



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 10:44 PM EDT

PDB ID : 8SCB
EMDB ID : EMD-40344
Title : Terminating ribosome with SRI-41315
Authors : Yip, M.C.J.; Coelho, J.P.L.; Oltion, K.; Tauton, J.; Shao, S.
Deposited on : 2023-04-05
Resolution : 2.50 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:

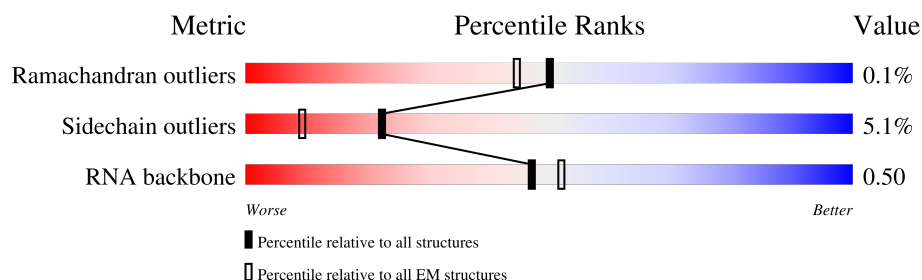
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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





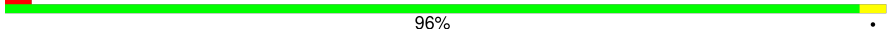

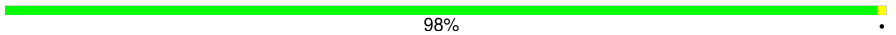
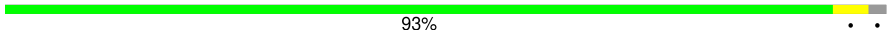

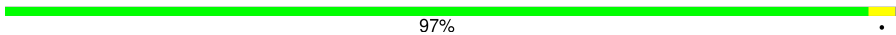

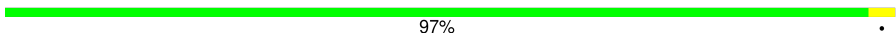
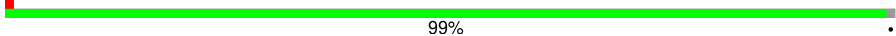




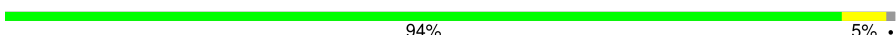
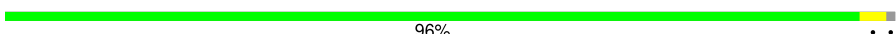



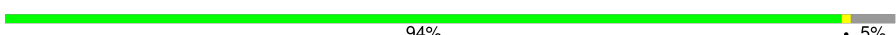
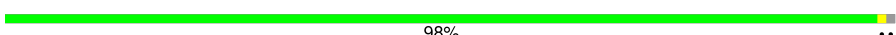

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	413	
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	

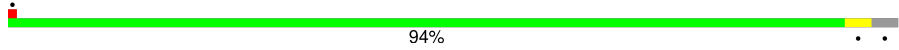

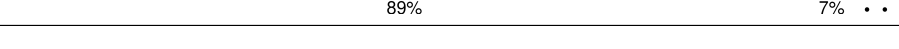
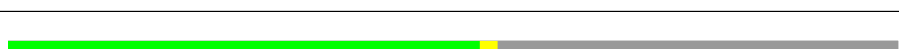

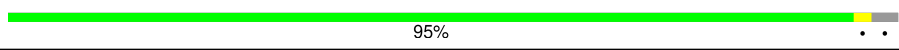
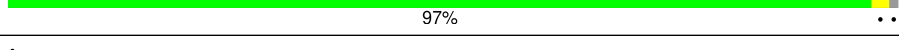




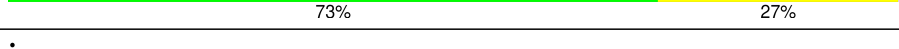

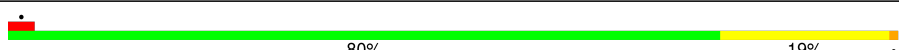


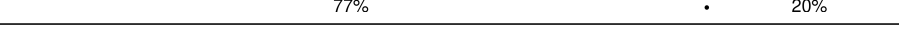







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Mol	Chain	Length	Quality of chain
9	I	214	 93% • 5%
10	J	178	 89% • 6%
11	L	211	 96% •
12	M	218	 63% 37%
13	N	204	 98% •
14	O	203	 93% • •
15	P	184	 81% • 17%
16	Q	188	 97% • •
17	R	196	 5% 88% • 9%
18	S	176	 97% •
19	T	160	 99% •
20	U	128	 73% • 23%
21	V	140	 92% • 7%
22	W	157	 39% • 60%
23	X	156	 73% • 26%
24	Y	145	 89% • 8%
25	Z	136	 94% • 5% •
26	a	148	 96% • •
27	b	245	 30% • 69%
28	c	115	 76% 6% 18%
29	d	125	 79% • 20%
30	e	135	 94% • 5%
31	f	110	 98% • •
32	g	117	 94% • •
33	h	123	 94% 5% •

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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	1	130	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	

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Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	

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Mol	Chain	Length	Quality of chain
84	gg	317	
85	hh	197	
86	ii	459	
87	jj	599	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
90	ZVM	ii	501	X	-	-	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 222478 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 Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called Ribosomal protein L3.

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 60S ribosomal protein L4.

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

- Molecule 4 is a protein called Ribosomal_L18_c domain-containing protein.

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 60S ribosomal protein L6.

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 60S ribosomal protein L7.

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 60S ribosomal protein L7a.

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 60S ribosomal protein L9.

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 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called 60S ribosomal protein L11.

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		

- Molecule 12 is a protein called 60S ribosomal protein L14.

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 Ribosomal protein L15.

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 Ribosomal protein L18.

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

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 17 is a protein called Ribosomal protein L19.

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
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		

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 Ribosomal protein L23.

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 60S ribosomal protein L24.

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 eL23.

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 60S ribosomal protein L27.

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

- Molecule 26 is a protein called 60S ribosomal protein L27a.

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 60S ribosomal protein L29.

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 60S ribosomal protein L34.

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 eL35.

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 60S ribosomal protein L36.

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 Ribosomal protein L37.

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 60S ribosomal protein L38.

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 Ubiquitin A-52 residue ribosomal protein fusion product 1.

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 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	190	Total	C	N	O	S	0	0
			1461	931	255	266	9		

- Molecule 44 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	141	Total	C	N	O	S	0	0
			1059	662	195	199	3		

- Molecule 45 is a protein called NC.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 46 is a RNA chain called P_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3530	Total	C	N	O	P	0	0
			75735	33780	13869	24556	3530		

- Molecule 49 is a RNA chain called 5S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a RNA chain called 5.8S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 51 is a RNA chain called 18S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1692	Total	C	N	O	P	0	0
			36134	16163	6486	11794	1691		

- Molecule 52 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 53 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	216	Total	C	N	O	S	0	0
			1674	1085	286	294	9		

- Molecule 55 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	221	Total	C	N	O	S	0	0
			1723	1098	311	307	7		

- Molecule 56 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	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 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	181	Total	C	N	O	S	0	0
			1441	902	273	259	7		

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	177	Total	C	N	O	S	0	0
			1425	912	258	254	1		

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	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 61 is a protein called uS4.

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

- Molecule 62 is a protein called S10_pectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	86	Total	C	N	O	S	0	0
			729	479	127	118	5		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	136	Total	C	N	O	S	0	0
			1123	717	210	190	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	122	Total	C	N	O	S	0	0
			939	588	166	176	9		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	OO	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	117	Total	C	N	O	S	0	0
			968	615	181	165	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	140	Total	C	N	O	S	0	0
			1117	710	211	193	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	118	Total	C	N	O	S	0	0
			962	604	179	176	3		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	138	Total	C	N	O	S	0	0
			1075	674	206	192	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 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	102	Total	C	N	O	S	0	0
			807	507	153	143	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	81	Total	C	N	O	S	0	0
			617	380	114	118	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 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	123	Total	C	N	O	S	0	0
			1006	637	197	167	5		

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ZZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	98	Total	C	N	O	S	0	0
			781	486	161	129	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 79 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bb	79	Total	C	N	O	S	0	0
			628	395	117	110	6		

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	47	Total	C	N	O	S	0	0
			380	231	86	62	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	63	Total	C	N	O	S	0	0
			527	336	99	86	6		

- Molecule 84 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	gg	304	Total	C	N	O	S	0	0
			2371	1496	414	449	12		

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	11	Total	C	N	O	P	0	0
			236	106	44	75	11		

- Molecule 86 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	expression tag	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495
ii	183	ALA	GLY	conflict	UNP P62495
ii	184	ALA	GLY	conflict	UNP P62495

- Molecule 87 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	578	Total	C	N	O	S	0	0
			4558	2914	780	835	29		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A	2	Total	Mg	0
			2	2	
88	I	2	Total	Mg	0
			2	2	
88	N	1	Total	Mg	0
			1	1	
88	P	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
88	e	1	Total 1	Mg 1	0
88	f	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	o	1	Total 1	Mg 1	0
88	2	2	Total 2	Mg 2	0
88	5	221	Total 221	Mg 221	0
88	7	6	Total 6	Mg 6	0
88	8	2	Total 2	Mg 2	0
88	9	64	Total 64	Mg 64	0
88	EE	1	Total 1	Mg 1	0
88	LL	1	Total 1	Mg 1	0
88	OO	1	Total 1	Mg 1	0
88	XX	1	Total 1	Mg 1	0
88	hh	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

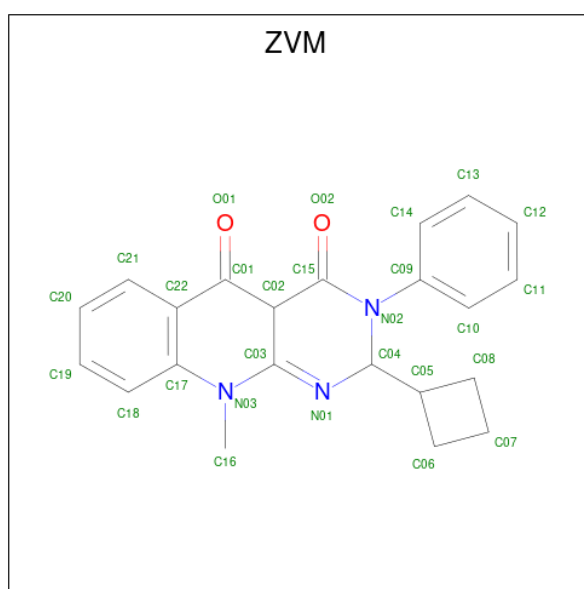
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0

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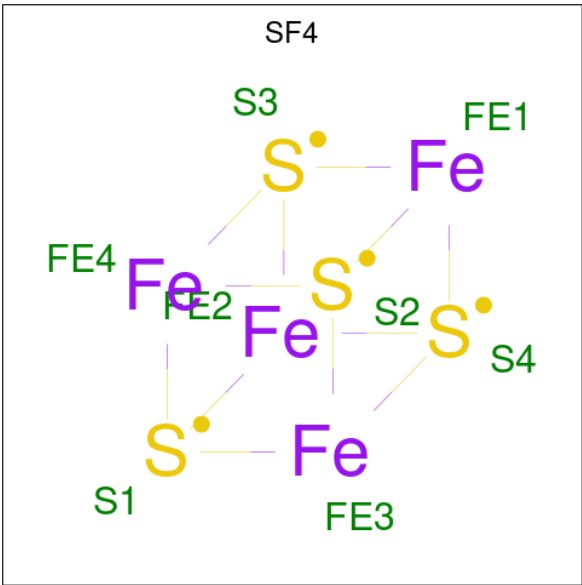
Mol	Chain	Residues	Atoms		AltConf
89	aa	1	Total	Zn	0
			1	1	
89	dd	1	Total	Zn	0
			1	1	
89	ff	1	Total	Zn	0
			1	1	

- Molecule 90 is (2S,4aS)-2-cyclobutyl-10-methyl-3-phenyl-2,10-dihydropyrimido[4,5-b]quinoline-4,5(3H,4aH)-dione (three-letter code: ZVM) (formula: C₂₂H₂₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
90	ii	1	Total	C	N	O	0
			27	22	3	2	

- Molecule 91 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
91	jj	1	Total	Fe	S	0
			8	4	4	
91	jj	1	Total	Fe	S	0
			8	4	4	

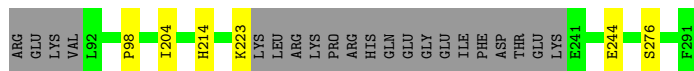
- Molecule 92 is water.

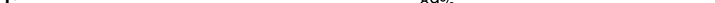
Mol	Chain	Residues	Atoms		AltConf
92	A	6	Total	O	0
			6	6	
92	B	2	Total	O	0
			2	2	
92	C	1	Total	O	0
			1	1	
92	F	1	Total	O	0
			1	1	
92	I	1	Total	O	0
			1	1	
92	L	1	Total	O	0
			1	1	
92	N	4	Total	O	0
			4	4	
92	Q	1	Total	O	0
			1	1	
92	R	1	Total	O	0
			1	1	
92	V	2	Total	O	0
			2	2	

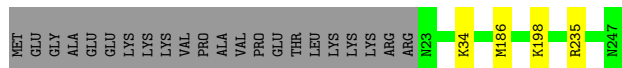
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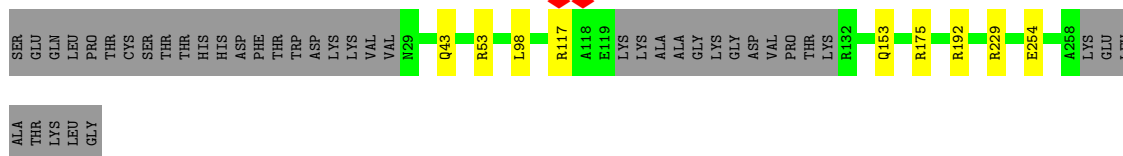
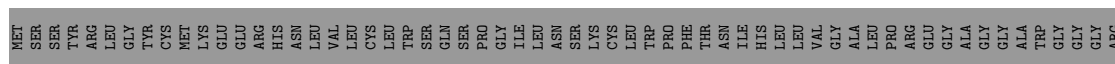
Mol	Chain	Residues	Atoms		AltConf
92	X	2	Total 2	O 2	0
92	a	5	Total 5	O 5	0
92	e	5	Total 5	O 5	0
92	j	1	Total 1	O 1	0
92	o	2	Total 2	O 2	0
92	5	723	Total 723	O 723	0
92	7	13	Total 13	O 13	0
92	8	8	Total 8	O 8	0
92	9	173	Total 173	O 173	0
92	II	1	Total 1	O 1	0
92	OO	1	Total 1	O 1	0
92	XX	1	Total 1	O 1	0
92	aa	1	Total 1	O 1	0
92	ii	2	Total 2	O 2	0



- Chain F:  89% 9%



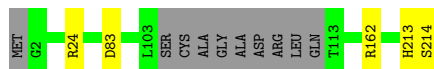
- Chain G: 66% 32%



- Chain H: 97%



- Chain I:  93% • 5%



- Chain J:  89% • 6%



- Chain L:  96%

A diagram of a protein structure represented as a horizontal bar. The bar is divided into segments by vertical lines. The segments are colored: the first and last segments are red, and the middle segments are yellow. The residues are labeled as follows: M1 (red), R29 (yellow), K53 (yellow), M93 (yellow), T102 (yellow), K164 (yellow), and F176 (red).

Chain T: 

Chain U: 73% 23%

MET	ALA	PRO	VAL	LYS	LEU	VAL	ALA	LYS	GLY	GLY	LYS	LYS	LYS	LYS	GLN	L18	K67	K93	R101	E108	F115	TLE	ASN	GLN	ASP	GLU	GLU	GLU	GLU	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain V:  92% • 7%

MET
SER
LYS
ARG
GLY
ARG
GLY
GLY
SER
SER
G11
K109
A140

Chain W:  39% 60%

[illegible]

Chain X: 73% 26%

MET	ALA	PRO	LYS	ALA	LYS	GLU	ALA	PRO	PRO	ALA	ALA	PRO	PRO	LYS	VAL	GLU	ALA	LYS	ALA	LYS	LYS	LEU	LYS	LYS	LYS	ALA	ALA	VAL	LEU	LYS	GLY	VAL	HIS	SER	HIS	LYS	LYS	LYS	LYS	I40	R53	D143	I155	ITF
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----

Chain Y: 89% 8%

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acids: M1, Q40, Y74, R115, E120, R121, G133, K134, TYR, LYS, GLU, GLU, THR, ILE, GLU, LYS, MET, GLN, GLU. G133 and K134 are highlighted with red diamonds.

- Molecule 25: 60S ribosomal protein L27

Chain Z:  94% 5%



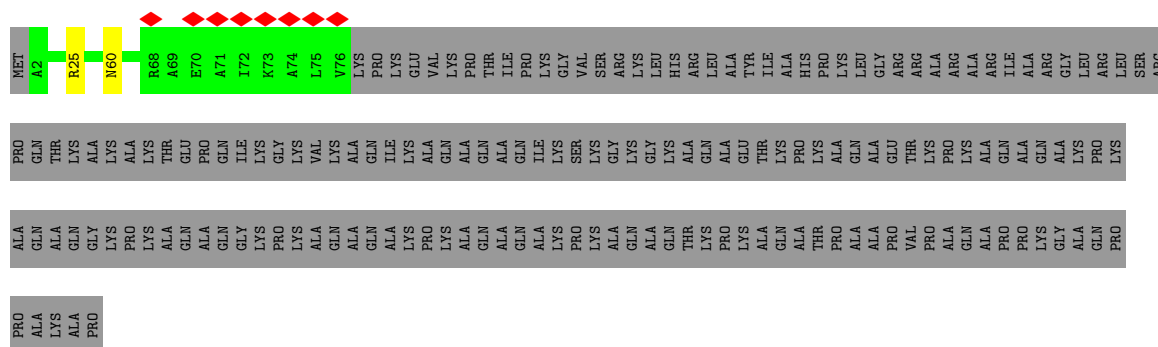
- Molecule 26: 60S ribosomal protein L27a

Chain a:  96%



- Molecule 27: 60S ribosomal protein L29

Chain b:  30% 69%



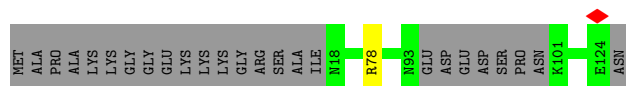
- Molecule 28: eL30

Chain c:  76% 6% 18%



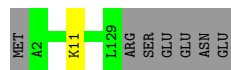
- Molecule 29: eL31

Chain d:  79% 20%



- Molecule 30: eL32

Chain e:  94% 5%



- Molecule 31: eL33

Chain f:  98% ..



