



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2024 – 01:22 PM EST

PDB ID : 8VFT
EMDB ID : EMD-43189
Title : Translating 80S rabbit ribosome stalled by emetine with eEF2
Authors : Murray, J.; Shao, S.
Deposited on : 2023-12-22
Resolution : 3.30 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:

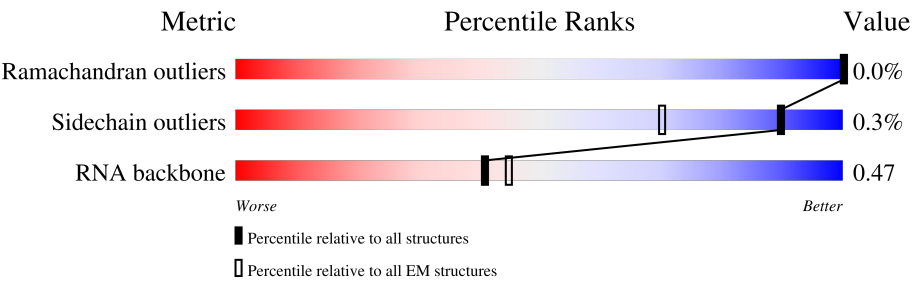
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	425	
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	

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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

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Mol	Chain	Length	Quality of chain
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	93	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	5	3543	
46	7	120	
47	8	156	
48	v	858	
49	9	1869	
50	AA	295	
51	BB	264	
52	CC	293	
53	DD	243	
54	EE	263	
55	FF	204	
56	GG	249	
57	HH	194	
58	II	208	

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Mol	Chain	Length	Quality of chain
59	JJ	194	
60	KK	165	
61	LL	158	
62	MM	132	
63	NN	151	
64	OO	168	
65	PP	145	
66	QQ	146	
67	RR	135	
68	SS	152	
69	TT	145	
70	UU	119	
71	VV	83	
72	WW	130	
73	XX	143	
74	YY	130	
75	ZZ	125	
76	aa	115	
77	bb	84	
78	cc	69	
79	dd	56	
80	ee	133	
81	ff	156	
82	gg	317	
83	3	75	

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Mol	Chain	Length	Quality of chain
84	w	6	<div><div></div><div>17%</div><div></div><div>100%</div></div>
85	2	76	<div><div></div><div>62%</div><div></div><div>84%</div><div></div><div>13%</div><div></div></div>

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 220911 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	0
			1891	1185	388	312	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	378	LYS	-	insertion	UNP G1SVW5
C	379	VAL	-	insertion	UNP G1SVW5
C	380	LYS	-	insertion	UNP G1SVW5
C	381	LYS	-	insertion	UNP G1SVW5
C	382	PRO	-	insertion	UNP G1SVW5
C	383	ARG	-	insertion	UNP G1SVW5
C	384	ALA	-	insertion	UNP G1SVW5
C	385	VAL	-	insertion	UNP G1SVW5
C	386	GLY	-	insertion	UNP G1SVW5
C	387	ILE	-	insertion	UNP G1SVW5
C	388	LYS	-	insertion	UNP G1SVW5
C	389	GLN	-	insertion	UNP G1SVW5

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	289	Total	C	N	O	S	0	0
			2361	1495	431	421	14		

- Molecule 5 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1726	1110	327	286	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	218	Total	C	N	O	S	0	0
			1768	1127	341	296	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	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 uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	208	Total	C	N	O	S	0	0
			1691	1072	327	279	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1336	846	249	235	6		

- Molecule 11 is a protein called eL13.

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

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	198	Total	C	N	O	S	0	0
			1621	1046	317	253	5		

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	179	Total	C	N	O	S	0	0
			1502	930	327	236	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	CYS	conflict	UNP G1TJR3
R	64	ARG	GLN	conflict	UNP G1TJR3

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Chain	Residue	Modelled	Actual	Comment	Reference
R	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 18 is a protein called eL20.

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

There are 23 discrepancies between the modelled and reference sequences:

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	98	Total	C	N	O	S	0	0
			800	514	139	145	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	LEU	VAL	conflict	UNP G1TSG1
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	62	SER	THR	conflict	UNP G1TSG1
U	63	LEU	ILE	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1
U	106	THR	SER	conflict	UNP G1TSG1
U	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	116	Total	C	N	O	S	0	0
			949	606	178	164	1		

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	464	130	132	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	100	Total	C	N	O	S	0	0
			833	530	163	138	2		

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	49	Total	C	N	O	S	0	0
			438	280	95	62	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	51	Total	C	N	O	S	0	0
			421	260	89	66	6		

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5	3529	Total	C	N	O	P	0	0
			75712	33770	13864	24549	3529		

- Molecule 46 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 47 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 48 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	835	Total	C	N	O	S	0	0
			6516	4144	1117	1211	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	847	GLY	-	insertion	UNP P55823

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 50 is a protein called uS2.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 51 is a protein called eS1.

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

- Molecule 52 is a protein called uS5.

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

- Molecule 53 is a protein called uS3.

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

- Molecule 54 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	EE	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
EE	25	GLY	SER	conflict	UNP G1TK17
EE	51	ARG	LYS	conflict	UNP G1TK17
EE	78	THR	ALA	conflict	UNP G1TK17
EE	156	VAL	MET	conflict	UNP G1TK17

- Molecule 55 is a protein called uS7.

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

- Molecule 56 is a protein called eS6.

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

- Molecule 57 is a protein called eS7.

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

- Molecule 58 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 59 is a protein called uS4.

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

- Molecule 60 is a protein called eS10.

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

- Molecule 61 is a protein called uS17.

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

- Molecule 62 is a protein called eS12.

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

- Molecule 63 is a protein called uS15.

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

- Molecule 64 is a protein called uS11.

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

- Molecule 65 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	PP	117	Total	C	N	O	S	0	0
			975	622	181	165	7		

- Molecule 66 is a protein called uS9.

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

- Molecule 67 is a protein called eS17.

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

- Molecule 68 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SS	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 69 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 70 is a protein called uS10.

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

- Molecule 71 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS8.

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

- Molecule 73 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	XX	138	Total	C	N	O	S	0	0
			1069	676	210	180	3		

- Molecule 74 is a protein called eS24.

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

- Molecule 75 is a protein called eS25.

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

- Molecule 76 is a protein called eS26.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 77 is a protein called eS27.

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

- Molecule 78 is a protein called eS28.

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

- Molecule 79 is a protein called uS14.

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

- Molecule 80 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	ee	34	Total	C	N	O	S	0	0
			289	175	70	43	1		

- Molecule 81 is a protein called eS31.

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

- Molecule 82 is a protein called RACK1.

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

- Molecule 83 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	74	Total	C	N	O	P	0	0
			1573	703	279	518	73		

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	w	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

- Molecule 85 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	2	74	Total	C	N	O	P	0	0
			1577	705	286	513	73		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	A	2	Total 2	Mg 2	0
86	I	2	Total 2	Mg 2	0
86	P	1	Total 1	Mg 1	0
86	V	1	Total 1	Mg 1	0
86	a	1	Total 1	Mg 1	0
86	e	1	Total 1	Mg 1	0
86	f	1	Total 1	Mg 1	0
86	g	1	Total 1	Mg 1	0
86	o	1	Total 1	Mg 1	0
86	5	198	Total 198	Mg 198	0
86	7	5	Total 5	Mg 5	0
86	8	1	Total 1	Mg 1	0
86	9	56	Total 56	Mg 56	0
86	QQ	1	Total 1	Mg 1	0
86	TT	1	Total 1	Mg 1	0
86	aa	1	Total 1	Mg 1	0
86	w	1	Total 1	Mg 1	0
86	2	1	Total 1	Mg 1	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

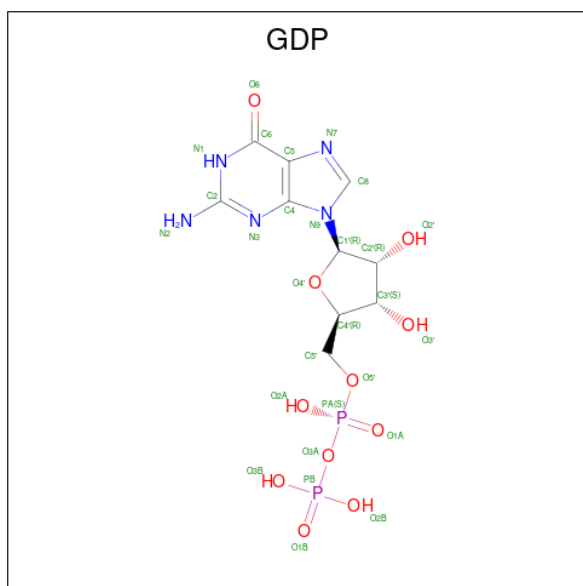
Mol	Chain	Residues	Atoms		AltConf
87	g	1	Total 1	Zn 1	0
87	j	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
87	m	1	Total	Zn	0
			1	1	
87	o	1	Total	Zn	0
			1	1	
87	p	1	Total	Zn	0
			1	1	
87	aa	1	Total	Zn	0
			1	1	
87	dd	1	Total	Zn	0
			1	1	
87	ff	1	Total	Zn	0
			1	1	

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



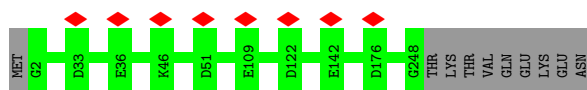


3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

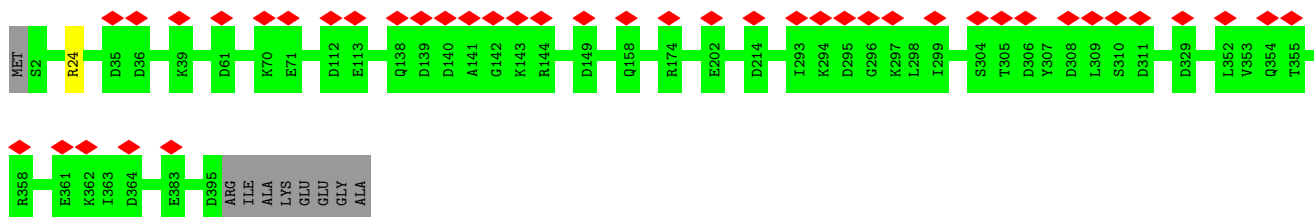
• Molecule 1: uL2

Chain A:  96%




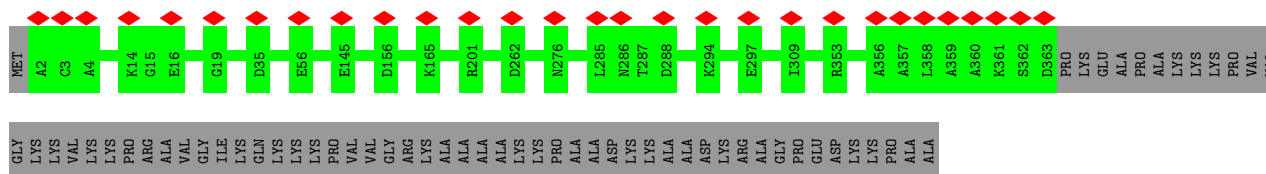
• Molecule 2: uL3

Chain B:  10% 98%



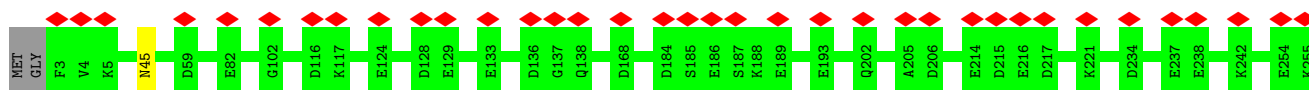
• Molecule 3: uL4

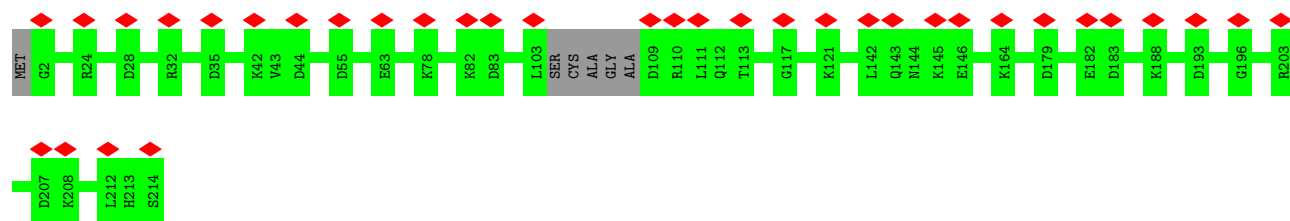
Chain C:  7% 85% 15%



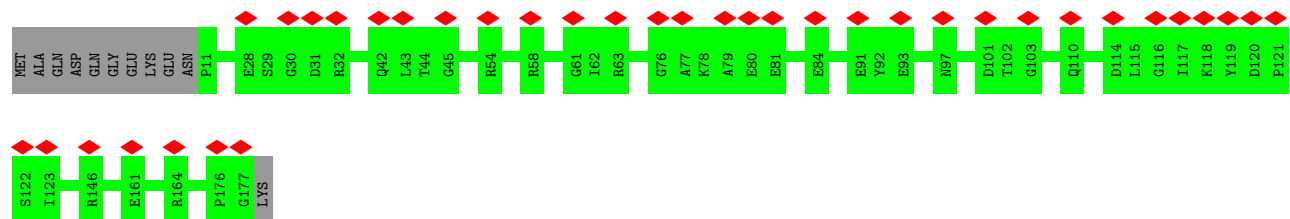
• Molecule 4: uL18

Chain D:  16% 97%

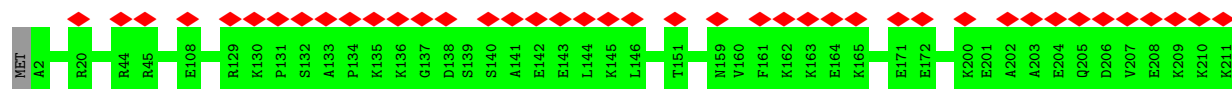




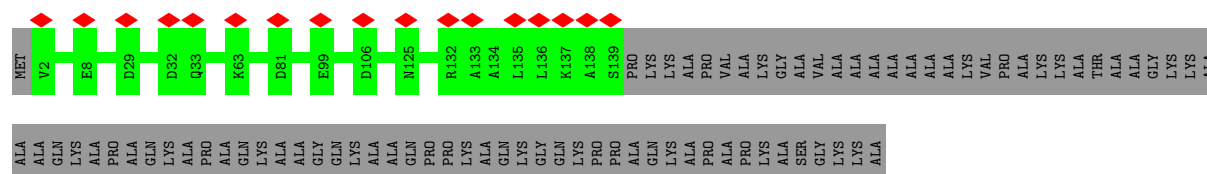
• Molecule 10: uL5



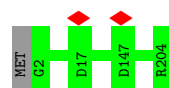
• Molecule 11: eL13



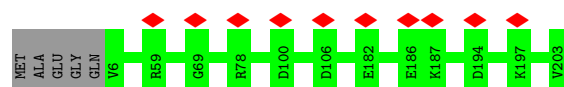
• Molecule 12: eL14




• Molecule 13: eL15

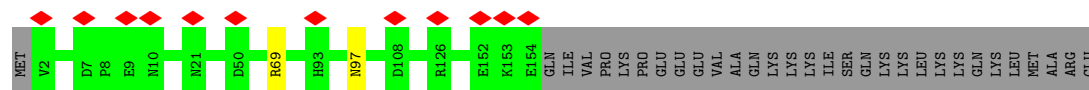


• Molecule 14: uL13



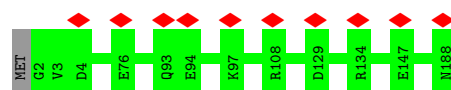
- Molecule 15: uL22

Chain P: 



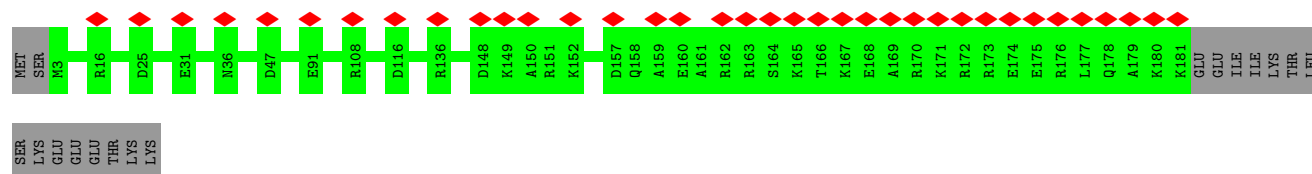
- Molecule 16: eL18

Chain Q: 



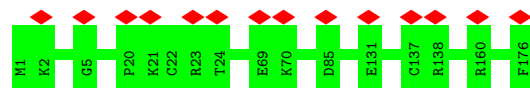
- Molecule 17: eL19

Chain R: 



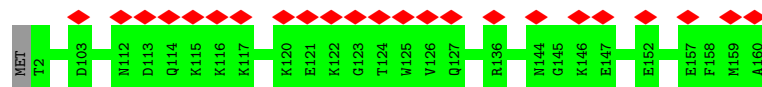
- Molecule 18: eL20

Chain S: 




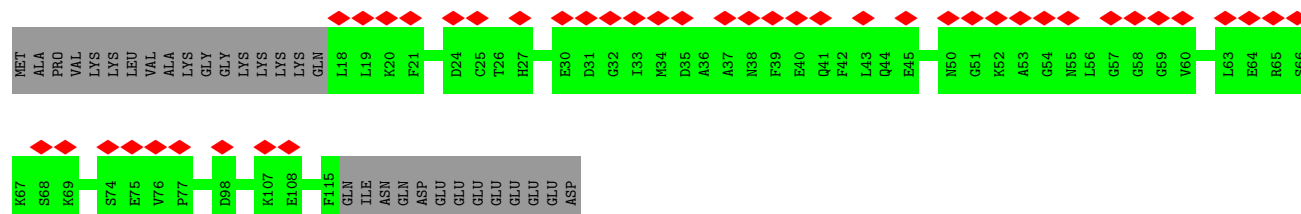
- Molecule 19: eL21

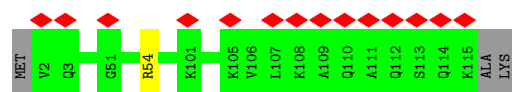
Chain T: 



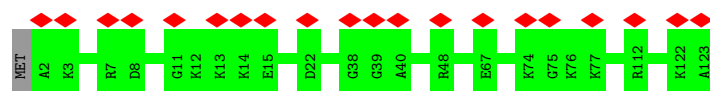
- Molecule 20: eL22

Chain U: 

