



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 07:39 PM EDT

PDB ID : 8VVT / pdb_00008vvt
EMDB ID : EMD-43568
Title : Mammalian ribosomes bound to Anisomycin in the rotated conformation
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.
Deposited on : 2024-01-31
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

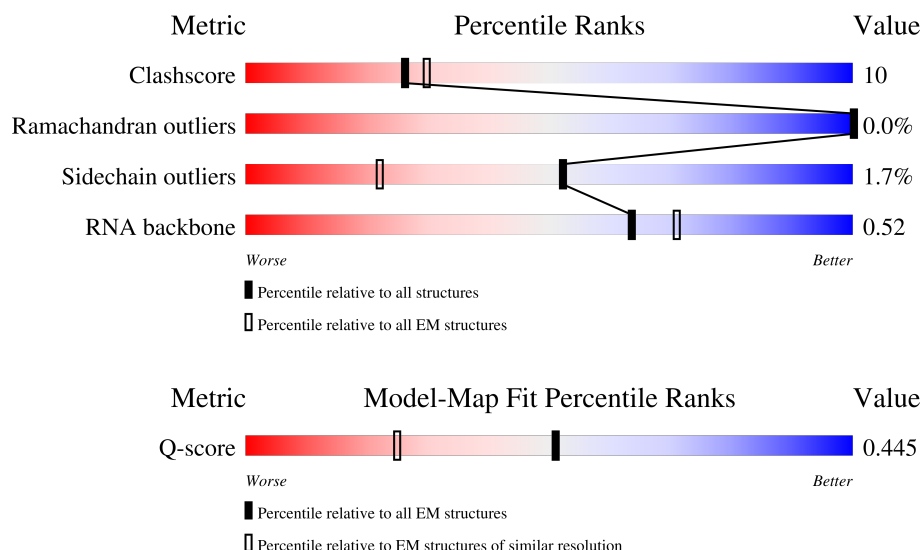
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



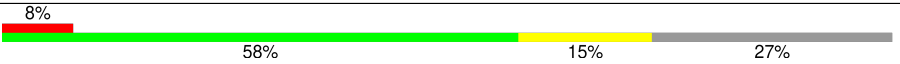
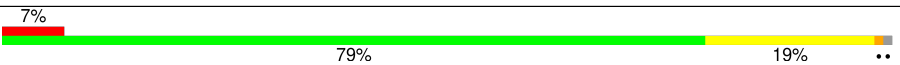
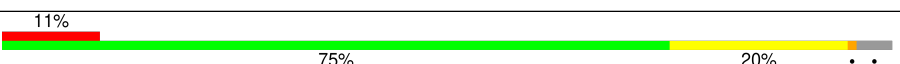
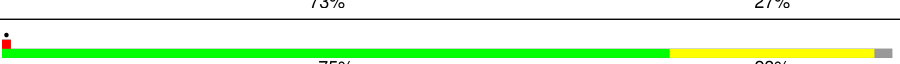
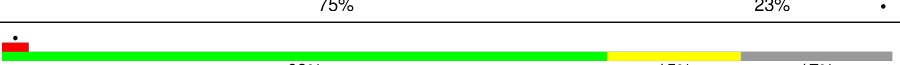
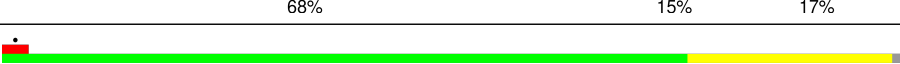
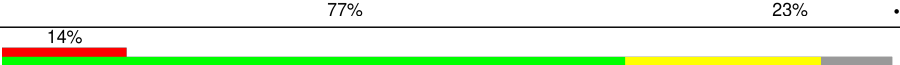
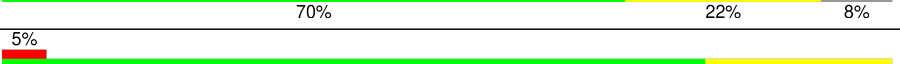
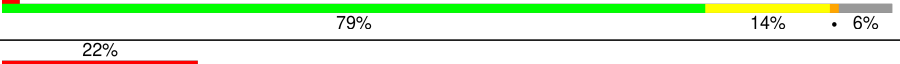
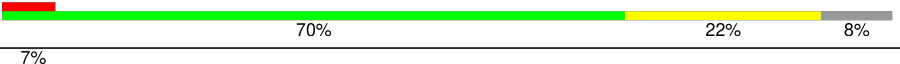
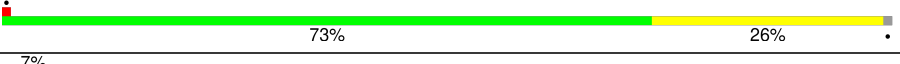
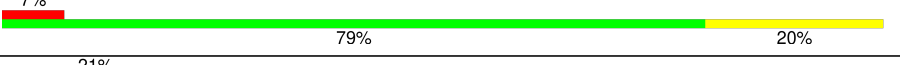
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	
2	B	403	
3	C	425	

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	218	
12	M	204	
13	N	203	
14	O	184	
15	P	188	
16	Q	196	
17	R	176	
18	S	160	
19	T	128	
20	U	140	
21	V	157	
22	W	156	
23	X	145	
24	Y	136	
25	Z	148	
26	K	211	
27	AB	295	
28	BB	264	

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Mol	Chain	Length	Quality of chain
29	CB	293	
30	WA	3635	
31	XA	120	
32	YA	156	
33	AA	245	
34	BA	115	
35	CA	125	
36	DA	135	
37	EA	110	
38	FA	117	
39	GA	123	
40	HA	105	
41	IA	97	
42	JA	70	
43	KA	51	
44	LA	102	
45	MA	25	
46	NA	106	
47	OA	92	
48	PA	137	
49	QA	318	
50	RA	165	
51	v	839	
52	w	46	
53	ZA	1869	

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Mol	Chain	Length	Quality of chain
54	DB	243	
55	EB	263	
56	FB	204	
57	GB	249	
58	HB	194	
59	IB	208	
60	JB	194	
61	KB	165	
62	LB	158	
63	MB	132	
64	NB	151	
65	OB	168	
66	PB	145	
67	QB	146	
68	RB	135	
69	SB	152	
70	TB	145	
71	UB	119	
72	VB	83	
73	WB	130	
74	XB	143	
75	YB	130	
76	ZB	125	
77	AC	115	
78	BC	84	

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Mol	Chain	Length	Quality of chain
79	CC	69	
80	DC	56	
81	EC	133	
82	FC	156	
83	GC	317	
84	b	394	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 221459 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 L8.

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 L5.

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	215	Total	C	N	O	S	0	0
			1720	1109	327	281	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		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- 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 L11.

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 L14.

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

- Molecule 12 is a protein called L15.

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

- Molecule 13 is a protein called uL13.

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

- Molecule 14 is a protein called uL22.

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

- Molecule 15 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	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
P	4	ASP	ASN	conflict	UNP G1TFE0
P	14	ARG	TRP	conflict	UNP G1TFE0
P	53	MET	LEU	conflict	UNP G1TFE0
P	58	ARG	TRP	conflict	UNP G1TFE0
P	75	ARG	GLN	conflict	UNP G1TFE0
P	80	ALA	PRO	conflict	UNP G1TFE0
P	86	VAL	ILE	conflict	UNP G1TFE0
P	104	ARG	HIS	conflict	UNP G1TFE0
P	110	ARG	CYS	conflict	UNP G1TFE0
P	137	VAL	GLY	conflict	UNP G1TFE0
P	157	GLY	ARG	conflict	UNP G1TFE0
P	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 16 is a protein called eL19.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	38	ARG	CYS	conflict	UNP G1TJR3
Q	64	ARG	GLN	conflict	UNP G1TJR3
Q	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 17 is a protein called eL20.

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

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	THR	conflict	UNP G1TTY7
R	18	PRO	-	insertion	UNP G1TTY7
R	19	THR	-	insertion	UNP G1TTY7
R	20	PRO	SER	conflict	UNP G1TTY7
R	22	CYS	SER	conflict	UNP G1TTY7
R	23	ARG	PRO	conflict	UNP G1TTY7
R	24	THR	ALA	conflict	UNP G1TTY7
R	49	SER	LEU	conflict	UNP G1TTY7
R	50	GLN	GLU	conflict	UNP G1TTY7
R	95	ARG	HIS	conflict	UNP G1TTY7
R	101	THR	ILE	conflict	UNP G1TTY7
R	102	THR	MET	conflict	UNP G1TTY7
R	104	GLY	SER	conflict	UNP G1TTY7
R	126	ILE	VAL	conflict	UNP G1TTY7
R	132	ILE	MET	conflict	UNP G1TTY7
R	135	SER	ALA	conflict	UNP G1TTY7
R	136	LYS	ARG	conflict	UNP G1TTY7
R	138	ARG	PRO	conflict	UNP G1TTY7
R	149	LYS	ARG	conflict	UNP G1TTY7
R	151	LYS	ARG	conflict	UNP G1TTY7
R	168	THR	TYR	conflict	UNP G1TTY7
R	169	THR	ALA	conflict	UNP G1TTY7
R	176	PHE	-	insertion	UNP G1TTY7

- Molecule 18 is a protein called eL21.

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

- Molecule 19 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	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
T	18	LEU	VAL	conflict	UNP G1TSG1
T	32	GLY	ARG	conflict	UNP G1TSG1
T	36	ALA	GLU	conflict	UNP G1TSG1
T	39	PHE	SER	conflict	UNP G1TSG1
T	54	GLY	ARG	conflict	UNP G1TSG1
T	60	VAL	ALA	conflict	UNP G1TSG1
T	62	SER	THR	conflict	UNP G1TSG1
T	63	LEU	ILE	conflict	UNP G1TSG1
T	97	ARG	HIS	conflict	UNP G1TSG1
T	106	THR	SER	conflict	UNP G1TSG1
T	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 20 is a protein called L23.

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

- Molecule 21 is a protein called L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	98	Total	C	N	O	S	0	0
			800	501	161	134	4		

- Molecule 22 is a protein called uL23.

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

- Molecule 23 is a protein called L26.

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

- Molecule 24 is a protein called L27.

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

- Molecule 25 is a protein called uL15.

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

- Molecule 26 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	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
K	46	ILE	-	insertion	UNP G1TPV0
K	47	ALA	-	insertion	UNP G1TPV0
K	48	PRO	-	insertion	UNP G1TPV0
K	49	ARG	-	insertion	UNP G1TPV0
K	50	PRO	-	insertion	UNP G1TPV0
K	51	ALA	-	insertion	UNP G1TPV0
K	52	ALA	-	insertion	UNP G1TPV0
K	53	GLY	-	insertion	UNP G1TPV0
K	54	PRO	-	insertion	UNP G1TPV0

- Molecule 27 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AB	217	Total	C	N	O	S	0	0
			1712	1087	300	317	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 28 is a protein called S3A.

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

- Molecule 29 is a protein called eS1.

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

- Molecule 30 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	WA	3541	Total	C	N	O	P	0	0
			76047	33931	13901	24674	3541		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	XA	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
XA	2	U	N	conflict	GB X06789.1
XA	36	C	N	conflict	GB X06789.1
XA	102	U	N	conflict	GB X06789.1
XA	112	U	N	conflict	GB X06789.1
XA	114	U	N	conflict	GB X06789.1
XA	119	U	C	conflict	GB X06789.1
XA	120	U	N	conflict	GB X06789.1

- Molecule 32 is a RNA chain called 5.8S rRNA.

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

- Molecule 33 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AA	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	BA	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	CA	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	DA	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	EA	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	FA	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	GA	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called L36.

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

- Molecule 41 is a protein called L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	IA	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	JA	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	24	LYS	ASN	conflict	UNP G1U001

- Molecule 43 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	KA	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	LA	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	MA	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	NA	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	OA	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	PA	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	QA	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 50 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RA	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	832	Total	C	N	O	S	0	0
			6489	4128	1111	1207	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	w	46	Total	C	N	O	0	0
			366	219	76	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ZA	1698	Total	C	N	O	P	0	0
			36263	16190	6509	11867	1697		

- Molecule 54 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DB	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	EB	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EB	25	GLY	SER	conflict	UNP G1TK17
EB	51	ARG	LYS	conflict	UNP G1TK17
EB	78	THR	ALA	conflict	UNP G1TK17
EB	156	VAL	MET	conflict	UNP G1TK17

- Molecule 56 is a protein called S5.

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

- Molecule 57 is a protein called S6.

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

- Molecule 58 is a protein called S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HB	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	IB	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
IB	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 60 is a protein called S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JB	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	KB	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LB	138	Total	C	N	O	S	0	0
			1137	725	214	192	6		

- Molecule 63 is a protein called S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	MB	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	NB	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	OB	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	PB	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 67 is a protein called S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	QB	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	RB	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	SB	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	TB	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
TB	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 71 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	UB	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	VB	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
VB	3	ASN	SER	conflict	UNP G1TM82
VB	4	ASP	ASN	conflict	UNP G1TM82
VB	33	GLN	PRO	conflict	UNP G1TM82
VB	50	PHE	SER	conflict	UNP G1TM82
VB	75	ALA	SER	conflict	UNP G1TM82
VB	76	ASP	HIS	conflict	UNP G1TM82
VB	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 73 is a protein called S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	WB	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	XB	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	YB	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	ZB	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	AC	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	28	ARG	CYS	conflict	UNP G1TFE8
AC	56	ALA	VAL	conflict	UNP G1TFE8
AC	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 78 is a protein called S27.

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

- Molecule 79 is a protein called S28.

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	DC	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called S30.

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

- Molecule 82 is a protein called S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	FC	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	GC	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 84 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	b	325	Total	C	N	O	S	0	0
			2422	1547	422	439	14		

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

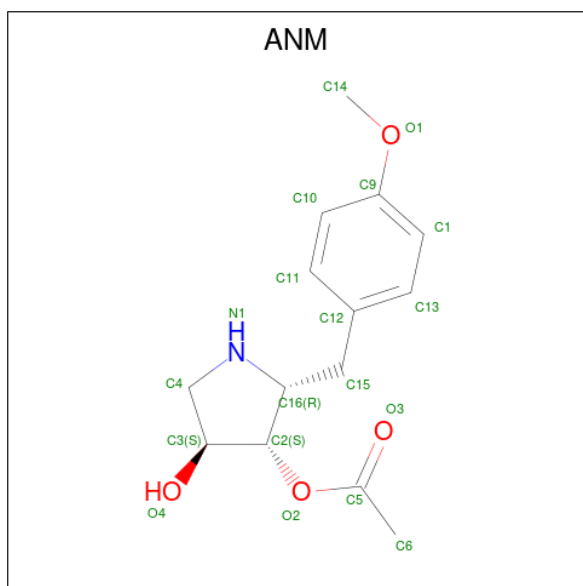
Mol	Chain	Residues	Atoms		AltConf
85	B	2	Total	Mg	0
			2	2	
85	I	1	Total	Mg	0
			1	1	
85	O	1	Total	Mg	0
			1	1	
85	U	1	Total	Mg	0
			1	1	
85	WA	110	Total	Mg	0
			110	110	
85	XA	4	Total	Mg	0
			4	4	
85	YA	1	Total	Mg	0
			1	1	
85	DA	1	Total	Mg	0
			1	1	
85	FA	1	Total	Mg	0
			1	1	
85	KA	1	Total	Mg	0
			1	1	
85	ZA	19	Total	Mg	0
			19	19	
85	TB	1	Total	Mg	0
			1	1	

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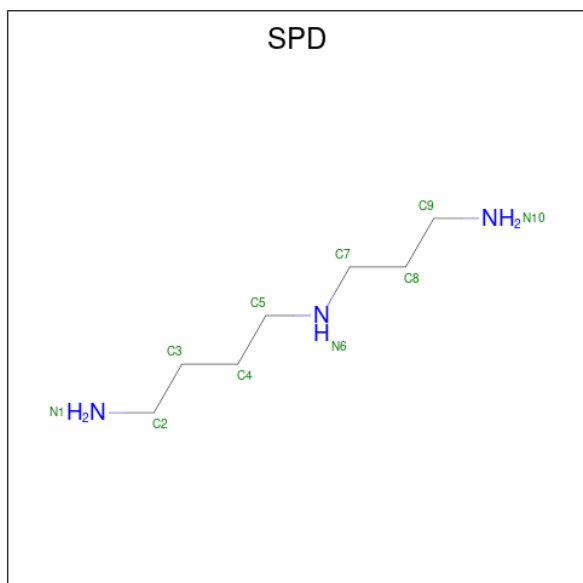
Mol	Chain	Residues	Atoms		AltConf
85	AC	1	Total	Mg	0
			1	1	

- Molecule 86 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
86	WA	1	Total	C	N	O	0
			19	14	1	4	

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

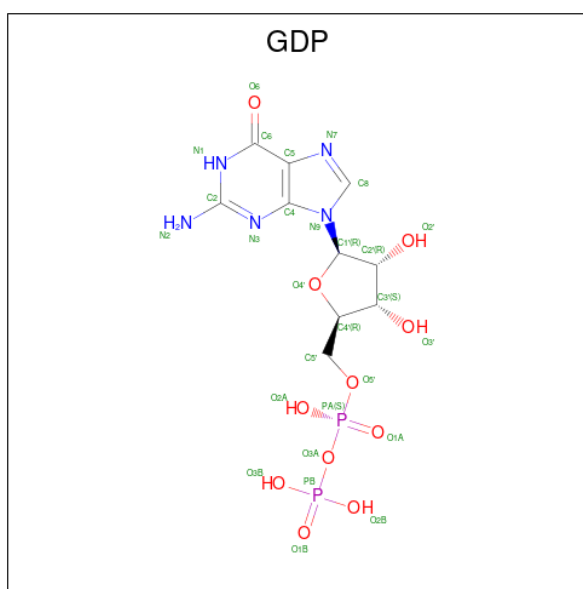


Mol	Chain	Residues	Atoms			AltConf
87	WA	1	Total	C	N	0
			10	7	3	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	FA	1	Total	Zn	0
			1	1	
88	IA	1	Total	Zn	0
			1	1	
88	LA	1	Total	Zn	0
			1	1	
88	NA	1	Total	Zn	0
			1	1	
88	OA	1	Total	Zn	0
			1	1	
88	AC	1	Total	Zn	0
			1	1	
88	DC	1	Total	Zn	0
			1	1	
88	FC	1	Total	Zn	0
			1	1	

- Molecule 89 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

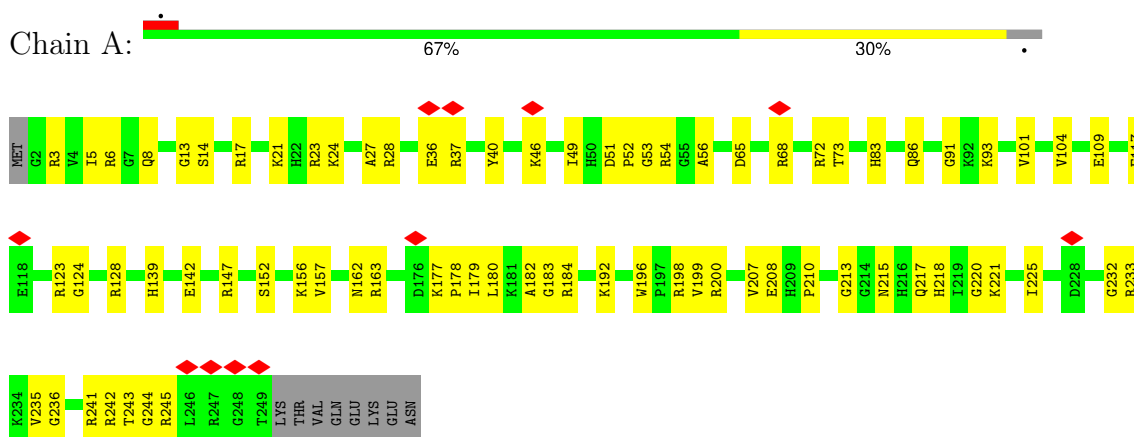


Mol	Chain	Residues	Atoms					AltConf
89	v	1	Total	C	N	O	P	0
			28	10	5	11	2	

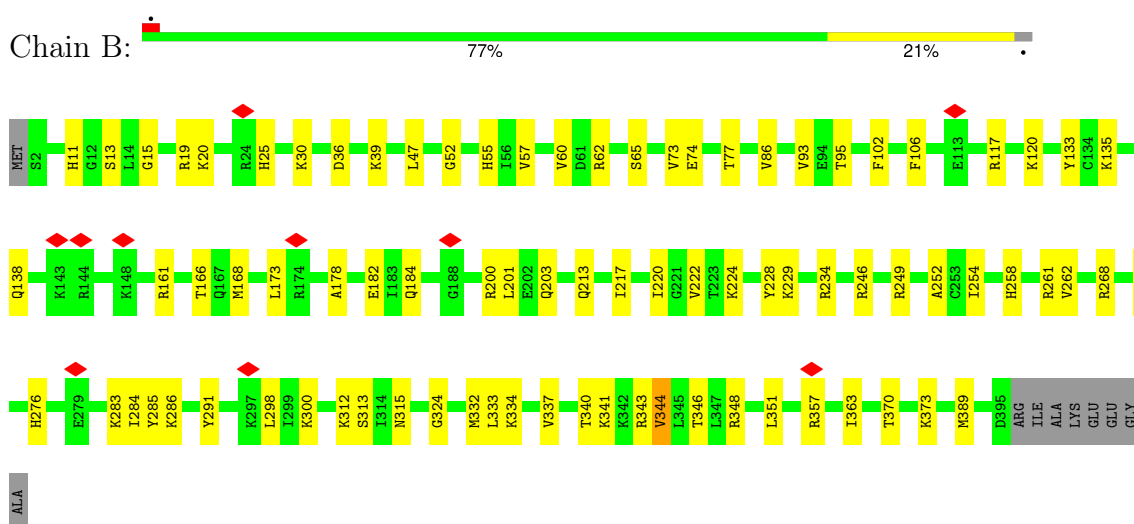
3 Residue-property plots

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: L8

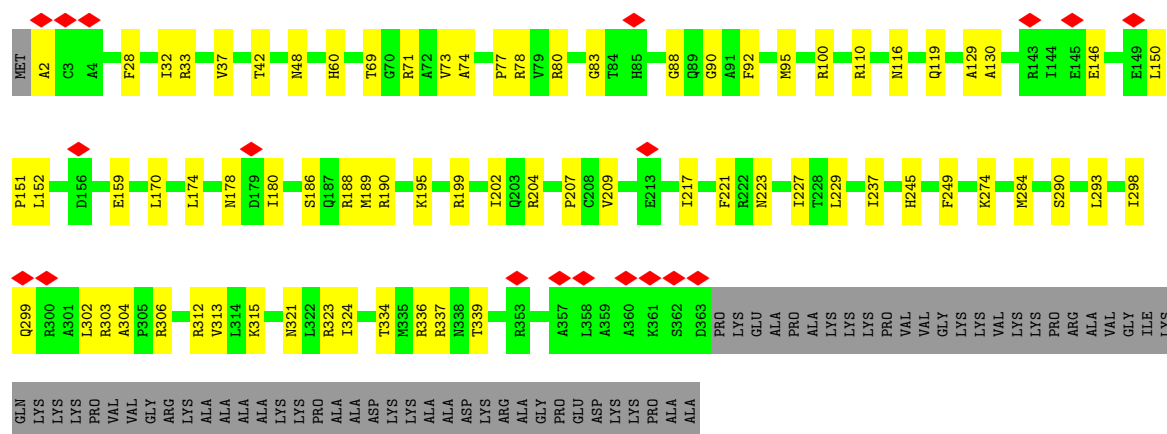


• Molecule 2: uL3

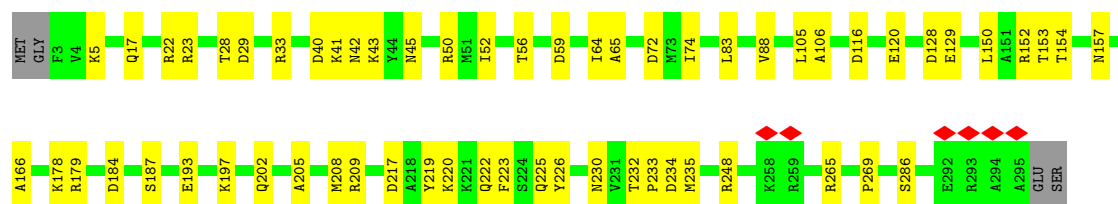
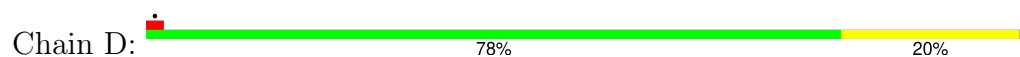


