



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 11:09 PM EST

PDB ID : 7UCK
EMDB ID : EMD-26445
Title : 80S translation initiation complex with ac4c(-1) mRNA and Harringtonine
Authors : Yang, R.; Arango, D.; Sturgill, D.; Oberdoerffer, S.
Deposited on : 2022-03-16
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

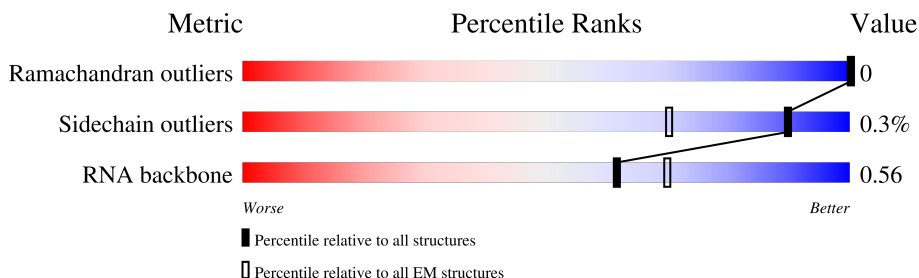
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



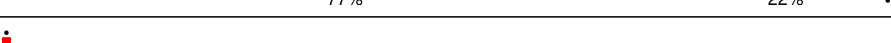


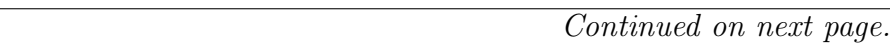

The reported resolution of this entry is 2.80 Å.

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



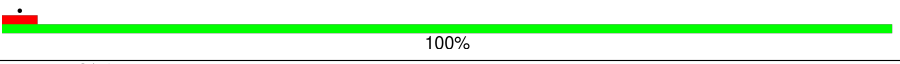
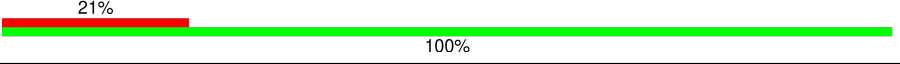

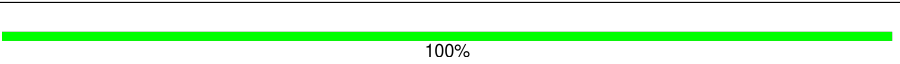
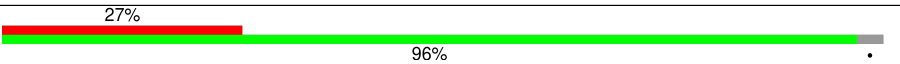
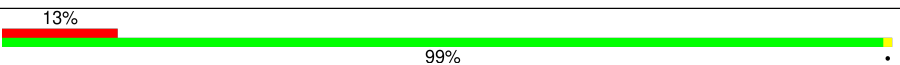
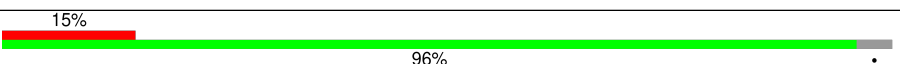
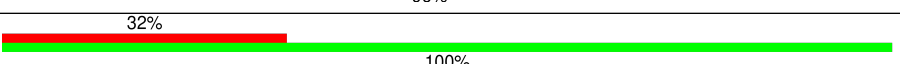
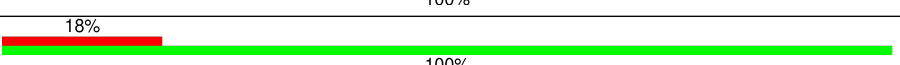
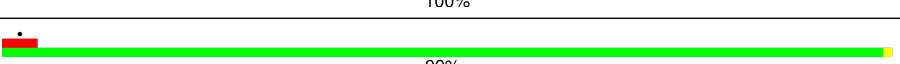
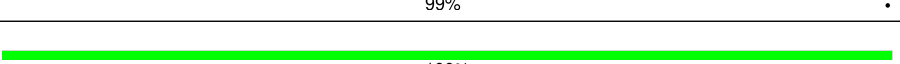
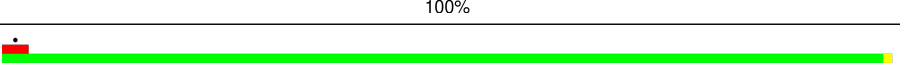
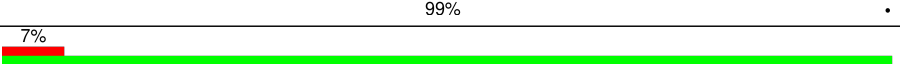
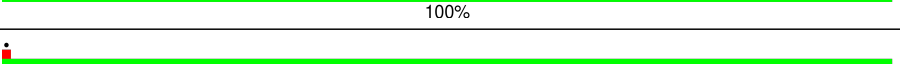
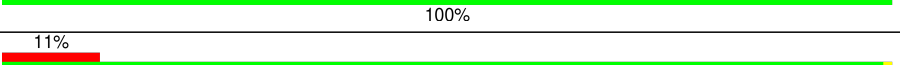
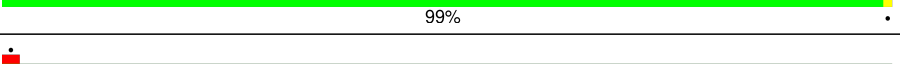

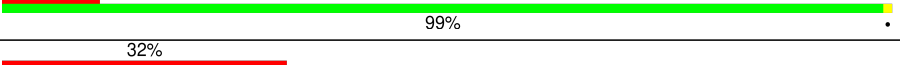
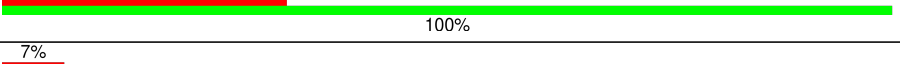
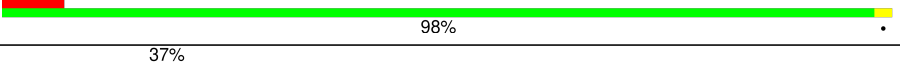
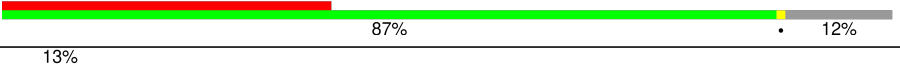
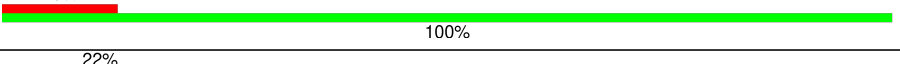
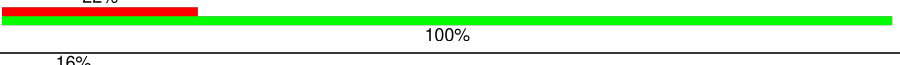
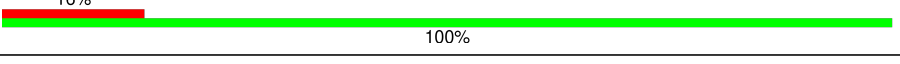
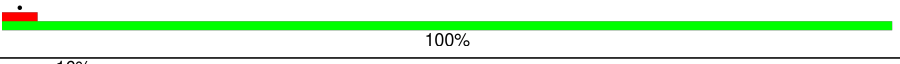
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	2	76	
2	1	6	
3	5	3546	
4	7	120	
5	8	156	
6	9	1698	
7	A	248	
8	B	394	

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Mol	Chain	Length	Quality of chain
9	C	360	
10	D	291	
11	E	251	
12	F	225	
13	G	234	
14	H	190	
15	I	213	
16	J	170	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	98	
27	V	131	
28	W	121	
29	X	118	
30	Y	134	
31	Z	135	
32	a	147	
33	b	116	

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Mol	Chain	Length	Quality of chain
34	c	98	9% 100%
35	d	107	12% 100%
36	e	128	• 100%
37	f	109	• 99% .
38	g	114	11% 99% .
39	h	122	17% 100%
40	i	102	15% 100%
41	j	86	• 100%
42	k	69	51% 100%
43	l	50	100%
44	m	51	16% 100%
45	n	25	100%
46	o	103	10% 99% .
47	p	91	• 100%
48	r	124	6% 100%
49	AA	217	18% 100%
50	BB	213	17% 100%
51	CC	221	9% 100%
52	DD	228	20% 99% .
53	EE	262	5% 100%
54	FF	191	13% 97% .
55	GG	237	30% 99% .
56	HH	189	52% 97% ..
57	II	206	14% 98% ..
58	JJ	185	11% 100%

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Mol	Chain	Length	Quality of chain
59	KK	96	
60	LL	151	
61	NN	149	
62	OO	136	
63	PP	120	
64	QQ	142	
65	RR	132	
66	SS	144	
67	TT	141	
68	UU	100	
69	VV	83	
70	WW	129	
71	XX	141	
72	YY	124	
73	ZZ	75	
74	Aa	101	
75	Bb	83	
76	Cc	62	
77	Dd	55	
78	Ee	55	
79	Gg	313	

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 210046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	72	Total	C	N	O	P	0	0
			1552	694	289	498	71		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	6	Total	C	N	O	P	0	0
			133	60	25	42	6		

- Molecule 3 is a RNA chain called 28s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	3546	Total	C	N	O	P	0	0
			76153	33978	13919	24710	3546		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 6 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 7 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	360	Total	C	N	O	S	0	0
			2870	1806	575	475	14		

- Molecule 10 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	291	Total	C	N	O	S	0	0
			2381	1506	436	425	14		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	227	Total	C	N	O	S	0	0
			1837	1172	354	307	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 15 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

There are 9 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

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

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

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

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 35 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	51	Total	C	N	O	S	0	0
			420	261	88	65	6		

- Molecule 45 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 46 is a protein called 60S ribosomal protein L36a.

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

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 49 is a protein called 40S_SA_C domain-containing protein.

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

- Molecule 50 is a protein called 40S ribosomal protein S3a.

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

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	73	MET	VAL	conflict	UNP G1TUT9
CC	101	SER	ALA	conflict	UNP G1TUT9
CC	119	GLY	ALA	conflict	UNP G1TUT9
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	215	MET	LEU	conflict	UNP G1TUT9
CC	227	ARG	TRP	conflict	UNP G1TUT9
CC	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 52 is a protein called 40S ribosomal protein S3.

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

- Molecule 53 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 54 is a protein called Ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S6.

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

- Molecule 56 is a protein called 40S ribosomal protein S7.

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

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	II	203	Total	C	N	O	S	0	0
			1668	1047	328	288	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 58 is a protein called 40S ribosomal protein S9.

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

- Molecule 59 is a protein called 40S ribosomal protein S10.

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

- Molecule 60 is a protein called 40S ribosomal protein S11.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14.

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

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 64 is a protein called 40S ribosomal protein S16.

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

- Molecule 65 is a protein called 40S ribosomal protein S17.

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

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 67 is a protein called 40S ribosomal protein S19.

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

- Molecule 68 is a protein called 40S ribosomal protein S20.

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

- Molecule 69 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 70 is a protein called 40S ribosomal protein S15a.

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

- Molecule 71 is a protein called 40S ribosomal protein S23.

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

- Molecule 72 is a protein called 40S ribosomal protein S24.

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

- Molecule 73 is a protein called 40S ribosomal protein S25.

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

- Molecule 74 is a protein called eS26.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	28	ARG	CYS	conflict	UNP G1TFE8
Aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 75 is a protein called 40S ribosomal protein S27.

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

- Molecule 76 is a protein called 40S ribosomal protein S28.

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

- Molecule 77 is a protein called 40S ribosomal protein S29.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

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

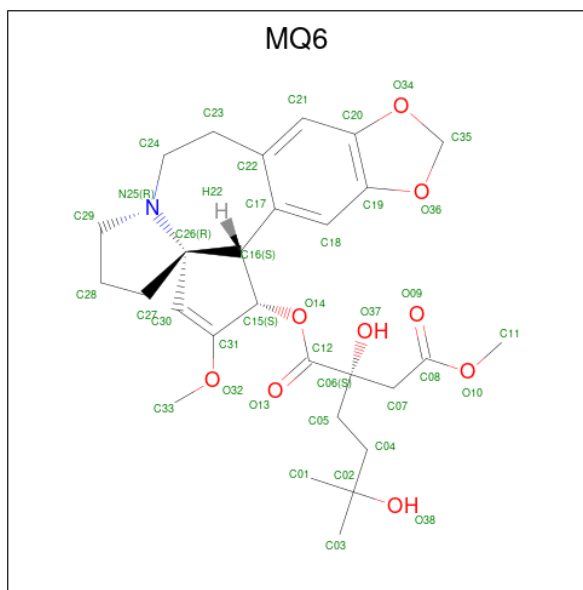
- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	5	196	Total 196	Mg 196	0
80	7	7	Total 7	Mg 7	0
80	8	8	Total 8	Mg 8	0
80	9	78	Total 78	Mg 78	0
80	A	1	Total 1	Mg 1	0
80	I	1	Total 1	Mg 1	0
80	P	1	Total 1	Mg 1	0
80	V	1	Total 1	Mg 1	0
80	a	1	Total 1	Mg 1	0
80	g	1	Total 1	Mg 1	0
80	j	1	Total 1	Mg 1	0
80	LL	1	Total 1	Mg 1	0

- Molecule 81 is Harringtonine (three-letter code: MQ6) (formula: $C_{28}H_{37}NO_9$).



Mol	Chain	Residues	Atoms				AltConf
81	5	1	Total	C	N	O	0
			38	28	1	9	

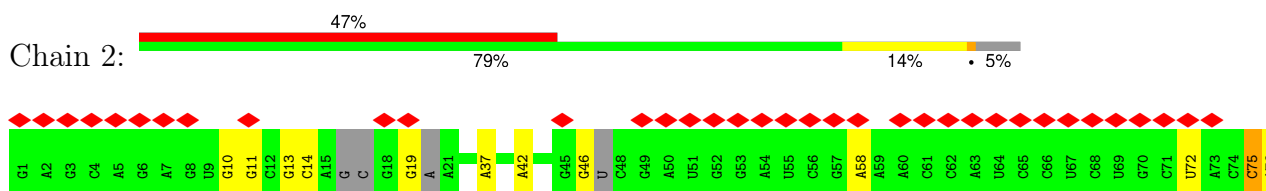
- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
82	g	1	Total	Zn	0
			1	1	
82	j	1	Total	Zn	0
			1	1	
82	m	1	Total	Zn	0
			1	1	
82	o	1	Total	Zn	0
			1	1	
82	p	1	Total	Zn	0
			1	1	
82	Aa	1	Total	Zn	0
			1	1	
82	Dd	1	Total	Zn	0
			1	1	

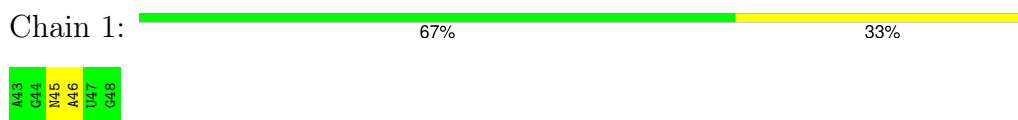
3 Residue-property plots [i](#)