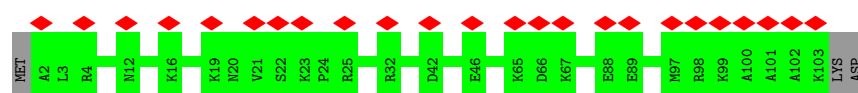




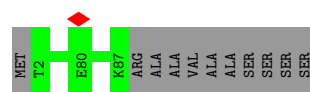
• Molecule 33: uL29



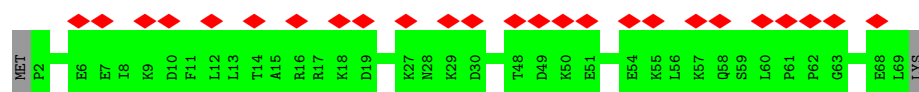
• Molecule 34: eL36



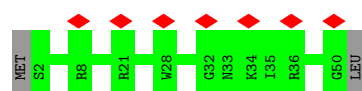
• Molecule 35: eL37



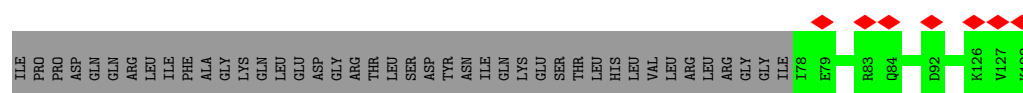
• Molecule 36: eL38



• Molecule 37: eL39

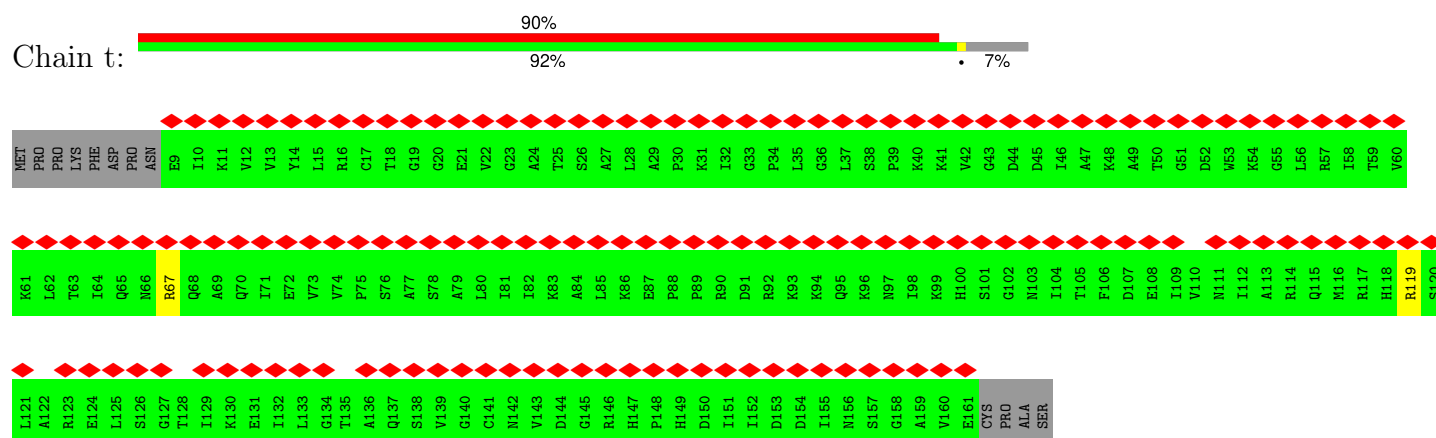


• Molecule 38: eL40

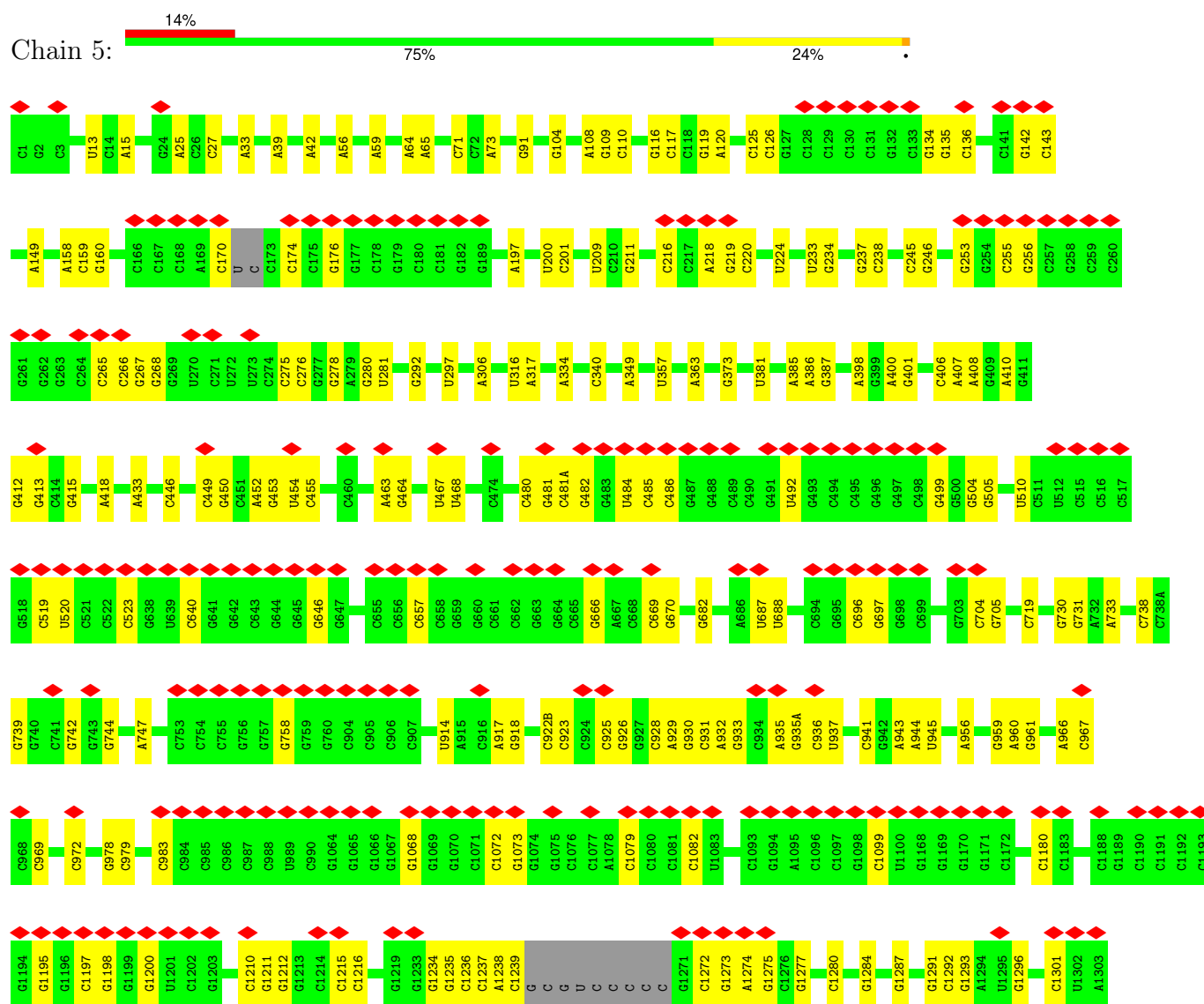


• Molecule 39: eL41

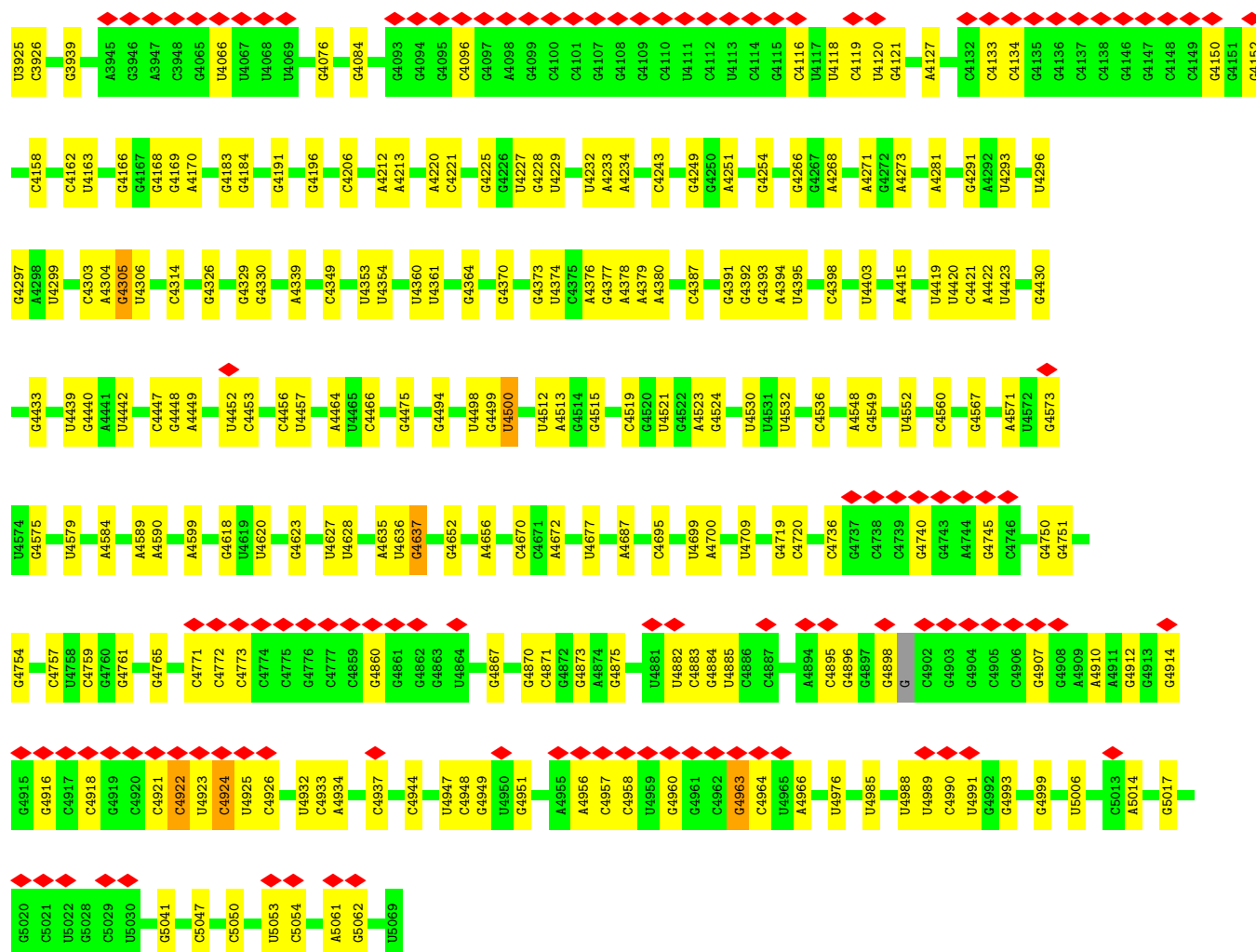
• Molecule 44: uL11



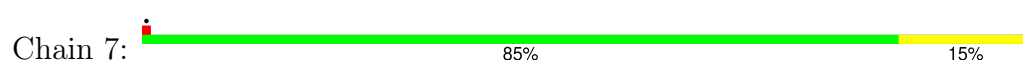
• Molecule 45: 28S rRNA



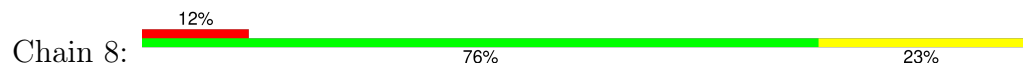




• Molecule 46: 5S rRNA

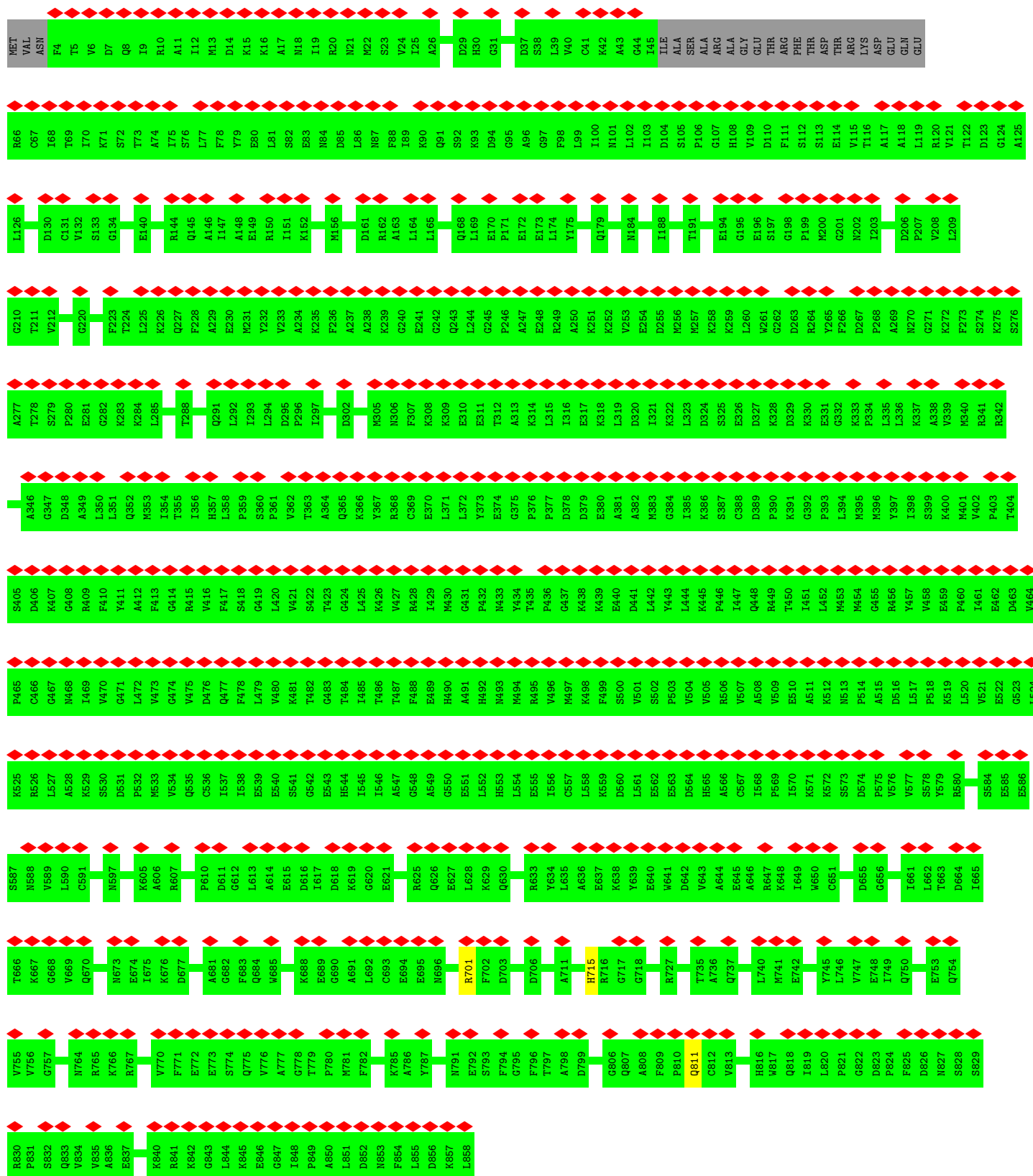


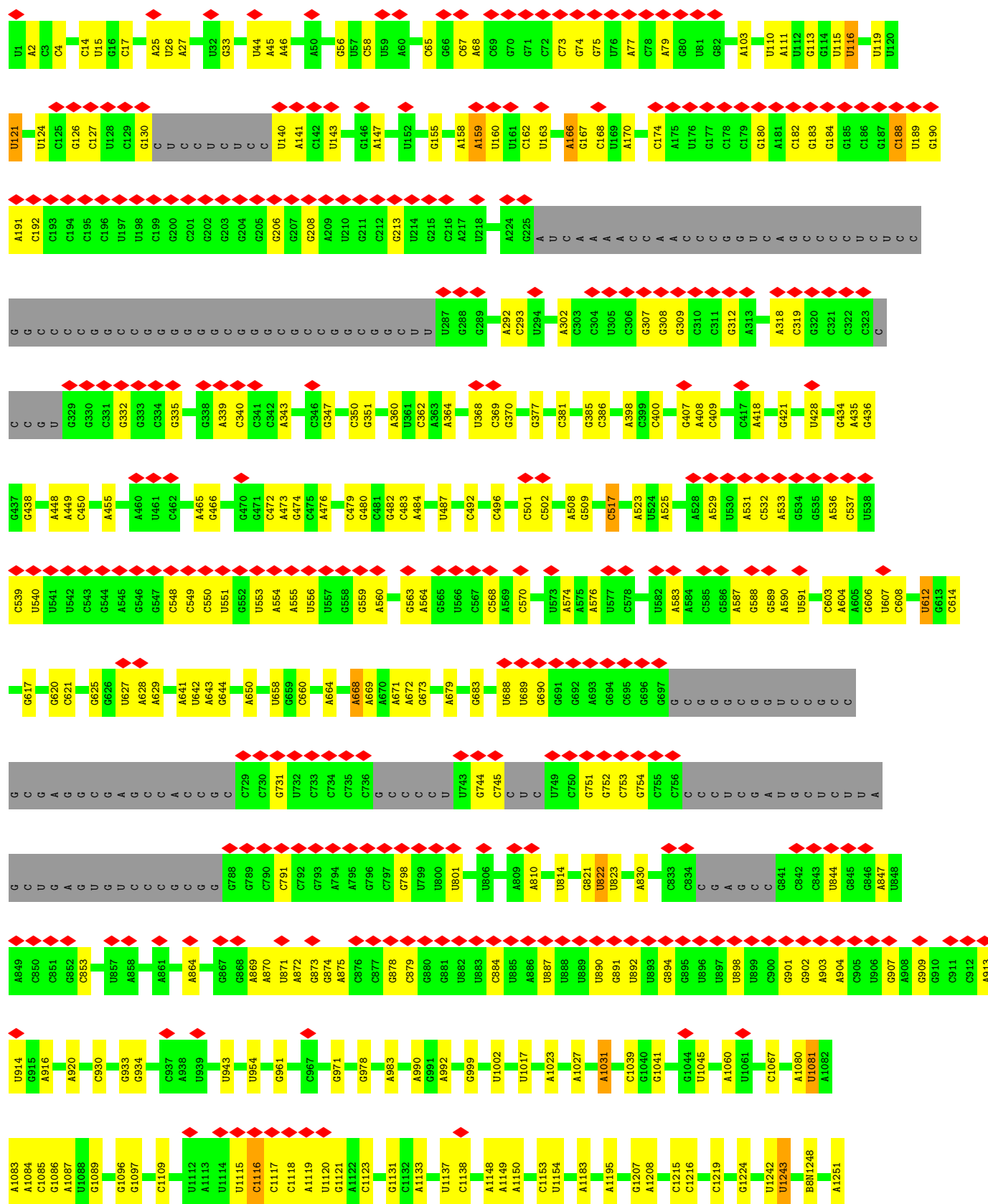
• Molecule 47: 5.8S rRNA

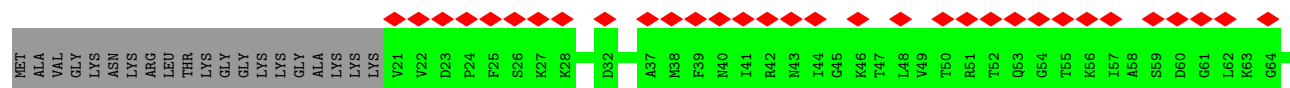


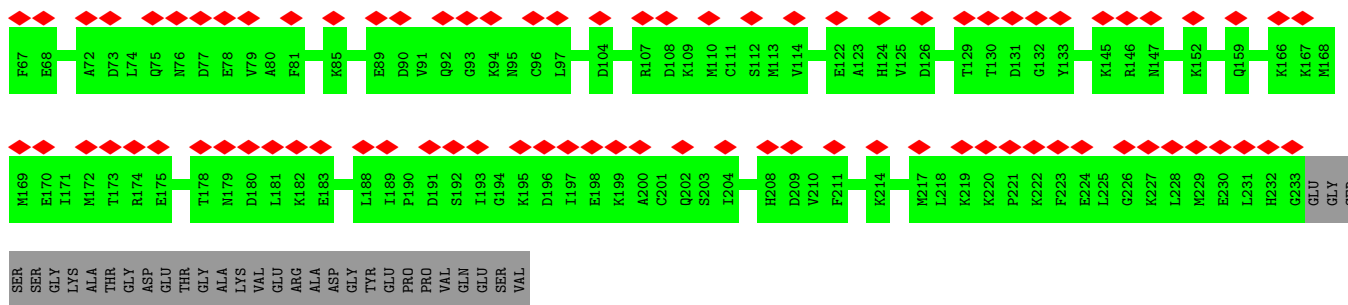
• Molecule 48: eEF2



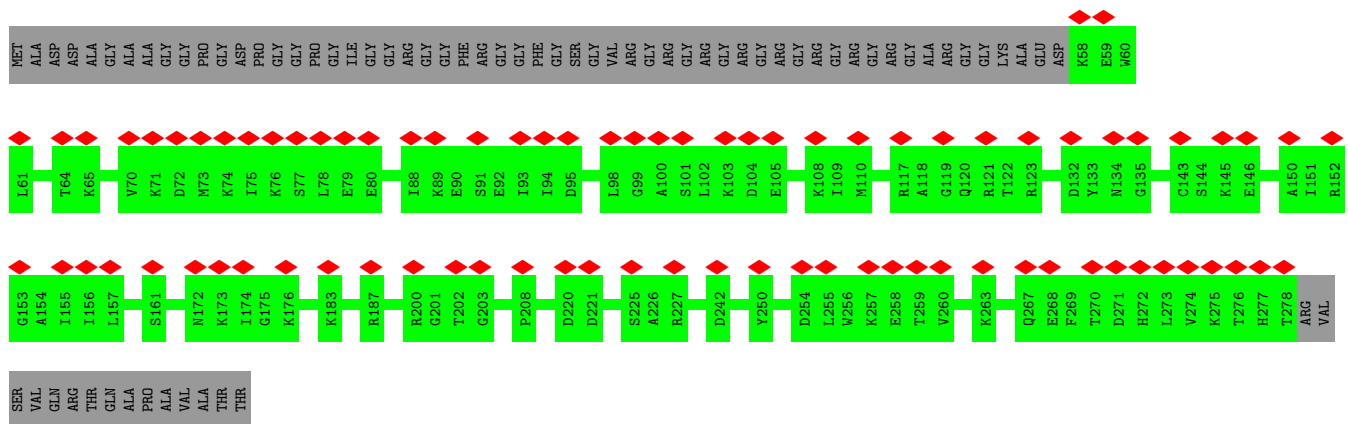
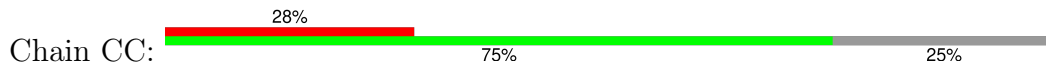