• Molecule 3: uL4

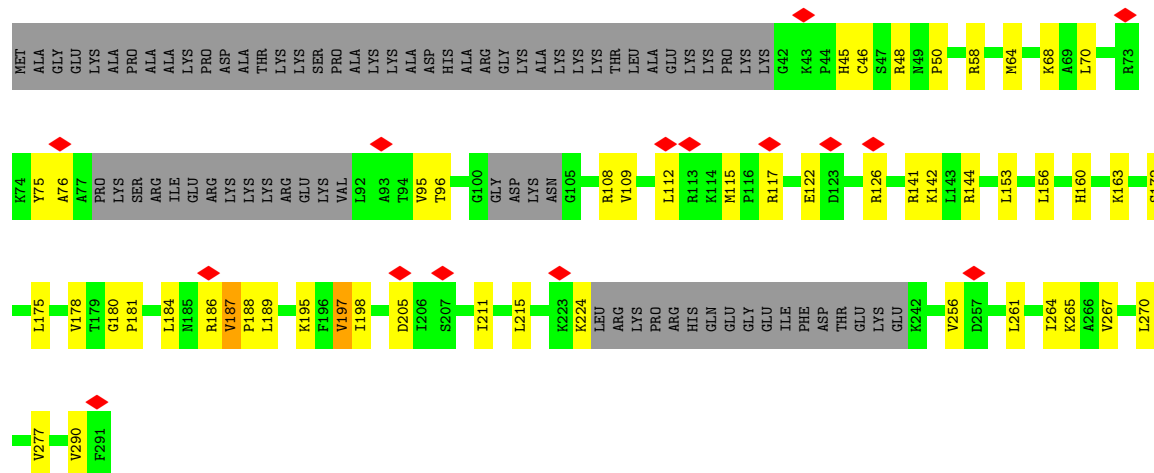




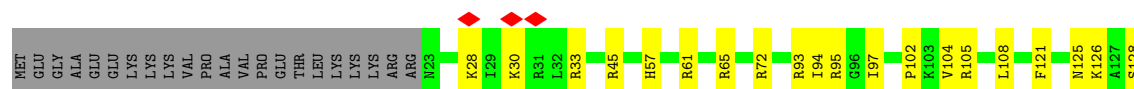
• Molecule 4: L5



• Molecule 5: L6

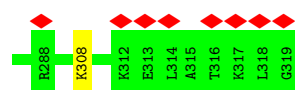
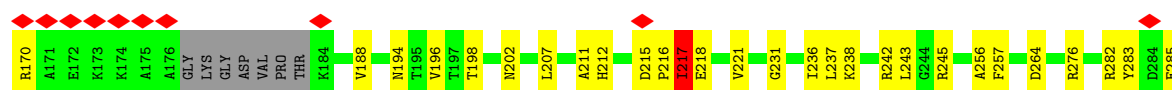
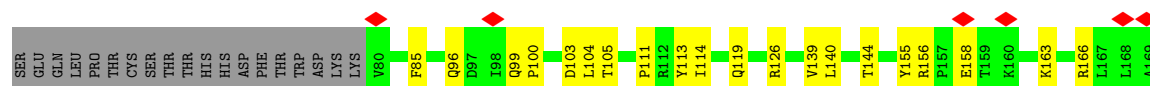
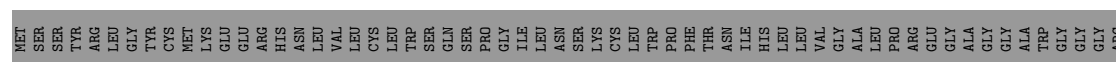


• Molecule 6: uL30

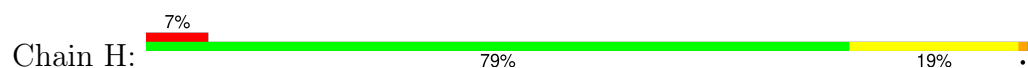




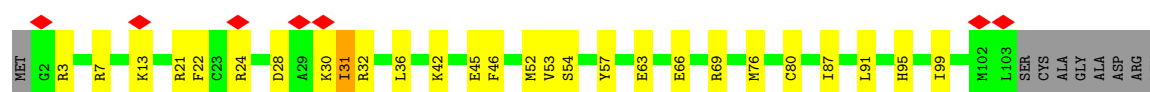
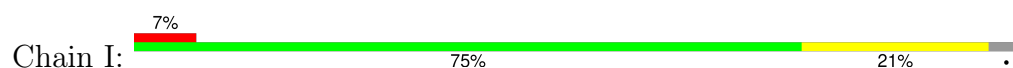
• Molecule 7: eL8



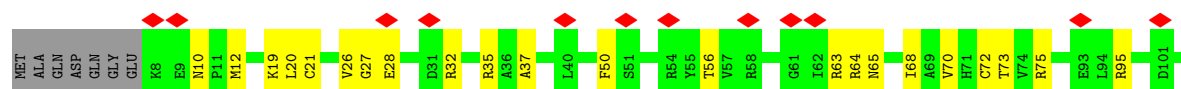
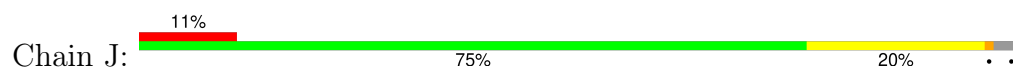
• Molecule 8: uL6



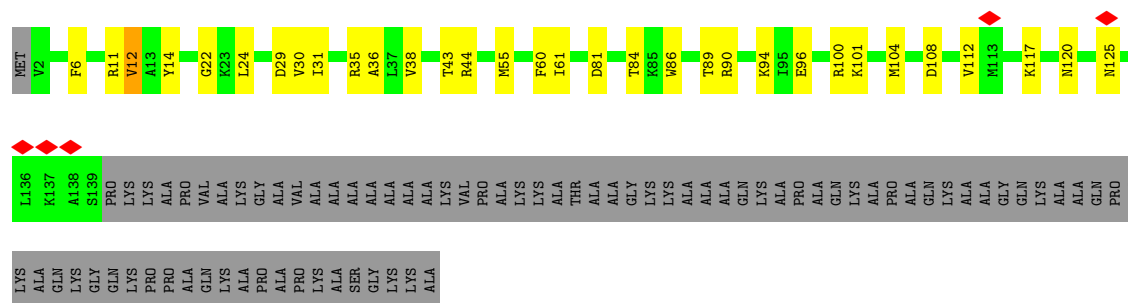
• Molecule 9: L10



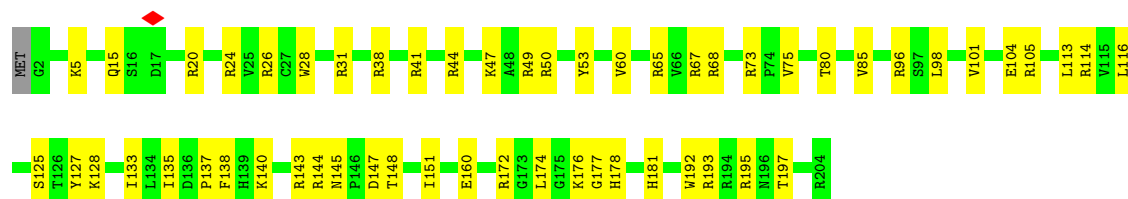
• Molecule 10: L11



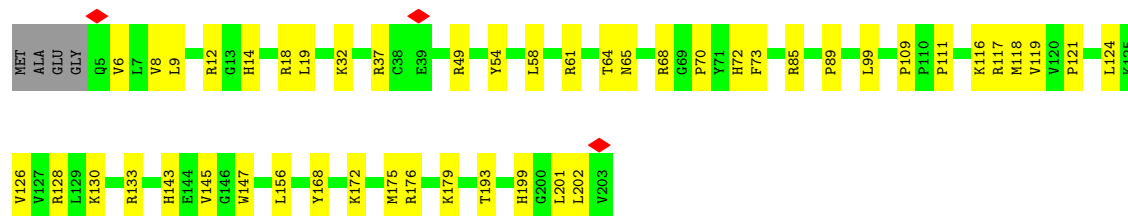
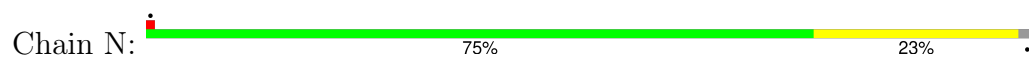
- Molecule 11: L14



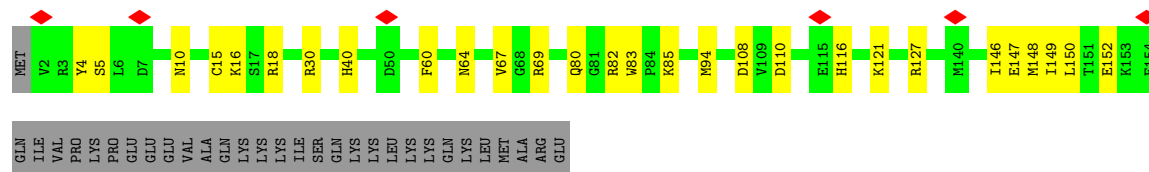
- Molecule 12: L15



- Molecule 13: uL13

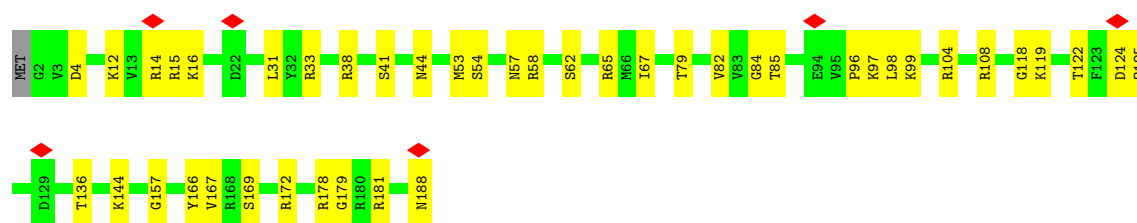


- Molecule 14: uL22



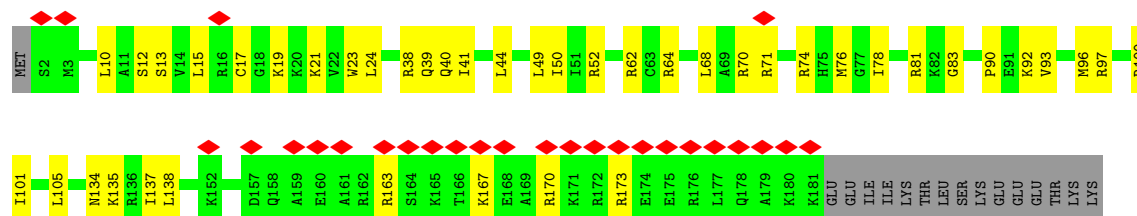
- Molecule 15: eL18

Chain P:  77% 23%



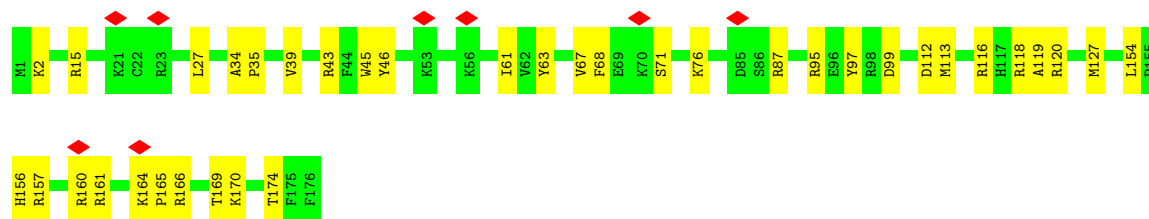
• Molecule 16: eL19

Chain Q:  14% 70% 22% 8%



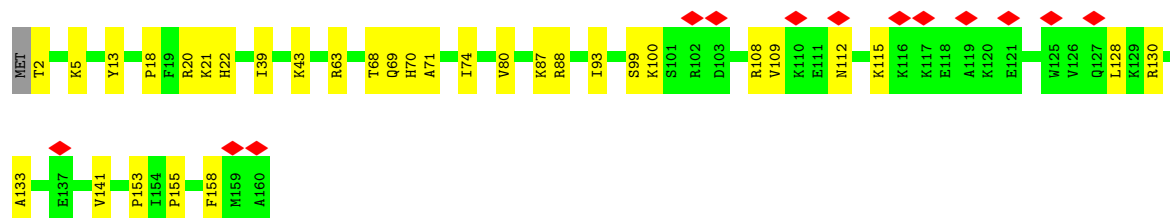
• Molecule 17: eL20

Chain R:  5% 79% 21%



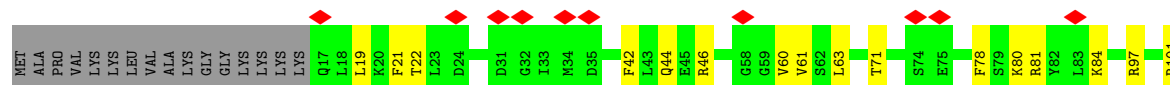
• Molecule 18: eL21

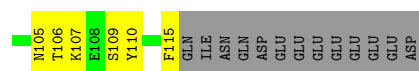
Chain S:  8% 79% 20%



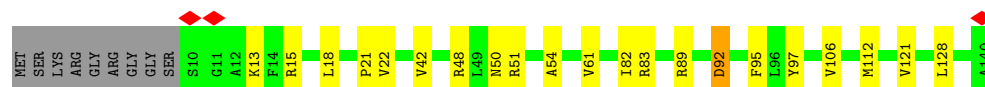
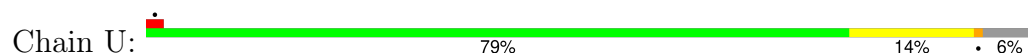
• Molecule 19: eL22

Chain T:  8% 60% 17% 23%

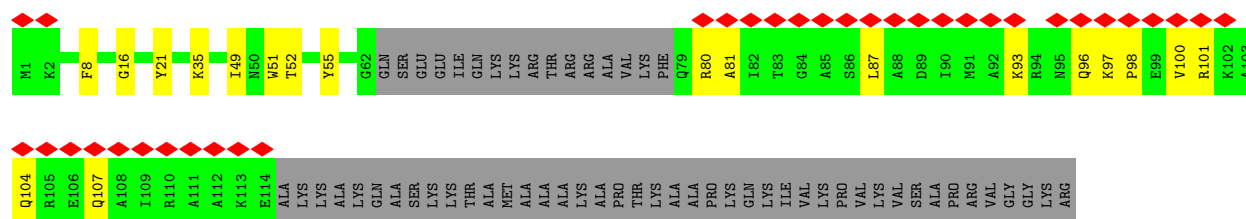




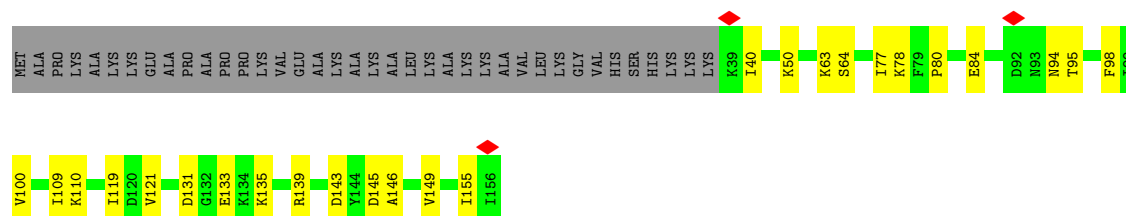
• Molecule 20: L23



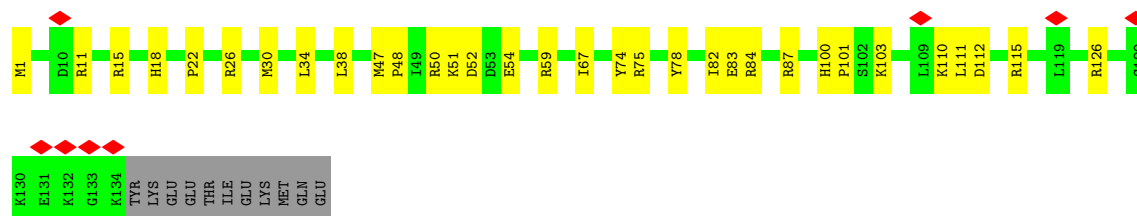
• Molecule 21: L24



• Molecule 22: uL23

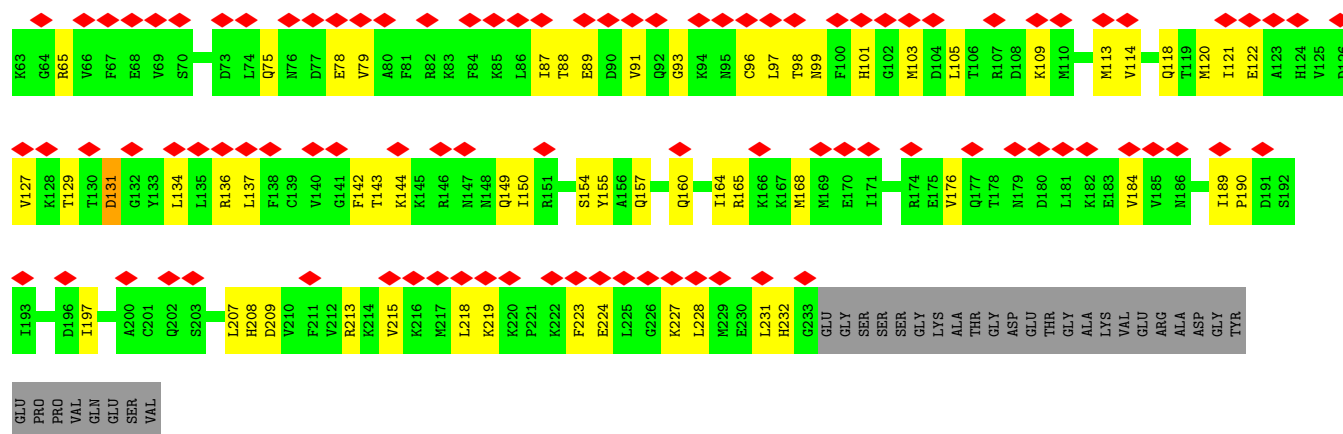


• Molecule 23: L26

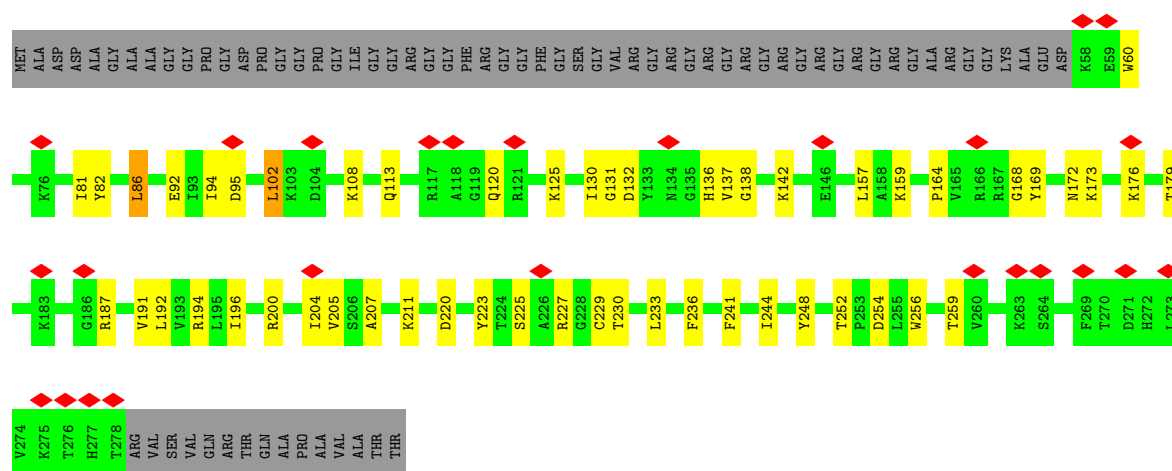


• Molecule 24: L27

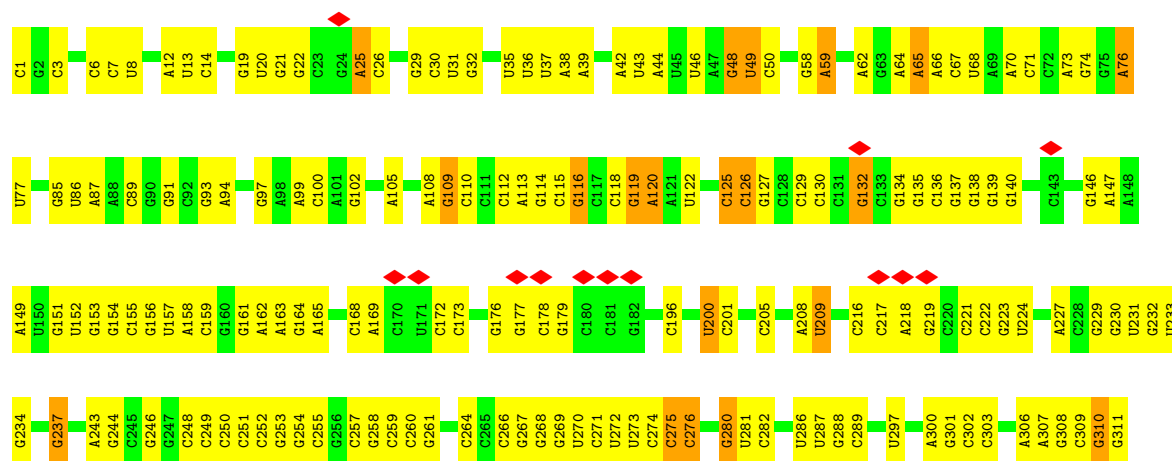


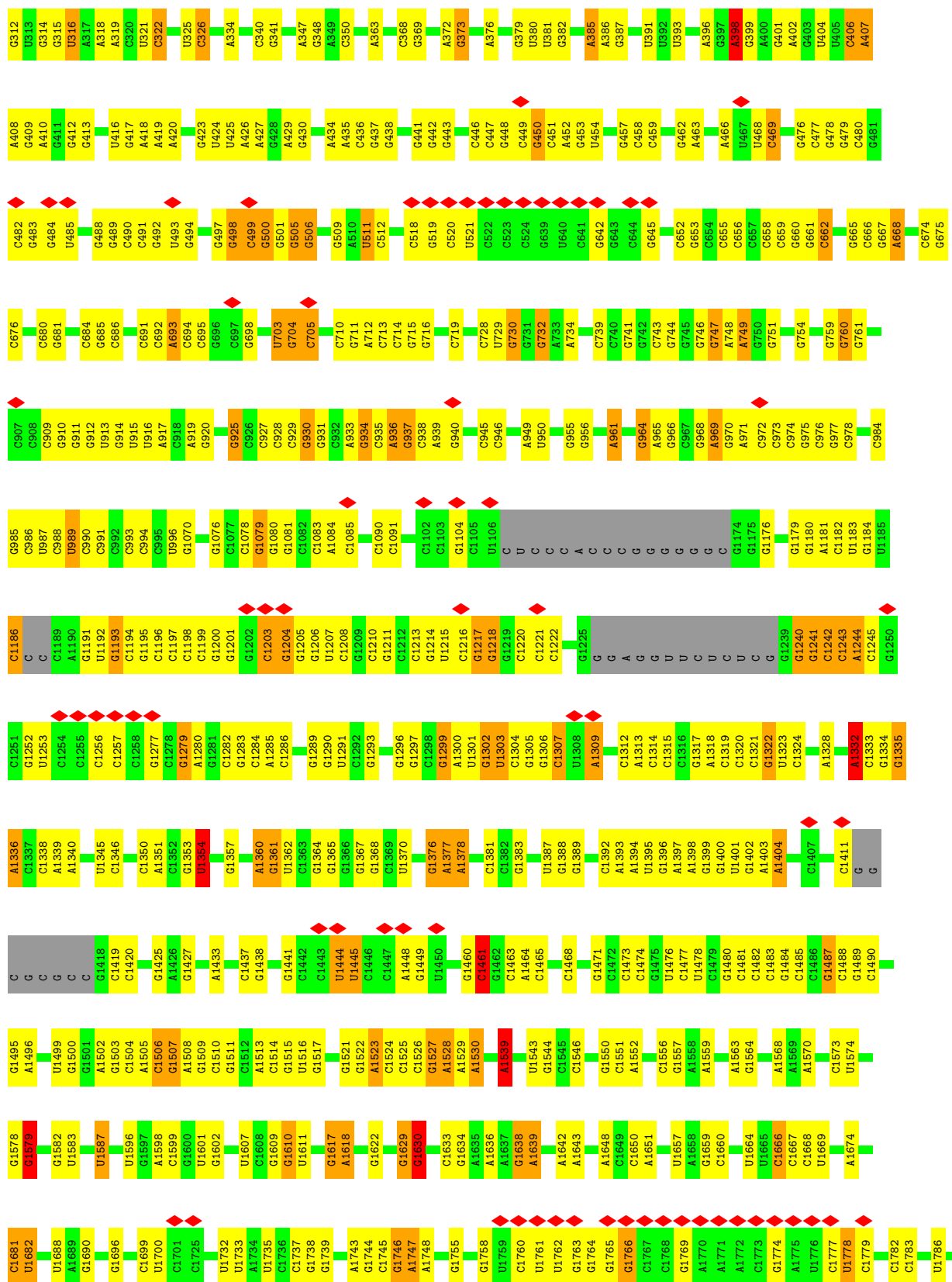


• Molecule 29: eS1



• Molecule 30: 28S rRNA

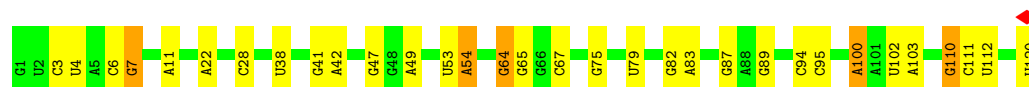
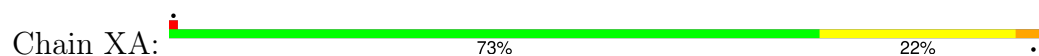