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

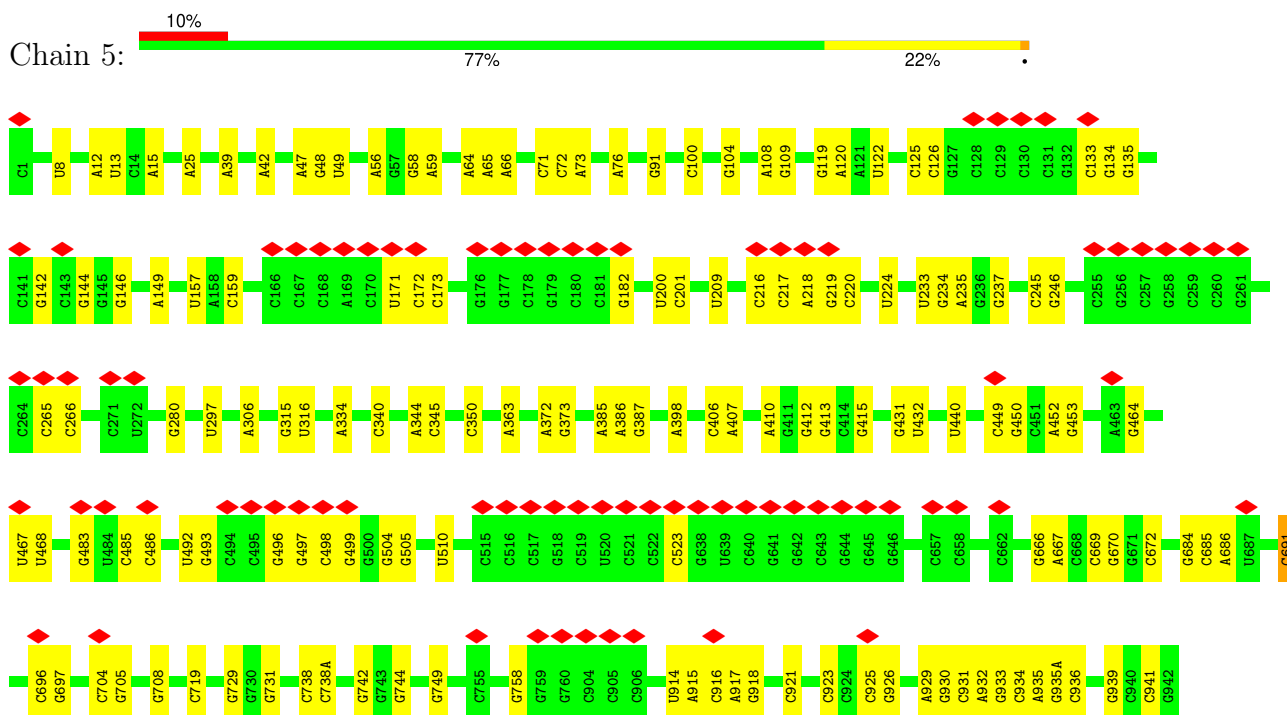
- Molecule 1: P-site tRNA



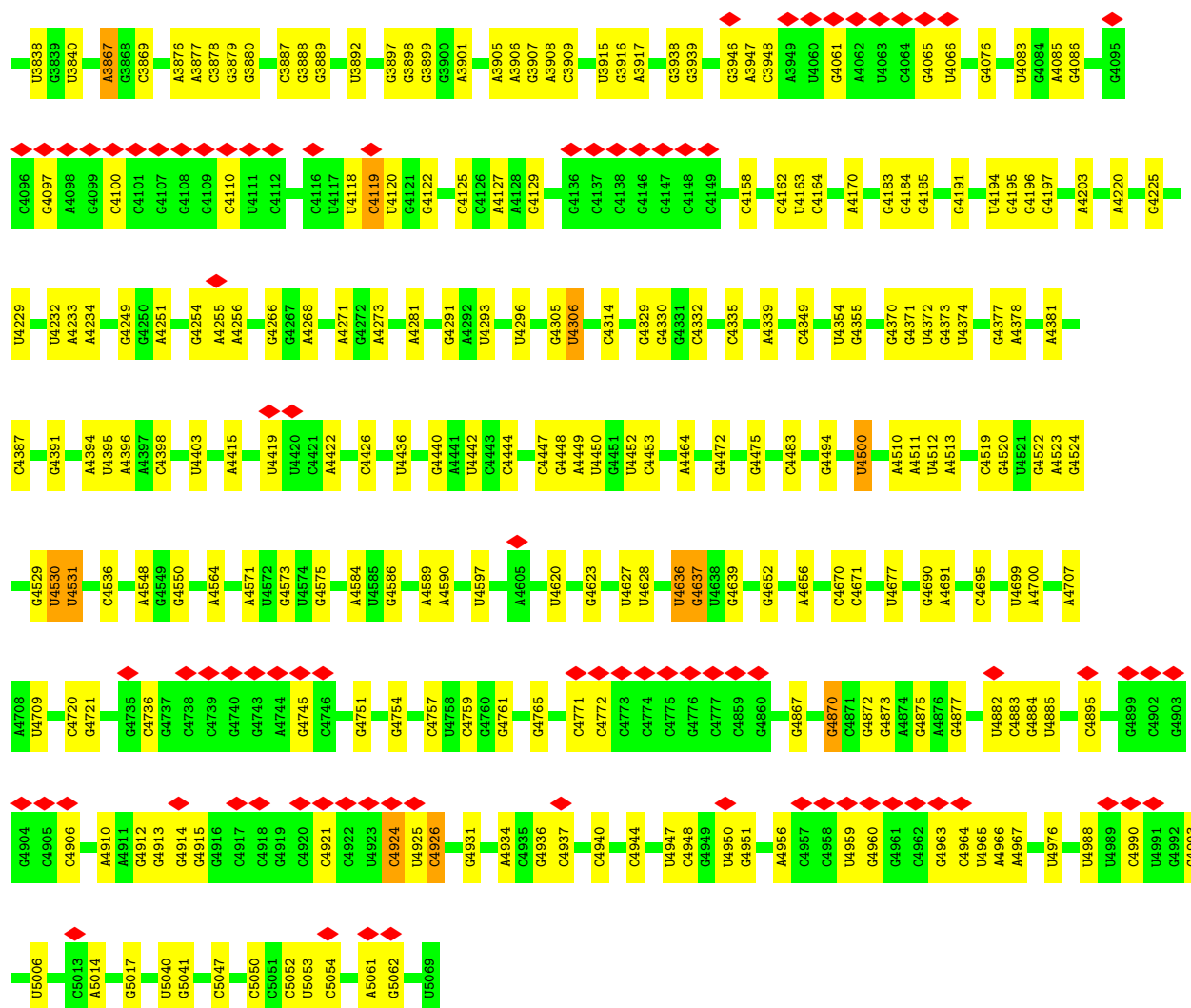
- Molecule 2: mRNA



- Molecule 3: 28s rRNA



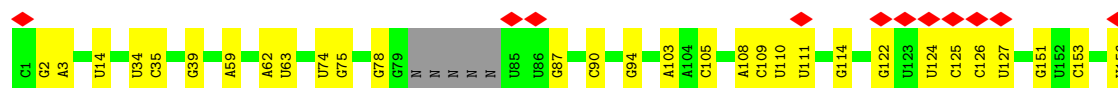
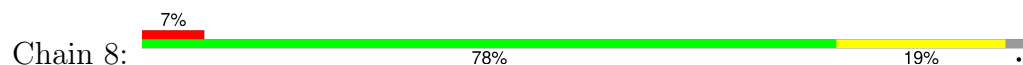
C3673	C3674	C3696	C3697	C3698	C3701	A3711	A3712	A3713	A3714	A3715	A3718	A3723	U3729	A3748	G3753	A3759	A3760	C3761	U3762	A3763	U3764	U3773	A3774	A3775	G3776	G3777	C3782	A3783	A3784	A3785	U3786	G3792	C3810	C3811	C3812	A3813	U3814	A3817	U3818	C3819	U3822	A3823	A3824	A3825																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U2763	U2769	U2769	C2772	C2773	C2786	A2787	A2788	A2789	A2790	A2798	C2804	C2805	A2806	A2814	A2815	U2826	C2827	G2842	C2855	C2861	C2867	C2875	A2898	G3603	A3604	C3605	U3606	G3615	C3618	C3619	G3625	C3626	A3635	U3644	A3648	A3662	A3663	A3664	G2714	G2715	C2716	A2725	G2726	U2740	A2743	A2744	G2753	G2754																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C2482	C2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	C2491	C2492	G2493	U2494	U2495	A2502	G2503	C2504	C2505	C2506	A2507	U2508	A2511	A2512	A2513	G2522	U2530	U2539	A2544	U2545	G2546	G2547	U2554	C2558	G2559	C2560	C2561	C2562	C2563	C2564	A2565	C2566	G2567	C2568	C2569	C2571	U2575	G2576	G2577																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
A2300	G2301	C2306	A2313	C2314	A2332	C2333	G2334	A2335	C2336	A2337	C2338	A2339	C2340	A2341	C2342	A2343	C2344	A2345	C2346	A2347	C2348	A2349	C2350	A2351	C2352	A2353	C2354	A2355	C2356	A2357	C2358	A2359	C2360	A2361	C2362	A2363	C2364	A2365	C2366	A2367	C2368	A2369	C2370	A2371	C2372	A2373	C2374	A2375	C2376	A2377	C2378	A2379	C2380	A2381	C2382	A2383	C2384	A2385	C2386	A2387	C2388	A2389	C2390	A2391	C2392	A2393	C2394	A2395	C2396	A2397	C2398	A2399	C2400	A2401	C2402	A2403	C2404	A2405	C2406	A2407	C2408	A2409	C2410	A2411	C2412	A2413	C2414	A2415	C2416	A2417	C2418	A2419	C2420	A2421	C2422	A2423	C2424	A2425	C2426	A2427	C2428	A2429	C2430	A2431	C2432	A2433	C2434	A2435	C2436	A2437	C2438	A2439	C2440	A2441	C2442	A2443	C2444	A2445	C2446	A2447	C2448	A2449	C2450	A2451	C2452	A2453	C2454	A2455	C2456	A2457	C2458	A2459	C2460	A2461	C2462	A2463	C2464	A2465	C2466	A2467	C2468	A2469	C2470	A2471	C2472	A2473	C2474	A2475	C2476	A2477	C2478	A2479	C2480	A2481	C2482	A2483	C2484	A2485	C2486	A2487	C2488	A2489	C2490	A2491	C2492	A2493	C2494	A2495	C2496	A2497	C2498	A2499	C2500	A2501	C2502	A2503	C2504	A2505	C2506	A2507	C2508	A2509	C2510	A2511	C2512	A2513	C2514	A2515	C2516	A2517	C2518	A2519	C2520	A2521	C2522	A2523	C2524	A2525	C2526	A2527	C2528	A2529	C2530	A2531	C2532	A2533	C2534	A2535	C2536	A2537	C2538	A2539	C2540	A2541	C2542	A2543	C2544	A2545	C2546	A2547	C2548	A2549	C2550	A2551	C2552	A2553	C2554	A2555	C2556	A2557	C2558	A2559	C2560	A2561	C2562	A2563	C2564	A2565	C2566	A2567	C2568	A2569	C2570	A2571	C2572	A2573	C2574	A2575	C2576	A2577	C2578	A2579	C2580	A2581	C2582	A2583	C2584	A2585	C2586	A2587	C2588	A2589	C2590	A2591	C2592	A2593	C2594	A2595	C2596	A2597	C2598	A2599	C2600	A2601	C2602	A2603	C2604	A2605	C2606	A2607	C2608	A2609	C2610	A2611	C2612	A2613	C2614	A2615	C2616	A2617	C2618	A2619	C2620	A2621	C2622	A2623	C2624	A2625	C2626	A2627	C2628	A2629	C2630	A2631	C2632	A2633	C2634	A2635	C2636	A2637	C2638	A2639	C2640	A2641	C2642	A2643	C2644	A2645	C2646	A2647	C2648	A2649	C2650	A2651	C2652	A2653	C2654	A2655	C2656	A2657	C2658	A2659	C2660	A2661	C2662	A2663	C2664	A2665	C2666	A2667	C2668	A2669	C2670	A2671	C2672	A2673	C2674	A2675	C2676	A2677	C2678	A2679	C2680	A2681	C2682	A2683	C2684	A2685	C2686	A2687	C2688	A2689	C2690	A2691	C2692	A2693	C2694	A2695	C2696	A2697	C2698	A2699	C2700	A2701	C2702	A2703	C2704	A2705	C2706	A2707	C2708	A2709	C2710	A2711	C2712	A2713	C2714	A2715	C2716	A2717	C2718	A2719	C2720	A2721	C2722	A2723	C2724	A2725	C2726	A2727	C2728	A2729	C2730	A2731	C2732	A2733	C2734	A2735	C2736	A2737	C2738	A2739	C2740	A2741	C2742	A2743	C2744	A2745	C2746	A2747	C2748	A2749	C2750	A2751	C2752	A2753	C2754	A2755	C2756	A2757	C2758	A2759	C2760	A2761	C2762	A2763	C2764	A2765	C2766	A2767	C2768	A2769	C2770	A2771	C2772	A2773	C2774	A2775	C2776	A2777	C2778	A2779	C2780	A2781	C2782	A2783	C2784	A2785	C2786	A2787	C2788	A2789	C2790	A2791	C2792	A2793	C2794	A2795	C2796	A2797	C2798	A2799	C2800	A2801	C2802	A2803	C2804	A2805	C2806	A2807	C2808	A2809	C2810	A2811	C2812	A2813	C2814	A2815	C2816	A2817	C2818	A2819	C2820	A2821	C2822	A2823	C2824	A2825	C2826	A2827	C2828	A2829	C2830	A2831	C2832	A2833	C2834	A2835	C2836	A2837	C2838	A2839	C2840	A2841	C2842	A2843	C2844	A2845	C2846	A2847	C2848	A2849	C2850	A2851	C2852	A2853	C2854	A2855	C2856	A2857	C2858	A2859	C2860	A2861	C2862	A2863	C2864	A2865	C2866	A2867	C2868	A2869	C2870	A2871	C2872	A2873	C2874	A2875	C2876	A2877	C2878	A2879	C2880	A2881	C2882	A2883	C2884	A2885	C2886	A2887	C2888	A2889	C2890	A2891	C2892	A2893	C2894	A2895	C2896	A2897	C2898	A2899	C2900	A2901	C2902	A2903	C2904	A2905	C2906	A2907	C2908	A2909	C2910	A2911	C2912	A2913	C2914	A2915	C2916	A2917	C2918	A2919	C2920	A2921	C2922	A2923	C2924	A2925	C2926	A2927	C2928	A2929	C2930	A2931	C2932	A2933	C2934	A2935	C2936	A2937	C2938	A2939	C2940	A2941	C2942	A2943	C2944	A2945	C2946	A2947	C2948	A2949	C2950	A2951	C2952	A2953	C2954	A2955	C2956	A2957	C2958	A2959	C2960	A2961	C2962	A2963	C2964	A2965	C2966	A2967	C2968	A2969	C2970	A2971	C2972	A2973	C2974	A2975	C2976	A2977	C2978	A2979	C2980	A2981	C2982	A2983	C2984	A2985	C2986	A2987	C2988	A2989	C2990	A2991	C2992	A2993	C2994	A2995	C2996	A2997	C2998	A2999	C3000	A3001	C3002	A3003	C3004	A3005	C3006	A3007	C3008	A3009	C3010	A3011	C3012	A3013	C3014	A3015	C3016	A3017	C3018	A3019	C3020	A3021	C3022	A3023	C3024	A3025	C3026	A3027	C3028	A3029	C3030	A3031	C3032	A3033	C3034	A3035	C3036	A3037	C3038	A3039	C3040	A3041	C3042	A3043	C3044	A3045	C3046	A3047	C3048	A3049	C3050	A3051	C3052	A3053	C3054	A3055	C3056	A3057	C3058	A3059	C3060	A3061	C3062	A3063	C3064	A3065	C3066	A3067	C3068	A3069	C3070	A3071	C3072	A3073	C3074	A3075	C3076	A3077	C3078	A3079	C3080	A3081	C3082	A3083	C3084	A3085	C3086	A3087	C3088	A3089	C3090	A3091	C3092	A3093	C3094	A3095	C3096	A3097	C3098	A3099	C3100	A3101	C3102	A3103	C3104	A3105	C3106	A3107	C3108	A3109	C3110	A3111	C3112	A3113	C3114	A3115	C3116	A3117	C3118	A3119	C3120	A3121	C3122	A3123	C3124	A3125	C3126	A3127	C3128	A3129	C3130	A3131	C3132	A3133	C3134	A3135	C3136	A3137	C3138	A3139	C3140	A3141	C3142	A3143	C3144	A3145	C3146	A3147	C3148	A3149	C3150	A3151	C3152	A3153	C3154	A3155	C3156	A3157	C3158	A3159	C3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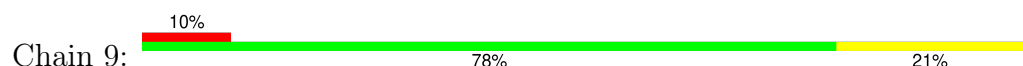
• Molecule 4: 5S rRNA

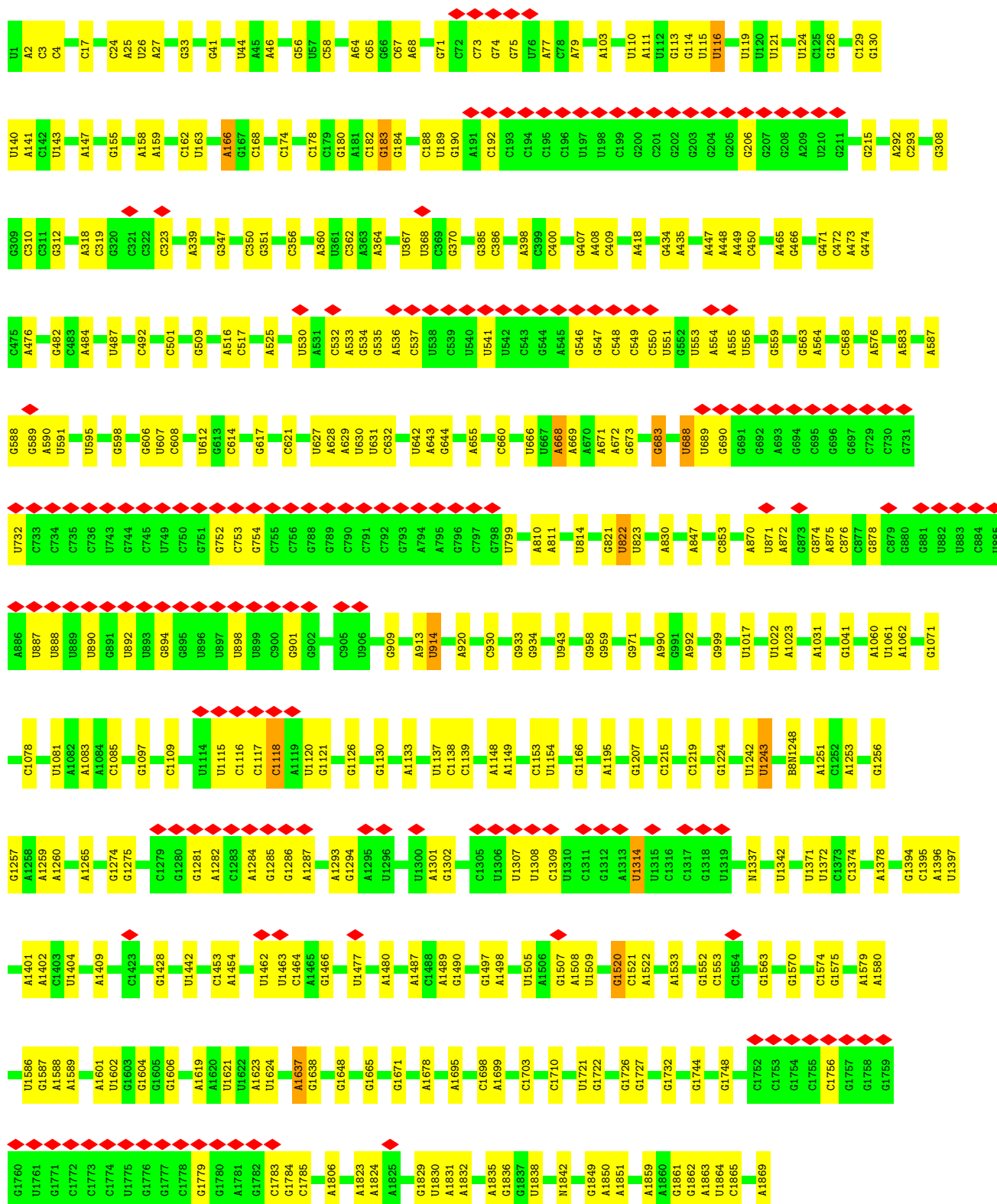


• Molecule 5: 5.8S rRNA



• Molecule 6: 18S rRNA

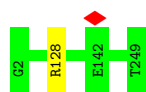




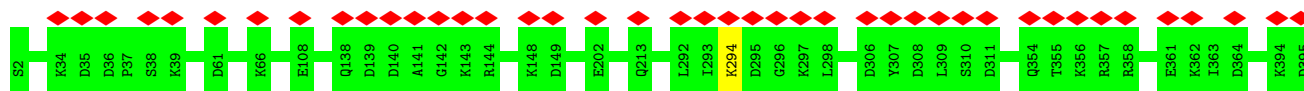
• Molecule 7: 60S ribosomal protein L8

Chain A:

