



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2024 – 11:55 pm BST

PDB ID : 7QIZ
EMDB ID : EMD-14004
Title : Specific features and methylation sites of a plant 80S ribosome
Authors : Cottilli, P.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-16
Resolution : 2.38 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

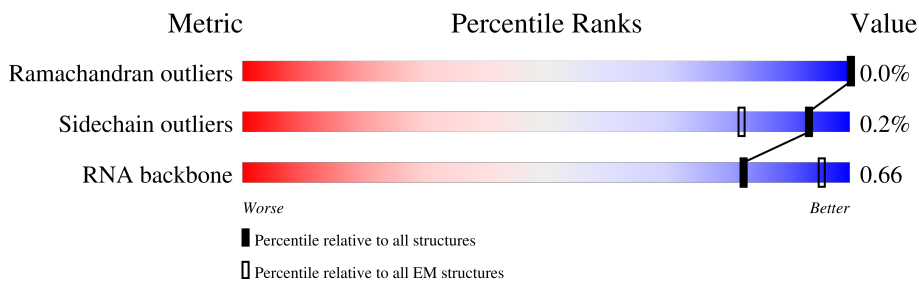
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.38 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.



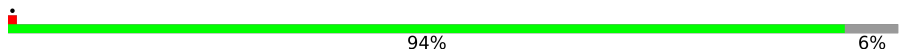

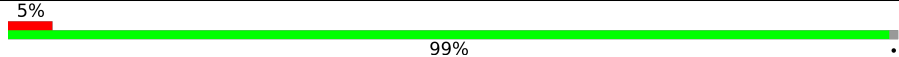
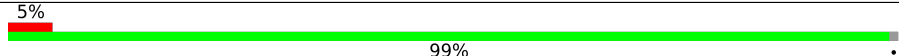
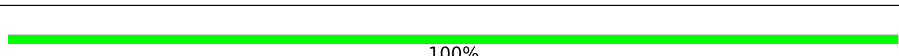
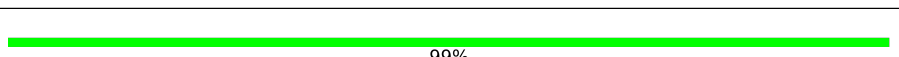
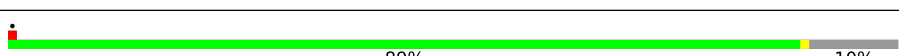
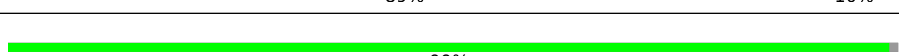
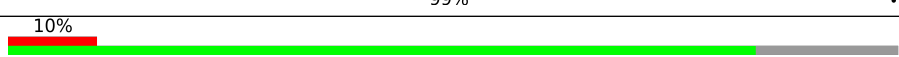

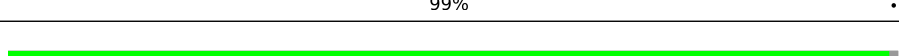


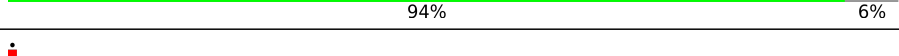
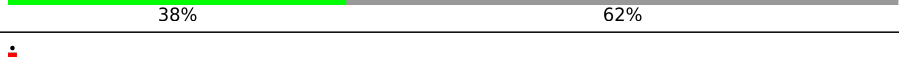

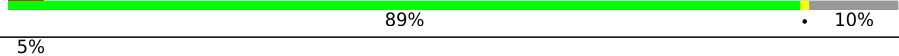
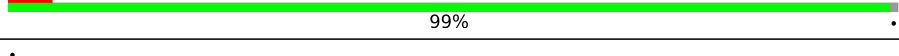
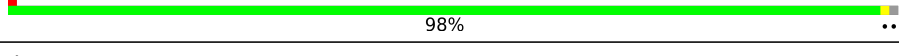
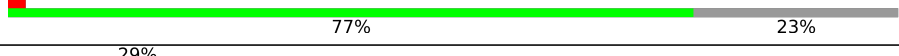

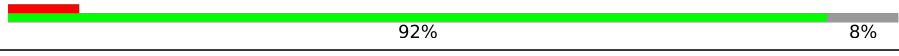
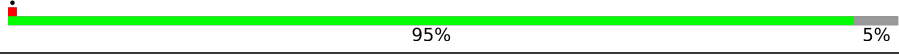
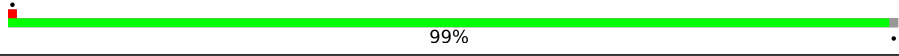
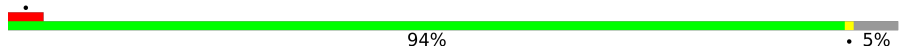
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	D	260	95%
2	F	406	95% 5%
3	E	389	99%
4	G	301	5% 92% 8%
5	H	229	6% 88% 12%
6	I	242	99%
7	J	258	9% 89% 11%
8	K	194	95% 5%

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Mol	Chain	Length	Quality of chain
9	L	220	 94% 6%
10	M	181	 10% 88% 12%
11	N	206	 5% 99%
12	O	133	 5% 99%
13	P	204	 100%
14	Q	206	 99%
15	R	173	 89% 10%
16	S	187	 99%
17	T	213	 10% 84% 16%
18	U	178	 99%
19	V	164	 99%
20	W	124	 20% 81% 19%
21	X	140	 94% 6%
22	Y	165	 38% 62%
23	Z	154	 76% 24%
24	a	146	 89% 10%
25	b	135	 5% 99%
26	c	148	 98%
27	d	60	 77% 23%
28	e	112	 29% 85% 15%
29	f	120	 8% 92% 8%
30	g	133	 95% 5%
31	h	112	 99%
32	i	120	 94% 5%
33	j	123	 99%

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Mol	Chain	Length	Quality of chain
34	k	110	91% 9%
35	l	95	92% 8%
36	m	69	99%
37	n	51	98%
38	o	128	41% 59%
39	p	105	94% 6%
40	q	92	99%
41	r	143	99%
42	s	2	50% 50%
43	2	3391	81% 10% 9%
44	5	120	92% 8%
45	8	165	86% 10%
46	S2	1808	77% 10% 12%
47	NA	239	9% 89% 11%
48	OA	211	88% 12%
49	PA	180	11% 51% 49%
50	QA	151	11% 83% 17%
51	RA	147	95% 5%
52	TA	152	93% 7%
53	UA	143	98%
54	VA	123	11% 85% 15%
55	WA	65	11% 98%
56	XA	56	89% 11%
57	YA	326	29% 97%
58	ZA	108	6% 69% 31%

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Mol	Chain	Length	Quality of chain
59	aA	14	100%
60	bA	3	100%
61	t	25	100%
62	u	296	68% 32%
63	v	260	15% 82% 17%
64	w	264	98%
65	x	191	29% 98%
66	y	220	83% 16%
67	z	159	92% 8%
68	AA	144	22% 83% 17%
69	BA	82	12% 100%
70	CA	142	99%
71	DA	127	77% 23%
72	EA	280	78% 21%
73	FA	249	20% 95% 5%
74	GA	197	5% 93% 7%
75	HA	151	99%
76	IA	150	5% 88% 12%
77	KA	133	8% 95% 5%
78	LA	86	10% 79% 21%
79	MA	62	5% 77% 23%
80	JA	130	99%

2 Entry composition i

There are 88 unique types of molecules in this entry. The entry contains 344910 atoms, of which 144985 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	D	251	3892	1201	1965	395	321	10	0	0

- Molecule 2 is a protein called Ribos_L4_asso_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	F	385	6099	1892	3104	563	530	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	162	VAL	ILE	conflict	UNP A0A3Q7HW81
F	170	ASN	VAL	conflict	UNP A0A3Q7HW81
F	277	GLN	LEU	conflict	UNP A0A3Q7HW81
F	366	ALA	GLN	conflict	UNP A0A3Q7HW81

- Molecule 3 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	386	6343	1984	3237	578	530	14	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	G	278	4537	1433	2278	409	412	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	PHE	LEU	conflict	UNP A0A3Q7H274

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Chain	Residue	Modelled	Actual	Comment	Reference
G	85	HIS	ARG	conflict	UNP A0A3Q7H274

- Molecule 5 is a protein called Ribosomal_L6e_N domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	H	201	3311	1030	1727	284	268	2	0	0

- Molecule 6 is a protein called Thaliana 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	I	239	4024	1259	2068	358	335	4	0	0

- Molecule 7 is a protein called Ribosomal_L7Ae domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	J	230	3845	1183	1999	341	314	8	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	10	SER	ALA	variant	UNP A0A3Q7GV73
J	18	ALA	SER	variant	UNP A0A3Q7GV73
J	21	LEU	VAL	variant	UNP A0A3Q7GV73

- Molecule 8 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	K	184	3023	932	1558	265	263	5	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	24	GLN	LEU	conflict	UNP A0A3Q7JDZ0
K	27	VAL	ILE	conflict	UNP A0A3Q7JDZ0
K	65	GLY	SER	conflict	UNP A0A3Q7JDZ0
K	69	THR	ALA	conflict	UNP A0A3Q7JDZ0
K	109	SER	THR	conflict	UNP A0A3Q7JDZ0

- Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	L	207	3362	1045	1709	327	271	10	0	0

- Molecule 10 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	M	160	2642	819	1344	244	228	7	0	0

- Molecule 11 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	N	204	3378	1036	1733	329	277	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	ARG	HIS	conflict	UNP A0A3Q7JCM5

- Molecule 12 is a protein called Ribosomal_L14e domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	O	132	2239	687	1167	200	181	4	0	0

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	P	203	3471	1068	1770	354	276	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	135	VAL	ILE	conflict	UNP A0A3Q7HQH0
P	137	GLN	SER	conflict	UNP A0A3Q7HQH0

- Molecule 14 is a protein called Pectinesterase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	Q	205	3418	1045	1775	320	270	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	206	TYR	GLU	variant	UNP A0A3Q7HGG4

- Molecule 15 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	R	155	2506	773	1258	245	225	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	46	SER	ARG	conflict	UNP A0A3Q7FNQ5

- Molecule 16 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	S	186	3013	924	1561	277	248	3	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	17	THR	ILE	conflict	UNP A0A3Q7I5W4
S	37	ALA	SER	conflict	UNP A0A3Q7I5W4
S	60	PRO	ALA	conflict	UNP A0A3Q7I5W4
S	68	ILE	VAL	conflict	UNP A0A3Q7I5W4
S	71	ALA	MET	conflict	UNP A0A3Q7I5W4
S	75	GLY	GLU	conflict	UNP A0A3Q7I5W4
S	79	VAL	ALA	conflict	UNP A0A3Q7I5W4
S	81	LEU	VAL	conflict	UNP A0A3Q7I5W4
S	100	CYS	THR	conflict	UNP A0A3Q7I5W4
S	103	LYS	ARG	conflict	UNP A0A3Q7I5W4
S	136	LEU	VAL	conflict	UNP A0A3Q7I5W4
S	153	PRO	LYS	conflict	UNP A0A3Q7I5W4

- Molecule 17 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	T	178	3126	929	1632	319	238	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	178	LYS	GLU	conflict	UNP A0A3Q7GQ29
T	179	LYS	GLU	conflict	UNP A0A3Q7GQ29

- Molecule 18 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	U	177	3056	971	1553	273	251	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	73	THR	LYS	conflict	UNP A0A3Q7IGB1
U	104	ALA	GLY	conflict	UNP A0A3Q7IGB1

- Molecule 19 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	V	163	2673	821	1365	258	226	3	0	0

- Molecule 20 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	W	101	1663	518	849	144	149	3	0	0

- Molecule 21 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	X	131	2032	623	1047	183	170	9	0	0

- Molecule 22 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	Y	62	1071	341	548	98	81	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	MET	-	initiating methionine	UNP A0A3Q7IN69

- Molecule 23 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	Z	117	1981	610	1030	170	169	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	55	SER	ASN	conflict	UNP A0A3Q7INK3
Z	61	VAL	ILE	conflict	UNP A0A3Q7INK3
Z	73	ALA	GLN	conflict	UNP A0A3Q7INK3
Z	74	ILE	VAL	conflict	UNP A0A3Q7INK3
Z	77	TYR	CYS	conflict	UNP A0A3Q7INK3
Z	101	LYS	HIS	conflict	UNP A0A3Q7INK3

- Molecule 24 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	a	132	2207	657	1144	218	185	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	25	VAL	LEU	conflict	UNP A0A3Q7FBC6
a	43	ASN	SER	conflict	UNP A0A3Q7FBC6
a	99	ASN	HIS	conflict	UNP A0A3Q7FBC6
a	105	VAL	ILE	conflict	UNP A0A3Q7FBC6

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	b	134	2275	708	1177	206	182	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	117	PHE	LEU	conflict	UNP A0A3Q7GZ83

- Molecule 26 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	c	147	2358	739	1204	224	188	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	82	VAL	LEU	conflict	UNP A0A3Q7GZ10
c	129	ILE	VAL	conflict	UNP A0A3Q7GZ10

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	d	46	775	235	388	88	63	1	0	0

- Molecule 28 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	e	95	1497	464	766	128	134	5	0	0

- Molecule 29 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	f	110	1841	558	951	171	159	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	76	VAL	ILE	conflict	UNP A0A3Q7JRW8

- Molecule 30 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	g	127	2173	662	1125	211	170	5	0	0

- Molecule 31 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	h	111	1839	573	937	172	153	4	0	0

- Molecule 32 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	i	114	1942	580	1015	194	152	1	0	0

- Molecule 33 is a protein called Similar to 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	j	122	2134	640	1137	191	165	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	67	ALA	LEU	conflict	UNP Q53U38
j	72	VAL	ALA	conflict	UNP Q53U38
j	100	SER	ALA	conflict	UNP Q53U38
j	112	MET	LEU	conflict	UNP Q53U38

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	k	100	1692	501	893	164	132	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	88	LYS	ARG	conflict	UNP A0A3Q7GUG2

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	l	87	1434	431	729	156	113	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	44	LEU	LYS	conflict	UNP A0A3Q7FV98

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	m	68	1163	358	605	99	98	3	0	0

- Molecule 37 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	n	50	927	285	479	96	65	2	0	0

- Molecule 38 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	o	52	901	268	470	91	66	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	113	ARG	LYS	conflict	UNP K4B017

- Molecule 39 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	p	99	1653	500	857	159	132	5	0	0

- Molecule 40 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	q	91	1455	443	746	136	125	5	0	0

- Molecule 41 is a protein called Ribosomal_L28e domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	r	142	2302	703	1185	210	202	2	0	0

- Molecule 42 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
42	s	2	64	19	22	8	13	2	0	0

- Molecule 43 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
43	2	3098	98740	29664	32316	12094	21568	3098	0	0

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
44	5	120	3796	1142	1237	459	838	120	0	0

- Molecule 45 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
45	8	159	5049	1517	1653	613	1107	159	0	0

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
46	S2	1584	50958	15153	17097	6050	11074	1584	0	0

- Molecule 47 is a protein called KH type-2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	NA	213	3429	1060	1751	307	302	9	0	0

- Molecule 48 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	OA	185	2965	912	1499	277	269	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
OA	37	GLY	ASP	conflict	UNP A0A3Q7IVL4
OA	43	MET	ILE	conflict	UNP A0A3Q7IVL4
OA	60	MET	THR	conflict	UNP A0A3Q7IVL4
OA	117	GLN	LEU	conflict	UNP A0A3Q7IVL4

- Molecule 49 is a protein called S10_pectin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	PA	92	1572	514	790	128	136	4	0	0

- Molecule 50 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	QA	126	2096	650	1078	190	173	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	75	GLN	PRO	conflict	UNP A0A3Q7F5X2

- Molecule 51 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	RA	140	2339	722	1204	220	189	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
RA	62	HIS	GLN	conflict	UNP A0A3Q7GDB0
RA	105	GLN	THR	conflict	UNP A0A3Q7GDB0

- Molecule 52 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	TA	142	2343	720	1189	227	202	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TA	67	LEU	VAL	conflict	UNP A0A3Q7FJL7

- Molecule 53 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
53	UA	140	2208	692	1104	215	194	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
UA	6	SER	ASN	conflict	UNP A0A3Q7FTS1
UA	14	ASP	GLU	conflict	UNP A0A3Q7FTS1

- Molecule 54 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
54	VA	104	1701	515	880	152	150	4	0	0

- Molecule 55 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
55	WA	64	1070	319	551	105	93	2	0	0

- Molecule 56 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
56	XA	50	805	253	400	82	64	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XA	13	ASN	TYR	conflict	UNP A0A3Q7ITW7

- Molecule 57 is a protein called Mitogen-activated protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
57	YA	317	4898	1554	2434	427	472	11	0	0

- Molecule 58 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
58	ZA	75	1228	373	636	108	108	3	0	0

- Molecule 59 is a RNA chain called tRNA_1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
59	aA	14	451	134	152	55	96	14	0	0

- Molecule 60 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
60	bA	3	95	28	33	10	21	3	0	0

- Molecule 61 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
61	t	25	527	145	289	62	28	3	0	0

- Molecule 62 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
62	u	202	3230	1024	1621	288	287	10	0	0

- Molecule 63 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
63	v	215	3570	1112	1810	322	318	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	39	GLU	GLY	conflict	UNP A0A3Q7I881
v	141	ALA	GLY	conflict	UNP A0A3Q7I881
v	169	VAL	ARG	conflict	UNP A0A3Q7I881
v	173	ARG	VAL	conflict	UNP A0A3Q7I881
v	185	VAL	ALA	conflict	UNP A0A3Q7I881
v	205	PHE	TYR	conflict	UNP A0A3Q7I881