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U2831	G2832	U2833	U2834	G2835	G2836	A2837	A2838	C2839	A2840	A2841	U2842	G2843	U2844	G2847	U2848	A2849	A2850	G2853	G2860	C2861	A2862	A2863	C2866	C2880	G2881	A2884	C2890	U2891	U2892	U2893	G2902	G2903	A3604	G3605	C3610	U3611	U3612	A3613	G3614	A3615	A3616	G3620	C3623	G3624	G3625	A3626	C3627	C3628	A3629																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2682	A2683	G2684	G2685	G2686	G2687	C2688	G2691	G2692	G2693	G2694	C2695	U2696	U2697	G2698	A2700	A2701	A2702	C2707	G2708	G2709	G2710	G2711	G2712	U2713	C2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2726	G2727	A2730	C2731	C2732	U2733	G2737	U2738	G2740	G2741	C2744	U2745	A2748	A2749	A2750	A2751	G2754																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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A1872	A1873	G1874	C1875	A1876	A1877	A1878	A1879	G1880	U1881	G1882	U1887	G1888	A1889	A1890	G1895	G1900	A1901	A1902	G1906	G1907	U1911	A1912	A1913	G1914	G1915	G1916	G1917	G1918	G1919	A1922	U1923	G1924	G1925	G1926	G1927	U1932	U1935	G1936	A1937	G1938	A1939	G1940	C1941	G1942	C1943	A1944	A1947	A1948	G1953																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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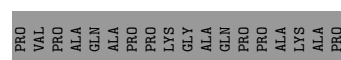
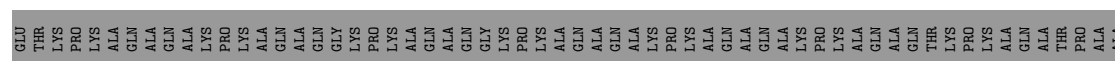
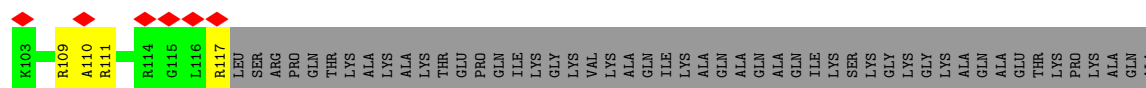
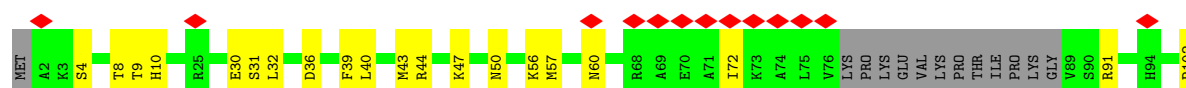
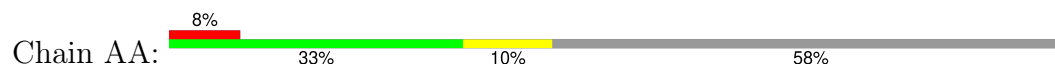
- Molecule 31: 5S rRNA



- Molecule 32: 5.8S rRNA

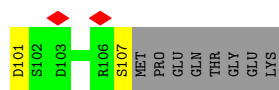


- Molecule 33: eL29

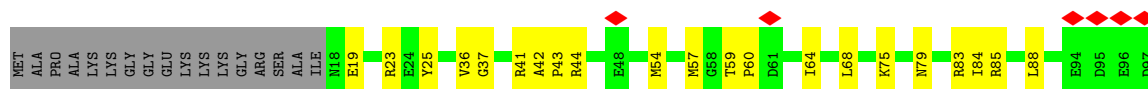


- Molecule 34: eL30

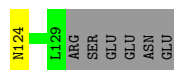
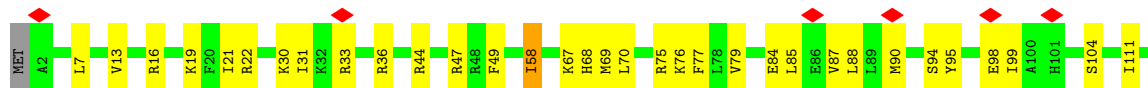




- Molecule 35: eL31



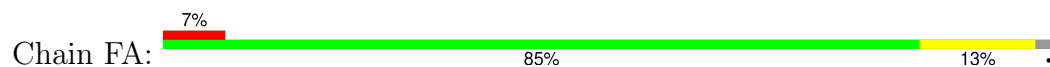
- Molecule 36: eL32



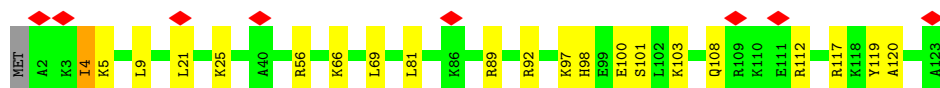
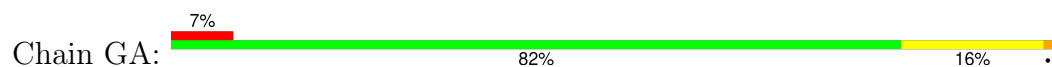
- Molecule 37: eL33



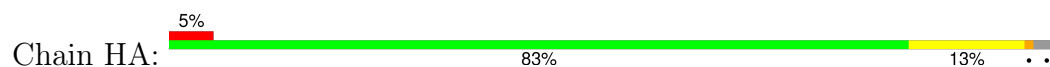
- Molecule 38: eL34



- Molecule 39: uL29



- Molecule 40: L36

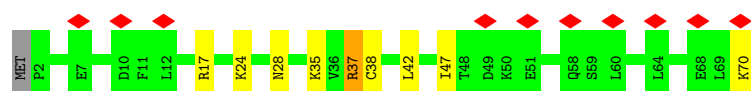
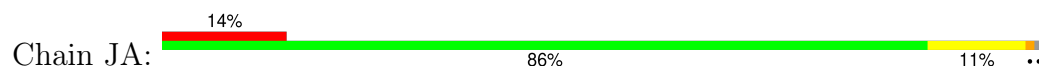




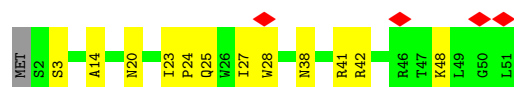
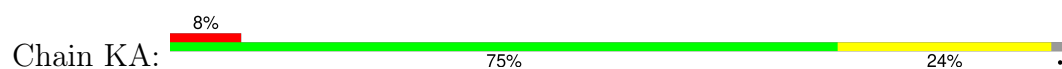
• Molecule 41: L37



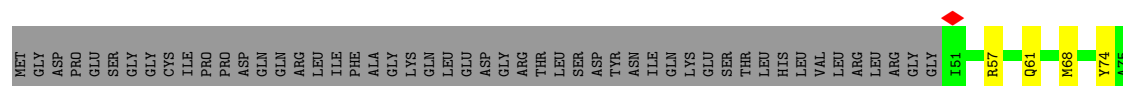
• Molecule 42: eL38



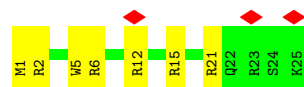
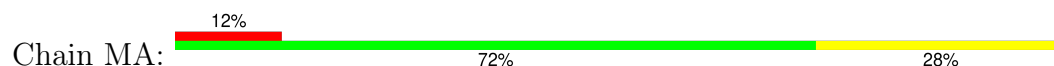
• Molecule 43: eL39



• Molecule 44: eL40



• Molecule 45: eL41

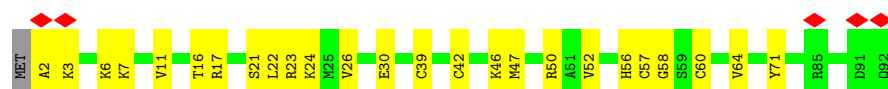
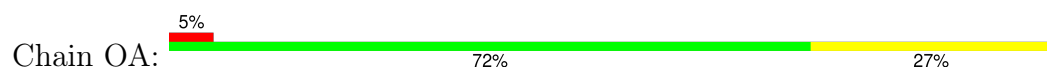


• Molecule 46: eL42

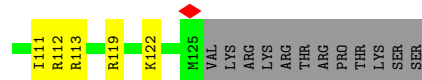
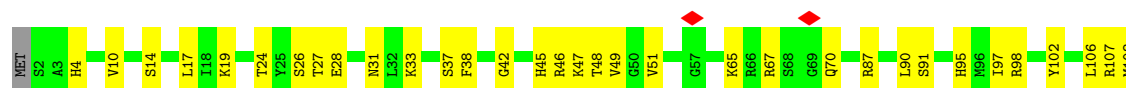




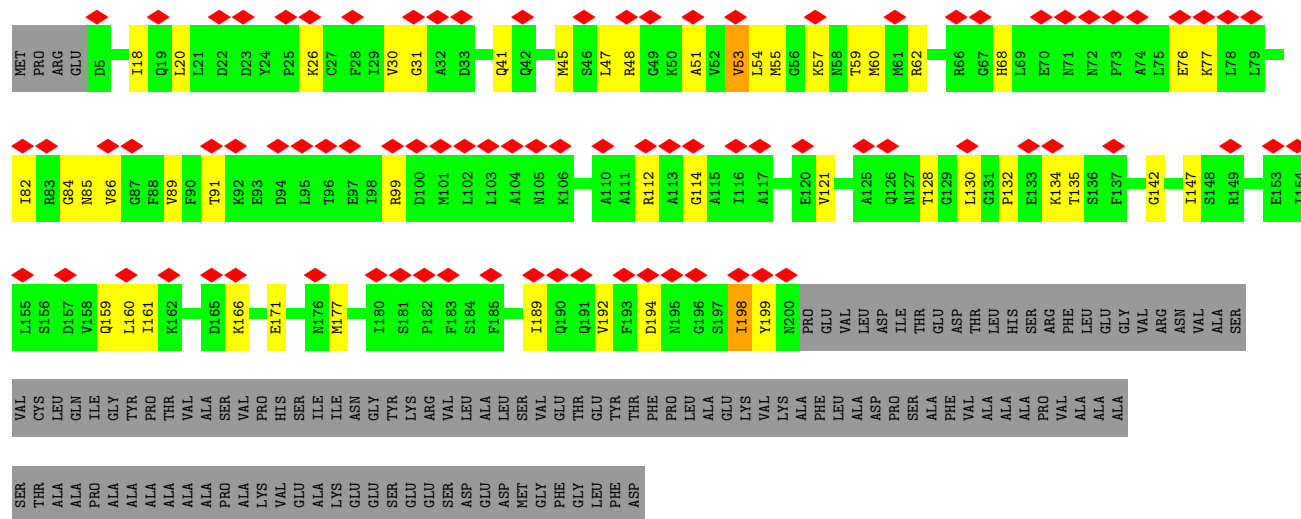
• Molecule 47: eL43



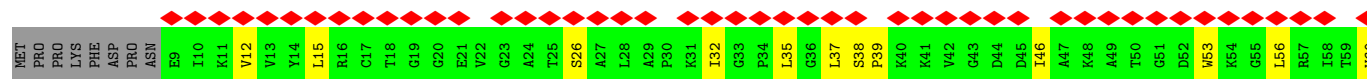
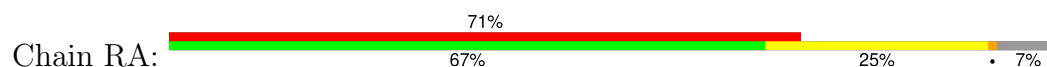
• Molecule 48: eL28

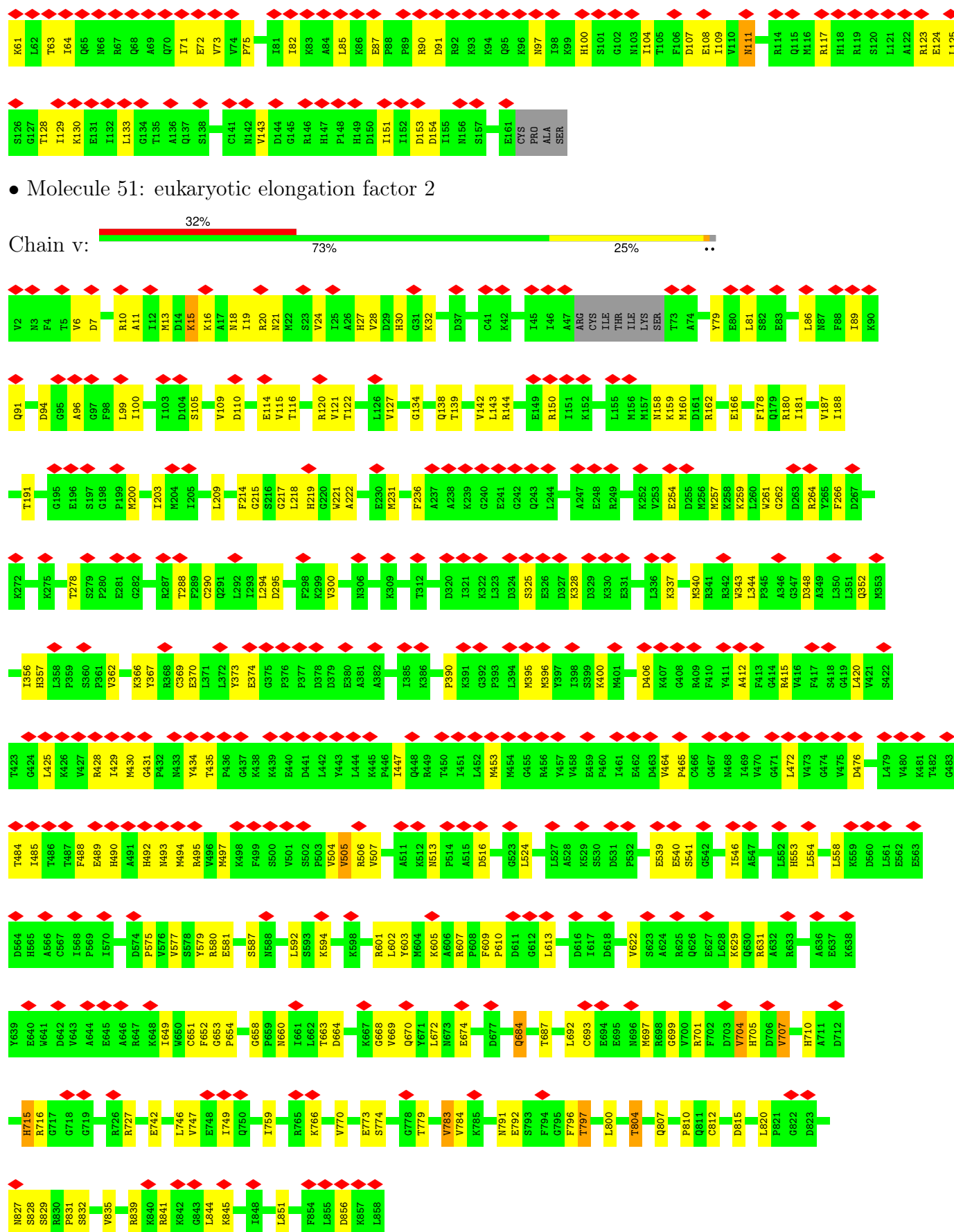


• Molecule 49: uL10

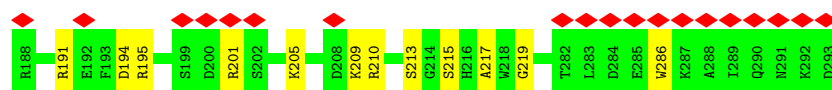
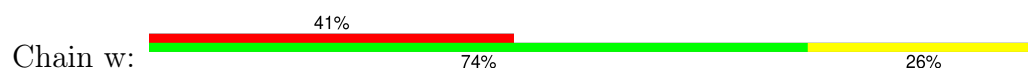


• Molecule 50: uL3

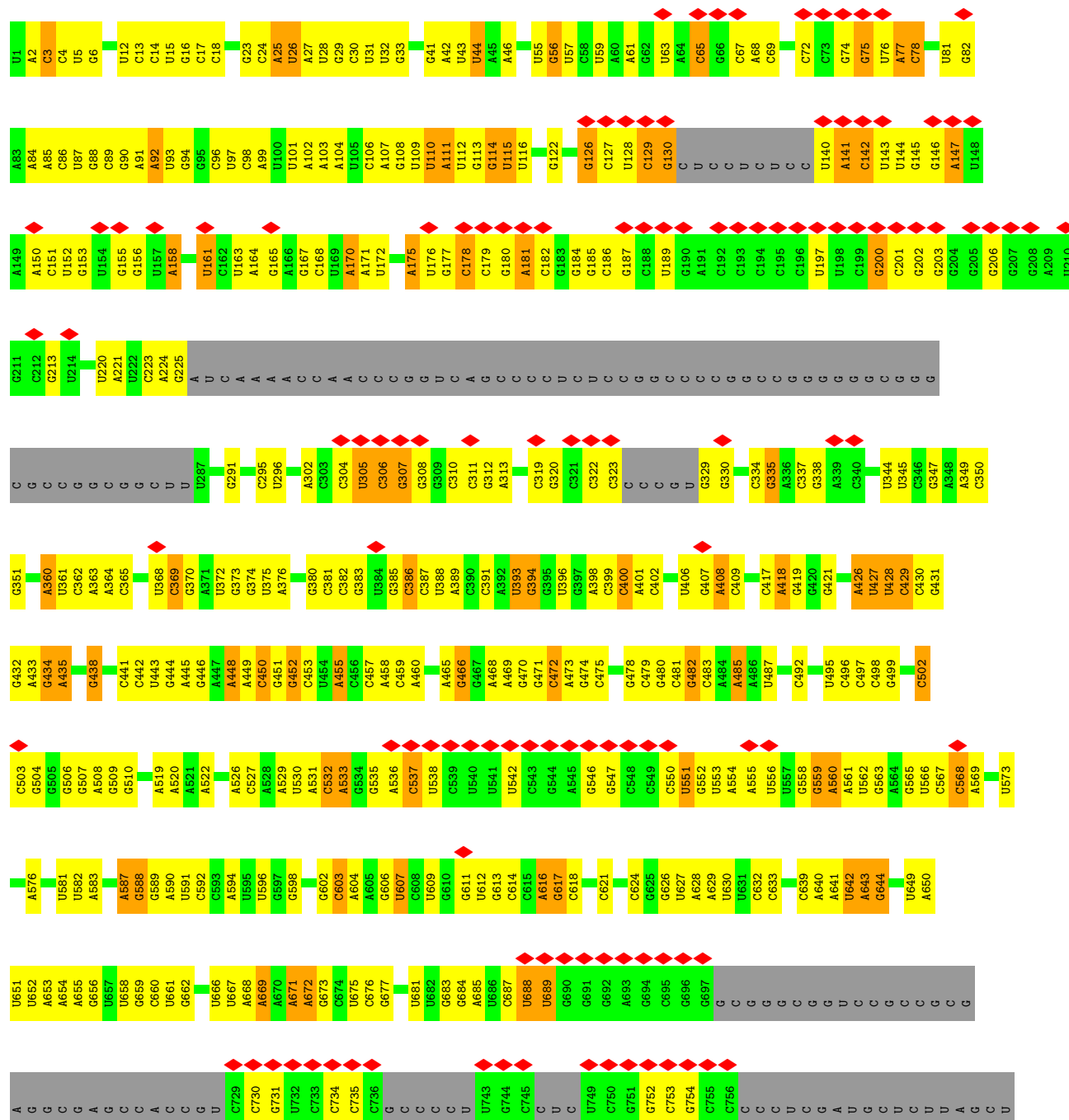




• Molecule 52: Serpine mRNA binding protein 1



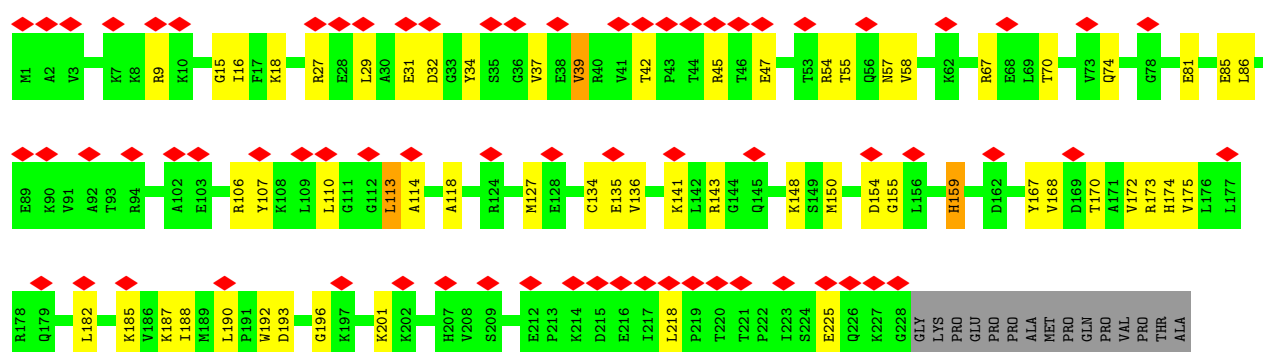
• Molecule 53: 18S rRNA



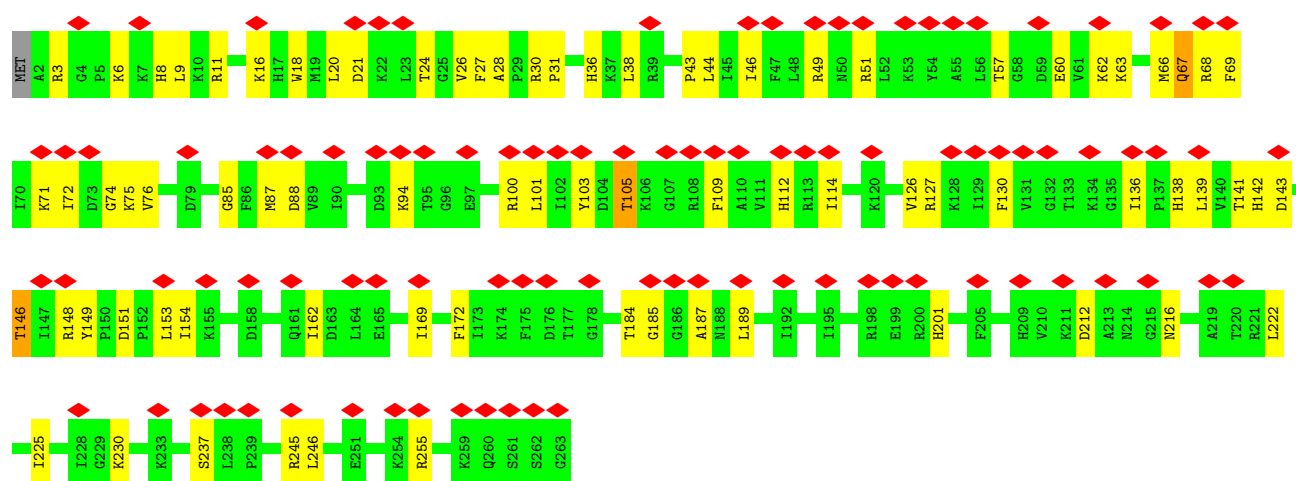
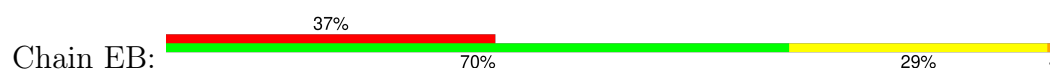




• Molecule 54: uS3

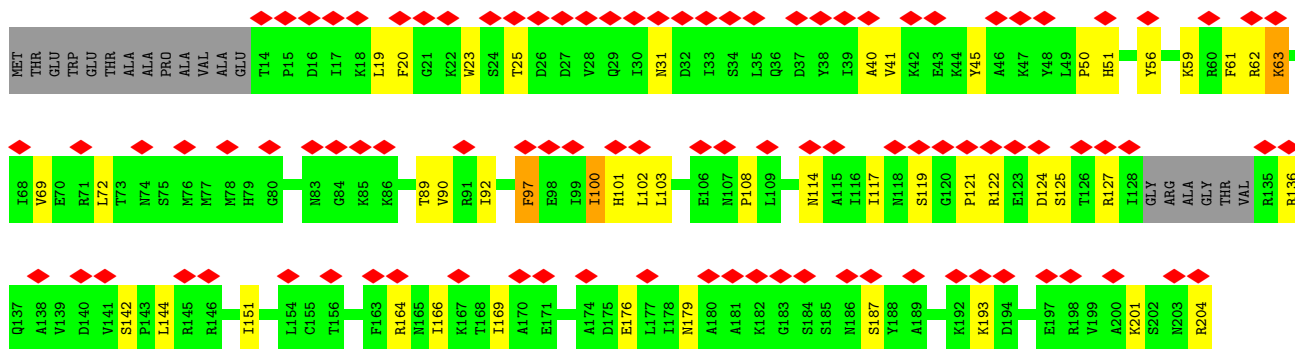


• Molecule 55: eS4

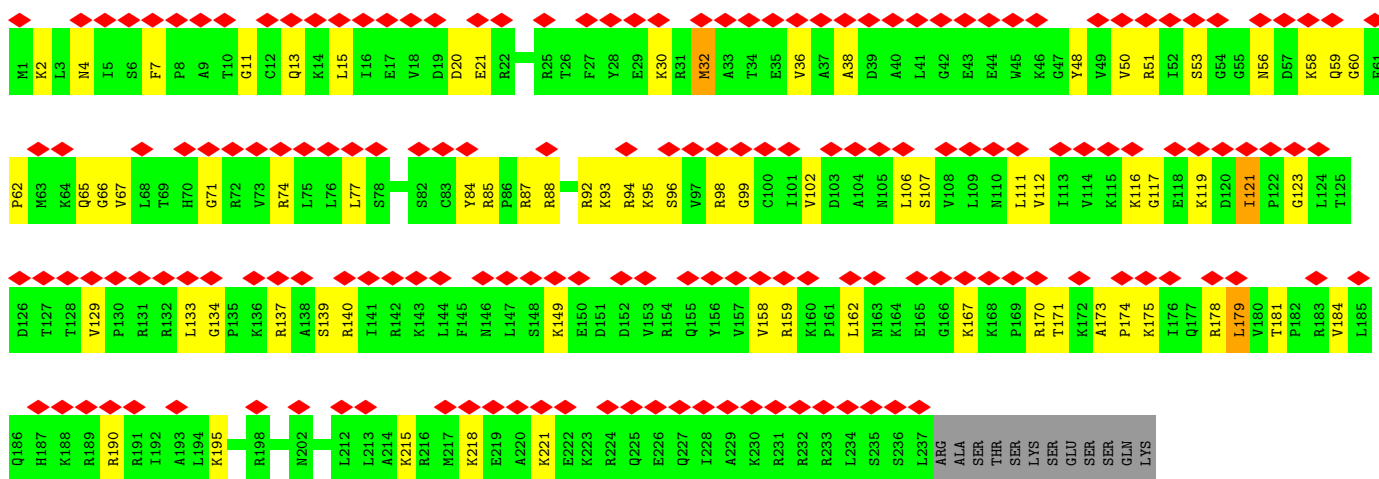


• Molecule 56: S5

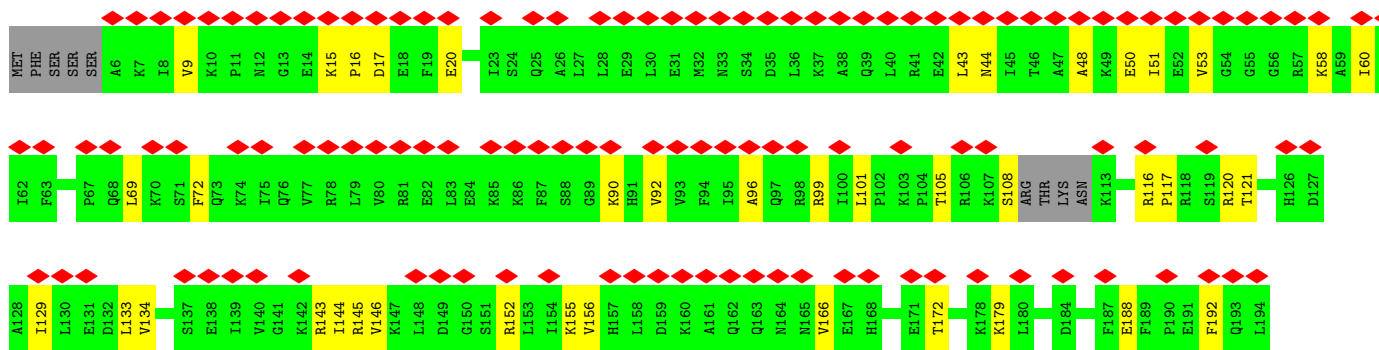
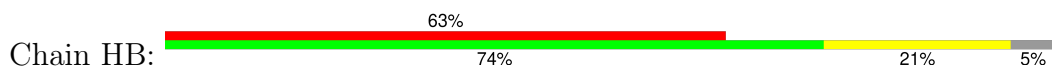