- Molecule 32: 60S ribosomal protein L34

Chain g:  94% ..



- Molecule 33: eL35

Chain h:  94% 5% ..




- Molecule 34: 60S ribosomal protein L36

Chain i:  94% ..




- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: 60S ribosomal protein L38

Chain k:  89% 7% ..



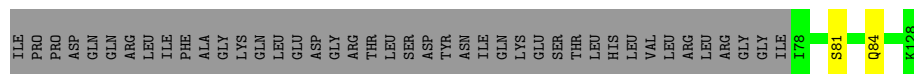
- Molecule 37: eL39

Chain l:  92% ..



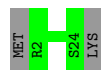
- Molecule 38: Ubiquitin A-52 residue ribosomal protein fusion product 1

Chain m:  53% 45%



- Molecule 39: eL41

Chain n:  92% 8%



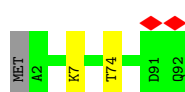
- Molecule 40: eL42

Chain o:  95%




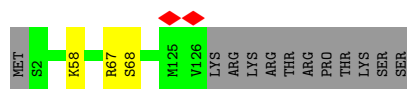
- Molecule 41: eL43

Chain p:  97%



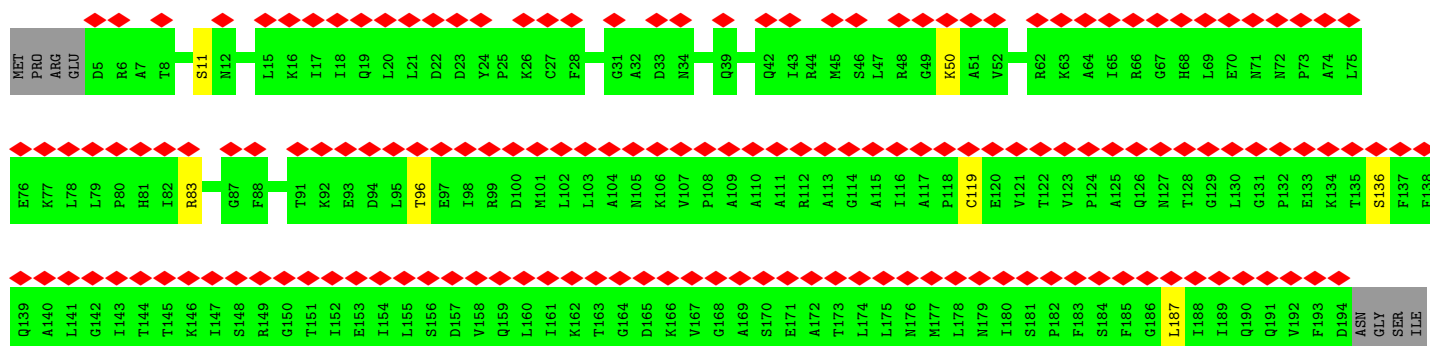
- Molecule 42: eL28

Chain r:  89% 9%

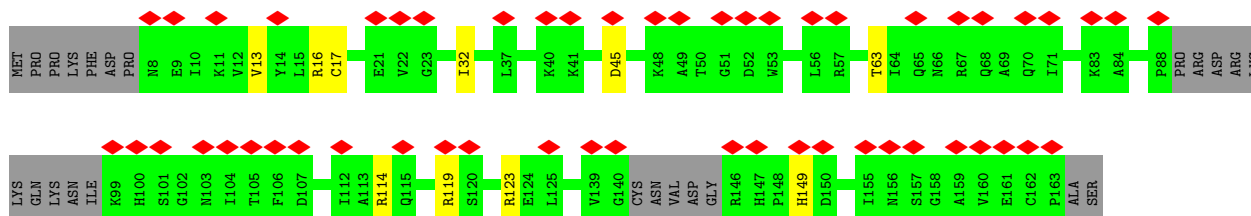
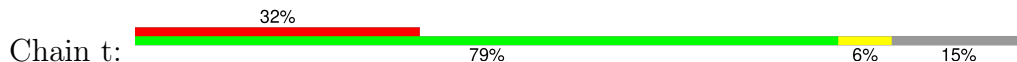


- Molecule 43: 60S acidic ribosomal protein P0

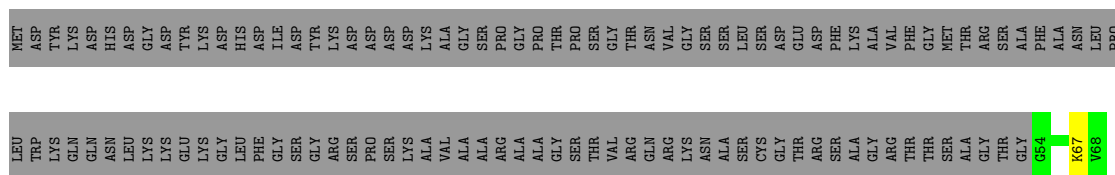
Chain s:  50% 58% 40%



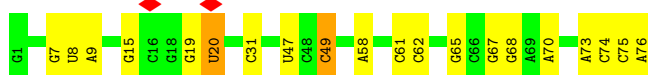
- Molecule 44: 60S ribosomal protein L12



- Molecule 45: NC



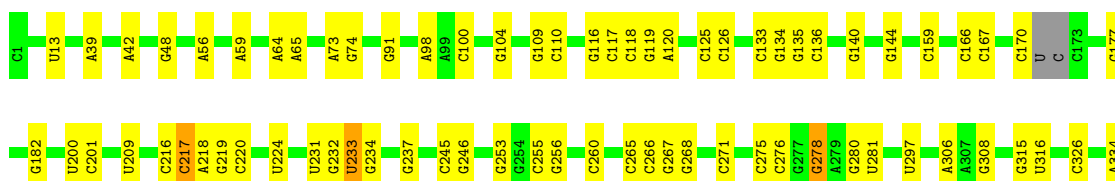
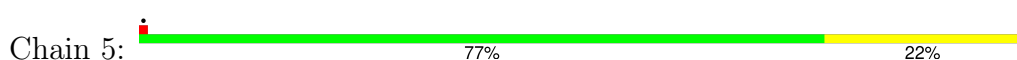
- Molecule 46: P tRNA



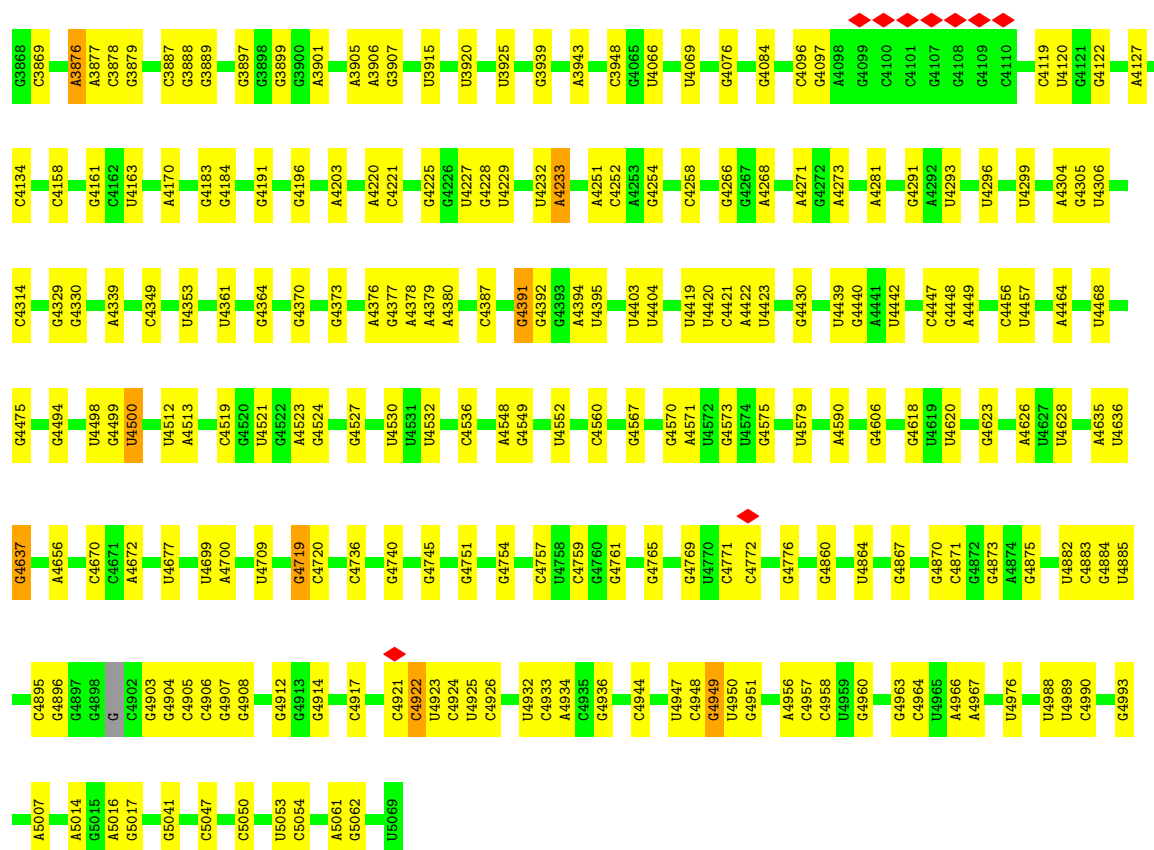
- Molecule 47: E tRNA



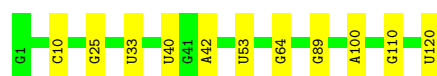
- Molecule 48: 28S rRNA



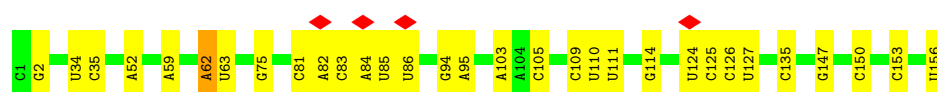
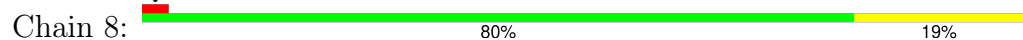




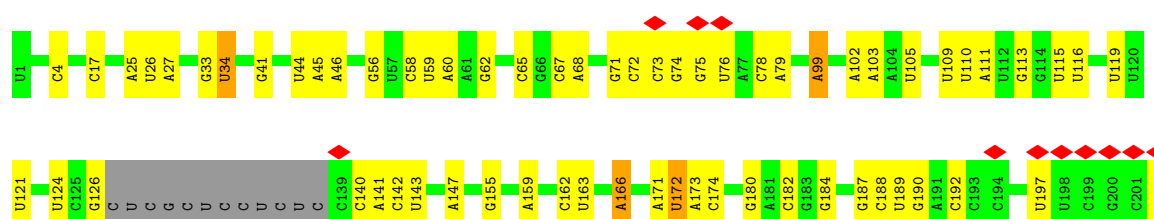
• Molecule 49: 5S_rRNA



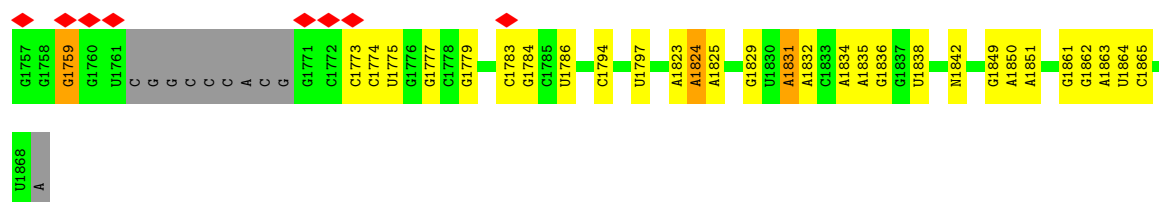
• Molecule 50: 5.8S_rRNA



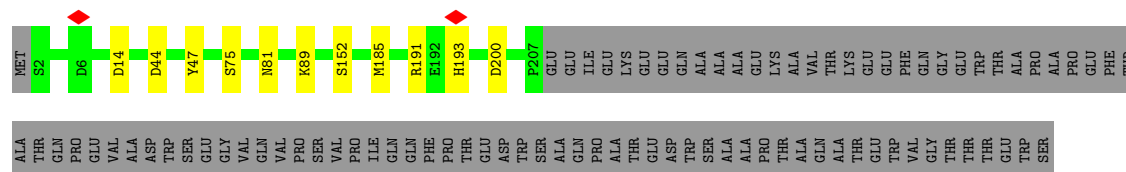
• Molecule 51: 18S_rRNA



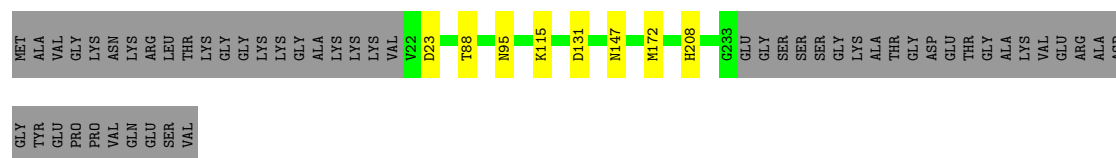
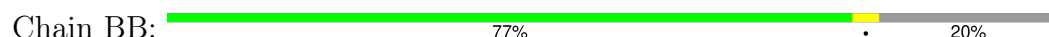




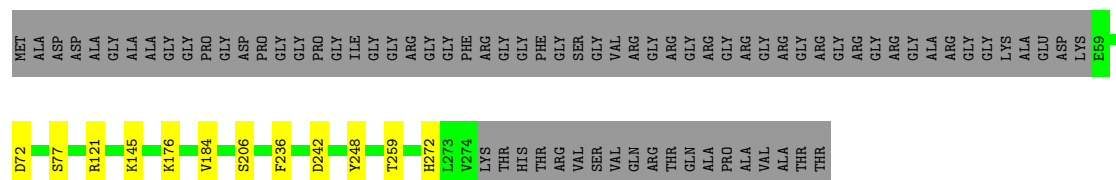
- Molecule 52: uS2 (SA)



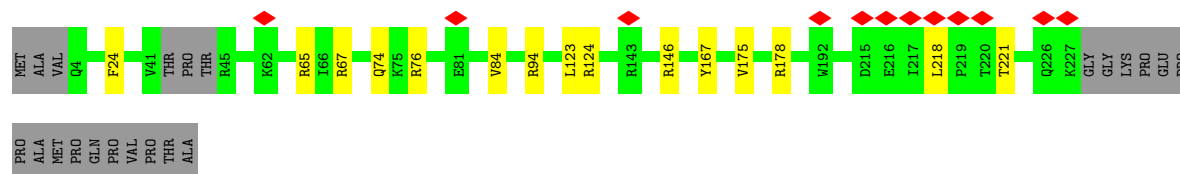
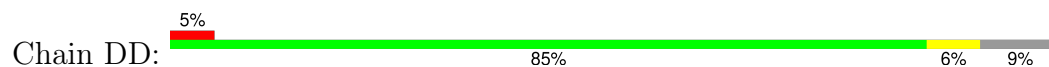
- Molecule 53: eS1



- Molecule 54: uS5



- Molecule 55: Ribosomal protein S3



- Molecule 56: eS4 (S4 X isoform)





