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
9	I	201/214 (94%)	199 (99%)	2 (1%)	0	100	100
10	J	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
11	L	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
12	M	136/218 (62%)	127 (93%)	9 (7%)	0	100	100
13	N	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
14	O	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
15	P	151/213 (71%)	147 (97%)	4 (3%)	0	100	100
16	Q	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
17	R	178/212 (84%)	173 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	174/224 (78%)	167 (96%)	7 (4%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
21	V	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
22	W	102/157 (65%)	100 (98%)	2 (2%)	0	100	100
23	X	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
24	Y	132/145 (91%)	132 (100%)	0	0	100	100
25	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
26	AA	215/295 (73%)	210 (98%)	5 (2%)	0	100	100
27	BB	211/264 (80%)	206 (98%)	5 (2%)	0	100	100
28	CC	219/293 (75%)	215 (98%)	4 (2%)	0	100	100
32	a	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
33	b	100/245 (41%)	99 (99%)	1 (1%)	0	100	100
34	c	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	d	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
36	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	112 (100%)	0	0	100	100
39	h	120/122 (98%)	120 (100%)	0	0	100	100
40	i	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
41	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	k	67/69 (97%)	67 (100%)	0	0	100	100
43	l	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
44	m	49/52 (94%)	42 (86%)	6 (12%)	1 (2%)	6	26
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
47	p	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
48	r	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
49	s	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
50	t	151/153 (99%)	134 (89%)	17 (11%)	0	100	100
51	v	834/839 (99%)	779 (93%)	54 (6%)	1 (0%)	48	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	w	22/26 (85%)	22 (100%)	0	0	100	100
54	DD	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
55	EE	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
56	FF	181/204 (89%)	170 (94%)	11 (6%)	0	100	100
57	GG	235/237 (99%)	231 (98%)	4 (2%)	0	100	100
58	HH	181/194 (93%)	176 (97%)	5 (3%)	0	100	100
59	II	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
60	JJ	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
61	KK	94/96 (98%)	87 (93%)	7 (7%)	0	100	100
62	LL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
63	MM	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
64	NN	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
65	OO	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
66	PP	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
67	QQ	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
68	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
69	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
71	UU	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
72	VV	81/83 (98%)	81 (100%)	0	0	100	100
73	WW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
74	XX	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	19	51
75	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
76	ZZ	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
77	aa	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
78	bb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
79	cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
80	dd	53/55 (96%)	53 (100%)	0	0	100	100
81	ee	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	ff	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
83	gg	311/313 (99%)	294 (94%)	17 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12372/13586 (91%)	11933 (96%)	436 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	v	288	THR
44	m	73	CYS
74	XX	62	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	185 (97%)	5 (3%)	41	68
2	B	342/348 (98%)	331 (97%)	11 (3%)	34	63
3	C	301/336 (90%)	290 (96%)	11 (4%)	29	59
4	D	247/250 (99%)	240 (97%)	7 (3%)	38	66
5	E	190/251 (76%)	184 (97%)	6 (3%)	34	63
6	F	196/218 (90%)	193 (98%)	3 (2%)	60	80
7	G	200/272 (74%)	193 (96%)	7 (4%)	31	61
8	H	169/171 (99%)	160 (95%)	9 (5%)	19	48
9	I	175/181 (97%)	168 (96%)	7 (4%)	27	58
10	J	143/149 (96%)	140 (98%)	3 (2%)	48	72
11	L	175/176 (99%)	166 (95%)	9 (5%)	20	49
12	M	117/161 (73%)	112 (96%)	5 (4%)	25	55
13	N	171/172 (99%)	166 (97%)	5 (3%)	37	65
14	O	171/173 (99%)	166 (97%)	5 (3%)	37	65
15	P	134/190 (70%)	129 (96%)	5 (4%)	29	59
16	Q	164/165 (99%)	162 (99%)	2 (1%)	67	83
17	R	159/191 (83%)	155 (98%)	4 (2%)	42	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	157/192 (82%)	152 (97%)	5 (3%)	34	63
19	T	139/140 (99%)	136 (98%)	3 (2%)	47	71
20	U	89/114 (78%)	87 (98%)	2 (2%)	47	71
21	V	101/107 (94%)	100 (99%)	1 (1%)	73	86
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	105 (99%)	1 (1%)	75	88
24	Y	124/135 (92%)	121 (98%)	3 (2%)	44	70
25	Z	117/118 (99%)	113 (97%)	4 (3%)	32	62
26	AA	180/245 (74%)	176 (98%)	4 (2%)	47	71
27	BB	194/231 (84%)	188 (97%)	6 (3%)	35	63
28	CC	187/225 (83%)	180 (96%)	7 (4%)	29	59
32	a	119/119 (100%)	118 (99%)	1 (1%)	79	89
33	b	84/184 (46%)	84 (100%)	0	100	100
34	c	84/84 (100%)	80 (95%)	4 (5%)	21	51
35	d	98/98 (100%)	93 (95%)	5 (5%)	20	49
36	e	114/114 (100%)	111 (97%)	3 (3%)	41	68
37	f	88/88 (100%)	85 (97%)	3 (3%)	32	62
38	g	98/98 (100%)	94 (96%)	4 (4%)	26	57
39	h	109/109 (100%)	106 (97%)	3 (3%)	38	66
40	i	86/86 (100%)	82 (95%)	4 (5%)	22	52
41	j	73/73 (100%)	71 (97%)	2 (3%)	40	67
42	k	64/64 (100%)	60 (94%)	4 (6%)	15	42
43	l	47/47 (100%)	45 (96%)	2 (4%)	25	55
44	m	47/47 (100%)	44 (94%)	3 (6%)	14	42
45	n	24/24 (100%)	23 (96%)	1 (4%)	25	56
46	o	91/91 (100%)	88 (97%)	3 (3%)	33	62
47	p	74/74 (100%)	70 (95%)	4 (5%)	18	47
48	r	108/108 (100%)	100 (93%)	8 (7%)	11	36
49	s	164/164 (100%)	151 (92%)	13 (8%)	10	34
50	t	126/126 (100%)	120 (95%)	6 (5%)	21	51
51	v	713/713 (100%)	658 (92%)	55 (8%)	10	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	w	23/23 (100%)	23 (100%)	0	100	100
54	DD	190/190 (100%)	182 (96%)	8 (4%)	25	56
55	EE	224/224 (100%)	212 (95%)	12 (5%)	18	47
56	FF	158/170 (93%)	152 (96%)	6 (4%)	28	59
57	GG	207/207 (100%)	202 (98%)	5 (2%)	44	70
58	HH	165/174 (95%)	155 (94%)	10 (6%)	15	43
59	II	178/178 (100%)	173 (97%)	5 (3%)	38	66
60	JJ	161/161 (100%)	160 (99%)	1 (1%)	84	91
61	KK	87/87 (100%)	84 (97%)	3 (3%)	32	62
62	LL	130/142 (92%)	126 (97%)	4 (3%)	35	63
63	MM	99/99 (100%)	94 (95%)	5 (5%)	20	49
64	NN	130/130 (100%)	127 (98%)	3 (2%)	45	70
65	OO	106/106 (100%)	104 (98%)	2 (2%)	52	75
66	PP	109/109 (100%)	106 (97%)	3 (3%)	38	66
67	QQ	117/117 (100%)	110 (94%)	7 (6%)	16	44
68	RR	119/119 (100%)	115 (97%)	4 (3%)	32	62
69	SS	125/125 (100%)	118 (94%)	7 (6%)	17	46
70	TT	111/111 (100%)	107 (96%)	4 (4%)	30	60
71	UU	92/92 (100%)	87 (95%)	5 (5%)	18	47
72	VV	67/67 (100%)	64 (96%)	3 (4%)	23	53
73	WW	112/112 (100%)	109 (97%)	3 (3%)	40	67
74	XX	113/113 (100%)	107 (95%)	6 (5%)	19	48
75	YY	107/107 (100%)	102 (95%)	5 (5%)	22	52
76	ZZ	66/66 (100%)	65 (98%)	1 (2%)	60	80
77	aa	88/88 (100%)	84 (96%)	4 (4%)	23	53
78	bb	75/75 (100%)	73 (97%)	2 (3%)	40	67
79	cc	55/55 (100%)	53 (96%)	2 (4%)	30	60
80	dd	48/48 (100%)	48 (100%)	0	100	100
81	ee	46/46 (100%)	44 (96%)	2 (4%)	25	55
82	ff	61/61 (100%)	59 (97%)	2 (3%)	33	62
83	gg	272/272 (100%)	257 (94%)	15 (6%)	18	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10776/11555 (93%)	10369 (96%)	407 (4%)	30 59

5 of 407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	v	344	LEU
55	EE	147	ILE
83	gg	174	VAL
51	v	420	LEU
51	v	770	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
51	v	803	ASN
72	VV	35	ASN
55	EE	161	GLN
61	KK	61	GLN
77	aa	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	5	3506/3635 (96%)	703 (20%)	50 (1%)
30	7	119/120 (99%)	15 (12%)	0
31	8	149/156 (95%)	24 (16%)	1 (0%)
53	9	1685/1698 (99%)	352 (20%)	17 (1%)
All	All	5459/5609 (97%)	1094 (20%)	68 (1%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	5	8	U
29	5	12	A
29	5	13	U
29	5	25	A
29	5	35	U

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	9	688	U
53	9	870	A
53	9	1489	A
29	5	1451	U
29	5	1446	U

