



Full wwPDB EM Validation Report ⓘ

Jul 25, 2022 – 09:36 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 Full wwPDB EM Validation 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:

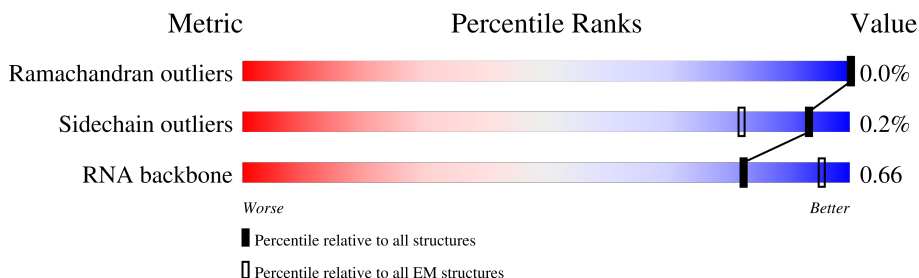
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

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	
2	F	406	
3	E	389	
4	G	301	
5	H	229	
6	I	242	
7	J	258	
8	K	194	

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

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Mol	Chain	Length	Quality of chain
34	k	110	
35	l	95	
36	m	69	
37	n	51	
38	o	128	
39	p	105	
40	q	92	
41	r	143	
42	s	2	
43	2	3391	
44	5	120	
45	8	165	
46	S2	1808	
47	NA	239	
48	OA	211	
49	PA	180	
50	QA	151	
51	RA	147	
52	TA	152	
53	UA	143	
54	VA	123	
55	WA	65	
56	XA	56	
57	YA	326	
58	ZA	108	

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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	15% 68% 32%
63	v	260	27% 82% 17%
64	w	264	11% 98% .
65	x	191	59% 98% .
66	y	220	10% 83% 16%
67	z	159	7% 92% . 8%
68	AA	144	44% 83% 17%
69	BA	82	24% 100%
70	CA	142	10% 99% ..
71	DA	127	6% 77% 23%
72	EA	280	12% 78% . 21%
73	FA	249	38% 95% 5%
74	GA	197	16% 93% 7%
75	HA	151	22% 99% .
76	IA	150	11% 88% 12%
77	KA	133	28% 95% 5%
78	LA	86	36% 79% 21%
79	MA	62	29% 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
1	D	251	Total	C	H	N	O	S	0	0
			3892	1201	1965	395	321	10		

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

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

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
3	E	386	Total	C	H	N	O	S	0	0
			6343	1984	3237	578	530	14		

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

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

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
5	H	201	Total	C	H	N	O	S	0	0
			3311	1030	1727	284	268	2		

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

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

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

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

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
8	K	184	Total	C	H	N	O	S	0	0
			3023	932	1558	265	263	5		

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
9	L	207	Total	C	H	N	O	S	0	0
			3362	1045	1709	327	271	10		

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

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

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

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

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
12	O	132	Total	C	H	N	O	S	0	0
			2239	687	1167	200	181	4		

- Molecule 13 is a protein called Ribosomal protein L15.

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

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
14	Q	205	Total	C	H	N	O	S	0	0
			3418	1045	1775	320	270	8		

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
15	R	155	Total	C	H	N	O	S	0	0
			2506	773	1258	245	225	5		

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
16	S	186	Total	C	H	N	O	S	0	0
			3013	924	1561	277	248	3		

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
17	T	178	Total	C	H	N	O	S	0	0
			3126	929	1632	319	238	8		

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
18	U	177	Total	C	H	N	O	S	0	0
			3056	971	1553	273	251	8		

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
19	V	163	Total	C	H	N	O	S	0	0
			2673	821	1365	258	226	3		

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

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

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

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

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

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

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
23	Z	117	Total	C	H	N	O	S	0	0
			1981	610	1030	170	169	2		

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
24	a	132	Total	C	H	N	O	S	0	0
			2207	657	1144	218	185	3		

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
25	b	134	Total	C	H	N	O	S	0	0
			2275	708	1177	206	182	2		

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
26	c	147	Total	C	H	N	O	S	0	0
			2358	739	1204	224	188	3		

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
27	d	46	Total	C	H	N	O	S	0	0
			775	235	388	88	63	1		

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

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

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

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

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
30	g	127	Total	C	H	N	O	S	0	0
			2173	662	1125	211	170	5		

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

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

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

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

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

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

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
34	k	100	Total	C	H	N	O	S	0	0
			1692	501	893	164	132	2		

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
35	l	87	Total	C	H	N	O	S	0	0
			1434	431	729	156	113	5		

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
36	m	68	Total	C	H	N	O	S	0	0
			1163	358	605	99	98	3		

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

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

- Molecule 38 is a protein called Ubiquitin.

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

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
39	p	99	Total	C	H	N	O	S	0	0
			1653	500	857	159	132	5		

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

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

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

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

- Molecule 42 is a RNA chain called tRNA.

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

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

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

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

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

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

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

- Molecule 46 is a RNA chain called 18S.

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

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

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

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

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

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
49	PA	92	Total	C	H	N	O	S	0	0
			1572	514	790	128	136	4		

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

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

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
51	RA	140	Total	C	H	N	O	S	0	0
			2339	722	1204	220	189	4		

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
52	TA	142	Total	C	H	N	O	S	0	0
			2343	720	1189	227	202	5		

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
53	UA	140	Total	C	H	N	O	S	0	0
			2208	692	1104	215	194	3		

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
54	VA	104	Total	C	H	N	O	S	0	0
			1701	515	880	152	150	4		

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

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

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

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

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
57	YA	317	Total	C	H	N	O	S	0	0
			4898	1554	2434	427	472	11		

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

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

- Molecule 59 is a RNA chain called tRNA_1.

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

- Molecule 60 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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
64	w	261	Total	C	H	N	O	S	0	0
			4264	1326	2180	389	361	8		

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
65	x	187	Total	C	H	N	O	S	0	0
			3103	962	1582	282	276	1		

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
66	y	184	Total	C	H	N	O	S	0	0
			3032	929	1539	296	264	4		

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
67	z	147	Total	C	H	N	O	S	0	0
			2381	737	1217	224	198	5		

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

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

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
69	BA	82	Total	C	H	N	O	S	0	0
			1257	391	617	116	128	5		

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
70	CA	141	Total	C	H	N	O	S	0	0
			2267	695	1167	215	187	3		

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

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

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

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

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

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

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

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

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

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

- Molecule 76 is a protein called Ribosomal protein S14.

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

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
77	KA	126	Total	C	H	N	O	S	0	0
			2136	654	1106	199	174	3		

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

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

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
79	MA	48	Total	C	H	N	O	S	0	0
			794	232	411	87	63	1		

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

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

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	0
			2	2	
81	E	1	Total	K	0
			1	1	
81	L	1	Total	K	0
			1	1	
81	N	2	Total	K	0
			2	2	
81	i	1	Total	K	0
			1	1	
81	p	1	Total	K	0
			1	1	
81	2	78	Total	K	0
			78	78	
81	8	4	Total	K	0
			4	4	
81	S2	26	Total	K	0
			26	26	

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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).

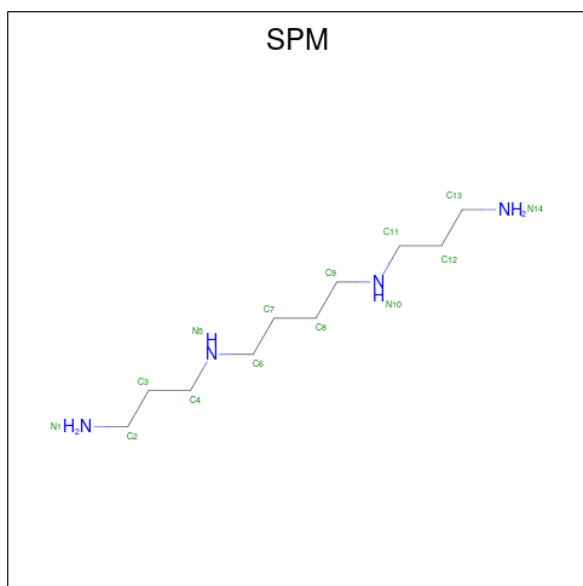
Mol	Chain	Residues	Atoms	AltConf
83	1	1	Total Zn 1 1	0

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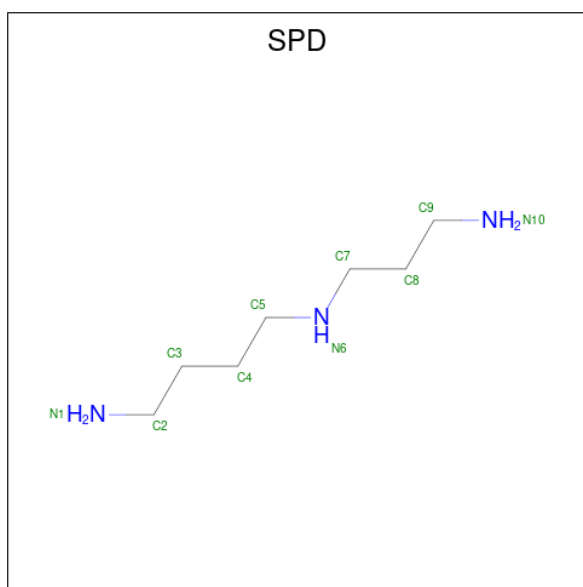
Mol	Chain	Residues	Atoms		AltConf
83	o	1	Total	Zn	0
			1	1	
83	p	1	Total	Zn	0
			1	1	
83	q	1	Total	Zn	0
			1	1	
83	XA	1	Total	Zn	0
			1	1	
83	DA	1	Total	Zn	0
			1	1	

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



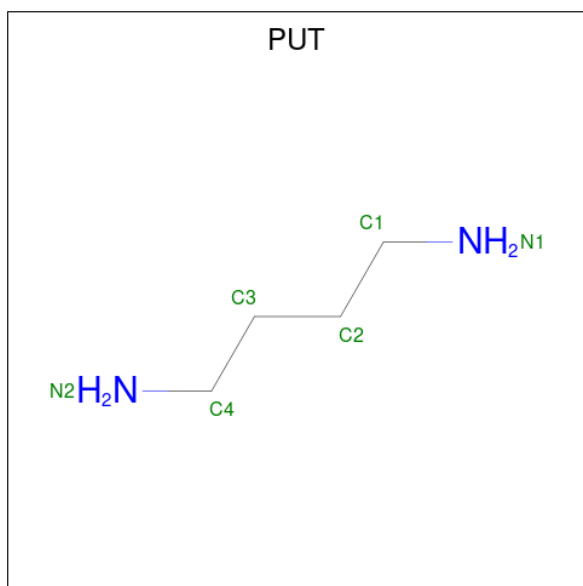
Mol	Chain	Residues	Atoms				AltConf
84	2	1	Total	C	H	N	0
			120	30	78	12	
84	2	1	Total	C	H	N	0
			120	30	78	12	
84	2	1	Total	C	H	N	0
			120	30	78	12	

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



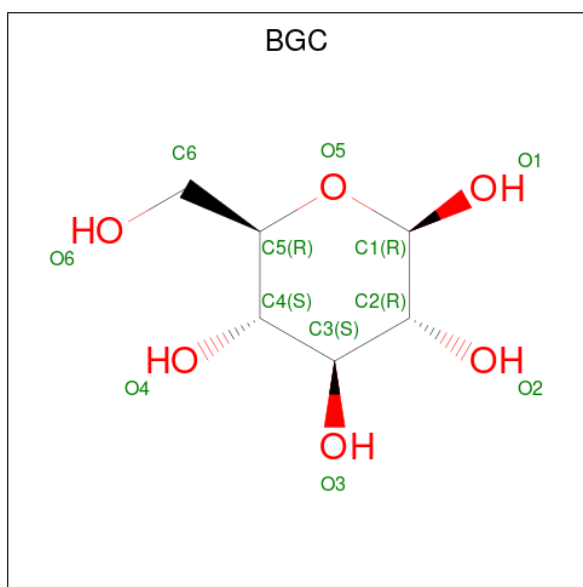
Mol	Chain	Residues	Atoms				AltConf
85	2	1	Total	C	H	N	0
			29	7	19	3	

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



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

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



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

- 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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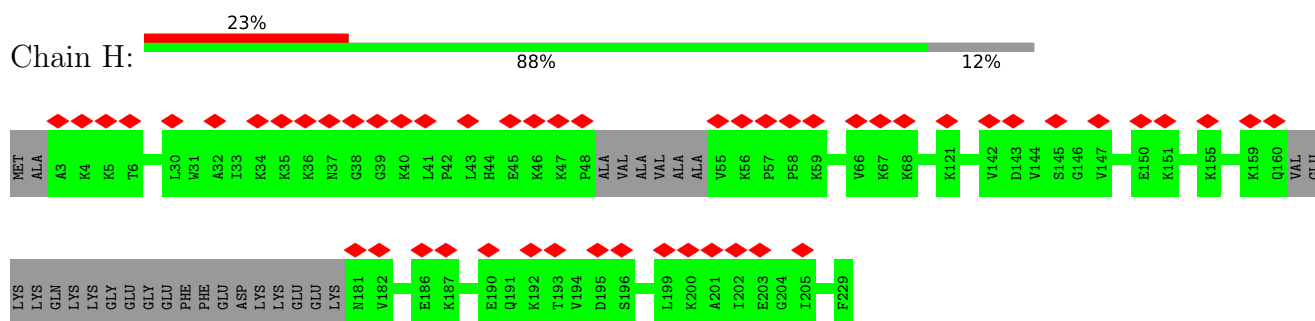
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Mol	Chain	Residues	Atoms		AltConf
88	l	29	Total 29	O 29	0
88	n	6	Total 6	O 6	0
88	o	2	Total 2	O 2	0
88	p	17	Total 17	O 17	0
88	q	8	Total 8	O 8	0
88	r	7	Total 7	O 7	0
88	s	4	Total 4	O 4	0
88	2	3141	Total 3141	O 3141	0
88	5	59	Total 59	O 59	0
88	8	115	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

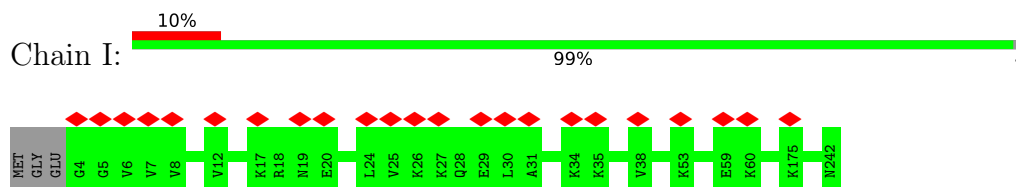
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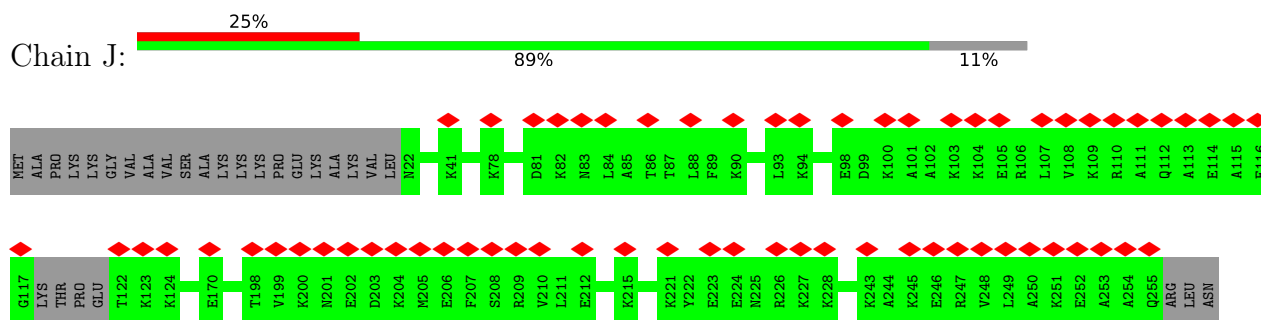
Mol	Chain	Residues	Atoms		AltConf
88	v	3	Total 3	O 3	0
88	w	6	Total 6	O 6	0
88	y	5	Total 5	O 5	0
88	z	24	Total 24	O 24	0
88	BA	2	Total 2	O 2	0
88	CA	13	Total 13	O 13	0
88	DA	15	Total 15	O 15	0
88	EA	2	Total 2	O 2	0
88	FA	2	Total 2	O 2	0
88	GA	12	Total 12	O 12	0
88	HA	6	Total 6	O 6	0
88	IA	5	Total 5	O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



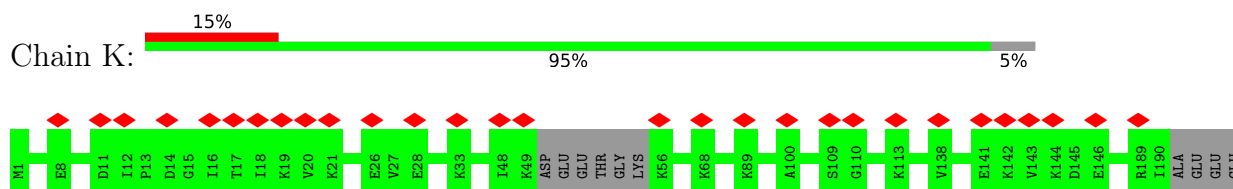
- Molecule 6: Thaliana 60S ribosomal protein L7