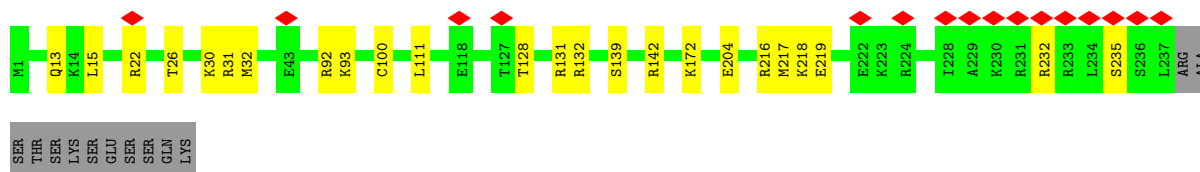
• Molecule 57: uS7

Chain FF: 81% 7% 11%



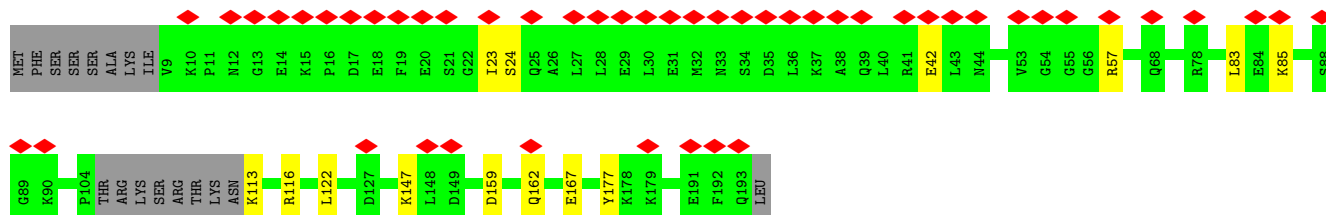
• Molecule 58: eS6

Chain GG: 6% 86% 10% 5%



• Molecule 59: eS7

Chain HH: 25% 84% 7% 9%



• Molecule 60: eS8

Chain II: 5% 93% 6%



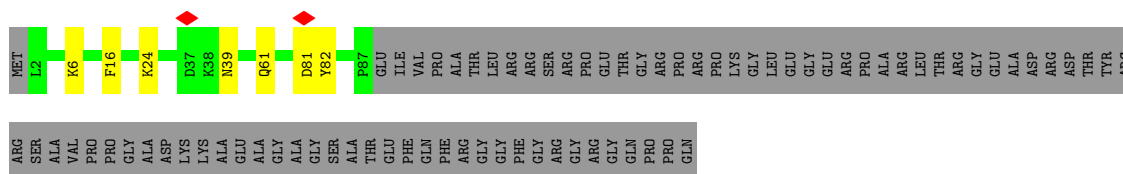
• Molecule 61: uS4

Chain JJ: 91% 5% 5%

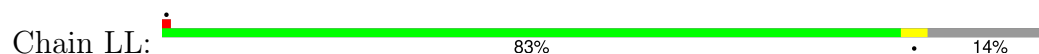


• Molecule 62: S10_pectin domain-containing protein

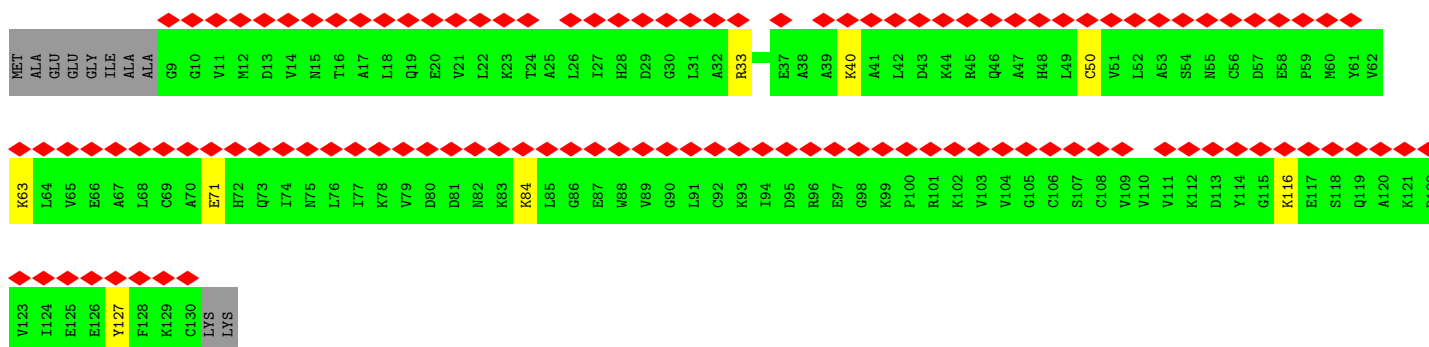
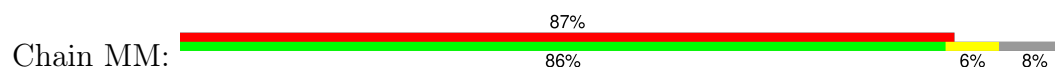
Chain KK: 48% 48%



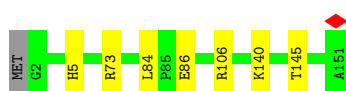
• Molecule 63: uS17



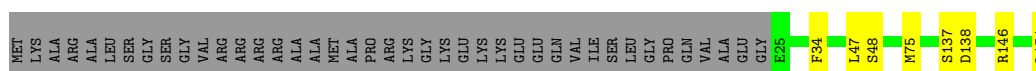
• Molecule 64: eS12



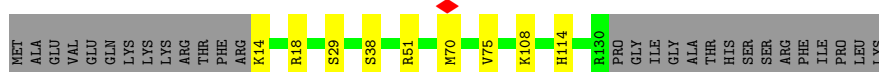
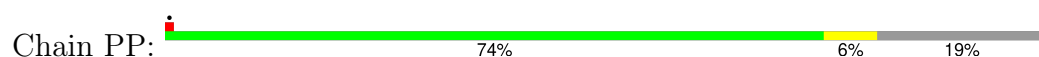
• Molecule 65: uS15



• Molecule 66: uS11



• Molecule 67: uS19




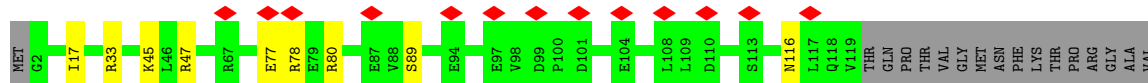
- Molecule 68: uS9

Chain QQ:  92%




- Molecule 69: eS17

Chain RR:  10% 81% 7% 13%



- Molecule 70: uS13

Chain SS:  86% 7% 8%




- Molecule 71: eS19

Chain TT:  92% 5%



- Molecule 72: uS10

Chain UU:  11% 82% 14%



- Molecule 73: eS21

Chain VV:  93% 5%



- Molecule 74: uS8

Chain WW:  95%



- Molecule 75: uS12

Chain XX:  95%



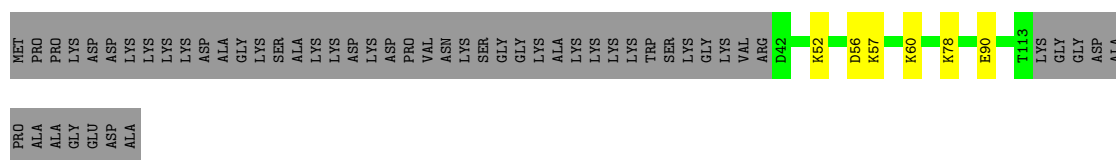
- Molecule 76: 40S ribosomal protein S24

Chain YY:  89% 5% 5%




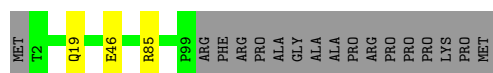
- Molecule 77: eS25

Chain ZZ:  53% 5% 42%



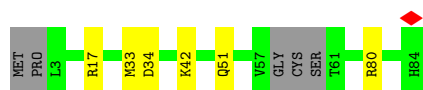
- Molecule 78: 40S ribosomal protein S26

Chain aa:  83% 15%




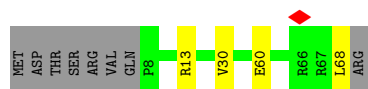
- Molecule 79: eS27

Chain bb:  87% 7% 6%




- Molecule 80: eS28

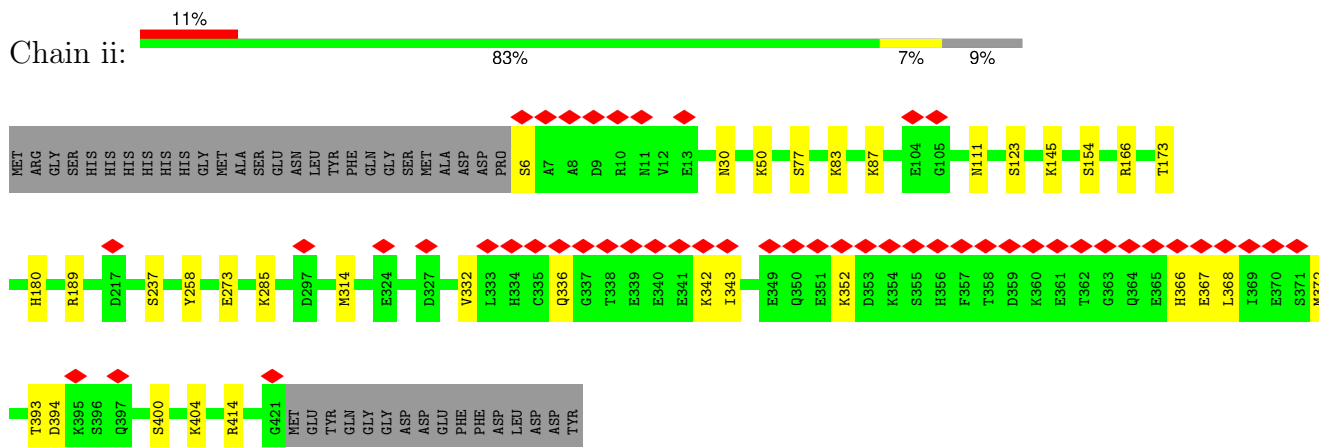
Chain cc:  83% 6% 12%



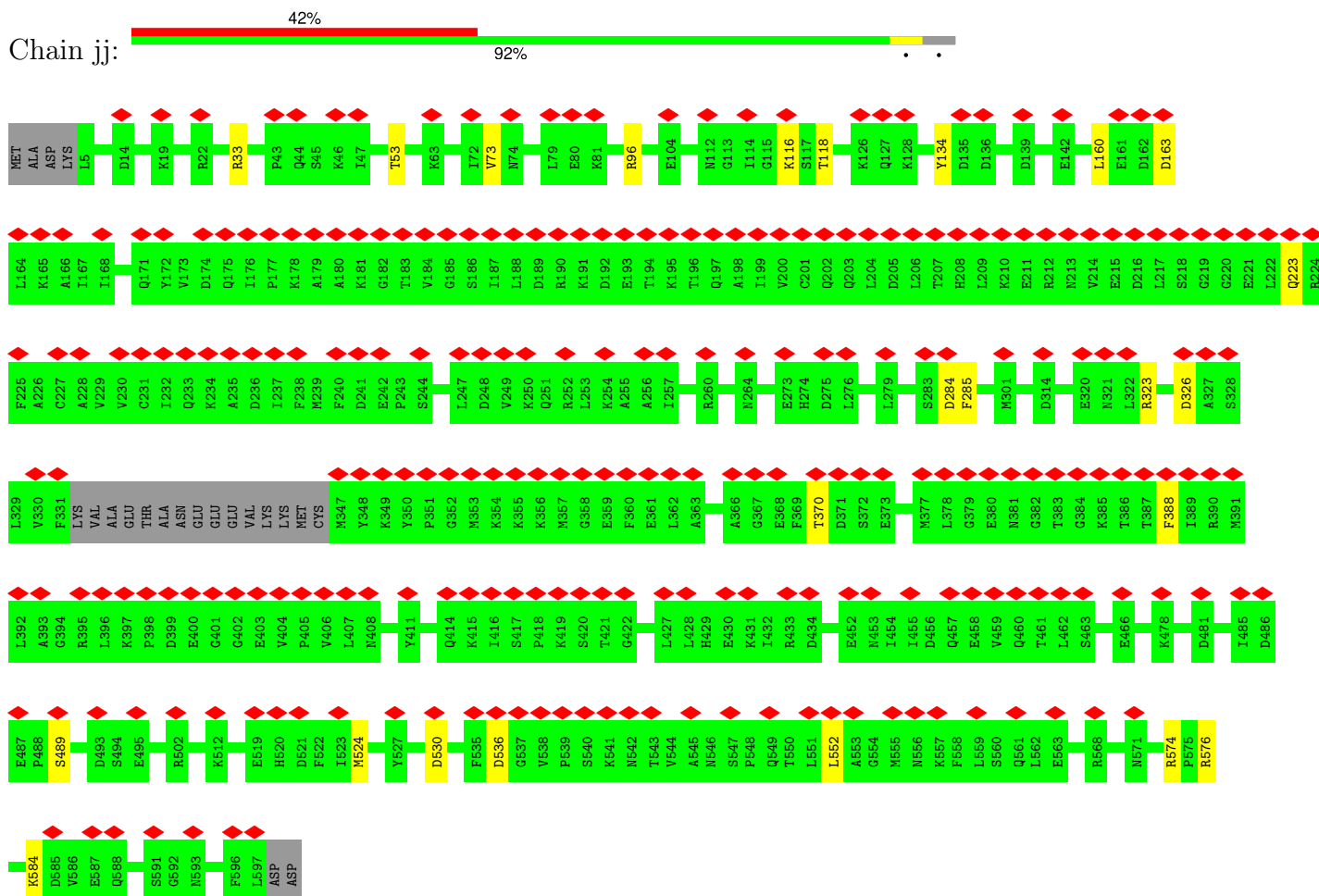
- Molecule 81: uS14

Chain dd:  84% 11% 5%

Chain ii:



Chain jj:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, OMC, OMU, B8N, 6MZ, ZVM, G7M, SF4, MA6, 1MA, UR3, 2MG, 5MC, UY1, MG, ZN, 4AC, B9B, A2M

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	0.39	0/1906	0.65	0/2556
2	B	0.39	0/3216	0.59	0/4311
3	C	0.38	0/2937	0.63	0/3946
4	D	0.38	0/2407	0.60	0/3224
5	E	0.37	0/1760	0.61	0/2362
6	F	0.40	0/1911	0.61	0/2549
7	G	0.36	0/1799	0.61	0/2424
8	H	0.36	0/1535	0.61	0/2063
9	I	0.37	0/1693	0.60	0/2260
10	J	0.36	0/1359	0.62	0/1817
11	L	0.36	0/1733	0.64	0/2316
12	M	0.36	0/1158	0.58	0/1547
13	N	0.42	0/1746	0.67	0/2338
14	O	0.37	0/1653	0.64	0/2210
15	P	0.39	0/1268	0.59	0/1700
16	Q	0.39	0/1539	0.68	0/2054
17	R	0.33	0/1518	0.65	0/2005
18	S	0.40	0/1501	0.63	0/2012
19	T	0.38	0/1326	0.59	0/1770
20	U	0.39	0/814	0.61	0/1092
21	V	0.38	0/987	0.61	0/1324
22	W	0.40	0/541	0.58	0/720
23	X	0.35	0/966	0.60	0/1301
24	Y	0.37	0/1132	0.62	0/1504
25	Z	0.41	0/1130	0.63	0/1507
26	a	0.41	0/1191	0.61	0/1590
27	b	0.39	0/619	0.57	0/818
28	c	0.39	0/742	0.58	0/995
29	d	0.36	0/846	0.62	0/1136
30	e	0.40	0/1071	0.62	0/1429
31	f	0.43	0/895	0.68	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.37	0/916	0.64	0/1220
33	h	0.35	0/1021	0.61	0/1348
34	i	0.35	0/841	0.64	0/1112
35	j	0.40	0/720	0.66	0/952
36	k	0.38	0/565	0.66	0/750
37	l	0.37	0/450	0.64	0/597
38	m	0.40	0/427	0.60	0/564
39	n	0.39	0/223	0.83	0/284
40	o	0.40	0/855	0.63	0/1128
41	p	0.37	0/718	0.60	0/953
42	r	0.38	0/1017	0.65	0/1364
43	s	0.31	0/1483	0.56	0/2000
44	t	0.29	0/1071	0.58	0/1444
45	1	0.37	0/129	0.58	0/173
46	2	0.55	0/1805	1.00	2/2809 (0.1%)
47	3	0.46	0/1777	0.99	0/2763
48	5	0.83	5/82331 (0.0%)	0.99	95/128398 (0.1%)
49	7	0.77	0/2858	0.88	0/4455
50	8	0.83	1/3675 (0.0%)	0.93	6/5725 (0.1%)
51	9	0.69	7/38943 (0.0%)	0.98	69/60686 (0.1%)
52	AA	0.34	0/1661	0.57	0/2259
53	BB	0.34	0/1749	0.58	0/2340
54	CC	0.35	0/1710	0.56	0/2312
55	DD	0.35	0/1749	0.60	0/2350
56	EE	0.35	0/2101	0.63	0/2828
57	FF	0.33	0/1461	0.57	0/1961
58	GG	0.33	0/1946	0.65	0/2590
59	HH	0.34	0/1447	0.60	0/1939
60	II	0.35	0/1715	0.64	0/2287
61	JJ	0.33	0/1550	0.64	0/2069
62	KK	0.36	0/752	0.59	0/1014
63	LL	0.37	0/1143	0.61	0/1529
64	MM	0.30	0/949	0.53	0/1274
65	NN	0.34	0/1232	0.59	0/1656
66	OO	0.39	0/969	0.71	0/1298
67	PP	0.33	0/986	0.63	0/1316
68	QQ	0.36	0/1134	0.62	0/1517
69	RR	0.34	0/973	0.61	0/1304
70	SS	0.33	0/1180	0.62	0/1581
71	TT	0.34	0/1093	0.60	0/1466
72	UU	0.32	0/817	0.62	0/1097
73	VV	0.34	0/623	0.61	0/833
74	WW	0.35	0/1051	0.59	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	XX	0.34	0/1116	0.61	0/1490
76	YY	0.35	0/1023	0.61	0/1359
77	ZZ	0.32	0/580	0.59	0/780
78	aa	0.36	0/794	0.64	0/1065
79	bb	0.33	0/640	0.58	0/856
80	cc	0.34	0/481	0.71	0/643
81	dd	0.35	0/455	0.65	0/603
82	ee	0.32	0/381	0.64	0/498
83	ff	0.34	0/538	0.64	0/713
84	gg	0.32	0/2427	0.58	0/3303
85	hh	0.63	0/264	0.95	0/409
86	ii	0.35	0/3333	0.59	0/4483
87	jj	0.31	0/4644	0.55	0/6272
All	All	0.63	13/233391 (0.0%)	0.85	172/341503 (0.1%)

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
57	FF	0	1
63	LL	0	1
All	All	0	2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	8	62	A	N9-C4	-7.30	1.33	1.37
48	5	978	G	N9-C4	-6.25	1.32	1.38
51	9	1675	A	N9-C4	-5.92	1.34	1.37
48	5	3775	A	N3-C4	-5.74	1.31	1.34
51	9	1130	G	N9-C4	-5.71	1.33	1.38