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

110 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
29	B8H	5	4302	29	19,22,23	6.87	8 (42%)	21,32,35	2.50	5 (23%)
53	A2M	9	1678	53	18,25,26	2.73	8 (44%)	20,36,39	2.03	4 (20%)
29	OMG	5	4202	29	19,26,27	2.56	7 (36%)	21,38,41	1.45	4 (19%)
29	JMH	5	1462	29	18,22,23	2.87	6 (33%)	23,32,35	1.40	3 (13%)
29	OMC	5	3875	29	19,22,23	3.04	8 (42%)	25,31,34	0.68	0
29	B8W	5	4135	29	18,26,27	1.52	2 (11%)	17,38,41	3.08	5 (29%)
53	5MC	9	1374	53	19,22,23	3.88	8 (42%)	26,32,35	1.06	2 (7%)
29	I4U	5	4200	29	20,24,25	3.51	8 (40%)	27,34,37	1.68	2 (7%)
29	E7G	5	2303	29	24,27,28	3.36	11 (45%)	28,40,43	2.40	9 (32%)
29	5MC	5	3788	29	19,22,23	3.88	8 (42%)	26,32,35	1.00	2 (7%)
29	OMG	5	2430	29	19,26,27	2.56	7 (36%)	21,38,41	1.47	4 (19%)
29	MHG	5	4377	29	29,32,33	3.60	10 (34%)	34,46,49	2.55	9 (26%)
29	OMC	5	2428	29,84	19,22,23	3.03	8 (42%)	25,31,34	0.74	0
29	A2M	5	4529	29,84	18,25,26	2.65	9 (50%)	20,36,39	2.01	3 (15%)
29	2MG	5	1523	29	18,26,27	2.19	5 (27%)	16,38,41	1.69	5 (31%)
29	OMG	5	2370	29	19,26,27	2.54	7 (36%)	21,38,41	1.47	4 (19%)
29	A2M	5	1332	29	18,25,26	2.72	9 (50%)	20,36,39	1.93	3 (15%)
29	A2M	5	2407	29,84	18,25,26	2.68	8 (44%)	20,36,39	1.92	3 (15%)
29	BGH	5	3905	29,84	25,29,30	4.54	18 (72%)	30,43,46	2.38	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PSU	5	3770	29	18,21,22	4.55	6 (33%)	21,30,33	2.94	5 (23%)
29	B8T	5	4677	29	19,22,23	3.30	8 (42%)	25,31,34	0.90	1 (4%)
29	1MA	5	1328	29,84	17,25,26	3.88	3 (17%)	17,37,40	1.75	3 (17%)
29	A2M	5	1540	29,84	18,25,26	2.71	8 (44%)	20,36,39	1.94	3 (15%)
29	UR3	5	4603	29	19,22,23	3.20	9 (47%)	26,32,35	1.56	4 (15%)
29	OMG	5	3798	29	19,26,27	2.55	7 (36%)	21,38,41	1.44	4 (19%)
29	OMU	5	4626	29	19,22,23	3.05	8 (42%)	25,31,34	1.81	5 (20%)
29	OMG	5	4643	29	19,26,27	2.55	7 (36%)	21,38,41	1.45	4 (19%)
29	OMG	5	4876	29	19,26,27	2.56	7 (36%)	21,38,41	1.48	4 (19%)
29	OMC	5	2867	29	19,22,23	3.06	8 (42%)	25,31,34	0.88	1 (4%)
29	B8W	5	4478	29	18,26,27	1.51	2 (11%)	17,38,41	3.10	6 (35%)
29	PSU	5	4409	29	18,21,22	4.55	7 (38%)	21,30,33	2.89	7 (33%)
29	A2M	5	1877	29,84	18,25,26	2.68	9 (50%)	20,36,39	1.89	3 (15%)
29	B8K	5	4696	29	24,28,29	3.33	12 (50%)	29,42,45	2.42	11 (37%)
29	7MG	5	1611	29	23,26,27	3.37	10 (43%)	27,39,42	2.21	9 (33%)
29	P7G	5	3886	29	24,28,29	3.59	10 (41%)	25,41,44	1.39	2 (8%)
29	PSU	5	4634	29	18,21,22	4.53	6 (33%)	21,30,33	3.05	5 (23%)
29	PSU	5	1683	29	18,21,22	4.57	7 (38%)	21,30,33	3.05	7 (33%)
29	OMG	5	1889	29	19,26,27	2.55	8 (42%)	21,38,41	1.49	4 (19%)
29	7MG	5	4556	29	23,26,27	3.39	10 (43%)	27,39,42	2.22	9 (33%)
29	PSU	5	2514	29	18,21,22	4.54	6 (33%)	21,30,33	2.99	5 (23%)
29	PSU	5	4299	29	18,21,22	4.53	7 (38%)	21,30,33	3.01	6 (28%)
29	UR3	5	4536	29	19,22,23	3.24	8 (42%)	26,32,35	1.60	3 (11%)
29	A2M	5	3791	29	18,25,26	2.81	9 (50%)	20,36,39	1.97	5 (25%)
29	B8W	5	4191	29	18,26,27	1.52	2 (11%)	17,38,41	3.18	6 (35%)
29	B9B	5	2760	29,84	20,28,29	1.76	2 (10%)	19,40,43	1.91	5 (26%)
29	OMG	5	373	29	19,26,27	2.54	7 (36%)	21,38,41	1.47	4 (19%)
29	A2M	5	398	29	18,25,26	2.65	8 (44%)	20,36,39	1.95	3 (15%)
3	MLZ	C	333	3	8,9,10	0.72	0	4,9,11	0.91	0
29	OMG	5	1528	29	19,26,27	2.55	7 (36%)	21,38,41	1.48	4 (19%)
29	OMC	5	3893	29	19,22,23	3.04	8 (42%)	25,31,34	0.72	0
53	PSU	9	1243	53	18,21,22	4.57	6 (33%)	21,30,33	2.87	5 (23%)
29	5MU	5	4089	29	19,22,23	8.30	7 (36%)	27,32,35	3.57	10 (37%)
29	PSU	5	3735	29	18,21,22	4.53	6 (33%)	21,30,33	2.98	5 (23%)
29	PSU	5	4537	29	18,21,22	4.52	6 (33%)	21,30,33	3.00	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	MLZ	m	72	44	8,9,10	0.72	0	4,9,11	0.80	0
29	P7G	5	1915	29	24,28,29	3.59	10 (41%)	25,41,44	1.22	2 (8%)
29	B8W	5	4535	29,84	18,26,27	1.50	2 (11%)	17,38,41	3.20	6 (35%)
29	PSU	5	1689	29	18,21,22	4.52	6 (33%)	21,30,33	3.01	6 (28%)
31	OMU	8	14	31,29	19,22,23	3.11	8 (42%)	25,31,34	1.84	5 (20%)
29	OMG	5	2779	29	19,26,27	2.58	7 (36%)	21,38,41	1.48	4 (19%)
29	OMG	5	4500	29	19,26,27	2.54	7 (36%)	21,38,41	1.47	4 (19%)
29	5MC	5	4453	29	19,22,23	3.85	8 (42%)	26,32,35	1.06	1 (3%)
29	B8H	5	3768	29	19,22,23	6.87	8 (42%)	21,32,35	2.47	5 (23%)
29	A2M	5	3873	29	18,25,26	2.71	9 (50%)	20,36,39	1.88	3 (15%)
51	DDE	v	715	51	15,20,21	2.21	4 (26%)	11,28,30	0.99	1 (9%)
29	P4U	5	1354	29,84	21,24,25	3.51	8 (38%)	28,33,36	1.52	2 (7%)
29	5MC	5	4341	29	19,22,23	3.90	8 (42%)	26,32,35	1.02	2 (7%)
29	B8H	5	1866	29	19,22,23	6.83	8 (42%)	21,32,35	2.46	5 (23%)
29	2MG	5	730	29	18,26,27	2.21	5 (27%)	16,38,41	1.60	4 (25%)
29	M7A	5	4570	29	19,25,26	1.61	2 (10%)	25,37,40	4.34	7 (28%)
29	OMG	5	4629	29	19,26,27	2.55	7 (36%)	21,38,41	1.46	4 (19%)
29	UR3	5	1872	29	19,22,23	3.20	8 (42%)	26,32,35	1.62	4 (15%)
29	A2M	5	1530	29	18,25,26	2.70	9 (50%)	20,36,39	1.92	4 (20%)
29	OMC	5	2371	29	19,22,23	3.03	8 (42%)	25,31,34	0.71	0
29	OMC	5	3915	29	19,22,23	3.03	8 (42%)	25,31,34	0.76	0
29	A2M	5	3729	29	18,25,26	2.70	9 (50%)	20,36,39	1.83	3 (15%)
29	OMC	5	4542	29	19,22,23	3.05	8 (42%)	25,31,34	0.77	0
29	A2M	5	2369	29,84	18,25,26	2.67	9 (50%)	20,36,39	1.94	3 (15%)
29	A2M	5	3831	29	18,25,26	2.67	9 (50%)	20,36,39	1.96	3 (15%)
29	B9H	5	2792	29	21,25,26	2.95	4 (19%)	22,35,38	1.59	5 (22%)
29	OMC	5	3707	29,84	19,22,23	3.02	8 (42%)	25,31,34	0.70	0
29	OMG	5	1631	29,84	19,26,27	2.56	7 (36%)	21,38,41	1.49	4 (19%)
29	2MG	5	4878	29	18,26,27	2.21	5 (27%)	16,38,41	1.98	5 (31%)
29	PSU	5	4506	29	18,21,22	4.54	7 (38%)	21,30,33	2.99	6 (28%)
29	7MG	5	2528	29	23,26,27	3.38	10 (43%)	27,39,42	2.21	9 (33%)
53	JMH	9	1219	53	18,22,23	2.97	6 (33%)	23,32,35	1.99	7 (30%)
29	E7G	5	1803	29	24,27,28	3.37	11 (45%)	28,40,43	2.37	9 (32%)
29	B8W	5	2386	29	18,26,27	1.51	2 (11%)	17,38,41	3.19	6 (35%)
29	PSU	5	4456	29,84	18,21,22	4.50	6 (33%)	21,30,33	3.03	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PSU	5	1588	29	18,21,22	4.52	6 (33%)	21,30,33	2.97	5 (23%)
29	OMU	5	4312	29	19,22,23	3.06	8 (42%)	25,31,34	1.81	5 (20%)
29	1MA	5	4421	29	17,25,26	3.91	3 (17%)	17,37,40	1.68	3 (17%)
29	A2M	5	3724	29	18,25,26	2.68	8 (44%)	20,36,39	1.93	3 (15%)
53	4AC	9	1337	53	21,24,25	3.71	9 (42%)	28,34,37	1.17	4 (14%)
29	6MZ	5	4226	29	17,25,26	1.39	2 (11%)	15,36,39	2.29	4 (26%)
29	OMC	5	2810	29	19,22,23	3.05	8 (42%)	25,31,34	0.72	0
53	B8N	9	1248	53	25,29,30	2.53	7 (28%)	28,42,45	2.07	5 (17%)
29	OMG	5	2056	29	19,26,27	2.53	7 (36%)	21,38,41	1.43	4 (19%)
29	B8K	5	3903	29	24,28,29	3.24	12 (50%)	29,42,45	2.36	11 (37%)
29	PSU	5	3721	29	18,21,22	4.55	6 (33%)	21,30,33	2.95	5 (23%)
29	B9B	5	1580	29	20,28,29	1.75	2 (10%)	19,40,43	1.91	4 (21%)
29	E6G	5	4361	29	19,27,28	1.78	2 (10%)	18,39,42	2.03	4 (22%)
29	B9B	5	237	29,84	20,28,29	1.75	2 (10%)	19,40,43	1.90	4 (21%)
29	PSU	5	4448	29	18,21,22	4.53	6 (33%)	21,30,33	2.99	7 (33%)
29	PSU	5	4642	29	18,21,22	4.53	6 (33%)	21,30,33	2.99	5 (23%)
29	B8T	5	4489	29	19,22,23	3.30	8 (42%)	25,31,34	0.88	1 (4%)
29	OMG	5	4376	29	19,26,27	2.53	7 (36%)	21,38,41	1.46	4 (19%)
29	OMG	5	1322	29	19,26,27	2.54	7 (36%)	21,38,41	1.48	4 (19%)
29	I4U	5	1665	29	20,24,25	3.53	8 (40%)	27,34,37	1.74	2 (7%)
29	A2M	5	4577	29	18,25,26	2.65	8 (44%)	20,36,39	1.93	3 (15%)