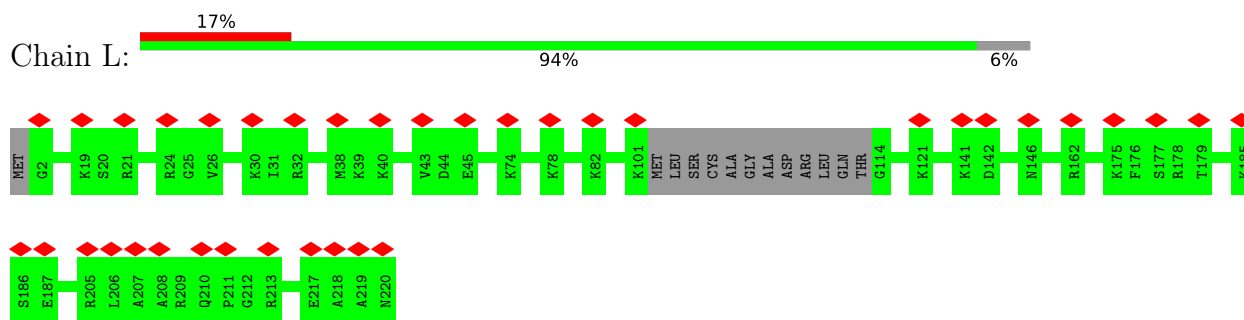
- Molecule 7: Ribosomal_L7Ae domain-containing protein



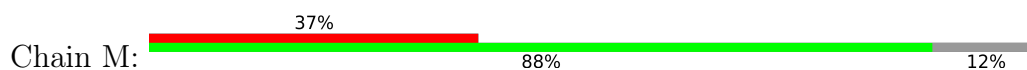
- Molecule 8: 60S ribosomal protein uL6

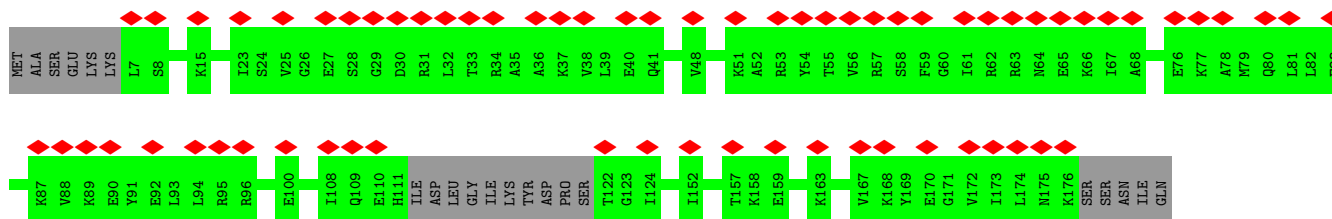


- Molecule 9: 60S ribosomal protein L10

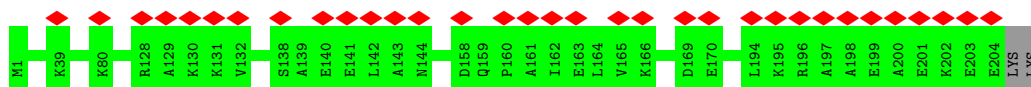


- Molecule 10: 60S ribosomal protein uL5

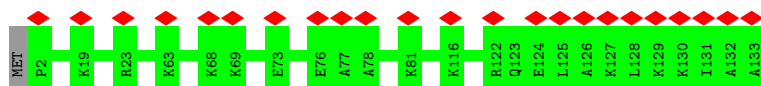




- Molecule 11: 60S ribosomal protein L13



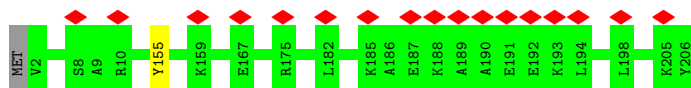
- Molecule 12: Ribosomal_L14e domain-containing protein



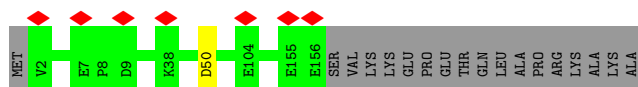
- Molecule 13: Ribosomal protein L15



- Molecule 14: Pectinesterase

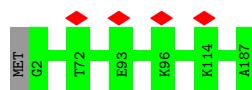


- Molecule 15: 50S ribosomal protein L22, chloroplastic

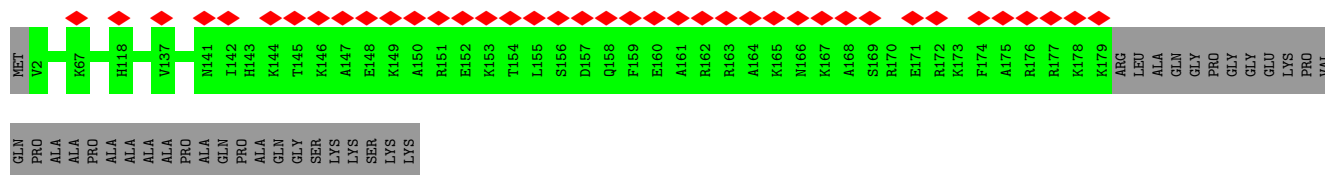
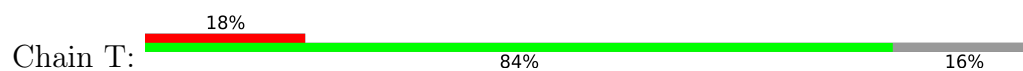


- Molecule 16: Ribosomal_L18e/L15P domain-containing protein

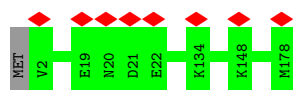




- Molecule 17: Ribosomal protein L19



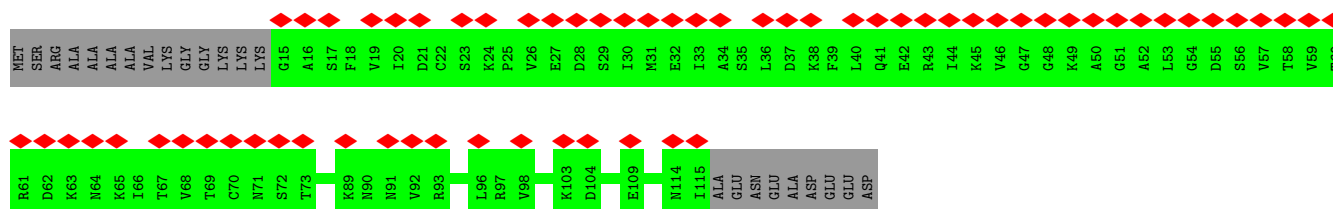
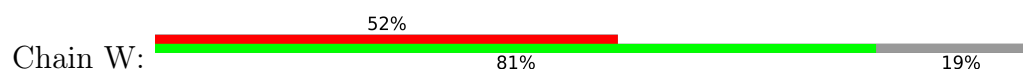
- Molecule 18: 60S ribosomal protein L18a



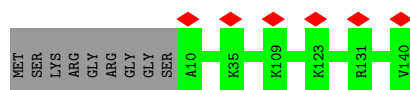
- Molecule 19: 60S ribosomal protein eL21



- Molecule 20: 60S ribosomal protein eL22

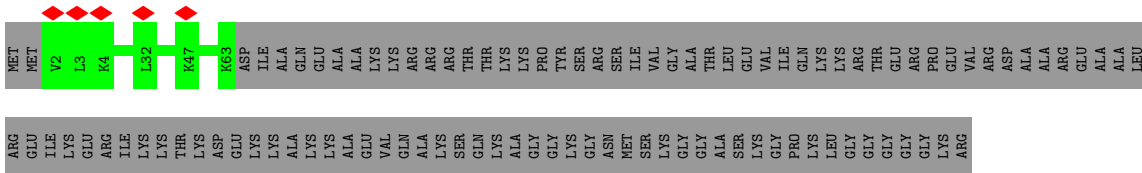


- Molecule 21: 60S ribosomal protein uL14

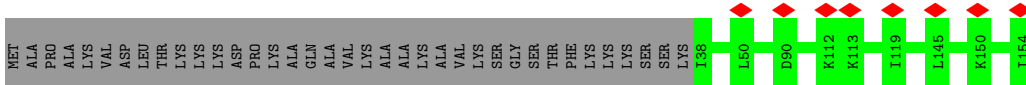
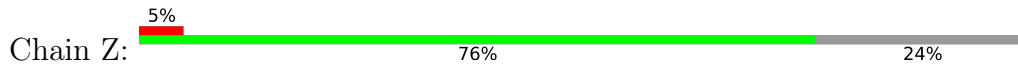


- Molecule 22: TRASH domain-containing protein

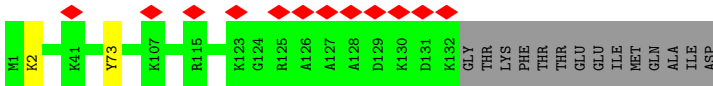
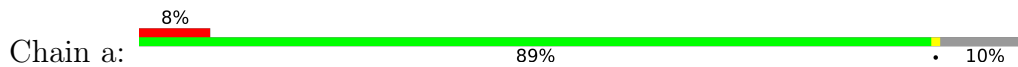




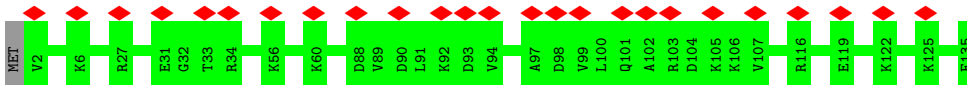
- Molecule 23: Ribosomal_L23eN domain-containing protein



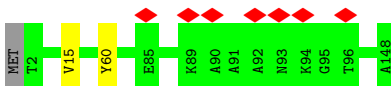
- Molecule 24: KOW domain-containing protein



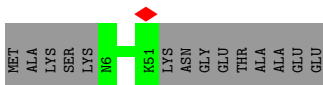
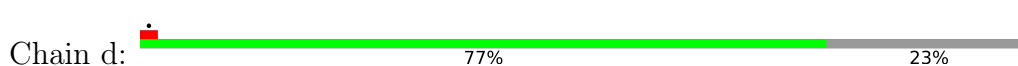
- Molecule 25: 60S ribosomal protein L27



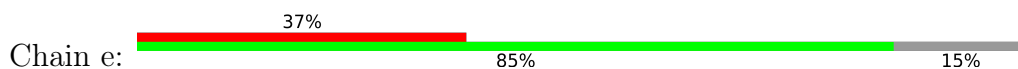
- Molecule 26: Ribosomal_L18e/L15P domain-containing protein

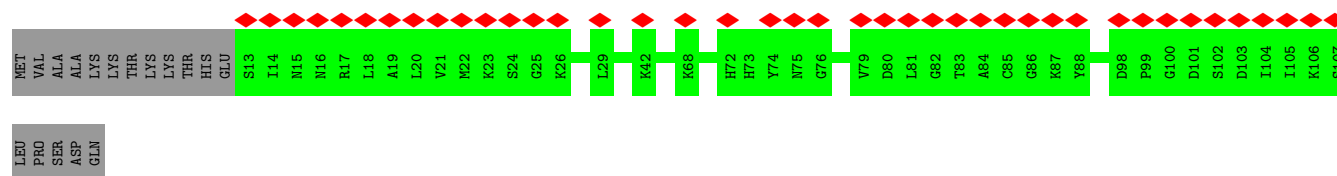


- Molecule 27: 60S ribosomal protein L29

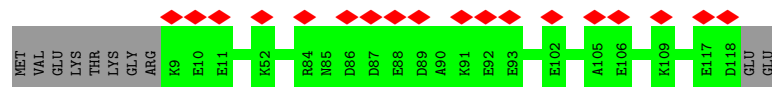


- Molecule 28: 60S ribosomal protein eL30

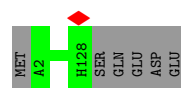




- Molecule 29: 60S ribosomal protein eL31



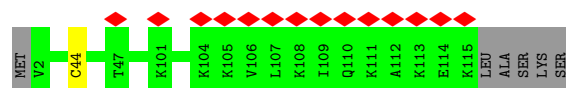
- Molecule 30: 60S ribosomal protein eL32



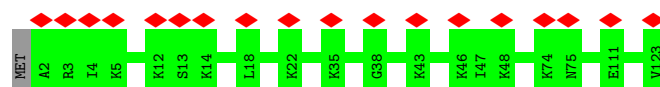
- Molecule 31: 60S ribosomal protein eL33



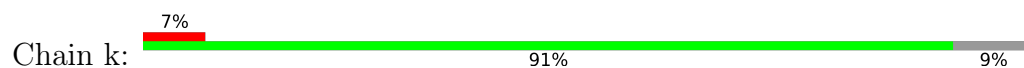
- Molecule 32: 60S ribosomal protein eL34

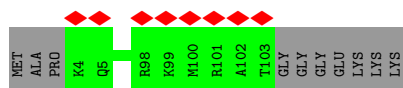


- Molecule 33: Similar to 60S ribosomal protein L35

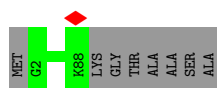


- Molecule 34: 60S ribosomal protein L36

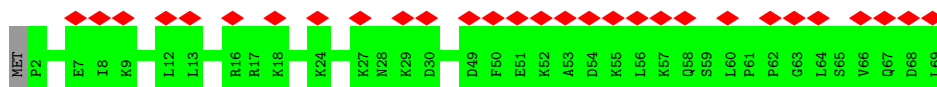
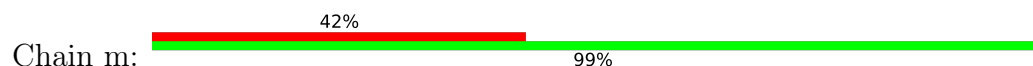




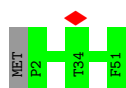
- Molecule 35: Ribosomal protein L37



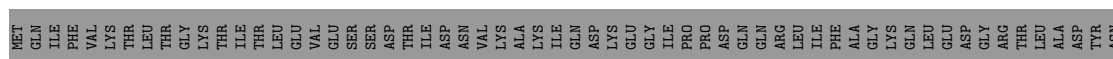
- Molecule 36: 60S ribosomal protein L38



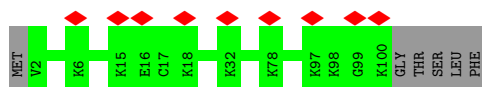
- Molecule 37: 60S ribosomal protein eL39