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	978	G	N3-C4-N9	-11.15	119.31	126.00
51	9	1779	G	N3-C4-N9	9.76	131.85	126.00
48	5	1612	G	N9-C4-C5	-9.75	101.50	105.40
48	5	255	C	N1-C2-O2	9.63	124.68	118.90
48	5	978	G	N3-C4-C5	9.42	133.31	128.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	FF	136	ARG	Sidechain
63	LL	118	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/257 (94%)	226 (93%)	16 (7%)	0	100	100
2	B	392/403 (97%)	376 (96%)	16 (4%)	0	100	100
3	C	360/413 (87%)	348 (97%)	12 (3%)	0	100	100
4	D	287/297 (97%)	270 (94%)	16 (6%)	1 (0%)	37	56
5	E	209/291 (72%)	189 (90%)	20 (10%)	0	100	100
6	F	223/247 (90%)	218 (98%)	5 (2%)	0	100	100
7	G	214/319 (67%)	202 (94%)	12 (6%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	200/214 (94%)	193 (96%)	7 (4%)	0	100	100
10	J	165/178 (93%)	151 (92%)	13 (8%)	1 (1%)	22	39
11	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
12	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
13	N	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
14	O	196/203 (97%)	187 (95%)	8 (4%)	1 (0%)	25	44
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
17	R	177/196 (90%)	172 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	96/128 (75%)	88 (92%)	8 (8%)	0	100	100
21	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
22	W	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
23	X	114/156 (73%)	108 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
25	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
26	a	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	19	35
27	b	73/245 (30%)	70 (96%)	3 (4%)	0	100	100
28	c	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
29	d	96/125 (77%)	94 (98%)	2 (2%)	0	100	100
30	e	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
31	f	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
32	g	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
33	h	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
34	i	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
35	j	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
36	k	66/70 (94%)	60 (91%)	5 (8%)	1 (2%)	8	16
37	l	47/51 (92%)	45 (96%)	2 (4%)	0	100	100
38	m	49/93 (53%)	47 (96%)	2 (4%)	0	100	100
39	n	21/25 (84%)	21 (100%)	0	0	100	100
40	o	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
41	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
42	r	123/137 (90%)	113 (92%)	10 (8%)	0	100	100
43	s	188/318 (59%)	163 (87%)	25 (13%)	0	100	100
44	t	135/165 (82%)	113 (84%)	21 (16%)	1 (1%)	19	35
45	1	13/130 (10%)	11 (85%)	2 (15%)	0	100	100
52	AA	204/295 (69%)	189 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BB	210/264 (80%)	200 (95%)	10 (5%)	0	100	100
54	CC	214/293 (73%)	202 (94%)	12 (6%)	0	100	100
55	DD	217/243 (89%)	196 (90%)	21 (10%)	0	100	100
56	EE	257/263 (98%)	231 (90%)	26 (10%)	0	100	100
57	FF	177/204 (87%)	163 (92%)	13 (7%)	1 (1%)	22	39
58	GG	235/249 (94%)	205 (87%)	29 (12%)	1 (0%)	30	49
59	HH	173/194 (89%)	146 (84%)	27 (16%)	0	100	100
60	II	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
61	JJ	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
62	KK	84/165 (51%)	76 (90%)	8 (10%)	0	100	100
63	LL	132/158 (84%)	125 (95%)	7 (5%)	0	100	100
64	MM	120/132 (91%)	91 (76%)	29 (24%)	0	100	100
65	NN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
66	OO	125/168 (74%)	121 (97%)	4 (3%)	0	100	100
67	PP	115/145 (79%)	106 (92%)	9 (8%)	0	100	100
68	QQ	138/146 (94%)	128 (93%)	10 (7%)	0	100	100
69	RR	116/135 (86%)	106 (91%)	10 (9%)	0	100	100
70	SS	138/152 (91%)	130 (94%)	8 (6%)	0	100	100
71	TT	136/145 (94%)	124 (91%)	12 (9%)	0	100	100
72	UU	100/119 (84%)	89 (89%)	11 (11%)	0	100	100
73	VV	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
76	YY	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
77	ZZ	70/125 (56%)	64 (91%)	6 (9%)	0	100	100
78	aa	96/115 (84%)	86 (90%)	10 (10%)	0	100	100
79	bb	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
80	cc	59/69 (86%)	54 (92%)	5 (8%)	0	100	100
81	dd	51/56 (91%)	45 (88%)	6 (12%)	0	100	100
82	ee	43/133 (32%)	37 (86%)	6 (14%)	0	100	100
83	ff	59/156 (38%)	49 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	gg	300/317 (95%)	252 (84%)	48 (16%)	0	100	100
86	ii	414/459 (90%)	380 (92%)	33 (8%)	1 (0%)	44	64
87	jj	574/599 (96%)	529 (92%)	44 (8%)	1 (0%)	44	64
All	All	12249/14542 (84%)	11407 (93%)	832 (7%)	10 (0%)	50	69

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	GG	128	THR
57	FF	33	ILE
86	ii	180	HIS
26	a	15	VAL
10	J	173	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/199 (94%)	181 (97%)	6 (3%)	34	60
2	B	336/348 (97%)	326 (97%)	10 (3%)	36	63
3	C	302/337 (90%)	291 (96%)	11 (4%)	30	56
4	D	245/250 (98%)	237 (97%)	8 (3%)	33	59
5	E	191/251 (76%)	183 (96%)	8 (4%)	25	49
6	F	196/215 (91%)	192 (98%)	4 (2%)	50	75
7	G	189/272 (70%)	180 (95%)	9 (5%)	21	43
8	H	169/171 (99%)	165 (98%)	4 (2%)	44	70
9	I	174/181 (96%)	169 (97%)	5 (3%)	37	64
10	J	140/149 (94%)	133 (95%)	7 (5%)	20	41
11	L	175/176 (99%)	168 (96%)	7 (4%)	27	51
12	M	117/161 (73%)	116 (99%)	1 (1%)	75	90
13	N	171/172 (99%)	168 (98%)	3 (2%)	54	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	170/173 (98%)	162 (95%)	8 (5%)	22	44
15	P	134/163 (82%)	130 (97%)	4 (3%)	36	63
16	Q	164/165 (99%)	159 (97%)	5 (3%)	36	63
17	R	158/175 (90%)	151 (96%)	7 (4%)	24	47
18	S	157/157 (100%)	152 (97%)	5 (3%)	34	60
19	T	139/140 (99%)	139 (100%)	0	100	100
20	U	88/114 (77%)	84 (96%)	4 (4%)	23	46
21	V	100/107 (94%)	99 (99%)	1 (1%)	73	88
22	W	55/126 (44%)	53 (96%)	2 (4%)	30	56
23	X	104/134 (78%)	102 (98%)	2 (2%)	52	77
24	Y	124/135 (92%)	119 (96%)	5 (4%)	27	51
25	Z	117/118 (99%)	110 (94%)	7 (6%)	16	33
26	a	119/120 (99%)	115 (97%)	4 (3%)	32	58
27	b	62/184 (34%)	60 (97%)	2 (3%)	34	60
28	c	80/98 (82%)	73 (91%)	7 (9%)	8	17
29	d	91/110 (83%)	90 (99%)	1 (1%)	70	87
30	e	114/121 (94%)	113 (99%)	1 (1%)	75	90
31	f	88/89 (99%)	87 (99%)	1 (1%)	70	87
32	g	98/100 (98%)	94 (96%)	4 (4%)	26	50
33	h	109/110 (99%)	103 (94%)	6 (6%)	18	37
34	i	86/89 (97%)	83 (96%)	3 (4%)	31	57
35	j	73/80 (91%)	67 (92%)	6 (8%)	9	19
36	k	63/65 (97%)	57 (90%)	6 (10%)	7	14
37	l	46/48 (96%)	44 (96%)	2 (4%)	25	48
38	m	47/84 (56%)	45 (96%)	2 (4%)	25	48
39	n	22/24 (92%)	22 (100%)	0	100	100
40	o	91/94 (97%)	89 (98%)	2 (2%)	47	73
41	p	74/75 (99%)	72 (97%)	2 (3%)	40	67
42	r	109/121 (90%)	106 (97%)	3 (3%)	38	65
43	s	159/258 (62%)	152 (96%)	7 (4%)	24	47
44	t	115/137 (84%)	106 (92%)	9 (8%)	10	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1	13/102 (13%)	12 (92%)	1 (8%)	10	22
52	AA	172/244 (70%)	161 (94%)	11 (6%)	14	30
53	BB	193/231 (84%)	185 (96%)	8 (4%)	26	50
54	CC	182/225 (81%)	170 (93%)	12 (7%)	14	28
55	DD	185/202 (92%)	170 (92%)	15 (8%)	9	20
56	EE	222/225 (99%)	210 (95%)	12 (5%)	18	37
57	FF	154/170 (91%)	140 (91%)	14 (9%)	7	16
58	GG	207/218 (95%)	184 (89%)	23 (11%)	5	10
59	HH	158/174 (91%)	144 (91%)	14 (9%)	8	17
60	II	178/180 (99%)	166 (93%)	12 (7%)	13	28
61	JJ	161/168 (96%)	152 (94%)	9 (6%)	17	36
62	KK	78/136 (57%)	71 (91%)	7 (9%)	8	16
63	LL	125/142 (88%)	121 (97%)	4 (3%)	34	60
64	MM	102/108 (94%)	94 (92%)	8 (8%)	10	21
65	NN	130/131 (99%)	123 (95%)	7 (5%)	18	37
66	OO	100/130 (77%)	92 (92%)	8 (8%)	10	20
67	PP	106/130 (82%)	97 (92%)	9 (8%)	8	18
68	QQ	116/121 (96%)	111 (96%)	5 (4%)	25	48
69	RR	107/121 (88%)	98 (92%)	9 (8%)	9	19
70	SS	122/132 (92%)	112 (92%)	10 (8%)	9	19
71	TT	109/115 (95%)	104 (95%)	5 (5%)	23	45
72	UU	93/107 (87%)	89 (96%)	4 (4%)	25	48
73	VV	65/67 (97%)	61 (94%)	4 (6%)	15	31
74	WW	112/113 (99%)	107 (96%)	5 (4%)	23	46
75	XX	113/115 (98%)	108 (96%)	5 (4%)	24	47
76	YY	107/112 (96%)	100 (94%)	7 (6%)	14	29
77	ZZ	64/103 (62%)	58 (91%)	6 (9%)	7	15
78	aa	85/98 (87%)	82 (96%)	3 (4%)	31	57
79	bb	72/76 (95%)	66 (92%)	6 (8%)	9	19
80	cc	54/62 (87%)	50 (93%)	4 (7%)	11	23
81	dd	47/49 (96%)	41 (87%)	6 (13%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	ee	39/106 (37%)	36 (92%)	3 (8%)	10	22
83	ff	59/140 (42%)	54 (92%)	5 (8%)	8	18
84	gg	263/275 (96%)	238 (90%)	25 (10%)	7	14
86	ii	358/394 (91%)	326 (91%)	32 (9%)	8	17
87	jj	508/526 (97%)	485 (96%)	23 (4%)	23	46
All	All	10707/12344 (87%)	10165 (95%)	542 (5%)	22	40

5 of 542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
84	gg	8	ARG
84	gg	131	LEU
84	gg	5	MET
87	jj	53	THR
44	t	17	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	8	GLN
62	KK	61	GLN
70	SS	97	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	0
47	3	72/75 (96%)	20 (27%)	0
48	5	3502/3543 (98%)	648 (18%)	72 (2%)
49	7	119/120 (99%)	11 (9%)	0
50	8	155/156 (99%)	29 (18%)	3 (1%)
51	9	1676/1869 (89%)	439 (26%)	36 (2%)
85	hh	10/197 (5%)	3 (30%)	0
All	All	5608/6036 (92%)	1170 (20%)	111 (1%)

5 of 1170 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	7	G
46	2	8	U
46	2	9	A
46	2	15	G
46	2	19	G

5 of 111 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	3876	A
51	9	1835	A
48	5	4947	U
51	9	1824	A
51	9	1408	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