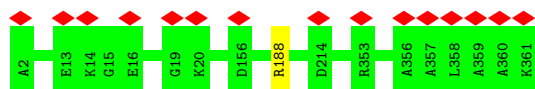
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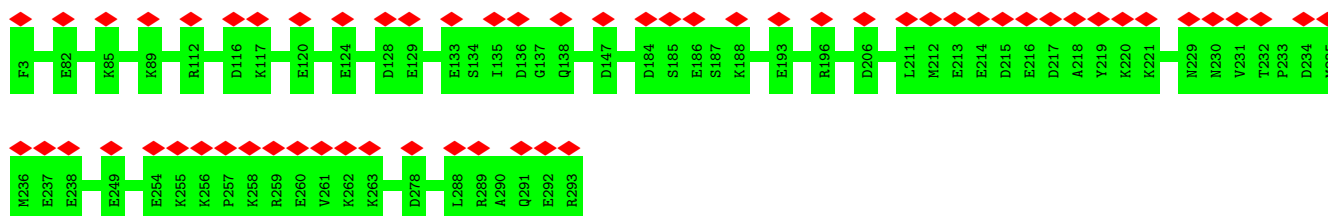
- Molecule 8: 60S ribosomal protein L3



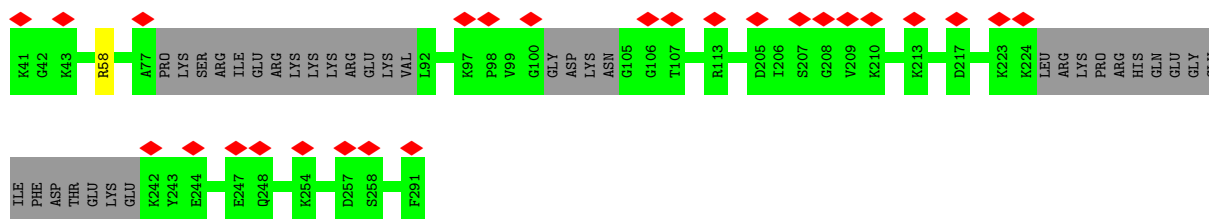
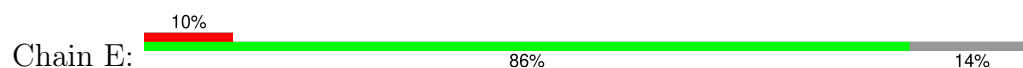
- Molecule 9: 60S ribosomal protein L4



- Molecule 10: Ribosomal_L18_c domain-containing protein



- Molecule 11: 60S ribosomal protein L6



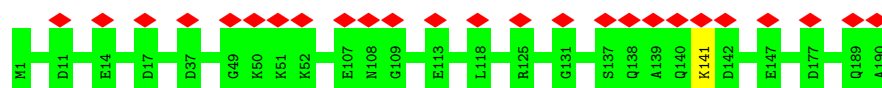
- Molecule 12: 60S ribosomal protein L7



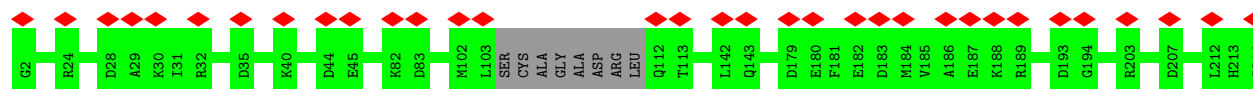
- Molecule 13: 60S ribosomal protein L7a



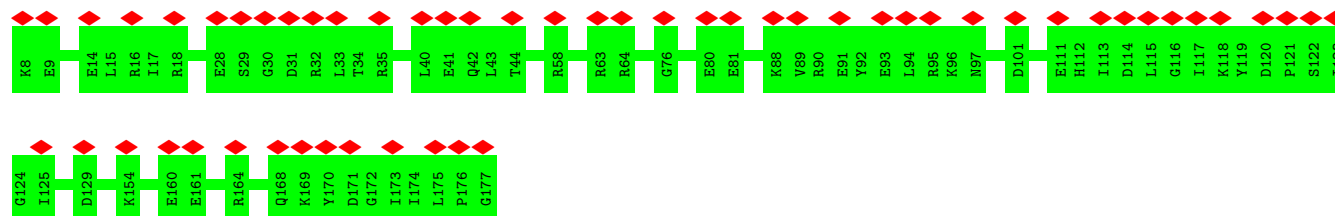
- Molecule 14: 60S ribosomal protein L9



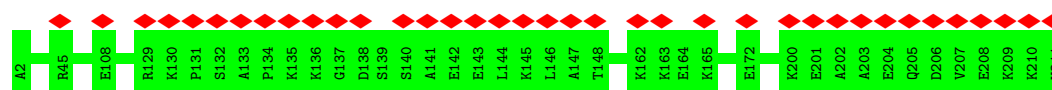
- Molecule 15: Ribosomal protein L10



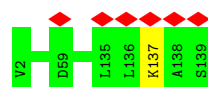
- Molecule 16: 60S ribosomal protein L11



- Molecule 17: 60S ribosomal protein L13

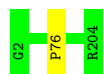


- Molecule 18: 60S ribosomal protein L14



- Molecule 19: 60S ribosomal protein L15

Chain N:  100%



- Molecule 20: 60S ribosomal protein L13a

Chain O:  99%



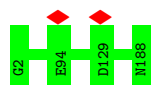
- Molecule 21: 60S ribosomal protein L17

Chain P:  100%



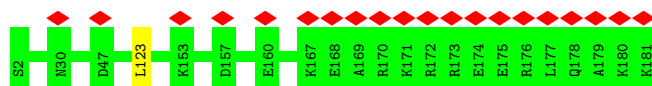
- Molecule 22: 60S ribosomal protein L18

Chain Q:  100%



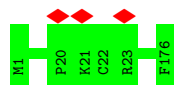
- Molecule 23: 60S ribosomal protein L19

Chain R:  99%



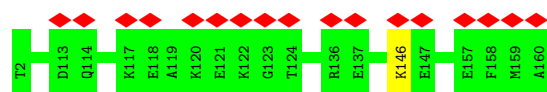
- Molecule 24: 60S ribosomal protein L18a

Chain S:  100%

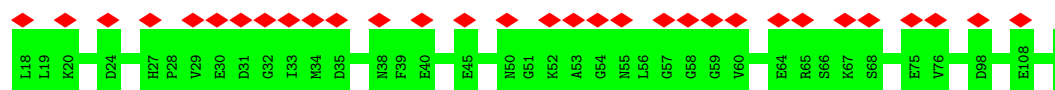


- Molecule 25: 60S ribosomal protein L21

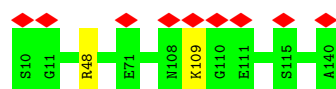
Chain T:  99%



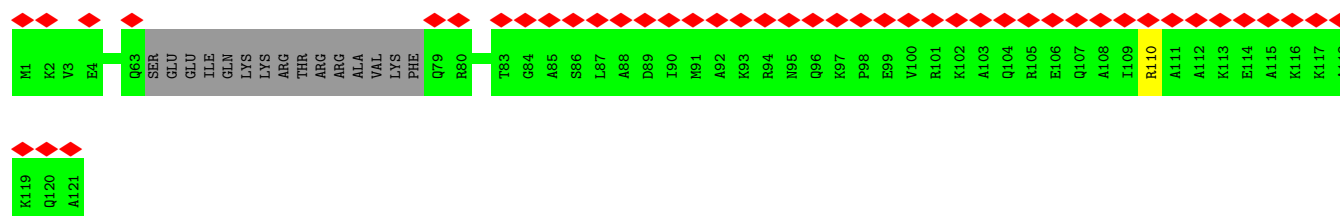
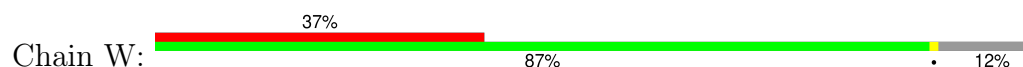
- Molecule 26: 60S ribosomal protein L22



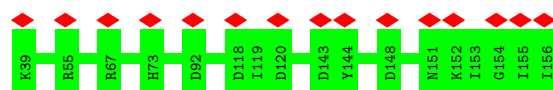
- Molecule 27: 60S ribosomal protein L23



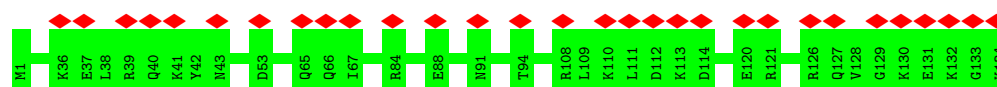
- Molecule 28: Ribosomal protein L24



- Molecule 29: 60S ribosomal protein L23a

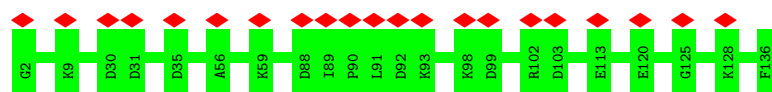


- Molecule 30: 60S ribosomal protein L26



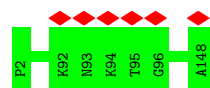
- Molecule 31: 60S ribosomal protein L27





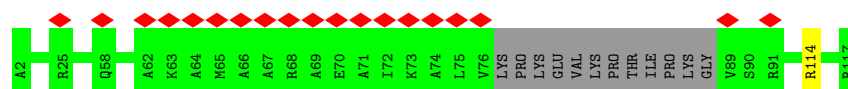
- Molecule 32: 60S ribosomal protein L27a

Chain a: 100%



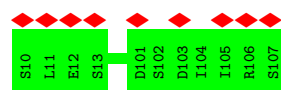
- Molecule 33: 60S ribosomal protein L29

Chain b: 16% 89% 10%



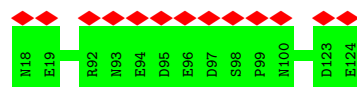
- Molecule 34: 60S ribosomal protein L30

Chain c: 9% 100%



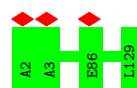
- Molecule 35: 60S ribosomal protein L31

Chain d: 12% 100%



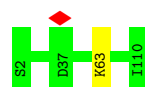
- Molecule 36: 60S ribosomal protein L32

Chain e: 100%

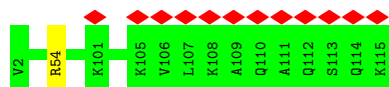


- Molecule 37: 60S ribosomal protein L35a

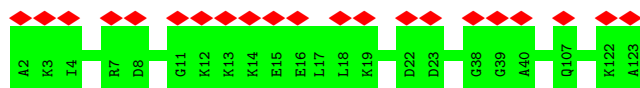
Chain f: 99%



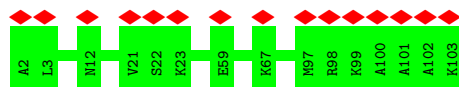
- Molecule 38: 60S ribosomal protein L34



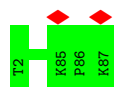
- Molecule 39: 60S ribosomal protein L35



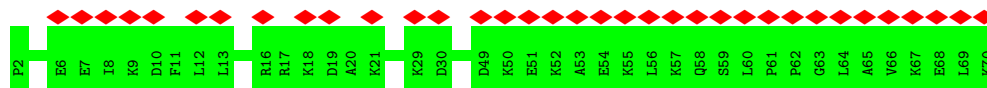
- Molecule 40: 60S ribosomal protein L36



- Molecule 41: 60S ribosomal protein L37



- Molecule 42: 60S ribosomal protein L38

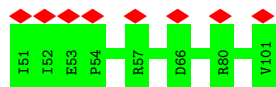


- Molecule 43: 60S ribosomal protein L39



There are no outlier residues recorded for this chain.

- Molecule 44: 60S ribosomal protein L40



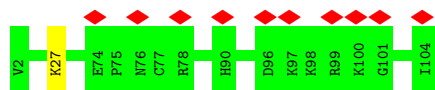
- Molecule 45: eL41

Chain n:  100%

There are no outlier residues recorded for this chain.

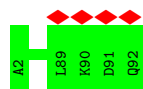
- Molecule 46: 60S ribosomal protein L36a

Chain o:  10%  99%



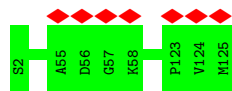
- Molecule 47: 60S ribosomal protein L37a

Chain p:  100%



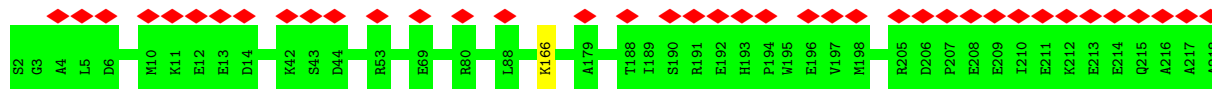
- Molecule 48: 60S ribosomal protein L28

Chain r:  6%  100%



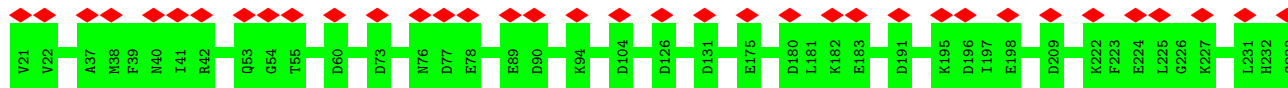
- Molecule 49: 40S_SA_C domain-containing protein

Chain AA:  18%  100%



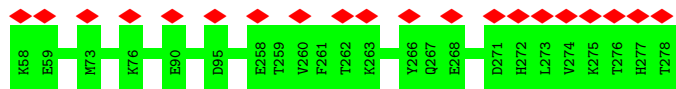
- Molecule 50: 40S ribosomal protein S3a

