Full wwPDB EM Validation Report (i)

May 31, 2022 – 02:32 am BST

PDB ID	:	7Q08
EMDB ID	:	EMD-13741
Title	:	Structure of Candida albicans 80S ribosome in complex with cycloheximide
Authors	:	Zgadzay, Y.; Kolosova, O.; Stetsenko, A.; Jenner, L.; Guskov, A.; Yusupova, G.; Yusupov, M.
Deposited on	:	2021-10-14
Resolution	:	2.56 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

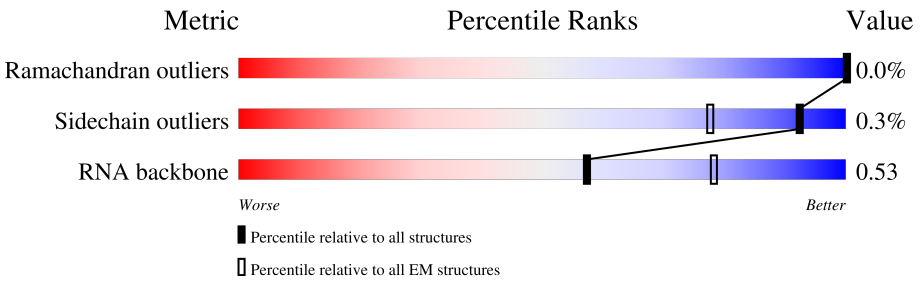
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.56 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1	3359	78% 17%
2	3	121	94% 6%
3	4	158	84% 16%
4	j	254	98%
5	k	389	99%
6	l	363	99%
7	m	298	98%
8	n	176	88% 12%

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Mol	Chain	Length	Quality of chain
9	o	241	97%
10	p	262	91% 9%
11	q	191	99%
12	r	220	95% 5%
13	s	174	98%
14	t	202	98%
15	u	131	98%
16	v	204	100%
17	w	200	100%
18	x	185	93% 7%
19	y	186	99%
20	z	190	94% 6%
21	0	172	99%
22	2	160	99%
23	5	124	81% 17%
24	6	137	96%
25	7	155	40% 59%
26	8	142	85% 15%
27	9	127	98%
28	AA	136	99%
29	AB	149	99%
30	AC	63	100%
31	AD	106	91% 9%
32	AE	112	97%
33	AF	131	95% 5%

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Mol	Chain	Length	Quality of chain
34	AG	107	99%
35	AH	122	92% 8%
36	AI	120	99%
37	AJ	99	98%
38	AK	90	94%
39	AL	78	99%
40	AM	51	98%
41	AN	52	100%
42	AO	25	92%
43	AP	106	96%
44	AQ	92	99%
45	i	267	16% 42% 58%
46	A	1787	69% 26% 5%
47	B	261	80% 20%
48	C	256	82% 16%
49	D	249	86% 13%
50	E	251	14% 88% 11%
51	F	262	99%
52	G	225	13% 92% 8%
53	H	236	5% 96%
54	I	186	11% 97%
55	J	206	11% 98%
56	K	189	5% 94% 6%
57	L	118	14% 78% 21%
58	M	155	5% 90% 9%

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Mol	Chain	Length	Quality of chain
59	N	143	62% 81% 19%
60	O	151	99%
61	P	132	95%
62	Q	142	31% 83% 17%
63	R	142	99%
64	S	137	12% 91% 9%
65	T	145	21% 98%
66	U	145	9% 97%
67	V	119	9% 82% 16%
68	W	87	100%
69	X	130	98%
70	Y	145	99%
71	Z	135	7% 98%
72	a	105	29% 69% 31%
73	b	119	84% 16%
74	c	82	5% 99%
75	d	67	24% 93% 7%
76	e	56	98%
77	f	63	11% 89% 11%
78	g	193	26% 36% 64%
79	h	317	25% 97%

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 199280 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3209	68595	30642	12317	22427	3209	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1153	463	842	121	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	585	1110	158	0	0

- Molecule 4 is a protein called Ribosomal 60S subunit protein L2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	j	249	1894	1185	377	330	2	1	0

- Molecule 5 is a protein called Ribosomal 60S subunit protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	k	386	3084	1955	584	538	7	1	0

- Molecule 6 is a protein called Ribosomal 60S subunit protein L4B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	l	361	2751	1729	529	490	3	0	0

- Molecule 7 is a protein called Ribosomal 60S subunit protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	m	292	2394	1526	416	450	2	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	n	155	1237	794	226	217	1	0

- Molecule 9 is a protein called Ribosomal 60S subunit protein L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	o	234	1893	1213	348	331	1	1	0

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	p	238	1839	1175	327	334	3	0	0