163 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$
48	OMG	5	4499	48	19,26,27	2.47	8 (42%)	21,38,41	1.51	4 (19%)
48	OMC	5	2422	48,88	19,22,23	2.93	8 (42%)	25,31,34	0.72	0
48	OMG	5	4494	48	19,26,27	2.27	8 (42%)	21,38,41	1.44	5 (23%)
48	OMG	5	2876	48	19,26,27	2.37	8 (42%)	21,38,41	1.38	3 (14%)
51	OMU	9	116	51	19,22,23	2.80	6 (31%)	25,31,34	1.78	5 (20%)
50	OMG	8	75	50	19,26,27	2.33	8 (42%)	21,38,41	1.48	5 (23%)
48	6MZ	5	4220	48	17,25,26	1.38	1 (5%)	15,36,39	2.33	3 (20%)
48	A2M	5	3830	48	18,25,26	4.29	6 (33%)	20,36,39	3.36	5 (25%)
48	A2M	5	3825	48	18,25,26	4.40	6 (33%)	20,36,39	3.08	4 (20%)
48	OMC	5	2351	48	19,22,23	2.74	8 (42%)	25,31,34	0.82	0
51	A2M	9	668	51,88	18,25,26	4.35	5 (27%)	20,36,39	3.65	7 (35%)
48	A2M	5	1871	48,88	18,25,26	4.28	6 (33%)	20,36,39	3.28	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	5	4579	48	17,20,22	1.05	1 (5%)	21,28,33	1.89	4 (19%)
48	A2M	5	4571	48	18,25,26	4.48	7 (38%)	20,36,39	3.46	4 (20%)
48	OMG	5	3627	48	19,26,27	2.38	8 (42%)	21,38,41	1.48	3 (14%)
48	OMG	5	4623	48	19,26,27	2.44	8 (42%)	21,38,41	1.56	4 (19%)
48	A2M	5	1326	48	18,25,26	4.34	7 (38%)	20,36,39	3.33	4 (20%)
48	OMC	5	3869	48	19,22,23	2.83	7 (36%)	25,31,34	0.76	0
51	MA6	9	1850	51	19,26,27	1.74	2 (10%)	18,38,41	4.28	4 (22%)
51	PSU	9	1692	51	17,20,22	1.14	1 (5%)	21,28,33	1.78	3 (14%)
51	OMC	9	1703	51	19,22,23	2.96	8 (42%)	25,31,34	0.80	0
48	OMC	5	2365	48	19,22,23	2.84	8 (42%)	25,31,34	0.67	0
48	PSU	5	3851	48	17,20,22	1.09	2 (11%)	21,28,33	2.06	4 (19%)
48	OMC	5	2824	48	19,22,23	2.84	8 (42%)	25,31,34	0.95	1 (4%)
51	PSU	9	109	51	17,20,22	1.20	1 (5%)	21,28,33	2.02	4 (19%)
48	2MG	5	1517	48	18,26,27	2.27	7 (38%)	16,38,41	2.49	5 (31%)
51	PSU	9	822	51	17,20,22	1.23	3 (17%)	21,28,33	2.24	6 (28%)
51	PSU	9	1045	51	17,20,22	1.15	2 (11%)	21,28,33	2.14	5 (23%)
51	OMC	9	174	51	19,22,23	2.91	8 (42%)	25,31,34	0.95	0
48	OMG	5	2364	48	19,26,27	2.38	8 (42%)	21,38,41	1.51	3 (14%)
51	PSU	9	609	51	17,20,22	1.08	1 (5%)	21,28,33	2.01	4 (19%)
48	A2M	5	3760	48,88	18,25,26	4.46	6 (33%)	20,36,39	3.38	3 (15%)
48	PSU	5	1781	48	17,20,22	1.13	2 (11%)	21,28,33	1.96	5 (23%)
48	B9B	5	237	48	20,28,29	1.70	2 (10%)	19,40,43	2.13	6 (31%)
51	A2M	9	1678	51	18,25,26	4.37	6 (33%)	20,36,39	3.58	4 (20%)
48	A2M	5	3724	48	18,25,26	4.48	6 (33%)	20,36,39	3.18	4 (20%)
48	PSU	5	4296	48	17,20,22	1.20	2 (11%)	21,28,33	1.96	3 (14%)
51	OMG	9	509	51,88	19,26,27	2.35	8 (42%)	21,38,41	1.38	4 (19%)
51	A2M	9	512	51	18,25,26	4.40	5 (27%)	20,36,39	3.66	4 (20%)
51	OMG	9	683	51	19,26,27	2.49	8 (42%)	21,38,41	1.69	4 (19%)
48	A2M	5	3785	48	18,25,26	4.13	6 (33%)	20,36,39	3.64	5 (25%)
48	OMC	5	3841	48	19,22,23	2.82	8 (42%)	25,31,34	0.90	0
48	OMU	5	4227	48	19,22,23	2.83	7 (36%)	25,31,34	1.85	5 (20%)
48	5MC	5	4447	48,88	19,22,23	3.54	8 (42%)	26,32,35	1.14	2 (7%)
48	PSU	5	4423	48	17,20,22	1.00	1 (5%)	21,28,33	1.98	4 (19%)
48	PSU	5	3639	48	17,20,22	1.16	1 (5%)	21,28,33	1.91	4 (19%)
48	OMG	5	2424	48	19,26,27	2.35	8 (42%)	21,38,41	1.48	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMC	5	3701	48,88	19,22,23	2.76	8 (42%)	25,31,34	1.04	1 (4%)
48	OMG	5	4618	48	19,26,27	2.34	8 (42%)	21,38,41	1.60	5 (23%)
48	PSU	5	1683	48,88	17,20,22	1.23	1 (5%)	21,28,33	2.02	4 (19%)
51	PSU	9	686	51	17,20,22	1.02	2 (11%)	21,28,33	2.29	6 (28%)
51	A2M	9	166	51	18,25,26	4.31	5 (27%)	20,36,39	3.35	4 (20%)
51	6MZ	9	1832	51,88	17,25,26	1.22	1 (5%)	15,36,39	2.34	2 (13%)
48	PSU	5	3920	48	17,20,22	1.05	1 (5%)	21,28,33	2.18	5 (23%)
51	OMG	9	436	51	19,26,27	2.43	8 (42%)	21,38,41	1.49	4 (19%)
51	PSU	9	649	51	17,20,22	1.06	1 (5%)	21,28,33	1.89	4 (19%)
51	PSU	9	1232	51	17,20,22	1.20	1 (5%)	21,28,33	1.93	3 (14%)
48	OMC	5	2861	48	19,22,23	2.94	8 (42%)	25,31,34	0.84	1 (4%)
48	PSU	5	4403	48	17,20,22	1.10	1 (5%)	21,28,33	1.88	4 (19%)
48	A2M	5	2363	48,88	18,25,26	4.39	5 (27%)	20,36,39	3.39	4 (20%)
48	OMG	5	3899	48	19,26,27	2.34	8 (42%)	21,38,41	1.42	3 (14%)
51	OMU	9	121	51	19,22,23	2.72	6 (31%)	25,31,34	1.90	6 (24%)
51	A2M	9	1383	51	18,25,26	4.47	6 (33%)	20,36,39	3.67	5 (25%)
48	PSU	5	4521	48,88	17,20,22	1.24	2 (11%)	21,28,33	2.25	7 (33%)
48	PSU	5	4442	48	17,20,22	1.09	1 (5%)	21,28,33	2.09	5 (23%)
48	A2M	5	400	48	18,25,26	4.35	8 (44%)	20,36,39	3.12	5 (25%)
51	PSU	9	1347	51	17,20,22	1.08	1 (5%)	21,28,33	2.00	5 (23%)
51	PSU	9	1643	51	17,20,22	1.03	1 (5%)	21,28,33	2.08	4 (19%)
51	PSU	9	1174	51	17,20,22	1.11	1 (5%)	21,28,33	2.07	4 (19%)
48	PSU	5	2508	48	17,20,22	1.07	1 (5%)	21,28,33	1.92	4 (19%)
48	A2M	5	1534	48,88	18,25,26	4.45	6 (33%)	20,36,39	3.42	6 (30%)
51	PSU	9	572	51	17,20,22	1.08	1 (5%)	21,28,33	1.95	4 (19%)
51	A2M	9	27	51	18,25,26	4.31	5 (27%)	20,36,39	3.32	3 (15%)
48	A2M	5	2787	48	18,25,26	4.30	7 (38%)	20,36,39	3.24	4 (20%)
51	PSU	9	1445	51	17,20,22	1.05	1 (5%)	21,28,33	1.84	4 (19%)
48	PSU	5	3715	48	17,20,22	1.13	3 (17%)	21,28,33	2.10	6 (28%)
48	5MC	5	3782	48,88	19,22,23	3.55	8 (42%)	26,32,35	1.14	2 (7%)
51	OMG	9	1490	51,88	19,26,27	2.32	7 (36%)	21,38,41	1.33	4 (19%)
48	PSU	5	1860	48	17,20,22	1.03	1 (5%)	21,28,33	1.92	4 (19%)
48	PSU	5	4628	48	17,20,22	1.22	2 (11%)	21,28,33	2.19	6 (28%)
48	UY1	5	3818	48,88	19,22,23	4.33	9 (47%)	21,31,34	2.11	5 (23%)
48	PSU	5	4500	48	17,20,22	1.11	3 (17%)	21,28,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	5	4457	48	17,20,22	1.15	1 (5%)	21,28,33	1.77	3 (14%)
48	OMC	5	4536	48	19,22,23	2.77	8 (42%)	25,31,34	0.86	0
51	PSU	9	1046	51	17,20,22	1.13	1 (5%)	21,28,33	1.92	5 (23%)
48	OMG	5	1316	48	19,26,27	2.37	8 (42%)	21,38,41	1.59	3 (14%)
48	OMG	5	1625	48,88	19,26,27	2.51	8 (42%)	21,38,41	1.71	4 (19%)
48	OMU	5	2837	48	19,22,23	2.84	6 (31%)	25,31,34	2.02	6 (24%)
48	PSU	5	4293	48	17,20,22	1.22	2 (11%)	21,28,33	1.88	4 (19%)
48	OMG	5	4392	48	19,26,27	2.27	8 (42%)	21,38,41	1.45	4 (19%)
51	OMU	9	172	51	19,22,23	2.85	7 (36%)	25,31,34	1.82	5 (20%)
51	A2M	9	159	51	18,25,26	4.48	7 (38%)	20,36,39	3.37	4 (20%)
48	PSU	5	4420	48	17,20,22	1.13	1 (5%)	21,28,33	2.06	4 (19%)
48	PSU	5	3695	48	17,20,22	1.05	1 (5%)	21,28,33	1.97	4 (19%)
48	UR3	5	4530	48	19,22,23	2.64	8 (42%)	26,32,35	1.50	4 (15%)
48	OMG	5	4228	48	19,26,27	2.33	8 (42%)	21,38,41	1.42	3 (14%)
51	OMU	9	1442	51	19,22,23	2.84	6 (31%)	25,31,34	1.83	4 (16%)
51	PSU	9	814	51	17,20,22	1.08	1 (5%)	21,28,33	2.05	5 (23%)
48	1MA	5	1322	48,88	17,25,26	3.52	5 (29%)	17,37,40	1.93	3 (17%)
51	PSU	9	1177	51	17,20,22	1.08	1 (5%)	21,28,33	1.77	4 (19%)
51	PSU	9	1238	51	17,20,22	1.22	2 (11%)	21,28,33	2.00	4 (19%)
48	PSU	5	1677	48	17,20,22	1.25	2 (11%)	21,28,33	2.17	4 (19%)
51	A2M	9	99	51,88	18,25,26	4.46	6 (33%)	20,36,39	3.36	4 (20%)
51	PSU	9	119	51	17,20,22	1.08	1 (5%)	21,28,33	2.02	5 (23%)
51	4AC	9	1842	51	21,24,25	3.00	10 (47%)	28,34,37	1.08	2 (7%)
48	OMU	5	4620	48	19,22,23	2.83	7 (36%)	25,31,34	1.87	5 (20%)
51	PSU	9	815	51	17,20,22	1.06	1 (5%)	21,28,33	2.17	5 (23%)
51	PSU	9	1081	51	17,20,22	1.14	1 (5%)	21,28,33	2.03	6 (28%)
48	PSU	5	4299	48	17,20,22	1.00	1 (5%)	21,28,33	1.94	3 (14%)
48	OMG	5	1522	48	19,26,27	2.38	8 (42%)	21,38,41	1.50	4 (19%)
51	A2M	9	468	51	18,25,26	4.44	7 (38%)	20,36,39	3.33	4 (20%)
48	OMG	5	3792	48	19,26,27	2.29	7 (36%)	21,38,41	1.41	4 (19%)
48	OMC	5	4456	48	19,22,23	2.80	8 (42%)	25,31,34	0.77	0
51	OMG	9	644	51	19,26,27	2.35	7 (36%)	21,38,41	1.33	3 (14%)
48	OMG	5	4196	48,46	19,26,27	2.41	8 (42%)	21,38,41	1.44	4 (19%)
48	PSU	5	4532	48	17,20,22	1.12	1 (5%)	21,28,33	1.76	3 (14%)
51	4AC	9	1337	51	21,24,25	3.09	10 (47%)	28,34,37	1.03	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMC	5	3887	48	19,22,23	2.78	7 (36%)	25,31,34	0.77	1 (4%)
51	OMU	9	1326	51	19,22,23	2.81	7 (36%)	25,31,34	1.95	5 (20%)
48	PSU	5	3762	48	17,20,22	1.14	1 (5%)	21,28,33	2.13	5 (23%)
48	PSU	5	3853	48	17,20,22	1.21	1 (5%)	21,28,33	2.19	5 (23%)
51	A2M	9	484	51	18,25,26	4.46	5 (27%)	20,36,39	3.56	3 (15%)
48	A2M	5	398	48	18,25,26	4.49	7 (38%)	20,36,39	3.29	3 (15%)
48	OMG	5	4637	48	19,26,27	2.35	8 (42%)	21,38,41	1.49	4 (19%)
51	OMG	9	1328	51	19,26,27	2.36	8 (42%)	21,38,41	1.41	4 (19%)
48	PSU	5	1862	48	17,20,22	1.11	1 (5%)	21,28,33	1.99	5 (23%)
51	B8N	9	1248	51	25,29,30	3.40	8 (32%)	28,42,45	2.31	7 (25%)
51	PSU	9	1004	51	17,20,22	1.13	1 (5%)	21,28,33	1.99	4 (19%)
51	OMC	9	1391	51	19,22,23	2.96	8 (42%)	25,31,34	0.97	1 (4%)
48	A2M	5	1524	48	18,25,26	4.25	6 (33%)	20,36,39	3.63	4 (20%)
48	PSU	5	3734	48	17,20,22	1.19	2 (11%)	21,28,33	1.93	5 (23%)
51	PSU	9	1244	51	17,20,22	1.17	1 (5%)	21,28,33	2.06	5 (23%)
51	PSU	9	105	51	17,20,22	1.14	1 (5%)	21,28,33	2.00	4 (19%)
51	MA6	9	1851	51	19,26,27	1.59	3 (15%)	18,38,41	4.96	4 (22%)
48	PSU	5	3764	48	17,20,22	1.18	1 (5%)	21,28,33	2.04	5 (23%)
51	PSU	9	801	51	17,20,22	1.25	2 (11%)	21,28,33	1.67	4 (19%)
48	A2M	5	3867	48	18,25,26	4.29	6 (33%)	20,36,39	3.26	3 (15%)
51	OMC	9	517	51	19,22,23	2.99	8 (42%)	25,31,34	0.82	0
48	OMU	5	4498	48	19,22,23	2.81	8 (42%)	25,31,34	1.93	5 (20%)
51	PSU	9	1367	51	17,20,22	1.15	1 (5%)	21,28,33	1.90	4 (19%)
48	PSU	5	1792	48	17,20,22	1.03	1 (5%)	21,28,33	1.89	3 (14%)
48	OMU	5	4306	48	19,22,23	2.86	7 (36%)	25,31,34	1.85	4 (16%)
48	PSU	5	2632	48	17,20,22	1.15	1 (5%)	21,28,33	1.97	4 (19%)
48	OMU	5	3925	48	19,22,23	2.81	7 (36%)	25,31,34	1.88	4 (16%)
51	OMU	9	428	51	19,22,23	2.87	7 (36%)	25,31,34	1.79	5 (20%)
51	PSU	9	34	51	17,20,22	1.16	1 (5%)	21,28,33	1.96	4 (19%)
48	PSU	5	4552	48	17,20,22	1.16	1 (5%)	21,28,33	1.93	4 (19%)
48	OMC	5	3808	48	19,22,23	2.74	8 (42%)	25,31,34	0.65	0
48	A2M	5	4523	48,88	18,25,26	4.30	6 (33%)	20,36,39	3.43	4 (20%)
48	OMG	5	373	48	19,26,27	2.36	8 (42%)	21,38,41	1.53	3 (14%)
51	G7M	9	1639	51,46	20,26,27	2.64	8 (40%)	16,39,42	1.10	2 (12%)
48	OMC	5	1340	48	19,22,23	2.97	8 (42%)	25,31,34	1.01	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMC	5	2804	48	19,22,23	2.79	8 (42%)	25,31,34	0.72	0
48	A2M	5	3718	48	18,25,26	4.47	6 (33%)	20,36,39	3.42	5 (25%)
48	PSU	5	1782	48	17,20,22	1.10	1 (5%)	21,28,33	2.01	5 (23%)
51	PSU	9	218	51	17,20,22	1.13	1 (5%)	21,28,33	2.28	7 (33%)
48	PSU	5	4361	48	17,20,22	1.11	1 (5%)	21,28,33	2.01	5 (23%)
48	OMG	5	4370	48	19,26,27	2.35	8 (42%)	21,38,41	1.51	4 (19%)
48	PSU	5	4353	48	17,20,22	1.12	2 (11%)	21,28,33	2.11	5 (23%)
51	PSU	9	863	51	17,20,22	0.99	1 (5%)	21,28,33	1.93	3 (14%)
51	A2M	9	1031	51	18,25,26	4.40	6 (33%)	20,36,39	3.24	4 (20%)
48	A2M	5	2815	48	18,25,26	4.30	6 (33%)	20,36,39	3.34	4 (20%)
48	PSU	5	1744	48,88	17,20,22	0.96	1 (5%)	21,28,33	2.01	4 (19%)

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
48	OMG	5	4499	48	-	1/5/27/28	0/3/3/3
48	OMC	5	2422	48,88	-	0/9/27/28	0/2/2/2
48	OMG	5	4494	48	-	1/5/27/28	0/3/3/3
48	OMG	5	2876	48	-	0/5/27/28	0/3/3/3
51	OMU	9	116	51	-	0/9/27/28	0/2/2/2
50	OMG	8	75	50	-	0/5/27/28	0/3/3/3
48	6MZ	5	4220	48	-	0/5/27/28	0/3/3/3
48	A2M	5	3830	48	-	0/5/27/28	0/3/3/3
48	A2M	5	3825	48	-	0/5/27/28	0/3/3/3
48	OMC	5	2351	48	-	1/9/27/28	0/2/2/2
51	A2M	9	668	51,88	-	2/5/27/28	0/3/3/3
48	A2M	5	1871	48,88	-	0/5/27/28	0/3/3/3
48	PSU	5	4579	48	-	0/6/24/26	0/2/2/2
48	A2M	5	4571	48	-	0/5/27/28	0/3/3/3
48	OMG	5	3627	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4623	48	-	0/5/27/28	0/3/3/3
48	A2M	5	1326	48	-	1/5/27/28	0/3/3/3
48	OMC	5	3869	48	-	0/9/27/28	0/2/2/2
51	MA6	9	1850	51	-	0/7/29/30	0/3/3/3
51	PSU	9	1692	51	-	0/6/24/26	0/2/2/2
51	OMC	9	1703	51	-	2/9/27/28	0/2/2/2
48	OMC	5	2365	48	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	5	3851	48	-	1/6/24/26	0/2/2/2
48	OMC	5	2824	48	-	0/9/27/28	0/2/2/2
51	PSU	9	109	51	-	0/6/24/26	0/2/2/2
48	2MG	5	1517	48	-	0/5/27/28	0/3/3/3
51	PSU	9	822	51	-	2/6/24/26	0/2/2/2
51	PSU	9	1045	51	-	2/6/24/26	0/2/2/2
51	OMC	9	174	51	-	0/9/27/28	0/2/2/2
48	OMG	5	2364	48	-	3/5/27/28	0/3/3/3
51	PSU	9	609	51	-	0/6/24/26	0/2/2/2
48	A2M	5	3760	48,88	-	3/5/27/28	0/3/3/3
48	PSU	5	1781	48	-	2/6/24/26	0/2/2/2
48	B9B	5	237	48	-	2/7/29/30	0/3/3/3
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
48	A2M	5	3724	48	-	0/5/27/28	0/3/3/3
48	PSU	5	4296	48	-	0/6/24/26	0/2/2/2
51	OMG	9	509	51,88	-	0/5/27/28	0/3/3/3
51	A2M	9	512	51	-	1/5/27/28	0/3/3/3
51	OMG	9	683	51	-	3/5/27/28	0/3/3/3
48	A2M	5	3785	48	-	2/5/27/28	0/3/3/3
48	OMC	5	3841	48	-	0/9/27/28	0/2/2/2
48	OMU	5	4227	48	-	0/9/27/28	0/2/2/2
48	5MC	5	4447	48,88	-	4/7/25/26	0/2/2/2
48	PSU	5	4423	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3639	48	-	0/6/24/26	0/2/2/2
48	OMG	5	2424	48	-	3/5/27/28	0/3/3/3
48	OMC	5	3701	48,88	-	4/9/27/28	0/2/2/2
48	OMG	5	4618	48	-	0/5/27/28	0/3/3/3
48	PSU	5	1683	48,88	-	0/6/24/26	0/2/2/2
51	PSU	9	686	51	-	0/6/24/26	0/2/2/2
51	A2M	9	166	51	-	2/5/27/28	0/3/3/3
51	6MZ	9	1832	51,88	-	2/5/27/28	0/3/3/3
48	PSU	5	3920	48	-	0/6/24/26	0/2/2/2
51	OMG	9	436	51	-	0/5/27/28	0/3/3/3
51	PSU	9	649	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1232	51	-	0/6/24/26	0/2/2/2
48	OMC	5	2861	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4403	48	-	0/6/24/26	0/2/2/2
48	A2M	5	2363	48,88	-	0/5/27/28	0/3/3/3
48	OMG	5	3899	48	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMU	9	121	51	-	1/9/27/28	0/2/2/2
51	A2M	9	1383	51	-	0/5/27/28	0/3/3/3
48	PSU	5	4521	48,88	-	0/6/24/26	0/2/2/2
48	PSU	5	4442	48	-	0/6/24/26	0/2/2/2
48	A2M	5	400	48	-	0/5/27/28	0/3/3/3
51	PSU	9	1347	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1643	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1174	51	-	0/6/24/26	0/2/2/2
48	PSU	5	2508	48	-	0/6/24/26	0/2/2/2
48	A2M	5	1534	48,88	-	2/5/27/28	0/3/3/3
51	PSU	9	572	51	-	0/6/24/26	0/2/2/2
51	A2M	9	27	51	-	0/5/27/28	0/3/3/3
48	A2M	5	2787	48	-	0/5/27/28	0/3/3/3
51	PSU	9	1445	51	-	1/6/24/26	0/2/2/2
48	PSU	5	3715	48	-	0/6/24/26	0/2/2/2
48	5MC	5	3782	48,88	-	0/7/25/26	0/2/2/2
51	OMG	9	1490	51,88	-	2/5/27/28	0/3/3/3
48	PSU	5	1860	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4628	48	-	0/6/24/26	0/2/2/2
48	UY1	5	3818	48,88	-	3/9/27/28	0/2/2/2
48	PSU	5	4500	48	-	2/6/24/26	0/2/2/2
48	PSU	5	4457	48	-	0/6/24/26	0/2/2/2
48	OMC	5	4536	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1046	51	-	0/6/24/26	0/2/2/2
48	OMG	5	1316	48	-	0/5/27/28	0/3/3/3
48	OMG	5	1625	48,88	-	1/5/27/28	0/3/3/3
48	OMU	5	2837	48	-	1/9/27/28	0/2/2/2
48	PSU	5	4293	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4392	48	-	0/5/27/28	0/3/3/3
51	OMU	9	172	51	-	2/9/27/28	0/2/2/2
51	A2M	9	159	51	-	0/5/27/28	0/3/3/3
48	PSU	5	4420	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3695	48	-	0/6/24/26	0/2/2/2
48	UR3	5	4530	48	-	0/7/25/26	0/2/2/2
48	OMG	5	4228	48	-	1/5/27/28	0/3/3/3
51	OMU	9	1442	51	-	2/9/27/28	0/2/2/2
51	PSU	9	814	51	-	0/6/24/26	0/2/2/2
48	1MA	5	1322	48,88	-	0/3/25/26	0/3/3/3
51	PSU	9	1177	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1238	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1677	48	-	0/6/24/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	9	99	51,88	-	2/5/27/28	0/3/3/3
51	PSU	9	119	51	-	0/6/24/26	0/2/2/2
51	4AC	9	1842	51	-	0/11/29/30	0/2/2/2
48	OMU	5	4620	48	-	0/9/27/28	0/2/2/2
51	PSU	9	815	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1081	51	-	0/6/24/26	0/2/2/2
48	PSU	5	4299	48	-	0/6/24/26	0/2/2/2
48	OMG	5	1522	48	-	0/5/27/28	0/3/3/3
51	A2M	9	468	51	-	1/5/27/28	0/3/3/3
48	OMG	5	3792	48	-	2/5/27/28	0/3/3/3
48	OMC	5	4456	48	-	0/9/27/28	0/2/2/2
51	OMG	9	644	51	-	1/5/27/28	0/3/3/3
48	OMG	5	4196	48,46	-	0/5/27/28	0/3/3/3
48	PSU	5	4532	48	-	0/6/24/26	0/2/2/2
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
48	OMC	5	3887	48	-	0/9/27/28	0/2/2/2
51	OMU	9	1326	51	-	0/9/27/28	0/2/2/2
48	PSU	5	3762	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3853	48	-	0/6/24/26	0/2/2/2
51	A2M	9	484	51	-	0/5/27/28	0/3/3/3
48	A2M	5	398	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4637	48	-	0/5/27/28	0/3/3/3
51	OMG	9	1328	51	-	1/5/27/28	0/3/3/3
48	PSU	5	1862	48	-	0/6/24/26	0/2/2/2
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
51	PSU	9	1004	51	-	0/6/24/26	0/2/2/2
51	OMC	9	1391	51	-	0/9/27/28	0/2/2/2
48	A2M	5	1524	48	-	1/5/27/28	0/3/3/3
48	PSU	5	3734	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1244	51	-	0/6/24/26	0/2/2/2
51	PSU	9	105	51	-	0/6/24/26	0/2/2/2
51	MA6	9	1851	51	-	3/7/29/30	0/3/3/3
48	PSU	5	3764	48	-	0/6/24/26	0/2/2/2
51	PSU	9	801	51	-	2/6/24/26	0/2/2/2
48	A2M	5	3867	48	-	1/5/27/28	0/3/3/3
51	OMC	9	517	51	-	0/9/27/28	0/2/2/2
48	OMU	5	4498	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1367	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1792	48	-	0/6/24/26	0/2/2/2
48	OMU	5	4306	48	-	0/9/27/28	0/2/2/2
48	PSU	5	2632	48	-	0/6/24/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	5	3925	48	-	0/9/27/28	0/2/2/2
51	OMU	9	428	51	-	4/9/27/28	0/2/2/2
51	PSU	9	34	51	-	4/6/24/26	0/2/2/2
48	PSU	5	4552	48	-	0/6/24/26	0/2/2/2
48	OMC	5	3808	48	-	0/9/27/28	0/2/2/2
48	A2M	5	4523	48,88	-	0/5/27/28	0/3/3/3
48	OMG	5	373	48	-	1/5/27/28	0/3/3/3
51	G7M	9	1639	51,46	-	2/3/25/26	0/3/3/3
48	OMC	5	1340	48	-	0/9/27/28	0/2/2/2
48	OMC	5	2804	48	-	0/9/27/28	0/2/2/2
48	A2M	5	3718	48	-	0/5/27/28	0/3/3/3
48	PSU	5	1782	48	-	0/6/24/26	0/2/2/2
51	PSU	9	218	51	-	0/6/24/26	0/2/2/2
48	PSU	5	4361	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4370	48	-	0/5/27/28	0/3/3/3
48	PSU	5	4353	48	-	0/6/24/26	0/2/2/2
51	PSU	9	863	51	-	2/6/24/26	0/2/2/2
51	A2M	9	1031	51	-	1/5/27/28	0/3/3/3
48	A2M	5	2815	48	-	2/5/27/28	0/3/3/3
48	PSU	5	1744	48,88	-	0/6/24/26	0/2/2/2