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
29	B8H	5	4302	29	-	0/7/25/26	0/2/2/2
53	A2M	9	1678	53	-	1/5/27/28	0/3/3/3
29	OMG	5	4202	29	-	0/5/27/28	0/3/3/3
29	JMH	5	1462	29	-	2/7/25/26	0/2/2/2
29	OMC	5	3875	29	-	0/9/27/28	0/2/2/2
29	B8W	5	4135	29	-	2/5/27/28	0/3/3/3
53	5MC	9	1374	53	-	0/7/25/26	0/2/2/2
29	I4U	5	4200	29	-	3/9/29/30	0/2/2/2
29	E7G	5	2303	29	-	3/9/39/40	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	5MC	5	3788	29	-	1/7/25/26	0/2/2/2
29	OMG	5	2430	29	-	2/5/27/28	0/3/3/3
29	MHG	5	4377	29	-	3/16/46/47	0/3/3/3
29	OMC	5	2428	29,84	-	2/9/27/28	0/2/2/2
29	A2M	5	4529	29,84	-	3/5/27/28	0/3/3/3
29	2MG	5	1523	29	-	0/5/27/28	0/3/3/3
29	OMG	5	2370	29	-	3/5/27/28	0/3/3/3
29	A2M	5	1332	29	-	1/5/27/28	0/3/3/3
29	A2M	5	2407	29,84	-	0/5/27/28	0/3/3/3
29	BGH	5	3905	29,84	-	3/13/43/44	0/3/3/3
29	PSU	5	3770	29	-	1/7/25/26	0/2/2/2
29	B8T	5	4677	29	-	2/7/27/28	0/2/2/2
29	1MA	5	1328	29,84	-	0/3/25/26	0/3/3/3
29	A2M	5	1540	29,84	-	1/5/27/28	0/3/3/3
29	UR3	5	4603	29	-	0/7/25/26	0/2/2/2
29	OMG	5	3798	29	-	2/5/27/28	0/3/3/3
29	OMU	5	4626	29	-	1/9/27/28	0/2/2/2
29	OMG	5	4643	29	-	3/5/27/28	0/3/3/3
29	OMG	5	4876	29	-	3/5/27/28	0/3/3/3
29	OMC	5	2867	29	-	0/9/27/28	0/2/2/2
29	B8W	5	4478	29	-	2/5/27/28	0/3/3/3
29	PSU	5	4409	29	-	2/7/25/26	0/2/2/2
29	A2M	5	1877	29,84	-	0/5/27/28	0/3/3/3
29	B8K	5	4696	29	-	0/11/41/42	0/3/3/3
29	7MG	5	1611	29	-	0/7/37/38	0/3/3/3
29	P7G	5	3886	29	-	2/10/40/41	0/3/3/3
29	PSU	5	4634	29	-	0/7/25/26	0/2/2/2
29	PSU	5	1683	29	-	1/7/25/26	0/2/2/2
29	OMG	5	1889	29	-	0/5/27/28	0/3/3/3
29	7MG	5	4556	29	-	0/7/37/38	0/3/3/3
29	PSU	5	2514	29	-	0/7/25/26	0/2/2/2
29	PSU	5	4299	29	-	2/7/25/26	0/2/2/2
29	UR3	5	4536	29	-	2/7/25/26	0/2/2/2
29	A2M	5	3791	29	-	2/5/27/28	0/3/3/3
29	B8W	5	4191	29	-	2/5/27/28	0/3/3/3
29	B9B	5	2760	29,84	-	3/7/29/30	0/3/3/3
29	OMG	5	373	29	-	1/5/27/28	0/3/3/3
29	A2M	5	398	29	-	3/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLZ	C	333	3	-	2/7/8/10	-
29	OMG	5	1528	29	-	0/5/27/28	0/3/3/3
29	OMC	5	3893	29	-	2/9/27/28	0/2/2/2
53	PSU	9	1243	53	-	2/7/25/26	0/2/2/2
29	5MU	5	4089	29	-	0/7/25/26	0/2/2/2
29	PSU	5	3735	29	-	2/7/25/26	0/2/2/2
29	PSU	5	4537	29	-	2/7/25/26	0/2/2/2
44	MLZ	m	72	44	-	2/7/8/10	-
29	P7G	5	1915	29	-	3/10/40/41	0/3/3/3
29	B8W	5	4535	29,84	-	4/5/27/28	0/3/3/3
29	PSU	5	1689	29	-	0/7/25/26	0/2/2/2
31	OMU	8	14	31,29	-	5/9/27/28	0/2/2/2
29	OMG	5	2779	29	-	2/5/27/28	0/3/3/3
29	OMG	5	4500	29	-	0/5/27/28	0/3/3/3
29	5MC	5	4453	29	-	4/7/25/26	0/2/2/2
29	B8H	5	3768	29	-	0/7/25/26	0/2/2/2
29	A2M	5	3873	29	-	4/5/27/28	0/3/3/3
51	DDE	v	715	51	-	7/20/21/23	0/1/1/1
29	P4U	5	1354	29,84	-	4/10/29/30	0/2/2/2
29	5MC	5	4341	29	-	3/7/25/26	0/2/2/2
29	B8H	5	1866	29	-	0/7/25/26	0/2/2/2
29	2MG	5	730	29	-	0/5/27/28	0/3/3/3
29	M7A	5	4570	29	-	0/7/37/38	0/3/3/3
29	OMG	5	4629	29	-	0/5/27/28	0/3/3/3
29	UR3	5	1872	29	-	0/7/25/26	0/2/2/2
29	A2M	5	1530	29	-	0/5/27/28	0/3/3/3
29	OMC	5	2371	29	-	0/9/27/28	0/2/2/2
29	OMC	5	3915	29	-	0/9/27/28	0/2/2/2
29	A2M	5	3729	29	-	1/5/27/28	0/3/3/3
29	OMC	5	4542	29	-	0/9/27/28	0/2/2/2
29	A2M	5	2369	29,84	-	0/5/27/28	0/3/3/3
29	A2M	5	3831	29	-	1/5/27/28	0/3/3/3
29	B9H	5	2792	29	-	0/12/47/48	0/2/2/2
29	OMC	5	3707	29,84	-	4/9/27/28	0/2/2/2
29	OMG	5	1631	29,84	-	2/5/27/28	0/3/3/3
29	2MG	5	4878	29	-	2/5/27/28	0/3/3/3
29	PSU	5	4506	29	-	3/7/25/26	0/2/2/2
29	7MG	5	2528	29	-	0/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	JMH	9	1219	53	-	1/7/25/26	0/2/2/2
29	E7G	5	1803	29	-	2/9/39/40	0/3/3/3
29	B8W	5	2386	29	-	4/5/27/28	0/3/3/3
29	PSU	5	4456	29,84	-	4/7/25/26	0/2/2/2
29	PSU	5	1588	29	-	2/7/25/26	0/2/2/2
29	OMU	5	4312	29	-	3/9/27/28	0/2/2/2
29	1MA	5	4421	29	-	1/3/25/26	0/3/3/3
29	A2M	5	3724	29	-	1/5/27/28	0/3/3/3
53	4AC	9	1337	53	-	0/11/29/30	0/2/2/2
29	6MZ	5	4226	29	-	0/5/27/28	0/3/3/3
29	OMC	5	2810	29	-	0/9/27/28	0/2/2/2
53	B8N	9	1248	53	-	2/16/34/35	0/2/2/2
29	OMG	5	2056	29	-	0/5/27/28	0/3/3/3
29	B8K	5	3903	29	-	3/11/41/42	0/3/3/3
29	PSU	5	3721	29	-	0/7/25/26	0/2/2/2
29	B9B	5	1580	29	-	3/7/29/30	0/3/3/3
29	E6G	5	4361	29	-	4/6/28/29	0/3/3/3
29	B9B	5	237	29,84	-	4/7/29/30	0/3/3/3
29	PSU	5	4448	29	-	2/7/25/26	0/2/2/2
29	PSU	5	4642	29	-	2/7/25/26	0/2/2/2
29	B8T	5	4489	29	-	0/7/27/28	0/2/2/2
29	OMG	5	4376	29	-	0/5/27/28	0/3/3/3
29	OMG	5	1322	29	-	1/5/27/28	0/3/3/3
29	I4U	5	1665	29	-	0/9/29/30	0/2/2/2
29	A2M	5	4577	29	-	1/5/27/28	0/3/3/3

The worst 5 of 769 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	4089	5MU	C4-C5	23.55	1.83	1.44
29	5	4089	5MU	C6-N1	17.77	1.68	1.38
29	5	3768	B8H	C6-C5	-15.88	1.12	1.35
29	5	4302	B8H	C6-C5	-15.81	1.12	1.35
29	5	1866	B8H	C6-C5	-15.64	1.12	1.35

The worst 5 of 463 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	4570	M7A	C5-C6-N6	14.78	148.85	123.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	4570	M7A	N6-C6-N1	-12.17	91.26	118.38
29	5	4089	5MU	C5-C4-N3	10.31	124.28	115.32
29	5	4089	5MU	C5-C6-N1	-9.16	113.36	123.31
29	5	4191	B8W	N2-C2-N3	7.94	130.19	117.79

There are no chirality outliers.