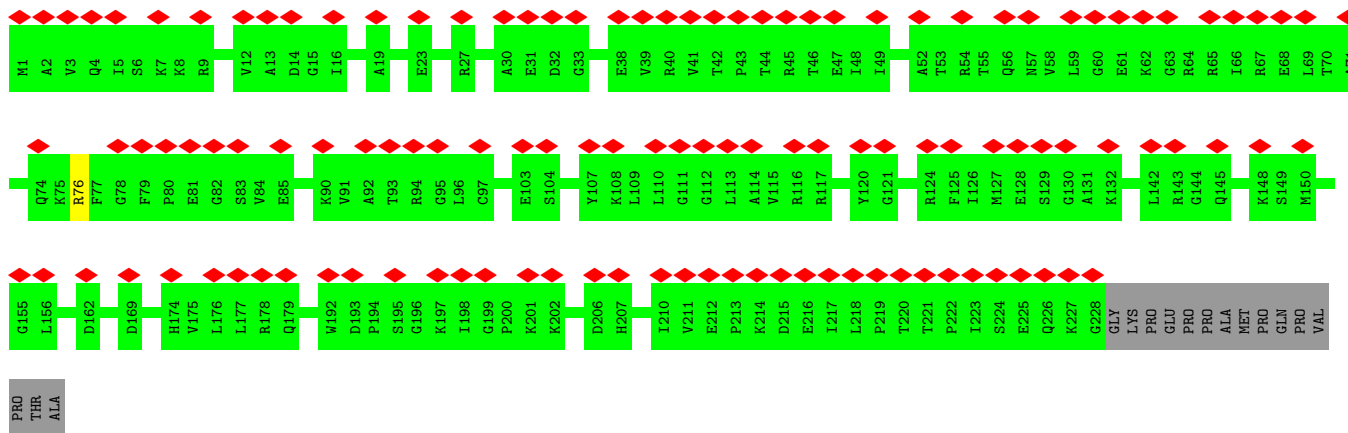




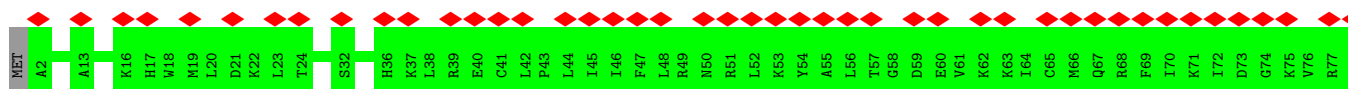
• Molecule 52: uS5

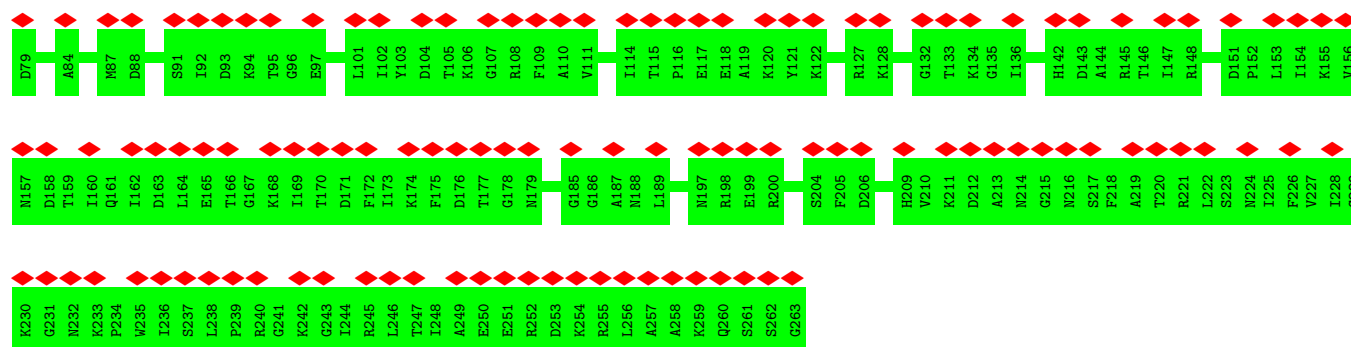


• Molecule 53: uS3

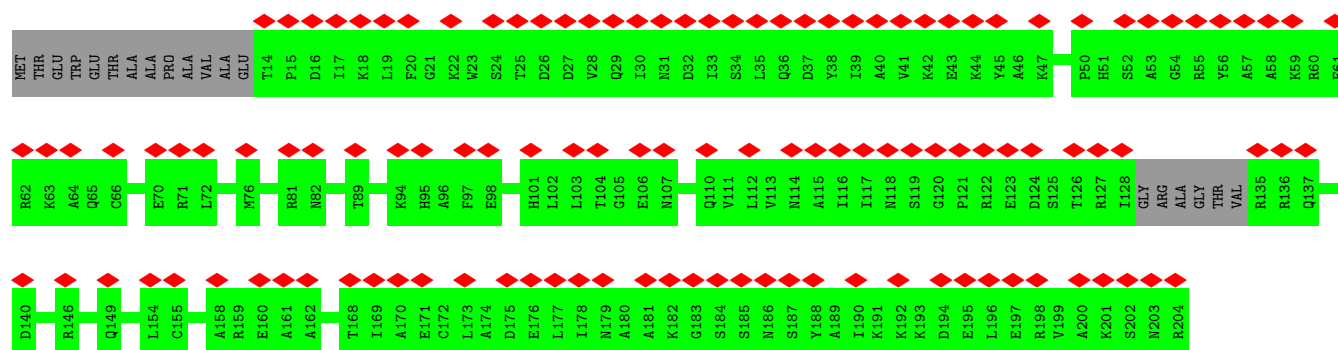
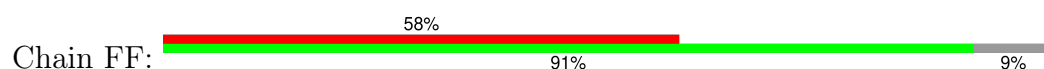


• Molecule 54: eS4

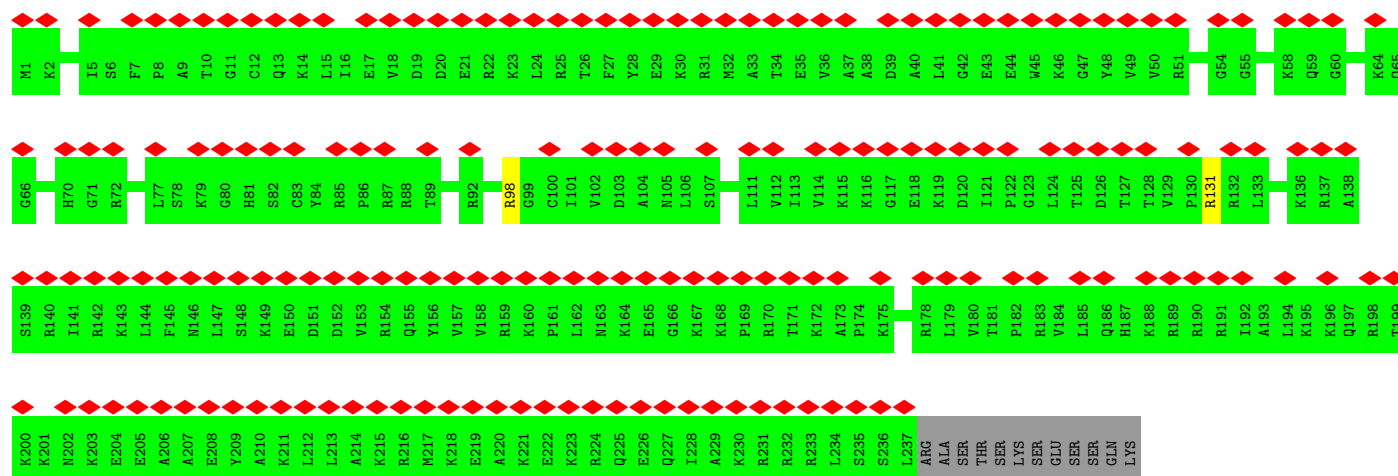
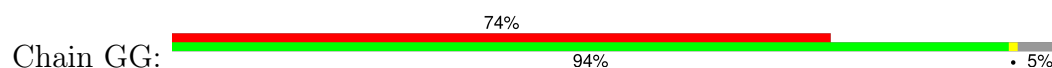




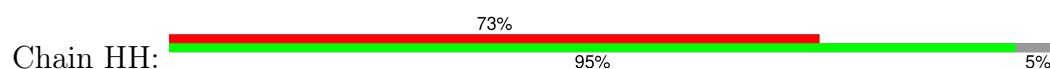
• Molecule 55: uS7

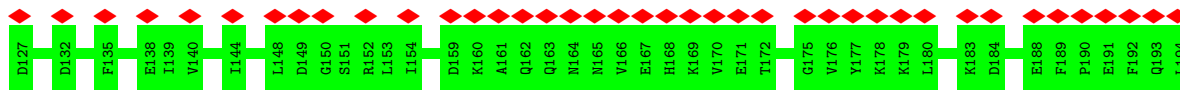


• Molecule 56: eS6

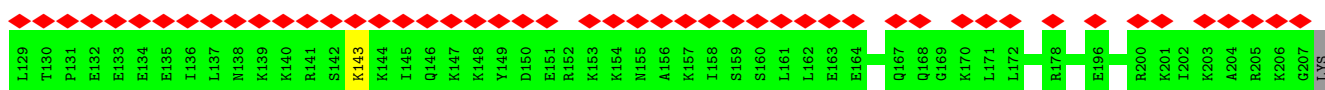
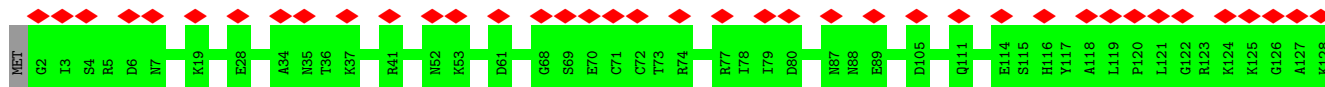
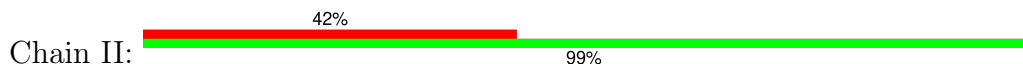


• Molecule 57: eS7

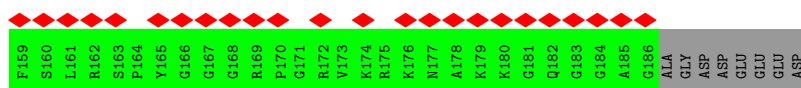
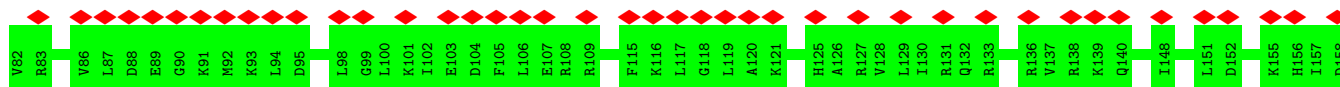
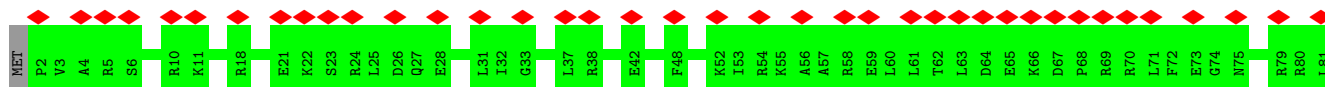




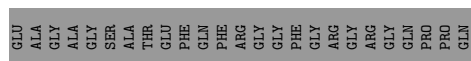
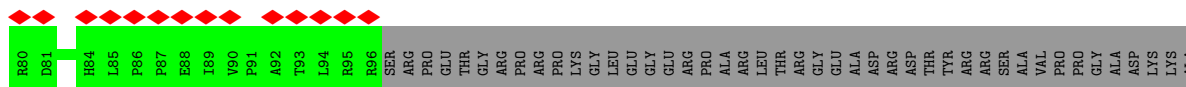
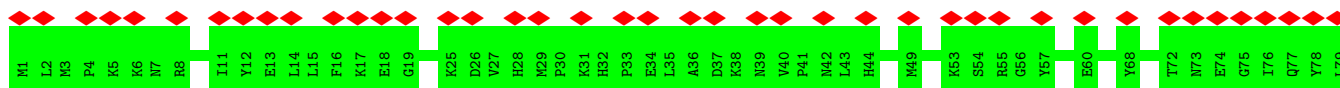
• Molecule 58: eS8



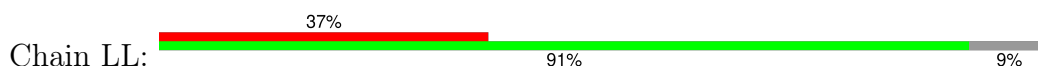
• Molecule 59: uS4

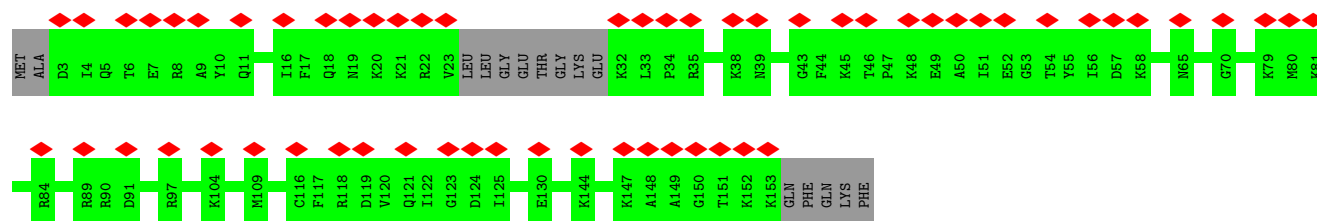


• Molecule 60: eS10

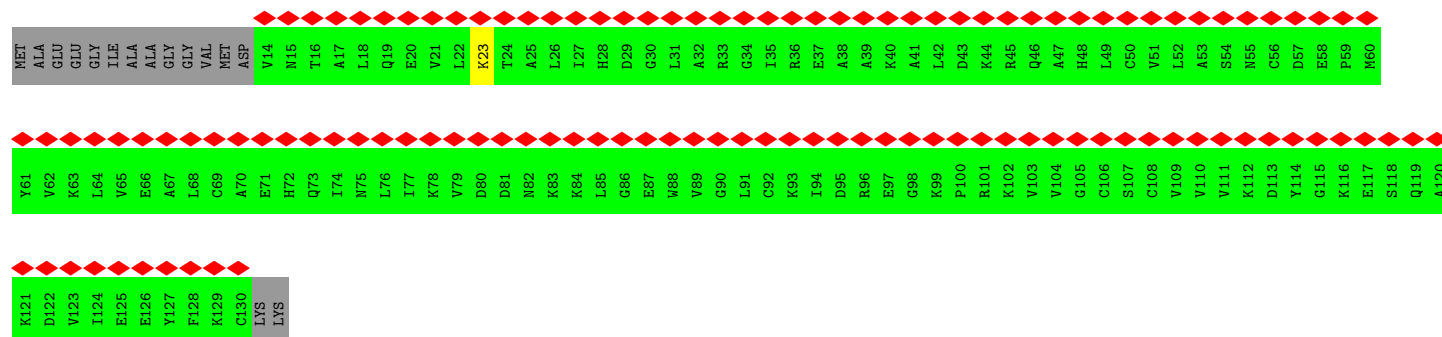
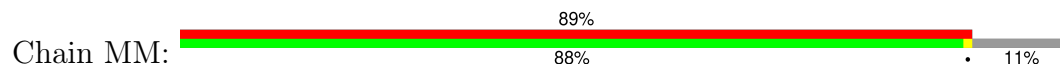


• Molecule 61: uS17

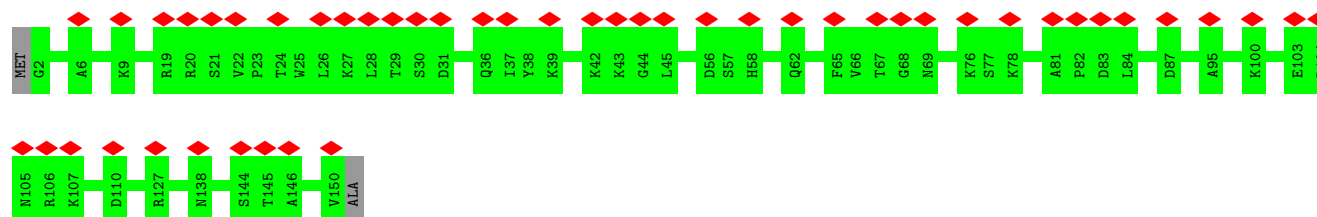




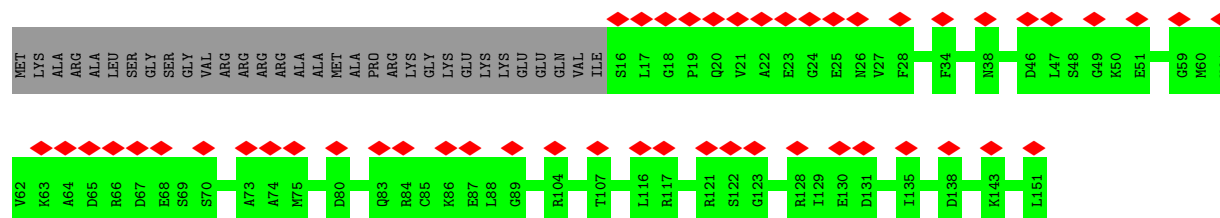
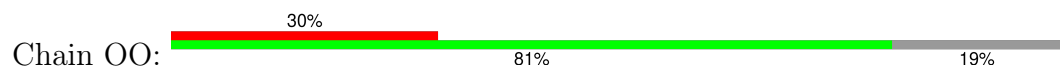
• Molecule 62: eS12



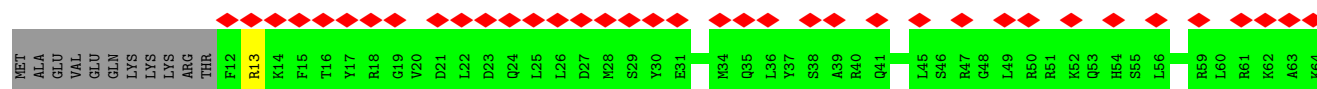
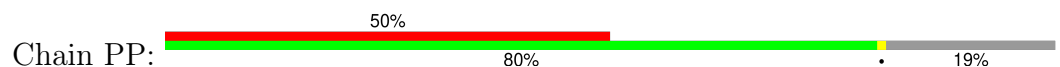
• Molecule 63: uS15