Chain BB:  17%  100%

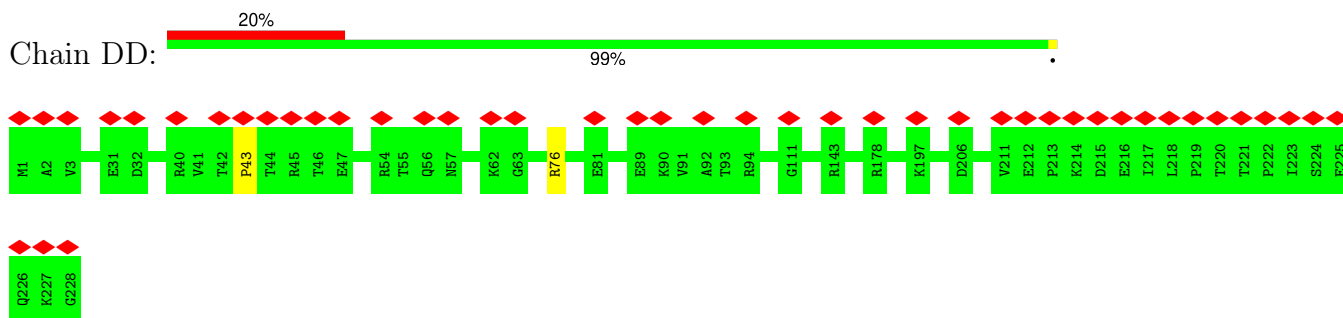


- Molecule 51: 40S ribosomal protein S2

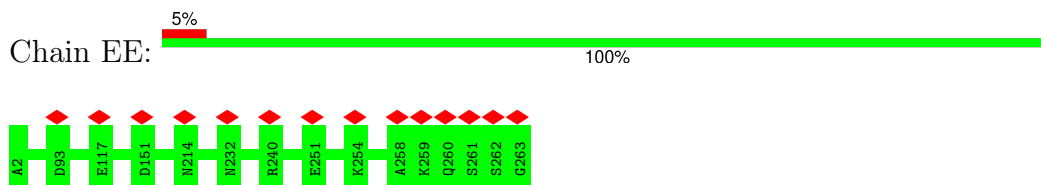
Chain CC:  9%  100%



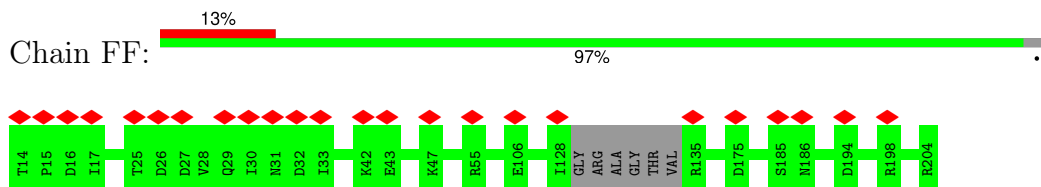
- Molecule 52: 40S ribosomal protein S3



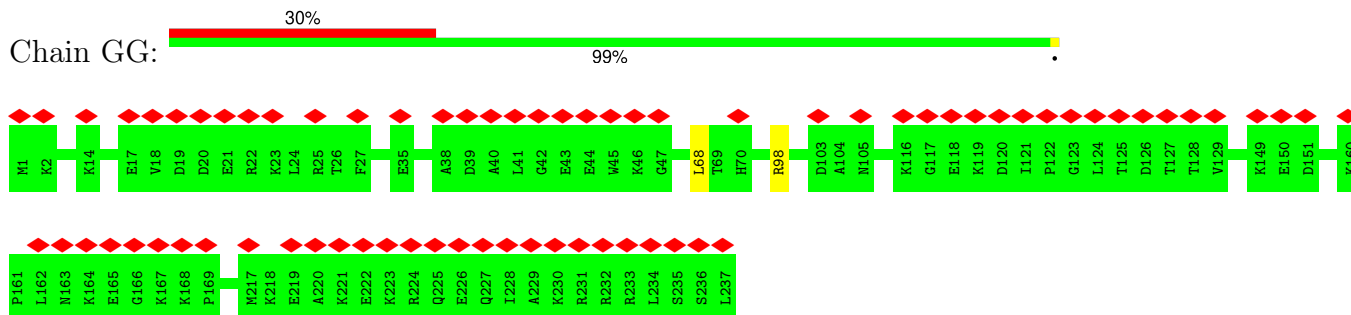
- Molecule 53: 40S ribosomal protein S4



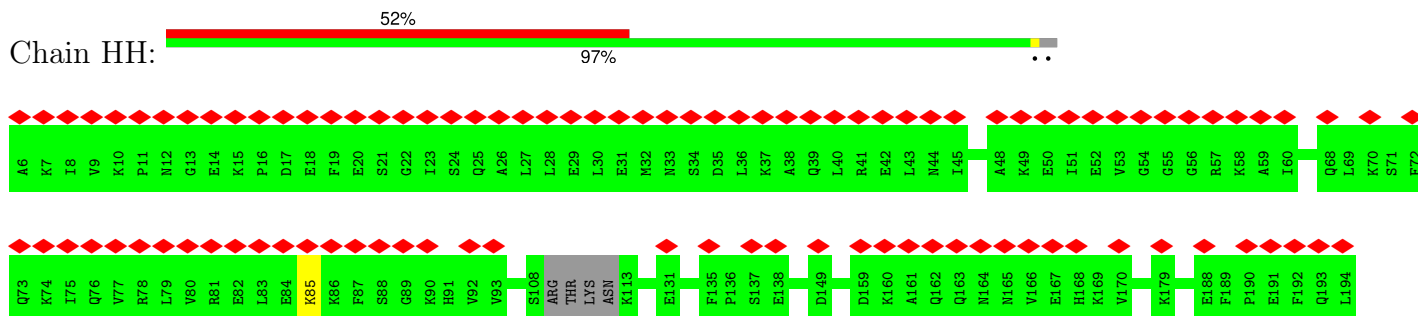
- Molecule 54: Ribosomal protein S5



- Molecule 55: 40S ribosomal protein S6

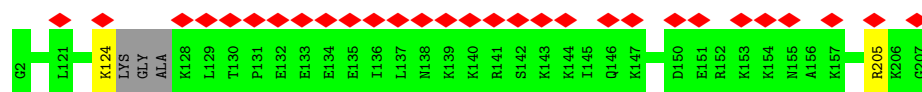


- Molecule 56: 40S ribosomal protein S7

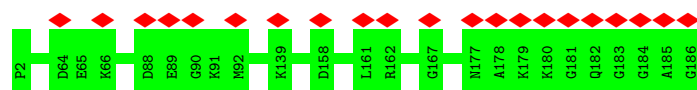


- Molecule 57: 40S ribosomal protein S8

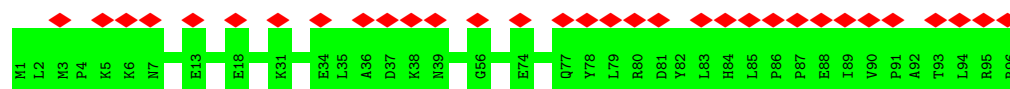




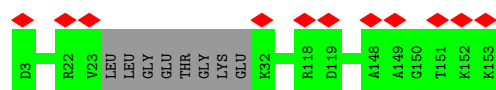
- Molecule 58: 40S ribosomal protein S9



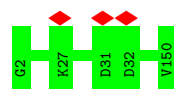
- Molecule 59: 40S ribosomal protein S10



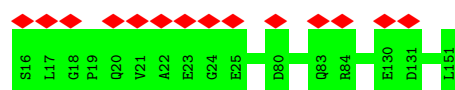
- Molecule 60: 40S ribosomal protein S11



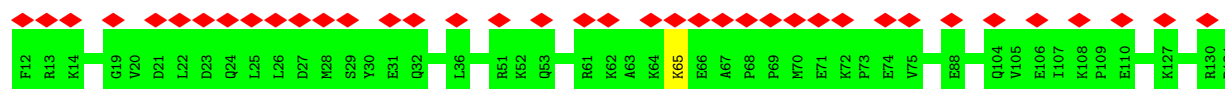
- Molecule 61: 40S ribosomal protein S13



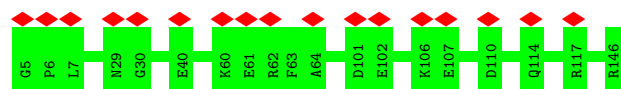
- Molecule 62: 40S ribosomal protein S14



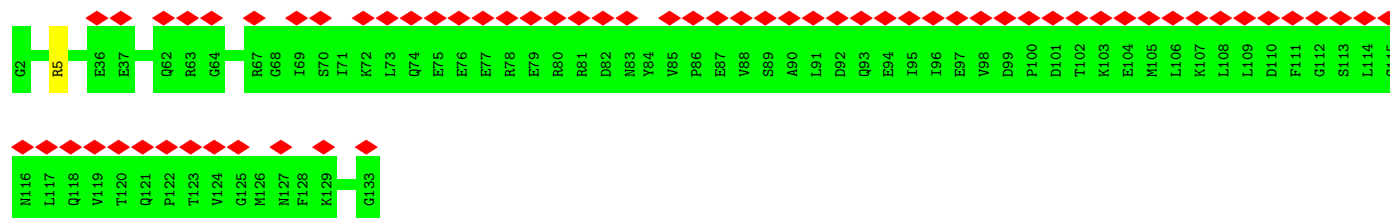
- Molecule 63: 40S ribosomal protein S15



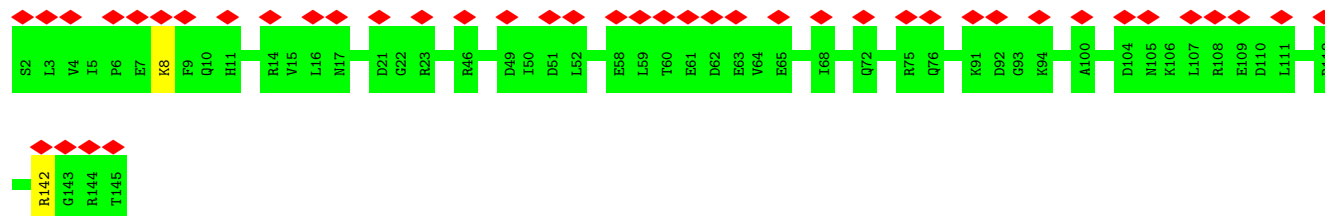
- Molecule 64: 40S ribosomal protein S16



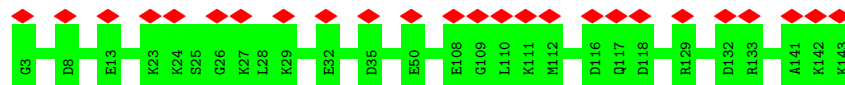
- Molecule 65: 40S ribosomal protein S17



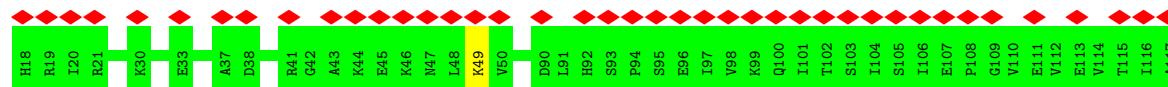
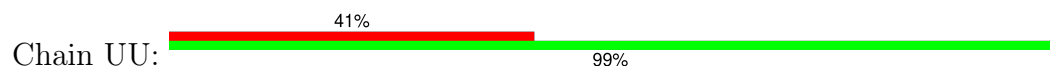
- Molecule 66: 40S ribosomal protein S18



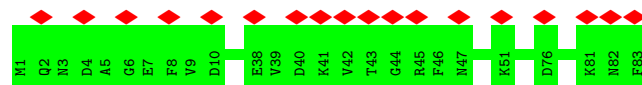
- Molecule 67: 40S ribosomal protein S19



- Molecule 68: 40S ribosomal protein S20



- Molecule 69: eS21



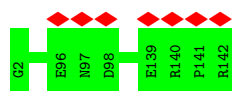
- Molecule 70: 40S ribosomal protein S15a

Chain WW:  100%

There are no outlier residues recorded for this chain.

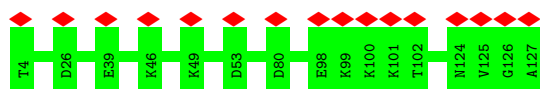
- Molecule 71: 40S ribosomal protein S23

Chain XX:  5%  100%



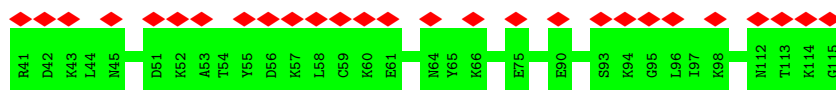
- Molecule 72: 40S ribosomal protein S24

Chain YY:  13%  100%



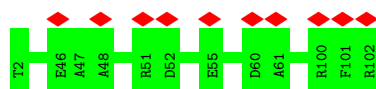
- Molecule 73: 40S ribosomal protein S25

Chain ZZ:  36%  100%



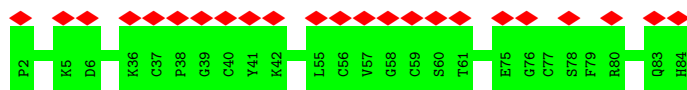
- Molecule 74: eS26

Chain Aa:  10%  100%



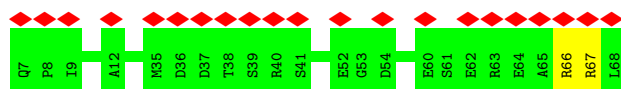
- Molecule 75: 40S ribosomal protein S27

Chain Bb:  28%  100%

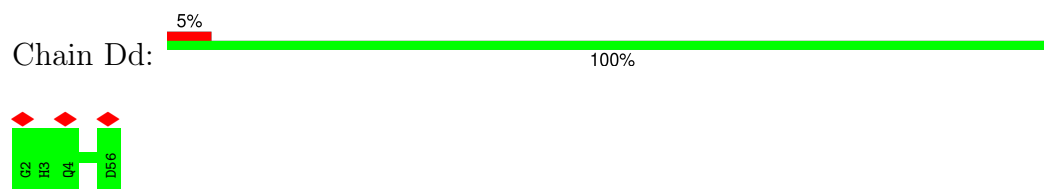


- Molecule 76: 40S ribosomal protein S28

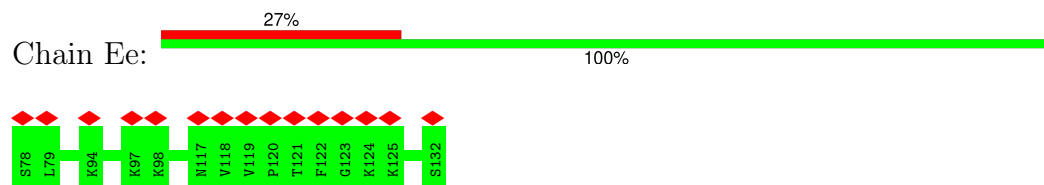
Chain Cc:  34%  97%



- Molecule 77: 40S ribosomal protein S29



- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107057	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	651.84, 651.84, 651.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.358, 1.358, 1.358	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, UR3, 4AC, PSU, BGH, MLZ, 5MU, OMG, MHG, OMC, P4U, B8H, B9H, T6A, B8W, B8Q, MG, OMU, B8T, M7A, 1MA, B9B, MA6, 2MG, I4U, P7G, 5MC, 6MZ, MMX, E6G, ZN, B8N, 7MG, MQ6, E7G, B8K

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	2	0.26	0/1698	0.86	4/2640 (0.2%)
2	1	0.23	0/122	0.72	0/186
3	5	0.35	0/82609	0.82	25/128762 (0.0%)
4	7	0.31	0/2858	0.76	0/4455
5	8	0.32	0/3559	0.77	0/5543
6	9	0.34	0/39730	0.82	28/61898 (0.0%)
7	A	0.30	0/1936	0.59	0/2596
8	B	0.29	0/3240	0.57	0/4339
9	C	0.29	0/2913	0.57	0/3913
10	D	0.28	0/2427	0.54	0/3250
11	E	0.27	0/1762	0.57	0/2362
12	F	0.29	0/1911	0.54	0/2549
13	G	0.29	0/1868	0.58	1/2514 (0.0%)
14	H	0.29	0/1535	0.59	0/2063
15	I	0.29	0/1702	0.57	0/2272
16	J	0.29	0/1385	0.61	0/1852
17	L	0.28	0/1733	0.60	0/2316
18	M	0.32	0/1158	0.59	0/1547
19	N	0.31	0/1746	0.62	0/2338
20	O	0.31	0/1662	0.56	0/2222
21	P	0.29	0/1268	0.57	0/1700
22	Q	0.29	0/1539	0.62	0/2054
23	R	0.28	0/1524	0.63	1/2013 (0.0%)
24	S	0.29	0/1501	0.57	0/2012
25	T	0.30	0/1326	0.53	0/1770
26	U	0.32	0/814	0.58	0/1092
27	V	0.29	0/993	0.55	0/1332
28	W	0.30	0/873	0.62	0/1158
29	X	0.27	0/984	0.55	0/1323
30	Y	0.30	0/1132	0.59	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Z	0.29	0/1130	0.54	0/1507
32	a	0.30	0/1191	0.56	0/1590
33	b	0.28	0/861	0.56	0/1138
34	c	0.29	0/771	0.53	0/1034
35	d	0.28	0/903	0.57	0/1216
36	e	0.31	0/1071	0.55	0/1429
37	f	0.30	0/895	0.58	0/1198
38	g	0.28	0/916	0.59	0/1220
39	h	0.27	0/1021	0.58	0/1348
40	i	0.26	0/841	0.58	0/1112
41	j	0.30	0/720	0.63	0/952
42	k	0.28	0/575	0.54	0/761
43	l	0.26	0/459	0.57	0/608
44	m	0.28	0/415	0.64	0/550
45	n	0.30	0/240	0.82	0/305
46	o	0.29	0/855	0.55	0/1128
47	p	0.27	0/718	0.52	0/953
48	r	0.28	0/1010	0.58	0/1354
49	AA	0.27	0/1747	0.51	0/2374
50	BB	0.28	0/1756	0.51	0/2350
51	CC	0.32	0/1753	0.53	0/2369
52	DD	0.27	0/1796	0.57	1/2417 (0.0%)
53	EE	0.29	0/2118	0.55	0/2849
54	FF	0.26	0/1492	0.52	0/2005
55	GG	0.26	0/1946	0.59	1/2590 (0.0%)
56	HH	0.27	0/1510	0.53	0/2022
57	II	0.28	0/1696	0.58	0/2261
58	JJ	0.28	0/1550	0.58	0/2069
59	KK	0.27	0/834	0.49	0/1125
60	LL	0.31	0/1195	0.56	0/1597
61	NN	0.27	0/1226	0.56	0/1649
62	OO	0.27	0/1029	0.59	0/1380
63	PP	0.32	0/1017	0.57	0/1358
64	QQ	0.27	0/1146	0.56	0/1534
65	RR	0.27	0/1082	0.54	0/1452
66	SS	0.28	0/1208	0.60	0/1618
67	TT	0.26	0/1115	0.52	0/1493
68	UU	0.25	0/805	0.58	0/1081
69	VV	0.29	0/643	0.56	0/860
70	WW	0.32	0/1051	0.59	0/1406
71	XX	0.29	0/1116	0.54	0/1490
72	YY	0.28	0/1028	0.56	0/1366
73	ZZ	0.25	0/604	0.55	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
74	Aa	0.28	0/828	0.58	0/1109
75	Bb	0.27	0/665	0.51	0/891
76	Cc	0.27	0/490	0.66	0/656
77	Dd	0.28	0/470	0.56	0/623
78	Ee	0.26	0/447	0.57	0/587
79	Gg	0.27	0/2493	0.55	0/3394
All	All	0.32	0/221956	0.73	61/325763 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	G	0	1
19	N	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	5	2022	C	N3-C2-O2	-7.78	116.45	121.90
3	5	1236	C	C2-N1-C1'	7.62	127.19	118.80
6	9	501	C	C2-N1-C1'	7.52	127.07	118.80
3	5	2019	C	N3-C2-O2	-7.34	116.76	121.90
6	9	356	C	C2-N1-C1'	7.27	126.80	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	215	ASP	Peptide
19	N	76	PRO	Peptide