- Molecule 64 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
64	w	261	4264	1326	2180	389	361	8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	48	LEU	MET	conflict	UNP A0A3Q7GQU3
w	91	THR	SER	conflict	UNP A0A3Q7GQU3
w	98	SER	ASN	conflict	UNP A0A3Q7GQU3
w	114	LEU	VAL	conflict	UNP A0A3Q7GQU3
w	119	ALA	SER	conflict	UNP A0A3Q7GQU3
w	165	ASP	GLU	conflict	UNP A0A3Q7GQU3
w	194	ILE	VAL	conflict	UNP A0A3Q7GQU3
w	195	LEU	ILE	conflict	UNP A0A3Q7GQU3
w	208	VAL	LEU	conflict	UNP A0A3Q7GQU3
w	232	SER	THR	conflict	UNP A0A3Q7GQU3
w	247	SER	THR	conflict	UNP A0A3Q7GQU3
w	256	MET	LEU	conflict	UNP A0A3Q7GQU3

- Molecule 65 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
65	x	187	3103	962	1582	282	276	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	13	ALA	ASP	conflict	UNP A0A3Q7H0E8
x	19	HIS	PHE	conflict	UNP A0A3Q7H0E8
x	22	SER	THR	conflict	UNP A0A3Q7H0E8
x	24	GLY	ALA	conflict	UNP A0A3Q7H0E8

- Molecule 66 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
66	y	184	3032	929	1539	296	264	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	18	LYS	GLN	conflict	UNP A0A3Q7HJ03
y	20	SER	THR	conflict	UNP A0A3Q7HJ03
y	66	PHE	TYR	conflict	UNP A0A3Q7HJ03
y	159	ASN	LYS	conflict	UNP A0A3Q7HJ03
y	162	ALA	LYS	conflict	UNP A0A3Q7HJ03
y	165	LYS	THR	conflict	UNP A0A3Q7HJ03
y	175	ALA	SER	conflict	UNP A0A3Q7HJ03
y	180	LEU	TYR	conflict	UNP A0A3Q7HJ03

- Molecule 67 is a protein called Ribosomal_S17_N domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
67	z	147	2381	737	1217	224	198	5	0	0

- Molecule 68 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
68	AA	119	1985	603	1024	176	177	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	87	GLU	ASP	conflict	UNP P49215

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
69	BA	82	1257	391	617	116	128	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	44	VAL	ARG	conflict	UNP A0A3Q7G7P4
BA	68	MET	LEU	conflict	UNP A0A3Q7G7P4

- Molecule 70 is a protein called 40S body ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
70	CA	141	2267	695	1167	215	187	3	0	0

- Molecule 71 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
71	DA	98	1628	495	831	164	130	8	0	0

- Molecule 72 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
72	EA	220	3515	1104	1809	303	291	8	0	0

- Molecule 73 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
73	FA	237	3934	1187	2028	374	337	8	0	0

- Molecule 74 is a protein called 40S body ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
74	GA	184	3130	965	1601	303	256	5	0	0

- Molecule 75 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
75	HA	150	2480	765	1285	224	204	2	0	0

- Molecule 76 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
76	IA	132	2031	612	1032	197	185	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IA	137	IAS	ASP	conflict	UNP Q38JI8

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
77	KA	126	2136	654	1106	199	174	3	0	0

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
78	LA	68	1098	341	558	101	95	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	19	LYS	ARG	conflict	UNP A0A1U8DQX3
LA	76	ILE	THR	conflict	UNP A0A1U8DQX3

- Molecule 79 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
79	MA	48	794	232	411	87	63	1	0	0

- Molecule 80 is a protein called 40S ribosomal protein S15a-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
80	JA	129	2062	650	1047	182	179	4	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	20	ALA	ARG	conflict	UNP A0A1U7YEG5
JA	23	ALA	ARG	conflict	UNP A0A1U7YEG5
JA	26	GLU	MET	conflict	UNP A0A1U7YEG5
JA	27	LEU	ILE	conflict	UNP A0A1U7YEG5
JA	49	ASP	GLU	conflict	UNP A0A1U7YEG5
JA	51	GLN	GLU	conflict	UNP A0A1U7YEG5
JA	58	VAL	SER	conflict	UNP A0A1U7YEG5
JA	84	ALA	LYS	conflict	UNP A0A1U7YEG5
JA	85	THR	GLU	conflict	UNP A0A1U7YEG5

- Molecule 81 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
81	D	2	Total K 2 2	0
81	E	1	Total K 1 1	0
81	L	1	Total K 1 1	0
81	N	2	Total K 2 2	0
81	i	1	Total K 1 1	0
81	p	1	Total K 1 1	0
81	2	78	Total K 78 78	0
81	8	4	Total K 4 4	0
81	S2	26	Total K 26 26	0

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Mol	Chain	Residues	Atoms	AltConf
81	TA	1	Total K 1 1	0
81	UA	1	Total K 1 1	0
81	XA	1	Total K 1 1	0

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
82	E	1	Total Mg 1 1	0
82	I	1	Total Mg 1 1	0
82	L	1	Total Mg 1 1	0
82	N	1	Total Mg 1 1	0
82	R	1	Total Mg 1 1	0
82	X	1	Total Mg 1 1	0
82	1	1	Total Mg 1 1	0
82	2	259	Total Mg 259 259	0
82	5	5	Total Mg 5 5	0
82	8	5	Total Mg 5 5	0
82	S2	86	Total Mg 86 86	0
82	TA	1	Total Mg 1 1	0
82	FA	1	Total Mg 1 1	0

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

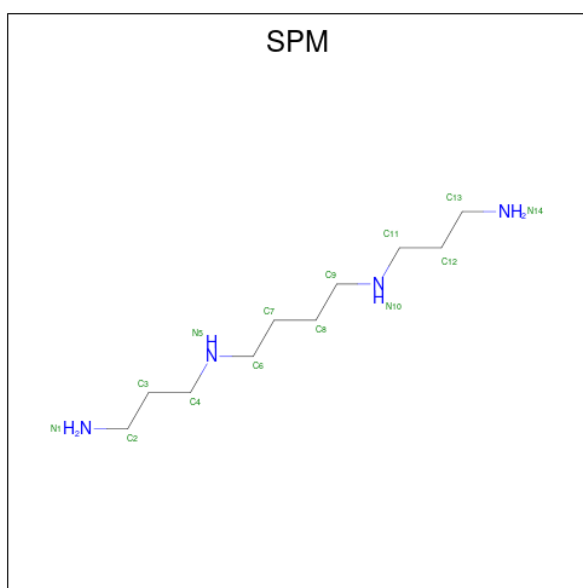
Mol	Chain	Residues	Atoms	AltConf
83	1	1	Total Zn 1 1	0

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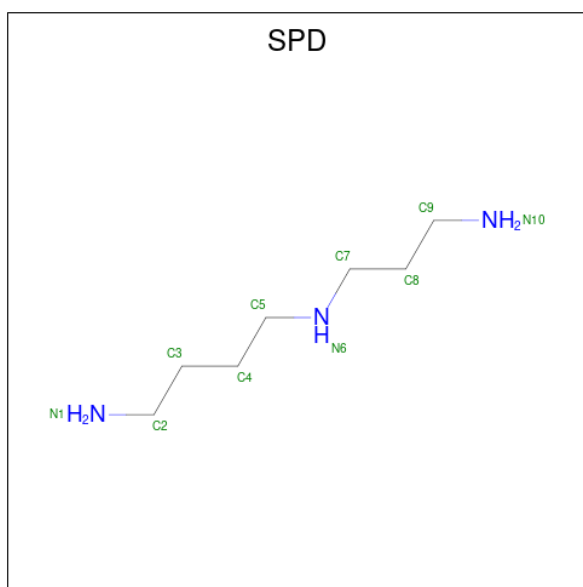
Mol	Chain	Residues	Atoms		AltConf
83	o	1	Total 1	Zn 1	0
83	p	1	Total 1	Zn 1	0
83	q	1	Total 1	Zn 1	0
83	XA	1	Total 1	Zn 1	0
83	DA	1	Total 1	Zn 1	0

- Molecule 84 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



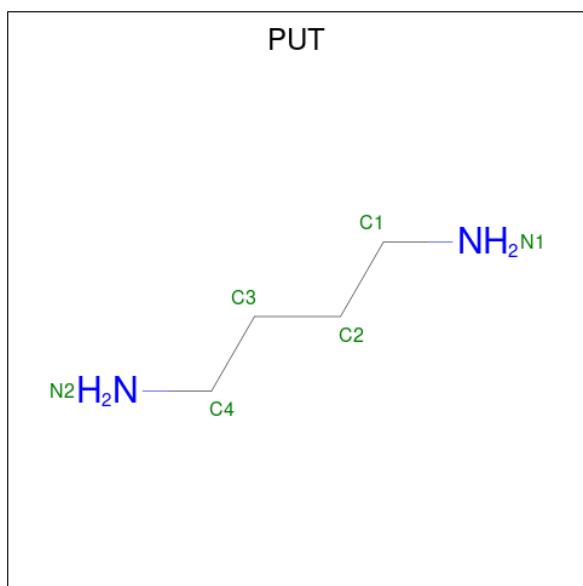
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
84	2	1	Total 40	C 10	H 26	N 4	0
84	2	1	Total 40	C 10	H 26	N 4	0
84	2	1	Total 40	C 10	H 26	N 4	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



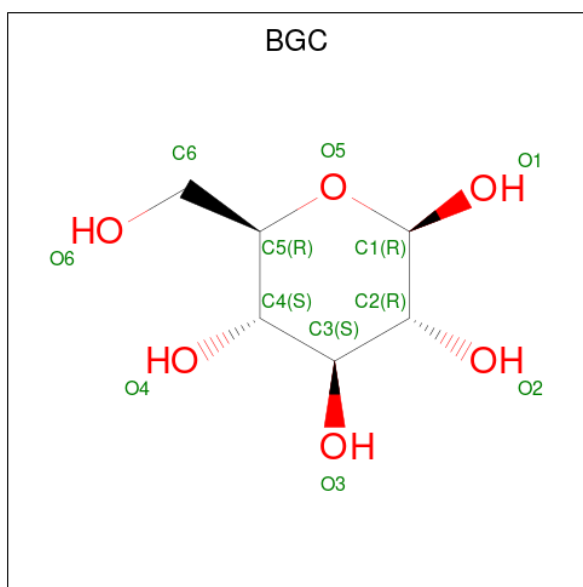
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
85	2	1	29	7	19	3	0

- Molecule 86 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
86	S2	1	18	4	12	2	0

- Molecule 87 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
87	NA	1	22	6	11	5	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	D	45	Total	O	0
			45	45	
88	F	53	Total	O	0
			53	53	
88	E	67	Total	O	0
			67	67	
88	G	17	Total	O	0
			17	17	
88	H	1	Total	O	0
			1	1	
88	I	26	Total	O	0
			26	26	
88	J	8	Total	O	0
			8	8	
88	K	1	Total	O	0
			1	1	
88	L	3	Total	O	0
			3	3	
88	M	1	Total	O	0
			1	1	
88	N	35	Total	O	0
			35	35	

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Mol	Chain	Residues	Atoms		AltConf
88	O	8	Total 8	O 8	0
88	P	47	Total 47	O 47	0
88	Q	20	Total 20	O 20	0
88	R	17	Total 17	O 17	0
88	S	21	Total 21	O 21	0
88	T	13	Total 13	O 13	0
88	U	8	Total 8	O 8	0
88	V	15	Total 15	O 15	0
88	X	7	Total 7	O 7	0
88	Y	3	Total 3	O 3	0
88	Z	4	Total 4	O 4	0
88	a	8	Total 8	O 8	0
88	b	4	Total 4	O 4	0
88	c	28	Total 28	O 28	0
88	d	10	Total 10	O 10	0
88	f	10	Total 10	O 10	0
88	g	29	Total 29	O 29	0
88	h	15	Total 15	O 15	0
88	i	11	Total 11	O 11	0
88	j	7	Total 7	O 7	0
88	k	5	Total 5	O 5	0

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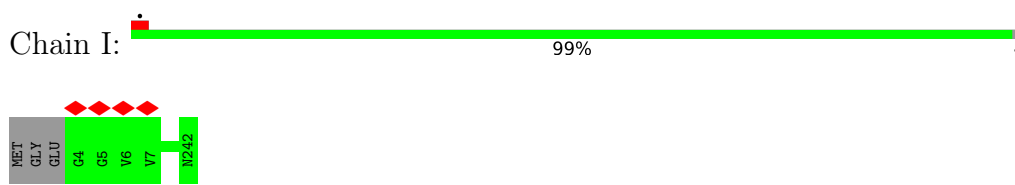
Mol	Chain	Residues	Atoms		AltConf
88	l	29	Total 29	O 29	0
88	n	6	Total 6	O 6	0
88	o	2	Total 2	O 2	0
88	p	17	Total 17	O 17	0
88	q	8	Total 8	O 8	0
88	r	7	Total 7	O 7	0
88	s	4	Total 4	O 4	0
88	2	3141	Total 3141	O 3141	0
88	5	59	Total 59	O 59	0
88	8	115	Total 115	O 115	0
88	S2	626	Total 626	O 626	0
88	OA	8	Total 8	O 8	0
88	QA	1	Total 1	O 1	0
88	RA	5	Total 5	O 5	0
88	TA	8	Total 8	O 8	0
88	UA	23	Total 23	O 23	0
88	VA	7	Total 7	O 7	0
88	WA	1	Total 1	O 1	0
88	XA	2	Total 2	O 2	0
88	ZA	4	Total 4	O 4	0
88	t	2	Total 2	O 2	0

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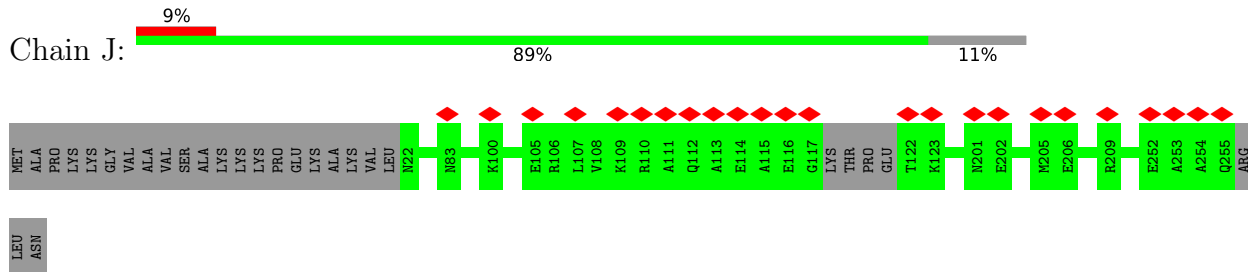
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Mol	Chain	Residues	Atoms		AltConf
88	v	3	Total 3	O 3	0
88	w	6	Total 6	O 6	0
88	y	5	Total 5	O 5	0
88	z	24	Total 24	O 24	0
88	BA	2	Total 2	O 2	0
88	CA	13	Total 13	O 13	0
88	DA	15	Total 15	O 15	0
88	EA	2	Total 2	O 2	0
88	FA	2	Total 2	O 2	0
88	GA	12	Total 12	O 12	0
88	HA	6	Total 6	O 6	0
88	IA	5	Total 5	O 5	0
88	LA	2	Total 2	O 2	0
88	MA	2	Total 2	O 2	0
88	JA	7	Total 7	O 7	0

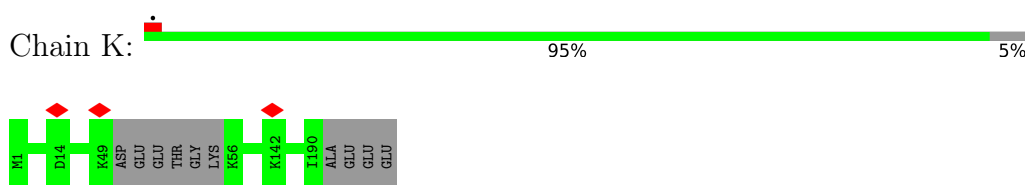
- Molecule 6: Thaliana 60S ribosomal protein L7



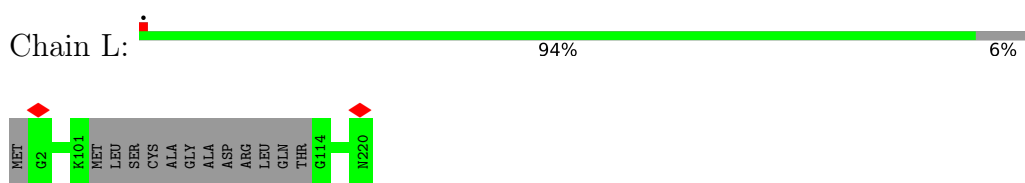
- Molecule 7: Ribosomal_L7Ae domain-containing protein



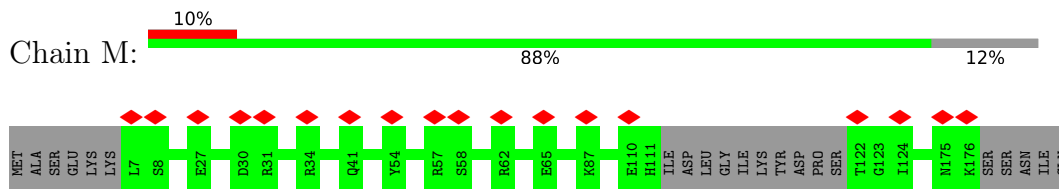
- Molecule 8: 60S ribosomal protein uL6



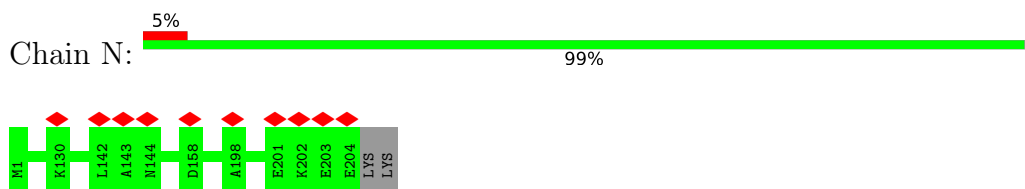
- Molecule 9: 60S ribosomal protein L10



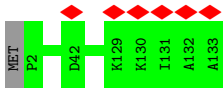
- Molecule 10: 60S ribosomal protein uL5