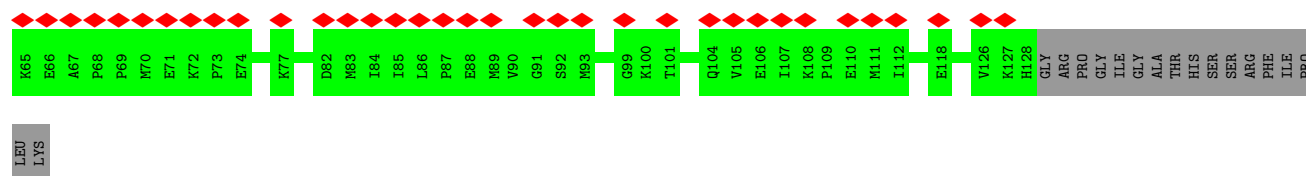


• Molecule 64: uS11



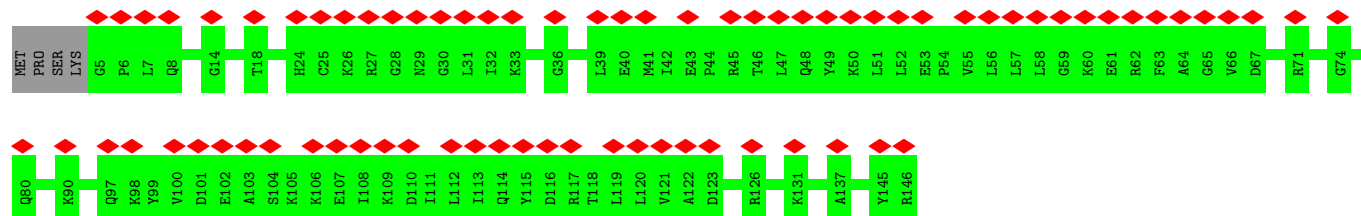
• Molecule 65: uS19





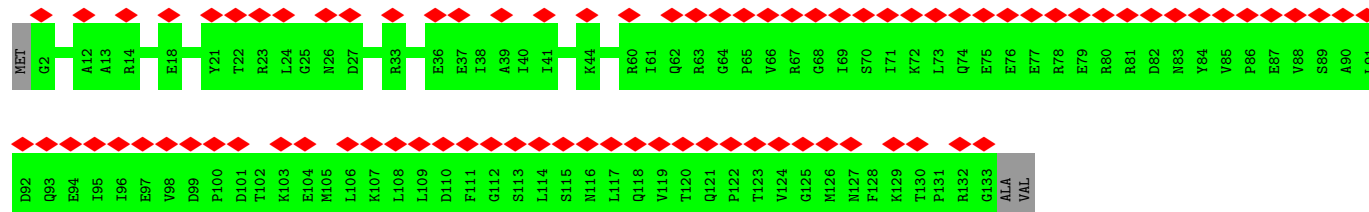
• Molecule 66: uS9

Chain QQ: 51% 97%



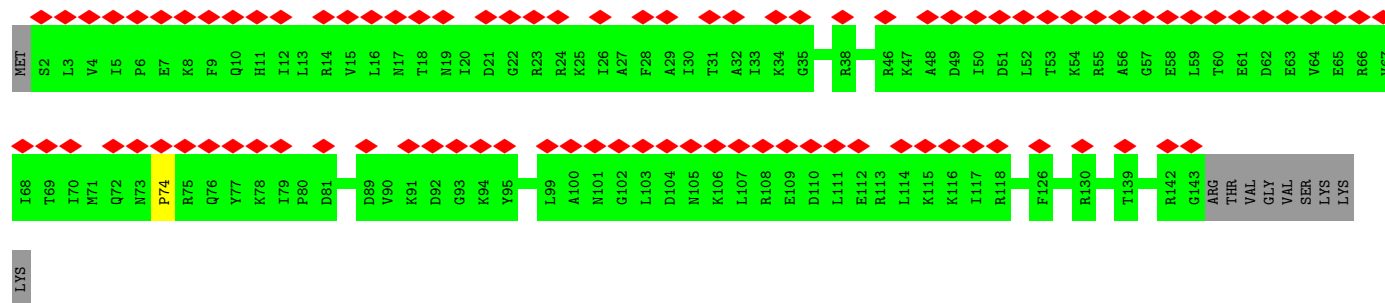
• Molecule 67: eS17

Chain RR: 63% 98%



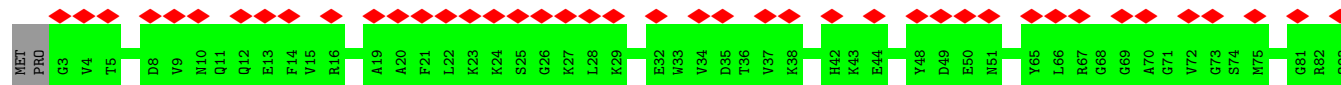
• Molecule 68: uS13

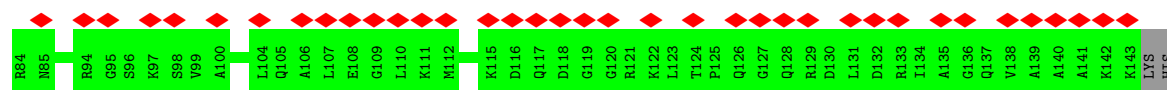
Chain SS: 61% 93% 7%



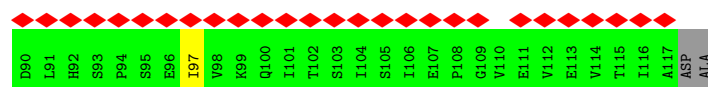
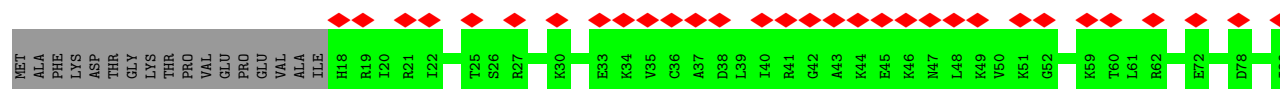
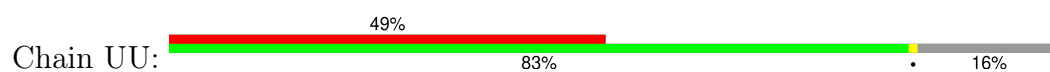
• Molecule 69: eS19

Chain TT: 54% 97%

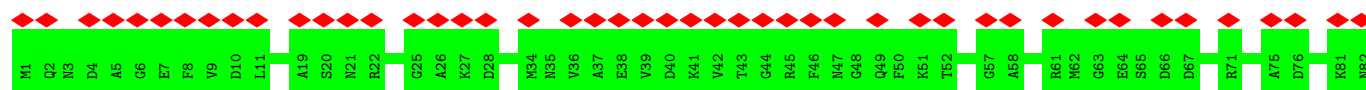




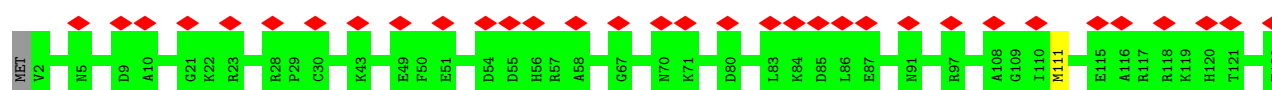
- Molecule 70: uS10



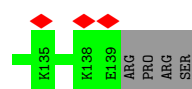
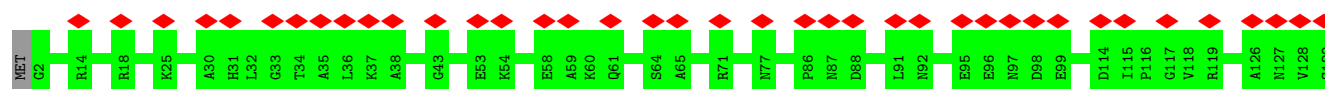
- Molecule 71: eS21



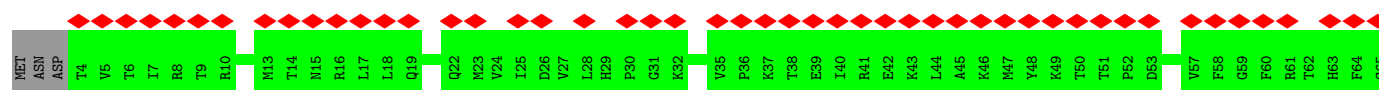
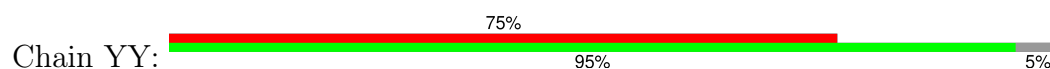
- Molecule 72: uS8

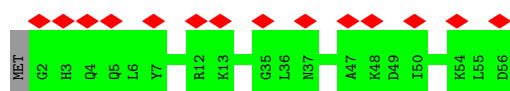


- Molecule 73: uS12

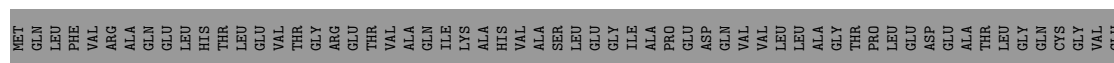


- Molecule 74: eS24

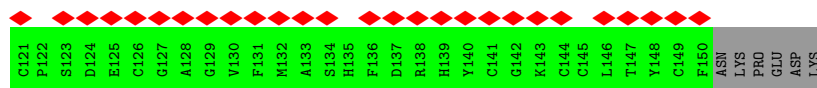
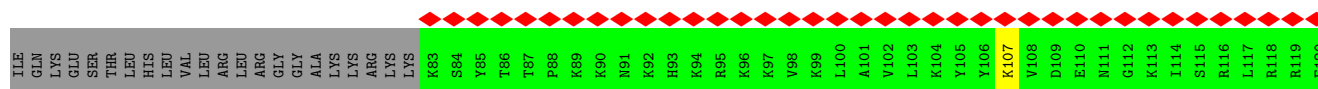
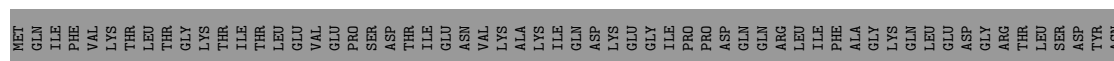
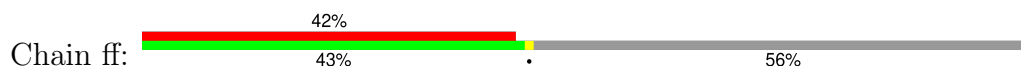




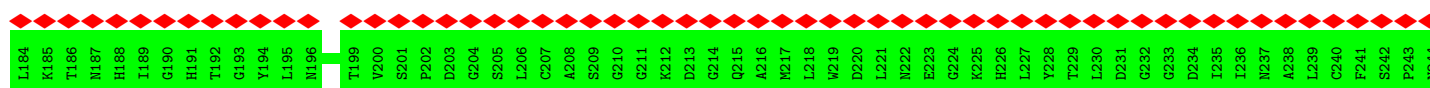
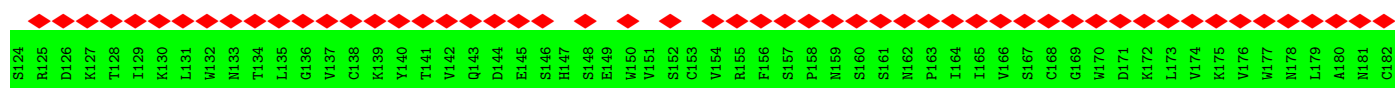
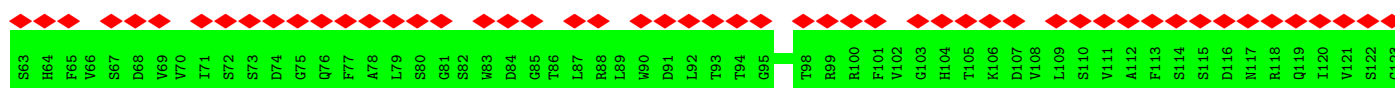
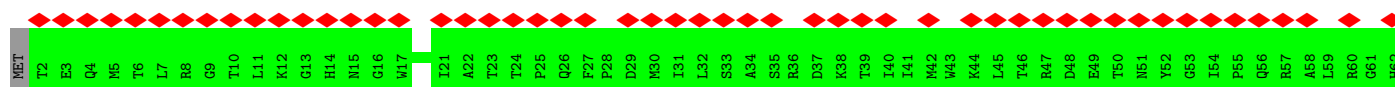
• Molecule 80: eS30



• Molecule 81: eS31

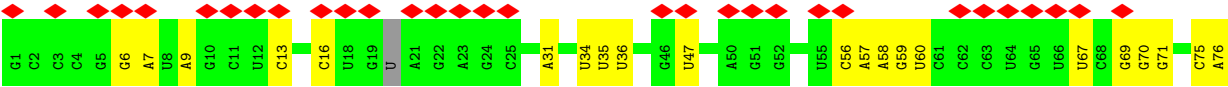


• Molecule 82: RACK1

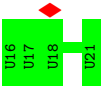




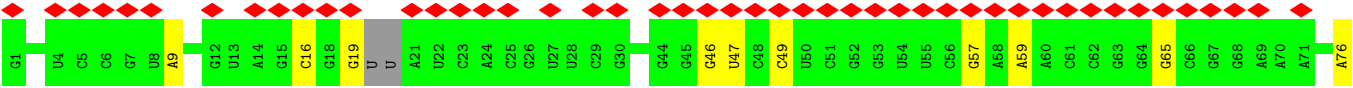
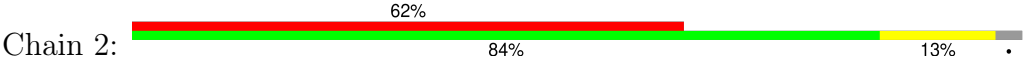
• Molecule 83: E-site tRNA



• Molecule 84: mRNA



• Molecule 85: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42975	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.943	Depositor
Minimum map value	-0.613	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (\AA)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, OMG, 1MA, PSU, DDE, OMU, 4AC, UY1, A2M, 5MU, GDP, B8N, OMC, B9B, 5MC, B8Q, ZN, MG, 2MG, M7A, 34G, UR3, E3C, 6MZ

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	0.44	0/1929	0.61	0/2586
2	B	0.44	0/3216	0.55	0/4311
3	C	0.43	0/2937	0.59	0/3946
4	D	0.40	0/2407	0.54	0/3224
5	E	0.36	0/1760	0.57	0/2362
6	F	0.46	0/1911	0.56	0/2549
7	G	0.37	0/1799	0.58	0/2424
8	H	0.41	0/1535	0.58	0/2063
9	I	0.42	0/1729	0.58	0/2308
10	J	0.37	0/1359	0.57	0/1817
11	L	0.37	0/1733	0.60	0/2316
12	M	0.40	0/1158	0.56	0/1547
13	N	0.48	0/1746	0.61	0/2338
14	O	0.42	0/1653	0.58	0/2210
15	P	0.46	0/1268	0.57	0/1700
16	Q	0.44	0/1539	0.65	0/2054
17	R	0.35	0/1518	0.60	0/2005
18	S	0.46	0/1501	0.59	0/2012
19	T	0.44	0/1326	0.55	0/1770
20	U	0.38	0/814	0.54	0/1092
21	V	0.42	0/987	0.56	0/1324
22	W	0.44	0/541	0.55	0/720
23	X	0.39	0/966	0.54	0/1301
24	Y	0.41	0/1132	0.60	0/1504
25	Z	0.40	0/1130	0.54	0/1507
26	a	0.47	0/1191	0.59	0/1590
27	b	0.35	0/619	0.54	0/818
28	c	0.44	0/742	0.51	0/995
29	d	0.40	0/846	0.59	0/1136
30	e	0.45	0/1071	0.59	0/1429
31	f	0.50	0/895	0.61	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.41	0/916	0.60	0/1220
33	h	0.36	0/1021	0.57	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.48	0/720	0.66	0/952
36	k	0.38	0/565	0.56	0/750
37	l	0.40	0/450	0.60	0/597
38	m	0.39	0/427	0.65	0/564
39	n	0.35	0/223	0.78	0/284
40	o	0.41	0/855	0.56	0/1128
41	p	0.44	0/718	0.58	0/953
42	r	0.42	0/1017	0.58	0/1364
43	s	0.27	0/1530	0.53	0/2064
44	t	0.26	0/1174	0.56	0/1582
45	5	0.78	0/82306	0.86	22/128361 (0.0%)
46	7	0.76	0/2858	0.79	0/4455
47	8	0.77	1/3675 (0.0%)	0.82	1/5725 (0.0%)
48	v	0.31	0/6623	0.54	0/8943
49	9	0.57	0/39726	0.83	11/61882 (0.0%)
50	AA	0.33	0/1747	0.53	0/2374
51	BB	0.32	0/1756	0.53	0/2350
52	CC	0.35	0/1753	0.54	0/2369
53	DD	0.33	0/1796	0.55	0/2417
54	EE	0.32	0/2118	0.57	0/2849
55	FF	0.30	0/1492	0.54	0/2005
56	GG	0.29	0/1946	0.59	0/2590
57	HH	0.30	0/1510	0.56	0/2022
58	II	0.34	0/1715	0.59	0/2287
59	JJ	0.31	0/1550	0.59	0/2069
60	KK	0.34	0/834	0.52	0/1125
61	LL	0.36	0/1195	0.57	0/1597
62	MM	0.27	0/918	0.52	0/1233
63	NN	0.31	0/1226	0.54	0/1649
64	OO	0.35	0/1029	0.62	0/1380
65	PP	0.33	0/994	0.55	0/1327
66	QQ	0.37	0/1146	0.58	0/1534
67	RR	0.31	0/1082	0.57	0/1452
68	SS	0.30	0/1190	0.60	0/1594
69	TT	0.31	0/1115	0.57	0/1493
70	UU	0.29	0/805	0.60	0/1081
71	VV	0.34	0/643	0.56	0/860
72	WW	0.35	0/1051	0.59	0/1406
73	XX	0.34	0/1086	0.56	0/1450
74	YY	0.31	0/1028	0.58	0/1366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	ZZ	0.30	0/604	0.53	0/810
76	aa	0.36	0/828	0.61	0/1109
77	bb	0.33	0/665	0.54	0/891
78	cc	0.28	0/490	0.65	0/656
79	dd	0.36	0/470	0.60	0/623
80	ee	0.27	0/289	0.74	0/374
81	ff	0.28	0/566	0.58	0/750
82	gg	0.29	0/2493	0.55	0/3394
83	3	0.47	0/1754	0.79	0/2725
84	w	0.45	0/131	0.73	0/200
85	2	0.43	0/1761	0.77	0/2739
All	All	0.59	1/233379 (0.0%)	0.75	34/341590 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
48	v	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	62	A	N9-C4	-5.65	1.34	1.37

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	1978	C	N3-C2-O2	-8.78	115.76	121.90
45	5	4924	C	N3-C2-O2	-8.60	115.88	121.90
45	5	2014	C	N1-C2-O2	-7.50	114.40	118.90
45	5	4305	G	N3-C2-N2	-7.43	114.70	119.90
45	5	1977	C	N1-C2-O2	6.85	123.01	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	v	701	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/257 (95%)	213 (87%)	32 (13%)	0	100	100
2	B	392/403 (97%)	356 (91%)	36 (9%)	0	100	100
3	C	360/425 (85%)	336 (93%)	24 (7%)	0	100	100
4	D	287/297 (97%)	274 (96%)	13 (4%)	0	100	100
5	E	209/291 (72%)	194 (93%)	15 (7%)	0	100	100
6	F	223/247 (90%)	207 (93%)	16 (7%)	0	100	100
7	G	214/319 (67%)	197 (92%)	17 (8%)	0	100	100
8	H	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
9	I	204/214 (95%)	189 (93%)	15 (7%)	0	100	100
10	J	165/178 (93%)	157 (95%)	8 (5%)	0	100	100
11	L	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
12	M	136/218 (62%)	128 (94%)	8 (6%)	0	100	100
13	N	201/204 (98%)	182 (90%)	19 (10%)	0	100	100
14	O	196/203 (97%)	187 (95%)	9 (5%)	0	100	100
15	P	151/184 (82%)	144 (95%)	7 (5%)	0	100	100
16	Q	185/188 (98%)	171 (92%)	14 (8%)	0	100	100
17	R	177/196 (90%)	168 (95%)	9 (5%)	0	100	100
18	S	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
19	T	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
20	U	96/128 (75%)	86 (90%)	10 (10%)	0	100	100
21	V	128/140 (91%)	118 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	61/157 (39%)	57 (93%)	4 (7%)	0	100	100
23	X	114/156 (73%)	106 (93%)	8 (7%)	0	100	100
24	Y	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
25	Z	133/136 (98%)	119 (90%)	14 (10%)	0	100	100
26	a	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
27	b	73/245 (30%)	66 (90%)	7 (10%)	0	100	100
28	c	92/115 (80%)	83 (90%)	9 (10%)	0	100	100
29	d	96/125 (77%)	93 (97%)	3 (3%)	0	100	100
30	e	126/135 (93%)	113 (90%)	13 (10%)	0	100	100
31	f	107/110 (97%)	97 (91%)	10 (9%)	0	100	100
32	g	112/117 (96%)	108 (96%)	4 (4%)	0	100	100
33	h	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
34	i	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
35	j	84/97 (87%)	77 (92%)	7 (8%)	0	100	100
36	k	66/70 (94%)	63 (96%)	3 (4%)	0	100	100
37	l	47/51 (92%)	42 (89%)	5 (11%)	0	100	100
38	m	49/93 (53%)	46 (94%)	3 (6%)	0	100	100
39	n	21/25 (84%)	21 (100%)	0	0	100	100
40	o	101/106 (95%)	92 (91%)	9 (9%)	0	100	100
41	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
42	r	123/137 (90%)	110 (89%)	13 (11%)	0	100	100
43	s	194/318 (61%)	170 (88%)	24 (12%)	0	100	100
44	t	151/165 (92%)	120 (80%)	31 (20%)	0	100	100
48	v	830/858 (97%)	724 (87%)	106 (13%)	0	100	100
50	AA	215/295 (73%)	190 (88%)	25 (12%)	0	100	100
51	BB	211/264 (80%)	194 (92%)	17 (8%)	0	100	100
52	CC	219/293 (75%)	200 (91%)	19 (9%)	0	100	100
53	DD	226/243 (93%)	212 (94%)	14 (6%)	0	100	100
54	EE	260/263 (99%)	233 (90%)	27 (10%)	0	100	100
55	FF	181/204 (89%)	171 (94%)	10 (6%)	0	100	100
56	GG	235/249 (94%)	221 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	HH	181/194 (93%)	166 (92%)	15 (8%)	0	100	100
58	II	204/208 (98%)	178 (87%)	26 (13%)	0	100	100
59	JJ	183/194 (94%)	170 (93%)	13 (7%)	0	100	100
60	KK	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
61	LL	139/158 (88%)	121 (87%)	18 (13%)	0	100	100
62	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
63	NN	147/151 (97%)	134 (91%)	13 (9%)	0	100	100
64	OO	134/168 (80%)	108 (81%)	26 (19%)	0	100	100
65	PP	115/145 (79%)	103 (90%)	12 (10%)	0	100	100
66	QQ	140/146 (96%)	125 (89%)	15 (11%)	0	100	100
67	RR	130/135 (96%)	119 (92%)	11 (8%)	0	100	100
68	SS	140/152 (92%)	126 (90%)	13 (9%)	1 (1%)	19	50
69	TT	139/145 (96%)	130 (94%)	9 (6%)	0	100	100
70	UU	98/119 (82%)	88 (90%)	9 (9%)	1 (1%)	13	42
71	VV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
72	WW	127/130 (98%)	112 (88%)	15 (12%)	0	100	100
73	XX	136/143 (95%)	125 (92%)	11 (8%)	0	100	100
74	YY	122/130 (94%)	112 (92%)	10 (8%)	0	100	100
75	ZZ	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
76	aa	99/115 (86%)	88 (89%)	11 (11%)	0	100	100
77	bb	81/84 (96%)	69 (85%)	12 (15%)	0	100	100
78	cc	60/69 (87%)	54 (90%)	6 (10%)	0	100	100
79	dd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
80	ee	32/133 (24%)	22 (69%)	7 (22%)	3 (9%)	0	3
81	ff	65/156 (42%)	56 (86%)	9 (14%)	0	100	100
82	gg	311/317 (98%)	269 (86%)	42 (14%)	0	100	100
All	All	12208/14224 (86%)	11108 (91%)	1095 (9%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
80	ee	96	GLU
80	ee	98	LYS