- Molecule 38: Ubiquitin

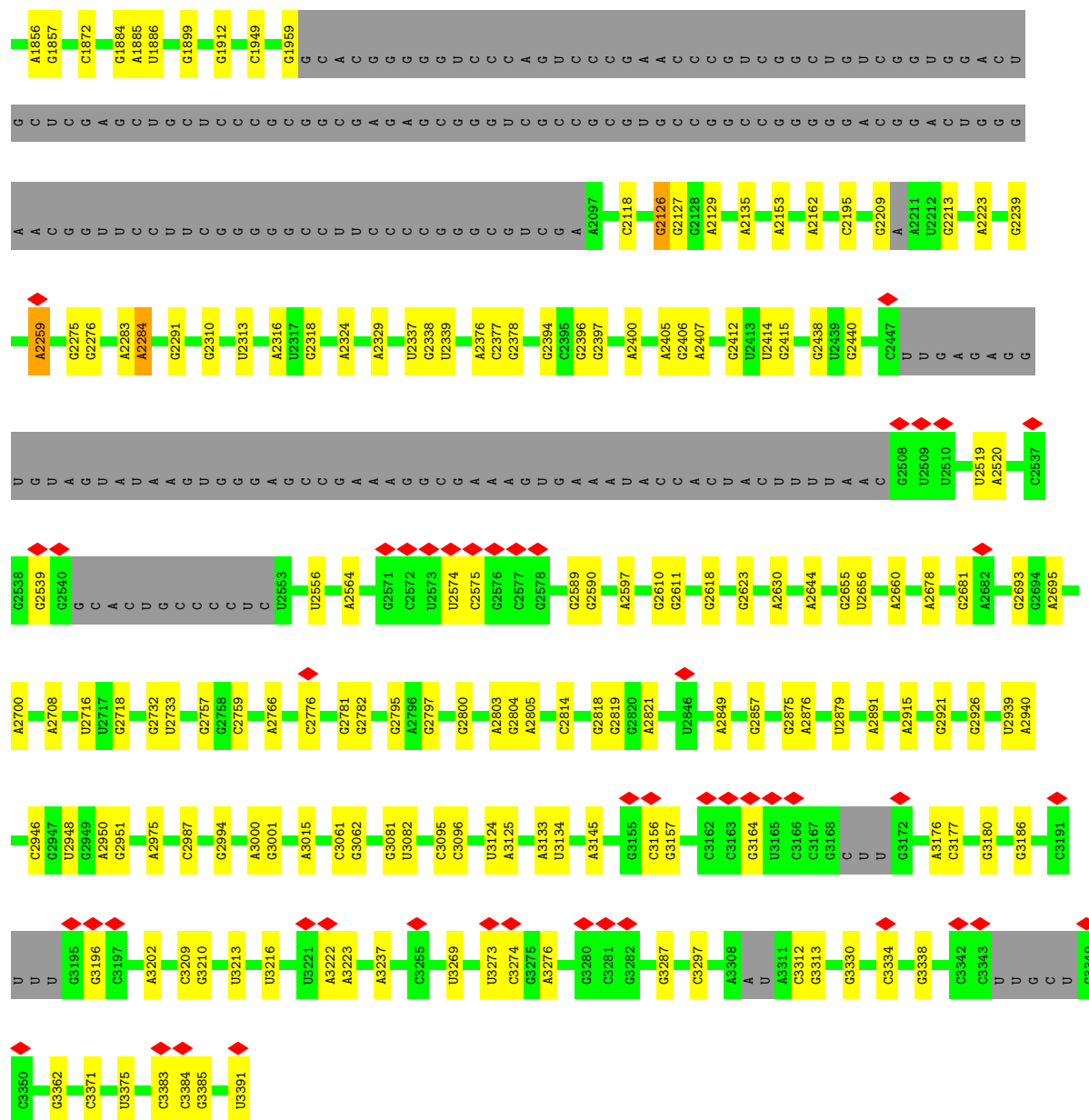


- Molecule 39: 60S ribosomal protein eL42

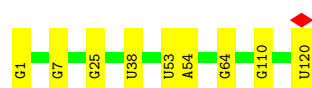


- Molecule 40: 60S ribosomal protein eL43

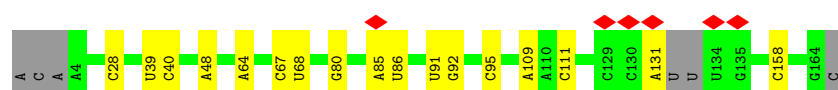
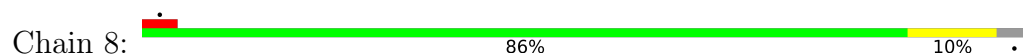


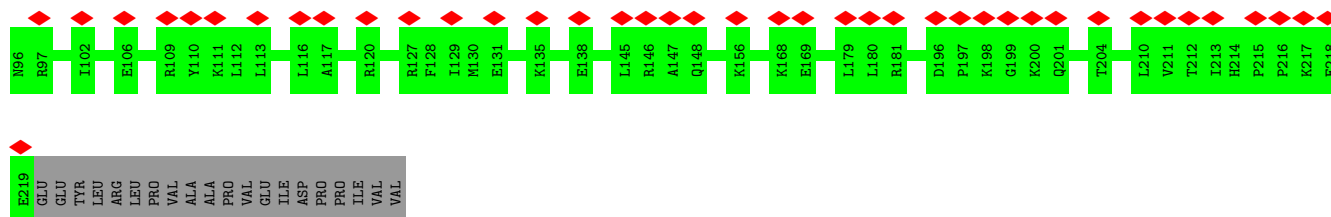


• Molecule 44: 5S rRNA

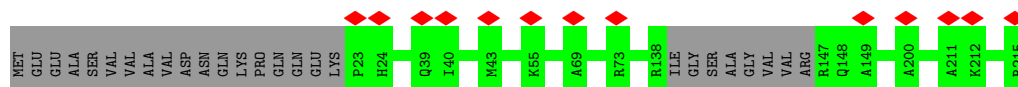
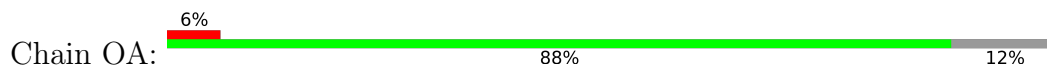


• Molecule 45: 5.8S rRNA

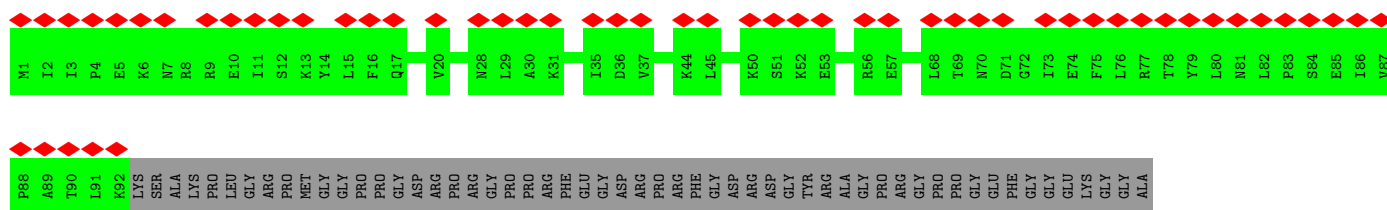




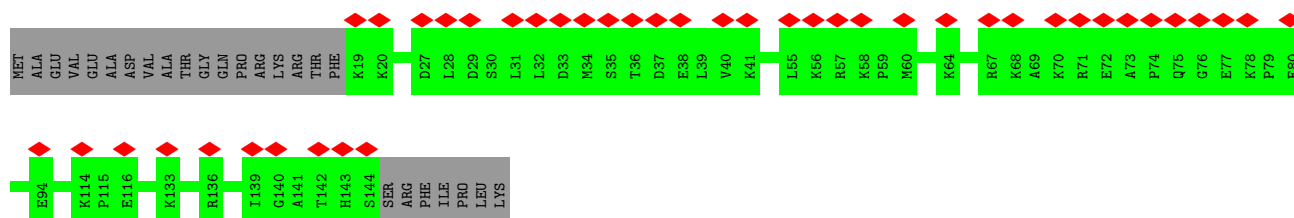
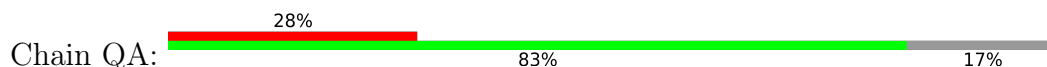
- Molecule 48: Ribosomal_S7 domain-containing protein



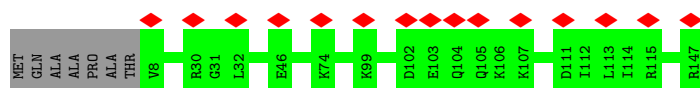
- Molecule 49: S10_ plectin domain-containing protein



- Molecule 50: 40S ribosomal protein uS19

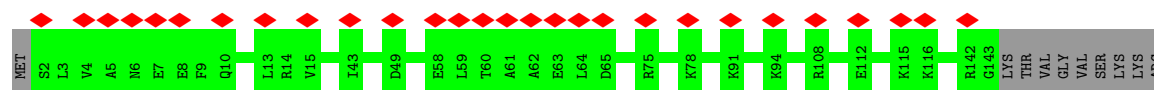


- Molecule 51: 40S ribosomal protein uS9

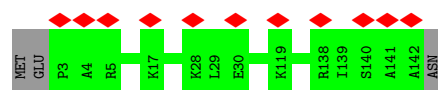


- Molecule 52: 40S ribosomal protein uS13

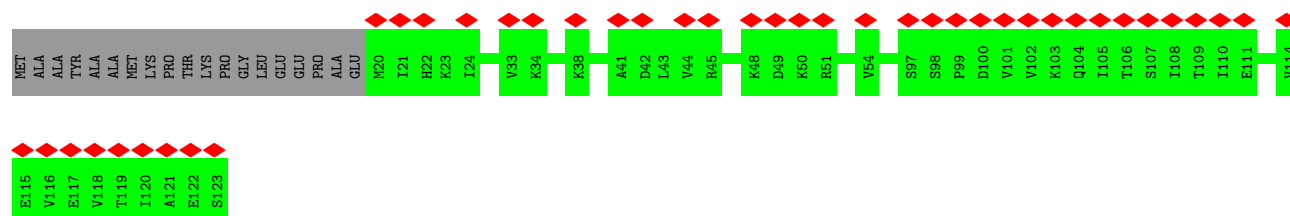
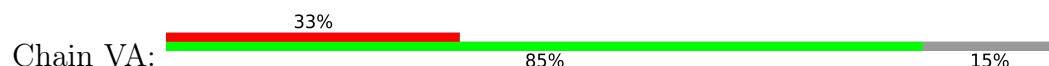




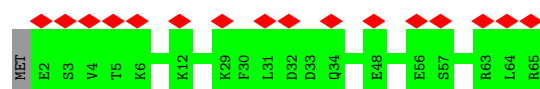
- Molecule 53: 40S ribosomal protein eS19



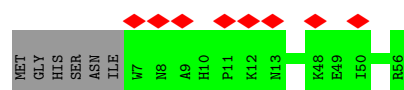
- Molecule 54: Ribosomal_S10 domain-containing protein



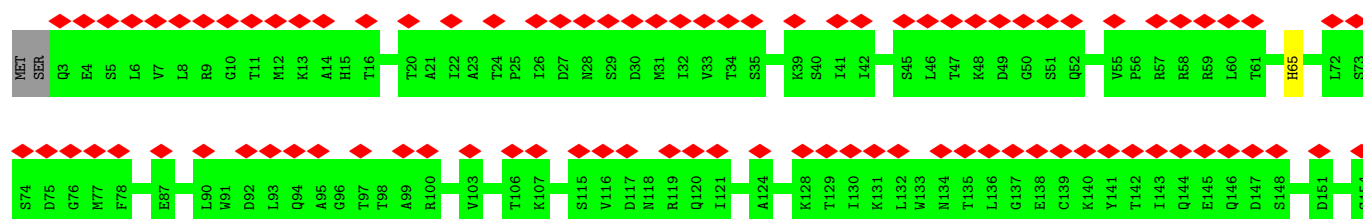
- Molecule 55: 40S ribosomal protein eS28

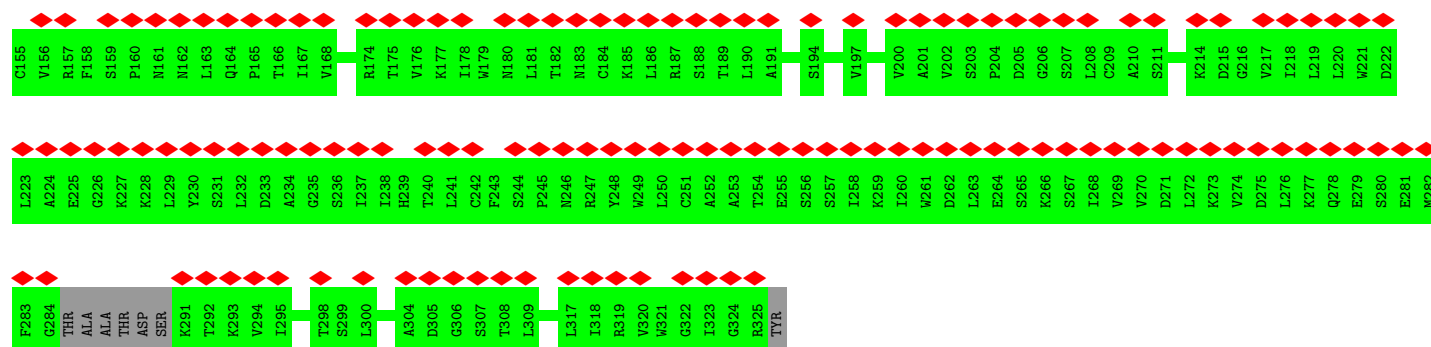


- Molecule 56: 40S ribosomal protein uS14

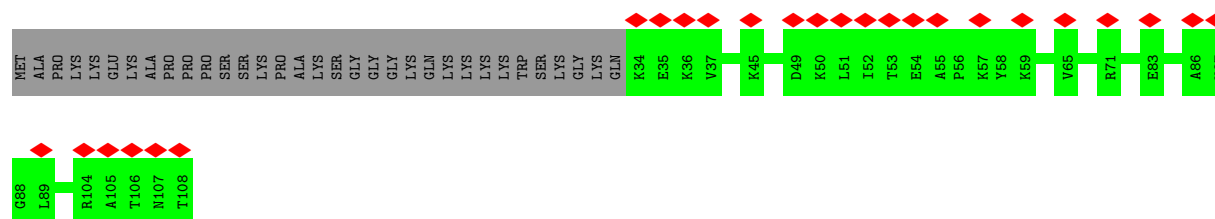


- Molecule 57: Mitogen-activated protein kinase





- Molecule 58: 40S ribosomal protein S25



- Molecule 59: tRNA_1



There are no outlier residues recorded for this chain.

- Molecule 60: mRNA

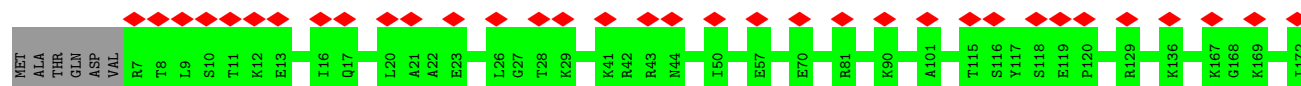


There are no outlier residues recorded for this chain.

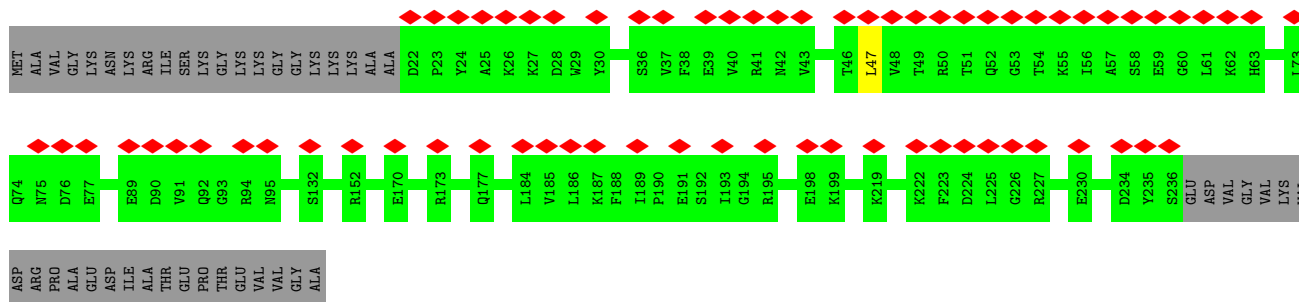
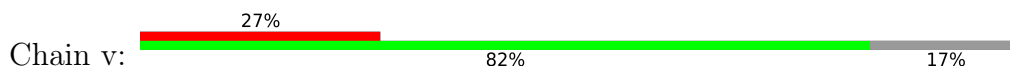
- Molecule 61: 60S ribosomal protein L41



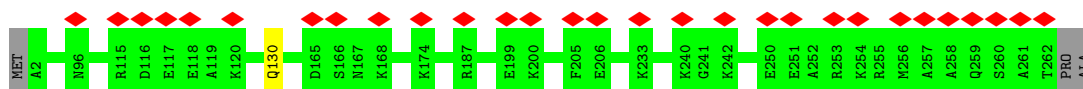
- Molecule 62: 40S ribosomal protein SA



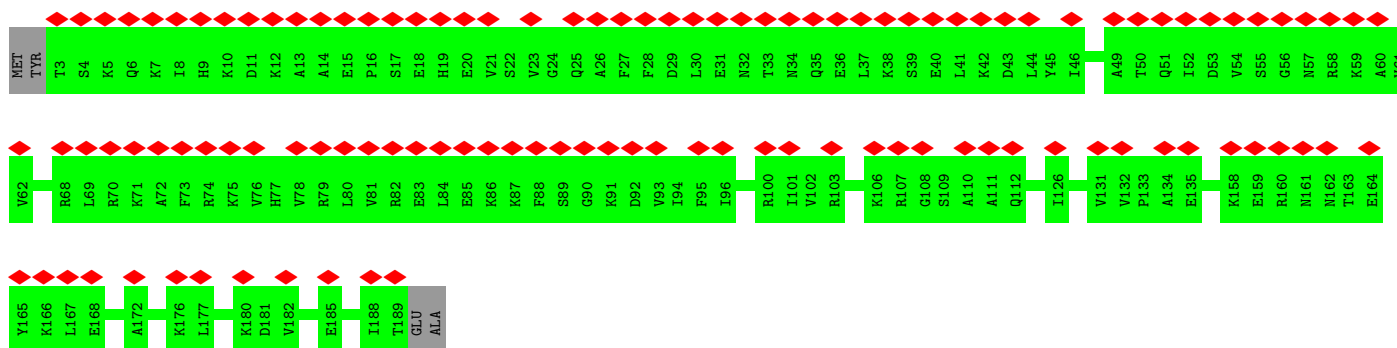
- Molecule 63: 40S ribosomal protein S3a