The worst 5 of 776 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1383	A2M	O4'-C1'	16.64	1.62	1.40
48	5	3724	A2M	O4'-C1'	16.59	1.62	1.40
51	9	99	A2M	O4'-C1'	16.56	1.62	1.40
48	5	398	A2M	O4'-C1'	16.55	1.62	1.40
51	9	159	A2M	O4'-C1'	16.48	1.62	1.40

The worst 5 of 617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1851	MA6	N1-C6-N6	-16.80	97.42	116.83
51	9	1850	MA6	N1-C6-N6	-13.95	100.72	116.83
51	9	512	A2M	C5-C6-N6	11.97	138.54	120.31
51	9	484	A2M	C5-C6-N6	11.70	138.13	120.31
51	9	1678	A2M	C5-C6-N6	11.45	137.75	120.31

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	5	237	B9B	C5-C6-O6-C61
48	5	237	B9B	N1-C6-O6-C61
48	5	1781	PSU	C3'-C4'-C5'-O5'
48	5	2424	OMG	O4'-C4'-C5'-O5'
48	5	2424	OMG	C1'-C2'-O2'-CM2

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 323 ligands modelled in this entry, 320 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
90	ZVM	ii	501	88	30,31,31	4.96	21 (70%)	32,46,46	3.11	7 (21%)
91	SF4	jj	602	87	0,12,12	-	-	-	-	-
91	SF4	jj	601	87	0,12,12	-	-	-	-	-

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
90	ZVM	ii	501	88	2/2/8/8	0/4/50/50	0/3/5/5
91	SF4	jj	602	87	-	-	0/6/5/5
91	SF4	jj	601	87	-	-	0/6/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	ii	501	ZVM	O01-C01	12.83	1.39	1.22
90	ii	501	ZVM	O02-C15	9.69	1.39	1.22
90	ii	501	ZVM	C13-C14	8.13	1.52	1.38
90	ii	501	ZVM	C10-C09	7.54	1.53	1.39
90	ii	501	ZVM	C03-N01	7.44	1.38	1.27

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	ii	501	ZVM	C05-C04-N01	11.95	121.33	109.91
90	ii	501	ZVM	O01-C01-C02	-9.29	118.89	126.79
90	ii	501	ZVM	C05-C04-N02	4.49	119.42	111.94
90	ii	501	ZVM	N02-C04-N01	4.29	119.25	113.37
90	ii	501	ZVM	C21-C22-C17	2.77	121.99	118.81

All (2) chirality outliers are listed below:

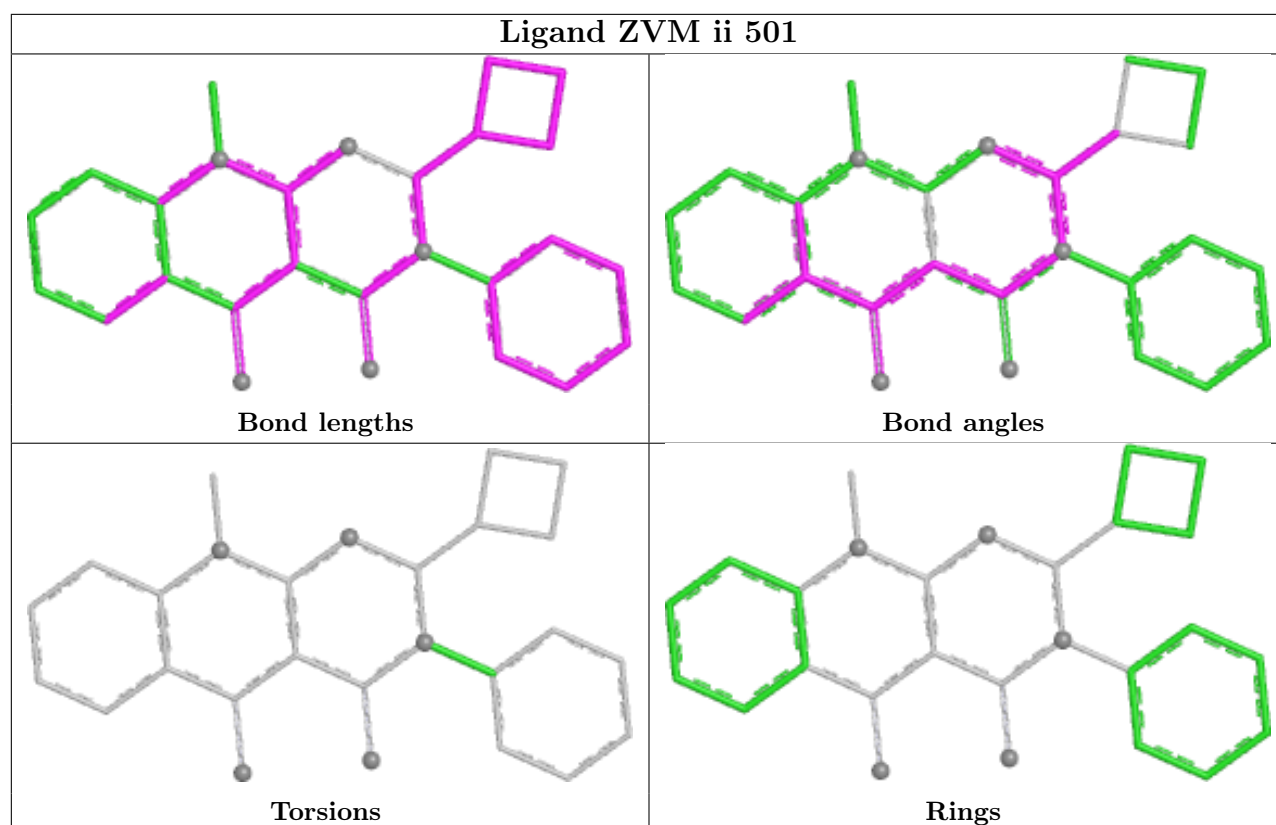
Mol	Chain	Res	Type	Atom
90	ii	501	ZVM	C04
90	ii	501	ZVM	C02

There are no torsion outliers.

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
48	5	23
51	9	3
47	3	2
46	2	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	41.98
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	16.99
1	5	1696:C	O3'	1720:C	P	16.41
1	5	990:C	O3'	1064:G	P	15.53

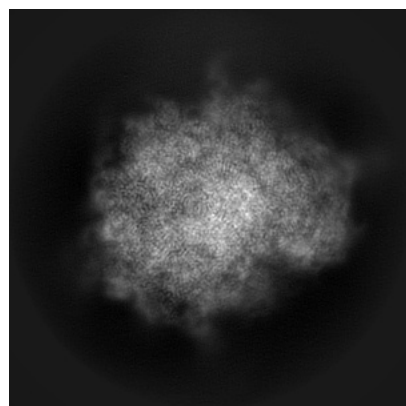
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40344. These allow visual inspection of the internal detail of the map and identification of artifacts.

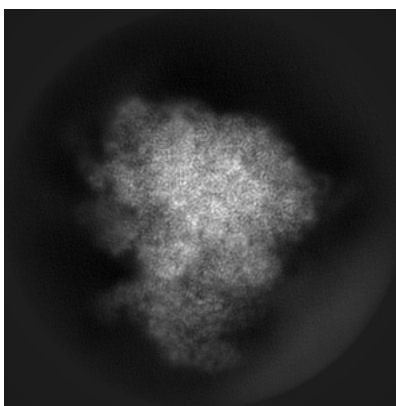
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

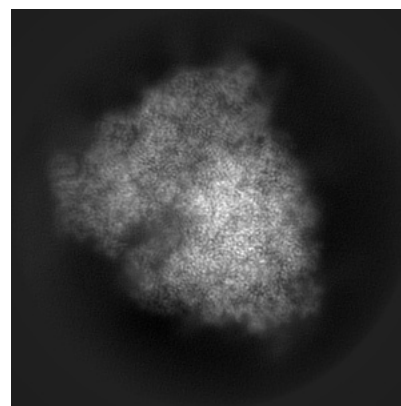
6.1.1 Primary map



X

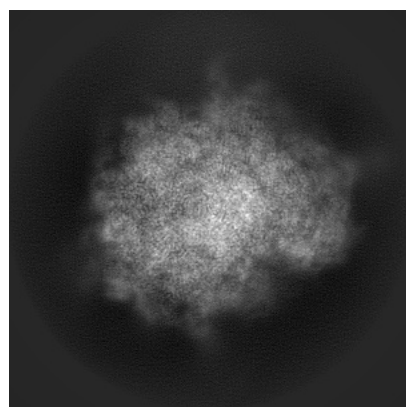


Y

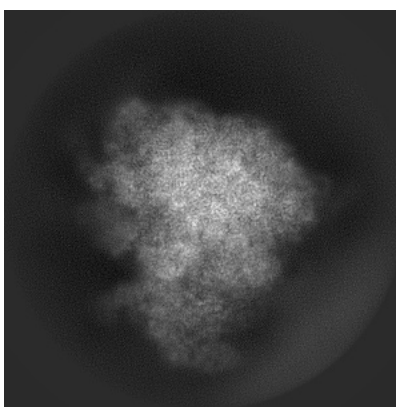


Z

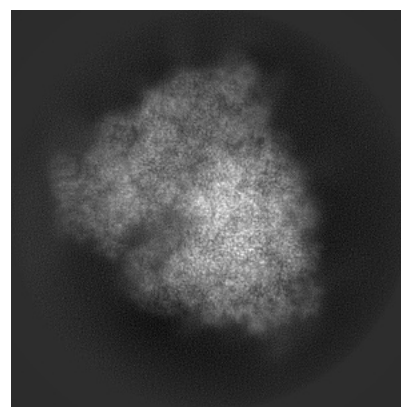
6.1.2 Raw map



X



Y

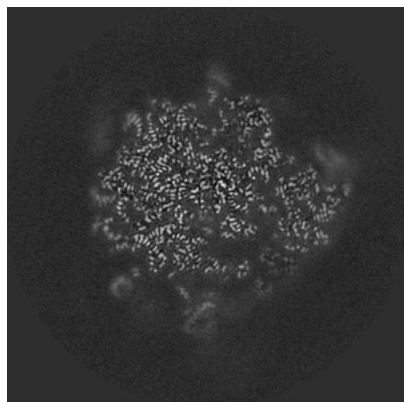


Z

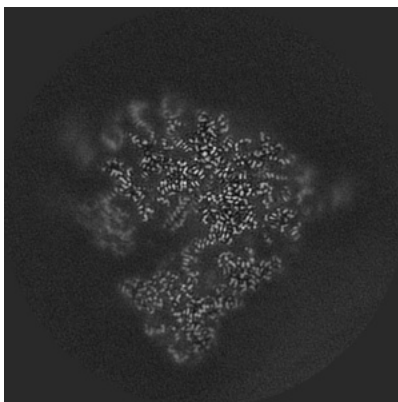
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

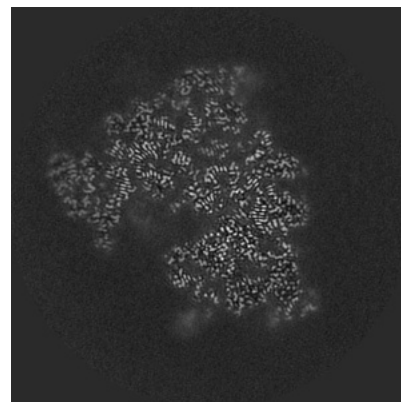
6.2.1 Primary map



X Index: 240

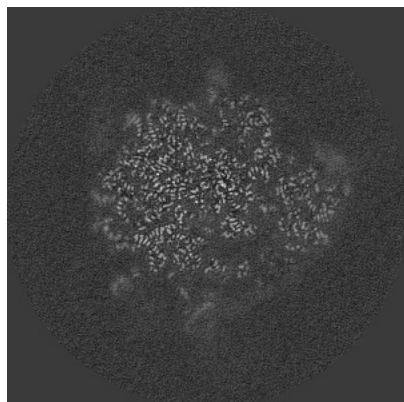


Y Index: 240

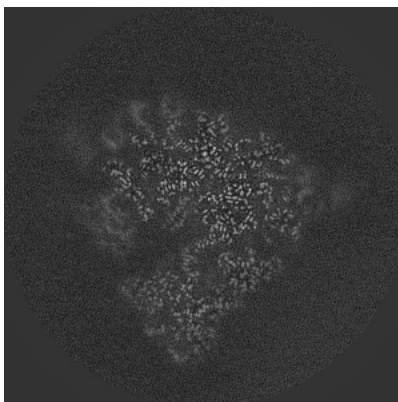


Z Index: 240

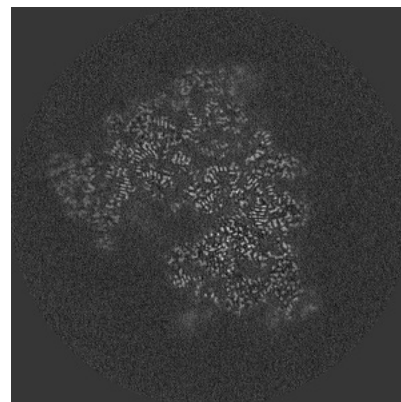
6.2.2 Raw map



X Index: 240



Y Index: 240

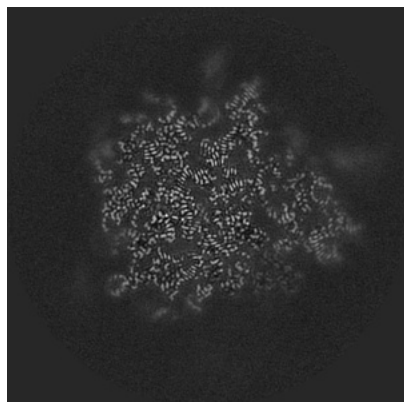


Z Index: 240

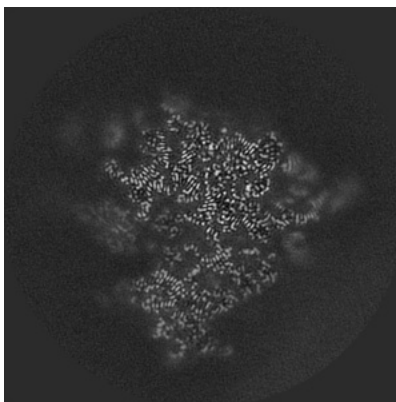
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