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Mol	Chain	Res	Type
70	UU	97	ILE
80	ee	97	LYS
68	SS	74	PRO

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	189/199 (95%)	189 (100%)	0	100	100
2	B	336/348 (97%)	335 (100%)	1 (0%)	91	94
3	C	302/347 (87%)	302 (100%)	0	100	100
4	D	245/250 (98%)	243 (99%)	2 (1%)	79	87
5	E	191/251 (76%)	190 (100%)	1 (0%)	86	91
6	F	196/215 (91%)	196 (100%)	0	100	100
7	G	189/272 (70%)	189 (100%)	0	100	100
8	H	169/171 (99%)	169 (100%)	0	100	100
9	I	178/181 (98%)	178 (100%)	0	100	100
10	J	140/149 (94%)	140 (100%)	0	100	100
11	L	175/176 (99%)	175 (100%)	0	100	100
12	M	117/161 (73%)	117 (100%)	0	100	100
13	N	171/172 (99%)	171 (100%)	0	100	100
14	O	170/173 (98%)	170 (100%)	0	100	100
15	P	134/163 (82%)	132 (98%)	2 (2%)	60	77
16	Q	164/165 (99%)	164 (100%)	0	100	100
17	R	158/175 (90%)	158 (100%)	0	100	100
18	S	157/157 (100%)	157 (100%)	0	100	100
19	T	139/140 (99%)	139 (100%)	0	100	100
20	U	88/114 (77%)	88 (100%)	0	100	100
21	V	100/107 (94%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W	55/126 (44%)	55 (100%)	0	100	100
23	X	104/134 (78%)	104 (100%)	0	100	100
24	Y	124/135 (92%)	122 (98%)	2 (2%)	58	76
25	Z	117/118 (99%)	117 (100%)	0	100	100
26	a	119/120 (99%)	119 (100%)	0	100	100
27	b	62/184 (34%)	62 (100%)	0	100	100
28	c	80/98 (82%)	79 (99%)	1 (1%)	65	79
29	d	91/110 (83%)	90 (99%)	1 (1%)	70	82
30	e	114/121 (94%)	114 (100%)	0	100	100
31	f	88/89 (99%)	88 (100%)	0	100	100
32	g	98/100 (98%)	97 (99%)	1 (1%)	73	84
33	h	109/110 (99%)	109 (100%)	0	100	100
34	i	86/89 (97%)	86 (100%)	0	100	100
35	j	73/80 (91%)	73 (100%)	0	100	100
36	k	63/65 (97%)	63 (100%)	0	100	100
37	l	46/48 (96%)	46 (100%)	0	100	100
38	m	47/84 (56%)	47 (100%)	0	100	100
39	n	22/24 (92%)	22 (100%)	0	100	100
40	o	91/94 (97%)	91 (100%)	0	100	100
41	p	74/75 (99%)	74 (100%)	0	100	100
42	r	109/121 (90%)	108 (99%)	1 (1%)	75	85
43	s	164/258 (64%)	164 (100%)	0	100	100
44	t	126/137 (92%)	124 (98%)	2 (2%)	58	76
48	v	710/729 (97%)	709 (100%)	1 (0%)	92	96
50	AA	180/245 (74%)	180 (100%)	0	100	100
51	BB	194/231 (84%)	194 (100%)	0	100	100
52	CC	187/225 (83%)	187 (100%)	0	100	100
53	DD	190/202 (94%)	189 (100%)	1 (0%)	86	91
54	EE	224/225 (100%)	224 (100%)	0	100	100
55	FF	158/170 (93%)	158 (100%)	0	100	100
56	GG	207/218 (95%)	205 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	HH	165/174 (95%)	165 (100%)	0	100	100
58	II	178/180 (99%)	177 (99%)	1 (1%)	84	90
59	JJ	161/168 (96%)	161 (100%)	0	100	100
60	KK	87/136 (64%)	87 (100%)	0	100	100
61	LL	130/142 (92%)	130 (100%)	0	100	100
62	MM	99/108 (92%)	98 (99%)	1 (1%)	73	84
63	NN	130/131 (99%)	130 (100%)	0	100	100
64	OO	106/130 (82%)	106 (100%)	0	100	100
65	PP	107/130 (82%)	106 (99%)	1 (1%)	75	85
66	QQ	117/121 (97%)	117 (100%)	0	100	100
67	RR	119/121 (98%)	119 (100%)	0	100	100
68	SS	123/132 (93%)	123 (100%)	0	100	100
69	TT	111/115 (96%)	111 (100%)	0	100	100
70	UU	92/107 (86%)	92 (100%)	0	100	100
71	VV	67/67 (100%)	67 (100%)	0	100	100
72	WW	112/113 (99%)	111 (99%)	1 (1%)	75	85
73	XX	110/115 (96%)	110 (100%)	0	100	100
74	YY	107/112 (96%)	107 (100%)	0	100	100
75	ZZ	66/103 (64%)	63 (96%)	3 (4%)	23	52
76	aa	88/98 (90%)	86 (98%)	2 (2%)	45	68
77	bb	75/76 (99%)	75 (100%)	0	100	100
78	cc	55/62 (89%)	55 (100%)	0	100	100
79	dd	48/49 (98%)	48 (100%)	0	100	100
80	ee	29/106 (27%)	29 (100%)	0	100	100
81	ff	61/140 (44%)	60 (98%)	1 (2%)	58	76
82	gg	272/275 (99%)	272 (100%)	0	100	100
All	All	10635/12062 (88%)	10607 (100%)	28 (0%)	90	94

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	v	811	GLN
81	ff	107	LYS

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Mol	Chain	Res	Type
56	GG	131	ARG
75	ZZ	64	ASN
56	GG	98	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
69	TT	91	HIS
63	NN	62	GLN
43	s	58	ASN
61	LL	106	HIS
38	m	120	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	5	3503/3543 (98%)	744 (21%)	61 (1%)
46	7	119/120 (99%)	17 (14%)	1 (0%)
47	8	155/156 (99%)	35 (22%)	2 (1%)
49	9	1674/1869 (89%)	412 (24%)	24 (1%)
83	3	70/75 (93%)	20 (28%)	1 (1%)
84	w	5/6 (83%)	0	0
85	2	71/76 (93%)	10 (14%)	0
All	All	5597/5845 (95%)	1238 (22%)	89 (1%)

5 of 1238 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	5	13	U
45	5	15	A
45	5	25	A
45	5	33	A
45	5	39	A

5 of 89 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	5	4884	G
49	9	553	U
45	5	4932	U

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Mol	Chain	Res	Type
49	9	140	U
49	9	870	A

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

136 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$
49	OMG	9	644	49	19,26,27	2.46	8 (42%)	21,38,41	1.41	4 (19%)
49	OMU	9	121	49	19,22,23	2.90	6 (31%)	25,31,34	1.90	6 (24%)
49	OMC	9	1703	49	19,22,23	3.01	8 (42%)	25,31,34	0.74	0
49	PSU	9	119	49	18,21,22	2.04	9 (50%)	21,30,33	1.93	4 (19%)
45	PSU	5	4353	45	17,20,22	2.16	9 (52%)	21,28,33	1.95	5 (23%)
45	5MC	5	4447	45	19,22,23	3.56	8 (42%)	26,32,35	1.25	3 (11%)
45	PSU	5	4552	45	17,20,22	2.31	8 (47%)	21,28,33	2.00	4 (19%)
45	A2M	5	4571	45	18,25,26	4.39	7 (38%)	20,36,39	3.27	5 (25%)
45	A2M	5	3830	45	18,25,26	4.28	6 (33%)	20,36,39	3.39	5 (25%)
49	A2M	9	27	49	18,25,26	4.41	7 (38%)	20,36,39	3.31	5 (25%)
45	PSU	5	1677	45	17,20,22	2.16	9 (52%)	21,28,33	1.90	4 (19%)
45	OMC	5	3701	86,45	19,22,23	2.92	8 (42%)	25,31,34	0.93	0
45	PSU	5	4457	45	17,20,22	2.20	9 (52%)	21,28,33	2.02	4 (19%)
45	OMG	5	4623	45	19,26,27	2.34	8 (42%)	21,38,41	1.39	3 (14%)
49	A2M	9	1678	49	18,25,26	4.47	7 (38%)	20,36,39	3.88	4 (20%)
47	OMG	8	75	47	19,26,27	2.42	8 (42%)	21,38,41	1.30	3 (14%)
49	PSU	9	1243	49	18,21,22	2.10	8 (44%)	21,30,33	2.01	4 (19%)
45	PSU	5	4296	45	17,20,22	2.14	8 (47%)	21,28,33	2.06	4 (19%)
45	PSU	5	3695	45	17,20,22	2.23	9 (52%)	21,28,33	1.86	3 (14%)
45	OMG	5	4618	45	19,26,27	2.41	8 (42%)	21,38,41	1.43	4 (19%)
45	A2M	5	1326	45	18,25,26	4.34	6 (33%)	20,36,39	3.51	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	UR3	9	1830	49	19,22,23	2.65	8 (42%)	26,32,35	1.56	4 (15%)
45	OMC	5	2351	45	19,22,23	2.82	8 (42%)	25,31,34	0.82	0
45	OMG	5	3627	45	19,26,27	2.39	8 (42%)	21,38,41	1.45	3 (14%)
49	A2M	9	668	86,49	18,25,26	4.21	6 (33%)	20,36,39	3.65	6 (30%)
45	PSU	5	1792	45	17,20,22	2.22	10 (58%)	21,28,33	1.95	4 (19%)
45	PSU	5	3920	45	17,20,22	2.25	8 (47%)	21,28,33	1.89	5 (23%)
45	A2M	5	3718	45	18,25,26	4.40	6 (33%)	20,36,39	3.36	4 (20%)
45	A2M	5	1524	45	18,25,26	4.34	6 (33%)	20,36,39	4.10	5 (25%)
45	PSU	5	4532	45	17,20,22	2.22	8 (47%)	21,28,33	1.95	4 (19%)
45	PSU	5	3639	45	17,20,22	2.27	8 (47%)	21,28,33	1.93	4 (19%)
45	A2M	5	2363	86,45	18,25,26	4.38	6 (33%)	20,36,39	3.50	4 (20%)
45	OMG	5	2424	45	19,26,27	2.45	8 (42%)	21,38,41	1.44	4 (19%)
45	A2M	5	1871	86,45	18,25,26	4.46	6 (33%)	20,36,39	3.39	4 (20%)
45	A2M	5	2815	45	18,25,26	4.36	6 (33%)	20,36,39	3.41	4 (20%)
49	A2M	9	484	49	18,25,26	4.39	7 (38%)	20,36,39	3.43	3 (15%)
49	MA6	9	1851	49	19,26,27	1.72	3 (15%)	18,38,41	4.76	4 (22%)
45	PSU	5	4628	45	17,20,22	2.26	9 (52%)	21,28,33	2.00	4 (19%)
49	5MU	9	814	49	19,22,23	1.42	6 (31%)	27,32,35	2.30	8 (29%)
45	A2M	5	3724	45	18,25,26	4.45	7 (38%)	20,36,39	3.30	4 (20%)
45	PSU	5	3764	45	17,20,22	2.15	9 (52%)	21,28,33	1.80	4 (19%)
45	5MC	5	3782	86,45	19,22,23	3.61	8 (42%)	26,32,35	1.08	2 (7%)
45	OMG	5	4494	45	19,26,27	2.41	8 (42%)	21,38,41	1.35	4 (19%)
49	OMC	9	174	49	19,22,23	3.05	8 (42%)	25,31,34	0.84	0
45	OMU	5	3925	45	19,22,23	2.68	6 (31%)	25,31,34	1.90	5 (20%)
45	PSU	5	3715	45	17,20,22	2.15	9 (52%)	21,28,33	1.92	4 (19%)
45	OMG	5	3792	45	19,26,27	2.44	8 (42%)	21,38,41	1.35	4 (19%)
45	PSU	5	4500	45	17,20,22	2.10	8 (47%)	21,28,33	1.90	4 (19%)
49	A2M	9	1031	49	18,25,26	4.38	7 (38%)	20,36,39	3.40	4 (20%)
45	PSU	5	2508	45	17,20,22	2.15	9 (52%)	21,28,33	1.93	4 (19%)
45	PSU	5	4361	45	17,20,22	2.25	8 (47%)	21,28,33	1.96	5 (23%)
45	A2M	5	4523	86,45	18,25,26	4.33	6 (33%)	20,36,39	3.32	4 (20%)
45	PSU	5	1860	45	17,20,22	2.09	9 (52%)	21,28,33	1.84	4 (19%)
45	OMC	5	3841	45	19,22,23	2.75	8 (42%)	25,31,34	0.92	1 (4%)
49	OMU	9	116	49	19,22,23	2.80	6 (31%)	25,31,34	1.74	6 (24%)
45	PSU	5	1862	45	17,20,22	2.23	9 (52%)	21,28,33	2.03	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	5	2837	45	19,22,23	2.81	6 (31%)	25,31,34	1.93	5 (20%)
45	PSU	5	4423	45	17,20,22	2.10	9 (52%)	21,28,33	1.90	4 (19%)
45	A2M	5	1534	86,45	18,25,26	4.24	7 (38%)	20,36,39	3.55	5 (25%)
45	OMG	5	1522	45	19,26,27	2.31	8 (42%)	21,38,41	1.37	3 (14%)
45	OMG	5	3899	45	19,26,27	2.38	8 (42%)	21,38,41	1.45	4 (19%)
45	OMC	5	2861	45	19,22,23	2.96	8 (42%)	25,31,34	0.78	0
49	A2M	9	166	49	18,25,26	4.41	6 (33%)	20,36,39	3.16	4 (20%)
49	PSU	9	612	49	18,21,22	2.12	9 (50%)	21,30,33	1.93	4 (19%)
45	PSU	5	3853	45	17,20,22	2.24	10 (58%)	21,28,33	2.02	3 (14%)
45	OMG	5	2364	45	19,26,27	2.39	8 (42%)	21,38,41	1.44	3 (14%)
49	B8N	9	1248	49	25,29,30	3.41	7 (28%)	28,42,45	2.11	7 (25%)
45	OMG	5	4392	45	19,26,27	2.31	8 (42%)	21,38,41	1.41	4 (19%)
45	PSU	5	4579	45	17,20,22	2.21	8 (47%)	21,28,33	1.85	4 (19%)
45	UY1	5	3818	86,45	19,22,23	4.33	9 (47%)	21,31,34	1.91	5 (23%)
45	PSU	5	4299	45	17,20,22	2.25	9 (52%)	21,28,33	1.98	5 (23%)
45	OMG	5	4499	45	19,26,27	2.50	8 (42%)	21,38,41	1.45	3 (14%)
49	5MC	9	1374	49	19,22,23	3.73	8 (42%)	26,32,35	0.99	2 (7%)
49	OMG	9	509	86,49	19,26,27	2.40	8 (42%)	21,38,41	1.27	3 (14%)
45	OMU	5	4306	45	19,22,23	2.73	6 (31%)	25,31,34	1.82	5 (20%)
49	B8Q	9	1219	86,49	18,22,23	2.76	4 (22%)	21,32,35	1.71	5 (23%)
45	OMG	5	4370	45	19,26,27	2.40	8 (42%)	21,38,41	1.41	3 (14%)
49	M7A	9	1806	49	19,25,26	1.76	4 (21%)	25,37,40	4.20	8 (32%)
49	E3C	9	568	49	19,23,24	3.30	6 (31%)	21,33,36	1.50	4 (19%)
45	OMC	5	3869	45	19,22,23	2.76	7 (36%)	25,31,34	0.95	2 (8%)
49	4AC	9	1842	49	21,24,25	3.29	10 (47%)	28,34,37	1.04	4 (14%)
49	MA6	9	1850	49	19,26,27	1.61	3 (15%)	18,38,41	4.90	4 (22%)
45	OMG	5	1316	45	19,26,27	2.39	8 (42%)	21,38,41	1.41	3 (14%)
45	PSU	5	3851	45	17,20,22	2.18	9 (52%)	21,28,33	1.95	5 (23%)
45	PSU	5	1781	45	17,20,22	2.16	10 (58%)	21,28,33	1.85	5 (23%)
45	1MA	5	1322	86,45	17,25,26	3.60	4 (23%)	17,37,40	1.85	3 (17%)
45	2MG	5	1517	45	18,26,27	2.30	7 (38%)	16,38,41	2.00	5 (31%)
45	OMU	5	4620	45	19,22,23	2.75	6 (31%)	25,31,34	1.98	5 (20%)
49	OMG	9	683	49	19,26,27	2.46	8 (42%)	21,38,41	1.40	3 (14%)
45	OMU	5	4227	45	19,22,23	2.78	6 (31%)	25,31,34	1.77	4 (16%)
45	A2M	5	398	45	18,25,26	4.41	6 (33%)	20,36,39	3.32	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	B9B	5	237	45	20,28,29	1.78	2 (10%)	19,40,43	2.37	5 (26%)
45	A2M	5	3760	45,49	18,25,26	4.39	7 (38%)	20,36,39	3.42	4 (20%)
45	PSU	5	4442	45	17,20,22	2.18	10 (58%)	21,28,33	1.93	4 (19%)
45	OMG	5	373	45	19,26,27	2.39	8 (42%)	21,38,41	1.38	4 (19%)
45	OMC	5	2422	86,45	19,22,23	2.94	8 (42%)	25,31,34	0.85	0
45	OMC	5	2824	45	19,22,23	2.85	8 (42%)	25,31,34	0.94	1 (4%)
45	6MZ	5	4220	45	17,25,26	1.50	2 (11%)	15,36,39	2.20	3 (20%)
45	PSU	5	4521	86,45	17,20,22	2.20	9 (52%)	21,28,33	1.94	4 (19%)
49	A2M	9	159	49	18,25,26	4.42	7 (38%)	20,36,39	3.42	4 (20%)
45	OMG	5	2876	45	19,26,27	2.44	8 (42%)	21,38,41	1.40	4 (19%)
45	PSU	5	1744	45	17,20,22	2.15	8 (47%)	21,28,33	2.07	4 (19%)
48	DDE	v	715	48	15,20,21	1.02	0	11,28,30	1.19	1 (9%)
45	PSU	5	4293	45	17,20,22	2.36	9 (52%)	21,28,33	2.01	4 (19%)
45	OMG	5	4637	45	19,26,27	2.47	8 (42%)	21,38,41	1.46	4 (19%)
45	PSU	5	2632	45	17,20,22	2.17	8 (47%)	21,28,33	1.98	4 (19%)
49	OMC	9	517	49	19,22,23	3.03	8 (42%)	25,31,34	0.84	0
45	PSU	5	1683	45	17,20,22	2.25	9 (52%)	21,28,33	1.98	4 (19%)
45	OMG	5	4196	85,45	19,26,27	2.36	8 (42%)	21,38,41	1.37	3 (14%)
45	OMG	5	4228	45	19,26,27	2.40	7 (36%)	21,38,41	1.41	3 (14%)
45	A2M	5	2787	45	18,25,26	4.27	6 (33%)	20,36,39	3.27	3 (15%)
45	A2M	5	3867	45	18,25,26	4.29	6 (33%)	20,36,39	3.60	5 (25%)
49	4AC	9	1337	49	21,24,25	3.31	10 (47%)	28,34,37	1.02	4 (14%)
49	PSU	9	822	49	18,21,22	2.07	8 (44%)	21,30,33	1.95	4 (19%)
45	PSU	5	3762	45	17,20,22	2.12	8 (47%)	21,28,33	1.98	4 (19%)
45	OMC	5	3887	45	19,22,23	2.89	8 (42%)	25,31,34	0.81	0
49	OMC	9	1710	49	19,22,23	2.99	8 (42%)	25,31,34	0.80	0
45	OMC	5	4456	45	19,22,23	2.89	8 (42%)	25,31,34	0.75	0
45	PSU	5	1782	45	17,20,22	2.13	9 (52%)	21,28,33	1.96	4 (19%)
45	OMC	5	1340	45	19,22,23	2.86	7 (36%)	25,31,34	1.00	1 (4%)
45	OMC	5	3808	45	19,22,23	2.90	8 (42%)	25,31,34	0.76	0
45	PSU	5	4403	45	17,20,22	2.31	10 (58%)	21,28,33	1.89	5 (23%)
45	A2M	5	400	45	18,25,26	4.33	6 (33%)	20,36,39	3.36	4 (20%)
45	OMU	5	4498	45	19,22,23	2.75	6 (31%)	25,31,34	1.88	5 (20%)
49	PSU	9	1081	49	18,21,22	2.19	10 (55%)	21,30,33	1.93	3 (14%)
45	PSU	5	4420	45	17,20,22	2.13	9 (52%)	21,28,33	1.86	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	UR3	5	4530	45	19,22,23	2.67	8 (42%)	26,32,35	1.64	4 (15%)
45	OMG	5	1625	45	19,26,27	2.45	8 (42%)	21,38,41	1.42	4 (19%)
49	6MZ	9	1832	86,49	17,25,26	1.37	2 (11%)	15,36,39	2.20	3 (20%)
45	A2M	5	3825	45	18,25,26	4.39	7 (38%)	20,36,39	3.16	4 (20%)
45	OMC	5	4536	45	19,22,23	2.81	8 (42%)	25,31,34	0.85	1 (4%)
49	PSU	9	823	49	18,21,22	2.09	9 (50%)	21,30,33	1.95	5 (23%)
45	OMC	5	2804	45	19,22,23	2.91	8 (42%)	25,31,34	0.83	0
45	PSU	5	3734	45	17,20,22	2.10	8 (47%)	21,28,33	1.87	4 (19%)
45	OMC	5	2365	45	19,22,23	2.98	8 (42%)	25,31,34	0.84	0
45	A2M	5	3785	45	18,25,26	4.18	6 (33%)	20,36,39	3.82	6 (30%)