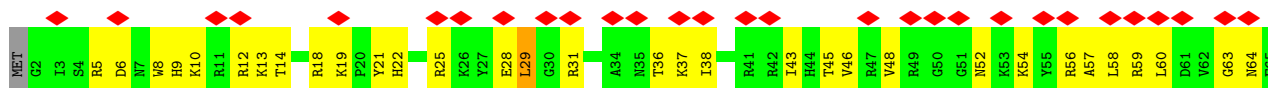
• Molecule 57: S6

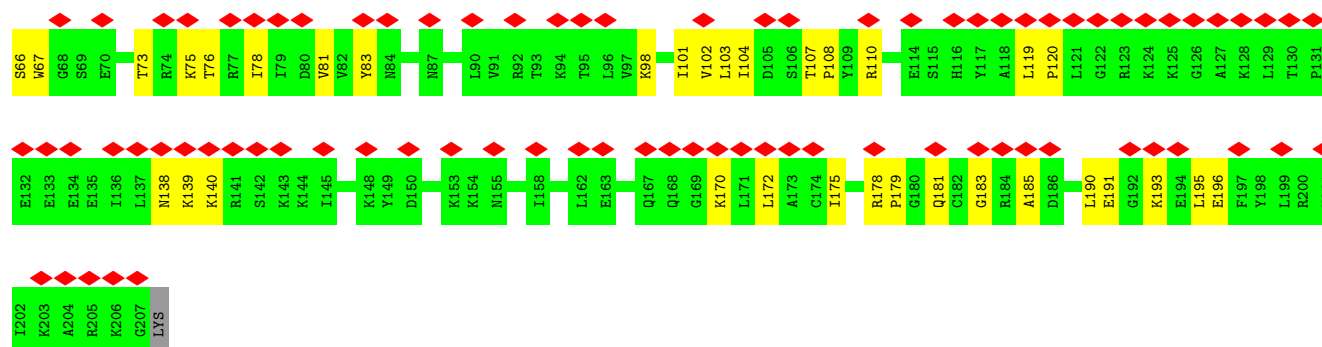


• Molecule 58: S7

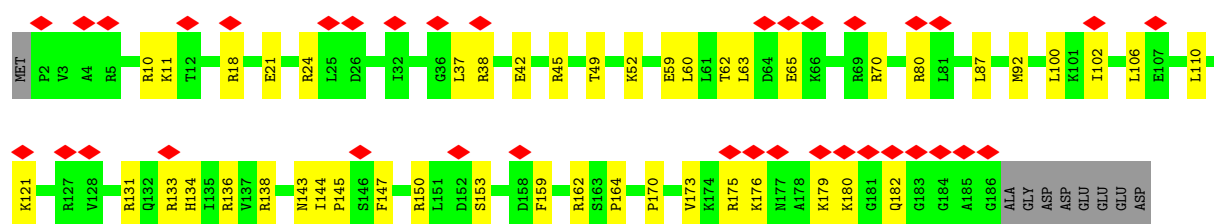
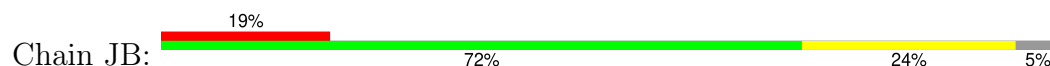


• Molecule 59: eS8

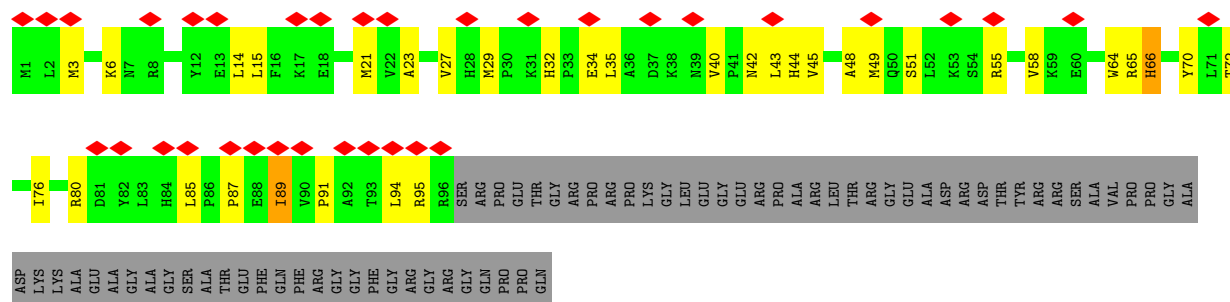




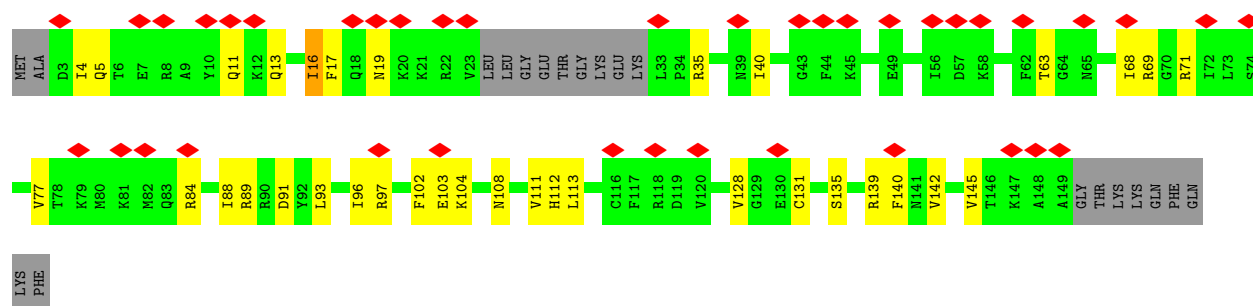
• Molecule 60: S9



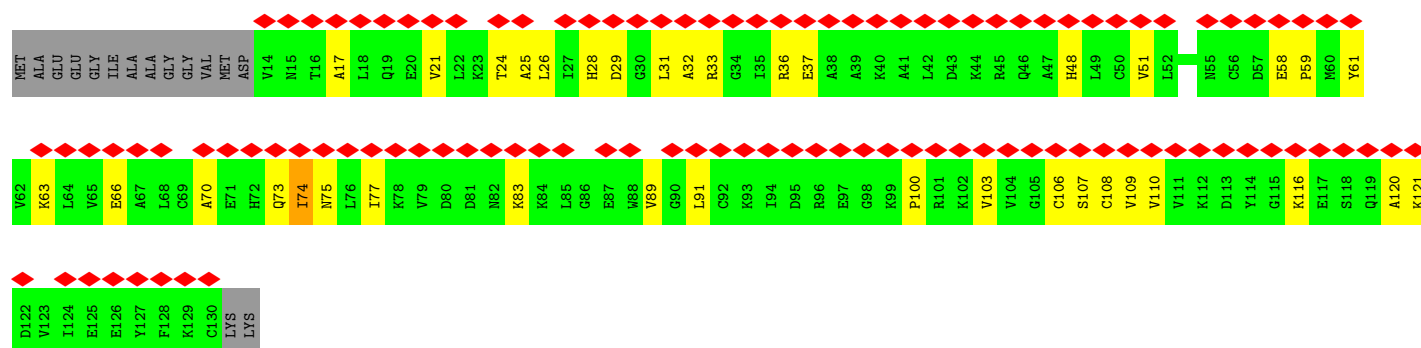
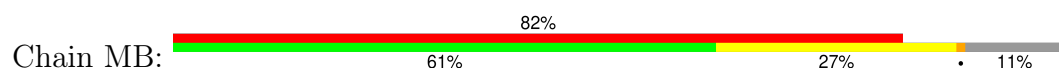
• Molecule 61: eS10



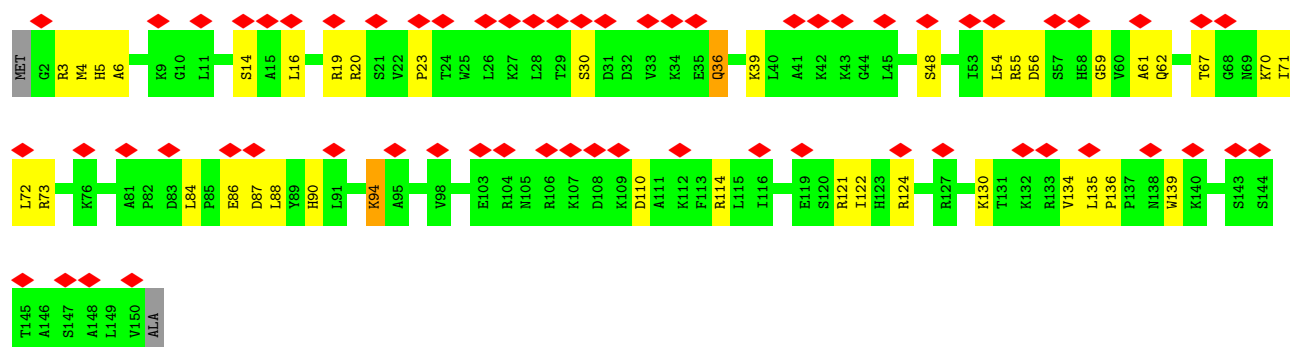
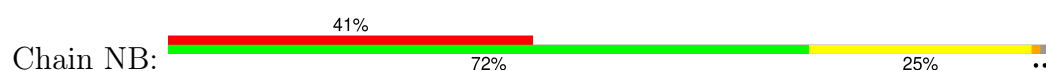
• Molecule 62: S11



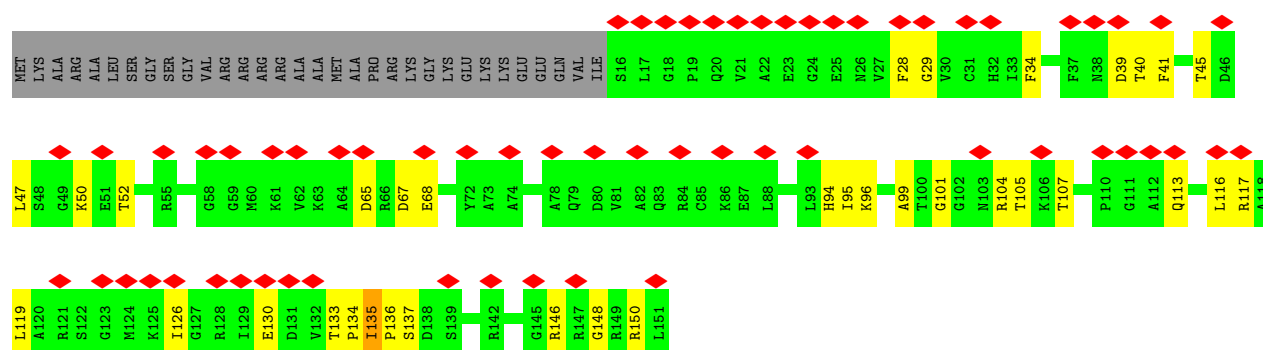
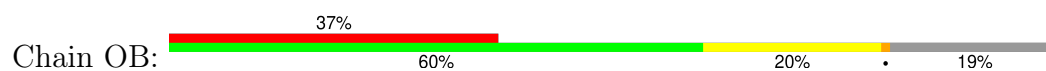
• Molecule 63: S12



• Molecule 64: uS15

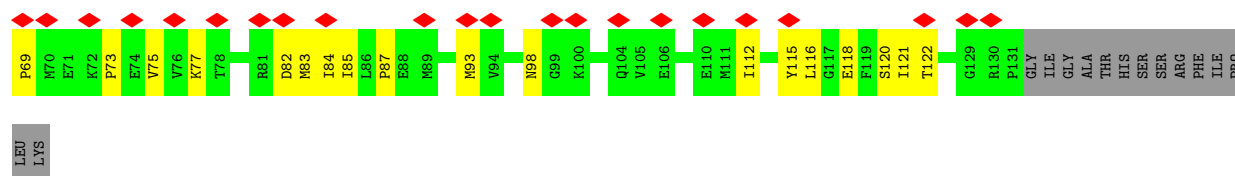


• Molecule 65: uS11

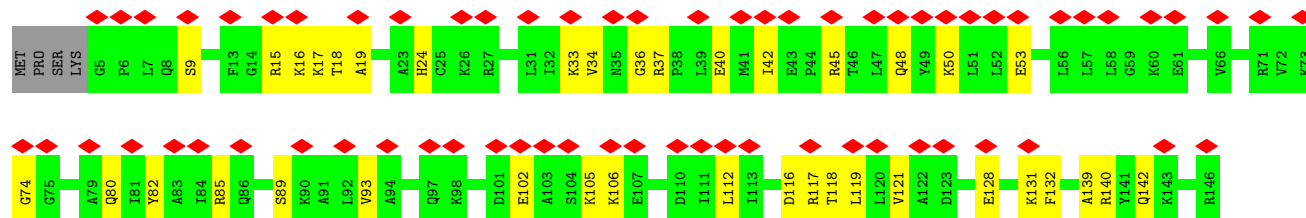
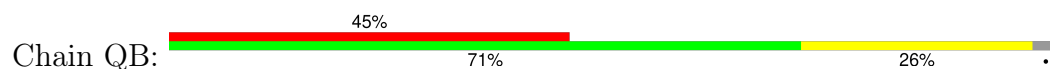


• Molecule 66: uS19

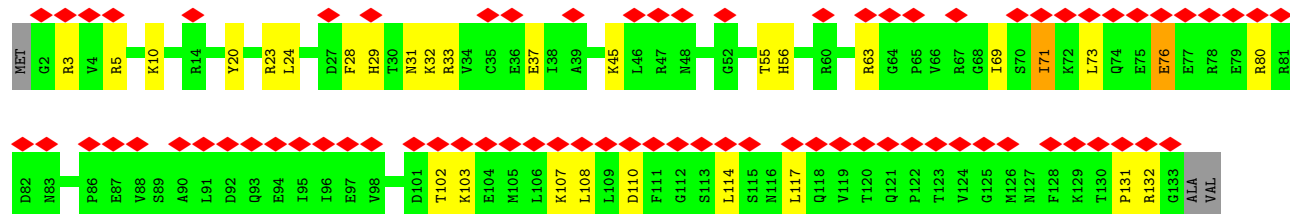
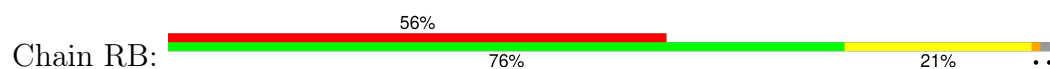




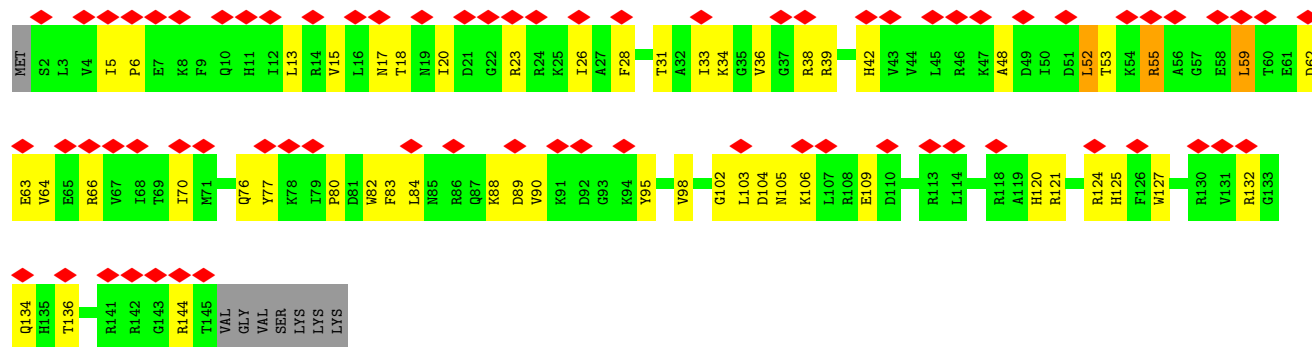
• Molecule 67: S16



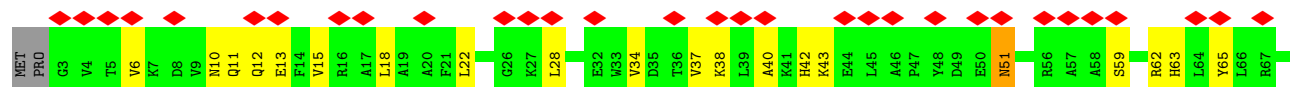
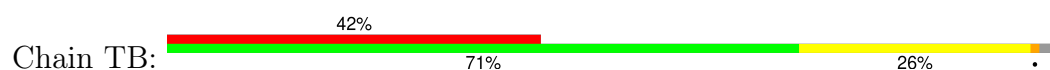
• Molecule 68: eS17



• Molecule 69: uS13

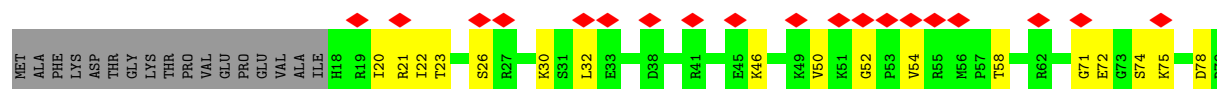
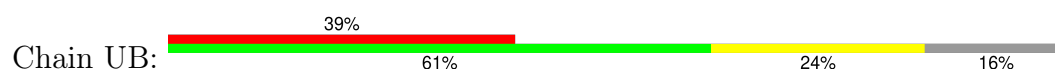


• Molecule 70: eS19

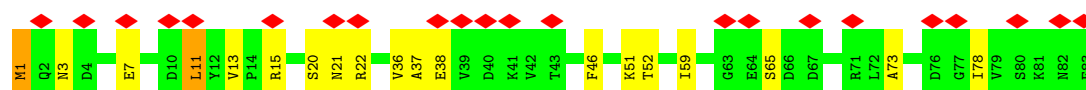
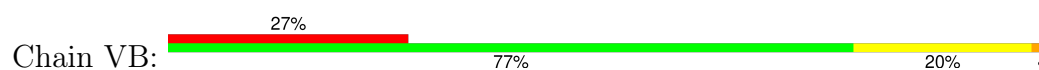




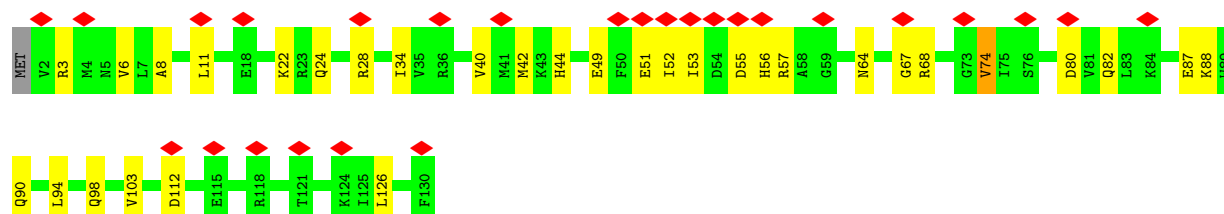
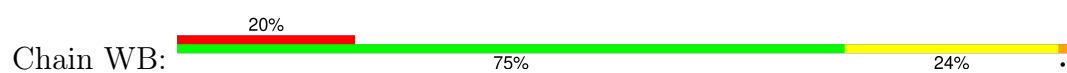
• Molecule 71: uS10



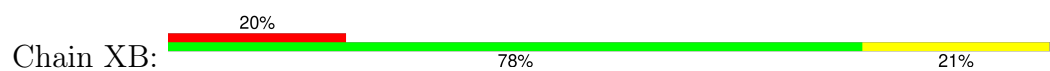
• Molecule 72: eS21



• Molecule 73: S15A

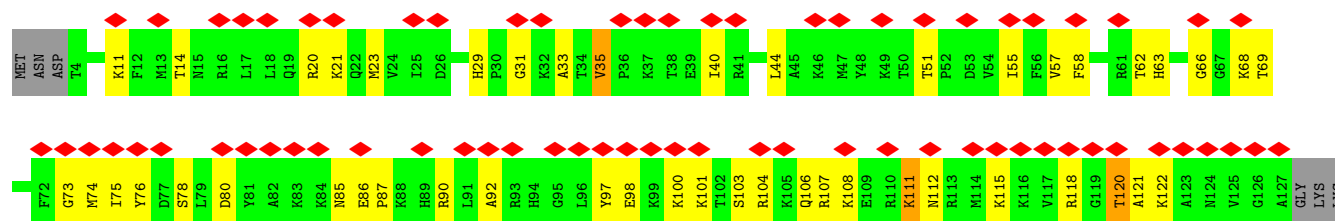


• Molecule 74: uS12

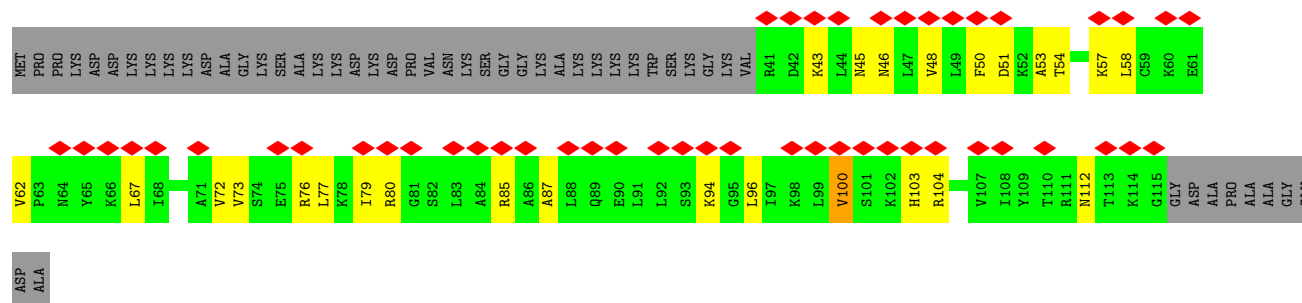


• Molecule 75: eS24

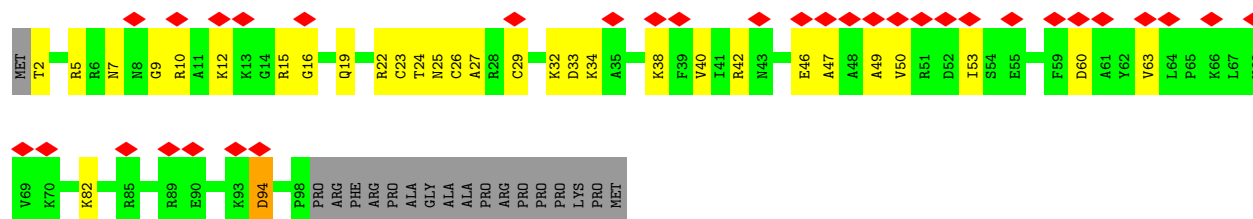




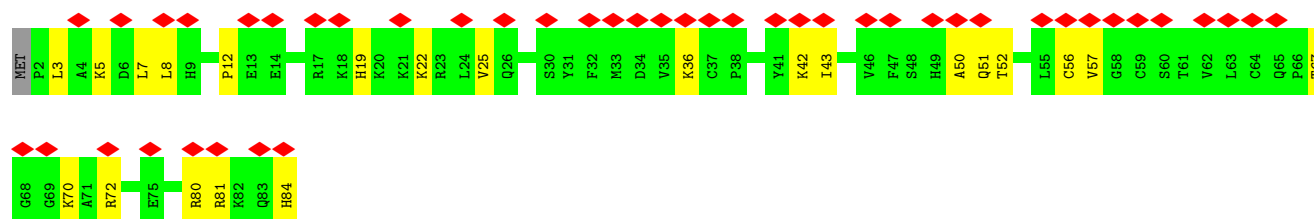
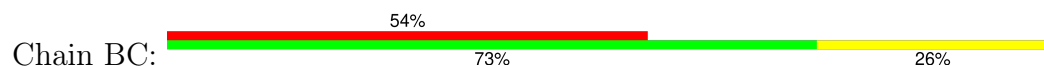
• Molecule 76: eS25