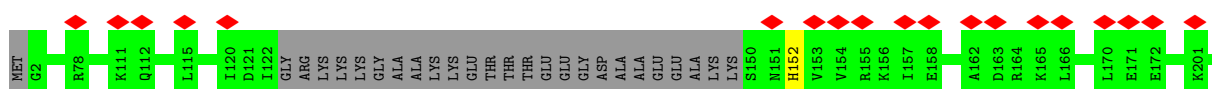
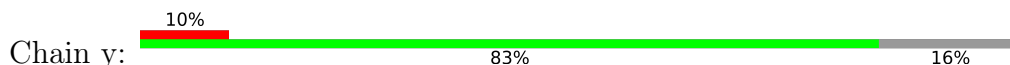
- Molecule 64: 40S ribosomal protein S4



- Molecule 65: 40S ribosomal protein S7

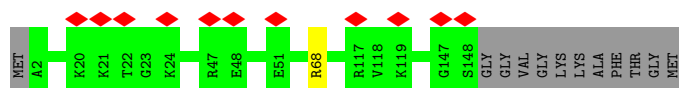
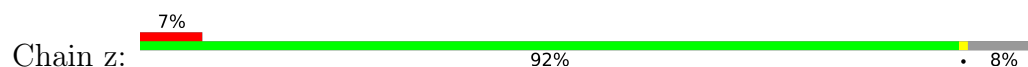


- Molecule 66: 40S ribosomal protein S8

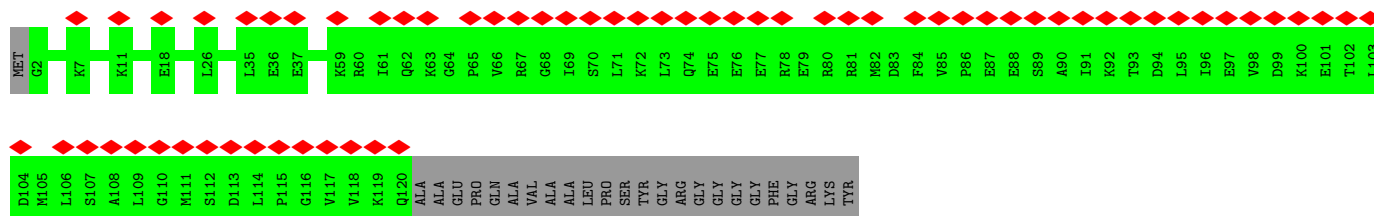
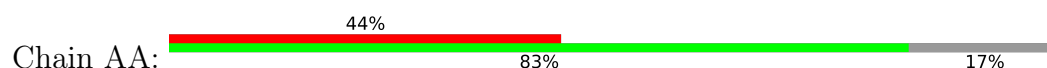




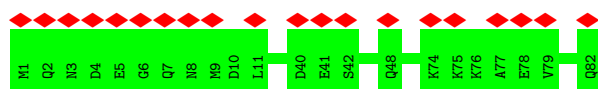
- Molecule 67: Ribosomal_S17_N domain-containing protein



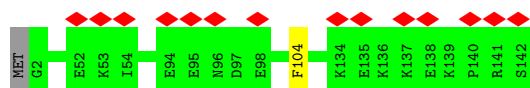
- Molecule 68: 40S ribosomal protein S17



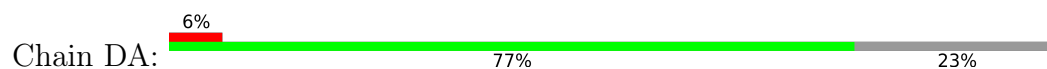
- Molecule 69: 40S ribosomal protein S21



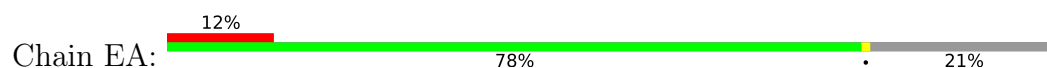
- Molecule 70: 40S body ribosomal protein uS12

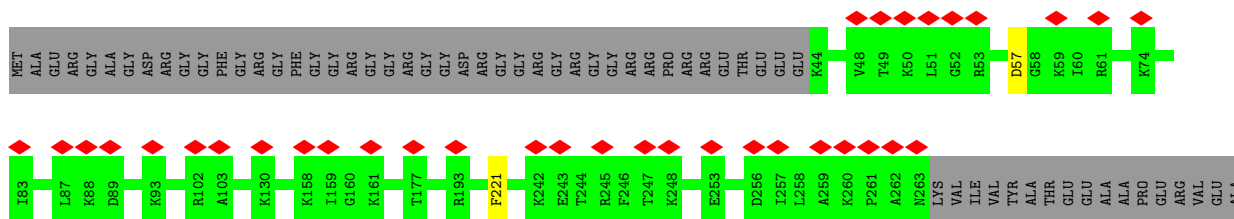


- Molecule 71: 40S ribosomal protein S26



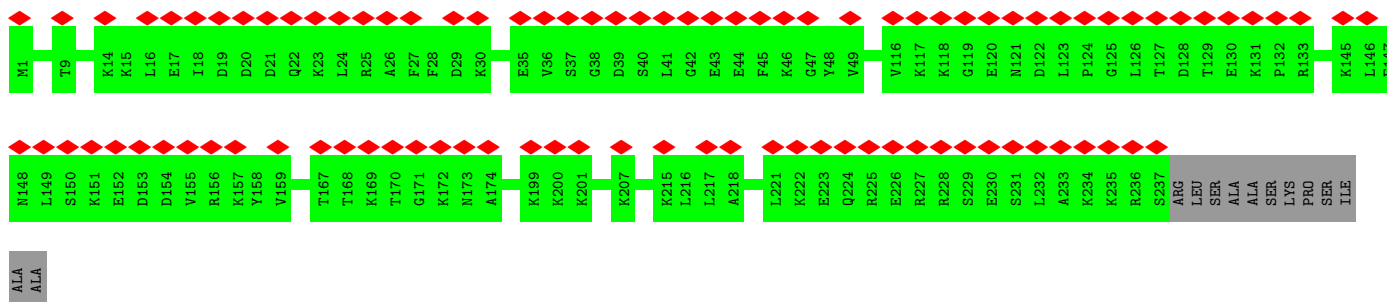
- Molecule 72: S5 DRBM domain-containing protein





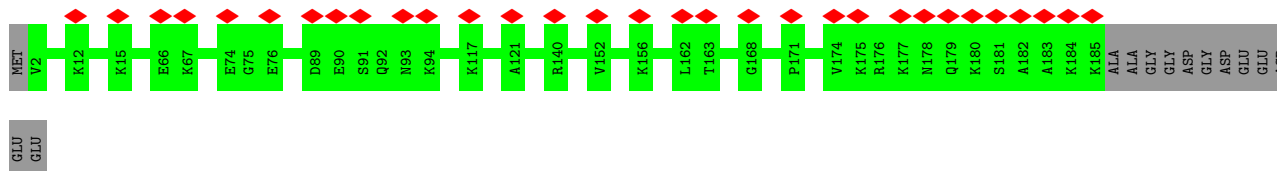
• Molecule 73: 40S ribosomal protein S6

Chain FA: 38% 95% 5%



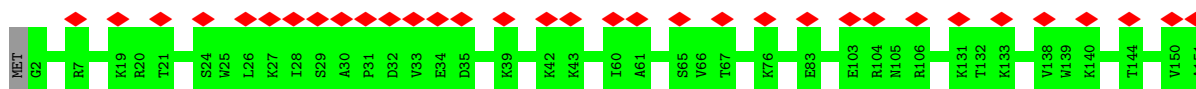
• Molecule 74: 40S body ribosomal protein uS4

Chain GA: 16% 93% 7%



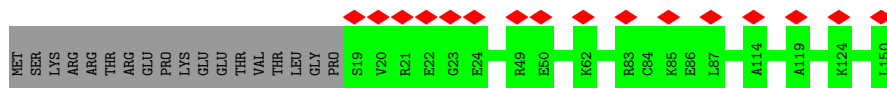
• Molecule 75: 30S ribosomal protein S15, chloroplastic

Chain HA: 22% 99% 0%



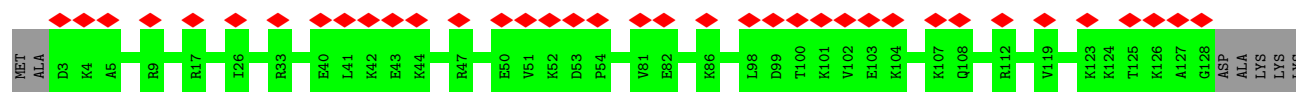
• Molecule 76: Ribosomal protein S14

Chain IA: 11% 88% 12%

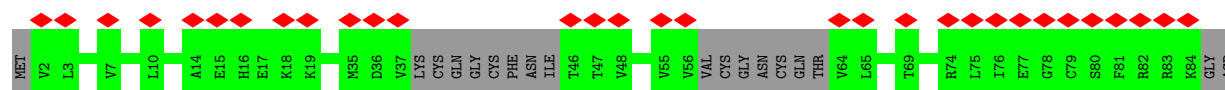
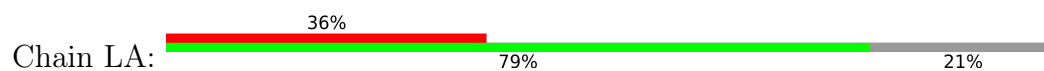


• Molecule 77: 40S ribosomal protein S24

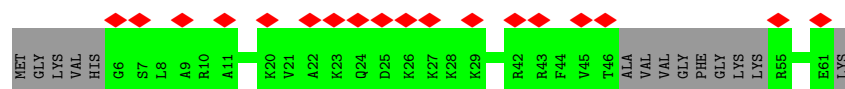
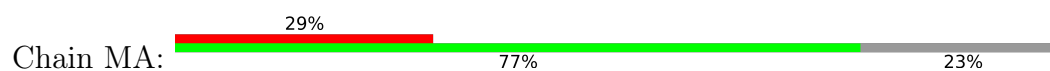
Chain KA: 28% 95% 5%



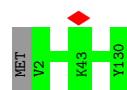
- Molecule 78: 40S ribosomal protein S27



- Molecule 79: 40S ribosomal protein S30



- Molecule 80: 40S ribosomal protein S15a-1



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: 6MZ, IAS, PUT, SPD, 1MA, OMU, UY1, HIC, OMG, MG, 4AC, THC, SPM, 5MC, MA6, I2T, OMC, PSU, ZN, K, A2M, 7MG, BGC, UR3

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 ⓘ

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

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	208	GLU
1	D	218	HIS
1	D	251	ARG
2	F	126	TYR
3	E	369	PHE
14	Q	155	TYR
15	R	50	ASP
24	a	2	LYS
24	a	73	TYR
26	c	60	TYR
32	i	44	CYS
57	YA	65	HIS
63	v	47	LEU
64	w	130	GLN
66	y	152	HIS
67	z	68	ARG
70	CA	104	PHE
72	EA	57	ASP
72	EA	221	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
9	L	123	GLN
17	T	40	ASN
41	r	103	ASN
41	r	104	GLN
47	NA	148	GLN
47	NA	177	HIS
51	RA	12	GLN
62	u	114	GLN
70	CA	60	GLN

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Mol	Chain	Res	Type
73	FA	7	ASN
78	LA	51	HIS
80	JA	51	GLN

5.3.3 RNA ⓘ

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%)

All (507) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
42	s	2	A
43	2	38	A
43	2	41	A
43	2	47	A
43	2	58	A
43	2	63	A
43	2	64	A
43	2	68	PSU
43	2	84	G
43	2	90	G
43	2	97	A
43	2	109	C
43	2	114	C
43	2	133	C
43	2	134	G
43	2	154	G
43	2	155	A
43	2	162	U
43	2	167	A
43	2	168	G
43	2	187	U
43	2	197	G

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Mol	Chain	Res	Type
43	2	216	A
43	2	258	G
43	2	262	A
43	2	283	U
43	2	292	A
43	2	320	A
43	2	326	U
43	2	373	G
43	2	394	A
43	2	396	A
43	2	398	U
43	2	418	G
43	2	419	A
43	2	436	C
43	2	445	C
43	2	446	C
43	2	465	G
43	2	483	U
43	2	484	C
43	2	488	U
43	2	489	C
43	2	525	A
43	2	538	C
43	2	539	G
43	2	542	A
43	2	544	G
43	2	550	G
43	2	571	U
43	2	589	U
43	2	590	C
43	2	591	C
43	2	592	G
43	2	600	U
43	2	603	G
43	2	607	C
43	2	608	U
43	2	609	G
43	2	620	A
43	2	629	U
43	2	632	G
43	2	636	U
43	2	660	A2M

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Mol	Chain	Res	Type
43	2	671	A
43	2	688	A
43	2	692	A
43	2	693	A
43	2	700	A
43	2	701	G
43	2	728	A
43	2	729	U
43	2	730	U
43	2	732	G
43	2	745	G
43	2	771	A
43	2	777	U
43	2	781	A
43	2	791	G
43	2	795	G
43	2	797	G
43	2	809	G
43	2	827	A2M
43	2	840	G
43	2	856	A
43	2	859	C
43	2	871	C
43	2	884	U
43	2	889	U
43	2	917	G
43	2	918	OMG
43	2	924	A
43	2	926	G
43	2	927	A
43	2	931	A
43	2	947	G
43	2	954	C
43	2	969	C
43	2	970	PSU
43	2	984	G
43	2	987	C
43	2	991	U
43	2	1013	C
43	2	1014	A
43	2	1022	G
43	2	1032	G

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Mol	Chain	Res	Type
43	2	1059	A
43	2	1076	A
43	2	1093	U
43	2	1107	G
43	2	1108	G
43	2	1109	A
43	2	1114	A
43	2	1115	G
43	2	1128	G
43	2	1142	G
43	2	1166	C
43	2	1170	A
43	2	1185	G
43	2	1191	C
43	2	1192	U
43	2	1202	C
43	2	1205	A
43	2	1213	C
43	2	1220	U
43	2	1233	A
43	2	1234	G
43	2	1297	G
43	2	1299	A
43	2	1319	G
43	2	1321	U
43	2	1328	U
43	2	1329	A
43	2	1360	A
43	2	1361	A
43	2	1362	G
43	2	1363	U
43	2	1364	G
43	2	1365	C
43	2	1366	C
43	2	1410	U
43	2	1430	G
43	2	1445	G
43	2	1448	OMC
43	2	1454	G
43	2	1457	A
43	2	1466	U
43	2	1492	A

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Mol	Chain	Res	Type
43	2	1513	G
43	2	1518	G
43	2	1547	G
43	2	1566	A
43	2	1571	G
43	2	1585	U
43	2	1592	A
43	2	1594	A
43	2	1598	A
43	2	1601	C
43	2	1602	G
43	2	1625	C
43	2	1633	U
43	2	1647	A
43	2	1649	G
43	2	1661	C
43	2	1691	U
43	2	1696	G
43	2	1729	G
43	2	1755	A
43	2	1756	G
43	2	1763	G
43	2	1802	G
43	2	1803	A
43	2	1820	A
43	2	1821	U
43	2	1827	C
43	2	1848	A
43	2	1856	A
43	2	1872	C
43	2	1884	G
43	2	1885	A
43	2	1886	U
43	2	1899	G
43	2	1912	G
43	2	1949	C
43	2	1959	G
43	2	2118	C
43	2	2126	OMG
43	2	2135	A
43	2	2153	A
43	2	2162	A

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Mol	Chain	Res	Type
43	2	2195	C
43	2	2209	G
43	2	2213	G
43	2	2259	A2M
43	2	2275	G
43	2	2276	G
43	2	2283	A
43	2	2284	A2M
43	2	2310	G
43	2	2313	U
43	2	2316	A
43	2	2318	G
43	2	2337	U
43	2	2338	G
43	2	2339	U
43	2	2376	A
43	2	2377	C
43	2	2378	G
43	2	2396	G
43	2	2397	G
43	2	2400	A
43	2	2405	A
43	2	2406	G
43	2	2407	A
43	2	2414	U
43	2	2415	G
43	2	2438	G
43	2	2440	G
43	2	2519	U
43	2	2520	A
43	2	2539	G
43	2	2556	U
43	2	2564	A
43	2	2574	U
43	2	2575	C
43	2	2589	G
43	2	2590	G
43	2	2597	A
43	2	2610	G
43	2	2611	G
43	2	2618	G
43	2	2630	A