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
8	B	392/394 (100%)	378 (96%)	14 (4%)	0	100	100
9	C	357/360 (99%)	347 (97%)	10 (3%)	0	100	100
10	D	289/291 (99%)	280 (97%)	9 (3%)	0	100	100
11	E	208/251 (83%)	198 (95%)	10 (5%)	0	100	100
12	F	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
13	G	223/234 (95%)	215 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
15	I	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
16	J	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
17	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
18	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
19	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
20	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	R	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
24	S	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
25	T	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
26	U	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
27	V	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
28	W	102/121 (84%)	99 (97%)	3 (3%)	0	100	100
29	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
30	Y	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
31	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	a	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
33	b	100/116 (86%)	97 (97%)	3 (3%)	0	100	100
34	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	d	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
36	e	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
41	j	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
42	k	67/69 (97%)	67 (100%)	0	0	100	100
43	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
44	m	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
47	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
48	r	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
49	AA	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
50	BB	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
51	CC	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
52	DD	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
53	EE	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
54	FF	181/191 (95%)	166 (92%)	15 (8%)	0	100	100
55	GG	235/237 (99%)	229 (97%)	6 (3%)	0	100	100
56	HH	181/189 (96%)	171 (94%)	10 (6%)	0	100	100
57	II	199/206 (97%)	190 (96%)	9 (4%)	0	100	100
58	JJ	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
59	KK	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
60	LL	139/151 (92%)	134 (96%)	5 (4%)	0	100	100
61	NN	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
62	OO	134/136 (98%)	132 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	PP	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
64	QQ	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
65	RR	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
66	SS	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
67	TT	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
68	UU	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
69	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
70	WW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
71	XX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
72	YY	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
73	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
74	Aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
75	Bb	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
76	Cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
77	Dd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
78	Ee	53/55 (96%)	53 (100%)	0	0	100	100
79	Gg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
All	All	10973/11241 (98%)	10587 (96%)	386 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
7	A	190/190 (100%)	189 (100%)	1 (0%)	86	95
8	B	342/342 (100%)	341 (100%)	1 (0%)	91	97
9	C	299/299 (100%)	298 (100%)	1 (0%)	91	97
10	D	247/247 (100%)	247 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	190/223 (85%)	189 (100%)	1 (0%)	86	95
12	F	196/196 (100%)	196 (100%)	0	100	100
13	G	196/201 (98%)	195 (100%)	1 (0%)	86	95
14	H	169/169 (100%)	168 (99%)	1 (1%)	84	95
15	I	175/180 (97%)	175 (100%)	0	100	100
16	J	143/143 (100%)	143 (100%)	0	100	100
17	L	175/175 (100%)	175 (100%)	0	100	100
18	M	117/117 (100%)	116 (99%)	1 (1%)	75	92
19	N	171/171 (100%)	171 (100%)	0	100	100
20	O	171/171 (100%)	169 (99%)	2 (1%)	67	89
21	P	134/134 (100%)	134 (100%)	0	100	100
22	Q	164/164 (100%)	164 (100%)	0	100	100
23	R	159/159 (100%)	159 (100%)	0	100	100
24	S	157/157 (100%)	157 (100%)	0	100	100
25	T	139/139 (100%)	138 (99%)	1 (1%)	81	94
26	U	88/88 (100%)	88 (100%)	0	100	100
27	V	101/101 (100%)	99 (98%)	2 (2%)	50	81
28	W	86/100 (86%)	85 (99%)	1 (1%)	67	89
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	124 (100%)	0	100	100
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	119 (100%)	0	100	100
33	b	84/95 (88%)	83 (99%)	1 (1%)	67	89
34	c	84/84 (100%)	84 (100%)	0	100	100
35	d	98/98 (100%)	98 (100%)	0	100	100
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	87 (99%)	1 (1%)	70	90
38	g	98/98 (100%)	97 (99%)	1 (1%)	73	91
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	k	64/64 (100%)	64 (100%)	0	100	100
43	l	47/47 (100%)	47 (100%)	0	100	100
44	m	46/46 (100%)	46 (100%)	0	100	100
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	90 (99%)	1 (1%)	70	90
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	108 (100%)	0	100	100
49	AA	180/181 (99%)	179 (99%)	1 (1%)	84	95
50	BB	194/194 (100%)	194 (100%)	0	100	100
51	CC	187/187 (100%)	187 (100%)	0	100	100
52	DD	190/190 (100%)	189 (100%)	1 (0%)	86	95
53	EE	224/224 (100%)	224 (100%)	0	100	100
54	FF	158/161 (98%)	158 (100%)	0	100	100
55	GG	207/207 (100%)	206 (100%)	1 (0%)	86	95
56	HH	165/169 (98%)	164 (99%)	1 (1%)	84	95
57	II	177/178 (99%)	175 (99%)	2 (1%)	70	90
58	JJ	161/161 (100%)	161 (100%)	0	100	100
59	KK	87/87 (100%)	87 (100%)	0	100	100
60	LL	130/136 (96%)	130 (100%)	0	100	100
61	NN	130/130 (100%)	130 (100%)	0	100	100
62	OO	106/106 (100%)	106 (100%)	0	100	100
63	PP	109/109 (100%)	108 (99%)	1 (1%)	75	92
64	QQ	117/117 (100%)	117 (100%)	0	100	100
65	RR	119/119 (100%)	118 (99%)	1 (1%)	79	93
66	SS	125/125 (100%)	123 (98%)	2 (2%)	58	85
67	TT	111/111 (100%)	111 (100%)	0	100	100
68	UU	92/92 (100%)	91 (99%)	1 (1%)	70	90
69	VV	67/67 (100%)	67 (100%)	0	100	100
70	WW	112/112 (100%)	112 (100%)	0	100	100
71	XX	113/113 (100%)	113 (100%)	0	100	100
72	YY	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	ZZ	66/66 (100%)	66 (100%)	0	100	100
74	Aa	88/88 (100%)	88 (100%)	0	100	100
75	Bb	75/75 (100%)	75 (100%)	0	100	100
76	Cc	55/55 (100%)	53 (96%)	2 (4%)	30	64
77	Dd	48/48 (100%)	48 (100%)	0	100	100
78	Ee	46/46 (100%)	46 (100%)	0	100	100
79	Gg	272/272 (100%)	269 (99%)	3 (1%)	70	90
All	All	9581/9664 (99%)	9548 (100%)	33 (0%)	90	97

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
76	Cc	66	ARG
76	Cc	67	ARG
79	Gg	280	LYS
28	W	110	ARG
27	V	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
67	TT	51	ASN
69	VV	2	GLN
79	Gg	226	HIS
25	T	54	HIS
24	S	146	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	68/76 (89%)	11 (16%)	0
2	1	4/6 (66%)	1 (25%)	0
3	5	3493/3546 (98%)	681 (19%)	55 (1%)
4	7	119/120 (99%)	10 (8%)	0
5	8	149/156 (95%)	29 (19%)	1 (0%)
6	9	1678/1698 (98%)	328 (19%)	18 (1%)
All	All	5511/5602 (98%)	1060 (19%)	74 (1%)

5 of 1060 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	10	G
1	2	11	G
1	2	13	G
1	2	14	C
1	2	19	G

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	9	110	U
6	9	1489	A
6	9	434	G
6	9	752	G
3	5	1370	G

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

139 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	$\# Z > 2$
3	OMC	5	3887	3	19,22,23	3.00	8 (42%)	25,31,34	0.77	0
6	PSU	9	612	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)
6	A2M	9	1678	6	18,25,26	3.55	7 (38%)	20,36,39	3.36	5 (25%)
3	BGH	5	3899	80,3	25,29,30	4.50	18 (72%)	30,43,46	2.48	13 (43%)
3	I4U	5	1659	3	20,24,25	3.43	8 (40%)	27,34,37	2.00	2 (7%)
3	OMC	5	3701	80,3	19,22,23	2.99	8 (42%)	25,31,34	0.72	0
3	5MC	5	4335	3	19,22,23	3.87	8 (42%)	26,32,35	1.08	2 (7%)
3	B8K	5	4690	3	24,28,29	3.27	11 (45%)	29,42,45	2.45	11 (37%)
3	B8T	5	4483	3	19,22,23	3.60	8 (42%)	25,31,34	0.91	1 (4%)
3	E7G	5	2297	3	24,27,28	3.57	11 (45%)	28,40,43	2.30	9 (32%)
3	PSU	5	4293	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	5	1524	3	18,25,26	3.61	6 (33%)	20,36,39	3.43	4 (20%)
3	B9H	5	2786	3	21,25,26	3.03	4 (19%)	22,35,38	1.47	3 (13%)
3	M7A	5	4564	3	19,25,26	1.60	2 (10%)	25,37,40	4.23	8 (32%)
3	OMC	5	3909	3	19,22,23	3.00	8 (42%)	25,31,34	0.96	1 (4%)
6	B8Q	9	1219	80,6	18,22,23	2.96	4 (22%)	21,32,35	2.32	7 (33%)
3	P7G	5	3880	3	24,28,29	3.62	11 (45%)	25,41,44	1.34	2 (8%)
3	PSU	5	4450	80,3	18,21,22	1.09	2 (11%)	21,30,33	2.03	5 (23%)
3	UR3	5	4530	3	19,22,23	2.85	7 (36%)	26,32,35	1.64	3 (11%)
3	OMU	5	4620	3	19,22,23	3.03	8 (42%)	25,31,34	1.78	4 (16%)
3	PSU	5	1683	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
3	B9B	5	1574	80,3	20,28,29	1.73	2 (10%)	19,40,43	7.22	5 (26%)
3	A2M	5	3785	3	18,25,26	3.65	7 (38%)	20,36,39	3.63	6 (30%)
3	OMG	5	4637	3	19,26,27	2.41	8 (42%)	21,38,41	1.46	4 (19%)
3	A2M	5	4523	80,3	18,25,26	3.58	7 (38%)	20,36,39	3.34	4 (20%)
6	OMG	9	644	6	19,26,27	2.39	8 (42%)	21,38,41	1.42	4 (19%)
3	PSU	5	1677	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
3	A2M	5	2401	80,3	18,25,26	3.60	7 (38%)	20,36,39	3.37	4 (20%)
6	B8N	9	1248	6	25,29,30	3.38	7 (28%)	28,42,45	2.00	7 (25%)
3	P4U	5	1348	3	21,24,25	3.41	8 (38%)	28,33,36	1.57	2 (7%)
3	B8H	5	4296	3	19,22,23	6.85	6 (31%)	21,32,35	2.51	5 (23%)
3	PSU	5	4403	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	5 (23%)
3	B8H	5	3762	3	19,22,23	6.83	6 (31%)	21,32,35	2.51	5 (23%)
3	PSU	5	3715	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	E6G	5	4355	3	19,27,28	2.25	2 (10%)	18,39,42	3.46	6 (33%)
3	B8W	5	4129	3	18,26,27	2.36	2 (11%)	17,38,41	2.74	8 (47%)
3	MHG	5	4371	3	29,32,33	3.55	11 (37%)	34,46,49	2.45	11 (32%)
6	UR3	9	1830	6	19,22,23	2.92	7 (36%)	26,32,35	1.72	4 (15%)
3	B8W	5	4529	80,3	18,26,27	2.36	2 (11%)	17,38,41	2.69	8 (47%)
3	OMG	5	1625	80,3	19,26,27	2.44	8 (42%)	21,38,41	1.45	4 (19%)
6	4AC	9	1337	6	21,24,25	3.19	9 (42%)	28,34,37	1.11	4 (14%)
6	PSU	9	119	6	18,21,22	1.02	1 (5%)	21,30,33	1.76	4 (19%)
6	OMU	9	116	6	19,22,23	3.06	8 (42%)	25,31,34	1.81	6 (24%)
3	OMG	5	373	3	19,26,27	2.39	8 (42%)	21,38,41	1.43	4 (19%)
3	A2M	5	1534	80,3	18,25,26	3.62	7 (38%)	20,36,39	3.41	4 (20%)
3	2MG	5	1517	3	18,26,27	2.50	7 (38%)	16,38,41	1.80	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	5	1871	80,3	18,25,26	3.58	7 (38%)	20,36,39	3.35	4 (20%)
3	B8Q	5	1456	3	18,22,23	2.89	6 (33%)	21,32,35	1.91	4 (19%)
6	OMG	9	509	80,6	19,26,27	2.39	8 (42%)	21,38,41	1.44	4 (19%)
3	A2M	5	1326	3	18,25,26	3.59	7 (38%)	20,36,39	3.29	4 (20%)
6	MA6	9	1850	6	19,26,27	1.92	4 (21%)	18,38,41	4.00	4 (22%)
3	OMG	5	4370	3	19,26,27	2.42	8 (42%)	21,38,41	1.43	4 (19%)
3	PSU	5	4636	3	18,21,22	1.12	1 (5%)	21,30,33	2.03	6 (28%)
3	B8W	5	2380	3	18,26,27	2.32	2 (11%)	17,38,41	2.63	6 (35%)
3	B8W	5	4472	3	18,26,27	2.35	2 (11%)	17,38,41	2.58	5 (29%)
3	OMU	5	4306	3	19,22,23	3.01	8 (42%)	25,31,34	1.82	5 (20%)
3	5MC	5	4447	3	19,22,23	3.76	8 (42%)	26,32,35	1.08	1 (3%)
3	A2M	5	3718	3	18,25,26	3.60	7 (38%)	20,36,39	3.28	5 (25%)
6	A2M	9	166	6	18,25,26	3.61	7 (38%)	20,36,39	3.31	6 (30%)
3	PSU	5	3729	3	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
3	7MG	5	4550	3	23,26,27	3.46	10 (43%)	27,39,42	2.11	9 (33%)
3	PSU	5	4442	3	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
6	PSU	9	1081	6	18,21,22	1.04	1 (5%)	21,30,33	1.82	5 (23%)
3	OMG	5	4494	3	19,26,27	2.43	8 (42%)	21,38,41	1.44	4 (19%)
3	B8T	5	4671	3	19,22,23	3.61	8 (42%)	25,31,34	0.90	1 (4%)
6	PSU	9	1243	6	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	5	4500	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
6	A2M	9	1031	6	18,25,26	3.59	7 (38%)	20,36,39	3.27	5 (25%)
3	OMG	5	1522	3	19,26,27	2.38	8 (42%)	21,38,41	1.44	3 (14%)
3	OMC	5	2804	3	19,22,23	2.96	8 (42%)	25,31,34	0.70	0
3	B9B	5	237	3	20,28,29	1.73	2 (10%)	19,40,43	7.09	5 (26%)
6	OMC	9	1703	6	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
3	E7G	5	1797	3	24,27,28	3.60	11 (45%)	28,40,43	2.33	9 (32%)
6	A2M	9	159	6	18,25,26	3.60	7 (38%)	20,36,39	3.32	5 (25%)
3	PSU	5	4628	3	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	1MA	5	1322	80,3	17,25,26	4.20	6 (35%)	17,37,40	1.94	3 (17%)
6	OMC	9	517	6	19,22,23	3.02	8 (42%)	25,31,34	0.77	0
3	6MZ	5	4220	3	17,25,26	1.48	2 (11%)	15,36,39	4.00	5 (33%)
6	OMC	9	1710	6	19,22,23	3.02	8 (42%)	25,31,34	0.76	0
3	B8H	5	1860	3	19,22,23	6.84	6 (31%)	21,32,35	2.48	5 (23%)
3	OMG	5	1316	3	19,26,27	2.37	8 (42%)	21,38,41	1.42	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	5	4571	3	18,25,26	3.61	7 (38%)	20,36,39	3.25	5 (25%)
3	OMG	5	4623	3	19,26,27	2.40	8 (42%)	21,38,41	1.46	4 (19%)
6	MMX	9	568	6	20,23,24	3.83	5 (25%)	21,33,36	2.90	5 (23%)
3	OMG	5	4196	3	19,26,27	2.40	8 (42%)	21,38,41	1.41	4 (19%)
1	T6A	2	37	1	26,34,35	1.90	7 (26%)	28,49,52	2.07	5 (17%)
3	B8W	5	4185	3	18,26,27	2.32	2 (11%)	17,38,41	2.62	5 (29%)
3	7MG	5	1605	3	23,26,27	3.48	10 (43%)	27,39,42	2.17	9 (33%)
5	OMU	8	14	3,5	19,22,23	3.07	8 (42%)	25,31,34	1.81	5 (20%)
6	A2M	9	668	80,6	18,25,26	3.66	6 (33%)	20,36,39	3.37	4 (20%)
6	5MU	9	814	6	19,22,23	4.96	7 (36%)	27,32,35	3.55	10 (37%)
3	OMG	5	2050	3	19,26,27	2.41	8 (42%)	21,38,41	1.43	4 (19%)
3	PSU	5	3764	3	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
6	4AC	9	1842	6	21,24,25	3.17	10 (47%)	28,34,37	1.05	4 (14%)
3	OMG	5	2424	3	19,26,27	2.44	8 (42%)	21,38,41	1.43	4 (19%)
44	MLZ	m	72	44	8,9,10	0.79	0	4,9,11	0.61	0
3	5MC	5	3782	3	19,22,23	3.79	8 (42%)	26,32,35	1.04	2 (7%)
2	4AC	1	45	2	21,24,25	3.28	9 (42%)	28,34,37	1.15	4 (14%)
3	5MU	5	4083	3	19,22,23	4.97	7 (36%)	27,32,35	3.61	10 (37%)
3	OMC	5	2365	3	19,22,23	2.97	8 (42%)	25,31,34	0.76	0
3	7MG	5	2522	3	23,26,27	3.47	10 (43%)	27,39,42	2.20	9 (33%)
3	2MG	5	4872	3	18,26,27	2.54	7 (38%)	16,38,41	2.43	6 (37%)
3	OMG	5	3792	3	19,26,27	2.42	8 (42%)	21,38,41	1.41	4 (19%)
3	PSU	5	2508	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	5 (23%)
3	A2M	5	2363	80,3	18,25,26	3.59	7 (38%)	20,36,39	3.32	5 (25%)
3	OMG	5	2773	3	19,26,27	2.44	8 (42%)	21,38,41	1.42	4 (19%)
6	OMU	9	121	6	19,22,23	3.05	8 (42%)	25,31,34	1.84	4 (16%)
3	OMG	5	2364	3	19,26,27	2.38	8 (42%)	21,38,41	1.43	4 (19%)
6	M7A	9	1806	6	19,25,26	1.64	2 (10%)	25,37,40	4.09	8 (32%)
6	MA6	9	1851	6	19,26,27	1.89	4 (21%)	18,38,41	4.16	4 (22%)
3	UR3	5	1866	3	19,22,23	2.86	6 (31%)	26,32,35	1.57	3 (11%)
6	PSU	9	823	6	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
6	A2M	9	27	80,6	18,25,26	3.59	7 (38%)	20,36,39	3.27	4 (20%)
3	A2M	5	3723	3	18,25,26	3.58	7 (38%)	20,36,39	3.29	5 (25%)
3	P7G	5	1909	3	24,28,29	3.70	11 (45%)	25,41,44	1.29	2 (8%)
3	2MG	5	729	3	18,26,27	2.51	6 (33%)	16,38,41	1.42	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	B8K	5	3897	3	24,28,29	3.18	11 (45%)	29,42,45	2.36	11 (37%)
3	OMC	5	4536	3	19,22,23	2.98	8 (42%)	25,31,34	0.80	0
6	5MC	9	1374	6	19,22,23	3.80	8 (42%)	26,32,35	1.02	2 (7%)
3	A2M	5	3867	3	18,25,26	3.61	7 (38%)	20,36,39	3.39	5 (25%)
3	B9B	5	2754	80,3	20,28,29	1.76	2 (10%)	19,40,43	7.54	4 (21%)
3	1MA	5	4415	3	17,25,26	4.30	6 (35%)	17,37,40	1.85	3 (17%)
3	OMC	5	2422	80,3	19,22,23	3.02	8 (42%)	25,31,34	0.75	0
3	A2M	5	3825	3	18,25,26	3.60	7 (38%)	20,36,39	3.24	5 (25%)
3	PSU	5	1582	3	18,21,22	1.04	1 (5%)	21,30,33	1.69	4 (19%)
3	UR3	5	4597	3	19,22,23	2.90	6 (31%)	26,32,35	1.53	3 (11%)
6	A2M	9	484	6	18,25,26	3.61	7 (38%)	20,36,39	3.31	4 (20%)
3	A2M	5	398	3	18,25,26	3.60	7 (38%)	20,36,39	3.25	5 (25%)
3	OMG	5	4870	3	19,26,27	2.46	8 (42%)	21,38,41	1.53	4 (19%)
3	OMC	5	3869	3	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
9	MLZ	C	333	9	8,9,10	0.84	0	4,9,11	0.70	0
6	6MZ	9	1832	80,6	17,25,26	1.44	2 (11%)	15,36,39	3.86	5 (33%)
3	OMG	5	1883	3	19,26,27	2.41	8 (42%)	21,38,41	1.48	4 (19%)
6	OMC	9	174	6	19,22,23	3.01	8 (42%)	25,31,34	0.73	0
3	OMC	5	2861	3	19,22,23	3.00	8 (42%)	25,31,34	0.75	0
3	PSU	5	4531	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
3	I4U	5	4194	3	20,24,25	3.40	8 (40%)	27,34,37	2.16	2 (7%)
6	OMG	9	683	6	19,26,27	2.44	8 (42%)	21,38,41	1.46	3 (14%)
6	PSU	9	822	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)