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	5	237	B9B	C5-C6-O6-C61
29	5	237	B9B	N1-C6-O6-C61
29	5	237	B9B	C3'-C4'-C5'-O5'
29	5	237	B9B	O4'-C4'-C5'-O5'
29	5	398	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

63 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5	4302	B8H	6	0
53	9	1678	A2M	3	0
29	5	1462	JMH	2	0
53	9	1374	5MC	1	0
29	5	4200	I4U	1	0
29	5	2303	E7G	1	0
29	5	2428	OMC	3	0
29	5	4529	A2M	1	0
29	5	1523	2MG	1	0
29	5	2370	OMG	1	0
29	5	1332	A2M	4	0
29	5	3905	BGH	1	0
29	5	4677	B8T	1	0
29	5	1328	1MA	1	0
29	5	1540	A2M	1	0
29	5	4603	UR3	1	0
29	5	4626	OMU	4	0
29	5	4478	B8W	1	0
29	5	1877	A2M	1	0
29	5	1611	7MG	2	0
29	5	4634	PSU	1	0
29	5	1889	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5	4556	7MG	1	0
29	5	4299	PSU	1	0
29	5	3791	A2M	1	0
29	5	2760	B9B	1	0
29	5	373	OMG	1	0
29	5	398	A2M	1	0
3	C	333	MLZ	1	0
29	5	1528	OMG	1	0
29	5	4089	5MU	5	0
29	5	3735	PSU	1	0
29	5	4537	PSU	1	0
44	m	72	MLZ	2	0
29	5	1915	P7G	1	0
29	5	1689	PSU	1	0
31	8	14	OMU	2	0
29	5	2779	OMG	2	0
29	5	4500	OMG	2	0
29	5	4453	5MC	1	0
29	5	3768	B8H	8	0
29	5	3873	A2M	2	0
51	v	715	DDE	4	0
29	5	1866	B8H	6	0
29	5	1872	UR3	2	0
29	5	2371	OMC	1	0
29	5	3729	A2M	5	0
29	5	4542	OMC	1	0
29	5	2369	A2M	2	0
29	5	1631	OMG	1	0
29	5	4878	2MG	2	0
29	5	4506	PSU	1	0
29	5	2528	7MG	2	0
53	9	1219	JMH	1	0
29	5	4312	OMU	1	0
29	5	3724	A2M	3	0
53	9	1337	4AC	5	0
29	5	4226	6MZ	2	0
29	5	2810	OMC	1	0
29	5	2056	OMG	1	0
29	5	4448	PSU	1	0
29	5	1322	OMG	2	0
29	5	4577	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 302 are monoatomic - leaving 1 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
86	GDP	v	902	-	25,30,30	3.75	15 (60%)	30,47,47	1.55	5 (16%)

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
86	GDP	v	902	-	-	7/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	v	902	GDP	O4'-C1'	8.07	1.51	1.40
86	v	902	GDP	C1'-N9	-6.57	1.32	1.50
86	v	902	GDP	O4'-C4'	-6.25	1.31	1.45
86	v	902	GDP	C2-N3	5.60	1.46	1.33
86	v	902	GDP	C3'-C4'	5.47	1.66	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	v	902	GDP	C8-N7-C5	3.97	109.31	102.55
86	v	902	GDP	C4'-O4'-C1'	-3.89	106.36	109.92
86	v	902	GDP	C5-C6-N1	3.16	120.10	114.07
86	v	902	GDP	C2-N1-C6	-2.85	119.89	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	v	902	GDP	O6-C6-C5	-2.16	120.04	124.32

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

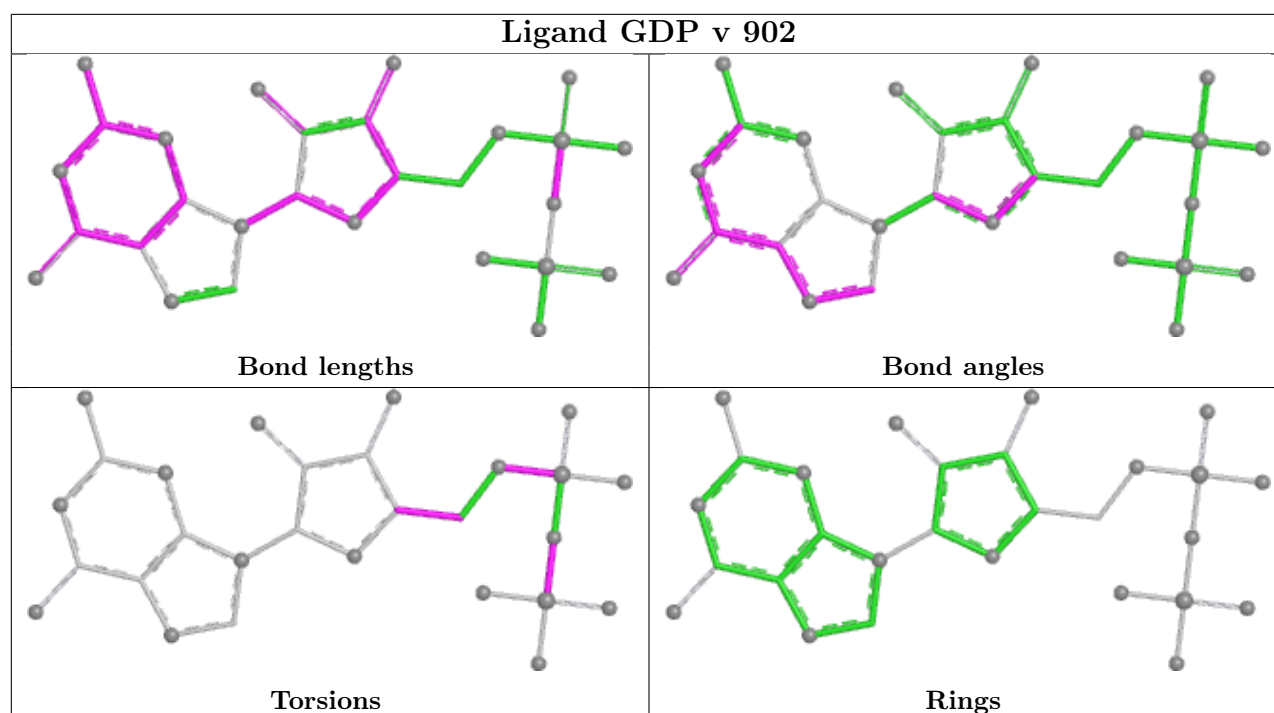
Mol	Chain	Res	Type	Atoms
86	v	902	GDP	PA-O3A-PB-O2B
86	v	902	GDP	PA-O3A-PB-O3B
86	v	902	GDP	C5'-O5'-PA-O2A
86	v	902	GDP	C3'-C4'-C5'-O5'
86	v	902	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	v	902	GDP	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	5	19
53	9	10
52	w	1
51	v	1

The worst 5 of 31 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	202:SER	C	282:THR	N	64.88
1	5	2119:G	O3'	2264:C	P	40.57
1	5	1258:C	O3'	1277:G	P	35.57
1	9	697:G	O3'	729:C	P	18.44
1	5	4144:C	O3'	4152:G	P	17.51

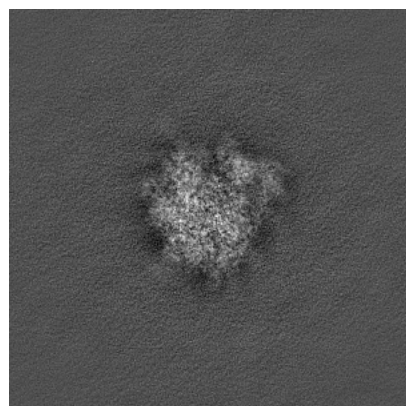
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43570. These allow visual inspection of the internal detail of the map and identification of artifacts.

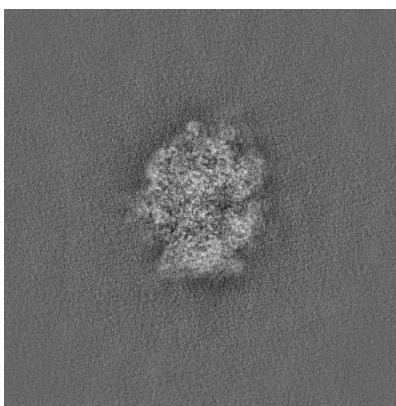
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

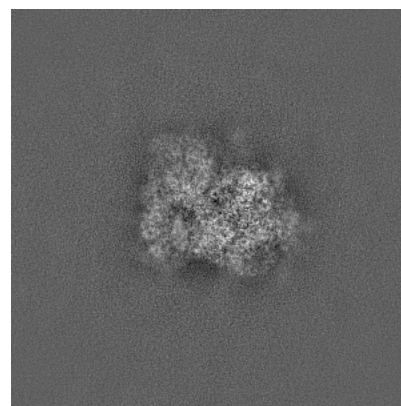
6.1.1 Primary map



X

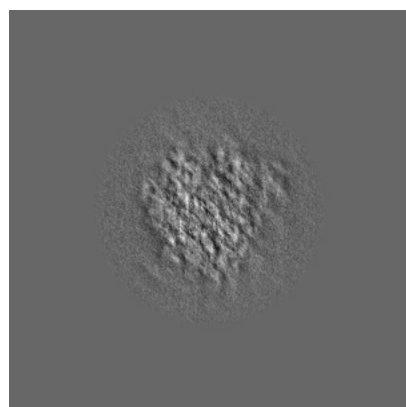


Y

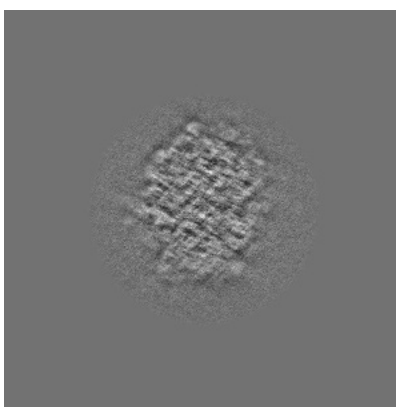


Z

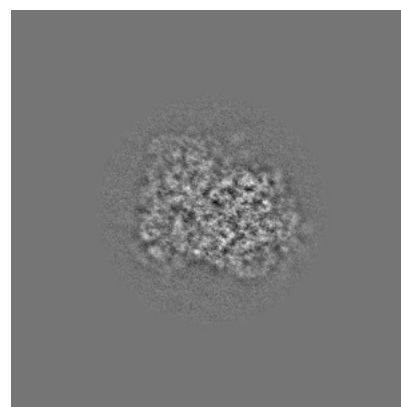
6.1.2 Raw map



X



Y

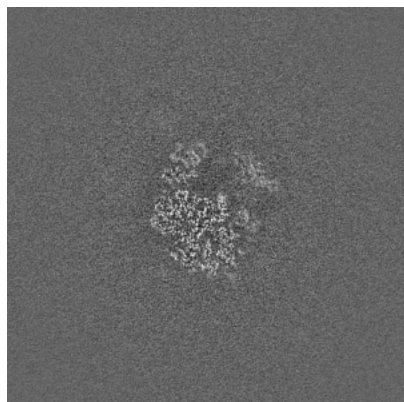


Z

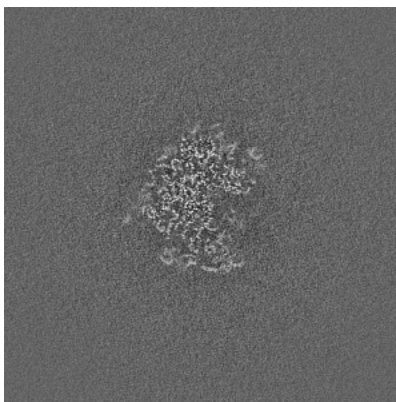
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