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Mol	Chain	Res	Type
43	2	2656	U
43	2	2660	A
43	2	2678	A
43	2	2681	G
43	2	2693	G
43	2	2695	A
43	2	2700	A
43	2	2708	A
43	2	2718	G
43	2	2732	G
43	2	2733	OMU
43	2	2757	G
43	2	2759	C
43	2	2766	A
43	2	2776	C
43	2	2781	G
43	2	2782	G
43	2	2800	G
43	2	2803	A
43	2	2804	G
43	2	2805	A
43	2	2814	C
43	2	2818	G
43	2	2821	A
43	2	2849	A
43	2	2857	G
43	2	2875	G
43	2	2876	A
43	2	2879	U
43	2	2891	A
43	2	2939	U
43	2	2940	A
43	2	2946	C
43	2	2951	G
43	2	2975	A
43	2	2987	C
43	2	2994	G
43	2	3000	A
43	2	3001	G
43	2	3015	A
43	2	3061	C
43	2	3062	G

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Mol	Chain	Res	Type
43	2	3081	G
43	2	3082	U
43	2	3095	C
43	2	3096	C
43	2	3125	A
43	2	3133	A
43	2	3134	U
43	2	3145	A
43	2	3156	C
43	2	3157	G
43	2	3164	G
43	2	3176	A
43	2	3177	C
43	2	3180	G
43	2	3186	G
43	2	3196	G
43	2	3202	A
43	2	3209	C
43	2	3210	G
43	2	3213	U
43	2	3216	U
43	2	3222	A
43	2	3223	A
43	2	3237	A
43	2	3269	U
43	2	3273	U
43	2	3274	C
43	2	3276	A
43	2	3287	G
43	2	3297	C
43	2	3312	C
43	2	3313	G
43	2	3330	G
43	2	3334	C
43	2	3338	G
43	2	3362	G
43	2	3371	C
43	2	3375	U
43	2	3383	C
43	2	3384	C
43	2	3385	G
43	2	3391	U

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Mol	Chain	Res	Type
44	5	7	G
44	5	25	G
44	5	38	U
44	5	53	U
44	5	54	A
44	5	64	G
44	5	110	G
44	5	120	U
45	8	28	C
45	8	39	U
45	8	40	C
45	8	64	A
45	8	67	C
45	8	68	U
45	8	85	A
45	8	86	U
45	8	91	U
45	8	92	G
45	8	95	C
45	8	109	A
45	8	111	C
45	8	131	A
45	8	158	C
46	S2	8	U
46	S2	25	C
46	S2	26	A
46	S2	34	G
46	S2	42	G
46	S2	45	U
46	S2	47	A
46	S2	59	G
46	S2	68	A
46	S2	105	A
46	S2	115	A
46	S2	128	G
46	S2	139	U
46	S2	151	A
46	S2	158	C
46	S2	164	C
46	S2	252	U
46	S2	253	C
46	S2	260	A

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Mol	Chain	Res	Type
46	S2	263	C
46	S2	275	C
46	S2	279	C
46	S2	318	C
46	S2	320	A
46	S2	341	G
46	S2	342	C
46	S2	365	C
46	S2	384	U
46	S2	394	G
46	S2	404	A
46	S2	405	A
46	S2	406	C
46	S2	408	G
46	S2	420	A
46	S2	421	A
46	S2	427	G
46	S2	428	C
46	S2	430	G
46	S2	438	G
46	S2	443	U
46	S2	448	C
46	S2	449	A
46	S2	452	C
46	S2	472	A
46	S2	481	A
46	S2	509	A
46	S2	510	U
46	S2	513	G
46	S2	518	A
46	S2	522	C
46	S2	537	A
46	S2	545	U
46	S2	574	G
46	S2	582	A
46	S2	597	A
46	S2	614	OMU
46	S2	622	A2M
46	S2	623	A
46	S2	625	A
46	S2	626	A
46	S2	641	U

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Mol	Chain	Res	Type
46	S2	642	U
46	S2	758	G
46	S2	759	A
46	S2	770	C
46	S2	782	C
46	S2	785	C
46	S2	786	G
46	S2	789	C
46	S2	790	U
46	S2	793	A
46	S2	816	A
46	S2	817	U
46	S2	818	A
46	S2	823	U
46	S2	859	A
46	S2	862	A
46	S2	866	A
46	S2	879	G
46	S2	936	A
46	S2	938	U
46	S2	963	U
46	S2	969	A
46	S2	973	A
46	S2	974	A
46	S2	1007	U
46	S2	1008	A
46	S2	1029	A
46	S2	1031	C
46	S2	1057	U
46	S2	1059	G
46	S2	1060	C
46	S2	1061	U
46	S2	1085	U
46	S2	1092	U
46	S2	1095	A
46	S2	1100	U
46	S2	1141	A
46	S2	1149	G
46	S2	1153	G
46	S2	1154	A
46	S2	1161	C
46	S2	1162	C

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Mol	Chain	Res	Type
46	S2	1167	G
46	S2	1170	G
46	S2	1188	U
46	S2	1197	A
46	S2	1199	A
46	S2	1202	G
46	S2	1203	G
46	S2	1205	A
46	S2	1210	PSU
46	S2	1220	A
46	S2	1221	G
46	S2	1247	A
46	S2	1304	PSU
46	S2	1317	U
46	S2	1318	U
46	S2	1319	C
46	S2	1324	A
46	S2	1377	C
46	S2	1395	U
46	S2	1404	U
46	S2	1407	G
46	S2	1418	U
46	S2	1419	U
46	S2	1420	U
46	S2	1432	A
46	S2	1433	OMG
46	S2	1440	G
46	S2	1441	A
46	S2	1450	G
46	S2	1451	A
46	S2	1464	C
46	S2	1465	A
46	S2	1476	A
46	S2	1491	G
46	S2	1495	U
46	S2	1500	G
46	S2	1503	U
46	S2	1518	G
46	S2	1522	A
46	S2	1523	A
46	S2	1528	U
46	S2	1530	A

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Mol	Chain	Res	Type
46	S2	1543	A
46	S2	1563	U
46	S2	1565	G
46	S2	1566	U
46	S2	1596	G
46	S2	1607	G
46	S2	1613	G
46	S2	1622	G
46	S2	1640	C
46	S2	1663	U
46	S2	1664	G
46	S2	1763	A
46	S2	1765	G
46	S2	1768	G
46	S2	1777	U
46	S2	1788	G
46	S2	1800	G
46	S2	1801	G
46	S2	1802	A
46	S2	1803	U
46	S2	1804	C
46	S2	1807	U
46	S2	1808	G