- Molecule 11: 60S ribosomal protein L13



- Molecule 12: Ribosomal_L14e domain-containing protein



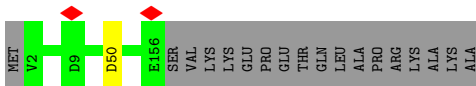
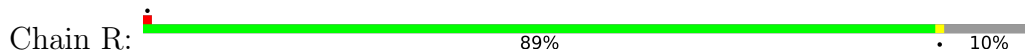
- Molecule 13: Ribosomal protein L15



- Molecule 14: Pectinesterase



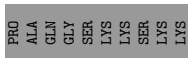
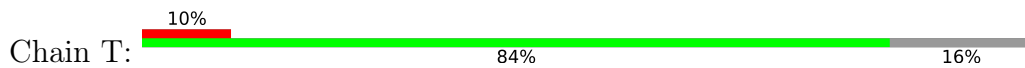
- Molecule 15: 50S ribosomal protein L22, chloroplastic



- Molecule 16: Ribosomal_L18e/L15P domain-containing protein

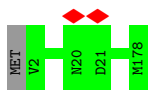


- Molecule 17: Ribosomal protein L19



- Molecule 18: 60S ribosomal protein L18a

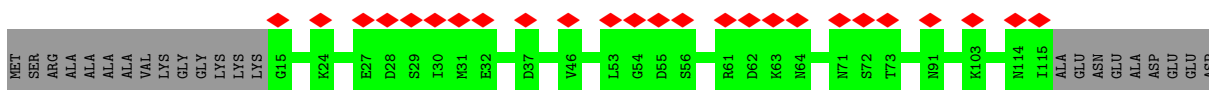
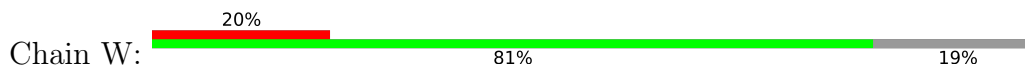




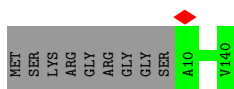
- Molecule 19: 60S ribosomal protein eL21



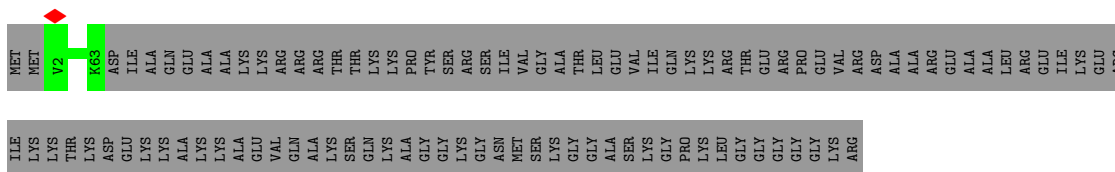
- Molecule 20: 60S ribosomal protein eL22



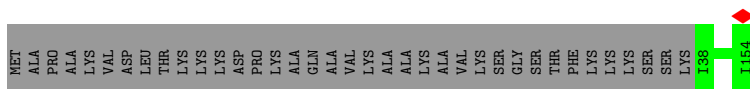
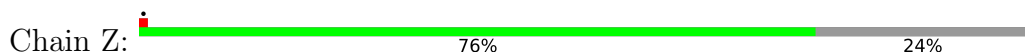
- Molecule 21: 60S ribosomal protein uL14



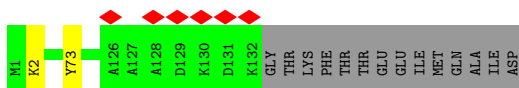
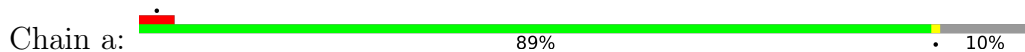
- Molecule 22: TRASH domain-containing protein



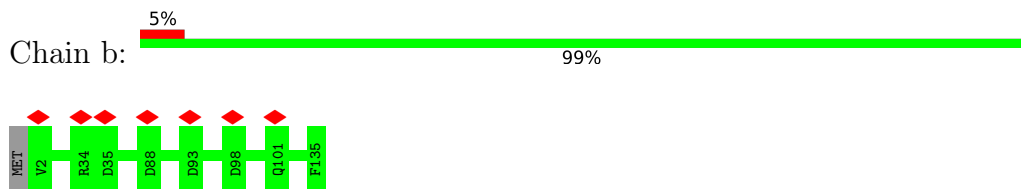
- Molecule 23: Ribosomal_L23eN domain-containing protein



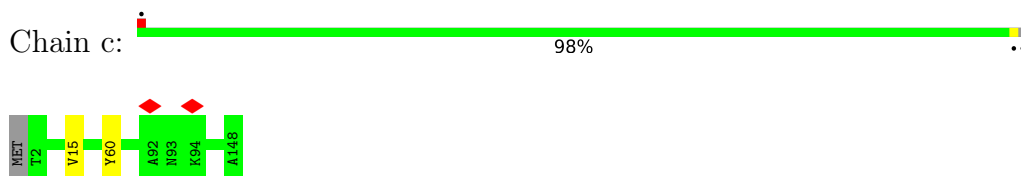
- Molecule 24: KOW domain-containing protein



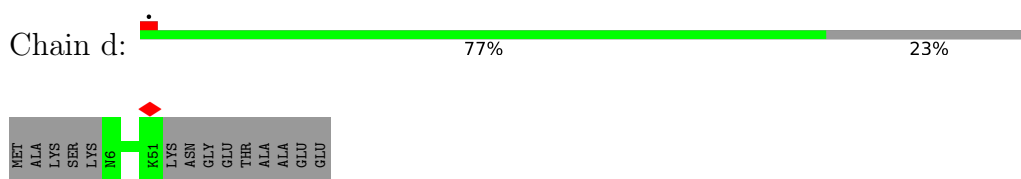
- Molecule 25: 60S ribosomal protein L27



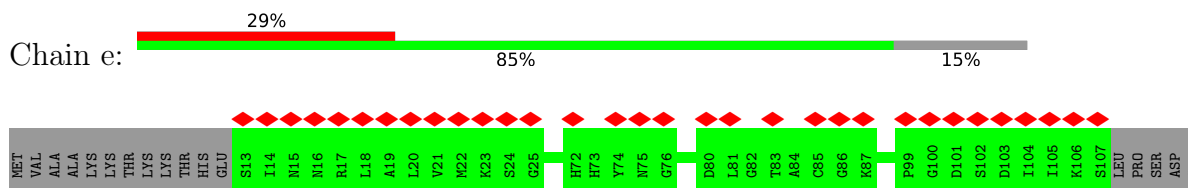
- Molecule 26: Ribosomal_L18e/L15P domain-containing protein



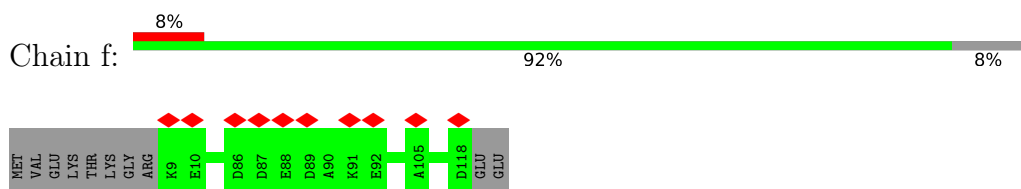
- Molecule 27: 60S ribosomal protein L29



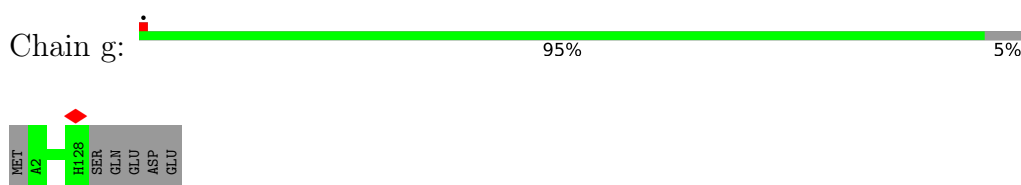
- Molecule 28: 60S ribosomal protein eL30



- Molecule 29: 60S ribosomal protein eL31



- Molecule 30: 60S ribosomal protein eL32

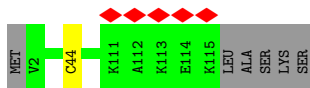


- Molecule 31: 60S ribosomal protein eL33

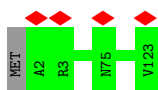




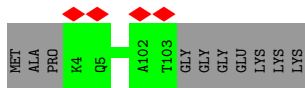
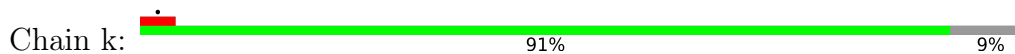
- Molecule 32: 60S ribosomal protein eL34



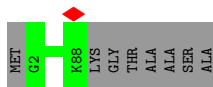
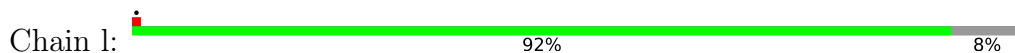
- Molecule 33: Similar to 60S ribosomal protein L35



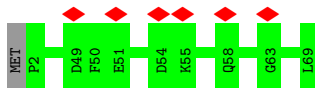
- Molecule 34: 60S ribosomal protein L36



- Molecule 35: Ribosomal protein L37



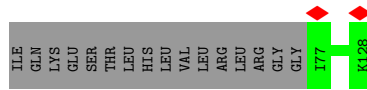
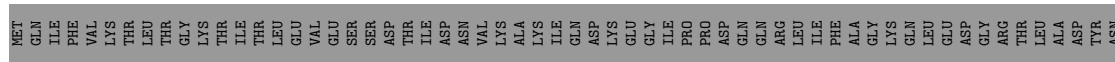
- Molecule 36: 60S ribosomal protein L38



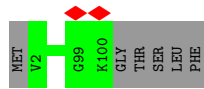
- Molecule 37: 60S ribosomal protein eL39



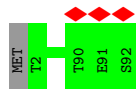
- Molecule 38: Ubiquitin



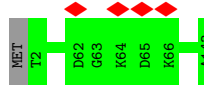
• Molecule 39: 60S ribosomal protein eL42



• Molecule 40: 60S ribosomal protein eL43



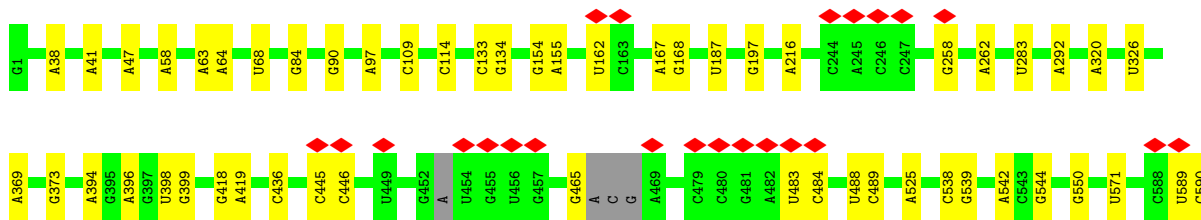
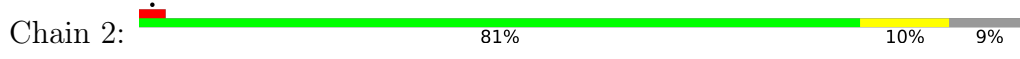
• Molecule 41: Ribosomal_L28e domain-containing protein

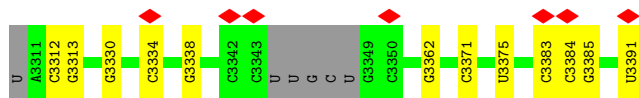


• Molecule 42: tRNA

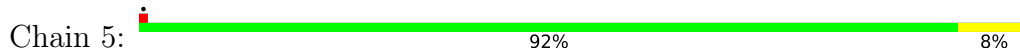


• Molecule 43: 25S rRNA

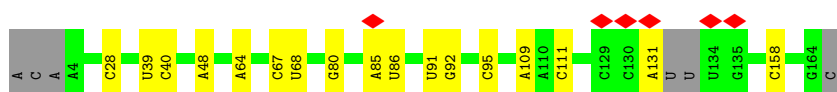
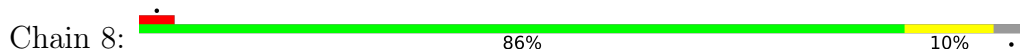




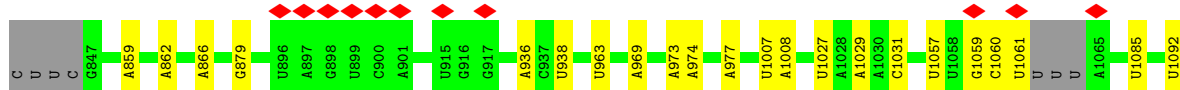
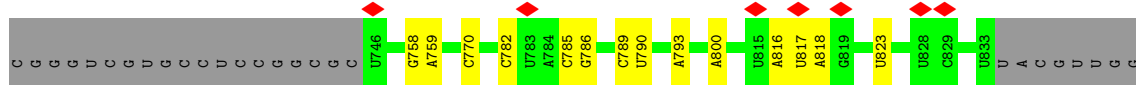
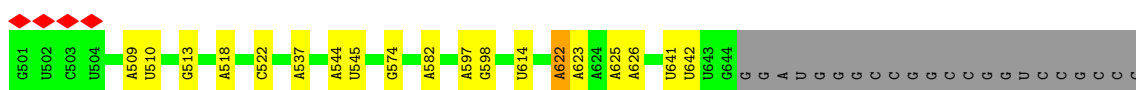
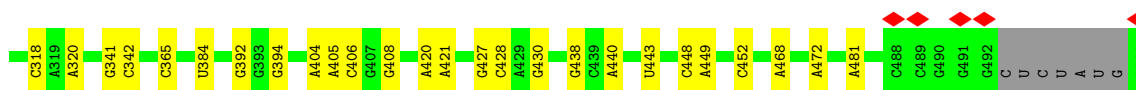
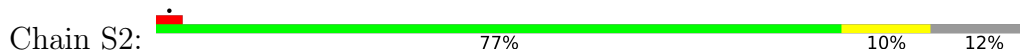
• Molecule 44: 5S rRNA

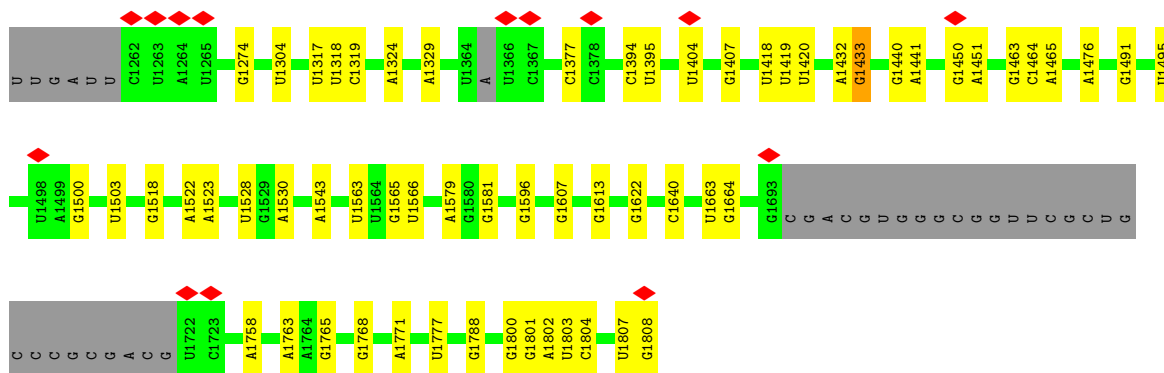


• Molecule 45: 5.8S rRNA

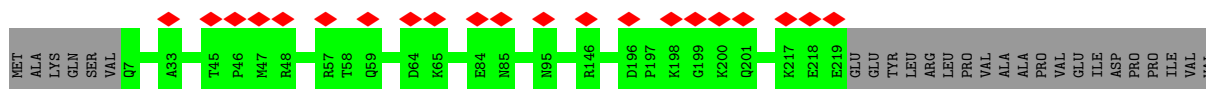
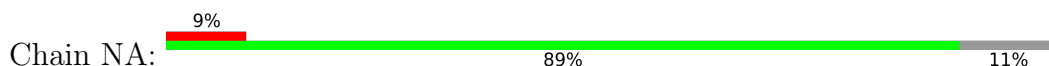


• Molecule 46: 18S

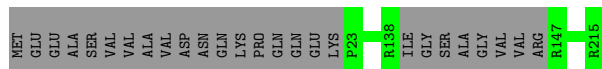
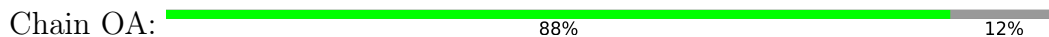




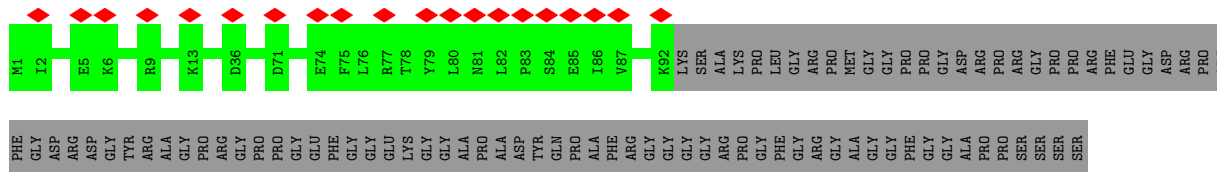
● Molecule 47: KH type-2 domain-containing protein