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
3	OMC	5	3887	3	-	1/9/27/28	0/2/2/2
6	PSU	9	612	6	-	0/7/25/26	0/2/2/2
6	A2M	9	1678	6	-	2/5/27/28	0/3/3/3
3	BGH	5	3899	80,3	-	0/13/43/44	0/3/3/3
3	I4U	5	1659	3	-	0/9/29/30	0/2/2/2
3	OMC	5	3701	80,3	-	4/9/27/28	0/2/2/2
3	5MC	5	4335	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B8K	5	4690	3	-	0/11/41/42	0/3/3/3
3	B8T	5	4483	3	-	0/7/27/28	0/2/2/2
3	E7G	5	2297	3	-	1/9/39/40	0/3/3/3
3	PSU	5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	5	1524	3	-	1/5/27/28	0/3/3/3
3	B9H	5	2786	3	-	2/12/47/48	0/2/2/2
3	M7A	5	4564	3	-	0/7/37/38	0/3/3/3
3	OMC	5	3909	3	-	2/9/27/28	0/2/2/2
6	B8Q	9	1219	80,6	-	2/7/42/43	0/2/2/2
3	P7G	5	3880	3	-	4/10/40/41	0/3/3/3
3	PSU	5	4450	80,3	-	1/7/25/26	0/2/2/2
3	UR3	5	4530	3	-	2/7/25/26	0/2/2/2
3	OMU	5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	5	1683	3	-	0/7/25/26	0/2/2/2
3	B9B	5	1574	80,3	-	3/7/29/30	0/3/3/3
3	A2M	5	3785	3	-	4/5/27/28	0/3/3/3
3	OMG	5	4637	3	-	2/5/27/28	0/3/3/3
3	A2M	5	4523	80,3	-	0/5/27/28	0/3/3/3
6	OMG	9	644	6	-	2/5/27/28	0/3/3/3
3	PSU	5	1677	3	-	3/7/25/26	0/2/2/2
3	A2M	5	2401	80,3	-	0/5/27/28	0/3/3/3
6	B8N	9	1248	6	-	1/16/34/35	0/2/2/2
3	P4U	5	1348	3	-	4/10/29/30	0/2/2/2
3	B8H	5	4296	3	-	2/7/25/26	0/2/2/2
3	PSU	5	4403	3	-	3/7/25/26	0/2/2/2
3	B8H	5	3762	3	-	2/7/25/26	0/2/2/2
3	PSU	5	3715	3	-	0/7/25/26	0/2/2/2
3	E6G	5	4355	3	-	4/6/28/29	0/3/3/3
3	B8W	5	4129	3	-	2/5/27/28	0/3/3/3
3	MHG	5	4371	3	-	6/16/46/47	0/3/3/3
6	UR3	9	1830	6	-	2/7/25/26	0/2/2/2
3	B8W	5	4529	80,3	-	2/5/27/28	0/3/3/3
3	OMG	5	1625	80,3	-	1/5/27/28	0/3/3/3
6	4AC	9	1337	6	-	1/11/29/30	0/2/2/2
6	PSU	9	119	6	-	0/7/25/26	0/2/2/2
6	OMU	9	116	6	-	3/9/27/28	0/2/2/2
3	OMG	5	373	3	-	1/5/27/28	0/3/3/3
3	A2M	5	1534	80,3	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2MG	5	1517	3	-	0/5/27/28	0/3/3/3
3	A2M	5	1871	80,3	-	0/5/27/28	0/3/3/3
3	B8Q	5	1456	3	-	0/7/42/43	0/2/2/2
6	OMG	9	509	80,6	-	0/5/27/28	0/3/3/3
3	A2M	5	1326	3	-	2/5/27/28	0/3/3/3
6	MA6	9	1850	6	-	0/7/29/30	0/3/3/3
3	OMG	5	4370	3	-	1/5/27/28	0/3/3/3
3	PSU	5	4636	3	-	4/7/25/26	0/2/2/2
3	B8W	5	2380	3	-	4/5/27/28	0/3/3/3
3	B8W	5	4472	3	-	2/5/27/28	0/3/3/3
3	OMU	5	4306	3	-	1/9/27/28	0/2/2/2
3	5MC	5	4447	3	-	0/7/25/26	0/2/2/2
3	A2M	5	3718	3	-	1/5/27/28	0/3/3/3
6	A2M	9	166	6	-	2/5/27/28	0/3/3/3
3	PSU	5	3729	3	-	2/7/25/26	0/2/2/2
3	7MG	5	4550	3	-	0/7/37/38	0/3/3/3
3	PSU	5	4442	3	-	0/7/25/26	0/2/2/2
6	PSU	9	1081	6	-	1/7/25/26	0/2/2/2
3	OMG	5	4494	3	-	1/5/27/28	0/3/3/3
3	B8T	5	4671	3	-	1/7/27/28	0/2/2/2
6	PSU	9	1243	6	-	2/7/25/26	0/2/2/2
3	PSU	5	4500	3	-	3/7/25/26	0/2/2/2
6	A2M	9	1031	6	-	1/5/27/28	0/3/3/3
3	OMG	5	1522	3	-	0/5/27/28	0/3/3/3
3	OMC	5	2804	3	-	0/9/27/28	0/2/2/2
3	B9B	5	237	3	-	5/7/29/30	0/3/3/3
6	OMC	9	1703	6	-	2/9/27/28	0/2/2/2
3	E7G	5	1797	3	-	2/9/39/40	0/3/3/3
6	A2M	9	159	6	-	2/5/27/28	0/3/3/3
3	PSU	5	4628	3	-	0/7/25/26	0/2/2/2
3	1MA	5	1322	80,3	-	0/3/25/26	0/3/3/3
6	OMC	9	517	6	-	1/9/27/28	0/2/2/2
3	6MZ	5	4220	3	-	1/5/27/28	0/3/3/3
6	OMC	9	1710	6	-	0/9/27/28	0/2/2/2
3	B8H	5	1860	3	-	2/7/25/26	0/2/2/2
3	OMG	5	1316	3	-	1/5/27/28	0/3/3/3
3	A2M	5	4571	3	-	0/5/27/28	0/3/3/3
3	OMG	5	4623	3	-	0/5/27/28	0/3/3/3
6	MMX	9	568	6	-	4/9/44/45	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	5	4196	3	-	1/5/27/28	0/3/3/3
1	T6A	2	37	1	-	2/19/41/42	0/3/3/3
3	B8W	5	4185	3	-	2/5/27/28	0/3/3/3
3	7MG	5	1605	3	-	0/7/37/38	0/3/3/3
5	OMU	8	14	3,5	-	1/9/27/28	0/2/2/2
6	A2M	9	668	80,6	-	2/5/27/28	0/3/3/3
6	5MU	9	814	6	-	1/7/25/26	0/2/2/2
3	OMG	5	2050	3	-	0/5/27/28	0/3/3/3
3	PSU	5	3764	3	-	2/7/25/26	0/2/2/2
6	4AC	9	1842	6	-	0/11/29/30	0/2/2/2
3	OMG	5	2424	3	-	2/5/27/28	0/3/3/3
44	MLZ	m	72	44	-	4/7/8/10	-
3	5MC	5	3782	3	-	0/7/25/26	0/2/2/2
2	4AC	1	45	2	-	0/11/29/30	0/2/2/2
3	5MU	5	4083	3	-	0/7/25/26	0/2/2/2
3	OMC	5	2365	3	-	0/9/27/28	0/2/2/2
3	7MG	5	2522	3	-	0/7/37/38	0/3/3/3
3	2MG	5	4872	3	-	1/5/27/28	0/3/3/3
3	OMG	5	3792	3	-	2/5/27/28	0/3/3/3
3	PSU	5	2508	3	-	0/7/25/26	0/2/2/2
3	A2M	5	2363	80,3	-	1/5/27/28	0/3/3/3
3	OMG	5	2773	3	-	0/5/27/28	0/3/3/3
6	OMU	9	121	6	-	1/9/27/28	0/2/2/2
3	OMG	5	2364	3	-	2/5/27/28	0/3/3/3
6	M7A	9	1806	6	-	0/7/37/38	0/3/3/3
6	MA6	9	1851	6	-	2/7/29/30	0/3/3/3
3	UR3	5	1866	3	-	0/7/25/26	0/2/2/2
6	PSU	9	823	6	-	0/7/25/26	0/2/2/2
6	A2M	9	27	80,6	-	1/5/27/28	0/3/3/3
3	A2M	5	3723	3	-	1/5/27/28	0/3/3/3
3	P7G	5	1909	3	-	2/10/40/41	0/3/3/3
3	2MG	5	729	3	-	0/5/27/28	0/3/3/3
3	B8K	5	3897	3	-	3/11/41/42	0/3/3/3
3	OMC	5	4536	3	-	0/9/27/28	0/2/2/2
6	5MC	9	1374	6	-	0/7/25/26	0/2/2/2
3	A2M	5	3867	3	-	3/5/27/28	0/3/3/3
3	B9B	5	2754	80,3	-	4/7/29/30	0/3/3/3
3	1MA	5	4415	3	-	1/3/25/26	0/3/3/3
3	OMC	5	2422	80,3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	5	3825	3	-	0/5/27/28	0/3/3/3
3	PSU	5	1582	3	-	1/7/25/26	0/2/2/2
3	UR3	5	4597	3	-	0/7/25/26	0/2/2/2
6	A2M	9	484	6	-	0/5/27/28	0/3/3/3
3	A2M	5	398	3	-	2/5/27/28	0/3/3/3
3	OMG	5	4870	3	-	3/5/27/28	0/3/3/3
3	OMC	5	3869	3	-	0/9/27/28	0/2/2/2
9	MLZ	C	333	9	-	1/7/8/10	-
6	6MZ	9	1832	80,6	-	2/5/27/28	0/3/3/3
3	OMG	5	1883	3	-	1/5/27/28	0/3/3/3
6	OMC	9	174	6	-	1/9/27/28	0/2/2/2
3	OMC	5	2861	3	-	1/9/27/28	0/2/2/2
3	PSU	5	4531	3	-	2/7/25/26	0/2/2/2
3	I4U	5	4194	3	-	1/9/29/30	0/2/2/2
6	OMG	9	683	6	-	2/5/27/28	0/3/3/3
6	PSU	9	822	6	-	0/7/25/26	0/2/2/2

The worst 5 of 845 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4296	B8H	C6-C5	-16.56	1.11	1.35
3	5	1860	B8H	C6-C5	-16.55	1.11	1.35
3	5	3762	B8H	C6-C5	-16.37	1.11	1.35
3	5	4415	1MA	C2-N3	15.92	1.48	1.28
3	5	4296	B8H	C4-N3	-15.63	1.09	1.38

The worst 5 of 607 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2754	B9B	O6-C6-N1	-31.66	93.18	120.23
3	5	1574	B9B	O6-C6-N1	-30.30	94.34	120.23
3	5	237	B9B	O6-C6-N1	-29.61	94.93	120.23
6	9	1851	MA6	N1-C6-N6	-14.81	99.73	116.83
3	5	4564	M7A	C5-C6-N6	14.20	147.88	123.75

There are no chirality outliers.

5 of 178 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	CD-CE-NZ-CM

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Mol	Chain	Res	Type	Atoms
3	5	237	B9B	C5-C6-O6-C61
3	5	237	B9B	N1-C6-O6-C61
3	5	237	B9B	C3'-C4'-C5'-O5'
3	5	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 are monoatomic - leaving 1 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	$\# Z > 2$
81	MQ6	5	5294	-	40,42,42	1.27	5 (12%)	40,65,65	2.64	9 (22%)

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
81	MQ6	5	5294	-	-	14/26/73/73	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5294	MQ6	O37-C06	-3.48	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5294	MQ6	O14-C12	2.40	1.38	1.34
81	5	5294	MQ6	C30-C31	2.16	1.35	1.32
81	5	5294	MQ6	C17-C16	2.11	1.54	1.51
81	5	5294	MQ6	C24-C23	-2.05	1.49	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	5	5294	MQ6	O37-C06-C05	-12.42	89.02	108.88
81	5	5294	MQ6	O37-C06-C07	6.16	123.42	109.38
81	5	5294	MQ6	O14-C12-C06	4.87	120.18	111.24
81	5	5294	MQ6	C23-C22-C21	-3.49	111.78	119.35
81	5	5294	MQ6	C28-C29-N25	2.58	107.64	103.94

There are no chirality outliers.