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
49	OMG	9	644	49	-	1/5/27/28	0/3/3/3
49	OMU	9	121	49	-	3/9/27/28	0/2/2/2
49	OMC	9	1703	49	-	2/9/27/28	0/2/2/2
49	PSU	9	119	49	-	1/7/25/26	0/2/2/2
45	PSU	5	4353	45	-	0/6/24/26	0/2/2/2
45	5MC	5	4447	45	-	4/7/25/26	0/2/2/2
45	PSU	5	4552	45	-	0/6/24/26	0/2/2/2
45	A2M	5	4571	45	-	0/5/27/28	0/3/3/3
45	A2M	5	3830	45	-	0/5/27/28	0/3/3/3
49	A2M	9	27	49	-	0/5/27/28	0/3/3/3
45	PSU	5	1677	45	-	4/6/24/26	0/2/2/2
45	OMC	5	3701	86,45	-	5/9/27/28	0/2/2/2
45	PSU	5	4457	45	-	0/6/24/26	0/2/2/2
45	OMG	5	4623	45	-	1/5/27/28	0/3/3/3
49	A2M	9	1678	49	-	2/5/27/28	0/3/3/3
47	OMG	8	75	47	-	2/5/27/28	0/3/3/3
49	PSU	9	1243	49	-	2/7/25/26	0/2/2/2
45	PSU	5	4296	45	-	0/6/24/26	0/2/2/2
45	PSU	5	3695	45	-	3/6/24/26	0/2/2/2
45	OMG	5	4618	45	-	1/5/27/28	0/3/3/3
45	A2M	5	1326	45	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	UR3	9	1830	49	-	2/7/25/26	0/2/2/2
45	OMC	5	2351	45	-	1/9/27/28	0/2/2/2
45	OMG	5	3627	45	-	1/5/27/28	0/3/3/3
49	A2M	9	668	86,49	-	0/5/27/28	0/3/3/3
45	PSU	5	1792	45	-	0/6/24/26	0/2/2/2
45	PSU	5	3920	45	-	0/6/24/26	0/2/2/2
45	A2M	5	3718	45	-	0/5/27/28	0/3/3/3
45	A2M	5	1524	45	-	2/5/27/28	0/3/3/3
45	PSU	5	4532	45	-	2/6/24/26	0/2/2/2
45	PSU	5	3639	45	-	0/6/24/26	0/2/2/2
45	A2M	5	2363	86,45	-	2/5/27/28	0/3/3/3
45	OMG	5	2424	45	-	2/5/27/28	0/3/3/3
45	A2M	5	1871	86,45	-	0/5/27/28	0/3/3/3
45	A2M	5	2815	45	-	1/5/27/28	0/3/3/3
49	A2M	9	484	49	-	0/5/27/28	0/3/3/3
49	MA6	9	1851	49	-	4/7/29/30	0/3/3/3
45	PSU	5	4628	45	-	0/6/24/26	0/2/2/2
49	5MU	9	814	49	-	0/7/25/26	0/2/2/2
45	A2M	5	3724	45	-	0/5/27/28	0/3/3/3
45	PSU	5	3764	45	-	0/6/24/26	0/2/2/2
45	5MC	5	3782	86,45	-	0/7/25/26	0/2/2/2
45	OMG	5	4494	45	-	0/5/27/28	0/3/3/3
49	OMC	9	174	49	-	3/9/27/28	0/2/2/2
45	OMU	5	3925	45	-	0/9/27/28	0/2/2/2
45	PSU	5	3715	45	-	0/6/24/26	0/2/2/2
45	OMG	5	3792	45	-	2/5/27/28	0/3/3/3
45	PSU	5	4500	45	-	2/6/24/26	0/2/2/2
49	A2M	9	1031	49	-	2/5/27/28	0/3/3/3
45	PSU	5	2508	45	-	1/6/24/26	0/2/2/2
45	PSU	5	4361	45	-	0/6/24/26	0/2/2/2
45	A2M	5	4523	86,45	-	0/5/27/28	0/3/3/3
45	PSU	5	1860	45	-	0/6/24/26	0/2/2/2
45	OMC	5	3841	45	-	1/9/27/28	0/2/2/2
49	OMU	9	116	49	-	4/9/27/28	0/2/2/2
45	PSU	5	1862	45	-	1/6/24/26	0/2/2/2
45	OMU	5	2837	45	-	0/9/27/28	0/2/2/2
45	PSU	5	4423	45	-	0/6/24/26	0/2/2/2
45	A2M	5	1534	86,45	-	2/5/27/28	0/3/3/3
45	OMG	5	1522	45	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMG	5	3899	45	-	0/5/27/28	0/3/3/3
45	OMC	5	2861	45	-	0/9/27/28	0/2/2/2
49	A2M	9	166	49	-	2/5/27/28	0/3/3/3
49	PSU	9	612	49	-	1/7/25/26	0/2/2/2
45	PSU	5	3853	45	-	0/6/24/26	0/2/2/2
45	OMG	5	2364	45	-	3/5/27/28	0/3/3/3
49	B8N	9	1248	49	-	10/16/34/35	0/2/2/2
45	OMG	5	4392	45	-	1/5/27/28	0/3/3/3
45	PSU	5	4579	45	-	0/6/24/26	0/2/2/2
45	UY1	5	3818	86,45	-	2/9/27/28	0/2/2/2
45	PSU	5	4299	45	-	0/6/24/26	0/2/2/2
45	OMG	5	4499	45	-	0/5/27/28	0/3/3/3
49	5MC	9	1374	49	-	0/7/25/26	0/2/2/2
49	OMG	9	509	86,49	-	0/5/27/28	0/3/3/3
45	OMU	5	4306	45	-	0/9/27/28	0/2/2/2
49	B8Q	9	1219	86,49	-	0/7/42/43	0/2/2/2
45	OMG	5	4370	45	-	2/5/27/28	0/3/3/3
49	M7A	9	1806	49	-	3/7/37/38	0/3/3/3
49	E3C	9	568	49	-	4/9/44/45	0/2/2/2
45	OMC	5	3869	45	-	3/9/27/28	0/2/2/2
49	4AC	9	1842	49	-	0/11/29/30	0/2/2/2
49	MA6	9	1850	49	-	3/7/29/30	0/3/3/3
45	OMG	5	1316	45	-	2/5/27/28	0/3/3/3
45	PSU	5	3851	45	-	0/6/24/26	0/2/2/2
45	PSU	5	1781	45	-	2/6/24/26	0/2/2/2
45	1MA	5	1322	86,45	-	0/3/25/26	0/3/3/3
45	2MG	5	1517	45	-	0/5/27/28	0/3/3/3
45	OMU	5	4620	45	-	2/9/27/28	0/2/2/2
49	OMG	9	683	49	-	0/5/27/28	0/3/3/3
45	OMU	5	4227	45	-	0/9/27/28	0/2/2/2
45	A2M	5	398	45	-	1/5/27/28	0/3/3/3
45	B9B	5	237	45	-	2/7/29/30	0/3/3/3
45	A2M	5	3760	45,49	-	1/5/27/28	0/3/3/3
45	PSU	5	4442	45	-	0/6/24/26	0/2/2/2
45	OMG	5	373	45	-	1/5/27/28	0/3/3/3
45	OMC	5	2422	86,45	-	1/9/27/28	0/2/2/2
45	OMC	5	2824	45	-	1/9/27/28	0/2/2/2
45	6MZ	5	4220	45	-	2/5/27/28	0/3/3/3
45	PSU	5	4521	86,45	-	0/6/24/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A2M	9	159	49	-	3/5/27/28	0/3/3/3
45	OMG	5	2876	45	-	2/5/27/28	0/3/3/3
45	PSU	5	1744	45	-	0/6/24/26	0/2/2/2
48	DDE	v	715	48	-	7/20/21/23	0/1/1/1
45	PSU	5	4293	45	-	0/6/24/26	0/2/2/2
45	OMG	5	4637	45	-	2/5/27/28	0/3/3/3
45	PSU	5	2632	45	-	0/6/24/26	0/2/2/2
49	OMC	9	517	49	-	3/9/27/28	0/2/2/2
45	PSU	5	1683	45	-	0/6/24/26	0/2/2/2
45	OMG	5	4196	85,45	-	0/5/27/28	0/3/3/3
45	OMG	5	4228	45	-	0/5/27/28	0/3/3/3
45	A2M	5	2787	45	-	0/5/27/28	0/3/3/3
45	A2M	5	3867	45	-	0/5/27/28	0/3/3/3
49	4AC	9	1337	49	-	0/11/29/30	0/2/2/2
49	PSU	9	822	49	-	2/7/25/26	0/2/2/2
45	PSU	5	3762	45	-	0/6/24/26	0/2/2/2
45	OMC	5	3887	45	-	1/9/27/28	0/2/2/2
49	OMC	9	1710	49	-	0/9/27/28	0/2/2/2
45	OMC	5	4456	45	-	0/9/27/28	0/2/2/2
45	PSU	5	1782	45	-	0/6/24/26	0/2/2/2
45	OMC	5	1340	45	-	0/9/27/28	0/2/2/2
45	OMC	5	3808	45	-	0/9/27/28	0/2/2/2
45	PSU	5	4403	45	-	0/6/24/26	0/2/2/2
45	A2M	5	400	45	-	0/5/27/28	0/3/3/3
45	OMU	5	4498	45	-	0/9/27/28	0/2/2/2
49	PSU	9	1081	49	-	5/7/25/26	0/2/2/2
45	PSU	5	4420	45	-	2/6/24/26	0/2/2/2
45	UR3	5	4530	45	-	0/7/25/26	0/2/2/2
45	OMG	5	1625	45	-	2/5/27/28	0/3/3/3
49	6MZ	9	1832	86,49	-	0/5/27/28	0/3/3/3
45	A2M	5	3825	45	-	2/5/27/28	0/3/3/3
45	OMC	5	4536	45	-	0/9/27/28	0/2/2/2
49	PSU	9	823	49	-	0/7/25/26	0/2/2/2
45	OMC	5	2804	45	-	2/9/27/28	0/2/2/2
45	PSU	5	3734	45	-	0/6/24/26	0/2/2/2
45	OMC	5	2365	45	-	2/9/27/28	0/2/2/2
45	A2M	5	3785	45	-	2/5/27/28	0/3/3/3

The worst 5 of 1013 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	5	3724	A2M	O4'-C1'	16.25	1.62	1.40
49	9	1678	A2M	O4'-C1'	16.25	1.62	1.40
45	5	3760	A2M	O4'-C1'	16.17	1.62	1.40
49	9	166	A2M	O4'-C1'	16.17	1.62	1.40
49	9	159	A2M	O4'-C1'	16.15	1.62	1.40

The worst 5 of 495 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	9	1850	MA6	N1-C6-N6	-17.26	96.89	116.83
49	9	1851	MA6	N1-C6-N6	-16.65	97.60	116.83
49	9	1806	M7A	C5-C6-N6	13.89	147.35	123.75
45	5	1534	A2M	C5-C6-N6	11.40	137.67	120.31
49	9	1806	M7A	N6-C6-N1	-11.38	93.02	118.38

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	v	715	DDE	CAU-CAT-CE1-NE2
48	v	715	DDE	CBI-CBW-NCB-CAB
48	v	715	DDE	CBI-CBW-NCB-CAC
48	v	715	DDE	CBI-CBW-NCB-CAA
48	v	715	DDE	CAU-CBW-NCB-CAB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 284 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	GDP	v	900	-	25,30,30	0.95	1 (4%)	30,47,47	1.21	3 (10%)
89	34G	9	1957	-	39,39,39	1.79	9 (23%)	51,56,56	2.39	22 (43%)

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
88	GDP	v	900	-	-	5/12/32/32	0/3/3/3
89	34G	9	1957	-	-	8/14/49/49	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	9	1957	34G	CBC-CBG	5.90	1.57	1.52
89	9	1957	34G	CBD-CBH	3.78	1.57	1.52
89	9	1957	34G	CAO-CBG	3.55	1.57	1.53
89	9	1957	34G	CAQ-NBI	2.80	1.51	1.47
89	9	1957	34G	CAM-CAX	2.78	1.55	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	9	1957	34G	CAN-NBI-CAQ	6.23	122.29	110.32
89	9	1957	34G	CAX-CBD-CBH	-5.74	114.17	121.58
89	9	1957	34G	CAW-CBC-CBG	-4.70	115.74	121.38
89	9	1957	34G	CAK-CAL-CAW	4.22	118.13	110.66
89	9	1957	34G	CAP-CBH-CBD	-4.03	107.34	113.07

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	v	900	GDP	C5'-O5'-PA-O3A
88	v	900	GDP	C5'-O5'-PA-O2A
89	9	1957	34G	CAA-CAJ-CBE-CAQ
89	9	1957	34G	CBF-CAO-CBG-NAR

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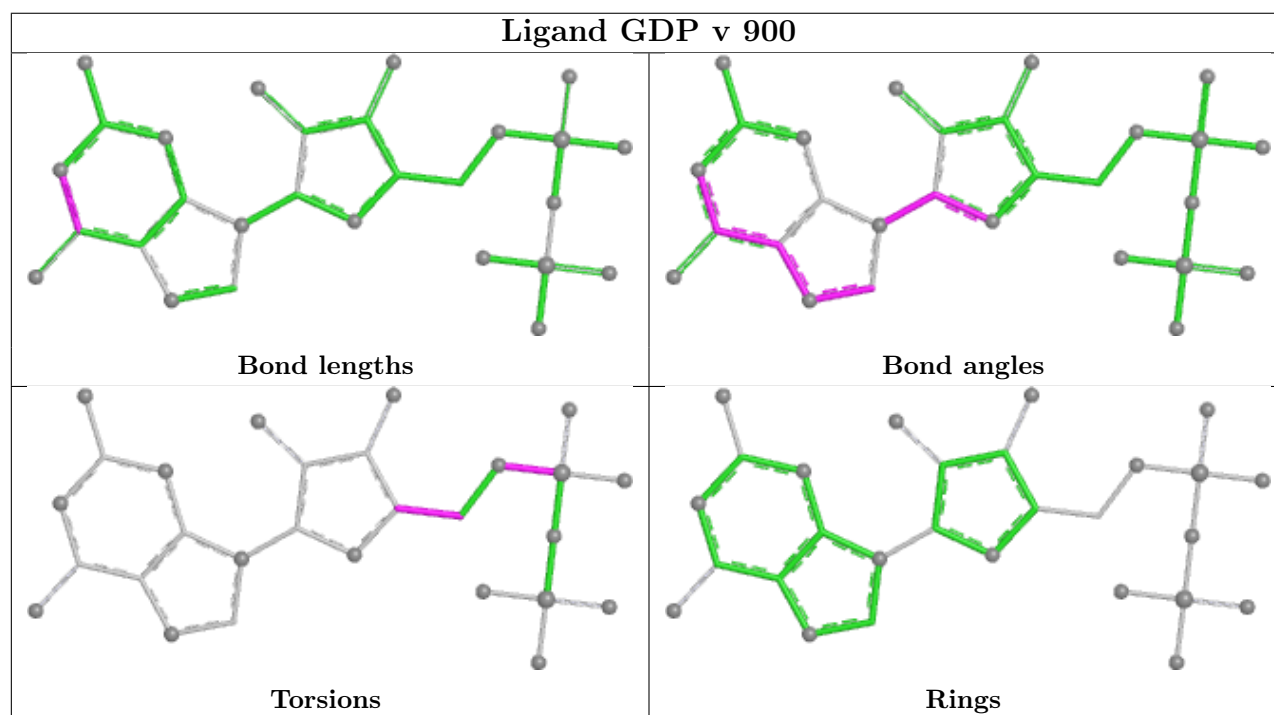
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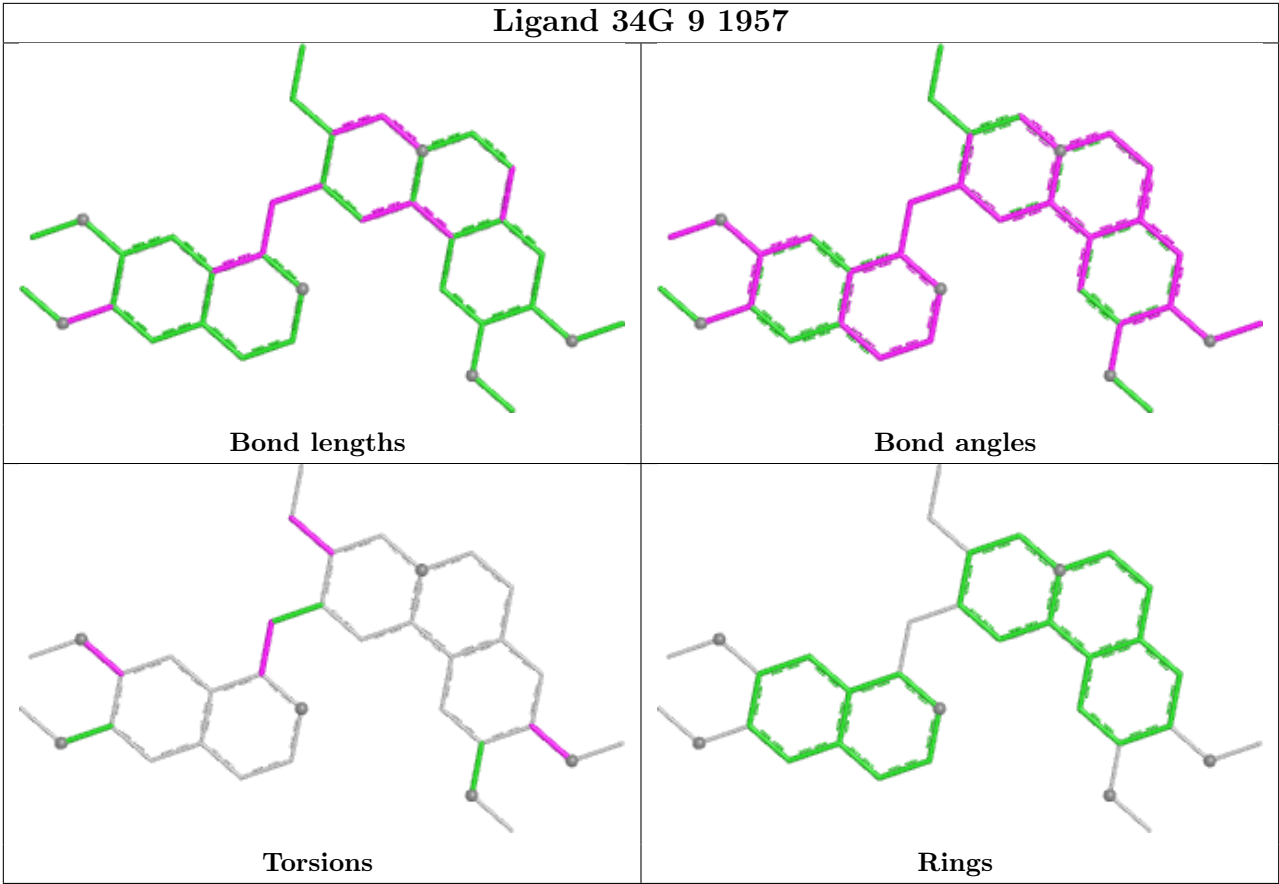
Mol	Chain	Res	Type	Atoms
89	9	1957	34G	CBF-CAO-CBG-CBC

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	5	21
49	9	4
83	3	2
85	2	1
81	ff	1

The worst 5 of 29 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	42.68
1	5	1219:G	O3'	1233:G	P	19.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	523:C	O3'	638:G	P	17.08
1	5	1406(C):G	O3'	1411:C	P	16.39
1	5	4138:C	O3'	4146:G	P	15.58

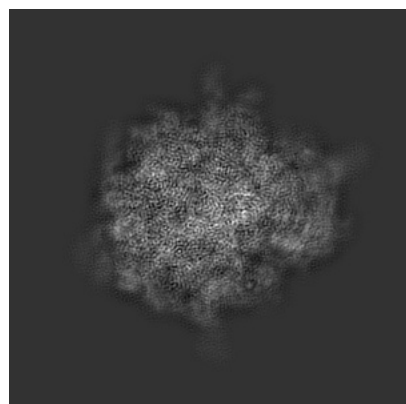
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43189. These allow visual inspection of the internal detail of the map and identification of artifacts.