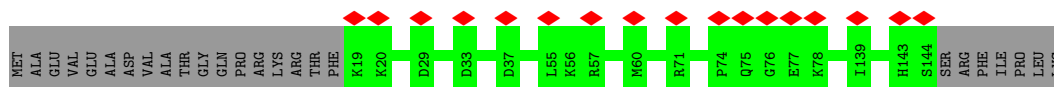
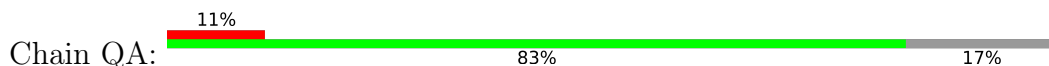
● Molecule 48: Ribosomal_S7 domain-containing protein



● Molecule 49: S10_pectin domain-containing protein

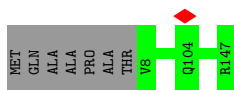


● Molecule 50: 40S ribosomal protein uS19

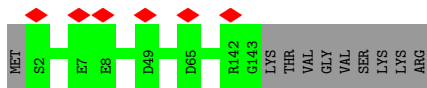


● Molecule 51: 40S ribosomal protein uS9

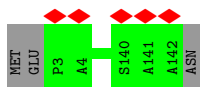




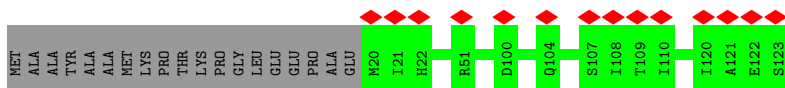
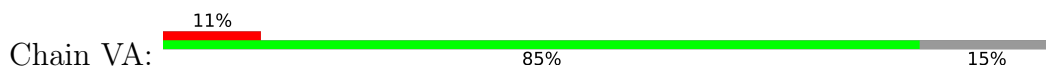
- Molecule 52: 40S ribosomal protein uS13



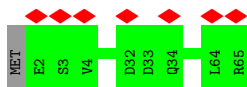
- Molecule 53: 40S ribosomal protein eS19



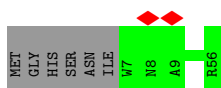
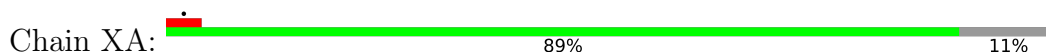
- Molecule 54: Ribosomal_S10 domain-containing protein



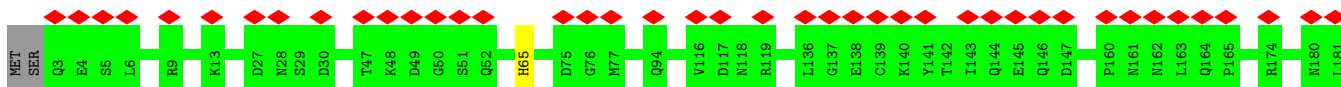
- Molecule 55: 40S ribosomal protein eS28

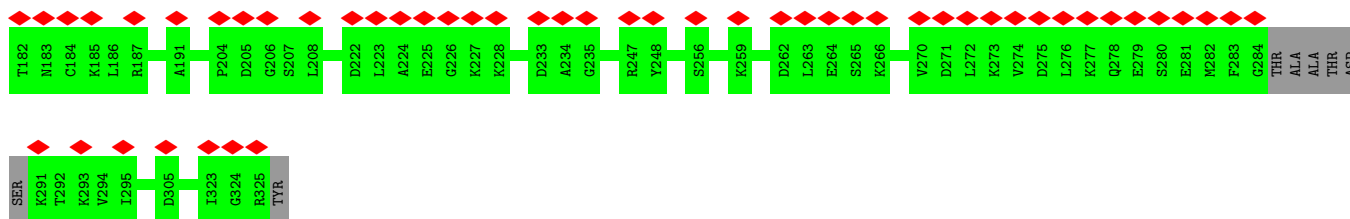


- Molecule 56: 40S ribosomal protein uS14

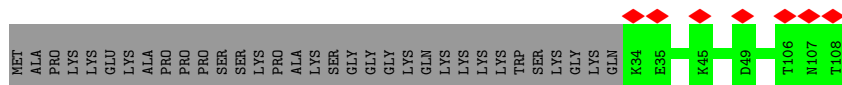


- Molecule 57: Mitogen-activated protein kinase





- Molecule 58: 40S ribosomal protein S25



- Molecule 59: tRNA_1



There are no outlier residues recorded for this chain.

- Molecule 60: mRNA

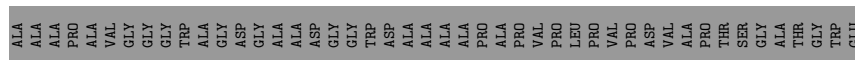
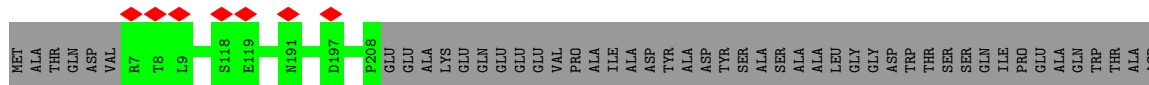


There are no outlier residues recorded for this chain.

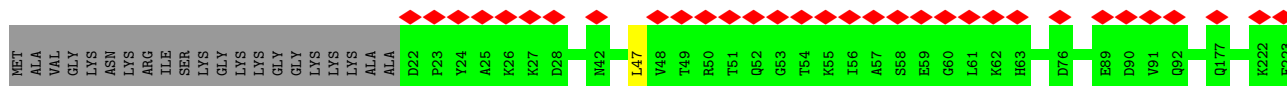
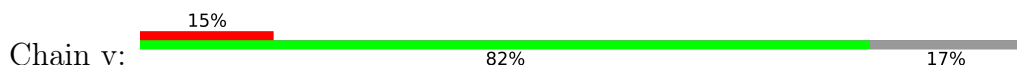
- Molecule 61: 60S ribosomal protein L41

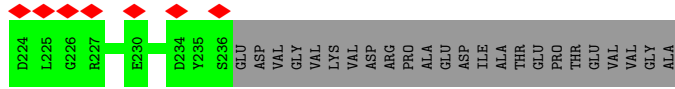


- Molecule 62: 40S ribosomal protein SA

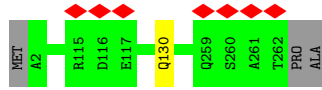


- Molecule 63: 40S ribosomal protein S3a

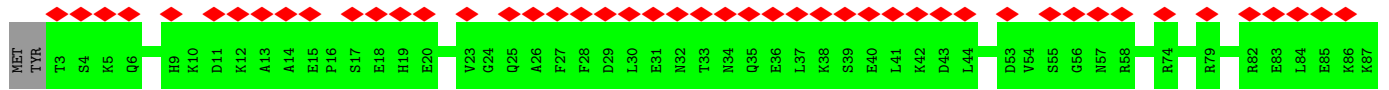




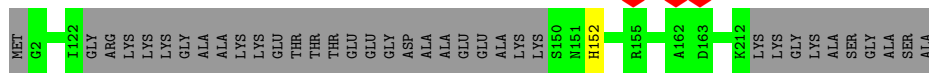
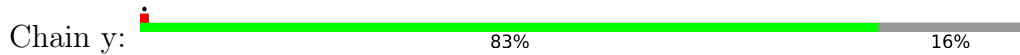
• Molecule 64: 40S ribosomal protein S4



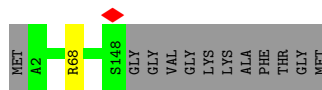
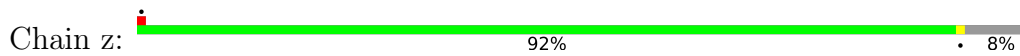
• Molecule 65: 40S ribosomal protein S7



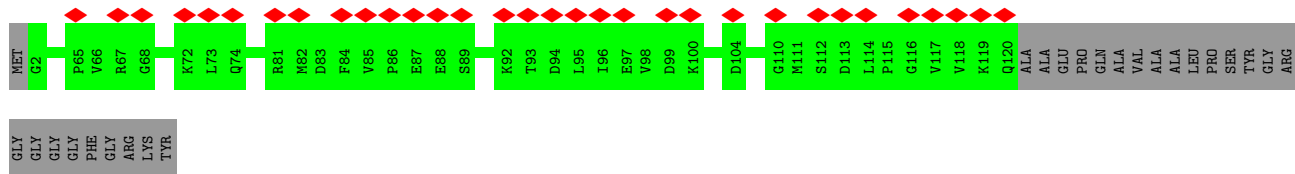
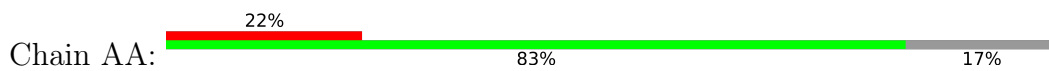
• Molecule 66: 40S ribosomal protein S8



• Molecule 67: Ribosomal_S17_N domain-containing protein



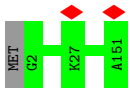
• Molecule 68: 40S ribosomal protein S17




• Molecule 69: 40S ribosomal protein S21

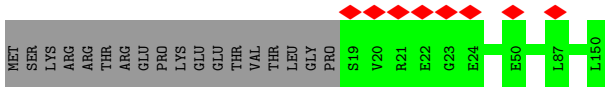
- Molecule 75: 30S ribosomal protein S15, chloroplastic

Chain HA:  99%



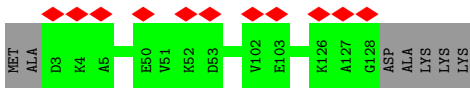
- Molecule 76: Ribosomal protein S14

Chain IA:  88% 12%




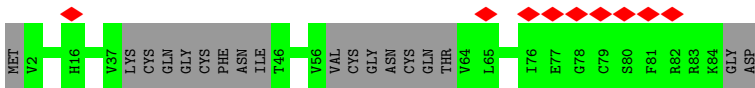
- Molecule 77: 40S ribosomal protein S24

Chain KA:  95% 5%




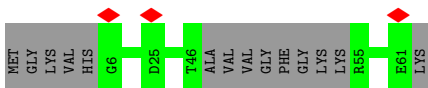
- Molecule 78: 40S ribosomal protein S27

Chain LA:  79% 21%



- Molecule 79: 40S ribosomal protein S30

Chain MA:  77% 23%



- Molecule 80: 40S ribosomal protein S15a-1

Chain JA:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335806	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 ($e^-/\text{\AA}^2$)	30.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.642	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0352	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, 4AC, 6MZ, MA6, PSU, THC, 7MG, BGC, 5MC, IAS, OMU, I2T, UY1, OMG, ZN, SPD, K, PUT, A2M, OMC, MG, SPM, UR3, HIC

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	D	0.24	0/1972	0.56	0/2651
2	F	0.23	0/3056	0.49	0/4123
3	E	0.24	0/3160	0.51	0/4230
4	G	0.24	0/2301	0.49	0/3087
5	H	0.24	0/1615	0.44	0/2163
6	I	0.24	0/1991	0.47	0/2669
7	J	0.23	0/1876	0.46	0/2513
8	K	0.23	0/1483	0.48	0/1982
9	L	0.24	0/1689	0.51	0/2258
10	M	0.23	0/1317	0.52	0/1758
11	N	0.24	0/1677	0.53	0/2249
12	O	0.23	0/1085	0.50	0/1448
13	P	0.23	0/1739	0.59	0/2330
14	Q	0.23	0/1672	0.50	0/2238
15	R	0.23	0/1273	0.51	0/1709
16	S	0.24	0/1477	0.53	0/1980
17	T	0.23	0/1513	0.55	0/1994
18	U	0.24	0/1543	0.49	0/2070
19	V	0.24	0/1332	0.54	0/1784
20	W	0.23	0/825	0.47	0/1106
21	X	0.25	0/1001	0.53	0/1345
22	Y	0.25	0/537	0.47	0/715
23	Z	0.23	0/966	0.47	0/1297
24	a	0.23	0/1076	0.57	0/1436
25	b	0.24	0/1118	0.50	0/1492
26	c	0.24	0/1183	0.49	0/1583
27	d	0.24	0/397	0.51	0/526
28	e	0.24	0/742	0.45	0/999
29	f	0.23	0/900	0.53	0/1202
30	g	0.23	0/1066	0.53	0/1425
31	h	0.25	0/922	0.53	0/1234

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.23	0/940	0.57	0/1253
33	j	0.23	0/1007	0.48	0/1339
34	k	0.23	0/808	0.52	0/1069
35	l	0.24	0/718	0.64	0/954
36	m	0.23	0/566	0.46	0/752
37	n	0.23	0/460	0.56	0/609
38	o	0.22	0/437	0.53	0/576
39	p	0.24	0/810	0.47	0/1069
40	q	0.23	0/718	0.53	0/952
41	r	0.23	0/1124	0.46	0/1504
42	s	0.18	0/46	0.67	0/69
43	2	0.19	0/71398	0.68	1/111346 (0.0%)
44	5	0.26	1/2860 (0.0%)	0.66	0/4454
45	8	0.18	0/3699	0.67	0/5762
46	S2	0.18	0/36046	0.67	1/56150 (0.0%)
47	NA	0.24	0/1702	0.50	0/2285
48	OA	0.23	0/1488	0.49	0/2005
49	PA	0.24	0/804	0.43	0/1087
50	QA	0.25	0/1039	0.51	0/1391
51	RA	0.23	0/1154	0.54	0/1540
52	TA	0.23	0/1171	0.51	0/1565
53	UA	0.23	0/1128	0.50	0/1515
54	VA	0.23	0/831	0.50	0/1118
55	WA	0.24	0/522	0.58	0/694
56	XA	0.24	0/416	0.52	0/555
57	YA	0.23	0/2516	0.48	0/3414
58	ZA	0.23	0/598	0.50	0/800
59	aA	0.13	0/334	0.63	0/518
60	bA	0.14	0/68	0.63	0/103
61	t	0.24	0/239	0.67	0/302
62	u	0.24	0/1645	0.47	0/2228
63	v	0.23	0/1790	0.50	0/2402
64	w	0.24	0/2124	0.51	0/2849
65	x	0.23	0/1547	0.50	0/2081
66	y	0.24	0/1516	0.54	0/2026
67	z	0.25	0/1189	0.52	0/1591
68	AA	0.24	0/971	0.48	0/1295
69	BA	0.24	0/649	0.46	0/871
70	CA	0.24	0/1119	0.51	0/1487
71	DA	0.24	0/810	0.55	0/1081
72	EA	0.24	0/1743	0.47	0/2350
73	FA	0.24	0/1930	0.53	0/2567
74	GA	0.24	0/1555	0.53	0/2078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	HA	0.24	0/1220	0.47	0/1639
76	IA	0.24	0/1002	0.56	0/1339
77	KA	0.24	0/1045	0.51	0/1385
78	LA	0.24	0/549	0.47	0/737
79	MA	0.23	0/387	0.56	0/508
80	JA	0.24	0/1033	0.48	0/1388
All	All	0.21	1/203975 (0.0%)	0.61	2/298248 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	1	G	OP3-P	-10.65	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	1565	C	C2-N1-C1'	5.39	124.73	118.80
46	S2	1394	C	C2-N1-C1'	5.11	124.42	118.80

There are no chirality outliers.

There are no planarity outliers.