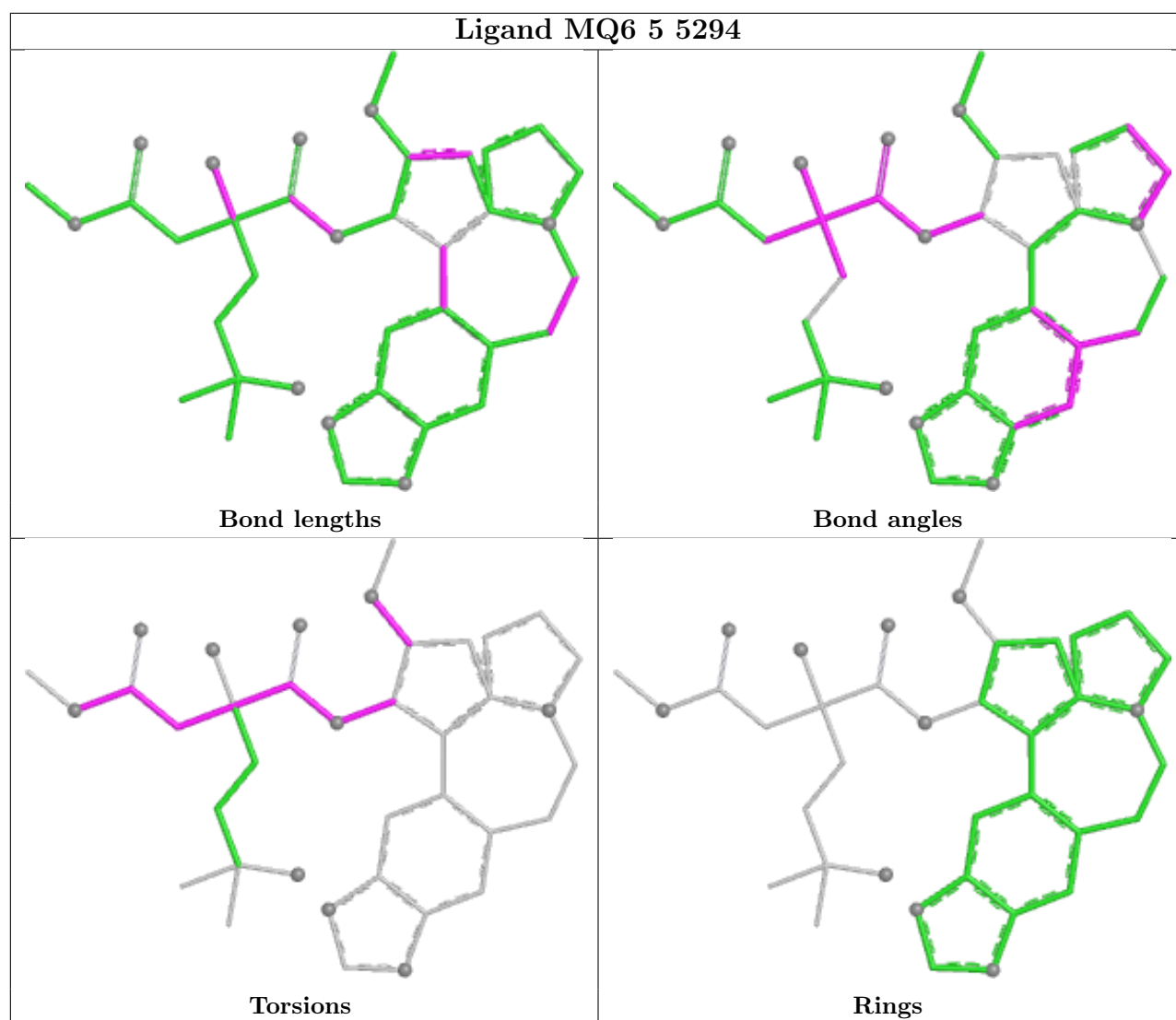
5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	5	5294	MQ6	C31-C15-O14-C12
81	5	5294	MQ6	C07-C06-C12-O13
81	5	5294	MQ6	C07-C06-C12-O14
81	5	5294	MQ6	C06-C12-O14-C15
81	5	5294	MQ6	C30-C31-O32-C33

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	5	24
6	9	11

The worst 5 of 35 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.43
1	5	1252:C	O3'	1271:G	P	35.31
1	5	1219:G	O3'	1233:G	P	20.31
1	5	4101:C	O3'	4107:G	P	17.50
1	5	1407:G	O3'	1410:C	P	17.49

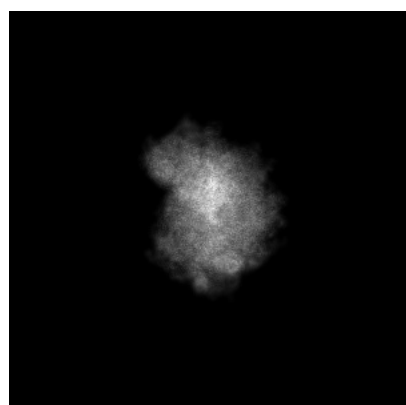
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26445. These allow visual inspection of the internal detail of the map and identification of artifacts.

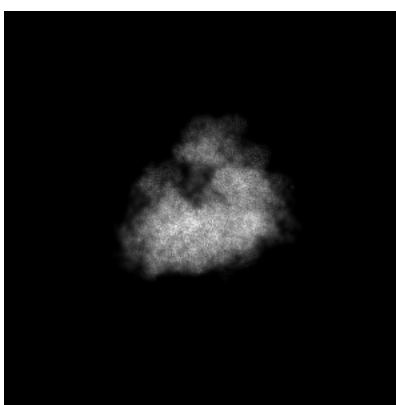
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

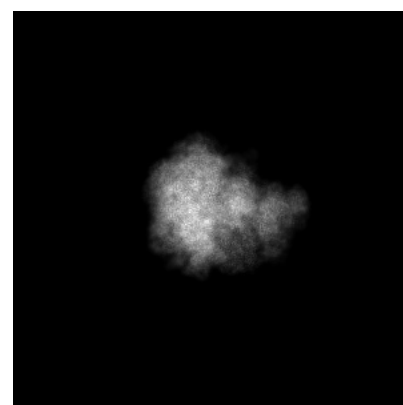
6.1.1 Primary map



X



Y

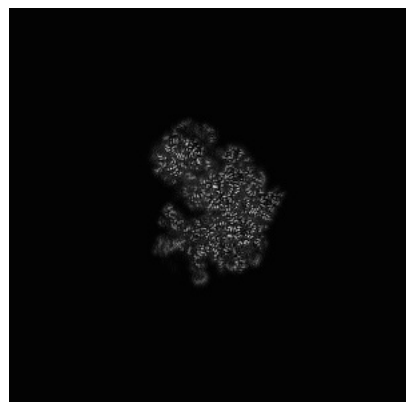


Z

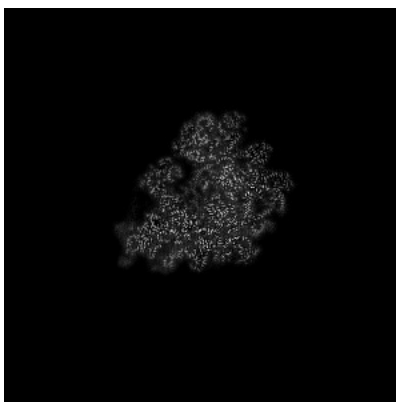
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

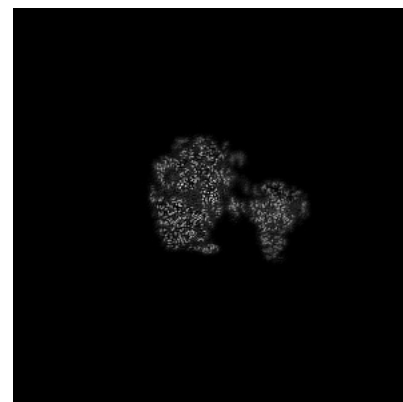
6.2.1 Primary map



X Index: 240



Y Index: 240

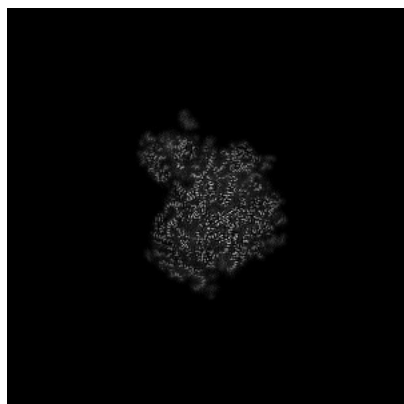


Z Index: 240

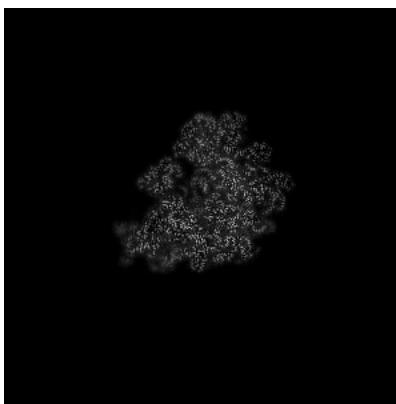
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

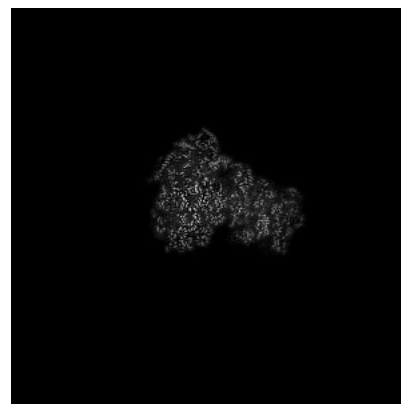
6.3.1 Primary map



X Index: 221



Y Index: 242

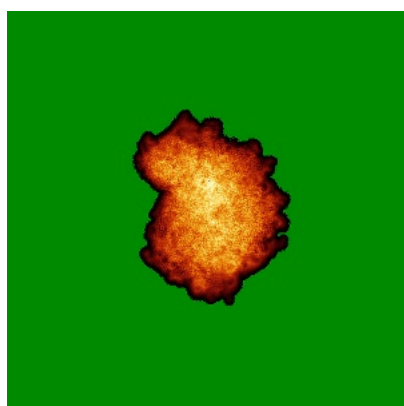


Z Index: 255

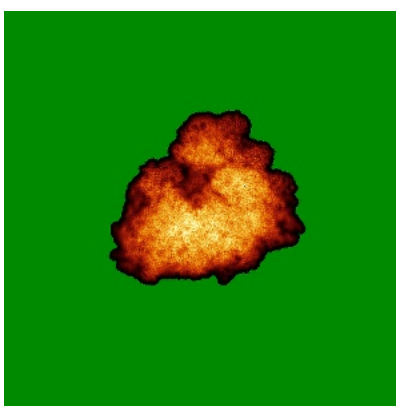
The images above show the largest variance slices of the map in three orthogonal directions.

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

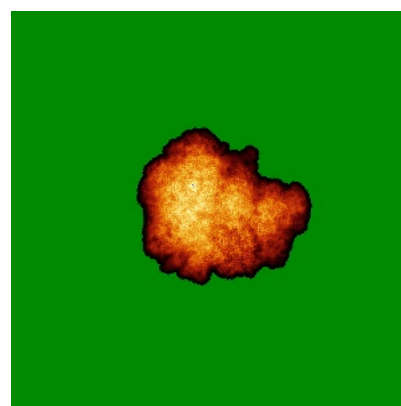
6.4.1 Primary map



X



Y

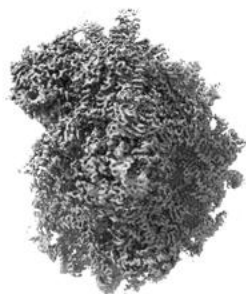


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

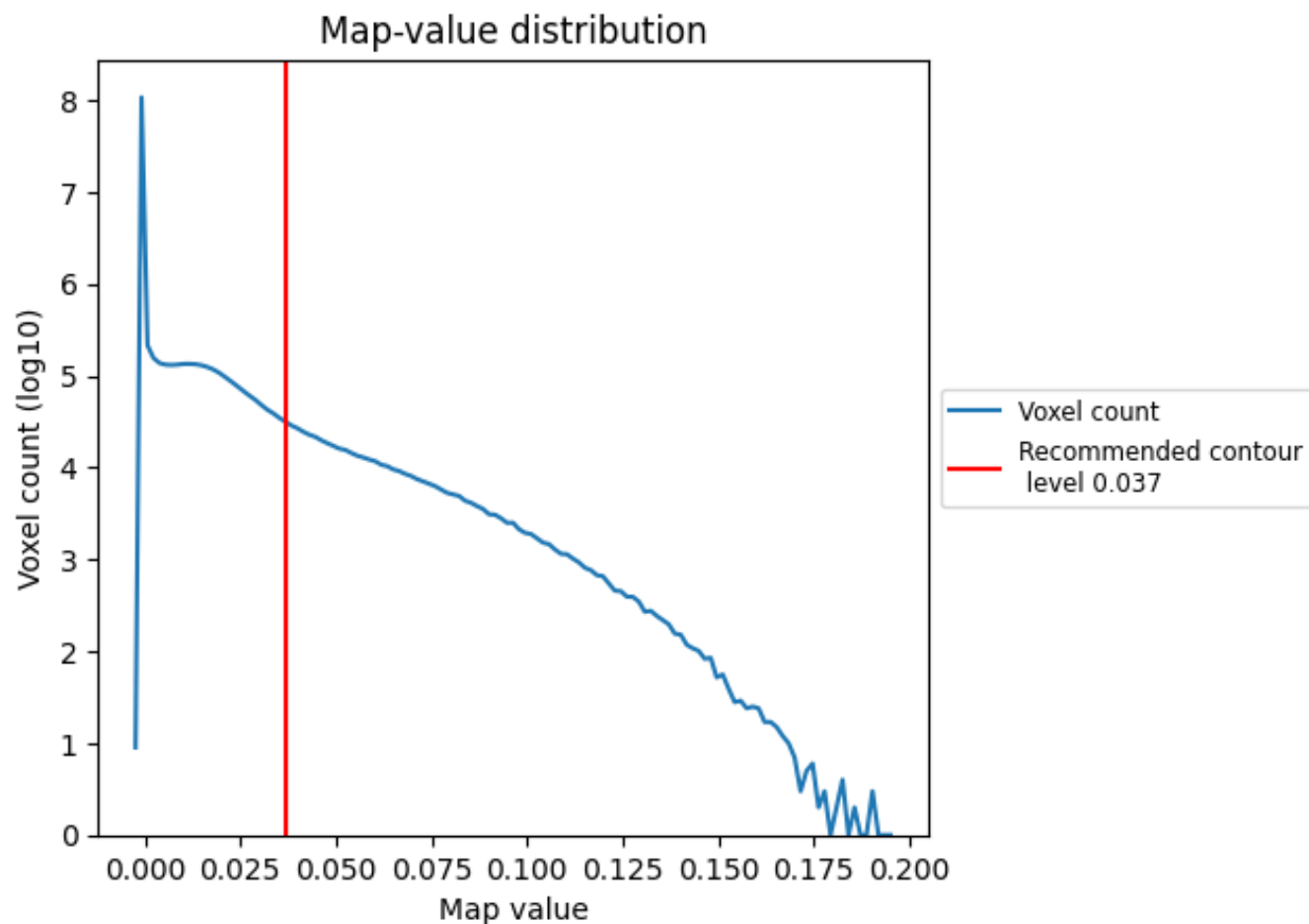
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

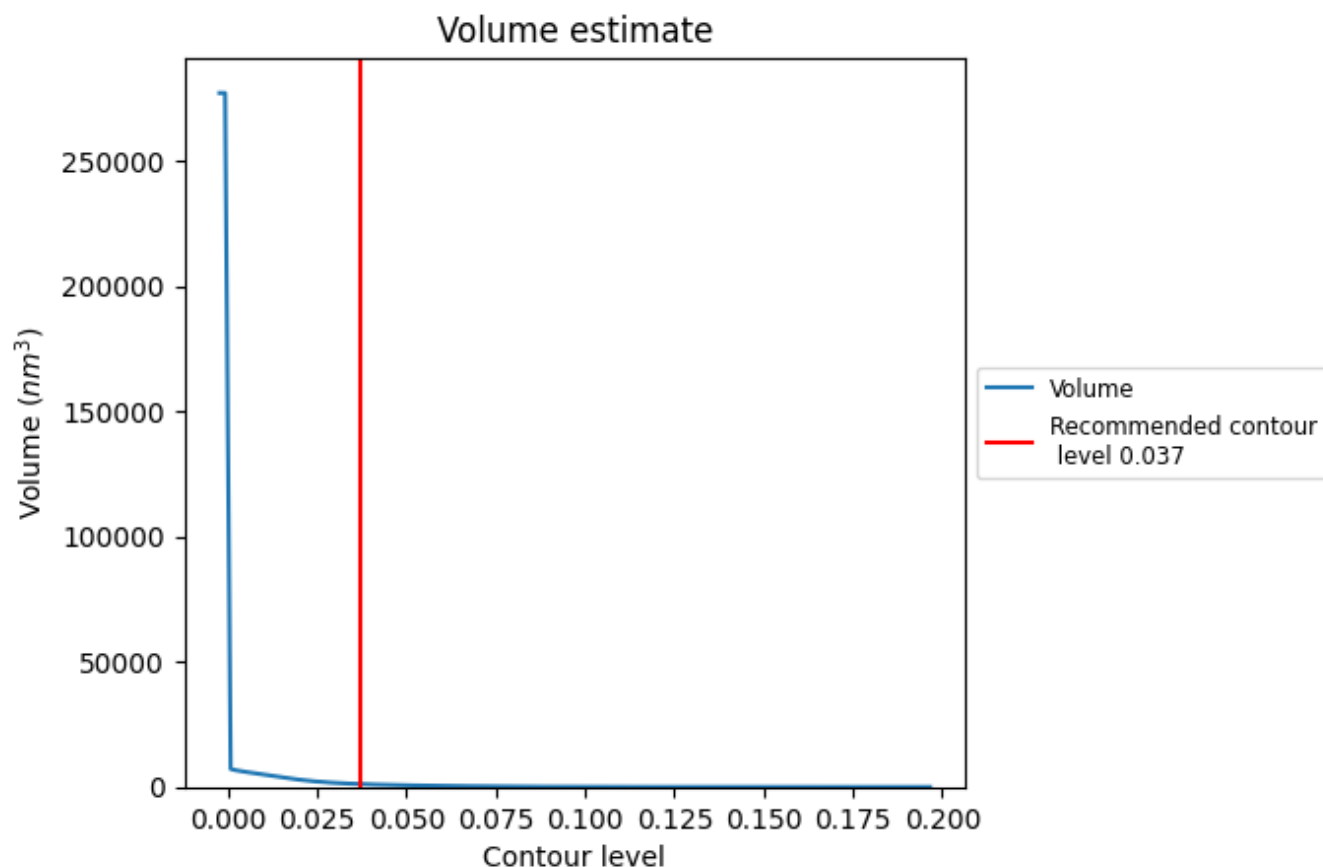
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