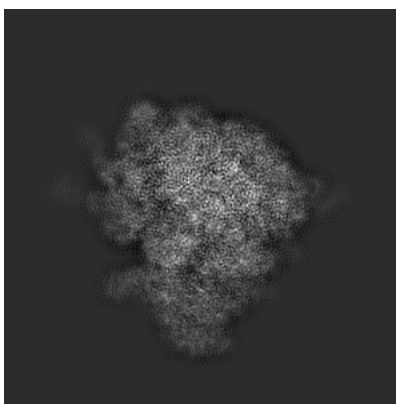
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

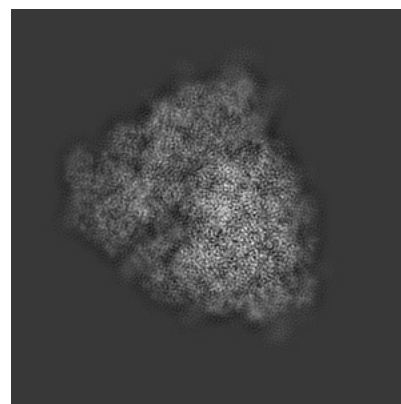
6.1.1 Primary map



X

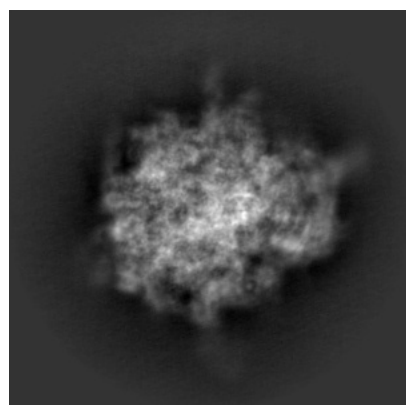


Y

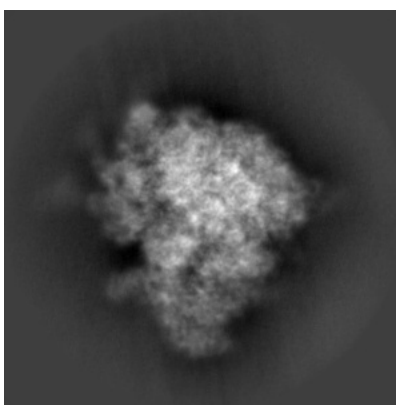


Z

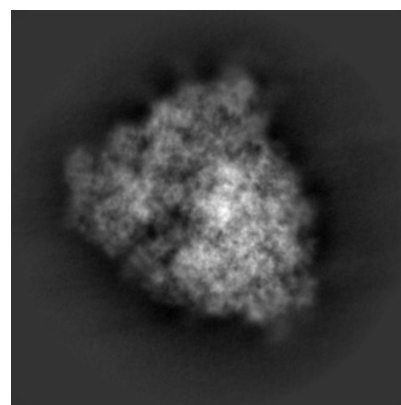
6.1.2 Raw map



X



Y

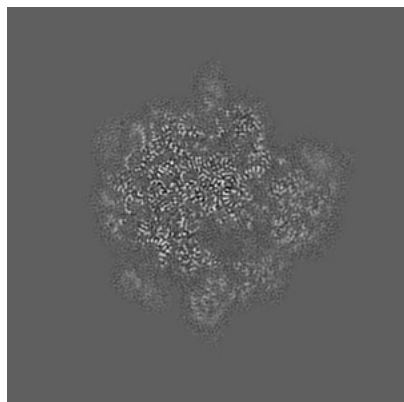


Z

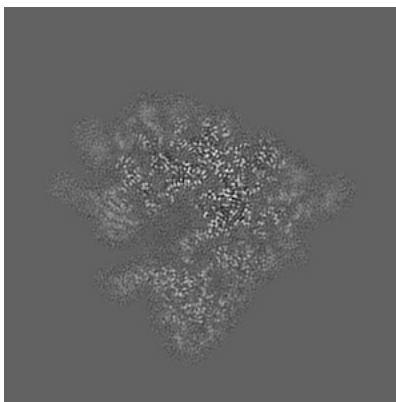
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

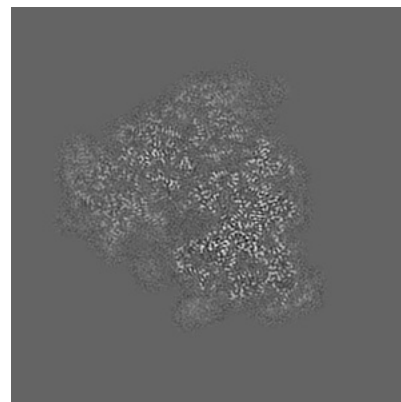
6.2.1 Primary map



X Index: 160

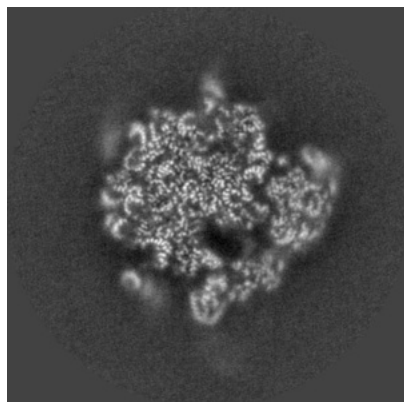


Y Index: 160

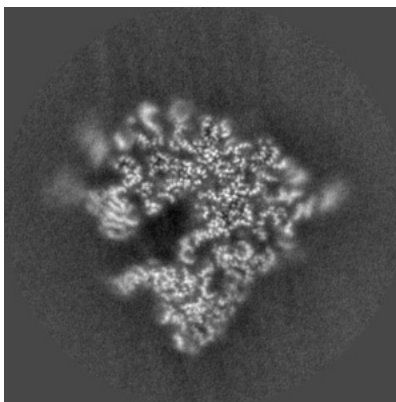


Z Index: 160

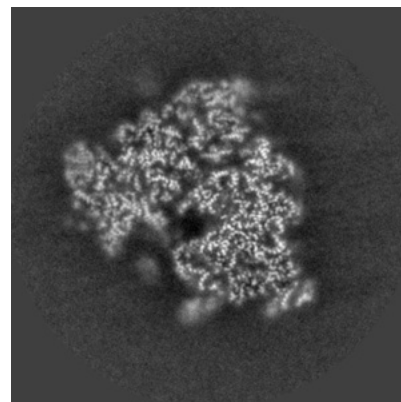
6.2.2 Raw map



X Index: 160



Y Index: 160

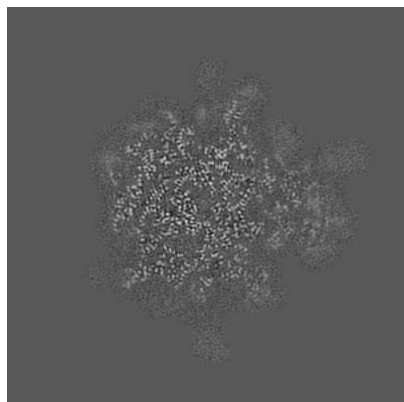


Z Index: 160

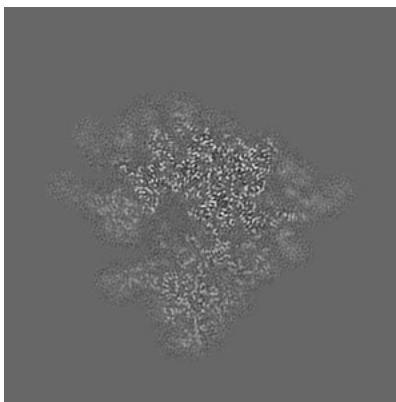
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

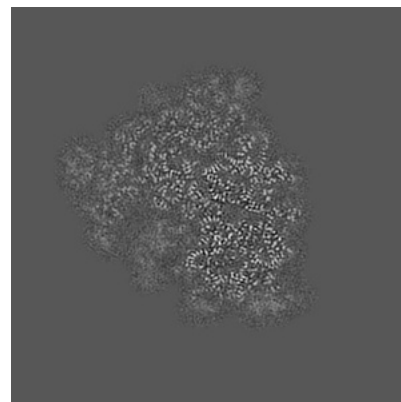
6.3.1 Primary map



X Index: 177

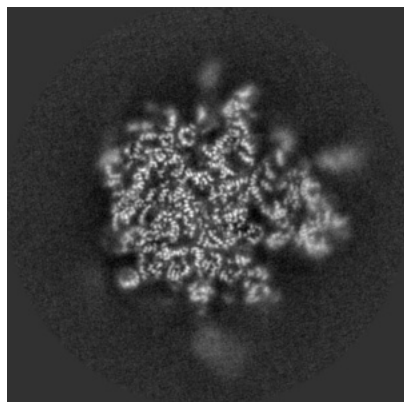


Y Index: 165

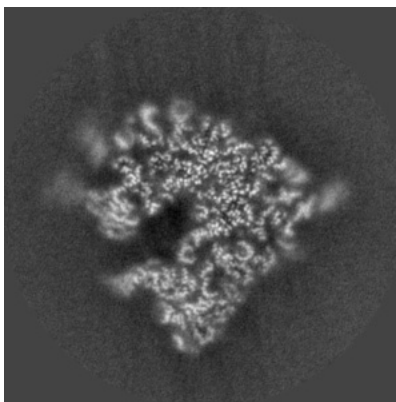


Z Index: 171

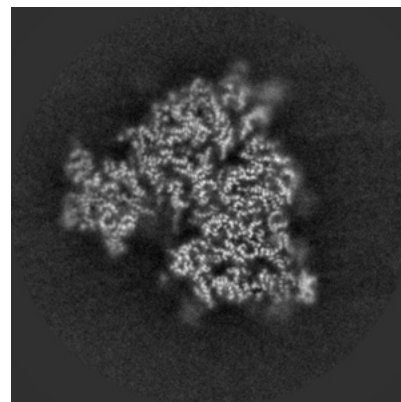
6.3.2 Raw map



X Index: 175



Y Index: 161

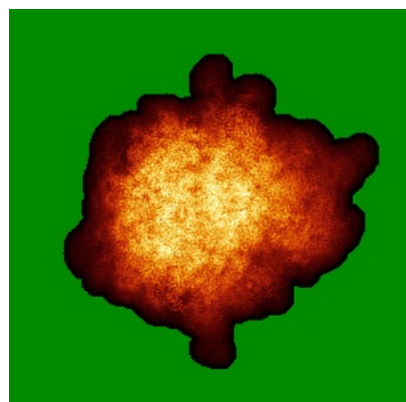


Z Index: 153

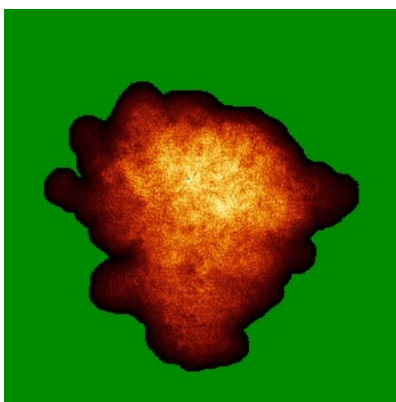
The images above show the largest variance slices of the map in three orthogonal directions.

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

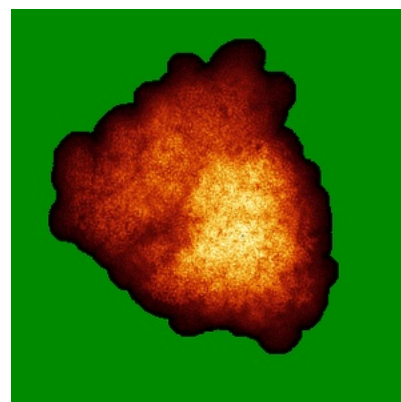
6.4.1 Primary map



X

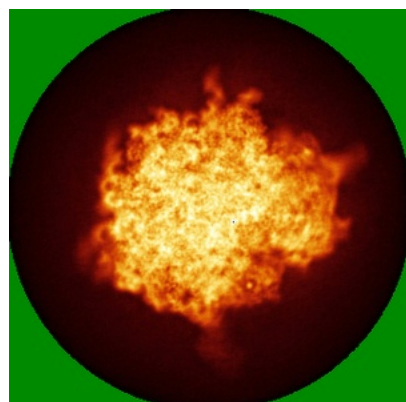


Y

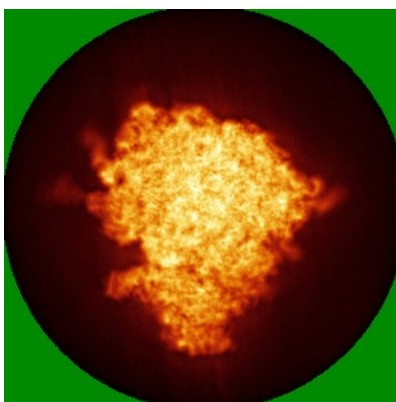


Z

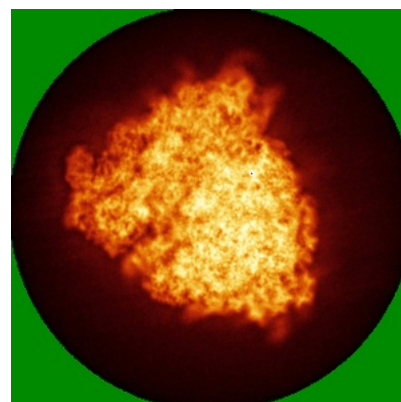
6.4.2 Raw map



X



Y

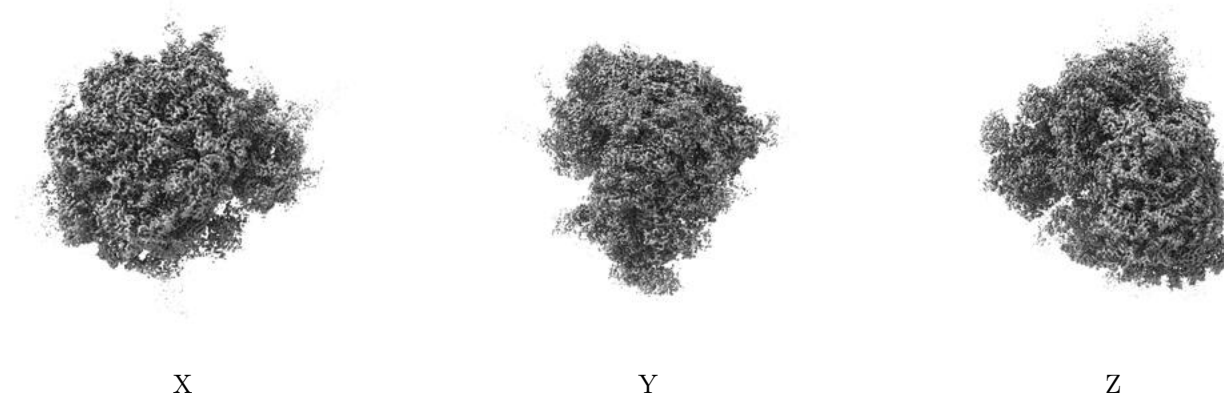


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

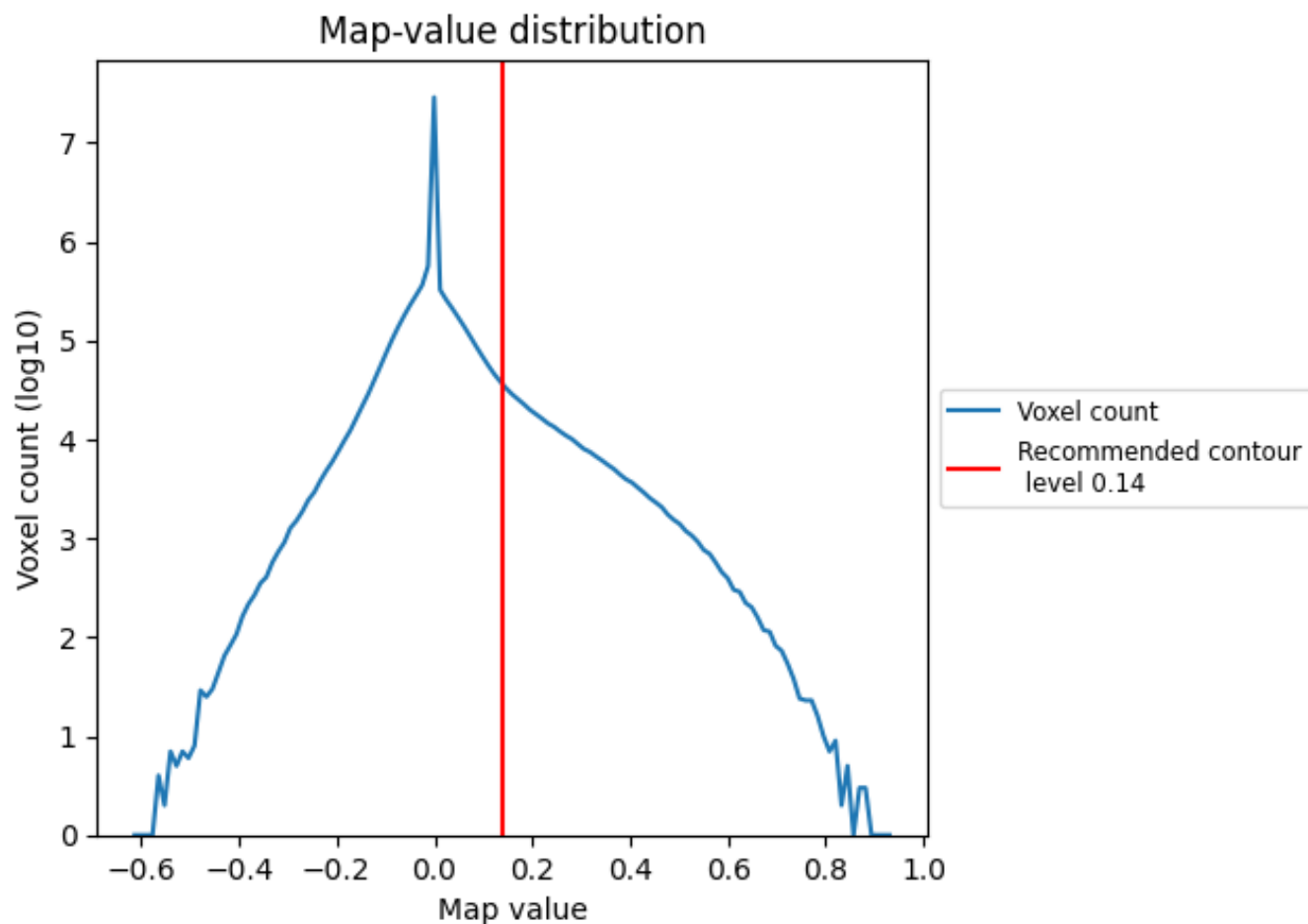
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

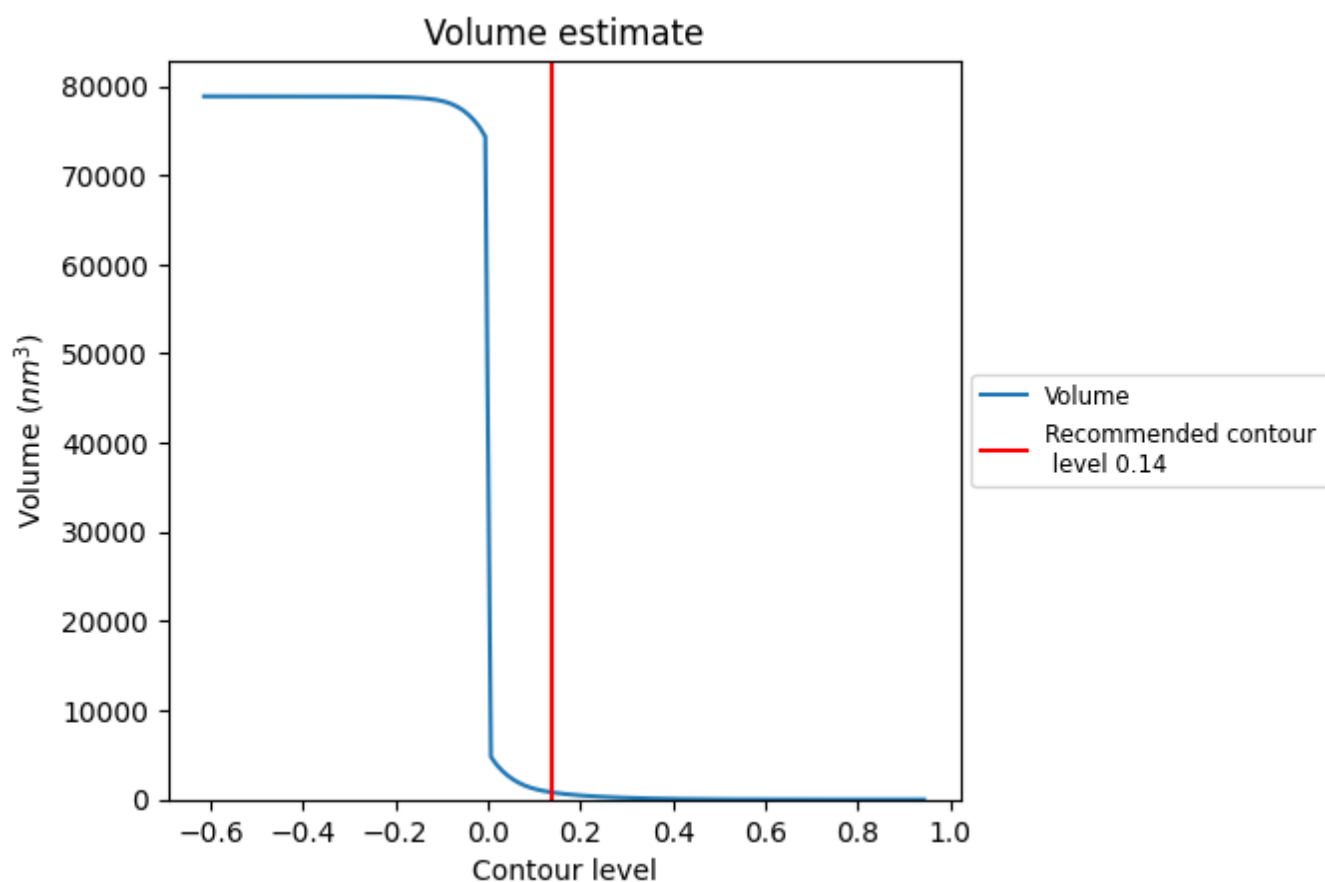
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