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	OMG	2	2926	43	18,26,27	0.90	1 (5%)	19,38,41	0.62	0
43	1MA	2	656	43,82	16,25,26	1.16	3 (18%)	18,37,40	0.83	1 (5%)
43	OMU	2	2925	43,82	19,22,23	0.28	0	26,31,34	0.47	0
46	OMG	S2	1433	46,82	18,26,27	0.92	2 (11%)	19,38,41	0.61	0
43	PSU	2	2317	43,81	18,21,22	0.47	0	22,30,33	0.59	0
46	7MG	S2	1581	46,59	22,26,27	1.21	1 (4%)	29,39,42	0.79	1 (3%)
46	OMU	S2	581	46	19,22,23	0.25	0	26,31,34	0.41	0
46	A2M	S2	440	46	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
43	PSU	2	2352	43,82	18,21,22	0.49	0	22,30,33	0.56	0
46	PSU	S2	306	46	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2948	43,82,81	18,21,22	0.53	0	22,30,33	0.62	1 (4%)
43	A2M	2	2329	43	18,25,26	0.67	0	18,36,39	0.84	1 (5%)
43	OMC	2	2840	43	19,22,23	0.27	0	26,31,34	0.37	0
46	OMG	S2	598	46	18,26,27	0.91	2 (11%)	19,38,41	0.63	0
43	PSU	2	2927	43	18,21,22	0.45	0	22,30,33	0.59	0
43	OMC	2	2952	43	19,22,23	0.27	0	26,31,34	0.37	0
43	OMU	2	144	43	19,22,23	0.25	0	26,31,34	0.40	0
46	A2M	S2	800	46	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
46	PSU	S2	208	46	18,21,22	0.46	0	22,30,33	0.57	0
46	I2T	S2	1194	46	24,29,30	0.59	0	29,42,45	0.61	0
46	PSU	S2	1308	46	18,21,22	0.45	0	22,30,33	0.38	0
41	THC	r	2	41	8,9,10	0.29	0	9,11,13	0.50	0
46	OMU	S2	1265	46	19,22,23	0.27	0	26,31,34	0.47	0
46	PSU	S2	300	46	18,21,22	0.47	0	22,30,33	0.55	0
46	OMU	S2	614	46,81	19,22,23	0.27	0	26,31,34	0.39	0
43	PSU	2	2435	43	18,21,22	0.47	0	22,30,33	0.56	0
46	OMU	S2	1263	46	19,22,23	0.27	0	26,31,34	0.44	0
46	OMU	S2	1012	46	19,22,23	0.29	0	26,31,34	0.51	0
43	PSU	2	1135	43	18,21,22	0.45	0	22,30,33	0.59	0
46	PSU	S2	383	46,82	18,21,22	0.46	0	22,30,33	0.56	0
43	OMG	2	2394	43	18,26,27	0.92	1 (5%)	19,38,41	0.60	0
46	PSU	S2	1027	46	18,21,22	0.52	0	22,30,33	0.63	1 (4%)
46	PSU	S2	949	46	18,21,22	0.50	0	22,30,33	0.54	0
43	OMG	2	2655	43	18,26,27	0.93	1 (5%)	19,38,41	0.68	0
46	PSU	S2	1535	46	18,21,22	0.46	0	22,30,33	0.56	0
43	A2M	2	2129	43	18,25,26	0.67	0	18,36,39	0.75	1 (5%)
43	OMG	2	399	43	18,26,27	0.89	1 (5%)	19,38,41	0.69	0
46	A2M	S2	28	46,82	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
43	PSU	2	2869	43	18,21,22	0.49	0	22,30,33	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A2M	2	946	43	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
43	PSU	2	1064	43,81	18,21,22	0.45	0	22,30,33	0.58	0
46	OMC	S2	1645	46	19,22,23	0.26	0	26,31,34	0.43	0
46	PSU	S2	1293	46	18,21,22	0.45	0	22,30,33	0.58	0
46	OMU	S2	1447	46	19,22,23	0.27	0	26,31,34	0.46	0
43	PSU	2	2257	43	18,21,22	0.47	0	22,30,33	0.58	0
46	PSU	S2	950	46	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2321	43,82	18,21,22	0.50	0	22,30,33	0.54	0
43	PSU	2	1134	43	18,21,22	0.47	0	22,30,33	0.58	0
43	PSU	2	1909	43,82,81	18,21,22	0.47	0	22,30,33	0.54	0
43	PSU	2	2617	43	18,21,22	0.49	0	22,30,33	0.56	0
46	UY1	S2	603	46	19,22,23	0.45	0	22,31,34	0.57	0
46	PSU	S2	912	46	18,21,22	0.46	0	22,30,33	0.57	0
46	4AC	S2	1283	46	21,24,25	0.30	0	29,34,37	0.36	0
43	PSU	2	1016	43,81	18,21,22	0.49	0	22,30,33	0.58	0
43	OMG	2	1857	43,81	18,26,27	0.94	2 (11%)	19,38,41	0.61	0
43	PSU	2	829	43	18,21,22	0.48	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	2296	43	19,22,23	0.29	0	26,31,34	0.44	0
43	OMG	2	2819	43	18,26,27	0.90	1 (5%)	19,38,41	0.61	0
46	PSU	S2	362	46	18,21,22	0.49	0	22,30,33	0.56	0
43	OMU	2	1068	43	19,22,23	0.30	0	26,31,34	0.53	0
43	PSU	2	35	43	18,21,22	0.44	0	22,30,33	0.56	0
43	PSU	2	2267	43	18,21,22	0.46	0	22,30,33	0.57	0
46	PSU	S2	255	46,82	18,21,22	0.48	0	22,30,33	0.58	0
46	PSU	S2	1538	46	18,21,22	0.46	0	22,30,33	0.56	0
46	PSU	S2	762	46	18,21,22	0.46	0	22,30,33	0.56	0
43	A2M	2	2915	43	18,25,26	0.64	0	18,36,39	0.76	1 (5%)
43	A2M	2	369	43	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
43	PSU	2	2959	43	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	970	43	18,21,22	0.53	0	22,30,33	0.64	1 (4%)
43	OMU	2	2887	43	19,22,23	0.29	0	26,31,34	0.55	0
46	PSU	S2	1184	46	18,21,22	0.47	0	22,30,33	0.55	0
43	OMG	2	2412	43	18,26,27	0.91	1 (5%)	19,38,41	0.67	0
43	PSU	2	1474	43	18,21,22	0.48	0	22,30,33	0.56	0
43	OMC	2	674	43	19,22,23	0.27	0	26,31,34	0.46	0
46	PSU	S2	809	46	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2898	43	18,21,22	0.52	0	22,30,33	0.53	0
43	OMG	2	1461	43	18,26,27	0.91	1 (5%)	19,38,41	0.65	0
43	OMC	2	2340	43	19,22,23	0.28	0	26,31,34	0.47	0
46	PSU	S2	1634	46	18,21,22	0.50	0	22,30,33	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMG	2	2126	43	18,26,27	0.96	2 (11%)	19,38,41	0.67	0
43	PSU	2	1230	43	18,21,22	0.45	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	PSU	2	378	43	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2830	43	18,21,22	0.49	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%)
46	OMC	S2	418	46	19,22,23	0.28	0	26,31,34	0.44	0
46	OMC	S2	1218	46	19,22,23	0.27	0	26,31,34	0.40	0
43	PSU	2	2748	43	18,21,22	0.48	0	22,30,33	0.55	0
43	OMU	2	675	43	19,22,23	0.30	0	26,31,34	0.52	0
43	OMC	2	2368	43	19,22,23	0.28	0	26,31,34	0.41	0
46	PSU	S2	753	46	18,21,22	0.48	0	22,30,33	0.57	0
43	OMC	2	2883	43	19,22,23	0.28	0	26,31,34	0.39	0
45	PSU	8	79	45	18,21,22	0.48	0	22,30,33	0.56	0
43	PSU	2	2228	43	18,21,22	0.53	0	22,30,33	0.52	0
43	OMC	2	2200	43,81	19,22,23	0.26	0	26,31,34	0.60	0
43	OMC	2	1849	43	19,22,23	0.28	0	26,31,34	0.39	0
45	A2M	8	48	45	18,25,26	0.67	0	18,36,39	0.81	1 (5%)
46	A2M	S2	1329	46	18,25,26	0.67	0	18,36,39	0.79	1 (5%)
46	MA6	S2	1790	46	19,26,27	0.76	0	18,38,41	0.56	0
43	A2M	2	2324	43	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
43	OMG	2	815	43	18,26,27	0.92	1 (5%)	19,38,41	0.66	0
43	PSU	2	2716	43	18,21,22	0.53	0	22,30,33	0.62	1 (4%)
46	6MZ	S2	1771	82,46,81	18,25,26	0.72	0	16,36,39	0.73	1 (6%)
46	OMG	S2	246	46	18,26,27	0.92	1 (5%)	19,38,41	0.64	0
46	PSU	S2	1210	46	18,21,22	0.46	0	22,30,33	0.40	0
46	PSU	S2	451	46,81	18,21,22	0.49	0	22,30,33	0.55	0
46	A2M	S2	977	46	18,25,26	0.68	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	5MC	2	2281	43,82	18,22,23	0.30	0	26,32,35	0.44	0
46	A2M	S2	544	46	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
43	PSU	2	1002	43	18,21,22	0.47	0	22,30,33	0.58	0
3	HIC	E	246	3	8,11,12	0.80	0	6,14,16	0.59	0
43	PSU	2	2214	43	18,21,22	0.49	0	22,30,33	0.55	0
43	OMG	2	2239	43	18,26,27	0.90	1 (5%)	19,38,41	0.62	0
43	PSU	2	2521	43	18,21,22	0.48	0	22,30,33	0.58	0
43	A2M	2	1460	43,82	18,25,26	0.67	0	18,36,39	0.78	1 (5%)
43	UR3	2	2957	43	19,22,23	0.30	0	26,32,35	0.32	0
46	4AC	S2	1781	46	21,24,25	0.29	0	29,34,37	0.30	0
43	PSU	2	2884	43	18,21,22	0.50	0	22,30,33	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMG	2	2398	43	18,26,27	0.89	0	19,38,41	0.71	0
43	OMG	2	2291	43	18,26,27	0.92	2 (11%)	19,38,41	0.59	0
43	OMU	2	44	43,81	19,22,23	0.28	0	26,31,34	0.38	0
46	PSU	S2	1190	46	18,21,22	0.46	0	22,30,33	0.58	0
43	5MC	2	2874	43,81	18,22,23	0.44	0	26,32,35	0.52	0
43	OMU	2	2739	43,82	19,22,23	0.29	0	26,31,34	0.46	0
46	PSU	S2	111	46,81	18,21,22	0.47	0	22,30,33	0.57	0
46	PSU	S2	1313	46	18,21,22	0.47	0	22,30,33	0.57	0
43	OMU	2	3305	43	19,22,23	0.29	0	26,31,34	0.42	0
46	PSU	S2	1120	46	18,21,22	0.48	0	22,30,33	0.56	0
43	OMU	2	2350	43,81	19,22,23	0.30	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
45	PSU	8	23	43,45	18,21,22	0.48	0	22,30,33	0.54	0
43	OMG	2	2127	43	18,26,27	0.93	1 (5%)	19,38,41	0.72	0
46	PSU	S2	103	46	18,21,22	0.49	0	22,30,33	0.56	0
43	OMG	2	2795	43	18,26,27	0.94	2 (11%)	19,38,41	0.61	0
43	PSU	2	2263	43	18,21,22	0.48	0	22,30,33	0.56	0
46	MA6	S2	1789	46	19,26,27	0.74	0	18,38,41	0.57	0
46	PSU	S2	584	46	18,21,22	0.49	0	22,30,33	0.58	0
43	OMC	2	1862	43	19,22,23	0.29	0	26,31,34	0.40	0
43	OMC	2	2963	43	19,22,23	0.29	0	26,31,34	0.47	0
43	OMU	2	2413	43,81	19,22,23	0.29	0	26,31,34	0.41	0
43	PSU	2	2419	43,82	18,21,22	0.49	0	22,30,33	0.56	0
43	PSU	2	2137	43,81	18,21,22	0.45	0	22,30,33	0.59	0
43	A2M	2	660	43	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
43	PSU	2	3114	43	18,21,22	0.47	0	22,30,33	0.55	0
45	OMG	8	80	45	18,26,27	0.91	1 (5%)	19,38,41	0.62	0
46	OMU	S2	1383	46,82	19,22,23	0.29	0	26,31,34	0.45	0
43	OMU	2	48	43	19,22,23	0.26	0	26,31,34	0.41	0
43	PSU	2	2847	43	18,21,22	0.48	0	22,30,33	0.57	0
43	OMU	2	2654	43	19,22,23	0.29	0	26,31,34	0.42	0
46	OMC	S2	38	46	19,22,23	0.28	0	26,31,34	0.48	0
43	PSU	2	2996	43	18,21,22	0.55	0	22,30,33	0.50	0
43	A2M	2	886	43	18,25,26	0.64	0	18,36,39	0.73	1 (5%)
43	OMU	2	1537	43,81	19,22,23	0.24	0	26,31,34	0.39	0
43	OMC	2	1448	43,82	19,22,23	0.29	0	26,31,34	0.39	0
46	PSU	S2	635	46	18,21,22	0.48	0	22,30,33	0.60	0
46	PSU	S2	1567	46	18,21,22	0.48	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%)
43	PSU	2	1133	43	18,21,22	0.46	0	22,30,33	0.55	0
43	OMU	2	2721	43	19,22,23	0.28	0	26,31,34	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMU	2	2733	43	19,22,23	0.30	0	26,31,34	0.45	0
46	A2M	S2	468	46	18,25,26	0.67	0	18,36,39	0.83	1 (5%)
43	PSU	2	2139	43	18,21,22	0.49	0	22,30,33	0.55	0
46	OMU	S2	1272	46,82	19,22,23	0.23	0	26,31,34	0.43	0
43	OMC	2	1852	43,82	19,22,23	0.26	0	26,31,34	0.42	0
43	OMU	2	1894	43,81	19,22,23	0.32	0	26,31,34	0.66	0
43	PSU	2	68	43	18,21,22	0.51	0	22,30,33	0.58	0
43	OMU	2	804	43	19,22,23	0.29	0	26,31,34	0.51	0
46	OMU	S2	123	46	19,22,23	0.29	0	26,31,34	0.46	0
46	PSU	S2	605	46	18,21,22	0.47	0	22,30,33	0.57	0
46	PSU	S2	258	46	18,21,22	0.46	0	22,30,33	0.56	0
46	OMC	S2	473	46	19,22,23	0.29	0	26,31,34	0.50	0
43	OMU	2	2116	43	19,22,23	0.24	0	26,31,34	0.42	0
43	A2M	2	2644	43	18,25,26	0.66	0	18,36,39	0.72	1 (5%)
43	OMC	2	1480	43	19,22,23	0.24	0	26,31,34	0.37	0
43	OMG	2	2921	43	18,26,27	0.95	2 (11%)	19,38,41	0.63	0
43	A2M	2	827	43,82	18,25,26	0.66	0	18,36,39	0.86	1 (5%)
43	OMC	2	2686	43	19,22,23	0.28	0	26,31,34	0.45	0
46	PSU	S2	1485	46	18,21,22	0.48	0	22,30,33	0.55	0
46	OMG	S2	1274	46,81	18,26,27	0.92	1 (5%)	19,38,41	0.63	0
46	PSU	S2	1002	46	18,21,22	0.48	0	22,30,33	0.55	0
43	PSU	2	2979	43	18,21,22	0.48	0	22,30,33	0.58	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
43	PSU	2	2261	43	18,21,22	0.51	0	22,30,33	0.53	0
46	PSU	S2	121	46	18,21,22	0.45	0	22,30,33	0.56	0
43	PSU	2	2269	43	18,21,22	0.46	0	22,30,33	0.57	0
43	A2M	2	1378	43,82	18,25,26	0.66	0	18,36,39	0.71	1 (5%)
43	OMU	2	2424	43	19,22,23	0.29	0	26,31,34	0.53	0
43	A2M	2	817	43	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
43	PSU	2	2858	43	18,21,22	0.48	0	22,30,33	0.56	0
76	IAS	IA	137	76	6,7,8	1.10	0	6,8,10	1.07	0
43	OMG	2	2623	43,82	18,26,27	0.91	2 (11%)	19,38,41	0.59	0
46	A2M	S2	1579	46	18,25,26	0.65	0	18,36,39	0.76	1 (5%)
43	OMG	2	918	43,81	18,26,27	0.95	2 (11%)	19,38,41	0.59	0
46	A2M	S2	622	46,82	18,25,26	0.64	0	18,36,39	0.75	1 (5%)
46	PSU	S2	1106	46	18,21,22	0.46	0	22,30,33	0.56	0
43	PSU	2	895	43	18,21,22	0.53	0	22,30,33	0.54	0
43	PSU	2	1482	43	18,21,22	0.50	0	22,30,33	0.55	0
43	A2M	2	1144	43,82	18,25,26	0.67	0	18,36,39	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	162	46	18,25,26	0.66	0	18,36,39	0.85	1 (5%)
43	A2M	2	2223	43	18,25,26	0.67	0	18,36,39	0.80	1 (5%)
46	OMG	S2	392	46	18,26,27	0.92	1 (5%)	19,38,41	0.62	0
43	PSU	2	1054	43	18,21,22	0.46	0	22,30,33	0.58	0
43	A2M	2	2950	43,82,81	18,25,26	0.68	0	18,36,39	0.88	1 (5%)
46	PSU	S2	1178	46	18,21,22	0.48	0	22,30,33	0.58	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
43	OMG	2	2926	43	-	0/5/27/28	0/3/3/3
43	1MA	2	656	43,82	-	0/3/25/26	0/3/3/3
43	OMU	2	2925	43,82	-	0/9/27/28	0/2/2/2
46	OMG	S2	1433	46,82	-	1/5/27/28	0/3/3/3
43	PSU	2	2317	43,81	-	1/7/25/26	0/2/2/2
46	7MG	S2	1581	46,59	-	0/7/37/38	0/3/3/3
46	OMU	S2	581	46	-	1/9/27/28	0/2/2/2
46	A2M	S2	440	46	-	0/5/27/28	0/3/3/3
43	PSU	2	2352	43,82	-	0/7/25/26	0/2/2/2
46	PSU	S2	306	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2948	43,82,81	-	1/7/25/26	0/2/2/2
43	A2M	2	2329	43	-	0/5/27/28	0/3/3/3
43	OMC	2	2840	43	-	0/9/27/28	0/2/2/2
46	OMG	S2	598	46	-	1/5/27/28	0/3/3/3
43	PSU	2	2927	43	-	1/7/25/26	0/2/2/2
43	OMC	2	2952	43	-	0/9/27/28	0/2/2/2
43	OMU	2	144	43	-	1/9/27/28	0/2/2/2
46	A2M	S2	800	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	208	46	-	0/7/25/26	0/2/2/2
46	I2T	S2	1194	46	-	1/16/34/35	0/2/2/2
46	PSU	S2	1308	46	-	0/7/25/26	0/2/2/2
41	THC	r	2	41	-	4/8/10/12	-
46	OMU	S2	1265	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	300	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	614	46,81	-	0/9/27/28	0/2/2/2
43	PSU	2	2435	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	1263	46	-	0/9/27/28	0/2/2/2
46	OMU	S2	1012	46	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PSU	2	1135	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	383	46,82	-	0/7/25/26	0/2/2/2
43	OMG	2	2394	43	-	1/5/27/28	0/3/3/3
46	PSU	S2	1027	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	949	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2655	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	1535	46	-	0/7/25/26	0/2/2/2
43	A2M	2	2129	43	-	0/5/27/28	0/3/3/3
43	OMG	2	399	43	-	0/5/27/28	0/3/3/3
46	A2M	S2	28	46,82	-	0/5/27/28	0/3/3/3
43	PSU	2	2869	43	-	0/7/25/26	0/2/2/2
43	A2M	2	946	43	-	0/5/27/28	0/3/3/3
43	PSU	2	1064	43,81	-	0/7/25/26	0/2/2/2
46	OMC	S2	1645	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1293	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	1447	46	-	0/9/27/28	0/2/2/2
43	PSU	2	2257	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	950	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2321	43,82	-	0/7/25/26	0/2/2/2
43	PSU	2	1134	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1909	43,82,81	-	0/7/25/26	0/2/2/2
43	PSU	2	2617	43	-	0/7/25/26	0/2/2/2
46	UY1	S2	603	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	912	46	-	0/7/25/26	0/2/2/2
46	4AC	S2	1283	46	-	0/11/29/30	0/2/2/2
43	PSU	2	1016	43,81	-	0/7/25/26	0/2/2/2
43	OMG	2	1857	43,81	-	0/5/27/28	0/3/3/3
43	PSU	2	829	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	2296	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2819	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	362	46	-	0/7/25/26	0/2/2/2
43	OMU	2	1068	43	-	0/9/27/28	0/2/2/2
43	PSU	2	35	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2267	43	-	0/7/25/26	0/2/2/2
46	PSU	S2	255	46,82	-	0/7/25/26	0/2/2/2
46	PSU	S2	1538	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	762	46	-	0/7/25/26	0/2/2/2
43	A2M	2	2915	43	-	0/5/27/28	0/3/3/3
43	A2M	2	369	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2959	43	-	0/7/25/26	0/2/2/2
43	PSU	2	970	43	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMU	2	2887	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1184	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2412	43	-	0/5/27/28	0/3/3/3
43	PSU	2	1474	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	809	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2898	43	-	0/7/25/26	0/2/2/2
43	OMG	2	1461	43	-	1/5/27/28	0/3/3/3
43	OMC	2	2340	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1634	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2126	43	-	3/5/27/28	0/3/3/3
43	PSU	2	1230	43	-	0/7/25/26	0/2/2/2
46	OMC	S2	140	46	-	0/9/27/28	0/2/2/2
43	PSU	2	378	43	-	0/7/25/26	0/2/2/2
43	PSU	2	2830	43	-	2/7/25/26	0/2/2/2
43	A2M	2	2284	43	-	2/5/27/28	0/3/3/3
46	OMC	S2	418	46	-	0/9/27/28	0/2/2/2
46	OMC	S2	1218	46	-	0/9/27/28	0/2/2/2
43	PSU	2	2748	43	-	0/7/25/26	0/2/2/2
43	OMU	2	675	43	-	0/9/27/28	0/2/2/2
43	OMC	2	2368	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	753	46	-	0/7/25/26	0/2/2/2
43	OMC	2	2883	43	-	0/9/27/28	0/2/2/2
45	PSU	8	79	45	-	0/7/25/26	0/2/2/2
43	PSU	2	2228	43	-	2/7/25/26	0/2/2/2
43	OMC	2	2200	43,81	-	4/9/27/28	0/2/2/2
43	OMC	2	1849	43	-	0/9/27/28	0/2/2/2
45	A2M	8	48	45	-	0/5/27/28	0/3/3/3
46	A2M	S2	1329	46	-	0/5/27/28	0/3/3/3
46	MA6	S2	1790	46	-	3/7/29/30	0/3/3/3
43	A2M	2	2324	43	-	0/5/27/28	0/3/3/3
43	OMG	2	815	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2716	43	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1771	82,46,81	-	0/5/27/28	0/3/3/3
46	OMG	S2	246	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	1210	46	-	2/7/25/26	0/2/2/2
46	PSU	S2	451	46,81	-	0/7/25/26	0/2/2/2
46	A2M	S2	977	46	-	0/5/27/28	0/3/3/3
43	A2M	2	2259	43	-	2/5/27/28	0/3/3/3
43	5MC	2	2281	43,82	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	S2	544	46	-	0/5/27/28	0/3/3/3
43	PSU	2	1002	43	-	0/7/25/26	0/2/2/2
3	HIC	E	246	3	-	1/5/6/8	0/1/1/1
43	PSU	2	2214	43	-	0/7/25/26	0/2/2/2
43	OMG	2	2239	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2521	43	-	0/7/25/26	0/2/2/2
43	A2M	2	1460	43,82	-	0/5/27/28	0/3/3/3
43	UR3	2	2957	43	-	0/7/25/26	0/2/2/2
46	4AC	S2	1781	46	-	2/11/29/30	0/2/2/2
43	PSU	2	2884	43	-	0/7/25/26	0/2/2/2
43	OMG	2	2398	43	-	0/5/27/28	0/3/3/3
43	OMG	2	2291	43	-	0/5/27/28	0/3/3/3
43	OMU	2	44	43,81	-	0/9/27/28	0/2/2/2
46	PSU	S2	1190	46	-	0/7/25/26	0/2/2/2
43	5MC	2	2874	43,81	-	2/7/25/26	0/2/2/2
43	OMU	2	2739	43,82	-	0/9/27/28	0/2/2/2
46	PSU	S2	111	46,81	-	0/7/25/26	0/2/2/2
46	PSU	S2	1313	46	-	0/7/25/26	0/2/2/2
43	OMU	2	3305	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1120	46	-	0/7/25/26	0/2/2/2
43	OMU	2	2350	43,81	-	0/9/27/28	0/2/2/2
43	OMG	2	2797	43	-	0/5/27/28	0/3/3/3
45	PSU	8	23	43,45	-	0/7/25/26	0/2/2/2
43	OMG	2	2127	43	-	0/5/27/28	0/3/3/3
46	PSU	S2	103	46	-	0/7/25/26	0/2/2/2
43	OMG	2	2795	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2263	43	-	0/7/25/26	0/2/2/2
46	MA6	S2	1789	46	-	0/7/29/30	0/3/3/3
46	PSU	S2	584	46	-	3/7/25/26	0/2/2/2
43	OMC	2	1862	43	-	0/9/27/28	0/2/2/2
43	OMC	2	2963	43	-	0/9/27/28	0/2/2/2
43	OMU	2	2413	43,81	-	0/9/27/28	0/2/2/2
43	PSU	2	2419	43,82	-	0/7/25/26	0/2/2/2
43	PSU	2	2137	43,81	-	0/7/25/26	0/2/2/2
43	A2M	2	660	43	-	1/5/27/28	0/3/3/3
43	PSU	2	3114	43	-	0/7/25/26	0/2/2/2
45	OMG	8	80	45	-	0/5/27/28	0/3/3/3
46	OMU	S2	1383	46,82	-	0/9/27/28	0/2/2/2
43	OMU	2	48	43	-	0/9/27/28	0/2/2/2
43	PSU	2	2847	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2654	43	-	0/9/27/28	0/2/2/2
46	OMC	S2	38	46	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PSU	2	2996	43	-	0/7/25/26	0/2/2/2
43	A2M	2	886	43	-	0/5/27/28	0/3/3/3
43	OMU	2	1537	43,81	-	0/9/27/28	0/2/2/2
43	OMC	2	1448	43,82	-	2/9/27/28	0/2/2/2
46	PSU	S2	635	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1567	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	1758	46	-	0/5/27/28	0/3/3/3
43	PSU	2	1133	43	-	0/7/25/26	0/2/2/2
43	OMU	2	2721	43	-	0/9/27/28	0/2/2/2
43	OMU	2	2733	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	2139	43	-	0/7/25/26	0/2/2/2
46	OMU	S2	1272	46,82	-	0/9/27/28	0/2/2/2
43	OMC	2	1852	43,82	-	1/9/27/28	0/2/2/2
43	OMU	2	1894	43,81	-	0/9/27/28	0/2/2/2
43	PSU	2	68	43	-	2/7/25/26	0/2/2/2
43	OMU	2	804	43	-	0/9/27/28	0/2/2/2
46	OMU	S2	123	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	605	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	258	46	-	0/7/25/26	0/2/2/2
46	OMC	S2	473	46	-	0/9/27/28	0/2/2/2
43	OMU	2	2116	43	-	0/9/27/28	0/2/2/2
43	A2M	2	2644	43	-	0/5/27/28	0/3/3/3
43	OMC	2	1480	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2921	43	-	0/5/27/28	0/3/3/3
43	A2M	2	827	43,82	-	2/5/27/28	0/3/3/3
43	OMC	2	2686	43	-	0/9/27/28	0/2/2/2
46	PSU	S2	1485	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	1274	46,81	-	0/5/27/28	0/3/3/3
46	PSU	S2	1002	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2979	43	-	0/7/25/26	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
43	PSU	2	2261	43	-	2/7/25/26	0/2/2/2
46	PSU	S2	121	46	-	0/7/25/26	0/2/2/2
43	PSU	2	2269	43	-	0/7/25/26	0/2/2/2
43	A2M	2	1378	43,82	-	0/5/27/28	0/3/3/3
43	OMU	2	2424	43	-	0/9/27/28	0/2/2/2
43	A2M	2	817	43	-	0/5/27/28	0/3/3/3
43	PSU	2	2858	43	-	0/7/25/26	0/2/2/2
76	IAS	IA	137	76	-	1/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	OMG	2	2623	43,82	-	0/5/27/28	0/3/3/3
46	A2M	S2	1579	46	-	0/5/27/28	0/3/3/3
43	OMG	2	918	43,81	-	1/5/27/28	0/3/3/3
46	A2M	S2	622	46,82	-	2/5/27/28	0/3/3/3
46	PSU	S2	1106	46	-	0/7/25/26	0/2/2/2
43	PSU	2	895	43	-	0/7/25/26	0/2/2/2
43	PSU	2	1482	43	-	0/7/25/26	0/2/2/2
43	A2M	2	1144	43,82	-	0/5/27/28	0/3/3/3
46	A2M	S2	162	46	-	0/5/27/28	0/3/3/3
43	A2M	2	2223	43	-	0/5/27/28	0/3/3/3
46	OMG	S2	392	46	-	0/5/27/28	0/3/3/3
43	PSU	2	1054	43	-	0/7/25/26	0/2/2/2
43	A2M	2	2950	43,82,81	-	0/5/27/28	0/3/3/3
46	PSU	S2	1178	46	-	0/7/25/26	0/2/2/2