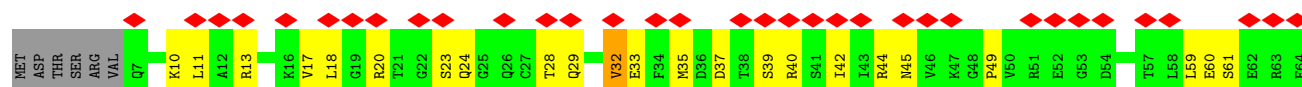
• Molecule 77: eS26

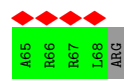


• Molecule 78: S27

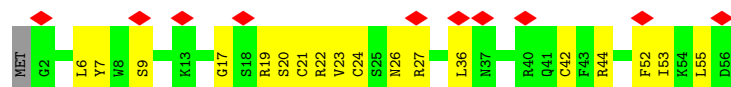


• Molecule 79: S28

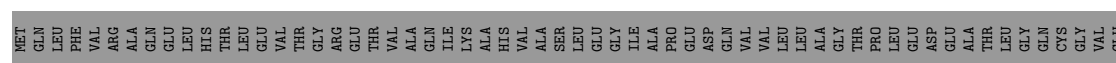
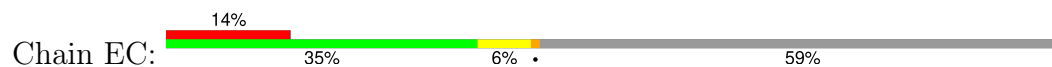




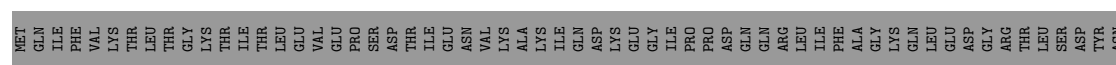
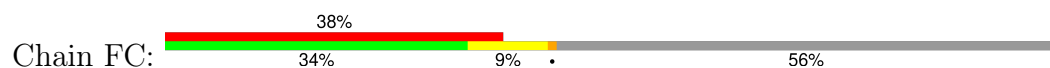
• Molecule 80: uS14



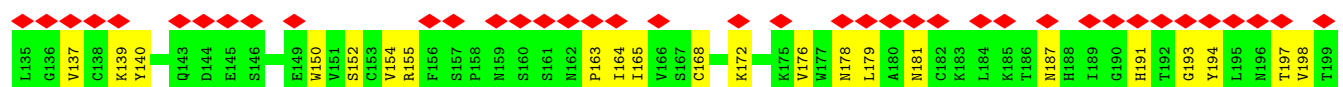
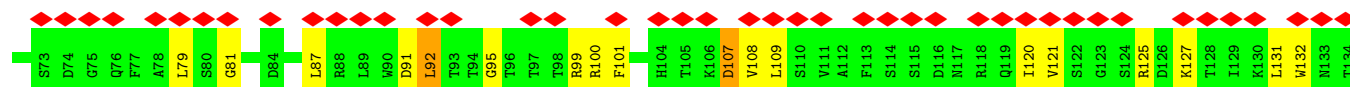
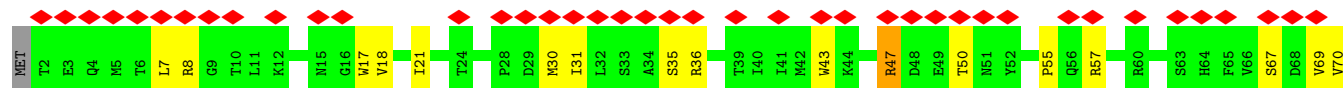
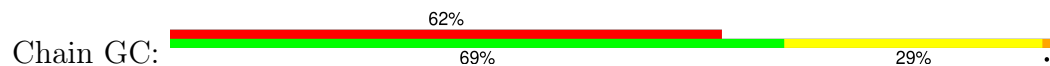
• Molecule 81: S30

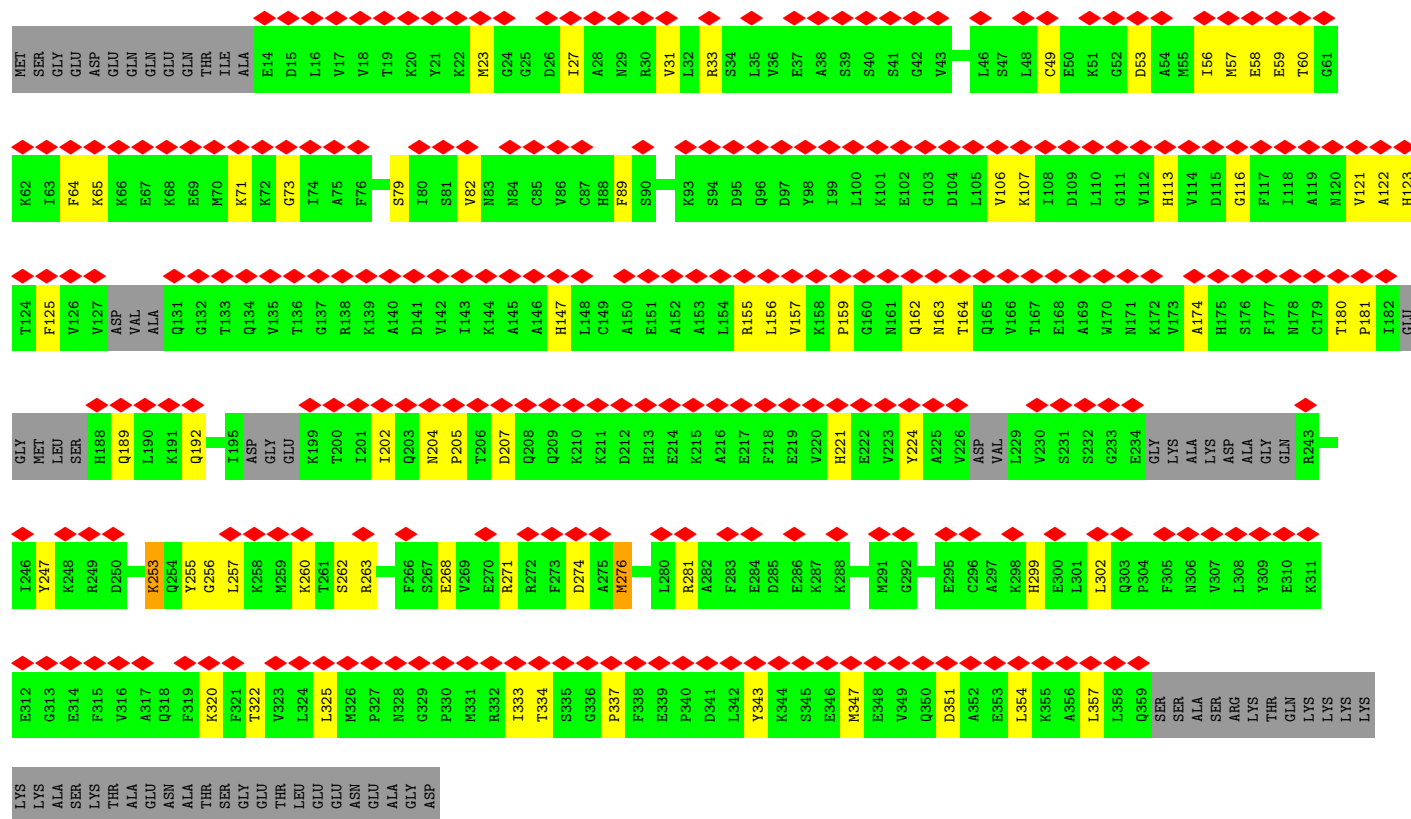


• Molecule 82: S27A



• Molecule 83: RACK1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10568	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 ($e^-/\text{\AA}^2$)	75	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	35.231	Depositor
Minimum map value	-21.911	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.532	Depositor
Recommended contour level	6.3	Depositor
Map size ($\text{\AA}$)	686.87994, 686.87994, 686.87994	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 7MG, I4U, 5MC, P4U, B8T, ZN, B9B, JMH, UR3, B8K, MLZ, 2MG, BGH, OMG, B8H, B9H, 1MA, MHG, SPD, M7A, A2M, PSU, OMU, P7G, OMC, B8W, 6MZ, B8N, 5MU, MG, 4AC, E7G, ANM, DDE, E6G, GDP

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	0.12	0/1936	0.27	0/2596
2	B	0.11	0/3240	0.24	0/4339
3	C	0.11	0/2927	0.22	0/3932
4	D	0.10	0/2437	0.22	0/3264
5	E	0.10	0/1753	0.23	0/2351
6	F	0.11	0/1911	0.23	0/2549
7	G	0.09	0/1910	0.22	0/2569
8	H	0.11	0/1535	0.23	0/2063
9	I	0.11	0/1702	0.21	0/2272
10	J	0.09	0/1385	0.22	0/1852
11	L	0.10	0/1158	0.22	0/1547
12	M	0.11	0/1746	0.23	0/2338
13	N	0.10	0/1662	0.23	0/2222
14	O	0.10	0/1268	0.23	0/1700
15	P	0.12	0/1539	0.24	0/2054
16	Q	0.08	0/1524	0.20	0/2013
17	R	0.11	0/1501	0.23	0/2012
18	S	0.10	0/1326	0.22	0/1770
19	T	0.09	0/823	0.24	0/1104
20	U	0.11	0/993	0.24	0/1332
21	V	0.09	0/813	0.22	0/1080
22	W	0.09	0/984	0.22	0/1323
23	X	0.10	0/1132	0.23	0/1504
24	Y	0.09	0/1130	0.24	0/1507
25	Z	0.11	0/1191	0.23	0/1590
26	K	0.10	0/1733	0.22	0/2316
27	AB	0.09	0/1749	0.22	0/2377
28	BB	0.08	0/1756	0.23	0/2350
29	CB	0.09	0/1753	0.24	0/2369
30	WA	0.14	0/82492	0.24	0/128582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	XA	0.11	0/2858	0.19	0/4455
32	YA	0.13	0/3559	0.21	0/5543
33	AA	0.08	0/861	0.20	0/1138
34	BA	0.09	0/771	0.19	0/1034
35	CA	0.11	0/903	0.25	0/1216
36	DA	0.11	0/1071	0.25	0/1429
37	EA	0.11	0/895	0.25	0/1198
38	FA	0.10	0/916	0.21	0/1220
39	GA	0.08	0/1021	0.19	0/1348
40	HA	0.09	0/841	0.21	0/1112
41	IA	0.11	0/720	0.25	0/952
42	JA	0.09	0/575	0.21	0/761
43	KA	0.11	0/459	0.26	0/608
44	LA	0.10	0/425	0.24	0/561
45	MA	0.08	0/240	0.21	0/305
46	NA	0.10	0/855	0.23	0/1128
47	OA	0.10	0/718	0.21	0/953
48	PA	0.09	0/1010	0.24	0/1354
49	QA	0.08	0/1530	0.21	0/2064
50	RA	0.08	0/1174	0.23	0/1582
51	v	0.10	0/6596	0.26	0/8909
52	w	0.09	0/372	0.25	0/492
53	ZA	0.10	0/40393	0.23	0/62941
54	DB	0.10	0/1796	0.25	0/2417
55	EB	0.09	0/2118	0.24	0/2849
56	FB	0.08	0/1492	0.23	0/2005
57	GB	0.08	0/1946	0.22	0/2590
58	HB	0.08	0/1510	0.21	0/2022
59	IB	0.09	0/1715	0.24	0/2287
60	JB	0.08	0/1550	0.20	0/2069
61	KB	0.09	0/834	0.26	0/1125
62	LB	0.09	0/1157	0.21	0/1549
63	MB	0.08	0/918	0.24	0/1233
64	NB	0.07	0/1226	0.20	0/1649
65	OB	0.08	0/1029	0.22	0/1380
66	PB	0.08	0/1017	0.21	0/1358
67	QB	0.09	0/1146	0.24	0/1534
68	RB	0.08	0/1082	0.20	0/1452
69	SB	0.09	0/1208	0.23	0/1618
70	TB	0.11	0/1115	0.23	0/1493
71	UB	0.08	0/805	0.21	0/1081
72	VB	0.08	0/643	0.22	0/860
73	WB	0.10	0/1051	0.24	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XB	0.09	0/1116	0.22	0/1490
75	YB	0.07	0/1028	0.22	0/1366
76	ZB	0.08	0/604	0.21	0/810
77	AC	0.10	0/786	0.23	0/1053
78	BC	0.09	0/665	0.24	0/891
79	CC	0.09	0/490	0.23	0/656
80	DC	0.09	0/470	0.22	0/623
81	EC	0.07	0/447	0.19	0/587
82	FC	0.07	0/567	0.20	0/753
83	GC	0.09	0/2493	0.24	0/3394
84	b	0.08	0/2462	0.22	0/3321
All	All	0.11	0/234258	0.23	0/342101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	65	0
2	B	3172	0	3310	68	0
3	C	2884	0	3053	54	0
4	D	2391	0	2424	44	0
5	E	1720	0	1874	36	0
6	F	1875	0	1995	39	0
7	G	1879	0	2027	38	0
8	H	1516	0	1597	23	0
9	I	1664	0	1712	29	0
10	J	1362	0	1399	26	0
11	L	1137	0	1211	22	0
12	M	1701	0	1749	43	0
13	N	1630	0	1778	37	0
14	O	1242	0	1274	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	1515	0	1633	37	0
16	Q	1508	0	1664	31	0
17	R	1462	0	1508	36	0
18	S	1298	0	1366	28	0
19	T	809	0	833	16	0
20	U	979	0	1039	16	0
21	V	800	0	833	14	0
22	W	967	0	1040	18	0
23	X	1115	0	1205	26	0
24	Y	1107	0	1182	27	0
25	Z	1162	0	1209	36	0
26	K	1702	0	1820	39	0
27	AB	1712	0	1713	35	0
28	BB	1729	0	1803	46	0
29	CB	1716	0	1806	34	0
30	WA	76047	0	38173	1359	0
31	XA	2558	0	1296	25	0
32	YA	3209	0	1631	74	0
33	AA	848	0	920	19	0
34	BA	761	0	794	14	0
35	CA	888	0	929	19	0
36	DA	1053	0	1147	26	0
37	EA	876	0	912	24	0
38	FA	906	0	998	12	0
39	GA	1013	0	1147	16	0
40	HA	830	0	916	13	0
41	IA	705	0	737	22	0
42	JA	569	0	637	6	0
43	KA	447	0	480	9	0
44	LA	430	0	465	6	0
45	MA	239	0	289	7	0
46	NA	842	0	912	21	0
47	OA	708	0	756	16	0
48	PA	994	0	1051	27	0
49	QA	1507	0	1564	32	0
50	RA	1160	0	1218	30	0
51	v	6489	0	6573	139	0
52	w	366	0	342	13	0
53	ZA	36263	0	18294	796	0
54	DB	1768	0	1866	41	0
55	EB	2076	0	2177	54	0
56	FB	1471	0	1522	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	GB	1923	0	2089	63	0
58	HB	1488	0	1582	27	0
59	IB	1686	0	1772	47	0
60	JB	1525	0	1640	34	0
61	KB	810	0	836	24	0
62	LB	1137	0	1200	24	0
63	MB	908	0	939	21	0
64	NB	1202	0	1289	36	0
65	OB	1016	0	1039	27	0
66	PB	997	0	1045	29	0
67	QB	1128	0	1195	32	0
68	RB	1068	0	1121	21	0
69	SB	1190	0	1249	38	0
70	TB	1097	0	1130	28	0
71	UB	795	0	862	20	0
72	VB	636	0	637	12	0
73	WB	1034	0	1080	28	0
74	XB	1098	0	1167	23	0
75	YB	1011	0	1083	35	0
76	ZB	598	0	656	19	0
77	AC	774	0	822	25	0
78	BC	651	0	672	19	0
79	CC	488	0	514	15	0
80	DC	459	0	448	15	0
81	EC	443	0	492	9	0
82	FC	555	0	566	14	0
83	GC	2436	0	2393	64	0
84	b	2422	0	2340	41	0
85	AC	1	0	0	0	0
85	B	2	0	0	0	0
85	DA	1	0	0	0	0
85	FA	1	0	0	0	0
85	I	1	0	0	0	0
85	KA	1	0	0	0	0
85	O	1	0	0	0	0
85	TB	1	0	0	0	0
85	U	1	0	0	0	0
85	WA	110	0	0	0	0
85	XA	4	0	0	0	0
85	YA	1	0	0	0	0
85	ZA	19	0	0	0	0
86	WA	19	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	WA	10	0	19	0	0
88	AC	1	0	0	0	0
88	DC	1	0	0	0	0
88	FA	1	0	0	0	0
88	FC	1	0	0	0	0
88	IA	1	0	0	0	0
88	LA	1	0	0	0	0
88	NA	1	0	0	0	0
88	OA	1	0	0	0	0
89	v	28	0	12	2	0
All	All	221459	0	167704	3842	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 10.

The worst 5 of 3842 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)
30:WA:4088:5MU:C4	30:WA:4088:5MU:C5	1.82	1.60
30:WA:4088:5MU:C6	30:WA:4088:5MU:N1	1.68	1.58
30:WA:4301:B8H:C5	30:WA:4301:B8H:C4	1.83	1.57
30:WA:3767:B8H:C4	30:WA:3767:B8H:C5	1.83	1.54
30:WA:1865:B8H:C4	30:WA:1865:B8H:C5	1.83	1.54

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%)	236 (96%)	10 (4%)	0	100	100
2	B	392/403 (97%)	377 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	359/425 (84%)	353 (98%)	6 (2%)	0	100	100
4	D	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
5	E	207/291 (71%)	200 (97%)	7 (3%)	0	100	100
6	F	223/247 (90%)	216 (97%)	7 (3%)	0	100	100
7	G	229/319 (72%)	224 (98%)	4 (2%)	1 (0%)	30	59
8	H	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
9	I	201/214 (94%)	199 (99%)	2 (1%)	0	100	100
10	J	168/178 (94%)	164 (98%)	3 (2%)	1 (1%)	21	51
11	L	136/218 (62%)	131 (96%)	5 (4%)	0	100	100
12	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
13	N	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
14	O	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
15	P	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
16	Q	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
17	R	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
18	S	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
19	T	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
20	U	129/140 (92%)	129 (100%)	0	0	100	100
21	V	94/157 (60%)	89 (95%)	5 (5%)	0	100	100
22	W	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
23	X	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
24	Y	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
25	Z	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
26	K	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
27	AB	215/295 (73%)	210 (98%)	5 (2%)	0	100	100
28	BB	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
29	CB	219/293 (75%)	218 (100%)	1 (0%)	0	100	100
33	AA	100/245 (41%)	96 (96%)	4 (4%)	0	100	100
34	BA	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
35	CA	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
36	DA	126/135 (93%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	EA	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
38	FA	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
39	GA	120/123 (98%)	120 (100%)	0	0	100	100
40	HA	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
41	IA	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
42	JA	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
43	KA	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
44	LA	49/102 (48%)	47 (96%)	2 (4%)	0	100	100
45	MA	23/25 (92%)	23 (100%)	0	0	100	100
46	NA	101/106 (95%)	97 (96%)	4 (4%)	0	100	100
47	OA	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
48	PA	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
49	QA	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
50	RA	151/165 (92%)	147 (97%)	4 (3%)	0	100	100
51	v	827/839 (99%)	802 (97%)	25 (3%)	0	100	100
52	w	42/46 (91%)	38 (90%)	4 (10%)	0	100	100
54	DB	226/243 (93%)	222 (98%)	4 (2%)	0	100	100
55	EB	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
56	FB	181/204 (89%)	174 (96%)	7 (4%)	0	100	100
57	GB	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
58	HB	181/194 (93%)	180 (99%)	1 (1%)	0	100	100
59	IB	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
60	JB	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
61	KB	94/165 (57%)	90 (96%)	4 (4%)	0	100	100
62	LB	134/158 (85%)	128 (96%)	6 (4%)	0	100	100
63	MB	115/132 (87%)	112 (97%)	2 (2%)	1 (1%)	14	41
64	NB	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
65	OB	134/168 (80%)	132 (98%)	2 (2%)	0	100	100
66	PB	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
67	QB	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
68	RB	130/135 (96%)	126 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	SB	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
70	TB	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
71	UB	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
72	VB	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
73	WB	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	XB	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
75	YB	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
76	ZB	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
77	AC	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
78	BC	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
79	CC	60/69 (87%)	60 (100%)	0	0	100	100
80	DC	53/56 (95%)	53 (100%)	0	0	100	100
81	EC	53/133 (40%)	53 (100%)	0	0	100	100
82	FC	66/156 (42%)	63 (96%)	3 (4%)	0	100	100
83	GC	311/317 (98%)	293 (94%)	18 (6%)	0	100	100
84	b	313/394 (79%)	302 (96%)	11 (4%)	0	100	100
All	All	12680/14654 (86%)	12346 (97%)	331 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	217	ILE
63	MB	74	ILE
10	J	10	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	186 (98%)	4 (2%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	342/348 (98%)	341 (100%)	1 (0%)	86	96
3	C	301/346 (87%)	300 (100%)	1 (0%)	86	96
4	D	247/250 (99%)	246 (100%)	1 (0%)	84	94
5	E	189/251 (75%)	184 (97%)	5 (3%)	40	73
6	F	196/215 (91%)	196 (100%)	0	100	100
7	G	200/272 (74%)	198 (99%)	2 (1%)	68	89
8	H	169/171 (99%)	167 (99%)	2 (1%)	63	86
9	I	175/181 (97%)	174 (99%)	1 (1%)	78	93
10	J	143/149 (96%)	142 (99%)	1 (1%)	76	92
11	L	117/161 (73%)	115 (98%)	2 (2%)	53	82
12	M	171/172 (99%)	170 (99%)	1 (1%)	78	93
13	N	171/173 (99%)	171 (100%)	0	100	100
14	O	134/163 (82%)	134 (100%)	0	100	100
15	P	164/165 (99%)	163 (99%)	1 (1%)	78	93
16	Q	159/175 (91%)	158 (99%)	1 (1%)	78	93
17	R	157/157 (100%)	157 (100%)	0	100	100
18	S	139/140 (99%)	137 (99%)	2 (1%)	59	85
19	T	89/114 (78%)	89 (100%)	0	100	100
20	U	101/107 (94%)	100 (99%)	1 (1%)	68	89
21	V	81/126 (64%)	81 (100%)	0	100	100
22	W	106/134 (79%)	105 (99%)	1 (1%)	70	90
23	X	124/135 (92%)	123 (99%)	1 (1%)	73	90
24	Y	117/118 (99%)	117 (100%)	0	100	100
25	Z	119/120 (99%)	119 (100%)	0	100	100
26	K	175/176 (99%)	172 (98%)	3 (2%)	53	82
27	AB	181/245 (74%)	178 (98%)	3 (2%)	53	82
28	BB	194/231 (84%)	192 (99%)	2 (1%)	68	89
29	CB	187/225 (83%)	184 (98%)	3 (2%)	55	83
33	AA	84/184 (46%)	82 (98%)	2 (2%)	43	75
34	BA	84/98 (86%)	82 (98%)	2 (2%)	43	75
35	CA	98/110 (89%)	97 (99%)	1 (1%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DA	114/121 (94%)	110 (96%)	4 (4%)	32	66
37	EA	88/89 (99%)	88 (100%)	0	100	100
38	FA	98/100 (98%)	97 (99%)	1 (1%)	68	89
39	GA	109/110 (99%)	108 (99%)	1 (1%)	70	90
40	HA	86/89 (97%)	85 (99%)	1 (1%)	63	86
41	IA	73/80 (91%)	71 (97%)	2 (3%)	39	73
42	JA	64/65 (98%)	62 (97%)	2 (3%)	35	69
43	KA	47/48 (98%)	47 (100%)	0	100	100
44	LA	47/89 (53%)	47 (100%)	0	100	100
45	MA	24/24 (100%)	24 (100%)	0	100	100
46	NA	91/94 (97%)	90 (99%)	1 (1%)	65	88
47	OA	74/75 (99%)	73 (99%)	1 (1%)	59	85
48	PA	108/121 (89%)	107 (99%)	1 (1%)	70	90
49	QA	164/258 (64%)	159 (97%)	5 (3%)	36	70
50	RA	126/137 (92%)	121 (96%)	5 (4%)	28	62
51	v	706/713 (99%)	687 (97%)	19 (3%)	39	73
52	w	37/37 (100%)	37 (100%)	0	100	100
54	DB	190/202 (94%)	183 (96%)	7 (4%)	30	64
55	EB	224/225 (100%)	218 (97%)	6 (3%)	39	73
56	FB	158/170 (93%)	153 (97%)	5 (3%)	34	68
57	GB	207/218 (95%)	202 (98%)	5 (2%)	43	75
58	HB	165/174 (95%)	164 (99%)	1 (1%)	78	93
59	IB	178/180 (99%)	176 (99%)	2 (1%)	65	88
60	JB	161/168 (96%)	158 (98%)	3 (2%)	50	79
61	KB	87/136 (64%)	85 (98%)	2 (2%)	44	76
62	LB	126/142 (89%)	124 (98%)	2 (2%)	55	83
63	MB	99/108 (92%)	95 (96%)	4 (4%)	28	62
64	NB	130/131 (99%)	128 (98%)	2 (2%)	57	84
65	OB	106/130 (82%)	105 (99%)	1 (1%)	70	90
66	PB	109/130 (84%)	107 (98%)	2 (2%)	51	80
67	QB	117/121 (97%)	114 (97%)	3 (3%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	RB	119/121 (98%)	113 (95%)	6 (5%)	22	53
69	SB	125/132 (95%)	121 (97%)	4 (3%)	34	68
70	TB	111/115 (96%)	106 (96%)	5 (4%)	24	58
71	UB	92/107 (86%)	89 (97%)	3 (3%)	33	67
72	VB	67/67 (100%)	62 (92%)	5 (8%)	12	37
73	WB	112/113 (99%)	110 (98%)	2 (2%)	51	80
74	XB	113/115 (98%)	110 (97%)	3 (3%)	39	73
75	YB	107/112 (96%)	103 (96%)	4 (4%)	30	64
76	ZB	66/103 (64%)	64 (97%)	2 (3%)	36	70
77	AC	84/98 (86%)	80 (95%)	4 (5%)	23	55
78	BC	75/76 (99%)	75 (100%)	0	100	100
79	CC	55/62 (89%)	51 (93%)	4 (7%)	13	38
80	DC	48/49 (98%)	48 (100%)	0	100	100
81	EC	46/106 (43%)	45 (98%)	1 (2%)	45	77
82	FC	61/140 (44%)	60 (98%)	1 (2%)	55	83
83	GC	272/275 (99%)	264 (97%)	8 (3%)	37	71
84	b	239/336 (71%)	231 (97%)	8 (3%)	33	67
All	All	11009/12423 (89%)	10817 (98%)	192 (2%)	52	82