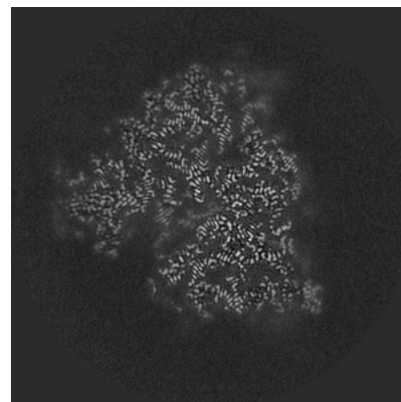
6.3.1 Primary map



X Index: 261

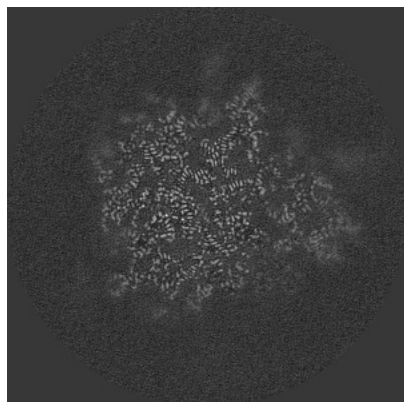


Y Index: 250

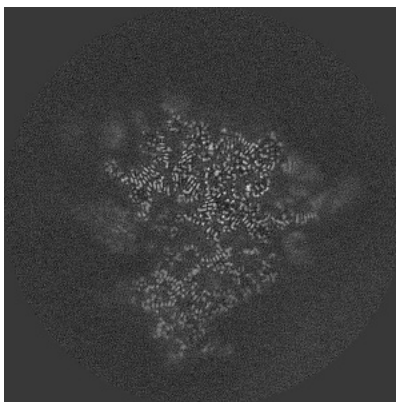


Z Index: 227

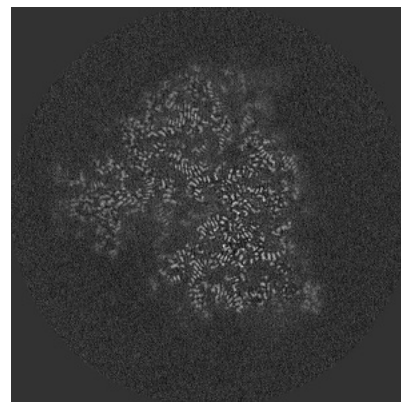
6.3.2 Raw map



X Index: 261



Y Index: 250

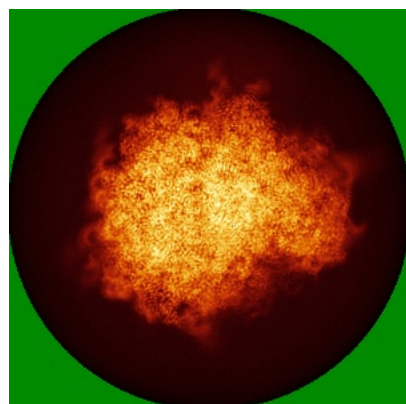


Z Index: 228

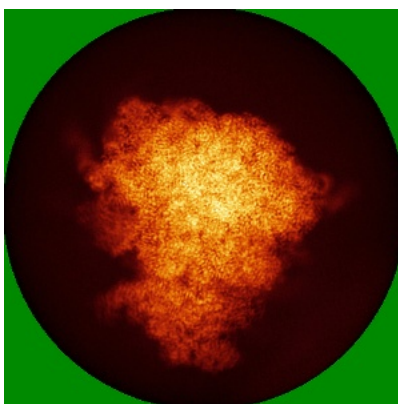
The images above show the largest variance slices of the map in three orthogonal directions.

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

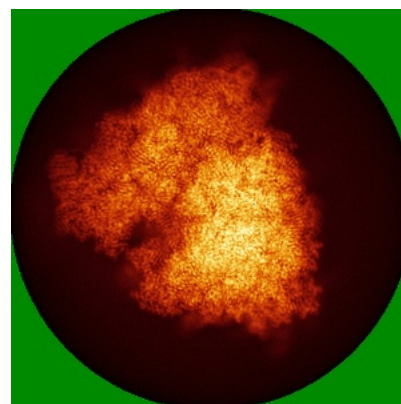
6.4.1 Primary map



X

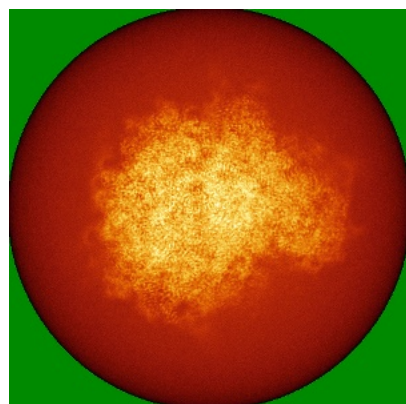


Y

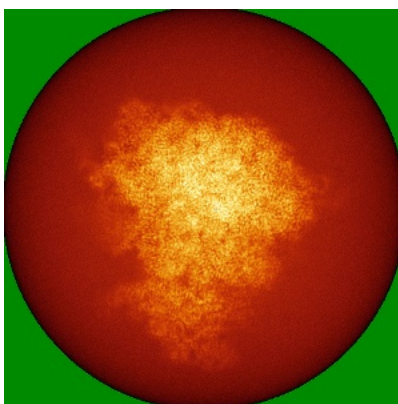


Z

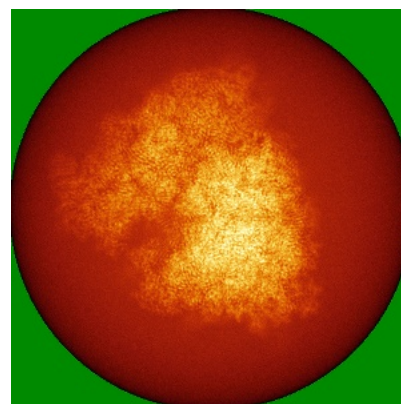
6.4.2 Raw map



X



Y

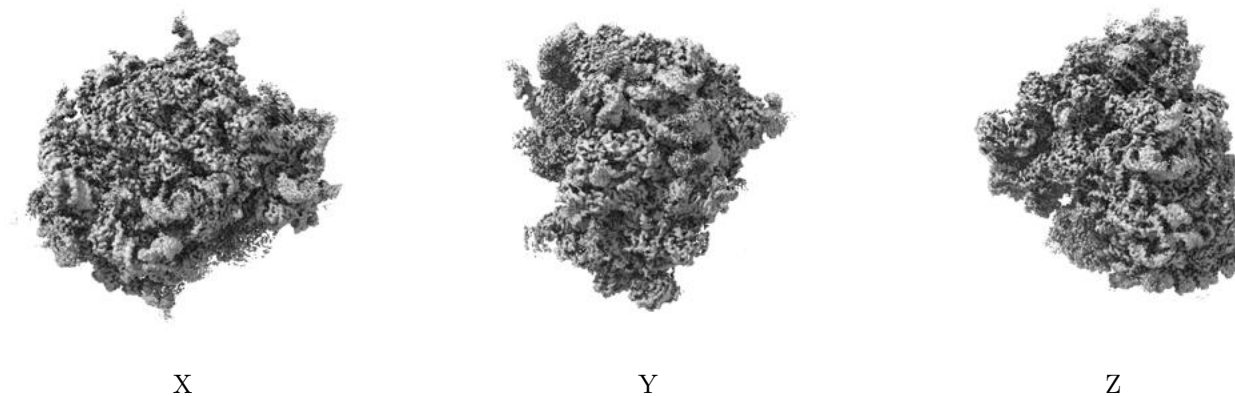


Z

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.

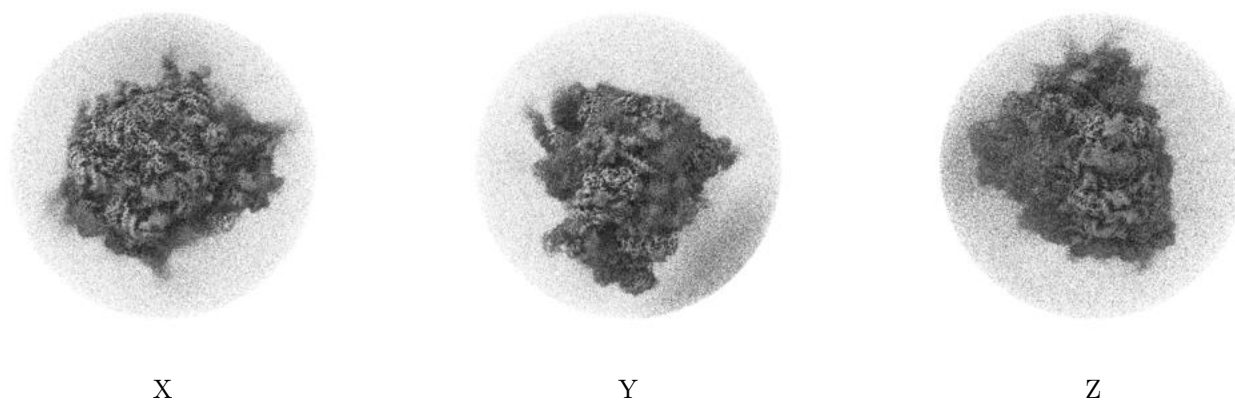
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

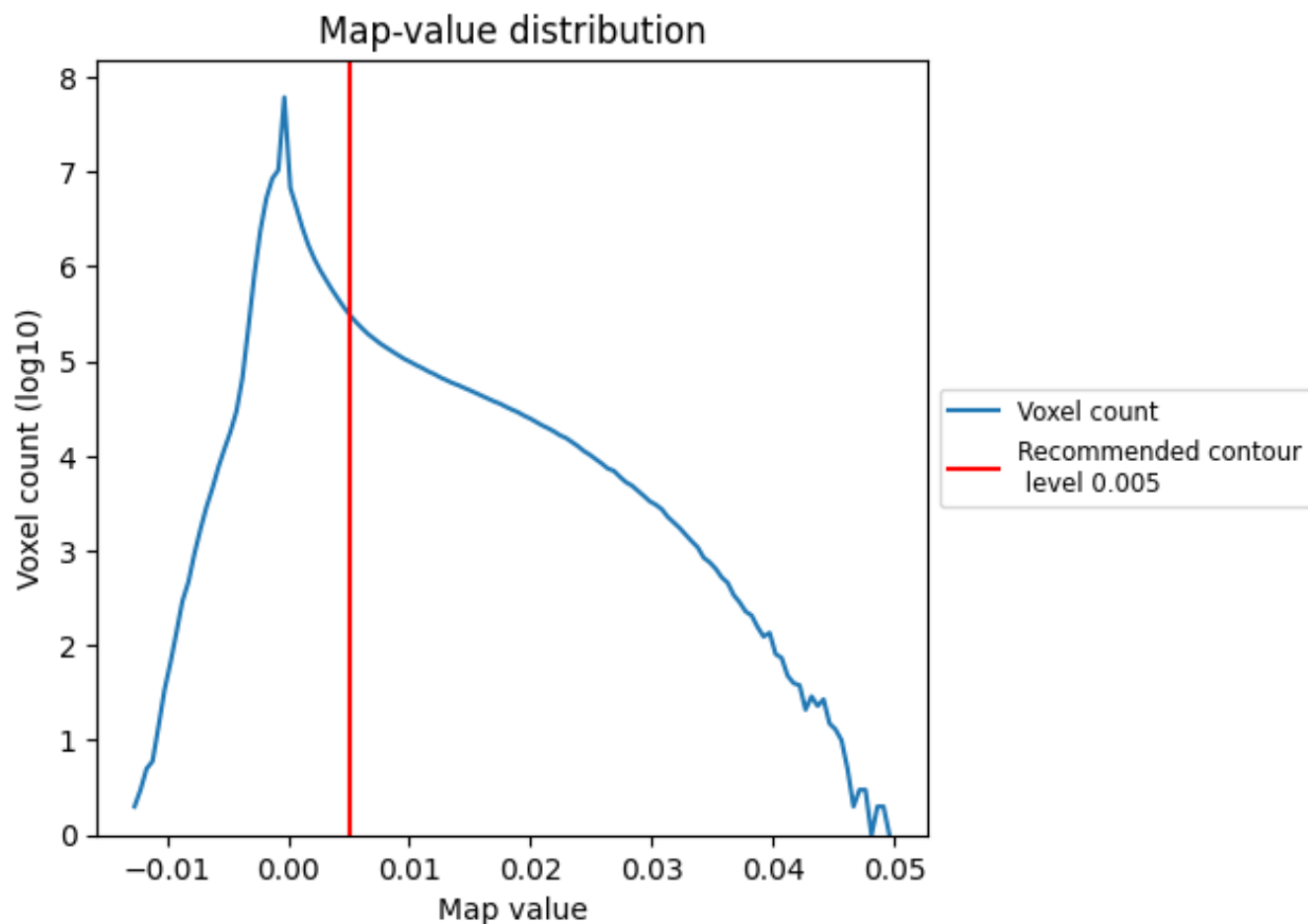
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

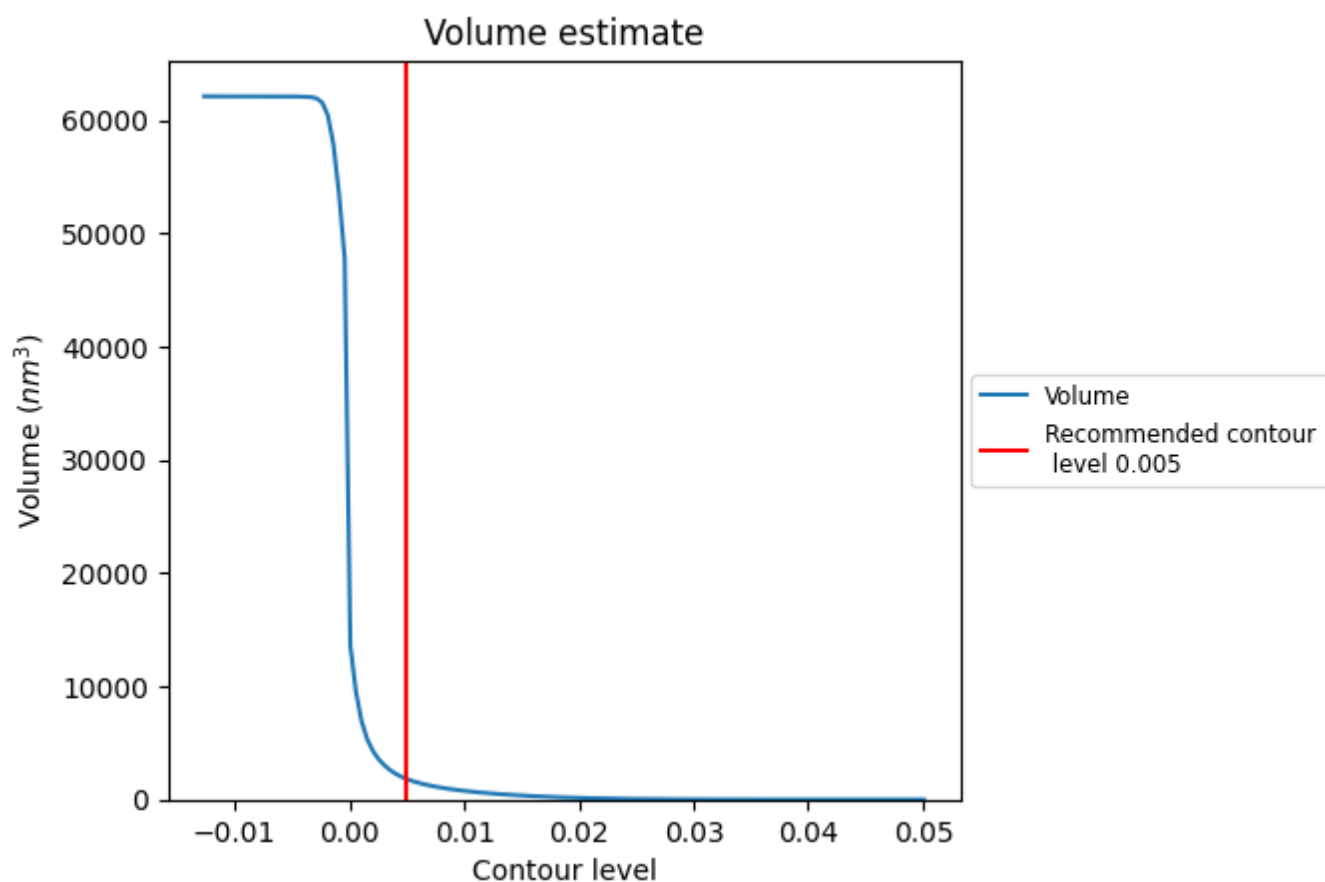
This section contains the results of statistical analysis of the map.

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.