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	D	249/260 (96%)	240 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	377/406 (93%)	374 (99%)	3 (1%)	0	100	100
3	E	383/389 (98%)	377 (98%)	6 (2%)	0	100	100
4	G	274/301 (91%)	272 (99%)	2 (1%)	0	100	100
5	H	195/229 (85%)	195 (100%)	0	0	100	100
6	I	237/242 (98%)	232 (98%)	5 (2%)	0	100	100
7	J	226/258 (88%)	225 (100%)	1 (0%)	0	100	100
8	K	180/194 (93%)	180 (100%)	0	0	100	100
9	L	203/220 (92%)	202 (100%)	1 (0%)	0	100	100
10	M	156/181 (86%)	155 (99%)	1 (1%)	0	100	100
11	N	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
12	O	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
13	P	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
14	Q	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
15	R	153/173 (88%)	151 (99%)	2 (1%)	0	100	100
16	S	184/187 (98%)	181 (98%)	3 (2%)	0	100	100
17	T	176/213 (83%)	176 (100%)	0	0	100	100
18	U	175/178 (98%)	175 (100%)	0	0	100	100
19	V	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
20	W	99/124 (80%)	99 (100%)	0	0	100	100
21	X	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
22	Y	60/165 (36%)	60 (100%)	0	0	100	100
23	Z	115/154 (75%)	114 (99%)	1 (1%)	0	100	100
24	a	130/146 (89%)	130 (100%)	0	0	100	100
25	b	132/135 (98%)	132 (100%)	0	0	100	100
26	c	145/148 (98%)	139 (96%)	5 (3%)	1 (1%)	22	30
27	d	44/60 (73%)	44 (100%)	0	0	100	100
28	e	93/112 (83%)	93 (100%)	0	0	100	100
29	f	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
30	g	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
31	h	109/112 (97%)	109 (100%)	0	0	100	100
32	i	112/120 (93%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	j	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	k	98/110 (89%)	98 (100%)	0	0	100	100
35	l	85/95 (90%)	84 (99%)	1 (1%)	0	100	100
36	m	66/69 (96%)	66 (100%)	0	0	100	100
37	n	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
38	o	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
39	p	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
40	q	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
41	r	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
47	NA	211/239 (88%)	209 (99%)	2 (1%)	0	100	100
48	OA	181/211 (86%)	177 (98%)	4 (2%)	0	100	100
49	PA	90/180 (50%)	88 (98%)	2 (2%)	0	100	100
50	QA	124/151 (82%)	122 (98%)	2 (2%)	0	100	100
51	RA	138/147 (94%)	136 (99%)	2 (1%)	0	100	100
52	TA	140/152 (92%)	138 (99%)	2 (1%)	0	100	100
53	UA	138/143 (96%)	138 (100%)	0	0	100	100
54	VA	102/123 (83%)	101 (99%)	1 (1%)	0	100	100
55	WA	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
56	XA	48/56 (86%)	48 (100%)	0	0	100	100
57	YA	313/326 (96%)	312 (100%)	1 (0%)	0	100	100
58	ZA	73/108 (68%)	73 (100%)	0	0	100	100
61	t	23/25 (92%)	23 (100%)	0	0	100	100
62	u	200/296 (68%)	200 (100%)	0	0	100	100
63	v	213/260 (82%)	213 (100%)	0	0	100	100
64	w	259/264 (98%)	258 (100%)	1 (0%)	0	100	100
65	x	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
66	y	180/220 (82%)	179 (99%)	1 (1%)	0	100	100
67	z	145/159 (91%)	145 (100%)	0	0	100	100
68	AA	117/144 (81%)	114 (97%)	3 (3%)	0	100	100
69	BA	80/82 (98%)	80 (100%)	0	0	100	100
70	CA	139/142 (98%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	DA	96/127 (76%)	96 (100%)	0	0	100	100
72	EA	218/280 (78%)	217 (100%)	1 (0%)	0	100	100
73	FA	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
74	GA	182/197 (92%)	182 (100%)	0	0	100	100
75	HA	148/151 (98%)	148 (100%)	0	0	100	100
76	IA	128/150 (85%)	127 (99%)	1 (1%)	0	100	100
77	KA	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
78	LA	62/86 (72%)	62 (100%)	0	0	100	100
79	MA	44/62 (71%)	43 (98%)	1 (2%)	0	100	100
80	JA	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
All	All	10784/12178 (89%)	10679 (99%)	104 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	c	15	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	194/199 (98%)	191 (98%)	3 (2%)	65	79
2	F	316/332 (95%)	315 (100%)	1 (0%)	92	97
3	E	330/332 (99%)	329 (100%)	1 (0%)	92	97
4	G	232/254 (91%)	232 (100%)	0	100	100
5	H	174/196 (89%)	174 (100%)	0	100	100
6	I	208/210 (99%)	208 (100%)	0	100	100
7	J	198/221 (90%)	198 (100%)	0	100	100
8	K	162/170 (95%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L	170/180 (94%)	170 (100%)	0	100	100
10	M	140/159 (88%)	140 (100%)	0	100	100
11	N	168/170 (99%)	168 (100%)	0	100	100
12	O	114/115 (99%)	114 (100%)	0	100	100
13	P	176/177 (99%)	176 (100%)	0	100	100
14	Q	174/176 (99%)	173 (99%)	1 (1%)	86	93
15	R	135/150 (90%)	134 (99%)	1 (1%)	84	92
16	S	153/154 (99%)	153 (100%)	0	100	100
17	T	157/179 (88%)	157 (100%)	0	100	100
18	U	163/164 (99%)	163 (100%)	0	100	100
19	V	139/140 (99%)	139 (100%)	0	100	100
20	W	91/106 (86%)	91 (100%)	0	100	100
21	X	103/109 (94%)	103 (100%)	0	100	100
22	Y	57/135 (42%)	57 (100%)	0	100	100
23	Z	106/135 (78%)	106 (100%)	0	100	100
24	a	118/130 (91%)	116 (98%)	2 (2%)	60	76
25	b	115/116 (99%)	115 (100%)	0	100	100
26	c	118/119 (99%)	117 (99%)	1 (1%)	81	91
27	d	41/51 (80%)	41 (100%)	0	100	100
28	e	82/97 (84%)	82 (100%)	0	100	100
29	f	96/105 (91%)	96 (100%)	0	100	100
30	g	115/121 (95%)	115 (100%)	0	100	100
31	h	97/98 (99%)	97 (100%)	0	100	100
32	i	99/104 (95%)	98 (99%)	1 (1%)	76	87
33	j	109/110 (99%)	109 (100%)	0	100	100
34	k	86/92 (94%)	86 (100%)	0	100	100
35	l	72/76 (95%)	72 (100%)	0	100	100
36	m	64/65 (98%)	64 (100%)	0	100	100
37	n	47/48 (98%)	47 (100%)	0	100	100
38	o	47/114 (41%)	47 (100%)	0	100	100
39	p	87/92 (95%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	q	73/74 (99%)	73 (100%)	0	100	100
41	r	122/123 (99%)	122 (100%)	0	100	100
47	NA	180/204 (88%)	180 (100%)	0	100	100
48	OA	157/178 (88%)	157 (100%)	0	100	100
49	PA	86/141 (61%)	86 (100%)	0	100	100
50	QA	111/132 (84%)	111 (100%)	0	100	100
51	RA	118/122 (97%)	118 (100%)	0	100	100
52	TA	122/131 (93%)	122 (100%)	0	100	100
53	UA	113/116 (97%)	113 (100%)	0	100	100
54	VA	96/109 (88%)	96 (100%)	0	100	100
55	WA	57/58 (98%)	57 (100%)	0	100	100
56	XA	42/47 (89%)	42 (100%)	0	100	100
57	YA	275/282 (98%)	274 (100%)	1 (0%)	91	96
58	ZA	65/91 (71%)	65 (100%)	0	100	100
61	t	24/24 (100%)	24 (100%)	0	100	100
62	u	170/229 (74%)	170 (100%)	0	100	100
63	v	196/229 (86%)	195 (100%)	1 (0%)	88	95
64	w	226/228 (99%)	225 (100%)	1 (0%)	91	96
65	x	168/171 (98%)	168 (100%)	0	100	100
66	y	158/181 (87%)	157 (99%)	1 (1%)	86	93
67	z	125/132 (95%)	124 (99%)	1 (1%)	81	91
68	AA	109/123 (89%)	109 (100%)	0	100	100
69	BA	68/68 (100%)	68 (100%)	0	100	100
70	CA	113/114 (99%)	112 (99%)	1 (1%)	78	89
71	DA	87/109 (80%)	87 (100%)	0	100	100
72	EA	185/222 (83%)	183 (99%)	2 (1%)	73	86
73	FA	206/214 (96%)	206 (100%)	0	100	100
74	GA	162/170 (95%)	162 (100%)	0	100	100
75	HA	130/131 (99%)	130 (100%)	0	100	100
76	IA	103/120 (86%)	103 (100%)	0	100	100
77	KA	109/114 (96%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	LA	63/78 (81%)	63 (100%)	0	100	100
79	MA	39/49 (80%)	39 (100%)	0	100	100
80	JA	108/109 (99%)	108 (100%)	0	100	100
All	All	9419/10324 (91%)	9400 (100%)	19 (0%)	93	97

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	y	152	HIS
72	EA	57	ASP
72	EA	221	PHE
70	CA	104	PHE
24	a	73	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
62	u	114	GLN
70	CA	60	GLN
80	JA	51	GLN
73	FA	7	ASN
41	r	104	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
42	s	1/2 (50%)	1 (100%)	0
43	2	3083/3391 (90%)	315 (10%)	2 (0%)
44	5	119/120 (99%)	8 (6%)	0
45	8	157/165 (95%)	15 (9%)	0
46	S2	1562/1808 (86%)	168 (10%)	1 (0%)
59	aA	13/14 (92%)	0	0
60	bA	2/3 (66%)	0	0
All	All	4937/5503 (89%)	507 (10%)	3 (0%)

5 of 507 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
42	s	2	A

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Mol	Chain	Res	Type
43	2	38	A
43	2	41	A
43	2	47	A
43	2	58	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	2	926	G
43	2	3124	U
46	S2	1463	G

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

207 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
43	PSU	2	2269	43	18,21,22	0.46	0	22,30,33	0.57	0
46	PSU	S2	762	46	18,21,22	0.46	0	22,30,33	0.56	0
43	OMC	2	2340	43	19,22,23	0.28	0	26,31,34	0.47	0
43	OMU	2	1068	43	19,22,23	0.30	0	26,31,34	0.53	0
43	PSU	2	2979	43	18,21,22	0.48	0	22,30,33	0.58	0
46	OMU	S2	1012	46	19,22,23	0.29	0	26,31,34	0.51	0
43	A2M	2	2915	43	18,25,26	0.64	0	18,36,39	0.76	1 (5%)
46	OMG	S2	598	46	18,26,27	0.91	2 (11%)	19,38,41	0.63	0
43	PSU	2	895	43	18,21,22	0.53	0	22,30,33	0.54	0
46	PSU	S2	103	46	18,21,22	0.49	0	22,30,33	0.56	0
46	4AC	S2	1781	46	21,24,25	0.29	0	29,34,37	0.30	0
46	OMU	S2	1263	46	19,22,23	0.27	0	26,31,34	0.44	0
46	OMC	S2	418	46	19,22,23	0.28	0	26,31,34	0.44	0
46	A2M	S2	977	46	18,25,26	0.68	0	18,36,39	0.78	1 (5%)
43	PSU	2	2267	43	18,21,22	0.46	0	22,30,33	0.57	0
43	OMU	2	2350	81,43	19,22,23	0.30	0	26,31,34	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMU	2	2413	81,43	19,22,23	0.29	0	26,31,34	0.41	0
43	PSU	2	2317	81,43	18,21,22	0.47	0	22,30,33	0.59	0
46	PSU	S2	1634	46	18,21,22	0.50	0	22,30,33	0.54	0
43	OMU	2	2887	43	19,22,23	0.29	0	26,31,34	0.55	0
43	PSU	2	2419	43,82	18,21,22	0.49	0	22,30,33	0.56	0
43	A2M	2	2324	43	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
43	PSU	2	2927	43	18,21,22	0.45	0	22,30,33	0.59	0
43	OMG	2	399	43	18,26,27	0.89	1 (5%)	19,38,41	0.69	0
46	PSU	S2	111	81,46	18,21,22	0.47	0	22,30,33	0.57	0
43	5MC	2	2874	81,43	18,22,23	0.44	0	26,32,35	0.52	0
46	I2T	S2	1194	46	24,29,30	0.59	0	29,42,45	0.61	0
43	PSU	2	1133	43	18,21,22	0.46	0	22,30,33	0.55	0
46	OMU	S2	1447	46	19,22,23	0.27	0	26,31,34	0.46	0
43	PSU	2	2228	43	18,21,22	0.53	0	22,30,33	0.52	0
43	PSU	2	2996	43	18,21,22	0.55	0	22,30,33	0.50	0
43	OMU	2	2733	43	19,22,23	0.30	0	26,31,34	0.45	0
46	A2M	S2	162	46	18,25,26	0.66	0	18,36,39	0.85	1 (5%)
43	A2M	2	2644	43	18,25,26	0.66	0	18,36,39	0.72	1 (5%)
43	PSU	2	2884	43	18,21,22	0.50	0	22,30,33	0.55	0
43	OMC	2	674	43	19,22,23	0.27	0	26,31,34	0.46	0
46	PSU	S2	1304	46	18,21,22	0.49	0	22,30,33	0.56	0
46	PSU	S2	1217	46	18,21,22	0.49	0	22,30,33	0.55	0
46	PSU	S2	1538	46	18,21,22	0.46	0	22,30,33	0.56	0
43	PSU	2	2352	43,82	18,21,22	0.49	0	22,30,33	0.56	0
46	4AC	S2	1283	46	21,24,25	0.30	0	29,34,37	0.36	0
46	PSU	S2	1178	46	18,21,22	0.48	0	22,30,33	0.58	0
46	PSU	S2	753	46	18,21,22	0.48	0	22,30,33	0.57	0
46	PSU	S2	635	46	18,21,22	0.48	0	22,30,33	0.60	0
43	PSU	2	2830	43	18,21,22	0.49	0	22,30,33	0.56	0
43	1MA	2	656	43,82	16,25,26	1.16	3 (18%)	18,37,40	0.83	1 (5%)
43	OMC	2	1849	43	19,22,23	0.28	0	26,31,34	0.39	0
43	OMG	2	918	81,43	18,26,27	0.95	2 (11%)	19,38,41	0.59	0
46	PSU	S2	1210	46	18,21,22	0.46	0	22,30,33	0.40	0
43	A2M	2	1460	43,82	18,25,26	0.67	0	18,36,39	0.78	1 (5%)
43	A2M	2	2259	43	18,25,26	0.65	0	18,36,39	0.74	1 (5%)
43	OMU	2	144	43	19,22,23	0.25	0	26,31,34	0.40	0
46	OMU	S2	1272	82,46	19,22,23	0.23	0	26,31,34	0.43	0
46	PSU	S2	949	46	18,21,22	0.50	0	22,30,33	0.54	0
46	PSU	S2	1027	46	18,21,22	0.52	0	22,30,33	0.63	1 (4%)
43	OMG	2	2623	43,82	18,26,27	0.91	2 (11%)	19,38,41	0.59	0
43	OMC	2	2686	43	19,22,23	0.28	0	26,31,34	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	1329	46	18,25,26	0.67	0	18,36,39	0.79	1 (5%)
46	OMC	S2	473	46	19,22,23	0.29	0	26,31,34	0.50	0
43	OMG	2	2127	43	18,26,27	0.93	1 (5%)	19,38,41	0.72	0
43	OMC	2	1862	43	19,22,23	0.29	0	26,31,34	0.40	0
43	OMG	2	2795	43	18,26,27	0.94	2 (11%)	19,38,41	0.61	0
45	A2M	8	48	45	18,25,26	0.67	0	18,36,39	0.81	1 (5%)
43	OMU	2	1537	81,43	19,22,23	0.24	0	26,31,34	0.39	0
46	PSU	S2	584	46	18,21,22	0.49	0	22,30,33	0.58	0
43	OMU	2	48	43	19,22,23	0.26	0	26,31,34	0.41	0
43	OMG	2	2797	43	18,26,27	0.93	1 (5%)	19,38,41	0.63	0
43	PSU	2	970	43	18,21,22	0.53	0	22,30,33	0.64	1 (4%)
43	PSU	2	1474	43	18,21,22	0.48	0	22,30,33	0.56	0
46	MA6	S2	1789	46	18,26,27	0.72	0	19,38,41	0.57	0
46	OMU	S2	123	46	19,22,23	0.29	0	26,31,34	0.46	0
46	PSU	S2	1002	46	18,21,22	0.48	0	22,30,33	0.55	0
46	PSU	S2	208	46	18,21,22	0.46	0	22,30,33	0.57	0
46	OMG	S2	1433	82,46	18,26,27	0.92	2 (11%)	19,38,41	0.61	0
46	OMC	S2	1218	46	19,22,23	0.27	0	26,31,34	0.40	0
43	OMU	2	675	43	19,22,23	0.30	0	26,31,34	0.52	0
43	PSU	2	2847	43	18,21,22	0.48	0	22,30,33	0.57	0
46	OMU	S2	1383	82,46	19,22,23	0.29	0	26,31,34	0.45	0
43	A2M	2	1378	43,82	18,25,26	0.66	0	18,36,39	0.71	1 (5%)
43	PSU	2	68	43	18,21,22	0.51	0	22,30,33	0.58	0
43	PSU	2	2959	43	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	1135	43	18,21,22	0.45	0	22,30,33	0.59	0
46	PSU	S2	912	46	18,21,22	0.46	0	22,30,33	0.57	0
46	A2M	S2	440	46	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
43	PSU	2	35	43	18,21,22	0.44	0	22,30,33	0.56	0
43	OMU	2	3305	43	19,22,23	0.29	0	26,31,34	0.42	0
46	PSU	S2	1293	46	18,21,22	0.45	0	22,30,33	0.58	0
46	PSU	S2	306	46	18,21,22	0.48	0	22,30,33	0.56	0
43	OMC	2	2963	43	19,22,23	0.29	0	26,31,34	0.47	0
43	PSU	2	2869	43	18,21,22	0.49	0	22,30,33	0.57	0
43	5MC	2	2281	43,82	18,22,23	0.30	0	26,32,35	0.44	0
43	PSU	2	2521	43	18,21,22	0.48	0	22,30,33	0.58	0
43	OMG	2	2291	43	18,26,27	0.92	2 (11%)	19,38,41	0.59	0
46	OMG	S2	246	46	18,26,27	0.92	1 (5%)	19,38,41	0.64	0
46	PSU	S2	1190	46	18,21,22	0.46	0	22,30,33	0.58	0
43	A2M	2	2329	43	18,25,26	0.67	0	18,36,39	0.84	1 (5%)
43	OMU	2	2739	43,82	19,22,23	0.29	0	26,31,34	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMU	2	2654	43	19,22,23	0.29	0	26,31,34	0.42	0
46	OMU	S2	1265	46	19,22,23	0.27	0	26,31,34	0.47	0
46	PSU	S2	1308	46	18,21,22	0.45	0	22,30,33	0.38	0
43	PSU	2	2321	43,82	18,21,22	0.50	0	22,30,33	0.54	0
43	OMC	2	2840	43	19,22,23	0.27	0	26,31,34	0.37	0
43	PSU	2	2139	43	18,21,22	0.49	0	22,30,33	0.55	0
46	PSU	S2	383	82,46	18,21,22	0.46	0	22,30,33	0.56	0
45	PSU	8	23	43,45	18,21,22	0.48	0	22,30,33	0.54	0
46	6MZ	S2	1771	81,82,46	18,25,26	0.72	0	16,36,39	0.73	1 (6%)
43	A2M	2	369	43	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
43	UR3	2	2957	43	19,22,23	0.30	0	26,32,35	0.32	0
43	PSU	2	1909	81,43,82	18,21,22	0.47	0	22,30,33	0.54	0
46	A2M	S2	800	46	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
46	PSU	S2	255	82,46	18,21,22	0.48	0	22,30,33	0.58	0
43	PSU	2	2898	43	18,21,22	0.52	0	22,30,33	0.53	0
46	OMU	S2	614	81,46	19,22,23	0.27	0	26,31,34	0.39	0
46	PSU	S2	1106	46	18,21,22	0.46	0	22,30,33	0.56	0
43	A2M	2	1144	43,82	18,25,26	0.67	0	18,36,39	0.87	1 (5%)
43	OMG	2	2412	43	18,26,27	0.91	1 (5%)	19,38,41	0.67	0
46	A2M	S2	28	82,46	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
43	OMC	2	2296	43	19,22,23	0.29	0	26,31,34	0.44	0
46	PSU	S2	605	46	18,21,22	0.47	0	22,30,33	0.57	0
46	PSU	S2	809	46	18,21,22	0.48	0	22,30,33	0.56	0
43	OMC	2	1480	43	19,22,23	0.24	0	26,31,34	0.37	0
43	OMC	2	2952	43	19,22,23	0.27	0	26,31,34	0.37	0
46	A2M	S2	468	46	18,25,26	0.67	0	18,36,39	0.83	1 (5%)
43	PSU	2	2435	43	18,21,22	0.47	0	22,30,33	0.56	0
46	7MG	S2	1581	59,46	22,26,27	1.21	1 (4%)	29,39,42	0.79	1 (3%)
46	OMC	S2	38	46	19,22,23	0.28	0	26,31,34	0.48	0
43	PSU	2	2263	43	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2748	43	18,21,22	0.48	0	22,30,33	0.55	0
46	PSU	S2	258	46	18,21,22	0.46	0	22,30,33	0.56	0
46	A2M	S2	1579	46	18,25,26	0.65	0	18,36,39	0.76	1 (5%)
43	PSU	2	1064	81,43	18,21,22	0.45	0	22,30,33	0.58	0
43	PSU	2	2194	43	18,21,22	0.54	0	22,30,33	0.52	0
43	OMC	2	2368	43	19,22,23	0.28	0	26,31,34	0.41	0
45	OMG	8	80	45	18,26,27	0.91	1 (5%)	19,38,41	0.62	0
43	A2M	2	946	43	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
43	A2M	2	2950	81,43,82	18,25,26	0.68	0	18,36,39	0.88	1 (5%)
46	PSU	S2	1535	46	18,21,22	0.46	0	22,30,33	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A2M	2	817	43	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
43	PSU	2	2137	81,43	18,21,22	0.45	0	22,30,33	0.59	0
43	A2M	2	2223	43	18,25,26	0.67	0	18,36,39	0.80	1 (5%)
46	PSU	S2	121	46	18,21,22	0.45	0	22,30,33	0.56	0
43	A2M	2	2284	43	18,25,26	0.66	0	18,36,39	0.87	1 (5%)
43	PSU	2	1230	43	18,21,22	0.45	0	22,30,33	0.58	0
46	MA6	S2	1790	46	18,26,27	0.75	0	19,38,41	0.57	0
43	OMU	2	2721	43	19,22,23	0.28	0	26,31,34	0.48	0
46	PSU	S2	1313	46	18,21,22	0.47	0	22,30,33	0.57	0
43	OMG	2	2126	43	18,26,27	0.96	2 (11%)	19,38,41	0.67	0
43	OMG	2	2655	43	18,26,27	0.93	1 (5%)	19,38,41	0.68	0
43	OMU	2	2116	43	19,22,23	0.24	0	26,31,34	0.42	0
43	A2M	2	2129	43	18,25,26	0.67	0	18,36,39	0.75	1 (5%)
43	PSU	2	1016	81,43	18,21,22	0.49	0	22,30,33	0.58	0
46	OMC	S2	140	46	19,22,23	0.28	0	26,31,34	0.45	0
43	A2M	2	827	43,82	18,25,26	0.66	0	18,36,39	0.86	1 (5%)
43	PSU	2	2858	43	18,21,22	0.48	0	22,30,33	0.56	0
43	A2M	2	886	43	18,25,26	0.64	0	18,36,39	0.73	1 (5%)
46	PSU	S2	950	46	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	1134	43	18,21,22	0.47	0	22,30,33	0.58	0
43	OMG	2	2921	43	18,26,27	0.95	2 (11%)	19,38,41	0.63	0
43	PSU	2	1482	43	18,21,22	0.50	0	22,30,33	0.55	0
46	PSU	S2	362	46	18,21,22	0.49	0	22,30,33	0.56	0
43	PSU	2	2617	43	18,21,22	0.49	0	22,30,33	0.56	0
43	OMC	2	2883	43	19,22,23	0.28	0	26,31,34	0.39	0
43	OMG	2	1857	81,43	18,26,27	0.94	2 (11%)	19,38,41	0.61	0
43	OMG	2	815	43	18,26,27	0.92	1 (5%)	19,38,41	0.66	0
46	PSU	S2	451	81,46	18,21,22	0.49	0	22,30,33	0.55	0
46	A2M	S2	1758	46	18,25,26	0.66	0	18,36,39	0.84	1 (5%)
46	PSU	S2	1485	46	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	2948	81,43,82	18,21,22	0.53	0	22,30,33	0.62	1 (4%)
41	THC	r	2	41	8,9,10	0.29	0	9,11,13	0.50	0
46	UY1	S2	603	46	19,22,23	0.45	0	22,31,34	0.57	0
76	IAS	IA	137	76	6,7,8	1.10	0	6,8,10	1.07	0
43	A2M	2	660	43	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
43	PSU	2	2261	43	18,21,22	0.51	0	22,30,33	0.53	0
43	PSU	2	2257	43	18,21,22	0.47	0	22,30,33	0.58	0
46	A2M	S2	544	46	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
46	PSU	S2	1184	46	18,21,22	0.47	0	22,30,33	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	1567	46	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	2716	43	18,21,22	0.53	0	22,30,33	0.62	1 (4%)
43	OMU	2	2424	43	19,22,23	0.29	0	26,31,34	0.53	0
46	OMG	S2	392	46	18,26,27	0.92	1 (5%)	19,38,41	0.62	0
43	PSU	2	1002	43	18,21,22	0.47	0	22,30,33	0.58	0
46	PSU	S2	300	46	18,21,22	0.47	0	22,30,33	0.55	0
46	PSU	S2	1120	46	18,21,22	0.48	0	22,30,33	0.56	0
43	OMC	2	1448	43,82	19,22,23	0.29	0	26,31,34	0.39	0
43	OMU	2	1894	81,43	19,22,23	0.32	0	26,31,34	0.66	0
43	OMG	2	2398	43	18,26,27	0.89	0	19,38,41	0.71	0
43	OMG	2	2819	43	18,26,27	0.90	1 (5%)	19,38,41	0.61	0
43	OMU	2	2925	43,82	19,22,23	0.28	0	26,31,34	0.47	0
45	PSU	8	79	45	18,21,22	0.48	0	22,30,33	0.56	0
3	HIC	E	246	3	8,11,12	0.80	0	6,14,16	0.59	0
43	OMG	2	2394	43	18,26,27	0.92	1 (5%)	19,38,41	0.60	0
43	OMG	2	2926	43	18,26,27	0.90	1 (5%)	19,38,41	0.62	0
43	OMG	2	2239	43	18,26,27	0.90	1 (5%)	19,38,41	0.62	0
46	OMC	S2	1645	46	19,22,23	0.26	0	26,31,34	0.43	0
46	OMG	S2	1274	81,46	18,26,27	0.92	1 (5%)	19,38,41	0.63	0
43	OMU	2	44	81,43	19,22,23	0.28	0	26,31,34	0.38	0
43	OMG	2	1461	43	18,26,27	0.91	1 (5%)	19,38,41	0.65	0
43	PSU	2	1054	43	18,21,22	0.46	0	22,30,33	0.58	0
43	OMU	2	804	43	19,22,23	0.29	0	26,31,34	0.51	0
43	PSU	2	2214	43	18,21,22	0.49	0	22,30,33	0.55	0
43	PSU	2	378	43	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	3114	43	18,21,22	0.47	0	22,30,33	0.55	0
46	OMU	S2	581	46	19,22,23	0.25	0	26,31,34	0.41	0
43	OMC	2	2200	81,43	19,22,23	0.26	0	26,31,34	0.60	0
43	PSU	2	829	43	18,21,22	0.48	0	22,30,33	0.58	0
43	OMC	2	1852	43,82	19,22,23	0.26	0	26,31,34	0.42	0
46	A2M	S2	622	82,46	18,25,26	0.64	0	18,36,39	0.75	1 (5%)