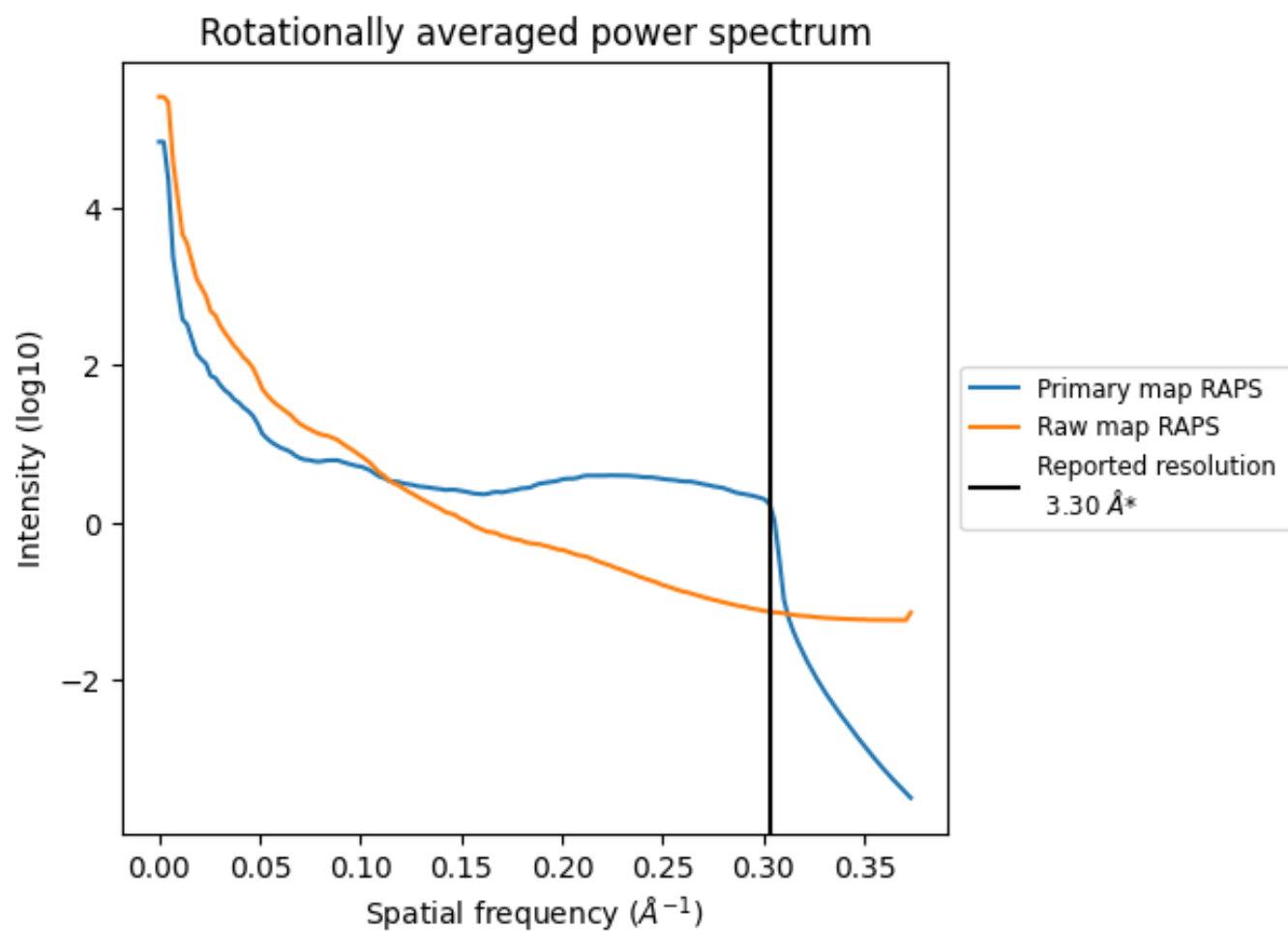
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 717 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 ⓘ

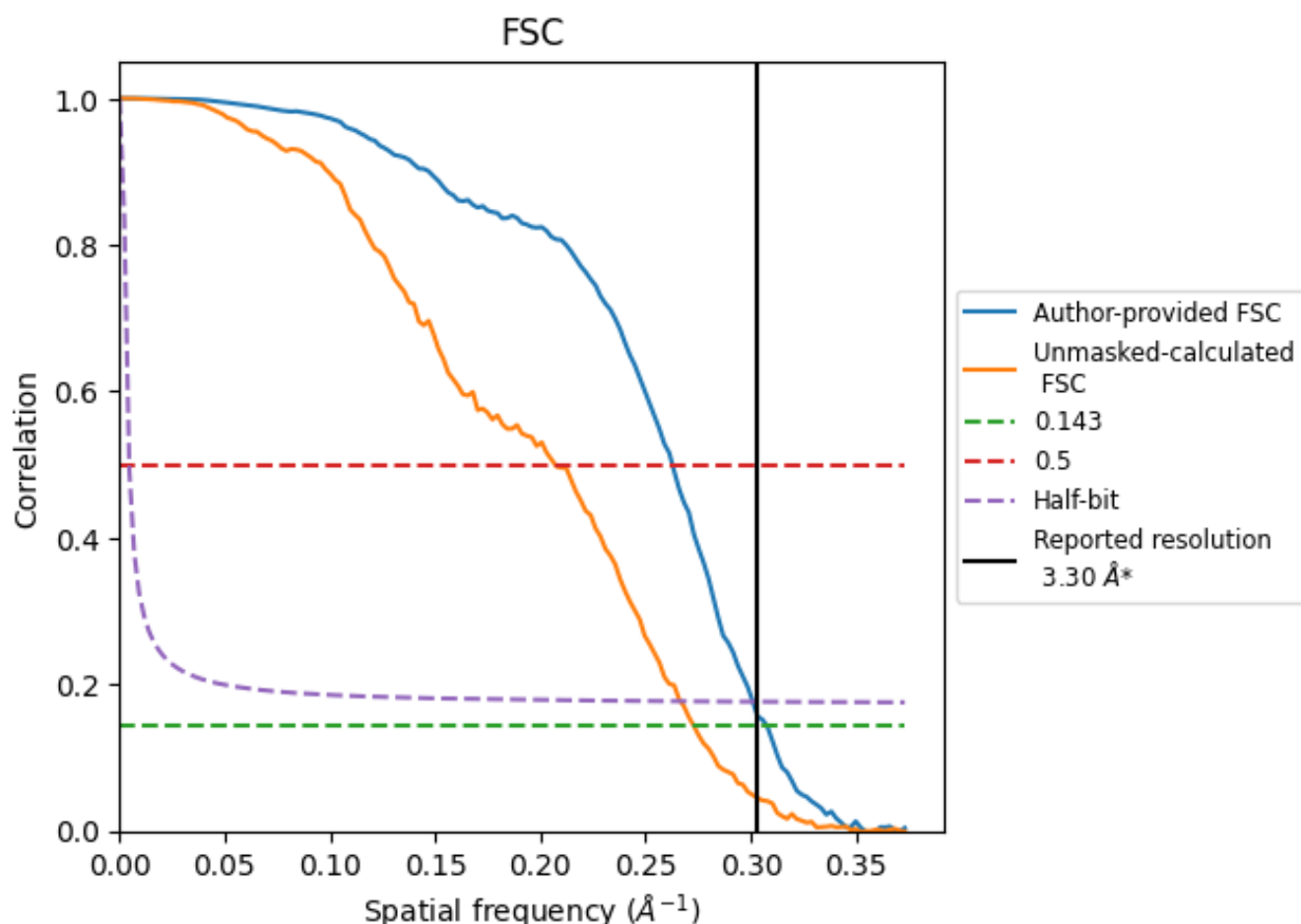


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

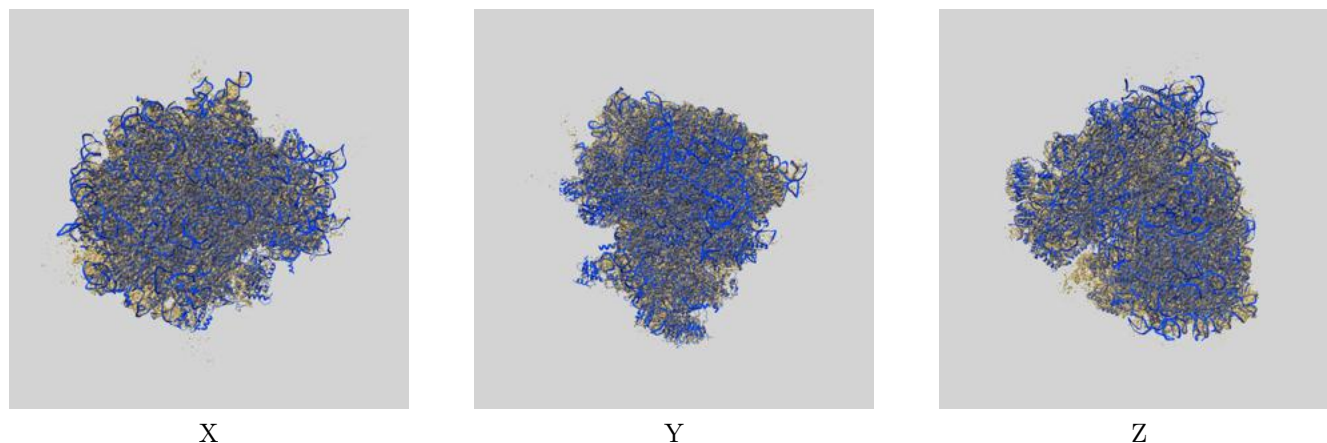
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.81	3.32
Unmasked-calculated*	3.67	4.83	3.75

*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 3.67 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

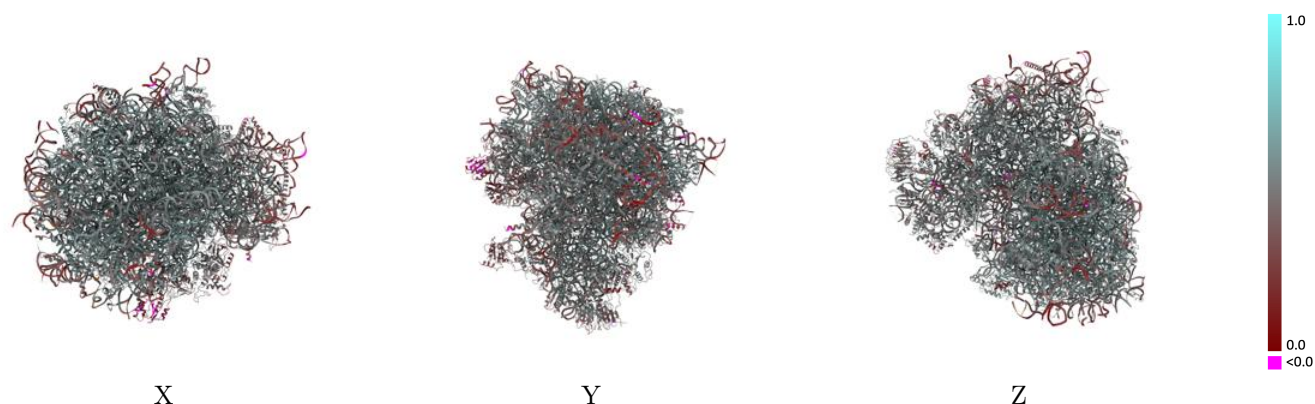
This section contains information regarding the fit between EMDB map EMD-43189 and PDB model 8VFT. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



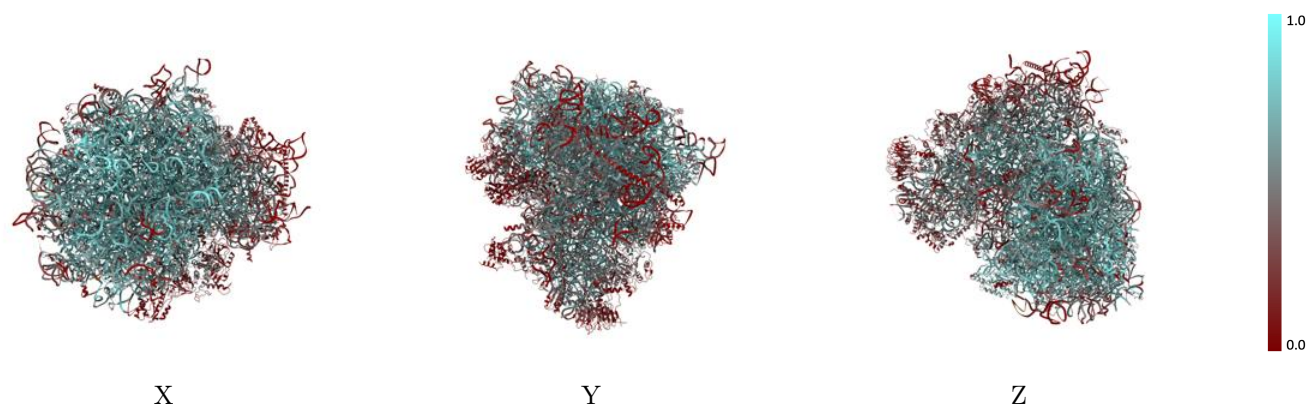
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



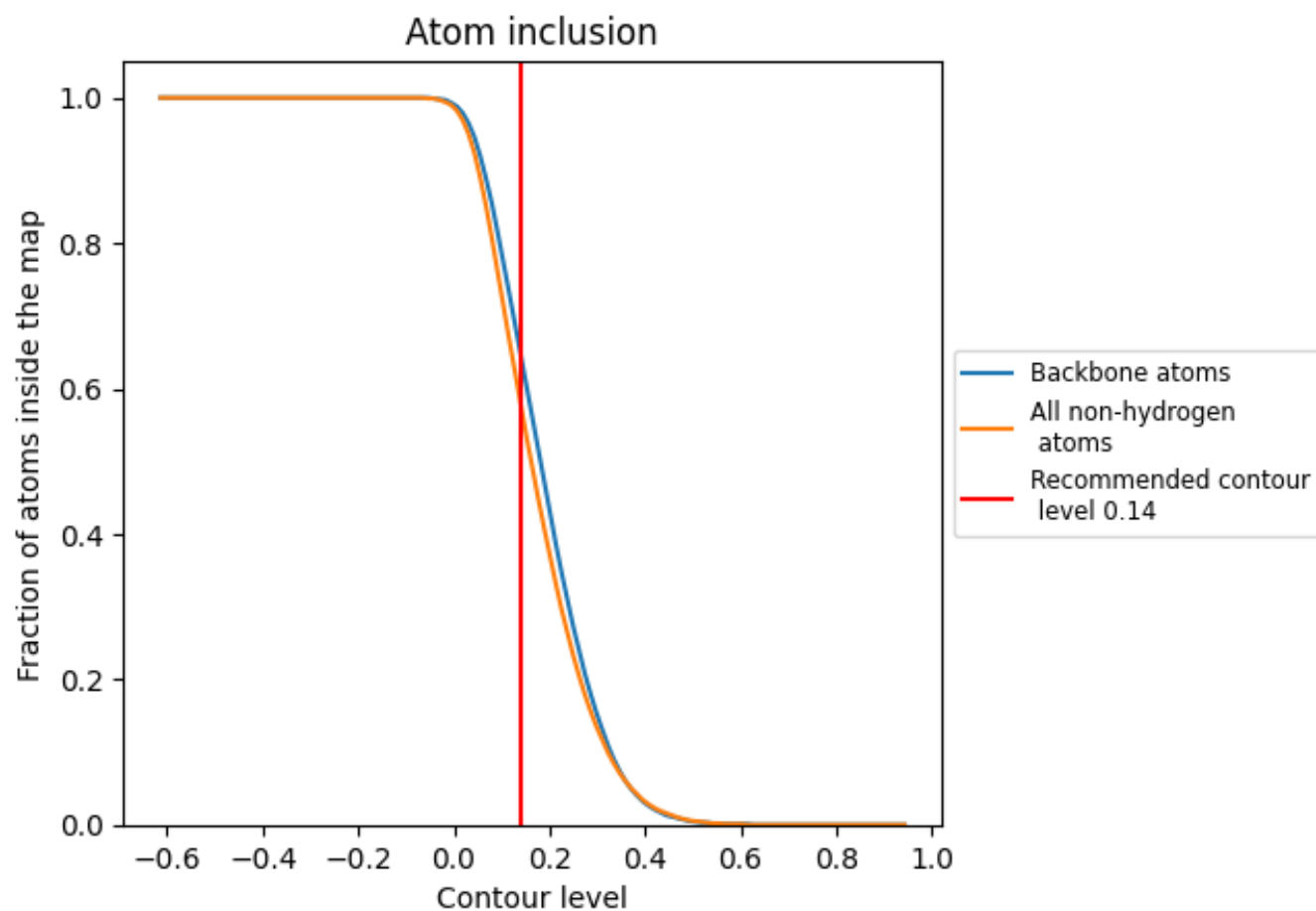
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.4930
2	 0.3500	 0.4200
3	 0.4350	 0.4340
5	 0.6930	 0.4940
7	 0.7890	 0.5260
8	 0.7080	 0.4960
9	 0.5590	 0.4610
A	 0.7070	 0.5670
AA	 0.4150	 0.4890
B	 0.6700	 0.5550
BB	 0.4020	 0.5080
C	 0.6780	 0.5510
CC	 0.4620	 0.5120
D	 0.6170	 0.5350
DD	 0.3760	 0.4750
E	 0.5970	 0.5400
EE	 0.3650	 0.4970
F	 0.6790	 0.5540
FF	 0.3350	 0.4700
G	 0.5580	 0.5160
GG	 0.2490	 0.4410
H	 0.6000	 0.5320
HH	 0.2380	 0.4450
I	 0.6260	 0.5460
II	 0.4180	 0.4990
J	 0.5640	 0.5180
JJ	 0.3930	 0.4810
KK	 0.3720	 0.4840
L	 0.5950	 0.5300
LL	 0.4630	 0.5200
M	 0.6370	 0.5390
MM	 0.0390	 0.3330
N	 0.7410	 0.5720
NN	 0.4830	 0.5180
O	 0.6940	 0.5570





















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Chain	Atom inclusion	Q-score
OO	 0.4600	 0.5040
P	 0.6860	 0.5550
PP	 0.3560	 0.4800
Q	 0.6790	 0.5640
QQ	 0.3790	 0.4830
R	 0.5880	 0.5230
RR	 0.3050	 0.4410
S	 0.6760	 0.5550
SS	 0.3380	 0.4590
T	 0.6100	 0.5370
TT	 0.3900	 0.4780
U	 0.4460	 0.4910
UU	 0.3400	 0.4720
V	 0.6350	 0.5550
VV	 0.3760	 0.4920
W	 0.6310	 0.5520
WW	 0.5080	 0.5230
X	 0.6310	 0.5450
XX	 0.5160	 0.5350
Y	 0.6280	 0.5450
YY	 0.2940	 0.4790
Z	 0.5880	 0.5300
ZZ	 0.2370	 0.4460
a	 0.7110	 0.5580
aa	 0.5270	 0.5200
b	 0.5230	 0.5030
bb	 0.3300	 0.4900
c	 0.6130	 0.5250
cc	 0.1260	 0.2290
d	 0.6470	 0.5440
dd	 0.5790	 0.5260
e	 0.6900	 0.5590
ee	 0.3970	 0.4730
f	 0.7300	 0.5720
ff	 0.0940	 0.3870
g	 0.6170	 0.5320
gg	 0.2000	 0.4340
h	 0.5960	 0.5370
i	 0.5650	 0.5080
j	 0.7430	 0.5650
k	 0.4970	 0.5040
l	 0.6720	 0.5390

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Chain	Atom inclusion	Q-score
m	 0.6490	 0.5560
n	 0.6520	 0.5460
o	 0.6280	 0.5600
p	 0.6210	 0.5410
r	 0.6690	 0.5510
s	 0.1230	 0.2650
t	 0.0660	 0.3450
v	 0.2620	 0.4440
w	 0.6280	 0.5140