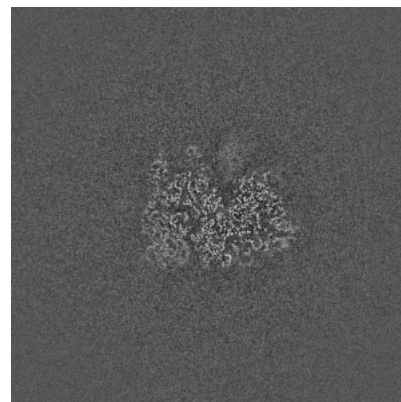
6.2.1 Primary map



X Index: 324

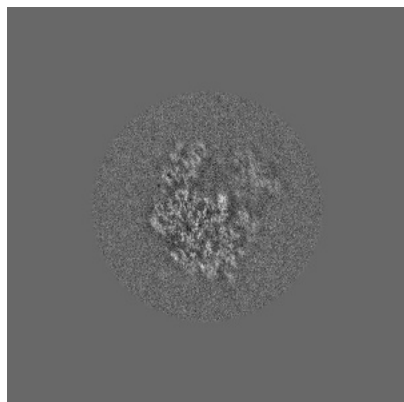


Y Index: 324

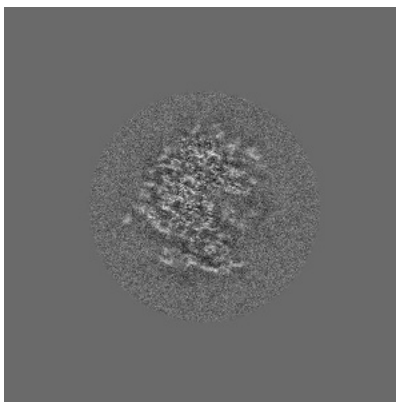


Z Index: 324

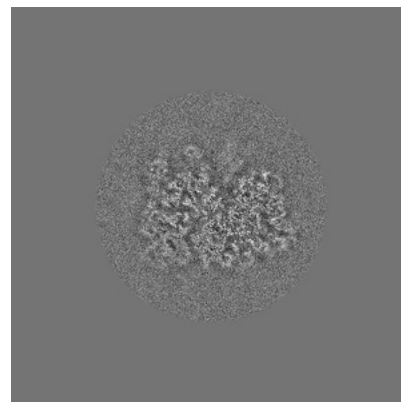
6.2.2 Raw map



X Index: 324



Y Index: 324

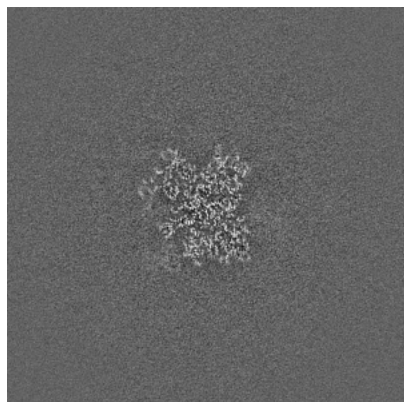


Z Index: 324

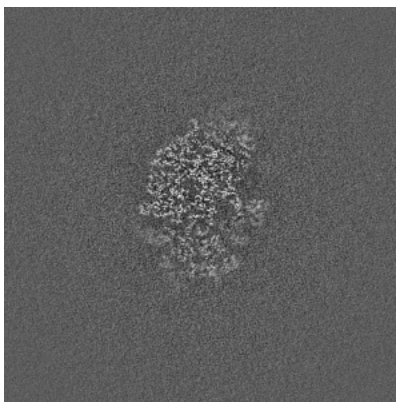
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

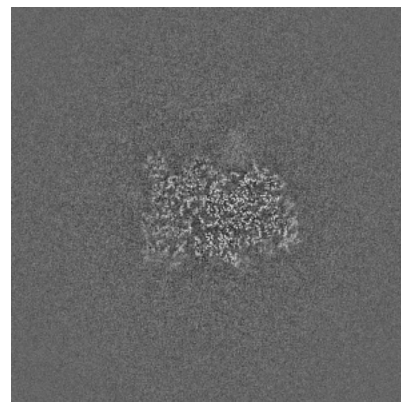
6.3.1 Primary map



X Index: 375

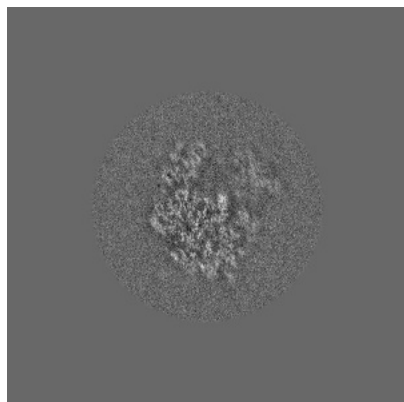


Y Index: 301

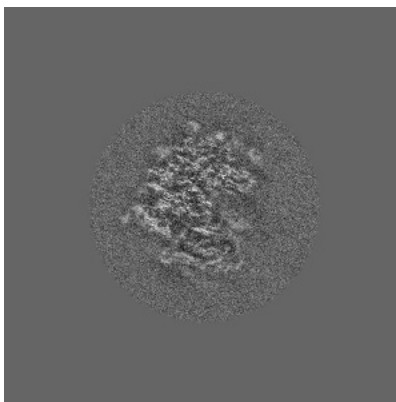


Z Index: 312

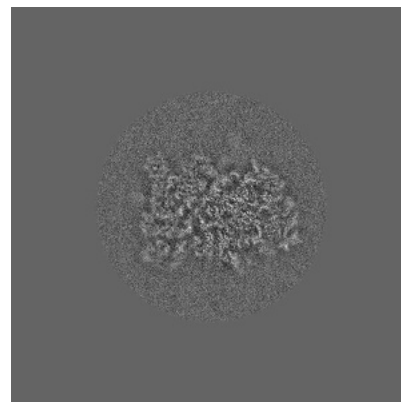
6.3.2 Raw map



X Index: 324



Y Index: 328

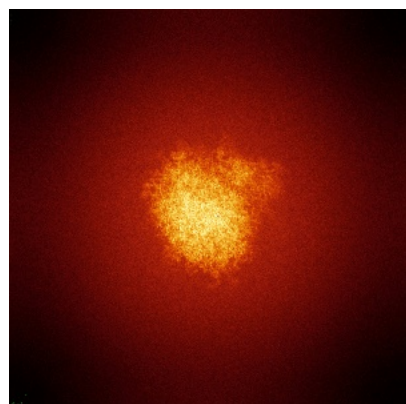


Z Index: 312

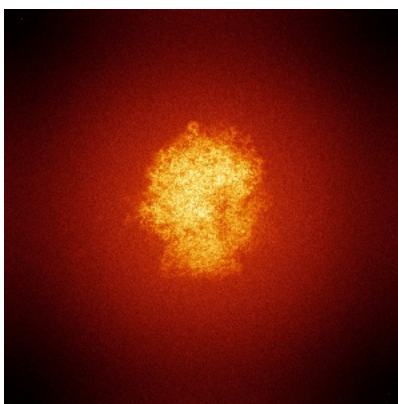
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