All (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
43	2	2921	OMG	C5-C6	-2.30	1.42	1.47
46	S2	1433	OMG	C5-C6	-2.28	1.42	1.47
43	2	1857	OMG	C5-C6	-2.28	1.42	1.47
43	2	2797	OMG	C5-C6	-2.28	1.42	1.47
43	2	2291	OMG	C5-C6	-2.25	1.42	1.47
43	2	2394	OMG	C5-C6	-2.25	1.42	1.47
46	S2	1274	OMG	C5-C6	-2.23	1.42	1.47
46	S2	246	OMG	C5-C6	-2.22	1.42	1.47
43	2	2623	OMG	C5-C6	-2.20	1.42	1.47
46	S2	392	OMG	C5-C6	-2.19	1.43	1.47
43	2	2127	OMG	C5-C6	-2.18	1.43	1.47
43	2	2412	OMG	C5-C6	-2.18	1.43	1.47
43	2	815	OMG	C5-C6	-2.17	1.43	1.47
46	S2	598	OMG	C5-C6	-2.15	1.43	1.47
43	2	2239	OMG	C5-C6	-2.13	1.43	1.47
43	2	2655	OMG	C5-C6	-2.13	1.43	1.47
43	2	1461	OMG	C5-C6	-2.12	1.43	1.47
43	2	2819	OMG	C5-C6	-2.11	1.43	1.47
43	2	656	1MA	C5-C4	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	2926	OMG	C5-C6	-2.10	1.43	1.47
43	2	2921	OMG	C8-N7	-2.09	1.31	1.35
43	2	656	1MA	C8-N7	-2.09	1.31	1.35
45	8	80	OMG	C5-C6	-2.08	1.43	1.47
43	2	1857	OMG	C8-N7	-2.07	1.31	1.35
43	2	918	OMG	C8-N7	-2.07	1.31	1.35
43	2	2795	OMG	C8-N7	-2.06	1.31	1.35
43	2	2126	OMG	C8-N7	-2.05	1.31	1.35
43	2	399	OMG	C5-C6	-2.02	1.43	1.47
43	2	2623	OMG	C8-N7	-2.02	1.31	1.35
46	S2	598	OMG	C8-N7	-2.01	1.31	1.35
46	S2	1433	OMG	C8-N7	-2.01	1.31	1.35
43	2	2291	OMG	C8-N7	-2.01	1.31	1.35

All (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
43	2	2950	A2M	C5-C6-N6	2.35	123.93	120.35
46	S2	544	A2M	C5-C6-N6	2.35	123.93	120.35
43	2	369	A2M	C5-C6-N6	2.35	123.92	120.35
43	2	2329	A2M	C5-C6-N6	2.34	123.92	120.35
46	S2	622	A2M	C5-C6-N6	2.34	123.91	120.35
43	2	1378	A2M	C5-C6-N6	2.34	123.91	120.35
43	2	2223	A2M	C5-C6-N6	2.34	123.91	120.35
43	2	817	A2M	C5-C6-N6	2.34	123.90	120.35
46	S2	28	A2M	C5-C6-N6	2.33	123.90	120.35
46	S2	1579	A2M	C5-C6-N6	2.33	123.90	120.35
46	S2	1329	A2M	C5-C6-N6	2.33	123.89	120.35
46	S2	440	A2M	C5-C6-N6	2.32	123.89	120.35
43	2	1460	A2M	C5-C6-N6	2.32	123.88	120.35
43	2	2259	A2M	C5-C6-N6	2.32	123.88	120.35
43	2	2324	A2M	C5-C6-N6	2.32	123.88	120.35
43	2	2644	A2M	C5-C6-N6	2.32	123.87	120.35
46	S2	162	A2M	C5-C6-N6	2.31	123.86	120.35
43	2	2284	A2M	C5-C6-N6	2.30	123.85	120.35
46	S2	468	A2M	C5-C6-N6	2.29	123.84	120.35
43	2	660	A2M	C5-C6-N6	2.28	123.82	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	2129	A2M	C5-C6-N6	2.27	123.81	120.35
43	2	1144	A2M	C5-C6-N6	2.27	123.81	120.35
45	8	48	A2M	C5-C6-N6	2.27	123.80	120.35
46	S2	1758	A2M	C5-C6-N6	2.26	123.79	120.35
43	2	2948	PSU	O4'-C1'-C2'	2.22	108.27	105.14
46	S2	1581	7MG	C5-C4-N9	2.22	109.22	106.35
43	2	2716	PSU	O4'-C1'-C2'	2.21	108.26	105.14
46	S2	977	A2M	C5-C6-N6	2.19	123.68	120.35
46	S2	1771	6MZ	C2-N1-C6	2.15	118.43	116.59
43	2	970	PSU	O4'-C1'-C2'	2.08	108.08	105.14
43	2	656	1MA	N1-C6-N6	2.04	124.97	119.77
46	S2	1027	PSU	O4'-C1'-C2'	2.03	108.01	105.14

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	246	HIC	CA-CB-CG-ND1
41	r	2	THC	N-CA-CB-OG1
41	r	2	THC	N-CA-CB-CG2
41	r	2	THC	C-CA-CB-OG1
41	r	2	THC	C-CA-CB-CG2
43	2	918	OMG	C3'-C2'-O2'-CM2
43	2	1852	OMC	C1'-C2'-O2'-CM2
43	2	2126	OMG	O4'-C4'-C5'-O5'
43	2	2259	A2M	O4'-C4'-C5'-O5'
46	S2	584	PSU	C2'-C1'-C5-C4
46	S2	1790	MA6	C5-C6-N6-C9
43	2	68	PSU	C3'-C4'-C5'-O5'
43	2	68	PSU	O4'-C4'-C5'-O5'
43	2	2126	OMG	C3'-C4'-C5'-O5'
43	2	2261	PSU	C3'-C4'-C5'-O5'
43	2	2261	PSU	O4'-C4'-C5'-O5'
43	2	2194	PSU	C3'-C4'-C5'-O5'
43	2	2194	PSU	O4'-C4'-C5'-O5'
43	2	2284	A2M	C3'-C4'-C5'-O5'
46	S2	622	A2M	O4'-C4'-C5'-O5'
46	S2	1304	PSU	O4'-C4'-C5'-O5'
43	2	2200	OMC	C2'-C1'-N1-C6
43	2	2284	A2M	O4'-C4'-C5'-O5'
46	S2	622	A2M	C3'-C4'-C5'-O5'
46	S2	1304	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2	2317	PSU	C4'-C5'-O5'-P
43	2	2200	OMC	O4'-C1'-N1-C6
43	2	2927	PSU	C4'-C5'-O5'-P
46	S2	1194	I2T	C32-C31-N3-C4
46	S2	468	A2M	O4'-C4'-C5'-O5'
43	2	2200	OMC	C2'-C1'-N1-C2
43	2	827	A2M	C4'-C5'-O5'-P
46	S2	598	OMG	C4'-C5'-O5'-P
46	S2	581	OMU	O4'-C4'-C5'-O5'
43	2	2228	PSU	C3'-C4'-C5'-O5'
43	2	2200	OMC	O4'-C1'-N1-C2
46	S2	1790	MA6	C5-C6-N6-C10
46	S2	1790	MA6	C4'-C5'-O5'-P
43	2	1448	OMC	C3'-C2'-O2'-CM2
43	2	660	A2M	C4'-C5'-O5'-P
43	2	2126	OMG	C4'-C5'-O5'-P
46	S2	1433	OMG	C4'-C5'-O5'-P
76	IA	137	IAS	CA-CB-CG-OD1
43	2	144	OMU	O4'-C4'-C5'-O5'
43	2	2830	PSU	O4'-C1'-C5-C4
43	2	2948	PSU	O4'-C1'-C5-C4
46	S2	584	PSU	O4'-C1'-C5-C4
46	S2	1210	PSU	O4'-C1'-C5-C4
43	2	2874	5MC	O4'-C1'-N1-C6
43	2	2874	5MC	C2'-C1'-N1-C6
43	2	2228	PSU	O4'-C4'-C5'-O5'
43	2	1448	OMC	O4'-C4'-C5'-O5'
43	2	2259	A2M	C3'-C4'-C5'-O5'
43	2	970	PSU	O4'-C1'-C5-C6
43	2	2830	PSU	O4'-C1'-C5-C6
46	S2	584	PSU	O4'-C1'-C5-C6
46	S2	1210	PSU	O4'-C1'-C5-C6
43	2	827	A2M	O4'-C4'-C5'-O5'
43	2	1461	OMG	O4'-C4'-C5'-O5'
46	S2	1781	4AC	N3-C4-N4-C7
46	S2	1781	4AC	C5-C4-N4-C7
43	2	2394	OMG	C3'-C4'-C5'-O5'

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
84	SPM	2	3482	-	13,13,13	0.28	0	12,12,12	0.94	0
84	SPM	2	3480	-	13,13,13	0.32	0	12,12,12	0.87	0
84	SPM	2	3479	-	13,13,13	0.29	0	12,12,12	0.90	0
87	BGC	NA	301	47	11,11,12	0.20	0	15,15,17	0.38	0
85	SPD	2	3481	-	9,9,9	0.26	0	8,8,8	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	-
84	SPM	2	3482	-	-	3/11/11/11	-
84	SPM	2	3480	-	-	0/11/11/11	-
84	SPM	2	3479	-	-	1/11/11/11	-
87	BGC	NA	301	47	-	1/2/19/22	0/1/1/1
85	SPD	2	3481	-	-	0/7/7/7	-

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.

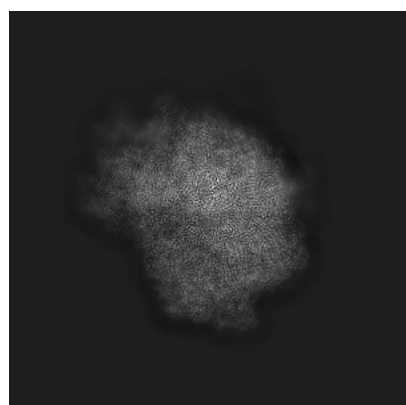
6 Map visualisation [i](#)

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.

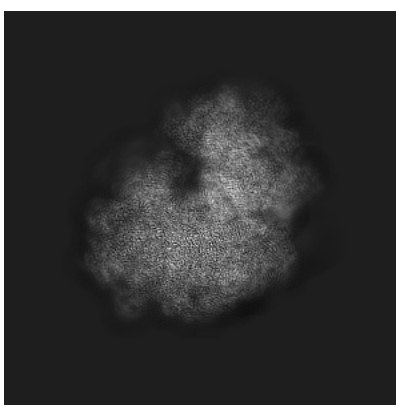
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

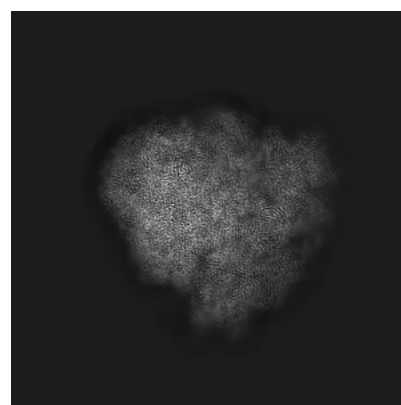
6.1.1 Primary map



X



Y

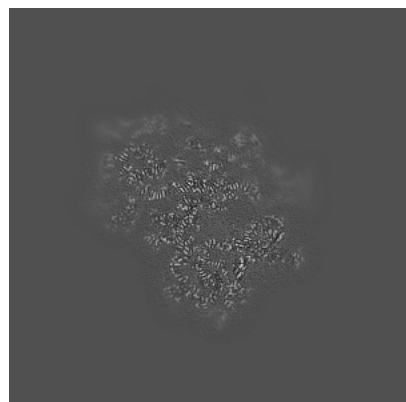


Z

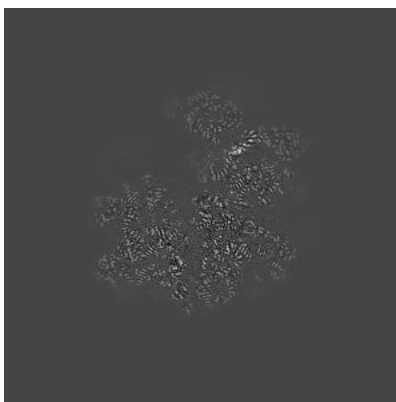
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

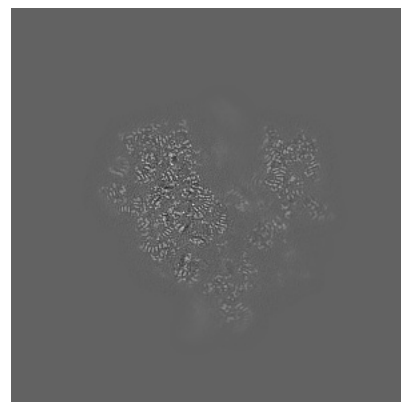
6.2.1 Primary map



X Index: 270



Y Index: 270

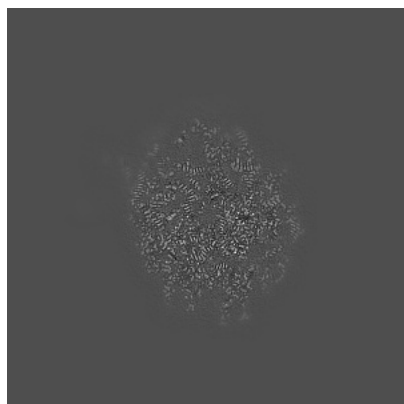


Z Index: 270

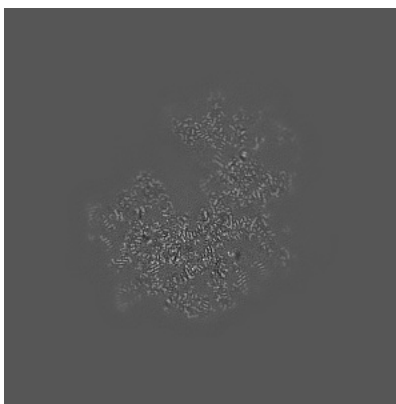
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

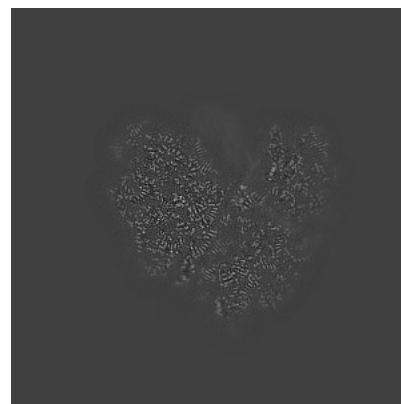
6.3.1 Primary map



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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