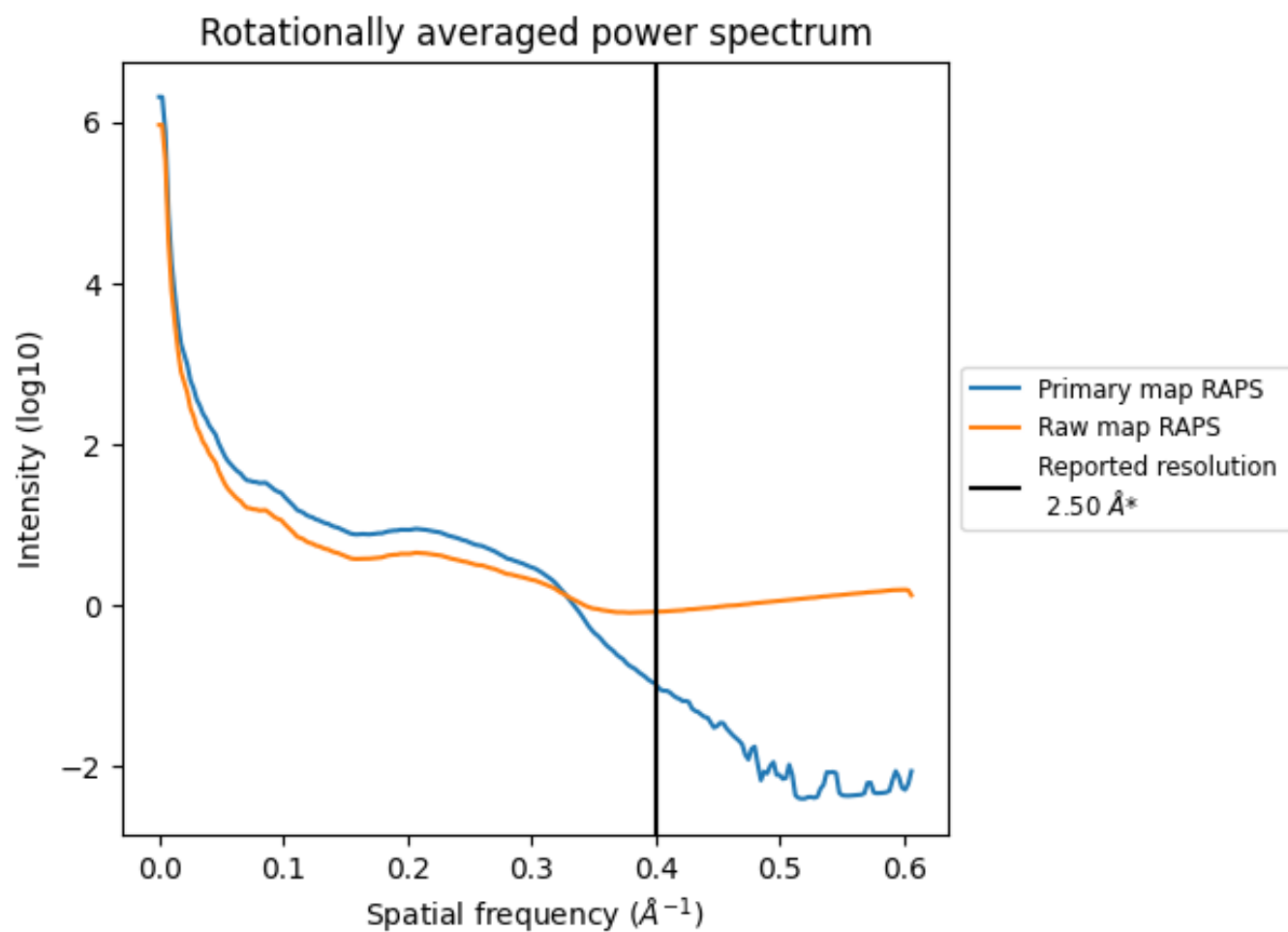
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1812 nm³; this corresponds to an approximate mass of 1637 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 ⓘ

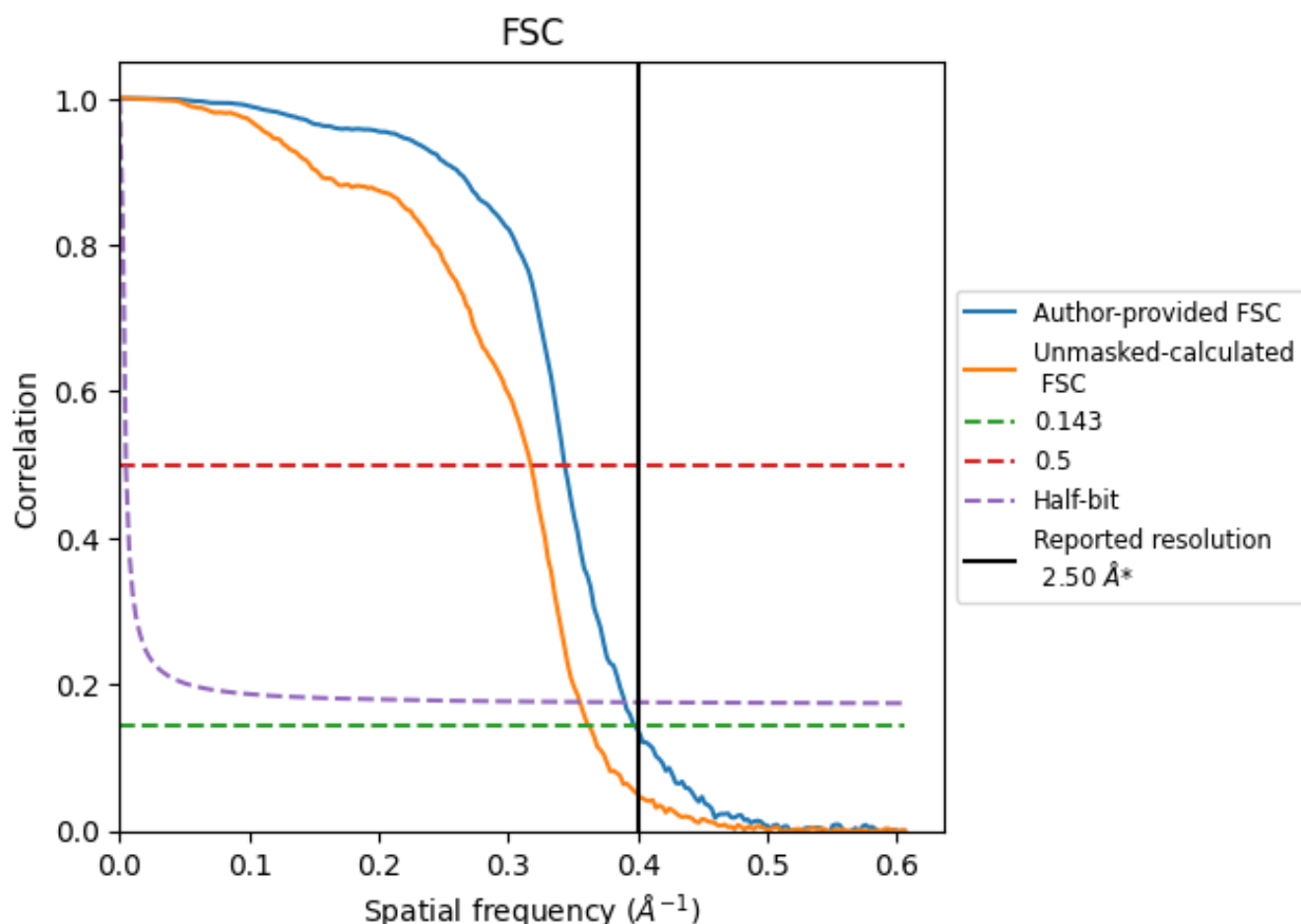


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

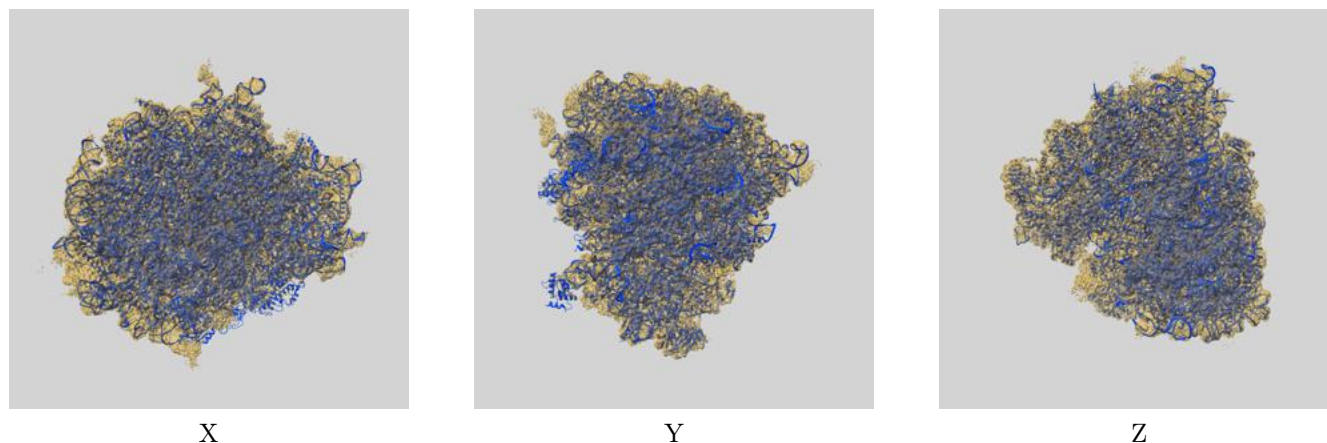
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.91	2.56
Unmasked-calculated*	2.76	3.15	2.81

*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 2.76 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

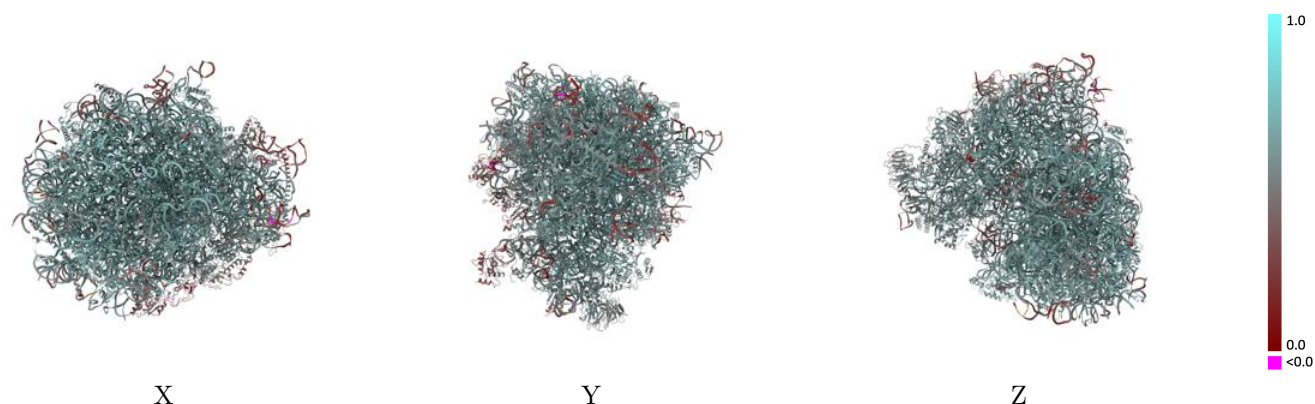
This section contains information regarding the fit between EMDB map EMD-40344 and PDB model 8SCB. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



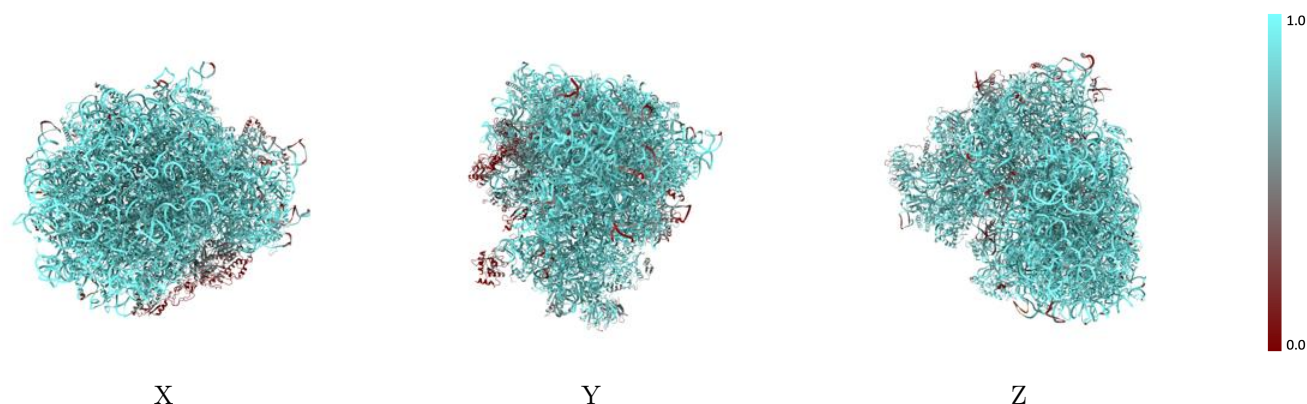
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



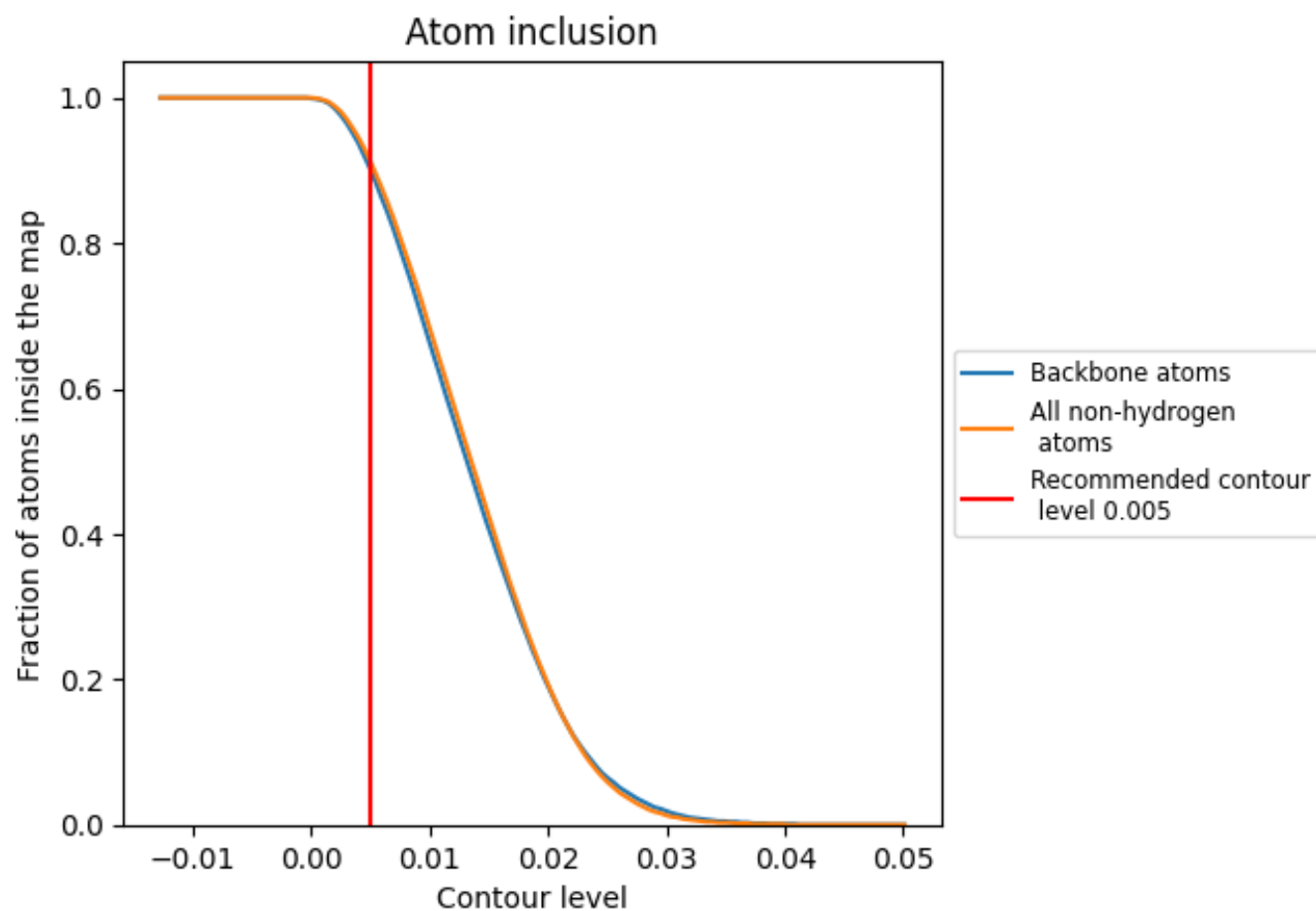
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.5890
1	 0.9590	 0.6230
2	 0.9490	 0.5410
3	 0.5710	 0.3940
5	 0.9750	 0.6070
7	 0.9950	 0.6350
8	 0.9630	 0.6010
9	 0.9380	 0.5680
A	 0.9860	 0.6570
AA	 0.8810	 0.5860
B	 0.9700	 0.6410
BB	 0.9000	 0.5920
C	 0.9670	 0.6410
CC	 0.9270	 0.6040
D	 0.9380	 0.6090
DD	 0.8180	 0.5420
E	 0.9520	 0.6100
EE	 0.9280	 0.5870
F	 0.9690	 0.6450
FF	 0.9060	 0.5780
G	 0.9140	 0.5970
GG	 0.7990	 0.5030
H	 0.9330	 0.6160
HH	 0.5830	 0.4750
I	 0.9590	 0.6300
II	 0.8730	 0.5680
J	 0.9180	 0.5910
JJ	 0.9020	 0.5760
KK	 0.8390	 0.5400
L	 0.9210	 0.6130
LL	 0.9440	 0.6250
M	 0.9470	 0.6130
MM	 0.1120	 0.3190
N	 0.9900	 0.6560
NN	 0.9280	 0.6010

























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Chain	Atom inclusion	Q-score
O	 0.9690	 0.6370
OO	 0.9570	 0.6170
P	 0.9640	 0.6460
PP	 0.8780	 0.5590
Q	 0.9730	 0.6490
QQ	 0.9080	 0.5780
R	 0.9000	 0.6030
RR	 0.7450	 0.5440
S	 0.9760	 0.6450
SS	 0.8830	 0.5660
T	 0.9440	 0.6210
TT	 0.9120	 0.5790
U	 0.8820	 0.5490
UU	 0.7490	 0.5170
V	 0.9730	 0.6440
VV	 0.8760	 0.5780
W	 0.9490	 0.6300
WW	 0.9550	 0.6150
X	 0.9530	 0.6240
XX	 0.9590	 0.6230
Y	 0.9390	 0.6220
YY	 0.8960	 0.5620
Z	 0.9460	 0.6140
ZZ	 0.8430	 0.5540
a	 0.9660	 0.6480
aa	 0.9420	 0.6160
b	 0.8450	 0.5830
bb	 0.8470	 0.5730
c	 0.9440	 0.6220
cc	 0.8400	 0.5680
d	 0.9650	 0.6330
dd	 0.9490	 0.5990
e	 0.9830	 0.6530
ee	 0.9060	 0.5680
f	 0.9790	 0.6560
ff	 0.2530	 0.3490
g	 0.9350	 0.6170
gg	 0.7550	 0.5030
h	 0.9380	 0.6160
hh	 0.9920	 0.6100
i	 0.9210	 0.6070
ii	 0.7390	 0.5290

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Chain	Atom inclusion	Q-score
j	 0.9940	 0.6520
jj	 0.4420	 0.5120
k	 0.8460	 0.5750
l	 0.9860	 0.6370
m	 0.9490	 0.6270
n	 0.9750	 0.6320
o	 0.9610	 0.6380
p	 0.9580	 0.6370
r	 0.9660	 0.6340
s	 0.1770	 0.2900
t	 0.4670	 0.3450