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	JB	102	ILE
70	TB	37	VAL
62	LB	145	VAL
67	QB	53	GLU
72	VB	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
73	WB	98	GLN
78	BC	19	HIS
84	b	161	ASN
26	K	104	ASN

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Mol	Chain	Res	Type
25	Z	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	WA	3517/3635 (96%)	662 (18%)	34 (0%)
31	XA	119/120 (99%)	11 (9%)	0
32	YA	149/156 (95%)	27 (18%)	1 (0%)
53	ZA	1688/1869 (90%)	373 (22%)	15 (0%)
All	All	5473/5780 (94%)	1073 (19%)	50 (0%)

5 of 1073 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	WA	12	A
30	WA	13	U
30	WA	25	A
30	WA	39	A
30	WA	42	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	WA	4237	U
53	ZA	110	U
53	ZA	1810	U
30	WA	4453	G
30	WA	4907	C

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
30	PSU	WA	4298	30	18,21,22	4.48	7 (38%)	21,30,33	2.83	5 (23%)
30	B8H	WA	1865	30	19,22,23	6.88	8 (42%)	21,32,35	2.48	5 (23%)
30	OMG	WA	2778	30	23,26,27	2.48	9 (39%)	32,38,41	2.13	11 (34%)
30	OMC	WA	4541	30	19,22,23	3.03	8 (42%)	25,31,34	0.74	0
30	7MG	WA	4555	30	23,26,27	3.34	10 (43%)	27,39,42	2.20	9 (33%)
30	B8T	WA	4676	30	19,22,23	3.28	8 (42%)	25,31,34	0.86	1 (4%)
30	P4U	WA	1354	30	21,24,25	3.49	8 (38%)	28,33,36	1.53	2 (7%)
30	P7G	WA	3885	30	24,28,29	3.53	10 (41%)	25,41,44	1.30	2 (8%)
30	OMG	WA	4375	30	23,26,27	2.45	9 (39%)	32,38,41	2.07	11 (34%)
51	DDE	v	715	51	18,20,21	2.11	5 (27%)	17,28,30	1.21	1 (5%)
30	A2M	WA	1332	30	22,25,26	2.65	11 (50%)	30,36,39	2.28	9 (30%)
30	I4U	WA	1664	30,85	20,24,25	3.51	8 (40%)	27,34,37	1.77	2 (7%)
30	5MC	WA	4452	30	19,22,23	3.82	8 (42%)	26,32,35	1.05	1 (3%)
30	PSU	WA	3769	30	18,21,22	4.53	6 (33%)	21,30,33	2.99	5 (23%)
30	UR3	WA	4602	30	19,22,23	3.19	9 (47%)	26,32,35	1.54	4 (15%)
30	B8W	WA	4190	30	23,26,27	2.19	6 (26%)	33,38,41	3.36	17 (51%)
30	OMG	WA	4642	30	23,26,27	2.47	9 (39%)	32,38,41	2.13	11 (34%)
32	OMU	YA	14	30,32	19,22,23	3.08	8 (42%)	25,31,34	1.84	5 (20%)
30	PSU	WA	4408	30	18,21,22	4.47	7 (38%)	21,30,33	2.98	6 (28%)
30	B8W	WA	2385	30	23,26,27	2.17	6 (26%)	33,38,41	3.39	16 (48%)
30	E6G	WA	4360	30	24,27,28	1.80	5 (20%)	34,39,42	2.42	13 (38%)
30	OMG	WA	2369	30	23,26,27	2.46	9 (39%)	32,38,41	2.11	11 (34%)
30	OMG	WA	1527	30	23,26,27	2.45	9 (39%)	32,38,41	2.10	11 (34%)
53	B8N	ZA	1248	53	25,29,30	2.49	5 (20%)	28,42,45	2.02	6 (21%)
30	OMC	WA	3914	30	19,22,23	3.01	8 (42%)	25,31,34	0.77	0
30	OMG	WA	3797	30	23,26,27	2.47	9 (39%)	32,38,41	2.12	11 (34%)
30	A2M	WA	3872	30	22,25,26	2.64	11 (50%)	30,36,39	2.30	9 (30%)
53	JMH	ZA	1219	53	18,22,23	2.90	6 (33%)	23,32,35	1.41	5 (21%)
30	OMC	WA	2866	30	19,22,23	3.04	8 (42%)	25,31,34	0.86	1 (4%)
30	OMG	WA	4875	30	23,26,27	2.46	9 (39%)	32,38,41	2.08	11 (34%)
30	PSU	WA	2513	30	18,21,22	4.53	6 (33%)	21,30,33	3.02	6 (28%)
30	PSU	WA	4455	30,85	18,21,22	4.48	6 (33%)	21,30,33	3.06	6 (28%)
30	JMH	WA	1461	30	18,22,23	2.86	6 (33%)	23,32,35	1.41	3 (13%)
30	A2M	WA	2406	30	22,25,26	2.66	11 (50%)	30,36,39	2.38	10 (33%)
30	A2M	WA	3728	30	22,25,26	2.66	11 (50%)	30,36,39	2.31	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	5MC	WA	4340	30	19,22,23	3.89	8 (42%)	26,32,35	1.03	2 (7%)
30	A2M	WA	4528	30,85	22,25,26	2.65	11 (50%)	30,36,39	2.39	10 (33%)
30	A2M	WA	1876	30	22,25,26	2.65	11 (50%)	30,36,39	2.43	10 (33%)
53	5MC	ZA	1374	53	19,22,23	3.88	8 (42%)	26,32,35	1.01	2 (7%)
30	OMU	WA	4625	30	19,22,23	3.03	8 (42%)	25,31,34	1.79	5 (20%)
30	PSU	WA	4641	30	18,21,22	4.70	6 (33%)	21,30,33	3.25	6 (28%)
30	OMG	WA	2429	30	23,26,27	2.46	9 (39%)	32,38,41	2.06	11 (34%)
30	E7G	WA	2302	30	24,27,28	3.33	11 (45%)	28,40,43	2.40	9 (32%)
30	B9B	WA	1579	30	25,28,29	1.77	6 (24%)	35,40,43	2.35	14 (40%)
30	B8H	WA	3767	-	19,22,23	6.87	8 (42%)	21,32,35	2.46	5 (23%)
53	4AC	ZA	1337	53	21,24,25	3.68	9 (42%)	28,34,37	1.20	4 (14%)
30	OMG	WA	2055	30	23,26,27	2.45	9 (39%)	32,38,41	2.06	11 (34%)
30	1MA	WA	4420	30	21,25,26	2.47	5 (23%)	30,37,40	1.93	8 (26%)
30	B8K	WA	4695	30	24,28,29	3.34	12 (50%)	29,42,45	2.45	11 (37%)
30	A2M	WA	3723	30	22,25,26	2.65	11 (50%)	30,36,39	2.30	10 (33%)
30	P7G	WA	1914	30	24,28,29	3.61	10 (41%)	25,41,44	1.33	2 (8%)
30	OMC	WA	2370	30	19,22,23	3.01	8 (42%)	25,31,34	0.70	0
30	2MG	WA	4877	30	23,26,27	2.61	7 (30%)	33,38,41	2.31	12 (36%)
30	I4U	WA	4199	30	20,24,25	3.51	8 (40%)	27,34,37	1.57	2 (7%)
30	OMG	WA	1630	30	23,26,27	2.46	9 (39%)	32,38,41	2.13	11 (34%)
30	2MG	WA	730	30	23,26,27	2.69	7 (30%)	33,38,41	2.38	12 (36%)
30	6MZ	WA	4225	30	22,25,26	2.44	4 (18%)	29,36,39	2.24	10 (34%)
30	1MA	WA	1328	30,85	21,25,26	2.45	4 (19%)	30,37,40	1.91	8 (26%)
30	5MU	WA	4088	30	19,22,23	8.29	7 (36%)	27,32,35	3.55	10 (37%)
30	A2M	WA	2368	30,85	22,25,26	2.65	11 (50%)	30,36,39	2.33	10 (33%)
30	B8W	WA	4134	30	23,26,27	2.16	6 (26%)	33,38,41	3.38	16 (48%)
30	OMG	WA	1888	30	23,26,27	2.48	9 (39%)	32,38,41	2.14	11 (34%)
30	OMC	WA	2427	30	19,22,23	3.04	8 (42%)	25,31,34	0.75	0
30	OMG	WA	1322	30	23,26,27	2.46	9 (39%)	32,38,41	2.12	11 (34%)
30	B8W	WA	4477	30	23,26,27	2.20	6 (26%)	33,38,41	3.33	15 (45%)
53	A2M	ZA	1678	53	22,25,26	2.67	11 (50%)	30,36,39	2.31	8 (26%)
30	5MC	WA	3787	30	19,22,23	3.83	8 (42%)	26,32,35	1.03	2 (7%)
30	OMC	WA	3892	30	19,22,23	3.03	8 (42%)	25,31,34	0.73	0
30	A2M	WA	1529	30	22,25,26	2.66	11 (50%)	30,36,39	2.33	8 (26%)
30	B9B	WA	237	30	25,28,29	1.77	5 (20%)	35,40,43	2.34	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMG	WA	4499	30	23,26,27	2.47	9 (39%)	32,38,41	2.13	11 (34%)
30	MHG	WA	4376	30	29,32,33	3.56	10 (34%)	34,46,49	2.53	11 (32%)
30	B8K	WA	3902	30	24,28,29	3.26	12 (50%)	29,42,45	2.36	10 (34%)
53	PSU	ZA	1243	53	18,21,22	4.54	6 (33%)	21,30,33	2.99	6 (28%)
30	PSU	WA	3734	30	18,21,22	4.54	6 (33%)	21,30,33	2.94	5 (23%)
30	B9H	WA	2791	30	21,25,26	2.90	5 (23%)	22,35,38	1.57	5 (22%)
30	A2M	WA	3790	30	22,25,26	2.69	11 (50%)	30,36,39	2.45	11 (36%)
30	E7G	WA	1802	30	24,27,28	3.35	11 (45%)	28,40,43	2.38	9 (32%)
30	A2M	WA	398	30	22,25,26	2.65	11 (50%)	30,36,39	2.33	10 (33%)
30	B8T	WA	4488	30	19,22,23	3.28	8 (42%)	25,31,34	0.87	1 (4%)
30	OMG	WA	4628	30	23,26,27	2.46	9 (39%)	32,38,41	2.07	11 (34%)
30	A2M	WA	4576	30	22,25,26	2.68	11 (50%)	30,36,39	2.35	10 (33%)
30	UR3	WA	1871	30	19,22,23	3.21	8 (42%)	26,32,35	1.59	4 (15%)
30	UR3	WA	4535	30	19,22,23	3.23	8 (42%)	26,32,35	1.60	3 (11%)
30	PSU	WA	1682	30	18,21,22	4.53	7 (38%)	21,30,33	3.04	7 (33%)
30	2MG	WA	1522	30	23,26,27	2.62	8 (34%)	33,38,41	2.28	13 (39%)
30	A2M	WA	3830	30	22,25,26	2.63	11 (50%)	30,36,39	2.31	10 (33%)
30	A2M	WA	1539	30,85	22,25,26	2.63	11 (50%)	30,36,39	2.31	10 (33%)
44	MLZ	LA	72	44	8,9,10	0.72	0	4,9,11	0.86	0
30	PSU	WA	4447	30	18,21,22	4.49	6 (33%)	21,30,33	2.89	6 (28%)
30	OMG	WA	373	30	23,26,27	2.46	9 (39%)	32,38,41	2.05	11 (34%)
30	PSU	WA	1587	30	18,21,22	4.50	7 (38%)	21,30,33	2.85	5 (23%)
30	B9B	WA	2759	30	25,28,29	1.76	5 (20%)	35,40,43	2.38	14 (40%)
30	B8H	WA	4301	30	19,22,23	6.85	8 (42%)	21,32,35	2.48	5 (23%)
30	OMG	WA	4201	30	23,26,27	2.45	9 (39%)	32,38,41	2.09	11 (34%)
30	OMC	WA	3874	30	19,22,23	3.00	8 (42%)	25,31,34	0.70	0
30	OMC	WA	2809	30	19,22,23	3.00	8 (42%)	25,31,34	0.69	0
30	7MG	WA	2527	30	23,26,27	3.37	10 (43%)	27,39,42	2.21	9 (33%)
30	OMC	WA	3706	30,85	19,22,23	3.02	8 (42%)	25,31,34	0.71	0
3	MLZ	C	333	3	8,9,10	0.68	0	4,9,11	0.84	0
30	PSU	WA	4505	30	18,21,22	4.50	6 (33%)	21,30,33	3.04	5 (23%)
30	PSU	WA	4633	30	18,21,22	4.51	6 (33%)	21,30,33	3.07	6 (28%)
30	BGH	WA	3904	30	25,29,30	4.54	17 (68%)	30,43,46	2.37	11 (36%)
30	PSU	WA	4536	30	18,21,22	4.56	6 (33%)	21,30,33	2.97	5 (23%)
30	M7A	WA	4569	30	19,25,26	1.57	2 (10%)	25,37,40	4.33	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	WA	3720	30	18,21,22	4.52	6 (33%)	21,30,33	2.97	5 (23%)
30	7MG	WA	1610	30	23,26,27	3.35	10 (43%)	27,39,42	2.22	9 (33%)
30	OMU	WA	4311	30	19,22,23	3.03	8 (42%)	25,31,34	1.82	5 (20%)
30	B8W	WA	4534	30	23,26,27	2.16	6 (26%)	33,38,41	3.42	16 (48%)
30	PSU	WA	1688	30	18,21,22	4.51	6 (33%)	21,30,33	3.06	6 (28%)

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
30	PSU	WA	4298	30	-	2/7/25/26	0/2/2/2
30	B8H	WA	1865	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	2778	30	-	2/9/27/28	0/3/3/3
30	OMC	WA	4541	30	-	0/9/27/28	0/2/2/2
30	7MG	WA	4555	30	-	2/7/37/38	0/3/3/3
30	B8T	WA	4676	30	-	5/7/27/28	0/2/2/2
30	P4U	WA	1354	30	-	4/10/29/30	0/2/2/2
30	P7G	WA	3885	30	-	2/10/40/41	0/3/3/3
30	OMG	WA	4375	30	-	0/9/27/28	0/3/3/3
51	DDE	v	715	51	-	4/20/21/23	0/1/1/1
30	A2M	WA	1332	30	-	1/9/27/28	0/3/3/3
30	I4U	WA	1664	30,85	-	0/9/29/30	0/2/2/2
30	5MC	WA	4452	30	-	4/7/25/26	0/2/2/2
30	PSU	WA	3769	30	-	0/7/25/26	0/2/2/2
30	UR3	WA	4602	30	-	0/7/25/26	0/2/2/2
30	B8W	WA	4190	30	-	2/9/27/28	0/3/3/3
30	OMG	WA	4642	30	-	3/9/27/28	0/3/3/3
32	OMU	YA	14	30,32	-	5/9/27/28	0/2/2/2
30	PSU	WA	4408	30	-	0/7/25/26	0/2/2/2
30	B8W	WA	2385	30	-	4/9/27/28	0/3/3/3
30	E6G	WA	4360	30	-	5/10/28/29	0/3/3/3
30	OMG	WA	2369	30	-	3/9/27/28	0/3/3/3
30	OMG	WA	1527	30	-	0/9/27/28	0/3/3/3
53	B8N	ZA	1248	53	-	3/16/34/35	0/2/2/2
30	OMC	WA	3914	30	-	0/9/27/28	0/2/2/2
30	OMG	WA	3797	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A2M	WA	3872	30	-	4/9/27/28	0/3/3/3
53	JMH	ZA	1219	53	-	0/7/25/26	0/2/2/2
30	OMC	WA	2866	30	-	1/9/27/28	0/2/2/2
30	OMG	WA	4875	30	-	3/9/27/28	0/3/3/3
30	PSU	WA	2513	30	-	0/7/25/26	0/2/2/2
30	PSU	WA	4455	30,85	-	3/7/25/26	0/2/2/2
30	JMH	WA	1461	30	-	0/7/25/26	0/2/2/2
30	A2M	WA	2406	30	-	0/9/27/28	0/3/3/3
30	A2M	WA	3728	30	-	3/9/27/28	0/3/3/3
30	5MC	WA	4340	30	-	2/7/25/26	0/2/2/2
30	A2M	WA	4528	30,85	-	1/9/27/28	0/3/3/3
30	A2M	WA	1876	30	-	0/9/27/28	0/3/3/3
53	5MC	ZA	1374	53	-	0/7/25/26	0/2/2/2
30	OMU	WA	4625	30	-	1/9/27/28	0/2/2/2
30	PSU	WA	4641	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	2429	30	-	2/9/27/28	0/3/3/3
30	E7G	WA	2302	30	-	2/9/39/40	0/3/3/3
30	B9B	WA	1579	30	-	3/11/29/30	0/3/3/3
30	B8H	WA	3767	-	-	3/7/25/26	0/2/2/2
53	4AC	ZA	1337	53	-	0/11/29/30	0/2/2/2
30	OMG	WA	2055	30	-	1/9/27/28	0/3/3/3
30	1MA	WA	4420	30	-	2/7/25/26	0/3/3/3
30	B8K	WA	4695	30	-	0/11/41/42	0/3/3/3
30	A2M	WA	3723	30	-	0/9/27/28	0/3/3/3
30	P7G	WA	1914	30	-	1/10/40/41	0/3/3/3
30	OMC	WA	2370	30	-	0/9/27/28	0/2/2/2
30	2MG	WA	4877	30	-	1/9/27/28	0/3/3/3
30	I4U	WA	4199	30	-	4/9/29/30	0/2/2/2
30	OMG	WA	1630	30	-	1/9/27/28	0/3/3/3
30	2MG	WA	730	30	-	0/9/27/28	0/3/3/3
30	6MZ	WA	4225	30	-	0/9/27/28	0/3/3/3
30	1MA	WA	1328	30,85	-	2/7/25/26	0/3/3/3
30	5MU	WA	4088	30	-	0/7/25/26	0/2/2/2
30	A2M	WA	2368	30,85	-	0/9/27/28	0/3/3/3
30	B8W	WA	4134	30	-	2/9/27/28	0/3/3/3
30	OMG	WA	1888	30	-	1/9/27/28	0/3/3/3
30	OMC	WA	2427	30	-	0/9/27/28	0/2/2/2
30	OMG	WA	1322	30	-	1/9/27/28	0/3/3/3
30	B8W	WA	4477	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	A2M	ZA	1678	53	-	1/9/27/28	0/3/3/3
30	5MC	WA	3787	30	-	1/7/25/26	0/2/2/2
30	OMC	WA	3892	30	-	3/9/27/28	0/2/2/2
30	A2M	WA	1529	30	-	1/9/27/28	0/3/3/3
30	B9B	WA	237	30	-	4/11/29/30	0/3/3/3
30	OMG	WA	4499	30	-	0/9/27/28	0/3/3/3
30	MHG	WA	4376	30	-	6/16/46/47	0/3/3/3
30	B8K	WA	3902	30	-	3/11/41/42	0/3/3/3
53	PSU	ZA	1243	53	-	2/7/25/26	0/2/2/2
30	PSU	WA	3734	30	-	2/7/25/26	0/2/2/2
30	B9H	WA	2791	30	-	1/12/47/48	0/2/2/2
30	A2M	WA	3790	30	-	4/9/27/28	0/3/3/3
30	E7G	WA	1802	30	-	2/9/39/40	0/3/3/3
30	A2M	WA	398	30	-	3/9/27/28	0/3/3/3
30	B8T	WA	4488	30	-	0/7/27/28	0/2/2/2
30	OMG	WA	4628	30	-	0/9/27/28	0/3/3/3
30	A2M	WA	4576	30	-	1/9/27/28	0/3/3/3
30	UR3	WA	1871	30	-	2/7/25/26	0/2/2/2
30	UR3	WA	4535	30	-	0/7/25/26	0/2/2/2
30	PSU	WA	1682	30	-	0/7/25/26	0/2/2/2
30	2MG	WA	1522	30	-	1/9/27/28	0/3/3/3
30	A2M	WA	3830	30	-	2/9/27/28	0/3/3/3
30	A2M	WA	1539	30,85	-	2/9/27/28	0/3/3/3
44	MLZ	LA	72	44	-	1/7/8/10	-
30	PSU	WA	4447	30	-	0/7/25/26	0/2/2/2
30	OMG	WA	373	30	-	1/9/27/28	0/3/3/3
30	PSU	WA	1587	30	-	2/7/25/26	0/2/2/2
30	B9B	WA	2759	30	-	2/11/29/30	0/3/3/3
30	B8H	WA	4301	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	4201	30	-	0/9/27/28	0/3/3/3
30	OMC	WA	3874	30	-	0/9/27/28	0/2/2/2
30	OMC	WA	2809	30	-	1/9/27/28	0/2/2/2
30	7MG	WA	2527	30	-	0/7/37/38	0/3/3/3
30	OMC	WA	3706	30,85	-	4/9/27/28	0/2/2/2
3	MLZ	C	333	3	-	4/7/8/10	-
30	PSU	WA	4505	30	-	3/7/25/26	0/2/2/2
30	PSU	WA	4633	30	-	0/7/25/26	0/2/2/2
30	BGH	WA	3904	30	-	0/13/43/44	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	WA	4536	30	-	0/7/25/26	0/2/2/2
30	M7A	WA	4569	30	-	0/7/37/38	0/3/3/3
30	PSU	WA	3720	30	-	0/7/25/26	0/2/2/2
30	7MG	WA	1610	30	-	0/7/37/38	0/3/3/3
30	OMU	WA	4311	30	-	0/9/27/28	0/2/2/2
30	B8W	WA	4534	30	-	0/9/27/28	0/3/3/3
30	PSU	WA	1688	30	-	0/7/25/26	0/2/2/2

The worst 5 of 880 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4088	5MU	C4-C5	23.43	1.82	1.44
30	WA	4088	5MU	C6-N1	17.74	1.68	1.38
30	WA	1865	B8H	C6-C5	-15.85	1.12	1.35
30	WA	4301	B8H	C6-C5	-15.75	1.12	1.35
30	WA	3767	B8H	C6-C5	-15.75	1.12	1.35

The worst 5 of 795 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	4569	M7A	C5-C6-N6	14.83	148.94	123.75
30	WA	4569	M7A	N6-C6-N1	-12.28	91.02	118.38
30	WA	4088	5MU	C5-C4-N3	10.30	124.28	115.32
30	WA	4088	5MU	C5-C6-N1	-9.05	113.48	123.31
30	WA	4641	PSU	N1-C2-N3	8.71	124.36	115.17

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	333	MLZ	CD-CE-NZ-CM
30	WA	237	B9B	C5-C6-O6-C61
30	WA	237	B9B	N1-C6-O6-C61
30	WA	237	B9B	O4'-C4'-C5'-O5'
30	WA	398	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