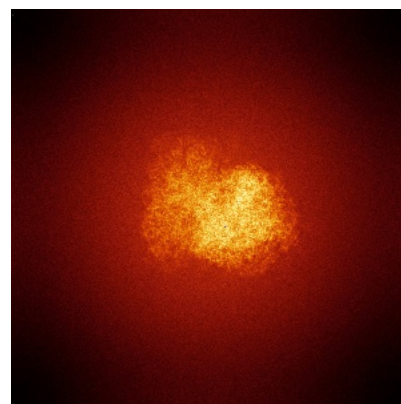
6.4.1 Primary map



X

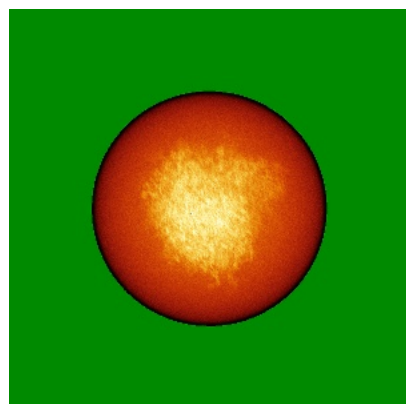


Y

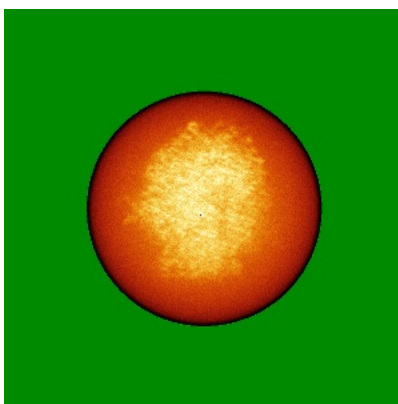


Z

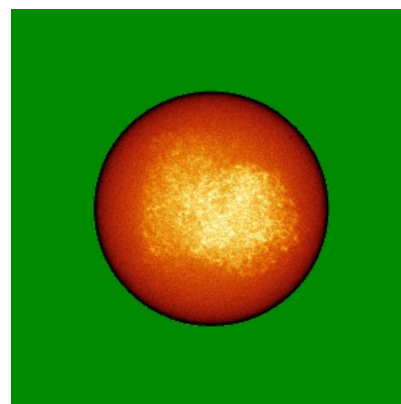
6.4.2 Raw map



X



Y

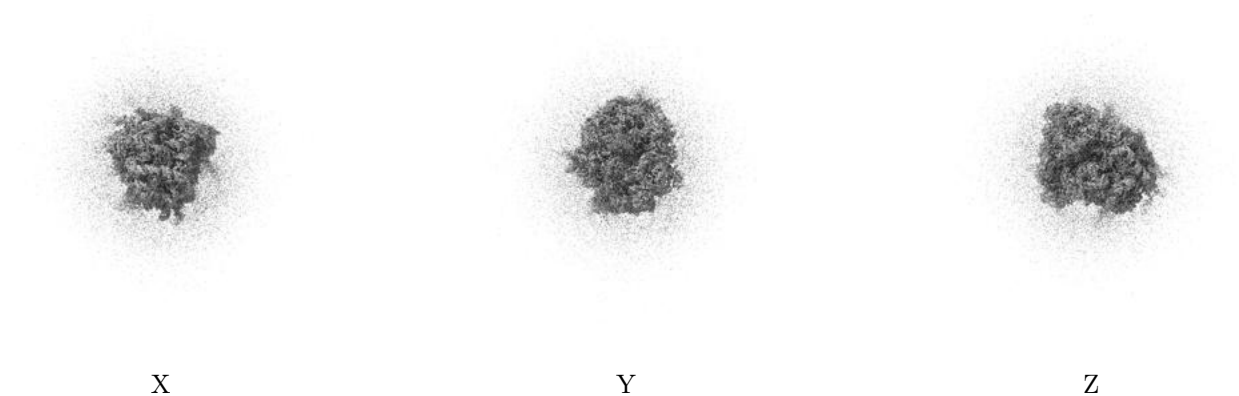


Z

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

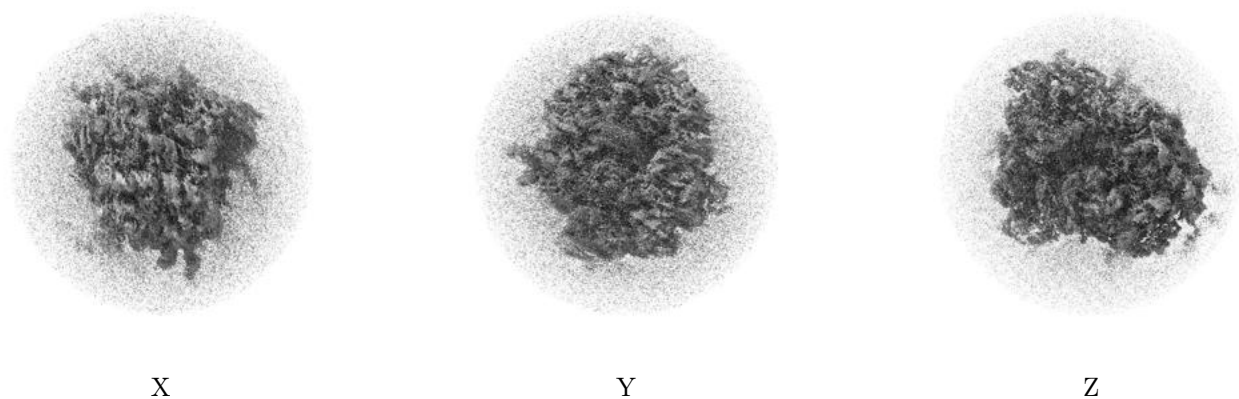
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

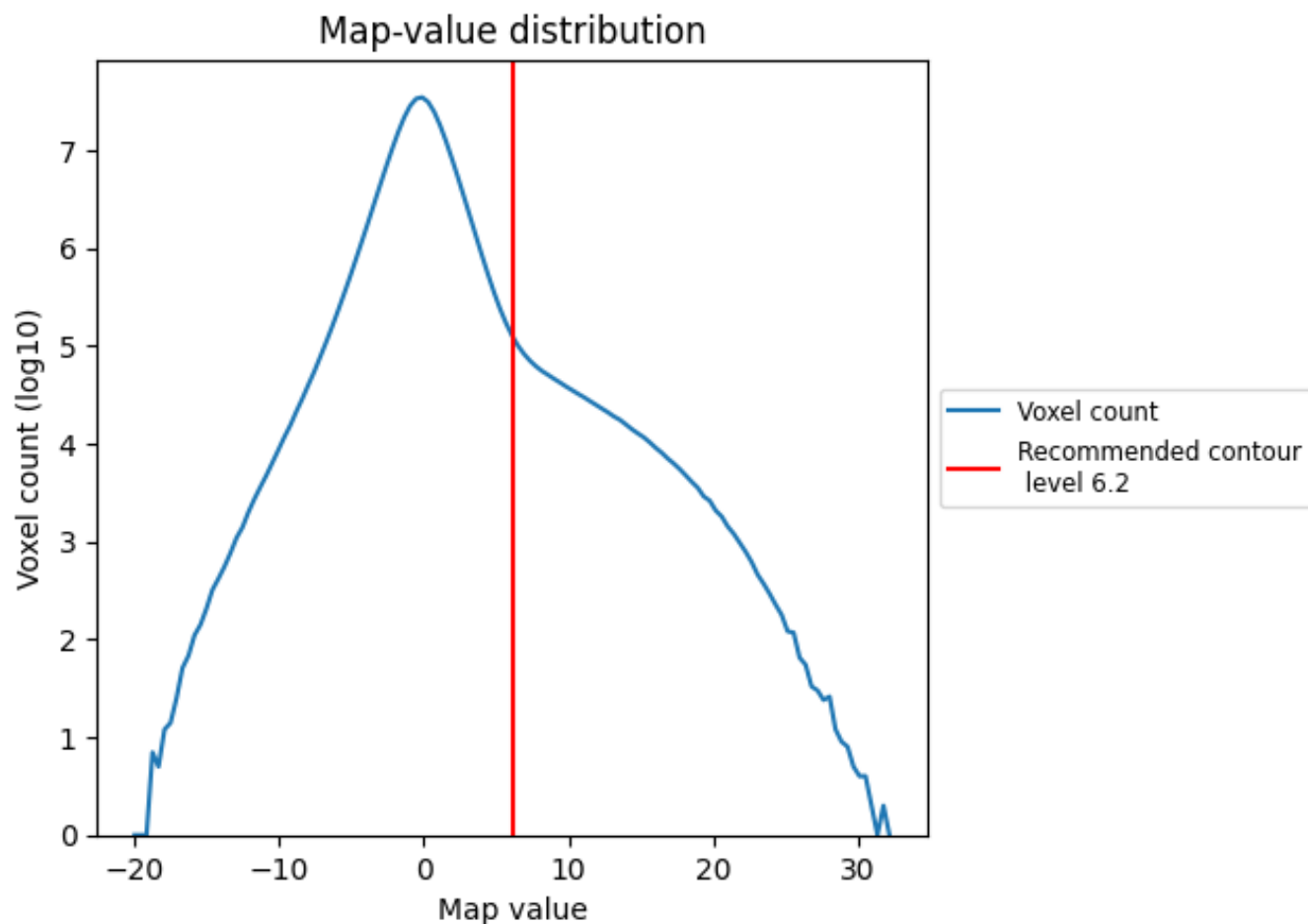
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

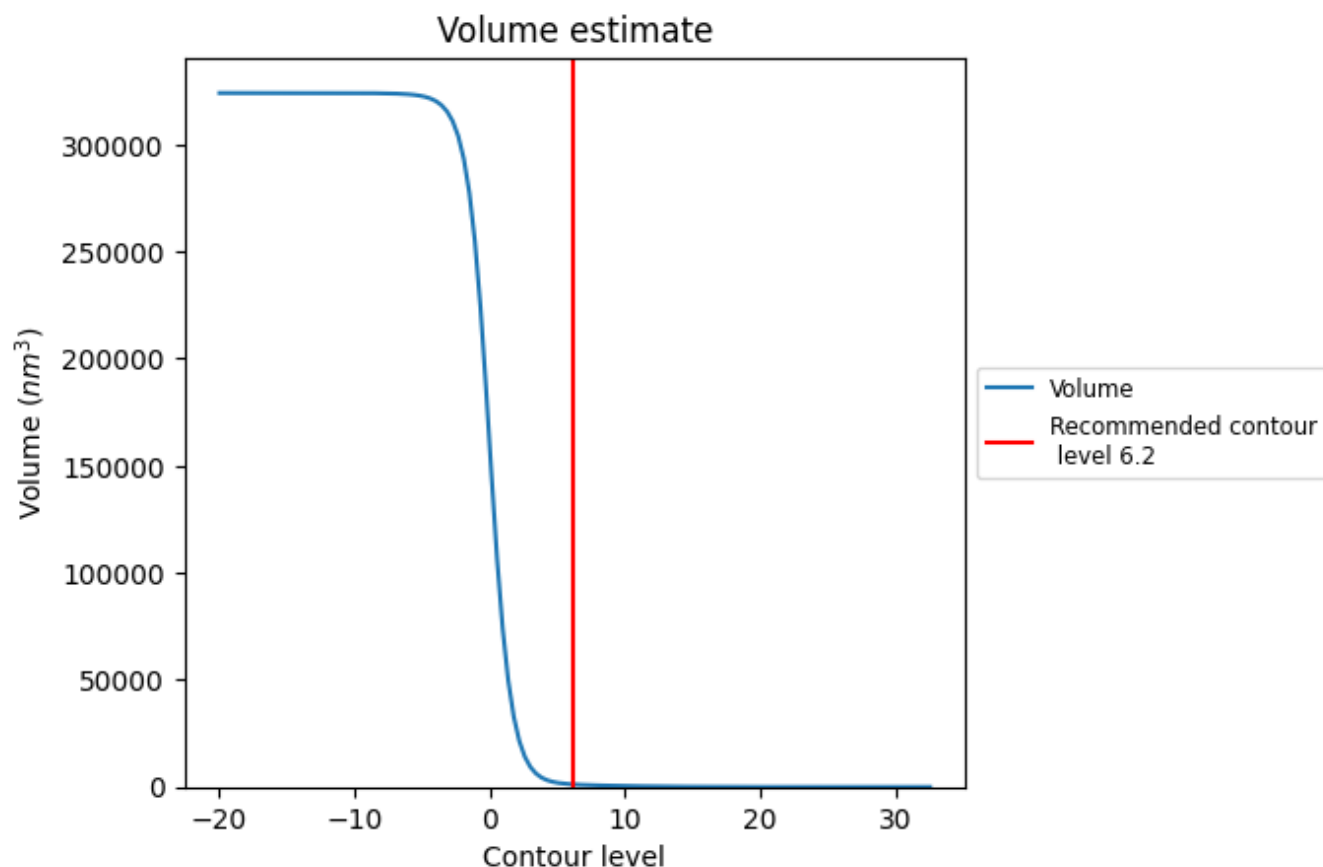
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