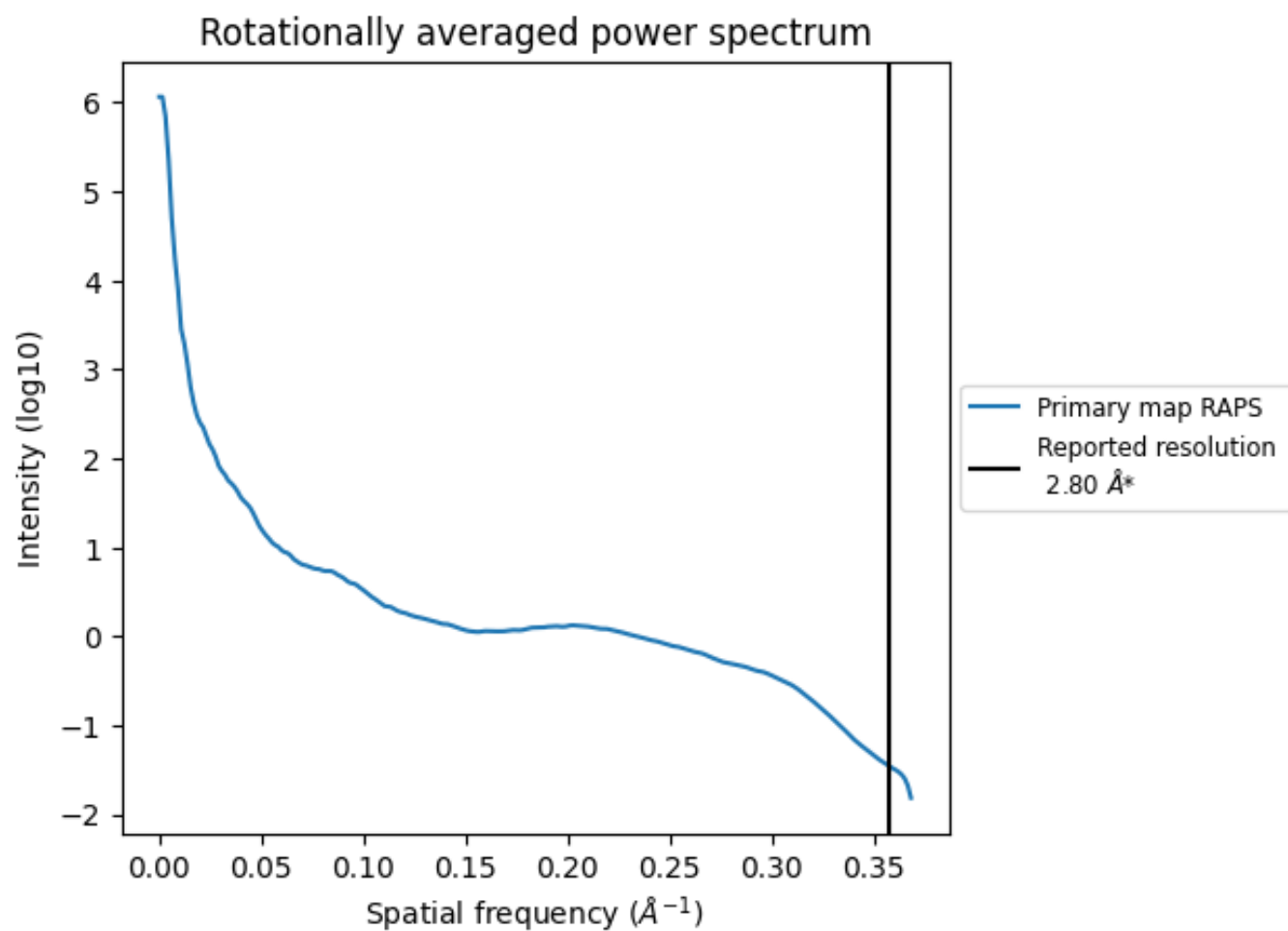
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1162 nm^3 ; this corresponds to an approximate mass of 1050 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 0.357 Å⁻¹

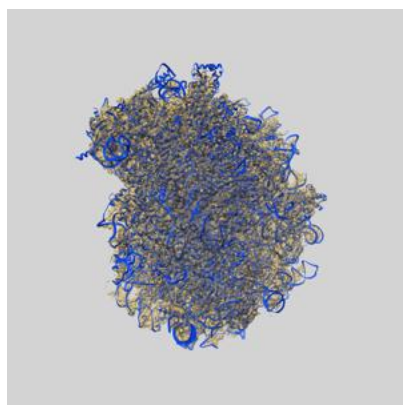
8 Fourier-Shell correlation

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

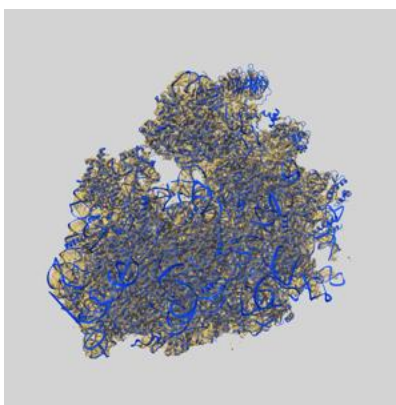
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26445 and PDB model 7UCK. Per-residue inclusion information can be found in section [3](#) on page [21](#).

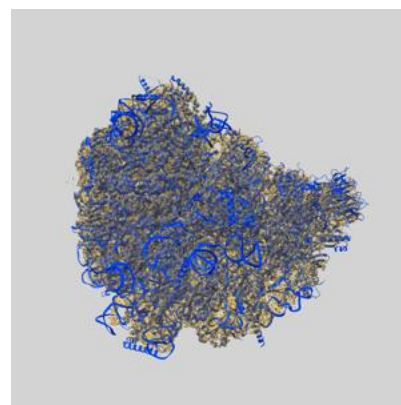
9.1 Map-model overlay [i](#)



X



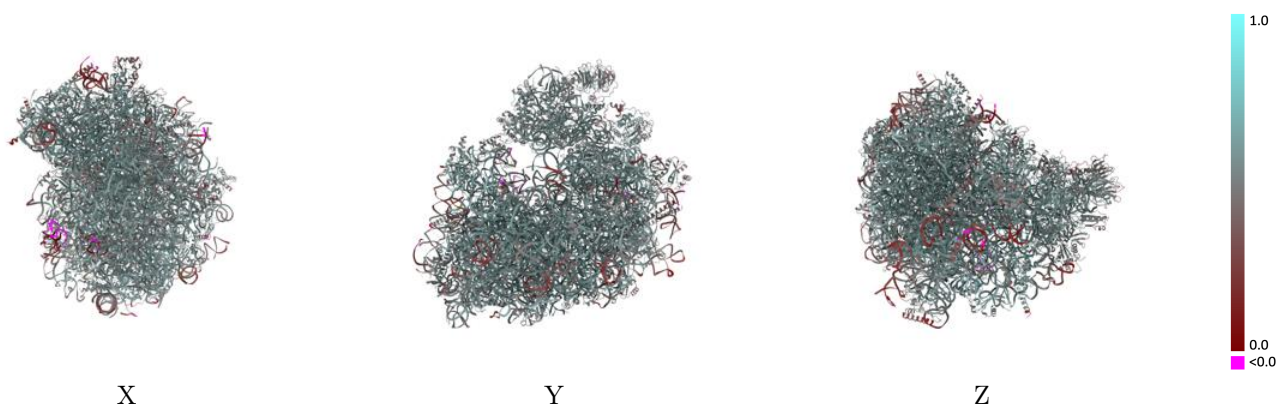
Y



Z

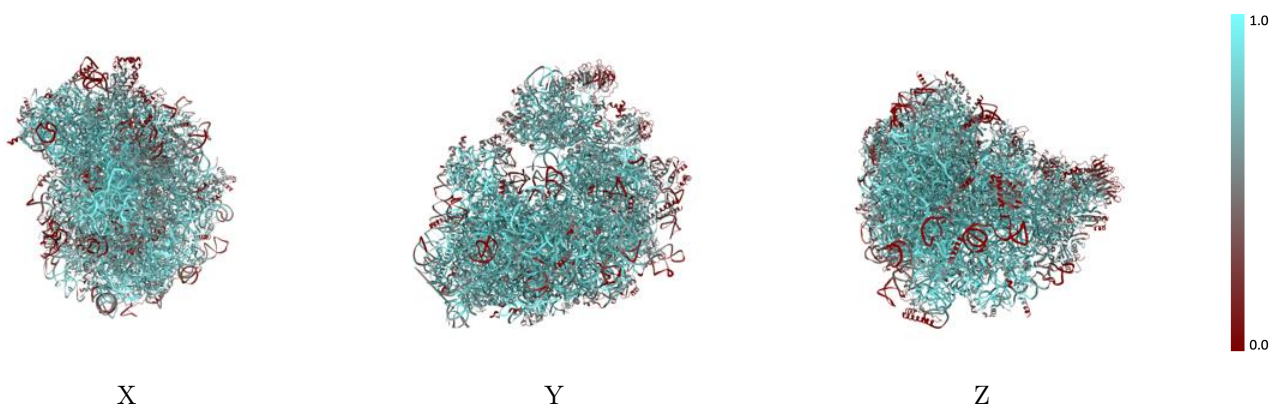
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



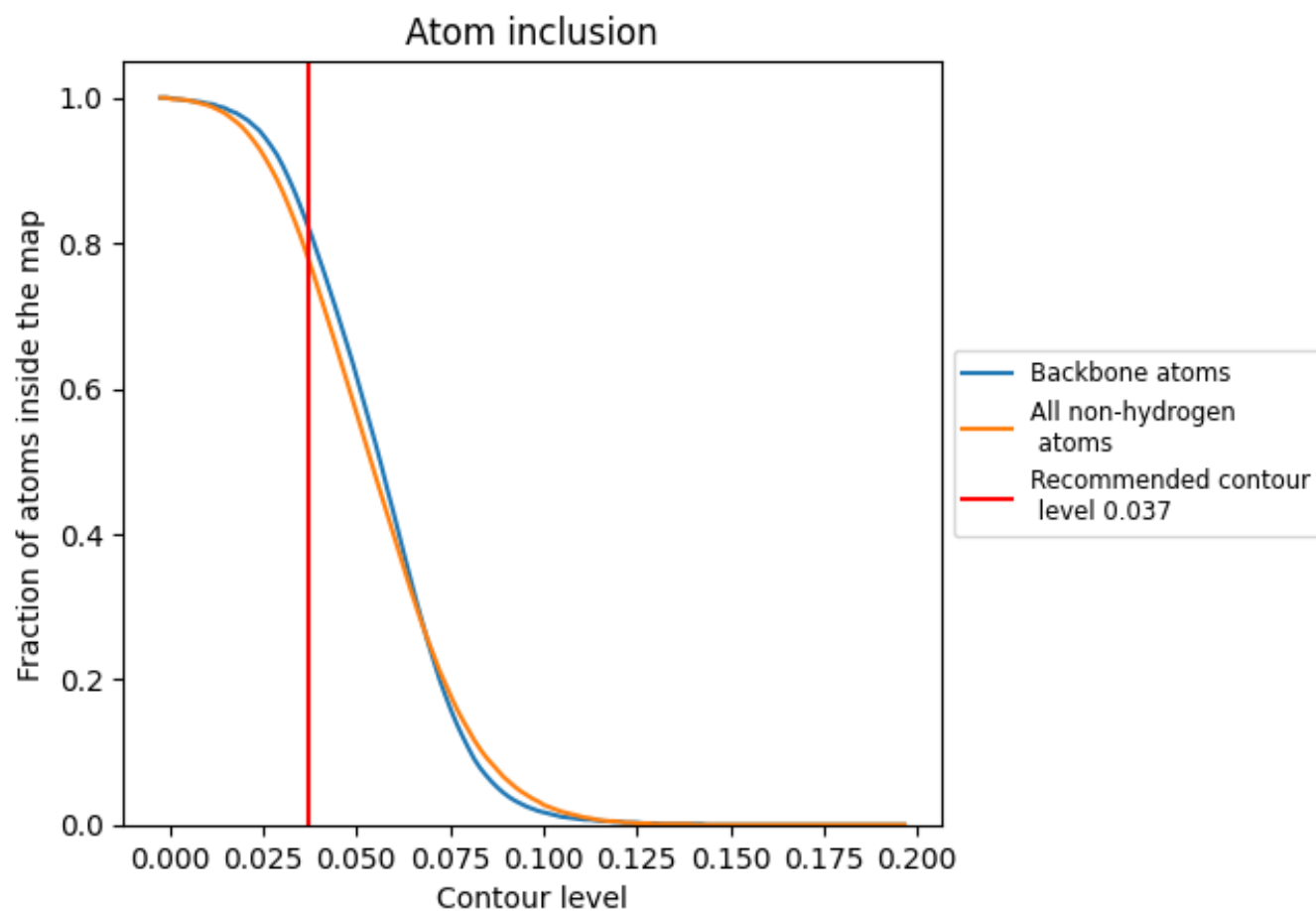
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.037).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5480
1	 0.9170	 0.5710
2	 0.4110	 0.5020
5	 0.8450	 0.5480
7	 0.9200	 0.5820
8	 0.8760	 0.5650
9	 0.8550	 0.5460
A	 0.8750	 0.5890
AA	 0.5810	 0.5490
Aa	 0.7760	 0.5540
B	 0.7290	 0.5740
BB	 0.6570	 0.5410
Bb	 0.5670	 0.5220
C	 0.8220	 0.5720
CC	 0.7270	 0.5640
Cc	 0.5130	 0.4950
D	 0.6320	 0.5460
DD	 0.5910	 0.5160
Dd	 0.8390	 0.5710
E	 0.7140	 0.5420
EE	 0.7840	 0.5690
Ee	 0.5750	 0.5190
F	 0.8690	 0.5750
FF	 0.6510	 0.5330
G	 0.5690	 0.5200
GG	 0.5460	 0.4980
Gg	 0.3380	 0.4730
H	 0.6070	 0.5480
HH	 0.3700	 0.4780
I	 0.6420	 0.5480
II	 0.7610	 0.5540
J	 0.5230	 0.5080
JJ	 0.7540	 0.5570
KK	 0.5340	 0.4910
L	 0.6920	 0.5400








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Chain	Atom inclusion	Q-score
LL	 0.8160	 0.5770
M	 0.7560	 0.5510
N	 0.9090	 0.5940
NN	 0.7920	 0.5700
O	 0.8140	 0.5680
OO	 0.7130	 0.5460
P	 0.7850	 0.5790
PP	 0.5230	 0.5030
Q	 0.8700	 0.5930
QQ	 0.7080	 0.5370
R	 0.7610	 0.5420
RR	 0.4210	 0.5000
S	 0.8200	 0.5780
SS	 0.5770	 0.5160
T	 0.7650	 0.5560
TT	 0.6660	 0.5380
U	 0.5400	 0.5040
UU	 0.5030	 0.4950
V	 0.7220	 0.5730
VV	 0.5920	 0.5590
W	 0.5160	 0.4740
WW	 0.8260	 0.5840
X	 0.6660	 0.5450
XX	 0.7820	 0.5750
Y	 0.6420	 0.5410
YY	 0.6530	 0.5350
Z	 0.6530	 0.5460
ZZ	 0.4490	 0.5020
a	 0.8650	 0.6000
b	 0.6970	 0.5320
c	 0.6910	 0.5390
d	 0.6980	 0.5630
e	 0.8580	 0.5920
f	 0.8930	 0.5900
g	 0.8020	 0.5640
h	 0.6180	 0.5280
i	 0.6680	 0.5350
j	 0.9140	 0.5980
k	 0.4520	 0.5000
l	 0.8270	 0.5740
m	 0.7100	 0.5630
n	 0.9130	 0.5840

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Chain	Atom inclusion	Q-score
o	 0.7530	 0.5730
p	 0.8010	 0.5630
r	 0.8140	 0.5810