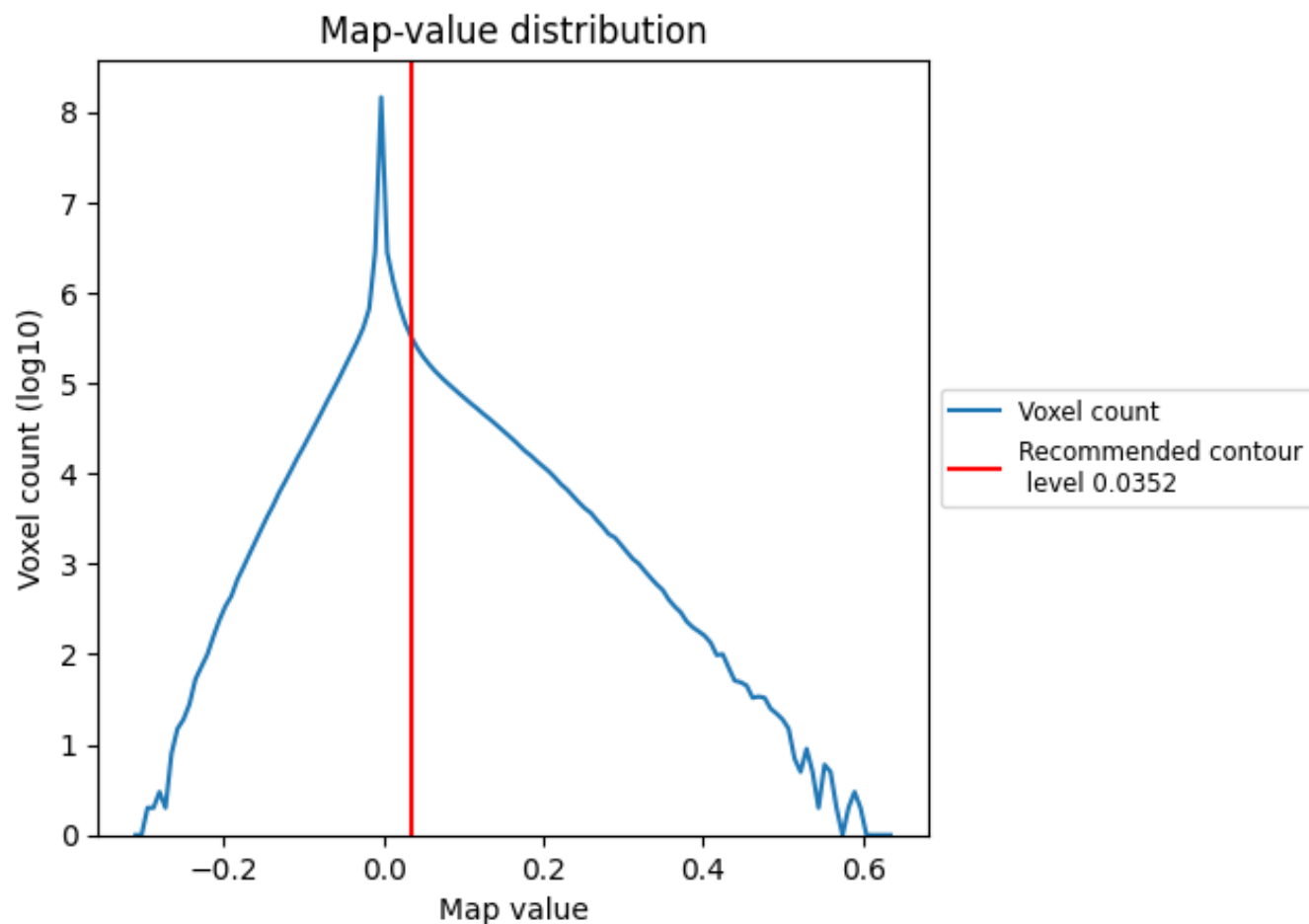
6.5 Mask visualisation

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

7 Map analysis [i](#)

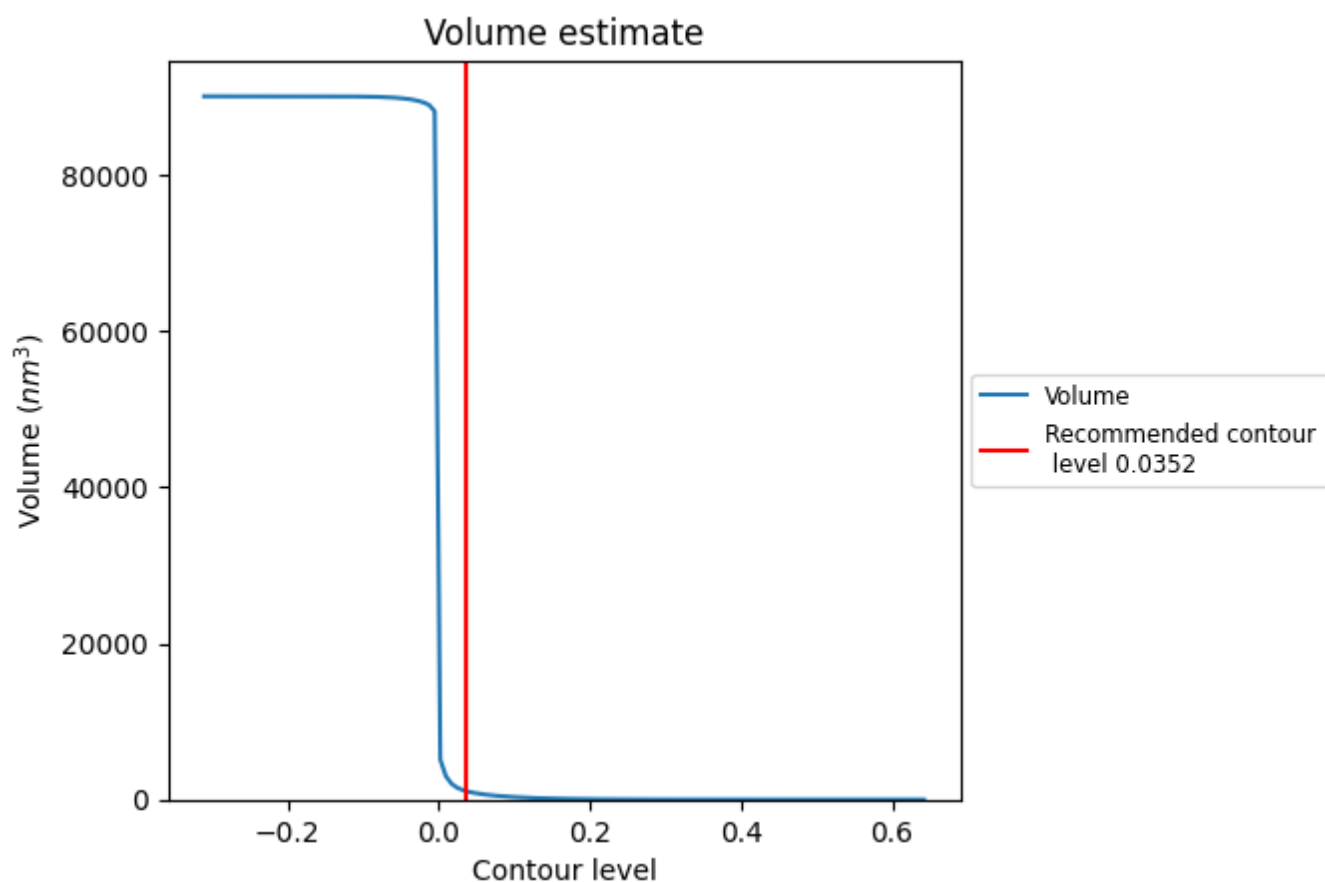
This section contains the results of statistical analysis of the map.

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.

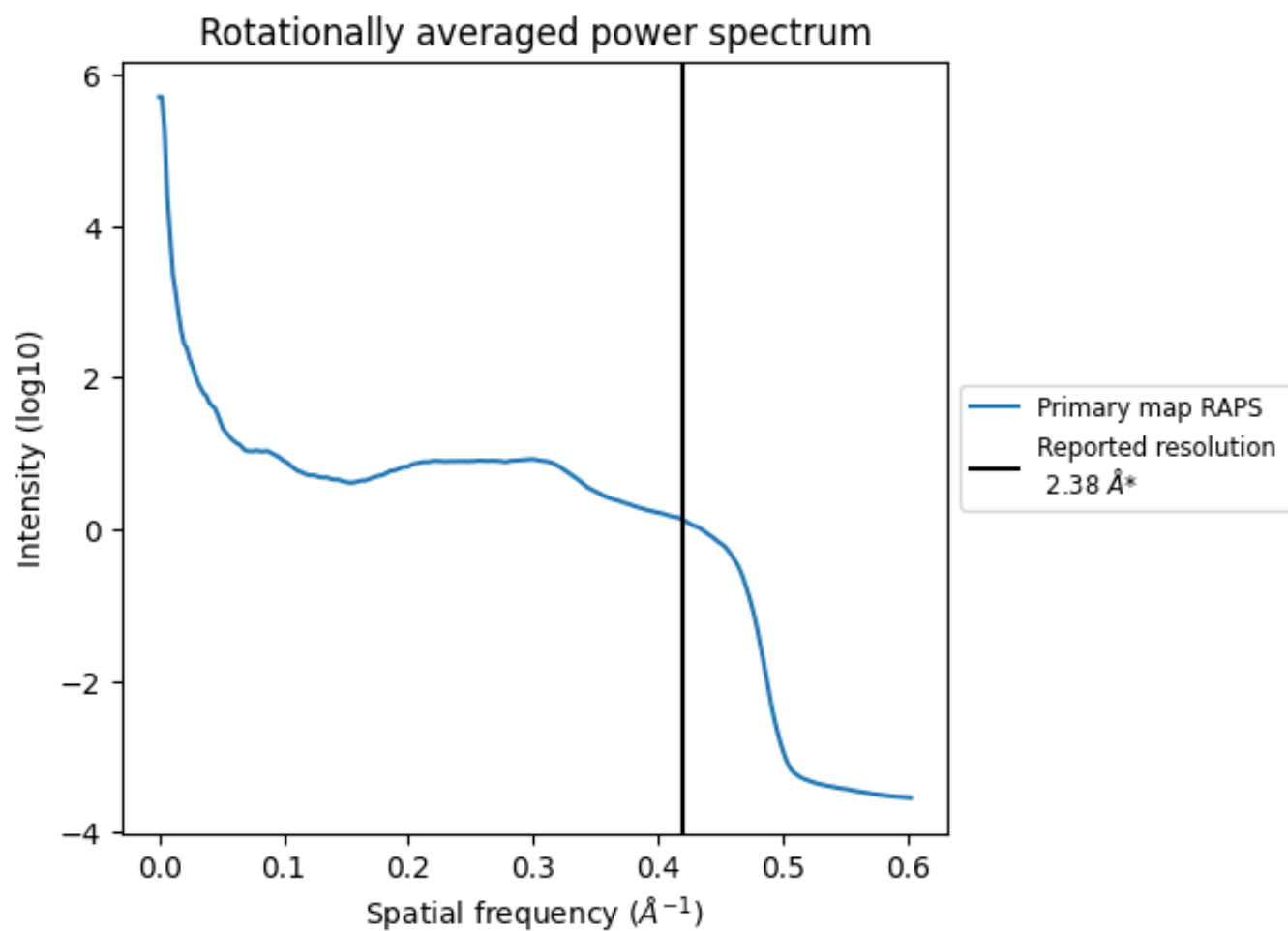
7.2 Volume estimate [i](#)



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 ⓘ



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

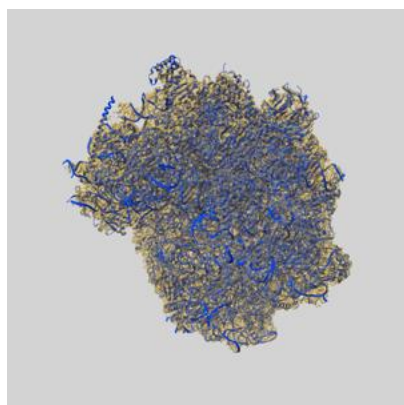
8 Fourier-Shell correlation ⓘ

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

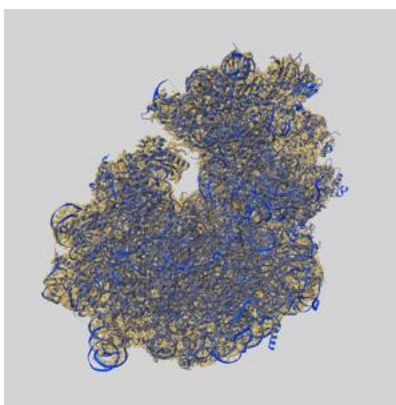
9 Map-model fit [i](#)

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](#).

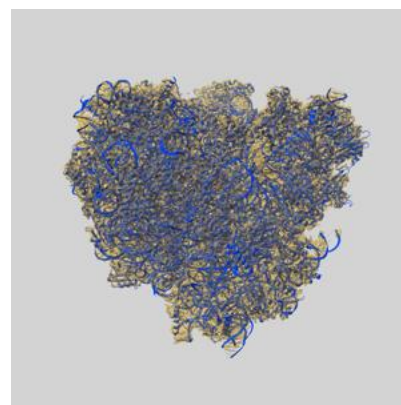
9.1 Map-model overlay [i](#)



X



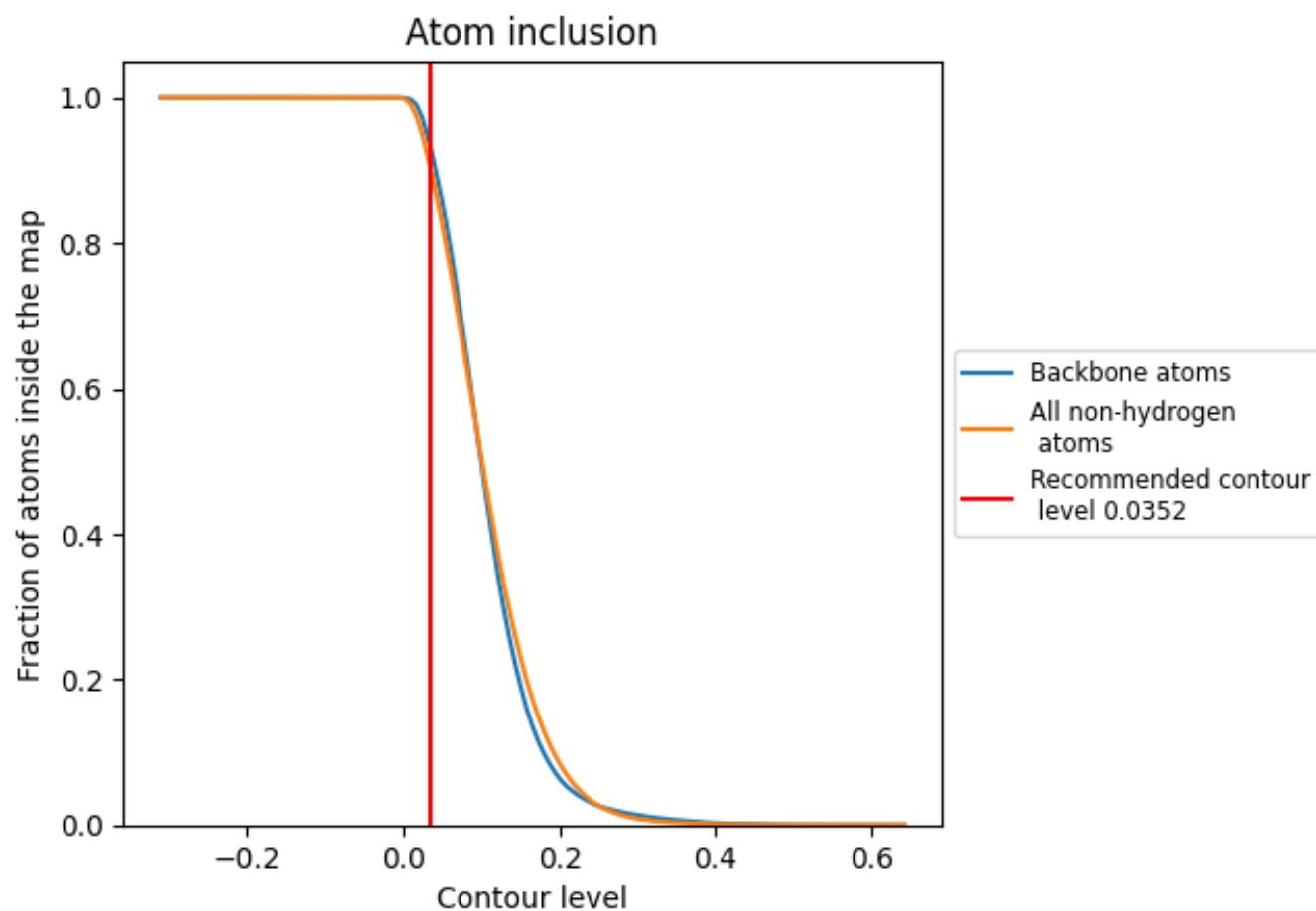
Y



Z

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 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.