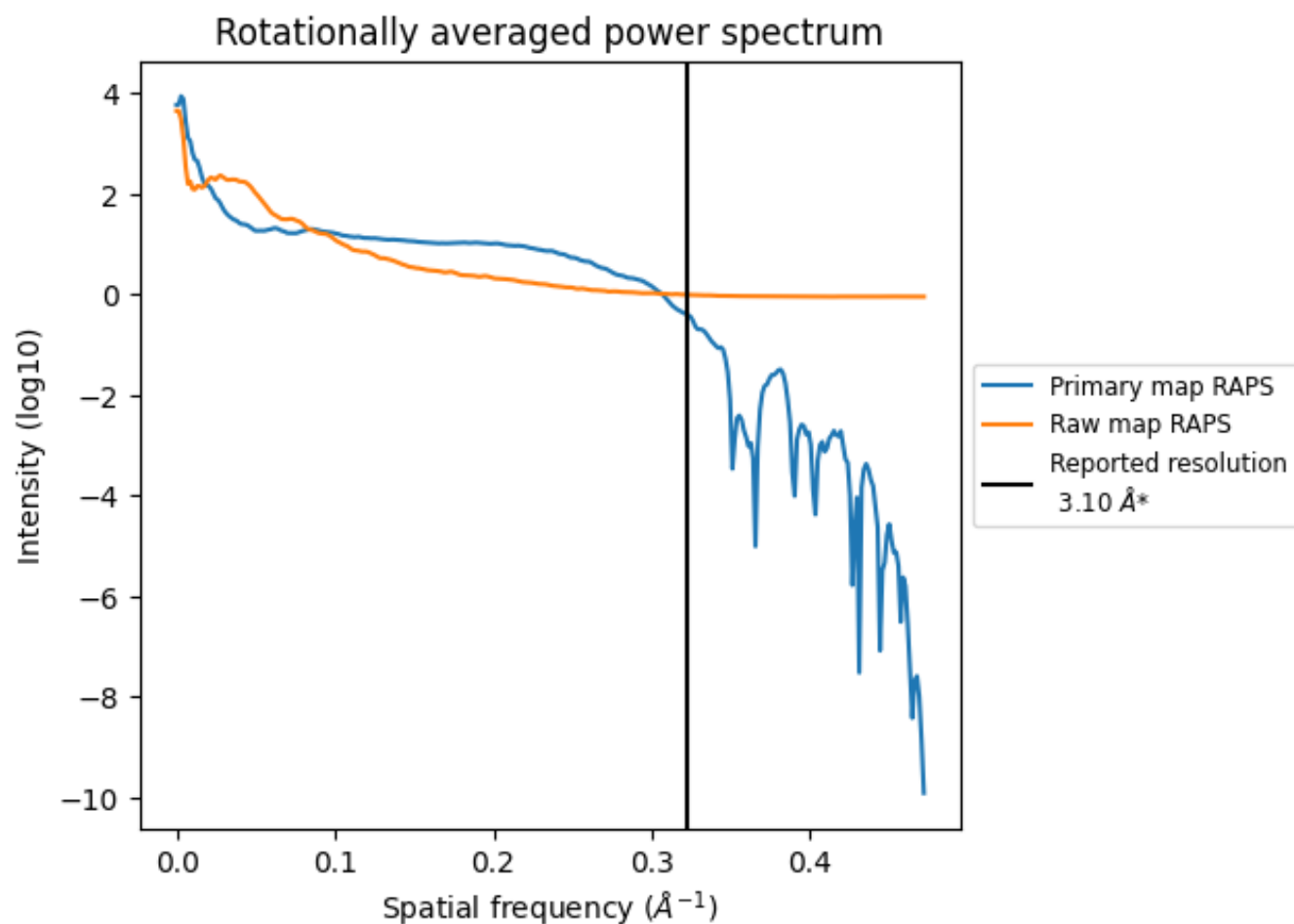
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1197 nm^3 ; this corresponds to an approximate mass of 1081 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 ⓘ

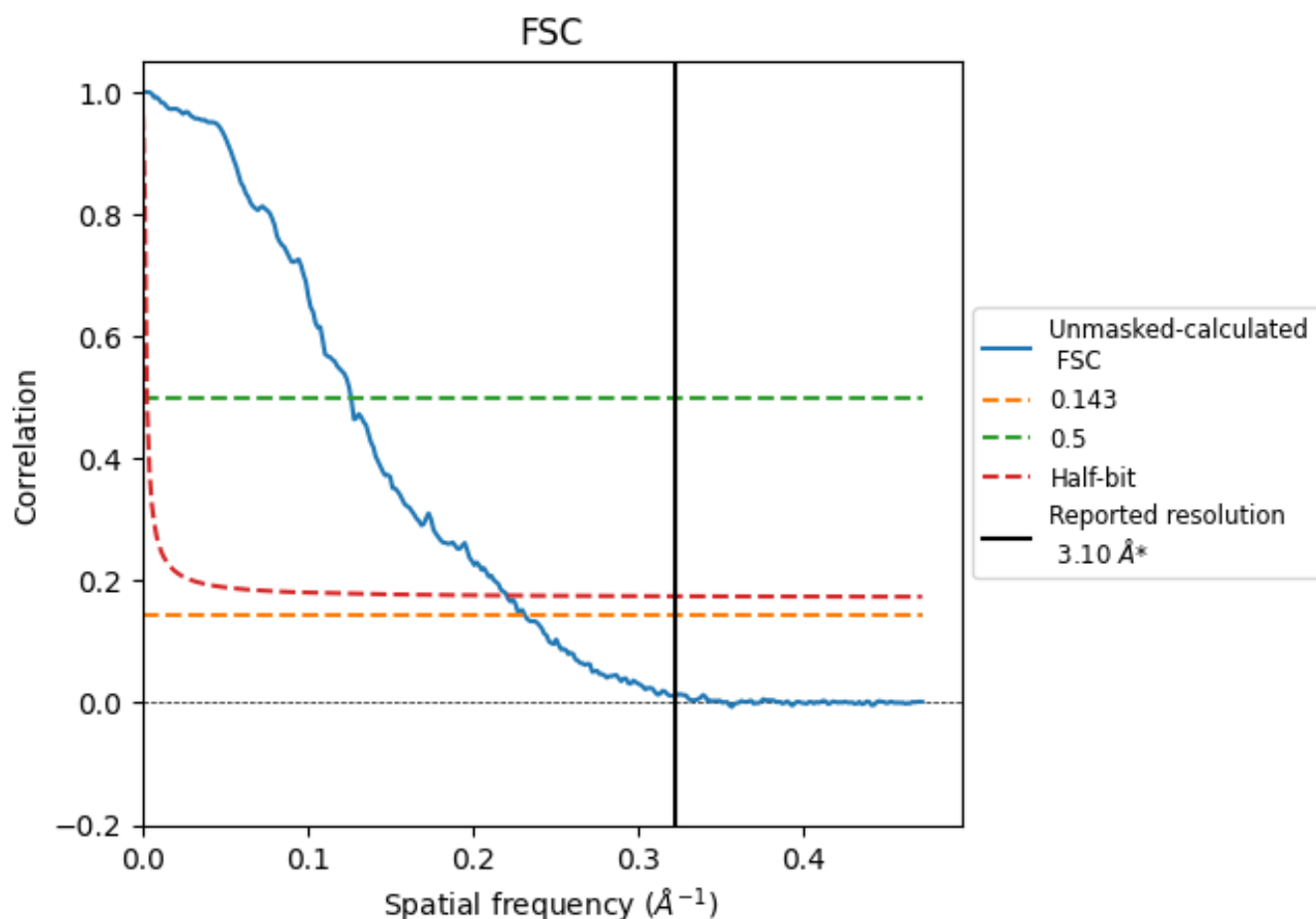


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

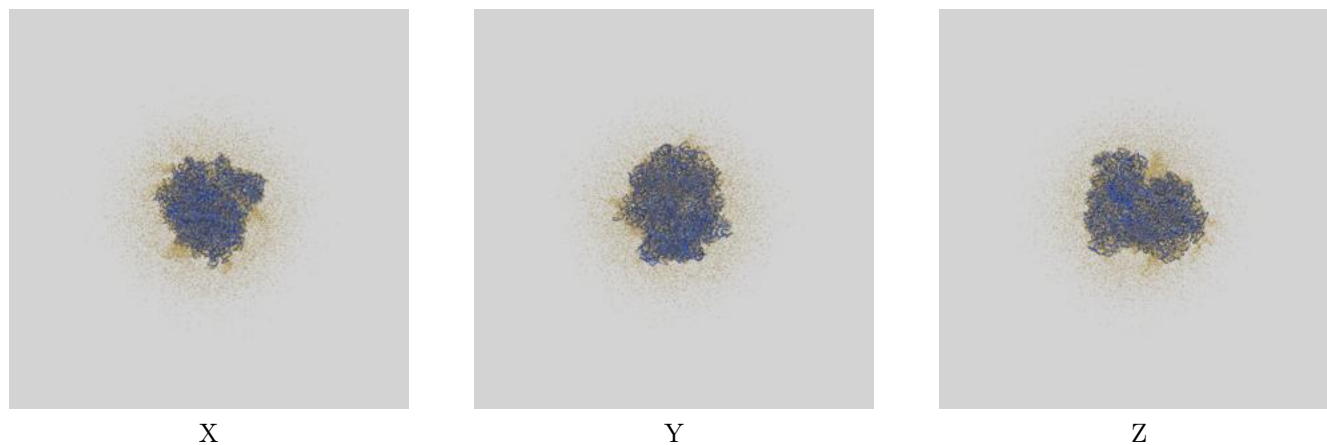
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	7.92	4.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