60 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	WA	4298	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	WA	1865	B8H	6	0
30	WA	2778	OMG	1	0
30	WA	4555	7MG	1	0
30	WA	1354	P4U	1	0
51	v	715	DDE	1	0
30	WA	1332	A2M	4	0
30	WA	4452	5MC	1	0
30	WA	4602	UR3	2	0
32	YA	14	OMU	3	0
30	WA	4360	E6G	2	0
30	WA	2369	OMG	1	0
30	WA	1527	OMG	1	0
30	WA	3872	A2M	2	0
53	ZA	1219	JMH	1	0
30	WA	2866	OMC	1	0
30	WA	1461	JMH	2	0
30	WA	3728	A2M	2	0
30	WA	4528	A2M	1	0
30	WA	1876	A2M	1	0
30	WA	4625	OMU	2	0
30	WA	4641	PSU	1	0
30	WA	1579	B9B	1	0
30	WA	3767	B8H	6	0
53	ZA	1337	4AC	4	0
30	WA	2055	OMG	2	0
30	WA	4695	B8K	1	0
30	WA	3723	A2M	3	0
30	WA	1914	P7G	1	0
30	WA	4877	2MG	3	0
30	WA	4199	I4U	1	0
30	WA	1630	OMG	1	0
30	WA	730	2MG	3	0
30	WA	4225	6MZ	3	0
30	WA	4088	5MU	5	0
30	WA	2368	A2M	1	0
30	WA	4134	B8W	1	0
30	WA	1888	OMG	1	0
30	WA	2427	OMC	1	0
30	WA	1322	OMG	1	0
30	WA	4477	B8W	2	0
53	ZA	1678	A2M	3	0
30	WA	4499	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	WA	3902	B8K	1	0
30	WA	3790	A2M	1	0
30	WA	398	A2M	1	0
30	WA	4628	OMG	2	0
30	WA	4576	A2M	1	0
30	WA	1871	UR3	3	0
30	WA	3830	A2M	1	0
30	WA	1539	A2M	1	0
30	WA	373	OMG	1	0
30	WA	2759	B9B	1	0
30	WA	4301	B8H	6	0
30	WA	2809	OMC	1	0
30	WA	2527	7MG	2	0
30	WA	4505	PSU	1	0
30	WA	3904	BGH	1	0
30	WA	4569	M7A	1	0
30	WA	1610	7MG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 155 ligands modelled in this entry, 152 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
89	GDP	v	900	-	29,30,30	3.26	17 (58%)	45,47,47	2.14	11 (24%)
86	ANM	WA	5199	-	20,20,20	4.08	7 (35%)	24,27,27	1.42	3 (12%)
87	SPD	WA	5200	-	9,9,9	0.27	0	8,8,8	0.32	0

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
89	GDP	v	900	-	-	4/16/32/32	0/3/3/3
86	ANM	WA	5199	-	-	0/10/23/23	0/2/2/2
87	SPD	WA	5200	-	-	1/7/7/7	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	WA	5199	ANM	C3-C2	-11.84	1.32	1.53
86	WA	5199	ANM	C16-N1	-8.82	1.30	1.47
86	WA	5199	ANM	C2-C16	7.39	1.68	1.53
89	v	900	GDP	C4-N3	6.60	1.49	1.34
89	v	900	GDP	O4'-C4'	-6.26	1.31	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	v	900	GDP	C1'-N9-C8	-6.61	107.96	126.73
86	WA	5199	ANM	O2-C5-C6	4.99	119.99	111.09
89	v	900	GDP	N9-C8-N7	-4.89	104.34	113.40
89	v	900	GDP	C5-C4-N3	-4.47	121.28	128.39
89	v	900	GDP	C1'-N9-C4	4.22	138.97	126.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

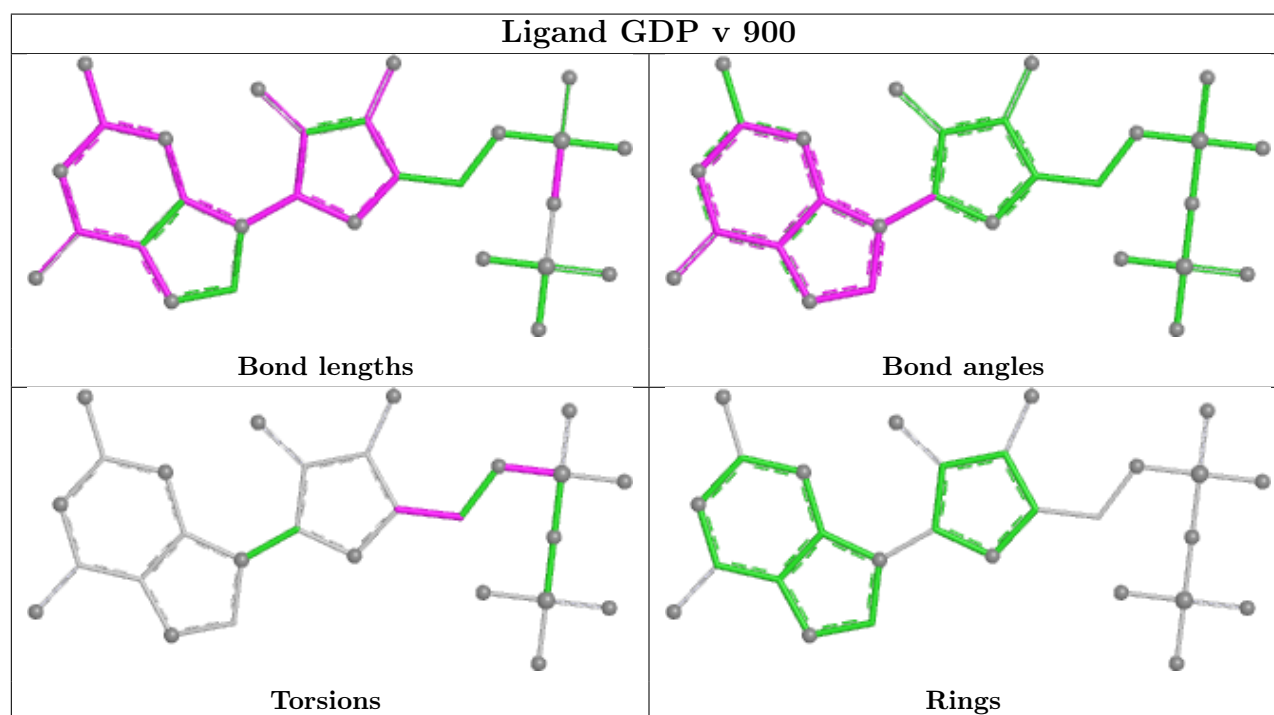
Mol	Chain	Res	Type	Atoms
89	v	900	GDP	C5'-O5'-PA-O3A
89	v	900	GDP	C5'-O5'-PA-O2A
87	WA	5200	SPD	N6-C7-C8-C9
89	v	900	GDP	O4'-C4'-C5'-O5'
89	v	900	GDP	C5'-O5'-PA-O1A

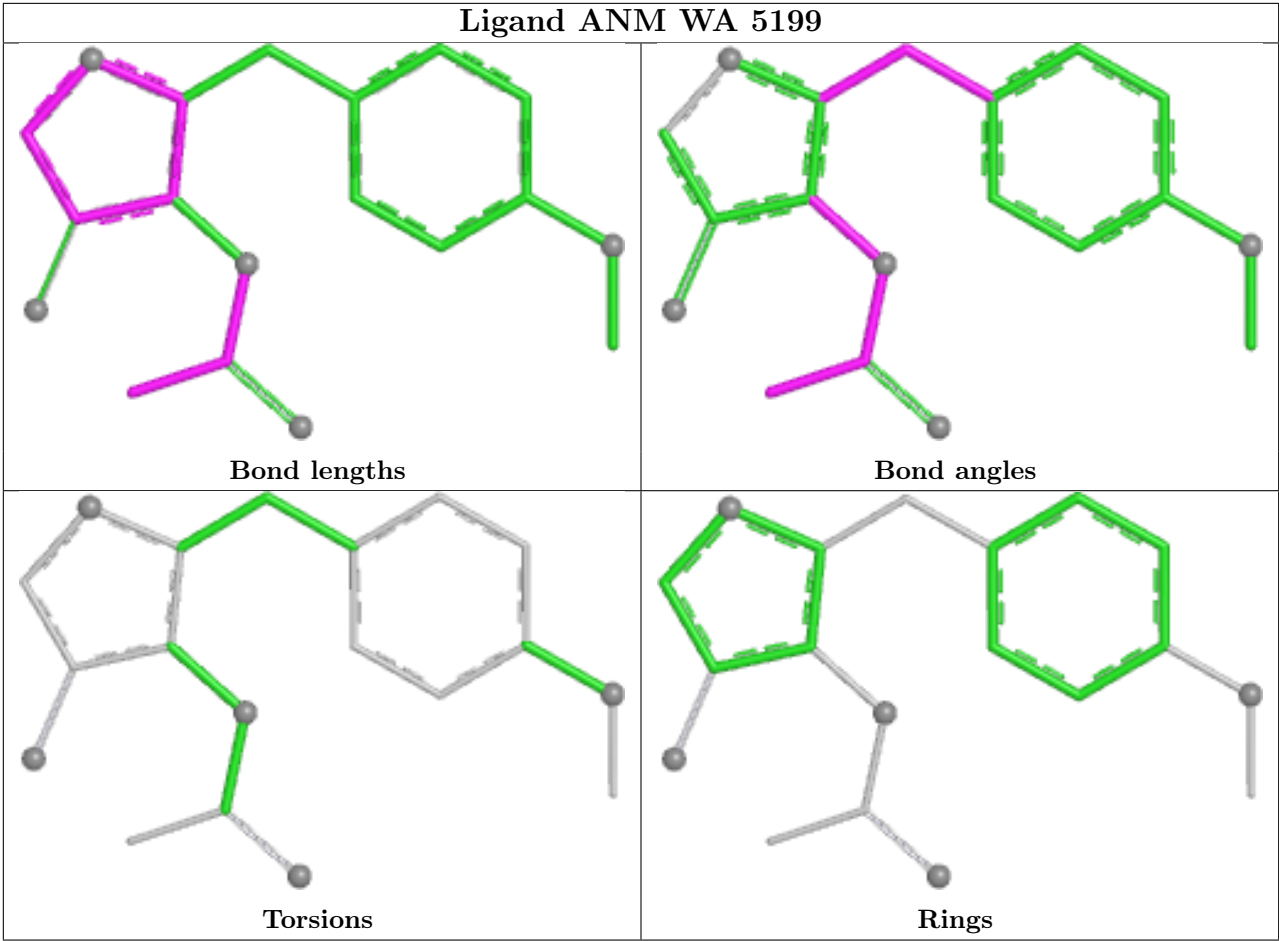
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	v	900	GDP	2	0
86	WA	5199	ANM	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	WA	19
52	w	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	221:VAL	C	282:THR	N	59.11
1	WA	2118:G	O3'	2263:C	P	40.34
1	WA	1258:C	O3'	1277:G	P	36.79
1	WA	2906:G	O3'	3602:G	P	19.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	WA	4106:C	O3'	4112:G	P	18.00

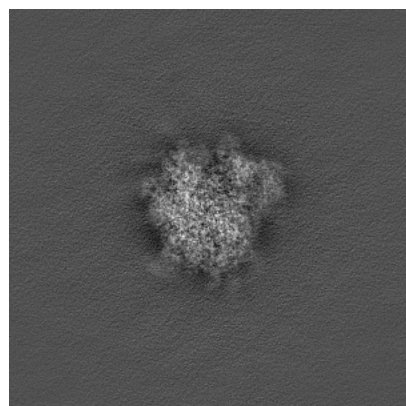
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43568. These allow visual inspection of the internal detail of the map and identification of artifacts.

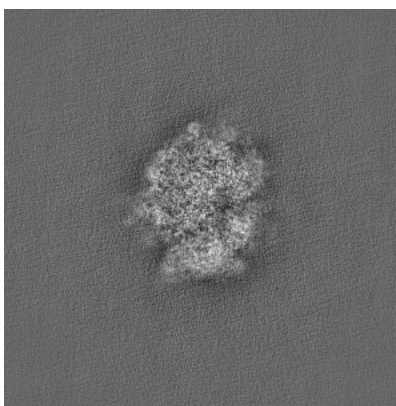
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

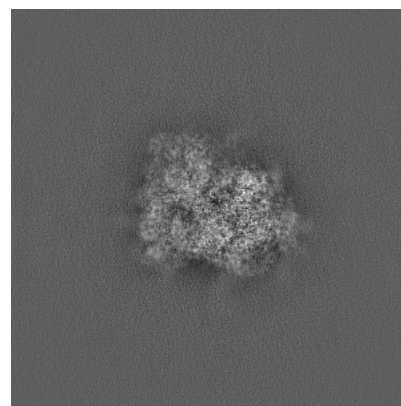
6.1.1 Primary map



X

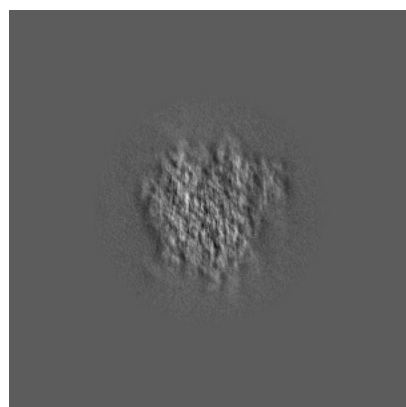


Y

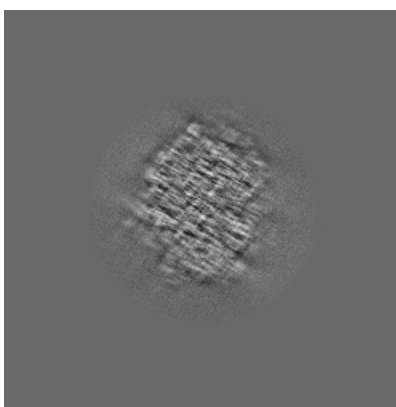


Z

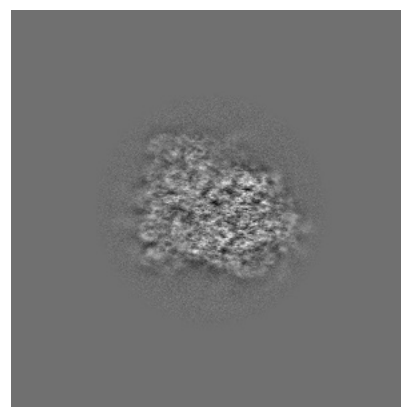
6.1.2 Raw map



X



Y

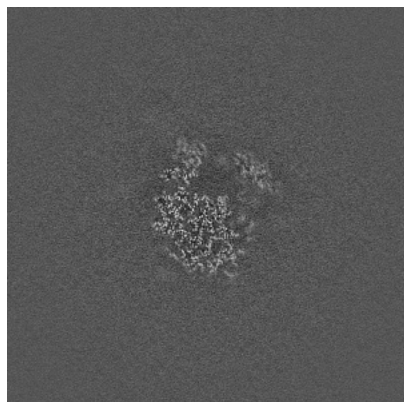


Z

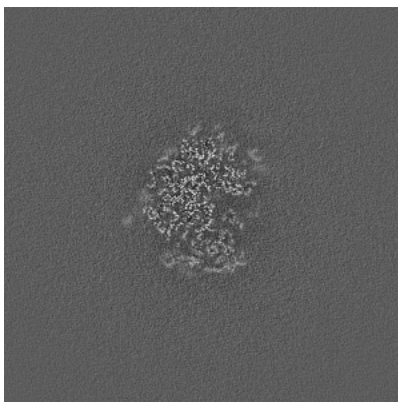
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

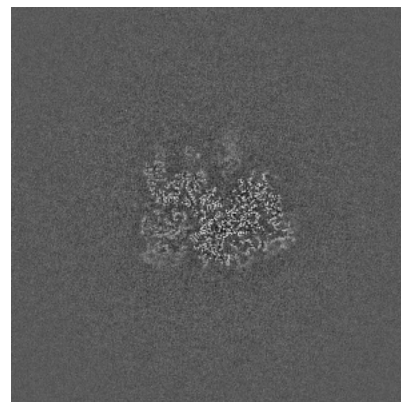
6.2.1 Primary map



X Index: 324

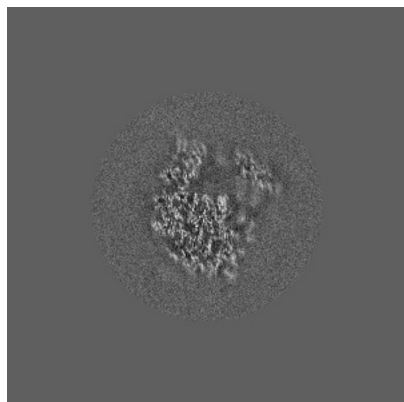


Y Index: 324

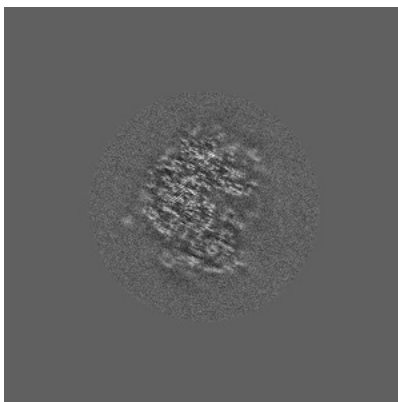


Z Index: 324

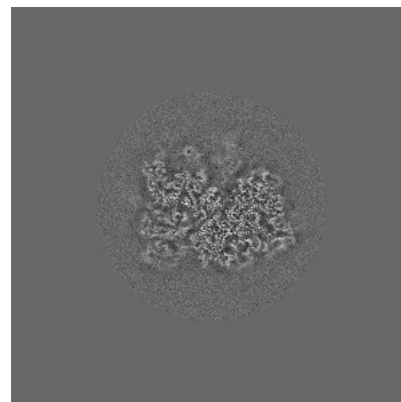
6.2.2 Raw map



X Index: 324



Y Index: 324

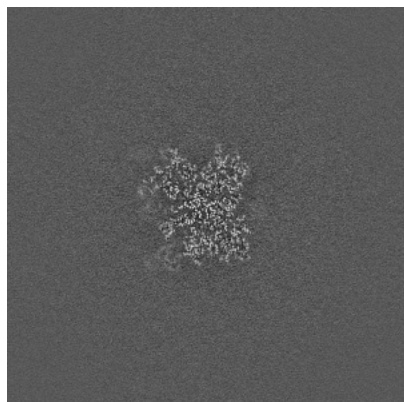


Z Index: 324

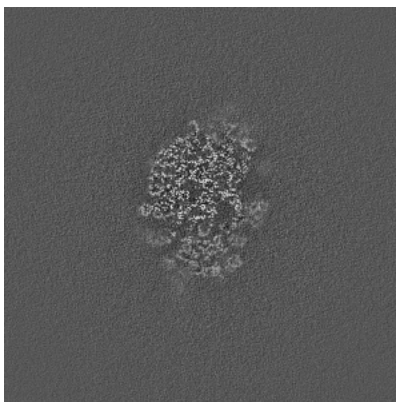
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

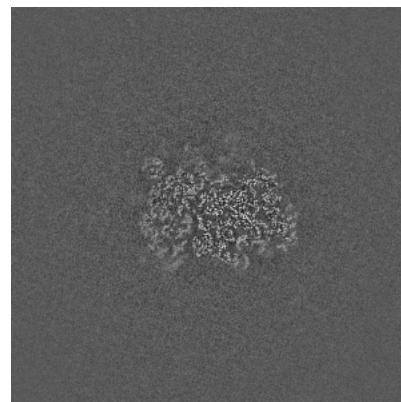
6.3.1 Primary map



X Index: 373

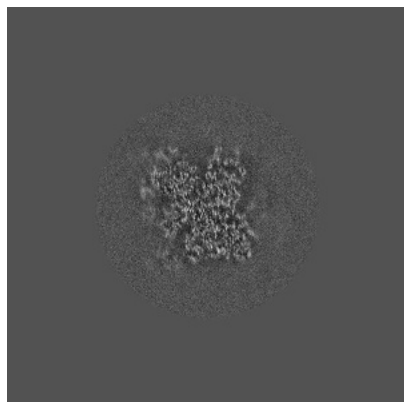


Y Index: 302

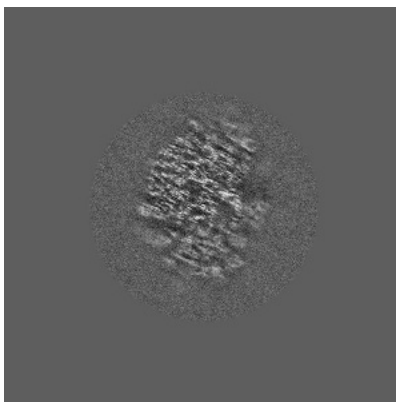


Z Index: 315

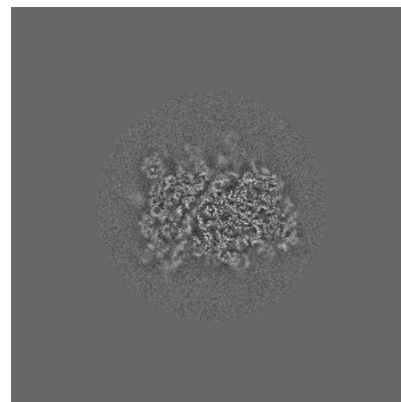
6.3.2 Raw map



X Index: 369



Y Index: 302

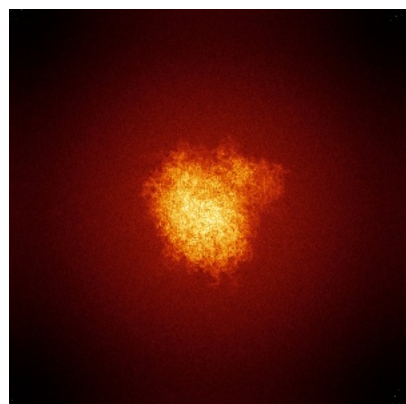


Z Index: 314

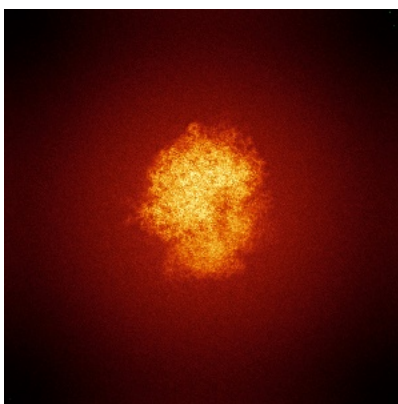
The images above show the largest variance slices of the map in three orthogonal directions.

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

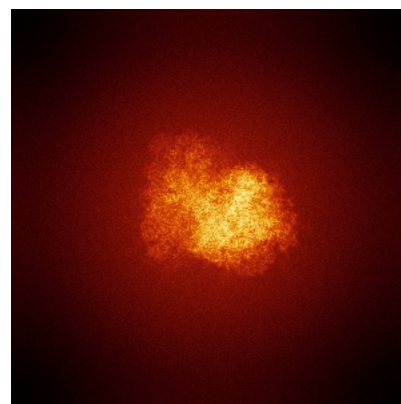
6.4.1 Primary map



X

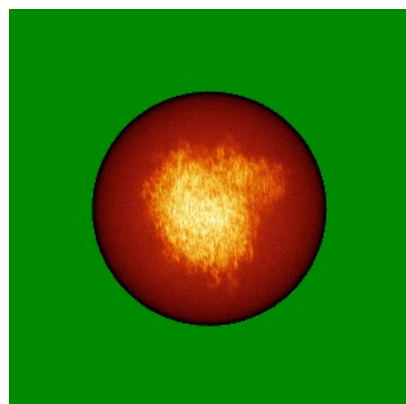


Y

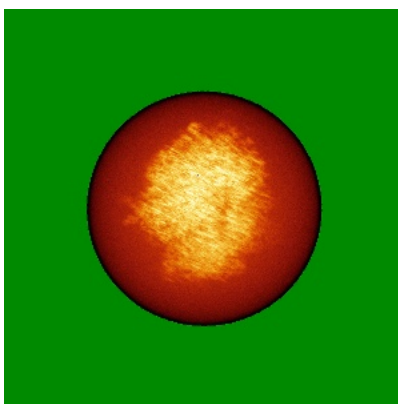


Z

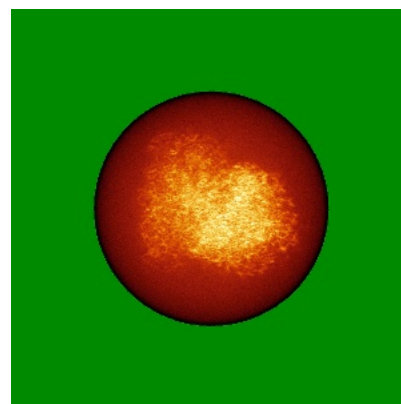
6.4.2 Raw map



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](#)

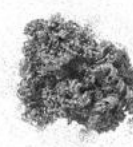
6.5.1 Primary map



X



Y



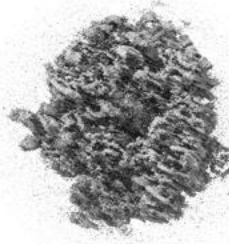
Z

The images above show the 3D surface view of the map at the recommended contour level 6.3. 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



X



Y



Z

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.