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
43	PSU	2	2269	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	762	46	-	0/7/25/26	0/2/2/2
43	OMC	2	2340	43	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMU	2	1068	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2979	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	1012	46	-	0/9/27/28	0/2/2/2
43	A2M	2	2915	43	-	0/5/27/28	0/3/3/3
46	OMG	S2	598	46	-	1/5/27/28	0/3/3/3
43	PSU	2	895	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	103	46	-	0/7/25/26	0/2/2/2
46	4AC	S2	1781	46	-	2/11/29/30	0/2/2/2
46	OMU	S2	1263	46	-	0/9/27/28	0/2/2/2
46	OMC	S2	418	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	977	46	-	0/5/27/28	0/3/3/3
43	PSU	2	2267	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2350	81,43	-	0/9/27/28	0/2/2/2
43	OMU	2	2413	81,43	-	0/9/27/28	0/2/2/2
43	PSU	2	2317	81,43	-	1/7/25/26	0/2/2/2
46	PSU	S2	1634	46	-	0/7/25/26	0/2/2/2
43	OMU	2	2887	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2419	43,82	-	0/7/25/26	0/2/2/2
43	A2M	2	2324	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2927	43	-	1/7/25/26	0/2/2/2
43	OMG	2	399	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	111	81,46	-	0/7/25/26	0/2/2/2
43	5MC	2	2874	81,43	-	2/7/25/26	0/2/2/2
46	I2T	S2	1194	46	-	1/16/34/35	0/2/2/2
43	PSU	2	1133	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	1447	46	-	0/9/27/28	0/2/2/2
43	PSU	2	2228	43	-	2/7/25/26	0/2/2/2
43	PSU	2	2996	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2733	43	-	0/9/27/28	0/2/2/2
46	A2M	S2	162	46	-	0/5/27/28	0/3/3/3
43	A2M	2	2644	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2884	43	-	0/7/25/26	0/2/2/2
43	OMC	2	674	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1304	46	-	2/7/25/26	0/2/2/2
46	PSU	S2	1217	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1538	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2352	43,82	-	0/7/25/26	0/2/2/2
46	4AC	S2	1283	46	-	0/11/29/30	0/2/2/2
46	PSU	S2	1178	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	753	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	635	46	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PSU	2	2830	43	-	2/7/25/26	0/2/2/2
43	1MA	2	656	43,82	-	0/3/25/26	0/3/3/3
43	OMC	2	1849	43	-	0/9/27/28	0/2/2/2
43	OMG	2	918	81,43	-	1/5/27/28	0/3/3/3
46	PSU	S2	1210	46	-	2/7/25/26	0/2/2/2
43	A2M	2	1460	43,82	-	0/5/27/28	0/3/3/3
43	A2M	2	2259	43	-	2/5/27/28	0/3/3/3
43	OMU	2	144	43	-	1/9/27/28	0/2/2/2
46	OMU	S2	1272	82,46	-	0/9/27/28	0/2/2/2
46	PSU	S2	949	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1027	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2623	43,82	-	0/5/27/28	0/3/3/3
43	OMC	2	2686	43	-	0/9/27/28	0/2/2/2
46	A2M	S2	1329	46	-	0/5/27/28	0/3/3/3
46	OMC	S2	473	46	-	0/9/27/28	0/2/2/2
43	OMG	2	2127	43	-	0/5/27/28	0/3/3/3
43	OMC	2	1862	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2795	43	-	0/5/27/28	0/3/3/3
45	A2M	8	48	45	-	0/5/27/28	0/3/3/3
43	OMU	2	1537	81,43	-	0/9/27/28	0/2/2/2
46	PSU	S2	584	46	-	3/7/25/26	0/2/2/2
43	OMU	2	48	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2797	43	-	0/5/27/28	0/3/3/3
43	PSU	2	970	43	-	1/7/25/26	0/2/2/2
43	PSU	2	1474	43	-	0/7/25/26	0/2/2/2
46	MA6	S2	1789	46	-	0/7/29/30	0/3/3/3
46	OMU	S2	123	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1002	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	208	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	1433	82,46	-	1/5/27/28	0/3/3/3
46	OMC	S2	1218	46	-	0/9/27/28	0/2/2/2
43	OMU	2	675	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2847	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	1383	82,46	-	0/9/27/28	0/2/2/2
43	A2M	2	1378	43,82	-	0/5/27/28	0/3/3/3
43	PSU	2	68	43	-	2/7/25/26	0/2/2/2
43	PSU	2	2959	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1135	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	912	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	440	46	-	0/5/27/28	0/3/3/3
43	PSU	2	35	43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMU	2	3305	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1293	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	306	46	-	0/7/25/26	0/2/2/2
43	OMC	2	2963	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2869	43	-	0/7/25/26	0/2/2/2
43	5MC	2	2281	43,82	-	0/7/25/26	0/2/2/2
43	PSU	2	2521	43	-	0/7/25/26	0/2/2/2
43	OMG	2	2291	43	-	0/5/27/28	0/3/3/3
46	OMG	S2	246	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	1190	46	-	0/7/25/26	0/2/2/2
43	A2M	2	2329	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2739	43,82	-	0/9/27/28	0/2/2/2
43	OMU	2	2654	43	-	0/9/27/28	0/2/2/2
46	OMU	S2	1265	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1308	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2321	43,82	-	0/7/25/26	0/2/2/2
43	OMC	2	2840	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2139	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	383	82,46	-	0/7/25/26	0/2/2/2
45	PSU	8	23	43,45	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1771	81,82,46	-	0/5/27/28	0/3/3/3
43	A2M	2	369	43	-	0/5/27/28	0/3/3/3
43	UR3	2	2957	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1909	81,43,82	-	0/7/25/26	0/2/2/2
46	A2M	S2	800	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	255	82,46	-	0/7/25/26	0/2/2/2
43	PSU	2	2898	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	614	81,46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1106	46	-	0/7/25/26	0/2/2/2
43	A2M	2	1144	43,82	-	0/5/27/28	0/3/3/3
43	OMG	2	2412	43	-	0/5/27/28	0/3/3/3
46	A2M	S2	28	82,46	-	0/5/27/28	0/3/3/3
43	OMC	2	2296	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	605	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	809	46	-	0/7/25/26	0/2/2/2
43	OMC	2	1480	43	-	0/9/27/28	0/2/2/2
43	OMC	2	2952	43	-	0/9/27/28	0/2/2/2
46	A2M	S2	468	46	-	1/5/27/28	0/3/3/3
43	PSU	2	2435	43	-	0/7/25/26	0/2/2/2
46	7MG	S2	1581	59,46	-	0/7/37/38	0/3/3/3
46	OMC	S2	38	46	-	0/9/27/28	0/2/2/2
43	PSU	2	2263	43	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PSU	2	2748	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	258	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	1579	46	-	0/5/27/28	0/3/3/3
43	PSU	2	1064	81,43	-	0/7/25/26	0/2/2/2
43	PSU	2	2194	43	-	2/7/25/26	0/2/2/2
43	OMC	2	2368	43	-	0/9/27/28	0/2/2/2
45	OMG	8	80	45	-	0/5/27/28	0/3/3/3
43	A2M	2	946	43	-	0/5/27/28	0/3/3/3
43	A2M	2	2950	81,43,82	-	0/5/27/28	0/3/3/3
46	PSU	S2	1535	46	-	0/7/25/26	0/2/2/2
43	A2M	2	817	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2137	81,43	-	0/7/25/26	0/2/2/2
43	A2M	2	2223	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	121	46	-	0/7/25/26	0/2/2/2
43	A2M	2	2284	43	-	2/5/27/28	0/3/3/3
43	PSU	2	1230	43	-	0/7/25/26	0/2/2/2
46	MA6	S2	1790	46	-	3/7/29/30	0/3/3/3
43	OMU	2	2721	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1313	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2126	43	-	3/5/27/28	0/3/3/3
43	OMG	2	2655	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2116	43	-	0/9/27/28	0/2/2/2
43	A2M	2	2129	43	-	0/5/27/28	0/3/3/3
43	PSU	2	1016	81,43	-	0/7/25/26	0/2/2/2
46	OMC	S2	140	46	-	0/9/27/28	0/2/2/2
43	A2M	2	827	43,82	-	2/5/27/28	0/3/3/3
43	PSU	2	2858	43	-	0/7/25/26	0/2/2/2
43	A2M	2	886	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	950	46	-	0/7/25/26	0/2/2/2
43	PSU	2	1134	43	-	0/7/25/26	0/2/2/2
43	OMG	2	2921	43	-	0/5/27/28	0/3/3/3
43	PSU	2	1482	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	362	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2617	43	-	0/7/25/26	0/2/2/2
43	OMC	2	2883	43	-	0/9/27/28	0/2/2/2
43	OMG	2	1857	81,43	-	0/5/27/28	0/3/3/3
43	OMG	2	815	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	451	81,46	-	0/7/25/26	0/2/2/2
46	A2M	S2	1758	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	1485	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2948	81,43,82	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	THC	r	2	41	-	4/8/10/12	-
46	UY1	S2	603	46	-	0/9/27/28	0/2/2/2
76	IAS	IA	137	76	-	1/7/7/8	-
43	A2M	2	660	43	-	1/5/27/28	0/3/3/3
43	PSU	2	2261	43	-	2/7/25/26	0/2/2/2
43	PSU	2	2257	43	-	0/7/25/26	0/2/2/2
46	A2M	S2	544	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	1184	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1567	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2716	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2424	43	-	0/9/27/28	0/2/2/2
46	OMG	S2	392	46	-	0/5/27/28	0/3/3/3
43	PSU	2	1002	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	300	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1120	46	-	0/7/25/26	0/2/2/2
43	OMC	2	1448	43,82	-	2/9/27/28	0/2/2/2
43	OMU	2	1894	81,43	-	0/9/27/28	0/2/2/2
43	OMG	2	2398	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2819	43	-	0/5/27/28	0/3/3/3
43	OMU	2	2925	43,82	-	0/9/27/28	0/2/2/2
45	PSU	8	79	45	-	0/7/25/26	0/2/2/2
3	HIC	E	246	3	-	1/5/6/8	0/1/1/1
43	OMG	2	2394	43	-	1/5/27/28	0/3/3/3
43	OMG	2	2926	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2239	43	-	0/5/27/28	0/3/3/3
46	OMC	S2	1645	46	-	0/9/27/28	0/2/2/2
46	OMG	S2	1274	81,46	-	0/5/27/28	0/3/3/3
43	OMU	2	44	81,43	-	0/9/27/28	0/2/2/2
43	OMG	2	1461	43	-	1/5/27/28	0/3/3/3
43	PSU	2	1054	43	-	0/7/25/26	0/2/2/2
43	OMU	2	804	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2214	43	-	0/7/25/26	0/2/2/2
43	PSU	2	378	43	-	0/7/25/26	0/2/2/2
43	PSU	2	3114	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	581	46	-	1/9/27/28	0/2/2/2
43	OMC	2	2200	81,43	-	4/9/27/28	0/2/2/2
43	PSU	2	829	43	-	0/7/25/26	0/2/2/2
43	OMC	2	1852	43,82	-	1/9/27/28	0/2/2/2
46	A2M	S2	622	82,46	-	2/5/27/28	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1581	7MG	C5-N7	5.00	1.41	1.35
43	2	656	1MA	C6-N6	2.96	1.35	1.27
43	2	2795	OMG	C5-C6	-2.37	1.42	1.47
43	2	918	OMG	C5-C6	-2.33	1.42	1.47
43	2	2126	OMG	C5-C6	-2.32	1.42	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	946	A2M	C5-C6-N6	2.39	123.99	120.35
43	2	2915	A2M	C5-C6-N6	2.38	123.97	120.35
46	S2	800	A2M	C5-C6-N6	2.37	123.95	120.35
43	2	886	A2M	C5-C6-N6	2.37	123.95	120.35
43	2	827	A2M	C5-C6-N6	2.36	123.94	120.35