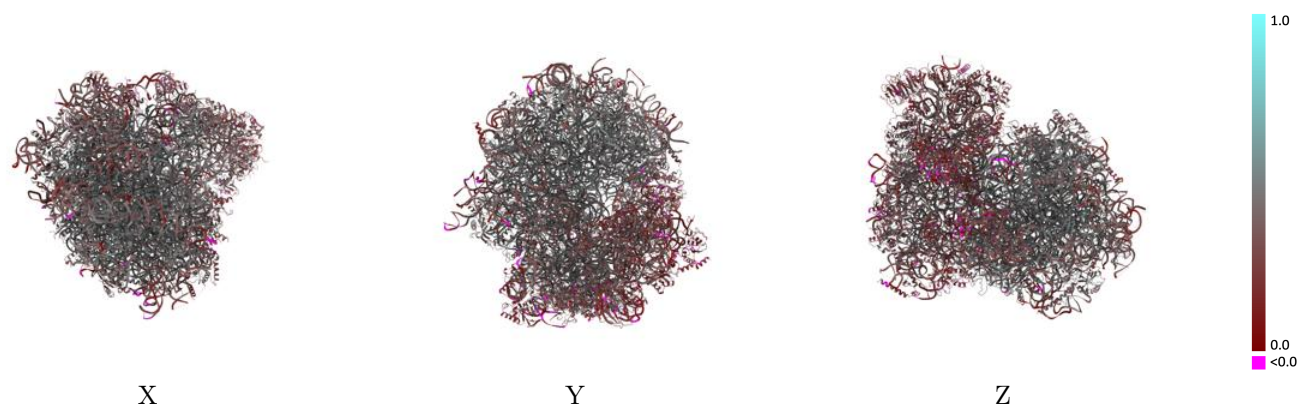
This section contains information regarding the fit between EMDB map EMD-43570 and PDB model 8VVV. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



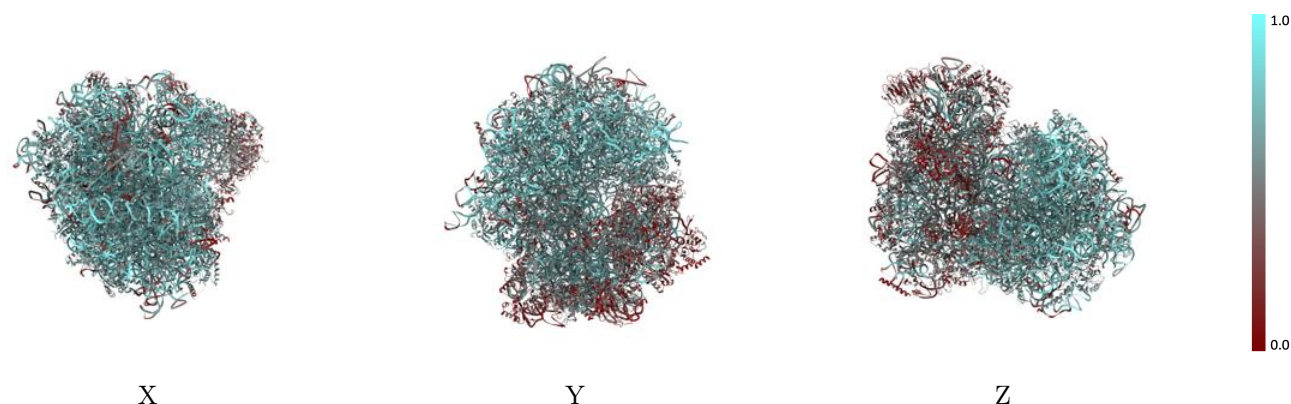
The images above show the 3D surface view of the map at the recommended contour level 6.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



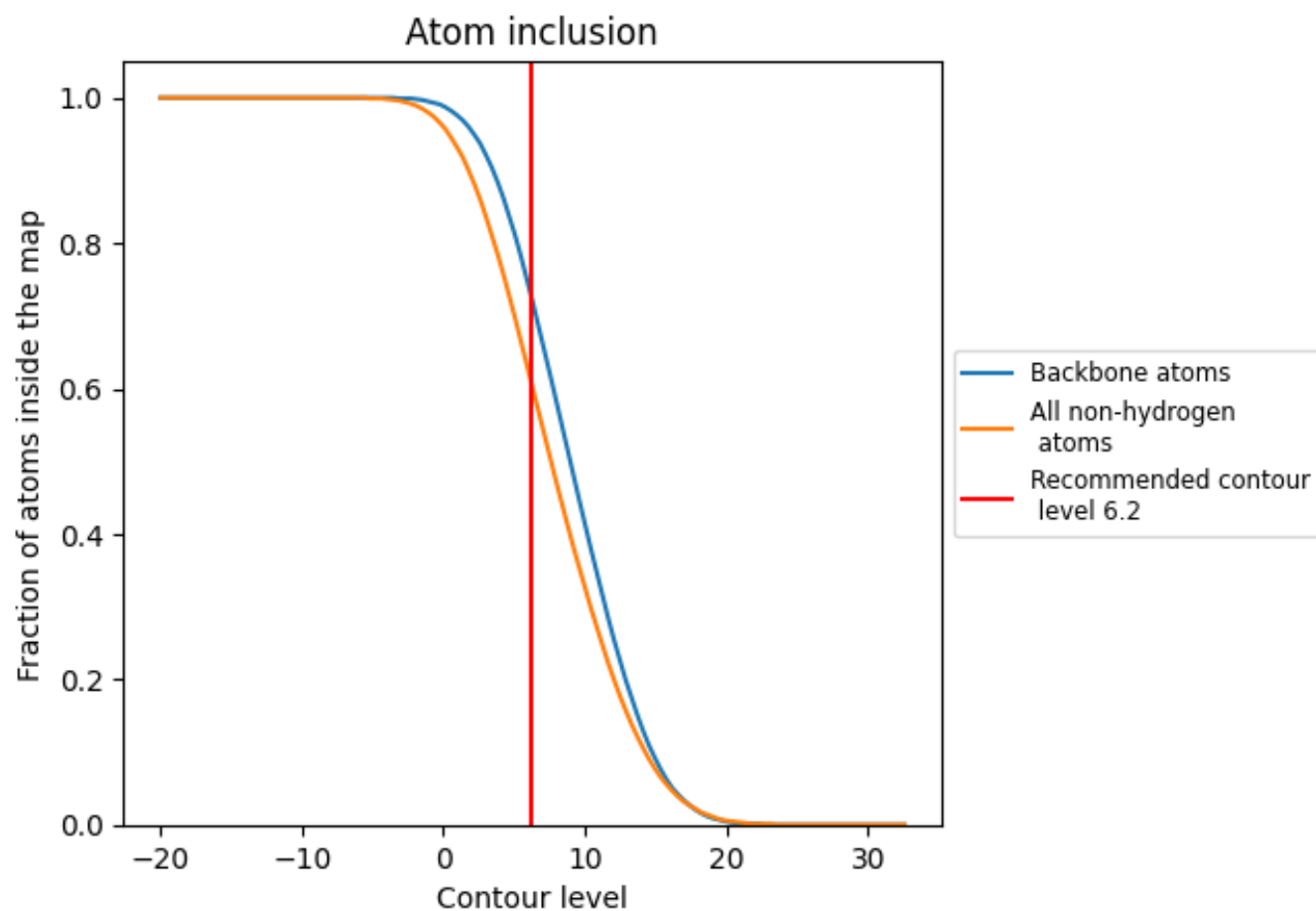
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (6.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.3940
5	 0.7490	 0.4260
7	 0.8260	 0.4590
8	 0.7640	 0.4240
9	 0.6070	 0.3590
A	 0.6270	 0.4830
AA	 0.4450	 0.3520
B	 0.6210	 0.4620
BB	 0.4280	 0.3620
C	 0.6260	 0.4600
CC	 0.4980	 0.3890
D	 0.6420	 0.4240
DD	 0.3480	 0.3260
E	 0.5830	 0.4270
EE	 0.4190	 0.3600
F	 0.6150	 0.4480
FF	 0.3510	 0.3090
G	 0.5870	 0.4000
GG	 0.3730	 0.3030
H	 0.5830	 0.4260
HH	 0.2830	 0.2920
I	 0.6080	 0.4490
II	 0.4470	 0.3660
J	 0.5760	 0.3910
JJ	 0.4800	 0.3510
KK	 0.2850	 0.2540
L	 0.6100	 0.4350
LL	 0.4830	 0.4190
M	 0.5990	 0.4180
MM	 0.1280	 0.1530
N	 0.6490	 0.4760
NN	 0.4910	 0.3850
O	 0.6330	 0.4520
OO	 0.4550	 0.3750
P	 0.6330	 0.4710

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PP	 0.3380	 0.2600
Q	 0.6190	 0.4700
QQ	 0.3320	 0.3060
R	 0.5790	 0.4060
RR	 0.2980	 0.3040
S	 0.6220	 0.4560
SS	 0.3320	 0.2910
T	 0.6140	 0.4580
TT	 0.3210	 0.2950
U	 0.5570	 0.3710
UU	 0.3000	 0.2960
V	 0.6080	 0.4660
VV	 0.4900	 0.3720
W	 0.4630	 0.3560
WW	 0.5000	 0.4100
X	 0.5940	 0.4430
XX	 0.4460	 0.3960
Y	 0.6180	 0.4360
YY	 0.3710	 0.3150
Z	 0.5960	 0.4240
ZZ	 0.2800	 0.2770
a	 0.6420	 0.4740
aa	 0.4780	 0.3880
b	 0.5150	 0.3950
bb	 0.3940	 0.3460
c	 0.5950	 0.4100
cc	 0.2940	 0.2930
d	 0.6070	 0.4350
dd	 0.4200	 0.3460
e	 0.6080	 0.4750
ee	 0.3710	 0.3090
f	 0.6370	 0.4800
ff	 0.1480	 0.2060
g	 0.6290	 0.4590
gg	 0.2470	 0.2550
h	 0.6080	 0.4210
i	 0.6010	 0.4160
j	 0.6420	 0.4710
k	 0.5420	 0.3880
l	 0.5970	 0.4710
m	 0.6020	 0.4250
n	 0.4910	 0.4160

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o	 0.6170	 0.4550
p	 0.6040	 0.4570
r	 0.6350	 0.4590
s	 0.3870	 0.2910
t	 0.2270	 0.1810
v	 0.3090	 0.2610
w	 0.1150	 0.2330