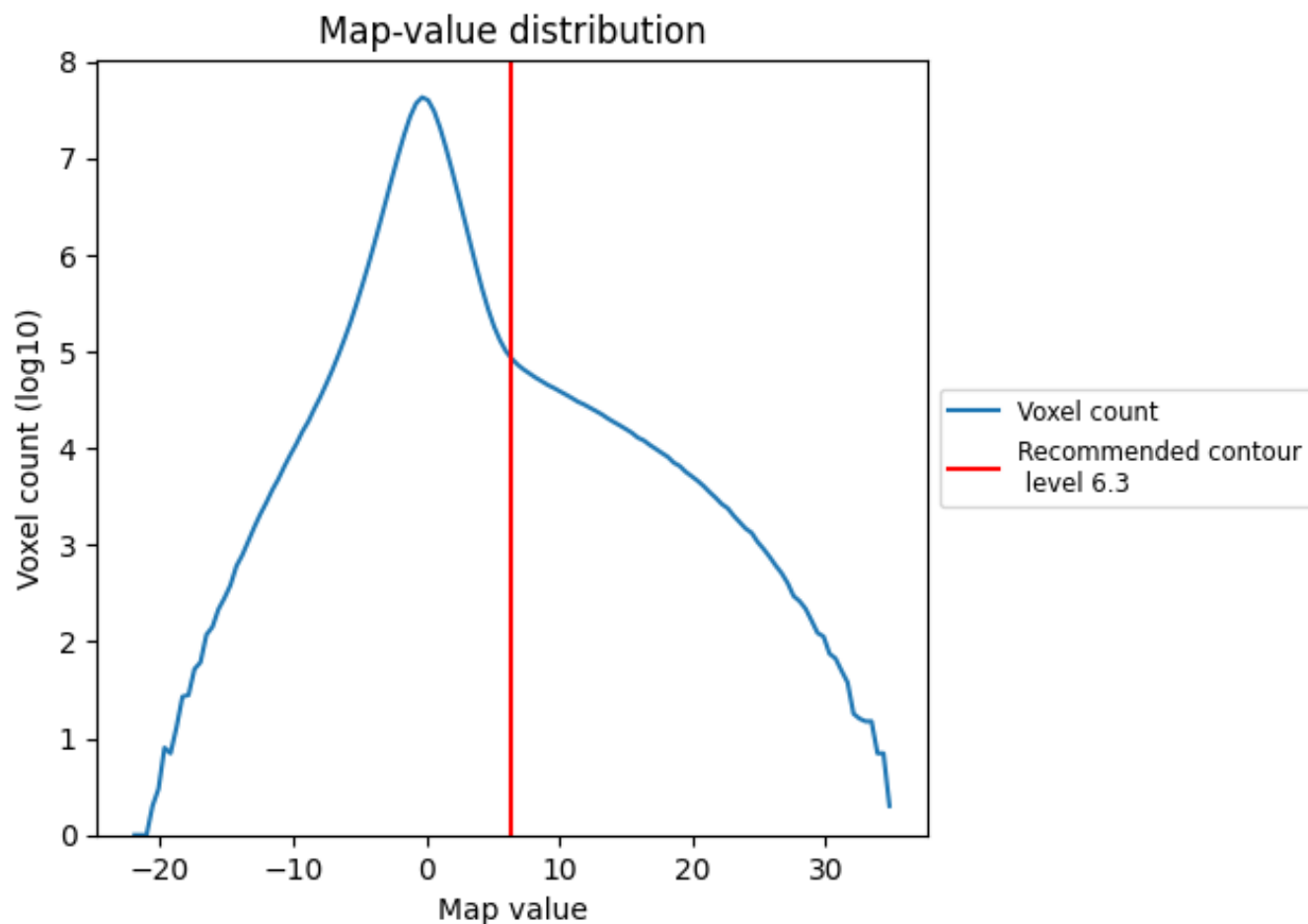
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

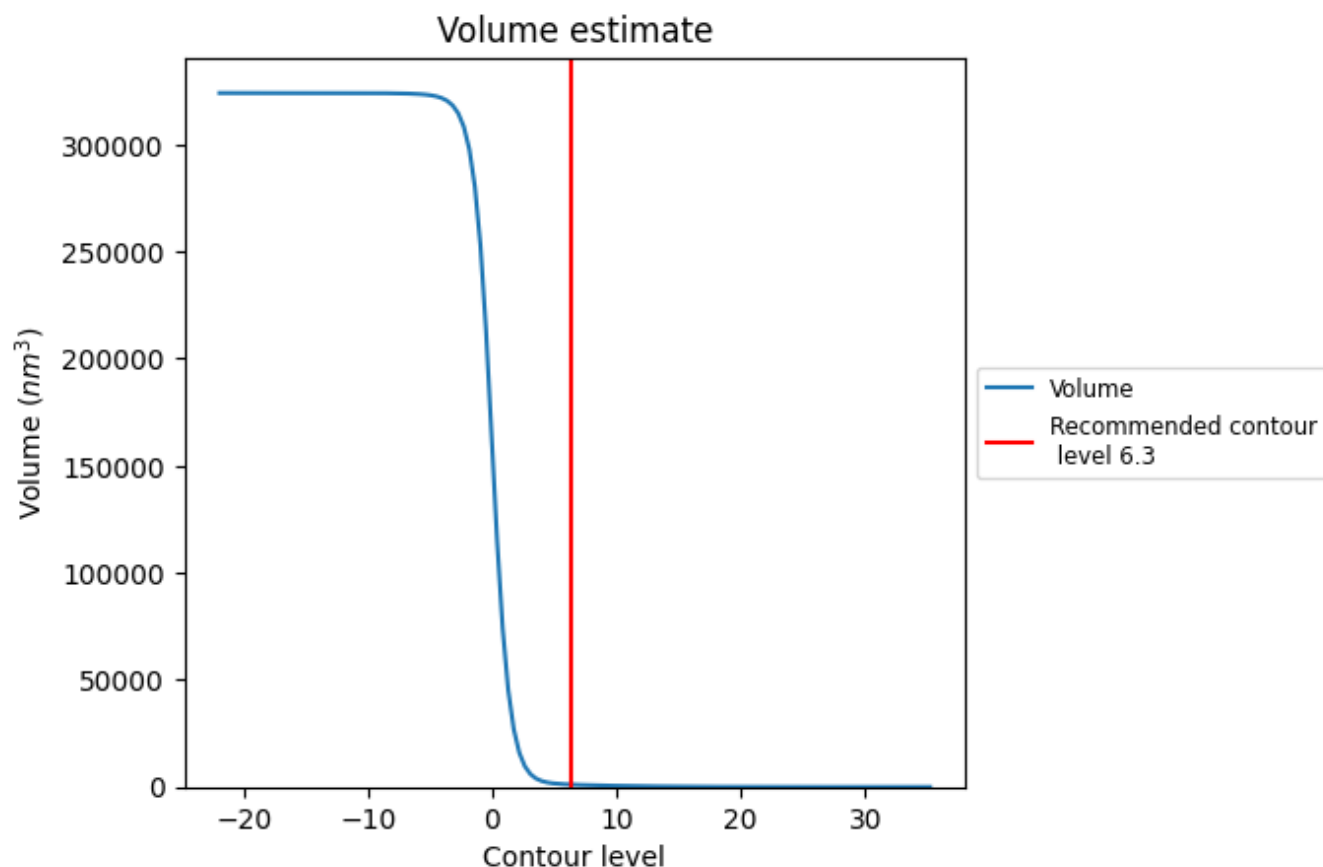
This section contains the results of statistical analysis of the map.

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.

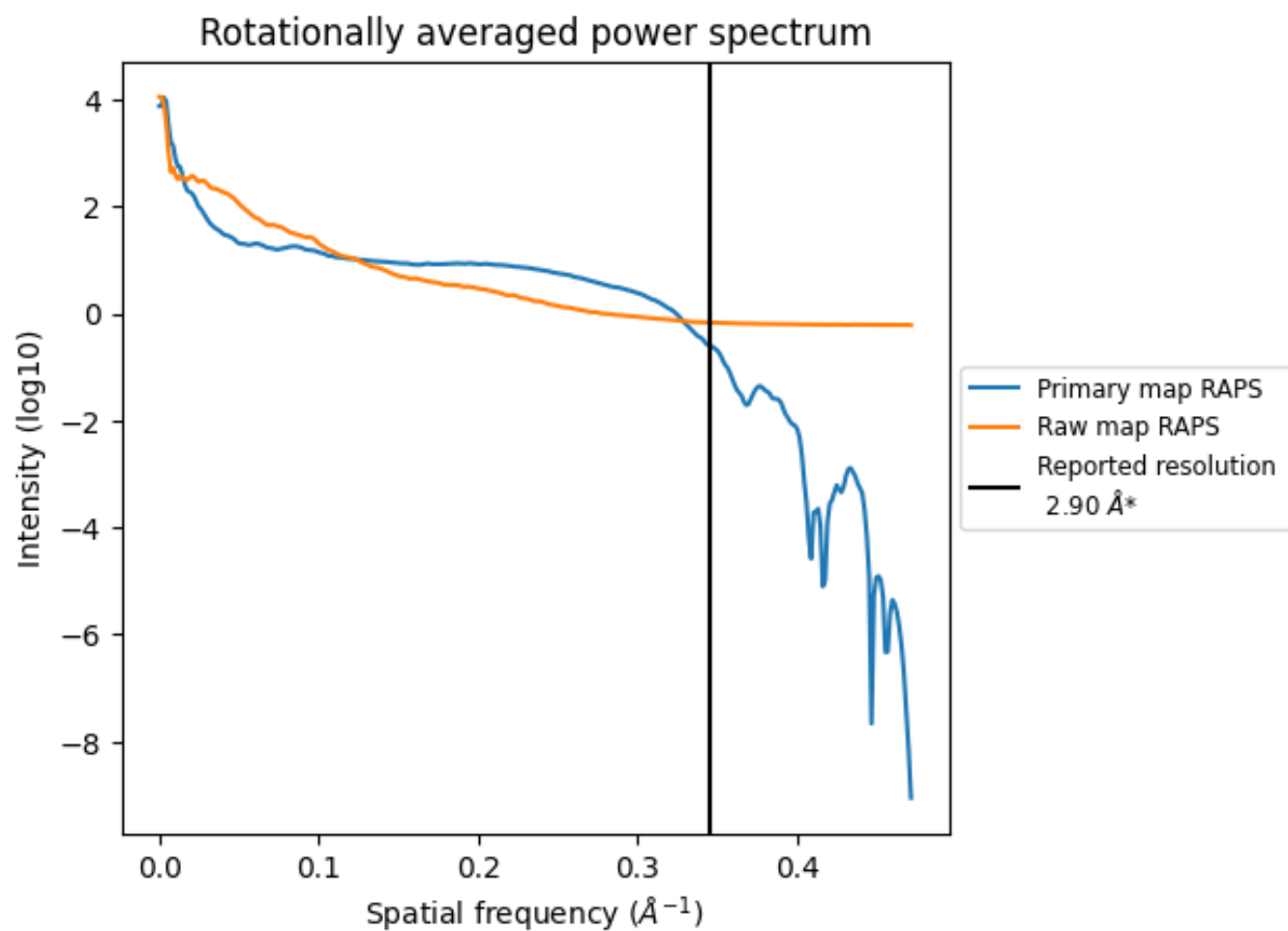
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1124 nm^3 ; this corresponds to an approximate mass of 1016 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 ⓘ

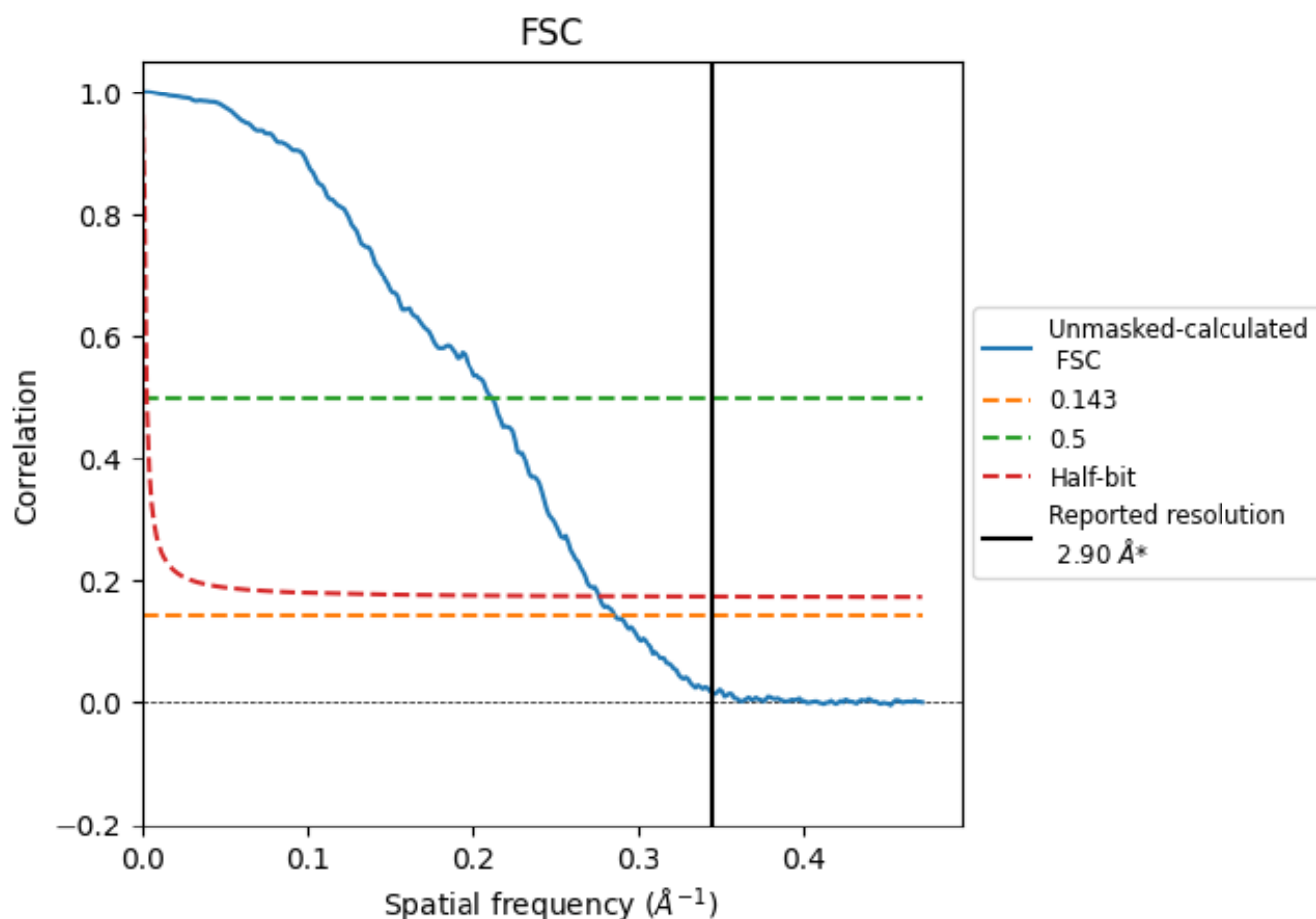


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

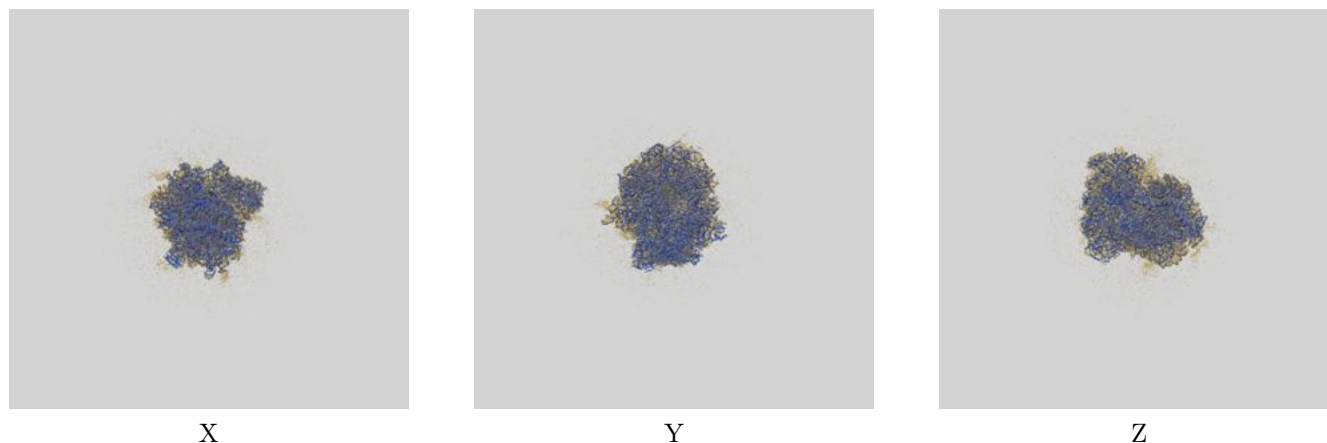
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	4.73	3.62

*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 3.50 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

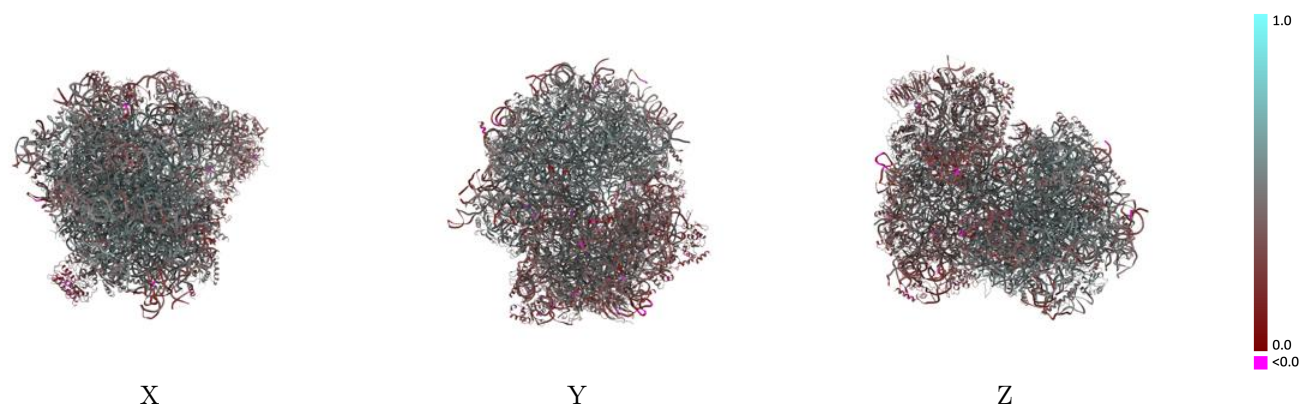
This section contains information regarding the fit between EMDB map EMD-43568 and PDB model 8VVT. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



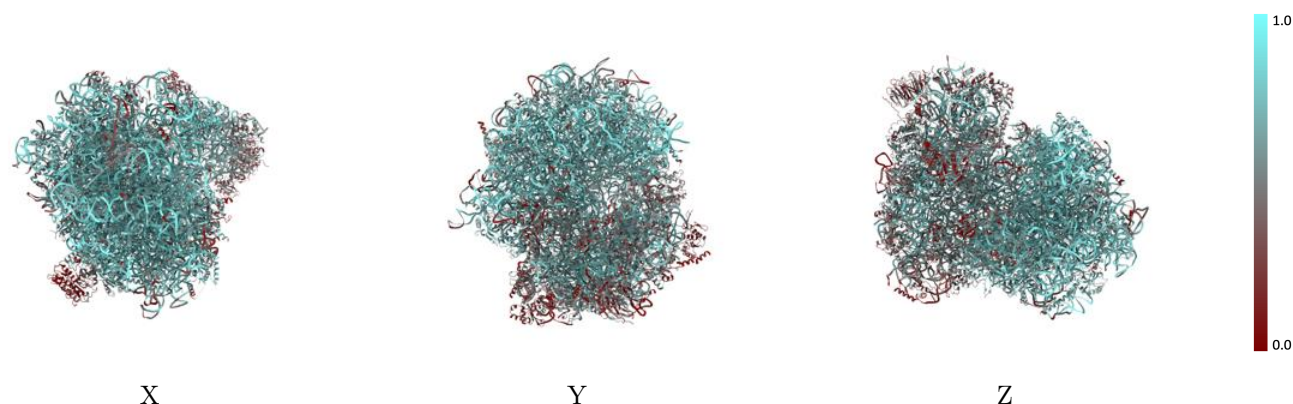
The images above show the 3D surface view of the map at the recommended contour level 6.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



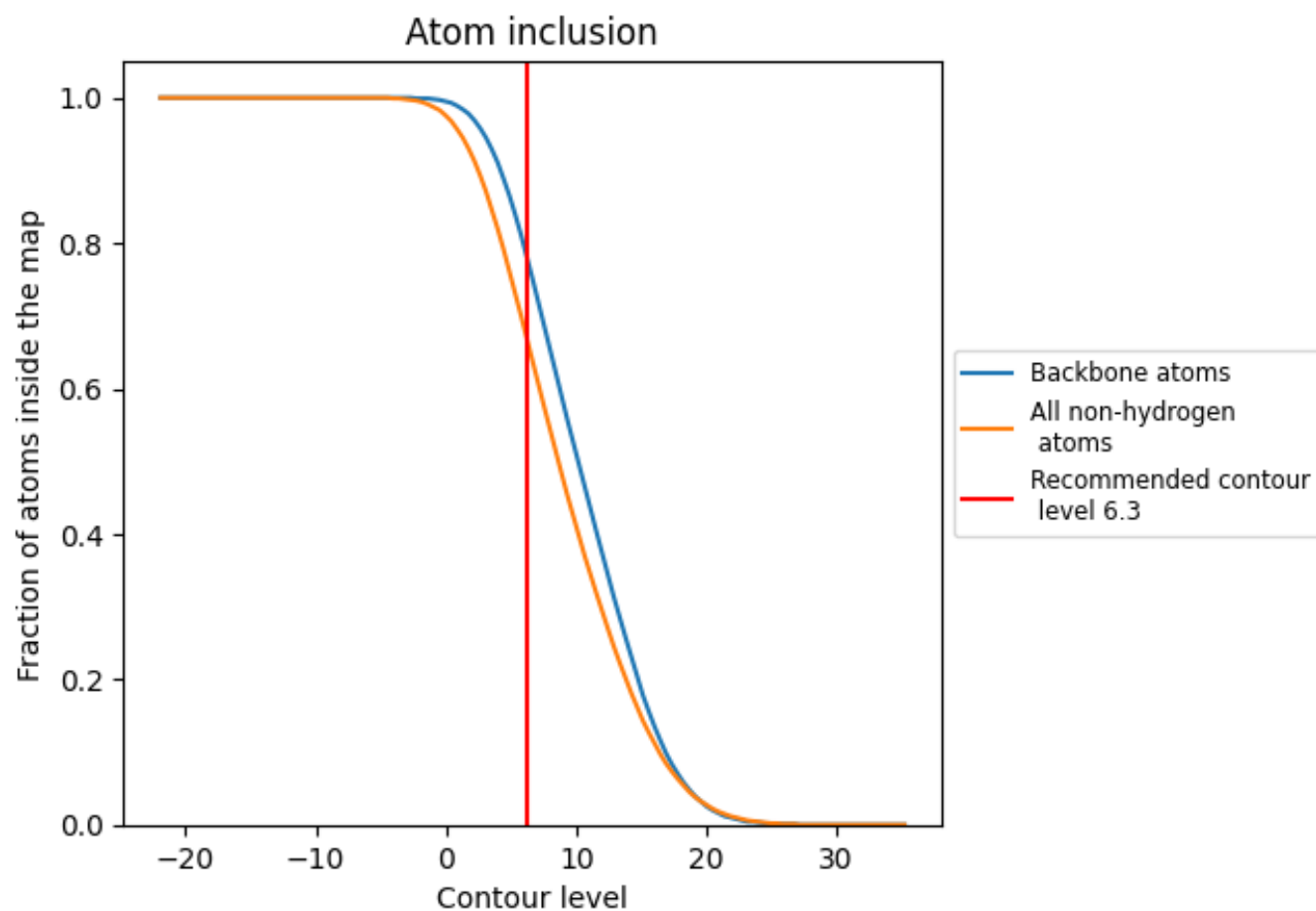
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 66% 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 (6.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.4450
A	 0.7030	 0.5280
AA	 0.6070	 0.4690
AB	 0.4930	 0.4000
AC	 0.5180	 0.4400
B	 0.7090	 0.5210
BA	 0.6500	 0.4650
BB	 0.3710	 0.3540
BC	 0.4080	 0.3690
C	 0.6840	 0.5120
CA	 0.6660	 0.4940
CB	 0.5770	 0.4450
CC	 0.3430	 0.3240
D	 0.7060	 0.4790
DA	 0.7090	 0.5320
DB	 0.5000	 0.4080
DC	 0.5750	 0.4240
E	 0.6630	 0.4880
EA	 0.7170	 0.5330
EB	 0.4640	 0.4010
EC	 0.4550	 0.4000
F	 0.6970	 0.5200
FA	 0.6840	 0.5080
FB	 0.3820	 0.3390
FC	 0.2130	 0.2950
G	 0.6390	 0.4500
GA	 0.6510	 0.4760
GB	 0.3000	 0.2970
GC	 0.3330	 0.3220
H	 0.6720	 0.4960
HA	 0.6860	 0.4700
HB	 0.3030	 0.3410
I	 0.6950	 0.5110
IA	 0.7490	 0.5330
IB	 0.3870	 0.3670



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Chain	Atom inclusion	Q-score
J	 0.6260	 0.4530
JA	 0.5980	 0.4450
JB	 0.5520	 0.4110
K	 0.6720	 0.4860
KA	 0.6590	 0.4890
KB	 0.4770	 0.3670
L	 0.7010	 0.4820
LA	 0.7100	 0.5090
LB	 0.4960	 0.4290
M	 0.7350	 0.5330
MA	 0.6010	 0.4850
MB	 0.1530	 0.2470
N	 0.7240	 0.5090
NA	 0.6780	 0.5150
NB	 0.4710	 0.4090
O	 0.7110	 0.5210
OA	 0.6780	 0.5170
OB	 0.4130	 0.3810
P	 0.7060	 0.5250
PA	 0.7170	 0.5130
PB	 0.5000	 0.3910
Q	 0.6180	 0.4650
QA	 0.4330	 0.3400
QB	 0.4220	 0.3680
R	 0.7050	 0.5180
RA	 0.2350	 0.2580
RB	 0.3420	 0.3540
S	 0.6830	 0.5080
SB	 0.4170	 0.3550
T	 0.6280	 0.4370
TB	 0.4560	 0.3660
U	 0.6770	 0.5230
UB	 0.4120	 0.3600
V	 0.5210	 0.4180
VB	 0.5260	 0.4070
W	 0.6890	 0.4960
WA	 0.7980	 0.4770
WB	 0.5440	 0.4550
X	 0.6770	 0.4910
XA	 0.8690	 0.5150
XB	 0.5600	 0.4650
Y	 0.6800	 0.4730

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Chain	Atom inclusion	Q-score
YA	 0.8030	 0.4820
YB	 0.4040	 0.3420
Z	 0.7460	 0.5270
ZA	 0.6580	 0.4000
ZB	 0.3430	 0.3220
b	 0.2020	 0.3040
v	 0.4930	 0.3890
w	 0.4460	 0.3970