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	246	HIC	CA-CB-CG-ND1
41	r	2	THC	N1-CA-CB-OG1
41	r	2	THC	N1-CA-CB-CG2
41	r	2	THC	C-CA-CB-OG1
41	r	2	THC	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 495 ligands modelled in this entry, 489 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PUT	S2	1927	-	5,5,5	0.14	0	4,4,4	0.18	0
87	BGC	NA	301	47	11,11,12	0.20	0	15,15,17	0.38	0
84	SPM	2	3482	-	13,13,13	0.28	0	12,12,12	0.94	0
84	SPM	2	3479	-	13,13,13	0.29	0	12,12,12	0.90	0
85	SPD	2	3481	-	9,9,9	0.26	0	8,8,8	0.87	0
84	SPM	2	3480	-	13,13,13	0.32	0	12,12,12	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PUT	S2	1927	-	-	0/3/3/3	-
87	BGC	NA	301	47	-	1/2/19/22	0/1/1/1
84	SPM	2	3482	-	-	3/11/11/11	-
84	SPM	2	3479	-	-	1/11/11/11	-
85	SPD	2	3481	-	-	0/7/7/7	-
84	SPM	2	3480	-	-	0/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	2	3482	SPM	N5-C6-C7-C8
87	NA	301	BGC	O5-C5-C6-O6
84	2	3479	SPM	C7-C8-C9-N10
84	2	3482	SPM	C3-C4-N5-C6
84	2	3482	SPM	C7-C6-N5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

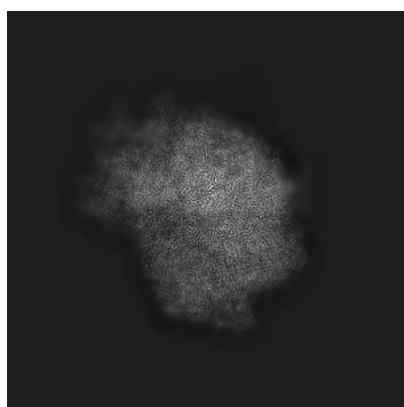
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14004. These allow visual inspection of the internal detail of the map and identification of artifacts.

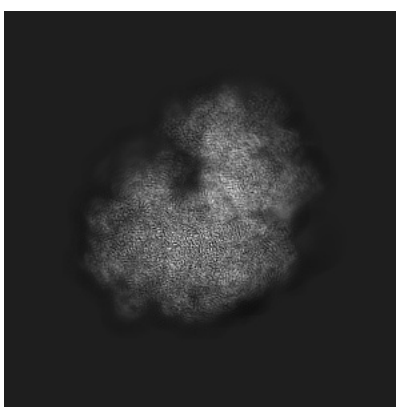
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

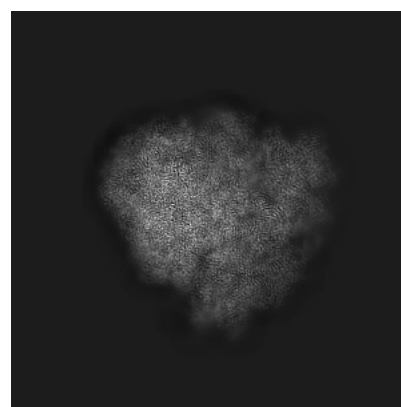
6.1.1 Primary map



X



Y

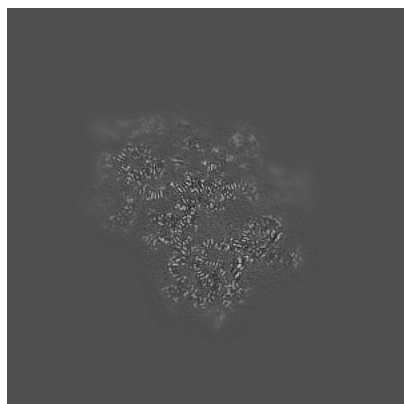


Z

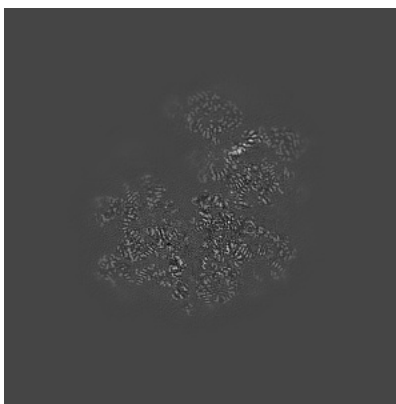
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

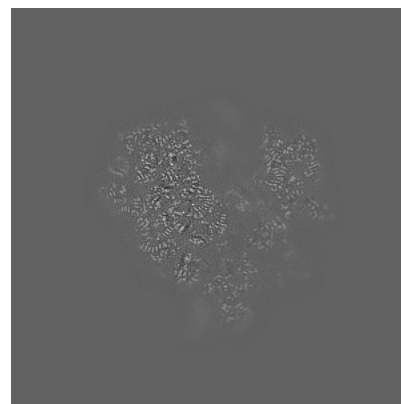
6.2.1 Primary map



X Index: 270



Y Index: 270

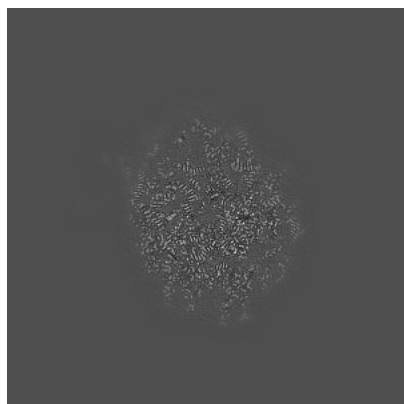


Z Index: 270

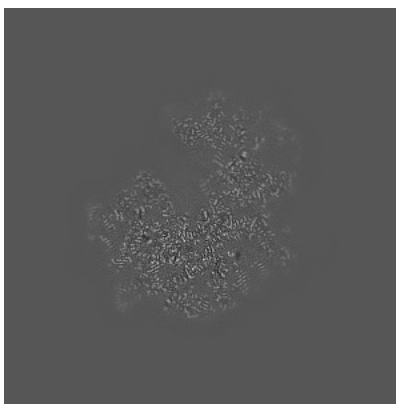
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

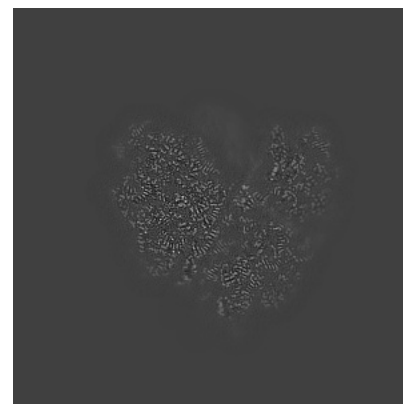
6.3.1 Primary map



X Index: 232



Y Index: 289

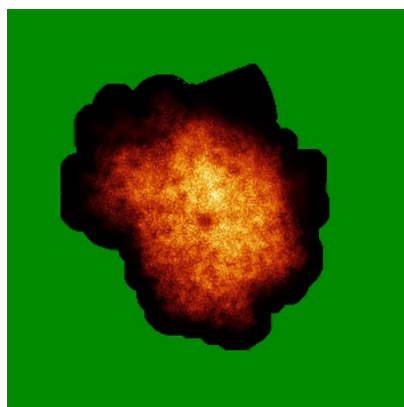


Z Index: 294

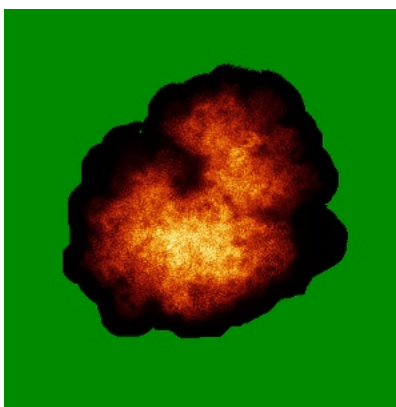
The images above show the largest variance slices of the map in three orthogonal directions.

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

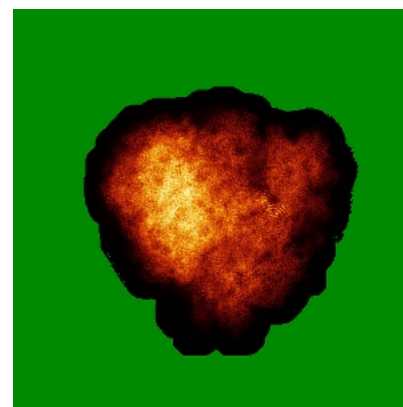
6.4.1 Primary map



X



Y

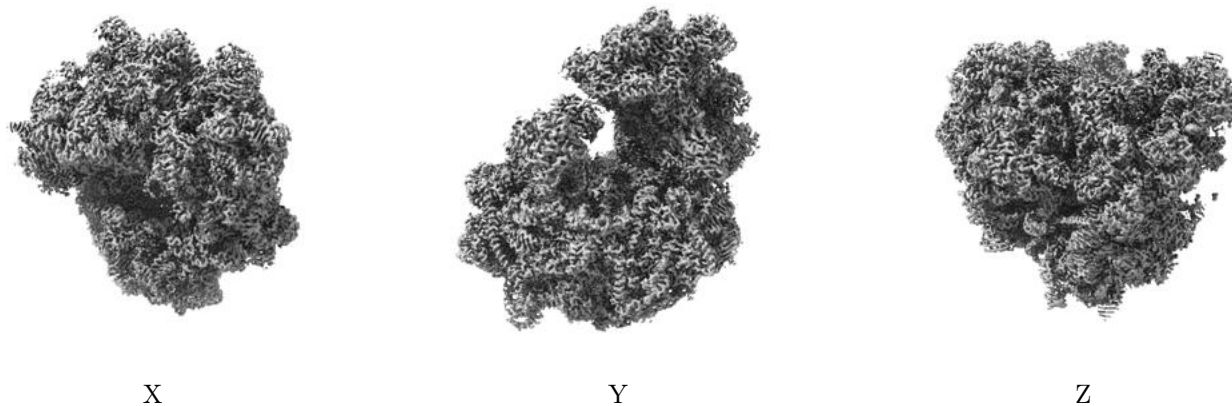


Z

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 0.0352. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

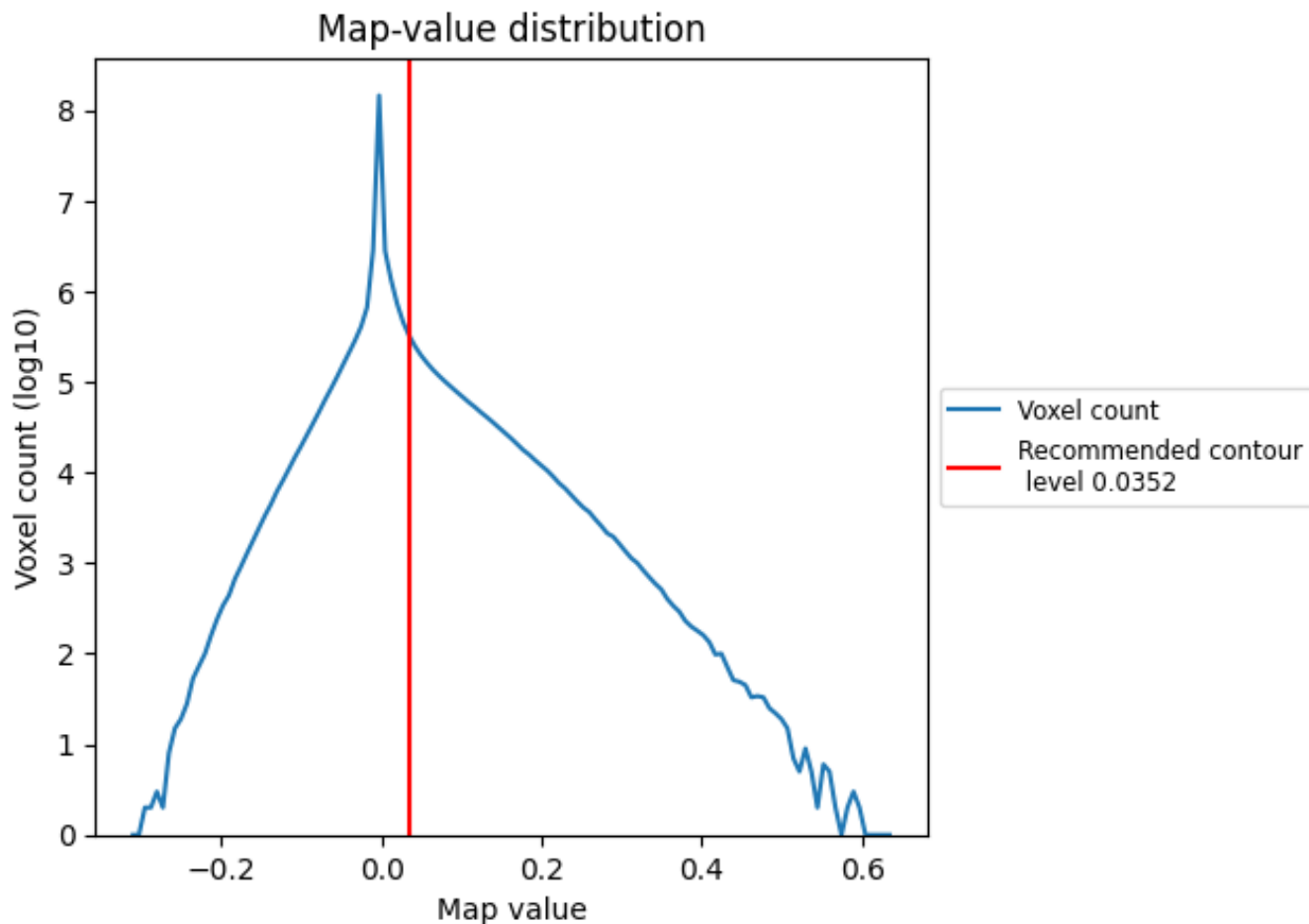
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

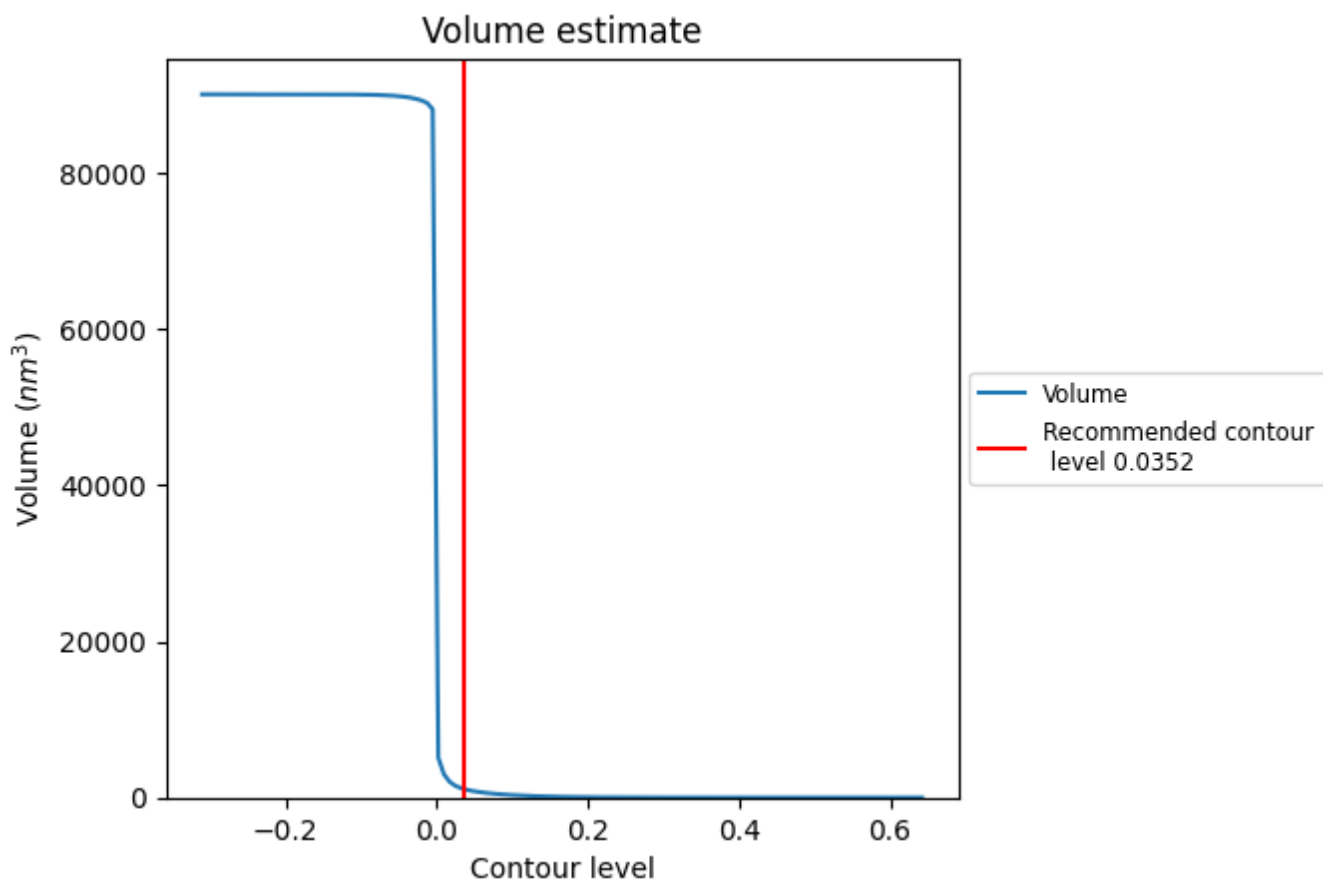
This section contains the results of statistical analysis of the map.

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.

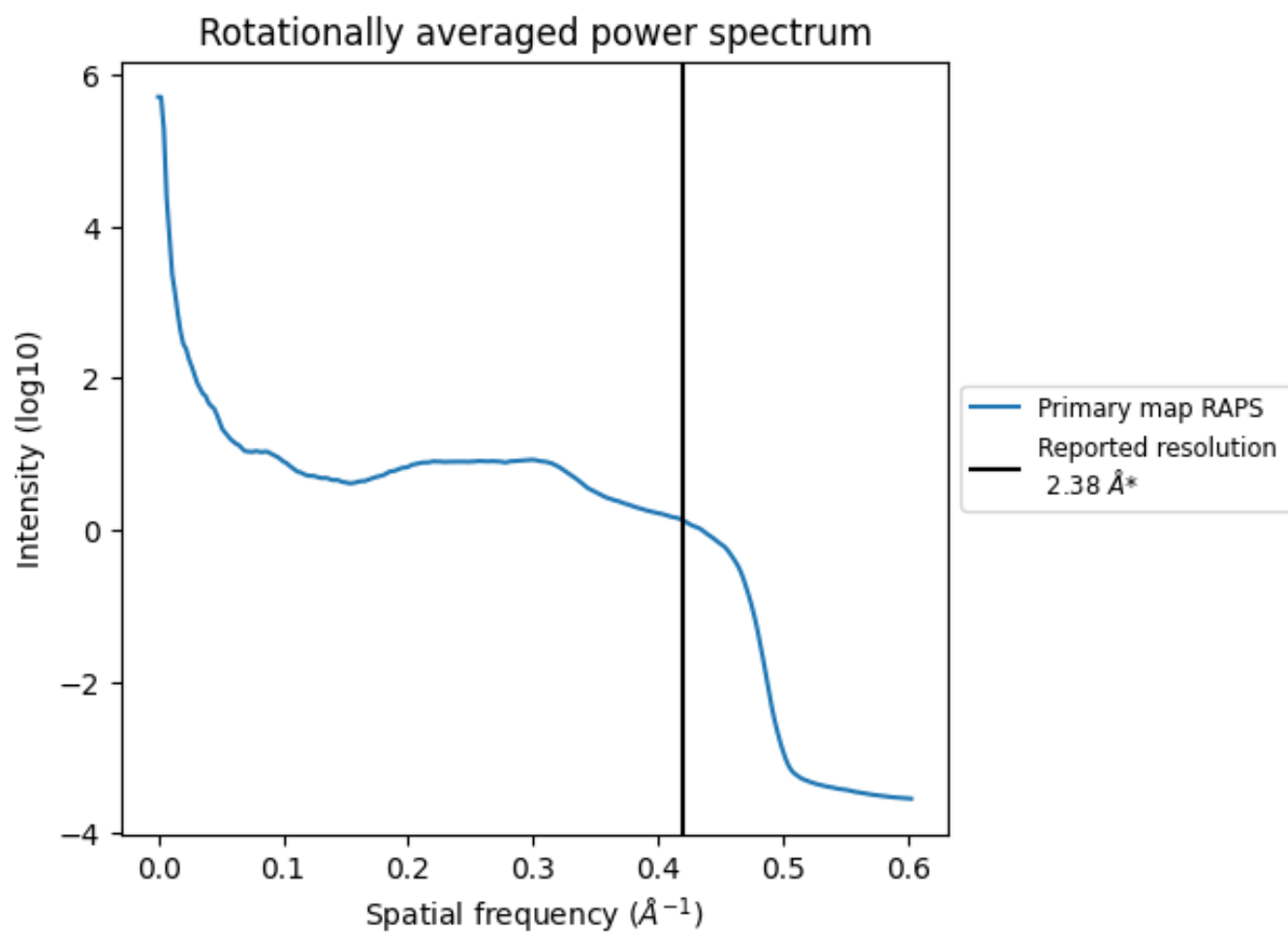
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1118 nm³; this corresponds to an approximate mass of 1010 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.420 Å⁻¹

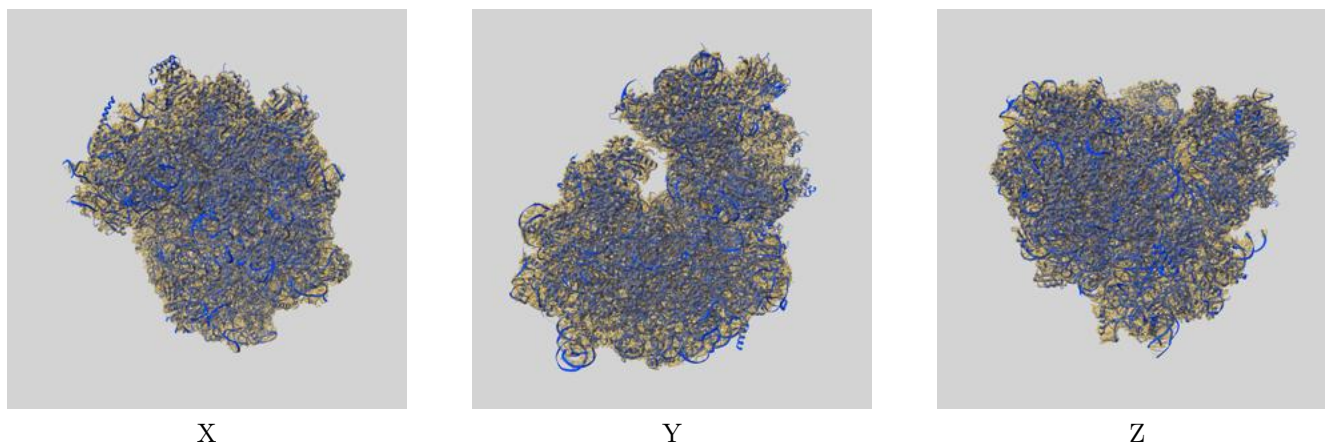
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

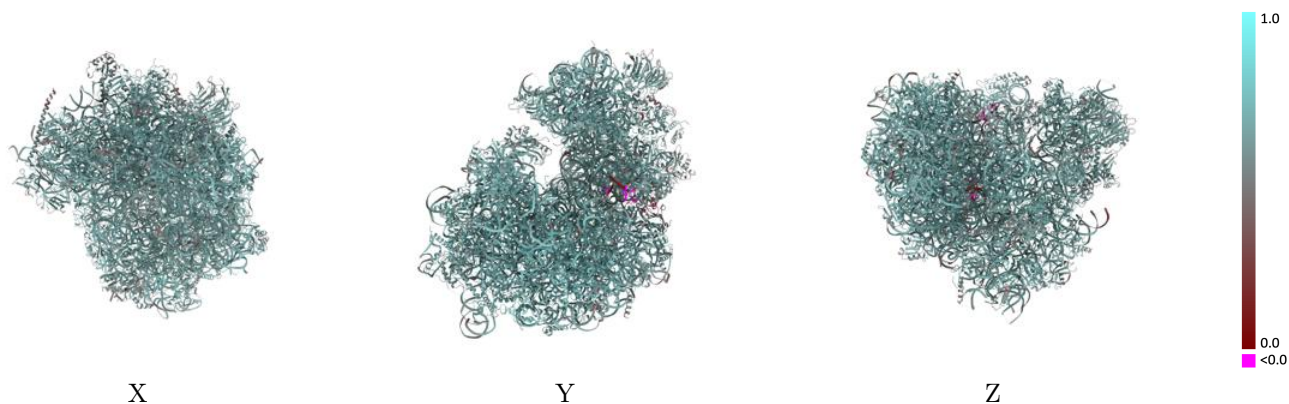
This section contains information regarding the fit between EMDB map EMD-14004 and PDB model 7QIZ. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)



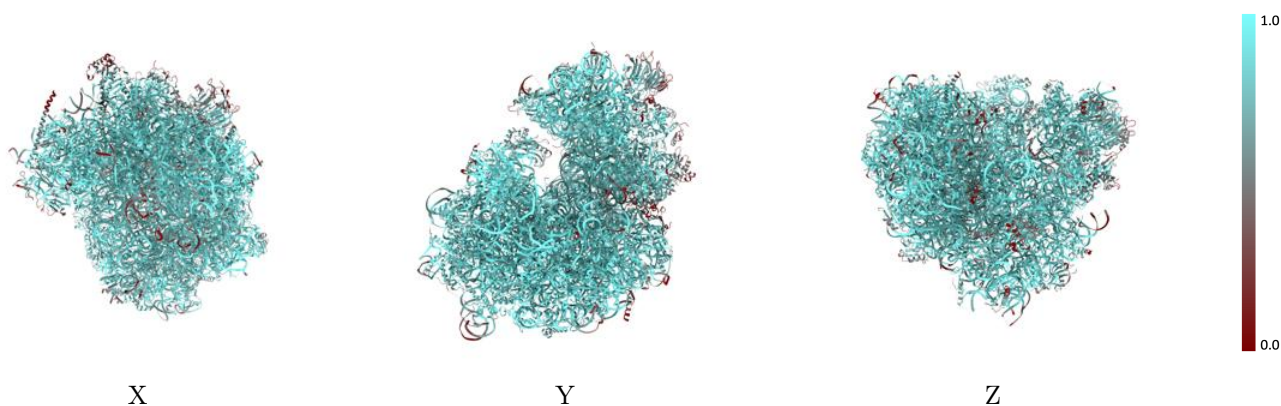
The images above show the 3D surface view of the map at the recommended contour level 0.0352 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



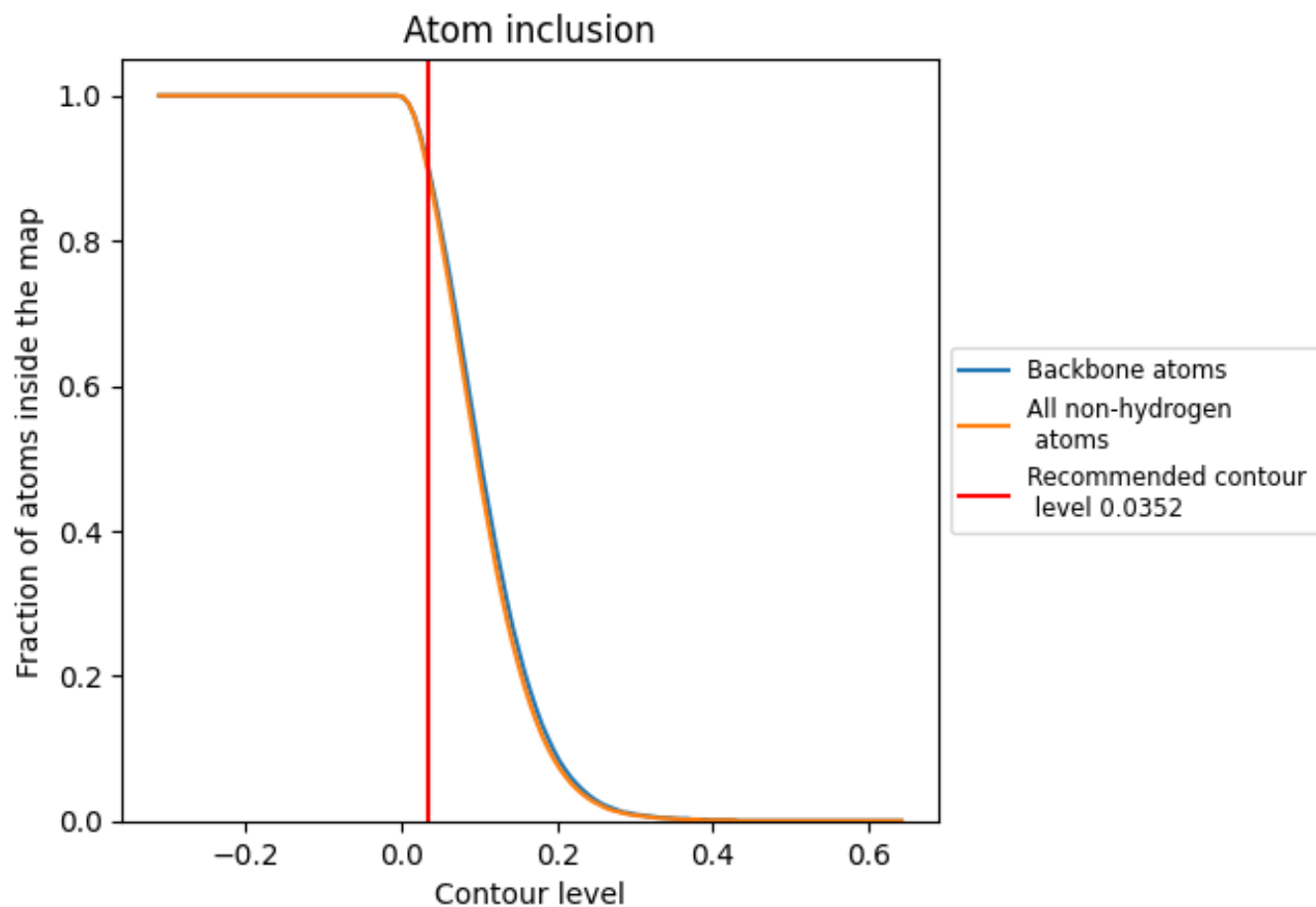
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0352).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.0352) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.6660
2	 0.9420	 0.6880
5	 0.9830	 0.6810
8	 0.9360	 0.6850
AA	 0.6460	 0.5600
BA	 0.7950	 0.6140
CA	 0.9010	 0.6680
D	 0.9710	 0.7270
DA	 0.9020	 0.6660
E	 0.9440	 0.7100
EA	 0.8700	 0.6310
F	 0.9220	 0.7020
FA	 0.6890	 0.5810
G	 0.8500	 0.6450
GA	 0.8560	 0.6310
H	 0.8180	 0.6340
HA	 0.8690	 0.6550
I	 0.9150	 0.6970
IA	 0.8680	 0.6090
J	 0.8060	 0.6380
JA	 0.9530	 0.6810
K	 0.8570	 0.6420
KA	 0.7700	 0.6120
L	 0.8820	 0.6560
LA	 0.7420	 0.6280
M	 0.7120	 0.5810
MA	 0.8000	 0.6040
N	 0.8830	 0.6770
NA	 0.7490	 0.6040
O	 0.8560	 0.6440
OA	 0.9010	 0.6530
P	 0.9910	 0.7410
PA	 0.6290	 0.5780
Q	 0.9320	 0.6970
QA	 0.7660	 0.6210



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Chain	Atom inclusion	Q-score
R	 0.9350	 0.7060
RA	 0.9100	 0.6630
S	 0.9670	 0.7210
S2	 0.9260	 0.6540
T	 0.8040	 0.6180
TA	 0.8560	 0.6410
U	 0.9470	 0.6990
UA	 0.9090	 0.6690
V	 0.9100	 0.6800
VA	 0.7480	 0.6080
W	 0.6250	 0.5720
WA	 0.7610	 0.5680
X	 0.9440	 0.7020
XA	 0.8930	 0.6700
Y	 0.9230	 0.6900
YA	 0.5600	 0.5750
Z	 0.9050	 0.6800
ZA	 0.7750	 0.6100
a	 0.8920	 0.6760
aA	 0.9200	 0.6430
b	 0.8610	 0.6470
bA	 0.9520	 0.6280
c	 0.9570	 0.7200
d	 0.9490	 0.7090
e	 0.6490	 0.4550
f	 0.8460	 0.6630
g	 0.9600	 0.7150
h	 0.9500	 0.7050
i	 0.8930	 0.6840
j	 0.8820	 0.6680
k	 0.8970	 0.6620
l	 0.9780	 0.7430
m	 0.7540	 0.6190
n	 0.9700	 0.7230
o	 0.8920	 0.6650
p	 0.9140	 0.6960
q	 0.9170	 0.6980
r	 0.9040	 0.6820
s	 1.0000	 0.7480
t	 0.9040	 0.6380
u	 0.8190	 0.6120
v	 0.7160	 0.5320

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Chain	Atom inclusion	Q-score
w	 0.8860	 0.6490
x	 0.5630	 0.5460
y	 0.8960	 0.6500
z	 0.9330	 0.6850