- Molecule 11 is a protein called Ribosomal 60S subunit protein L9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	q	190	1519	958	276	281	4	0	0

- Molecule 12 is a protein called Ribosomal 60S subunit protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	r	208	1689	1069	322	291	7	0	0

- Molecule 13 is a protein called Ribosomal 60S subunit protein L11B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	s	172	1385	864	262	255	4	1	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	t	200	1610	1009	318	283	0	0

- Molecule 15 is a protein called Ribosomal 60S subunit protein L14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	u	130	1029	660	193	175	1	0	0

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	v	203	1713	1075	356	280	2	0	0

- Molecule 17 is a protein called Ribosomal 60S subunit protein L16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	w	199	1590	1025	294	269	2	0	0

- Molecule 18 is a protein called Ribosomal 60S subunit protein L17B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	x	172	1375	850	279	246	0	0

- Molecule 19 is a protein called Ribosomal 60S subunit protein L18A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	y	185	1478	930	302	246	3	0

- Molecule 20 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	z	179	1462	904	311	244	3	1	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	0	171	1442	933	262	244	3	2	0

- Molecule 22 is a protein called Ribosomal 60S subunit protein L21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	2	159	1276	807	244	223	2	2	0

- Molecule 23 is a protein called Ribosomal 60S subunit protein L22B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	5	103	848	553	139	156	2	0

- Molecule 24 is a protein called Ribosomal 60S subunit protein L23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	6	131	986	621	186	171	8	1	0

- Molecule 25 is a protein called Ribosomal 60S subunit protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	7	63	524	334	103	86	1	0	0

- Molecule 26 is a protein called Ribosomal 60S subunit protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	8	121	974	622	175	176	1	0	0

- Molecule 27 is a protein called Ribosomal 60S subunit protein L26B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	9	126	989	618	190	181	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AA	135	1087	705	197	183	2	0	0

- Molecule 29 is a protein called Ribosomal 60S subunit protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AB	148	1170	741	231	197	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AC	63	509	317	109	82	1	1	0

- Molecule 31 is a protein called Ribosomal 60S subunit protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AD	96	729	469	121	137	2	0	0

- Molecule 32 is a protein called Ribosomal 60S subunit protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AE	109	889	562	167	158	2	0	0

- Molecule 33 is a protein called Ribosomal 60S subunit protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	AF	125	1015	649	197	168	1	1	0

- Molecule 34 is a protein called Ribosomal 60S subunit protein L33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AG	106	867	558	166	142	1	3	0

- Molecule 35 is a protein called Ribosomal 60S subunit protein L34B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AH	112	913	567	188	154	4	4	0

- Molecule 36 is a protein called Ribosomal 60S subunit protein L35A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	AI	119	990	629	195	166	1	0

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AJ	98	772	481	158	131	2	1	0

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AK	86	677	413	148	110	6	0	0

- Molecule 39 is a protein called Ribosomal 60S subunit protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	AL	77	623	398	116	109	1	0

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	AM	50	446	280	100	66	1	0

- Molecule 41 is a protein called Rpl40bp.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AN	52	427	265	89	67	6	1	0

- Molecule 42 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AO	24	227	138	61	27	1	0	0

- Molecule 43 is a protein called Ribosomal 60S subunit protein L42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	AP	103	843	533	168	137	5	2	0

- Molecule 44 is a protein called Ribosomal 60S subunit protein L43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	AQ	91	698	430	140	124	4	0	0

- Molecule 45 is a protein called HABP4_PAI-RBP1 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	i	113	853	512	155	186	0	0

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	A	1692	36083	16130	6412	11849	1692	0	0

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	B	208	1627	1041	284	297	5	0	0

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	C	214	1724	1094	313	313	4	0	0

- Molecule 49 is a protein called Ribosomal 40S subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	D	216	1620	1033	287	295	5	0	0

- Molecule 50 is a protein called Ribosomal 40S subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	E	223	1707	1087	311	305	4	0	0

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	F	260	2055	1306	386	358	5	0	0

- Molecule 52 is a protein called Ribosomal 40S subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	G	206	1614	1008	301	301	4	0	0

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	H	226	1820	1133	351	330	6	0	0

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	I	182	1466	939	264	263	0	0

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	J	203	1579	973	322	283	1	0	0

- Molecule 56 is a protein called Ribosomal 40S subunit protein S9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	K	178	1453	918	286	248	1	0	0

- Molecule 57 is a protein called Ribosomal 40S subunit protein S10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	L	93	783	511	129	142	1	0	0

- Molecule 58 is a protein called Ribosomal 40S subunit protein S11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	M	141	1129	722	212	192	3	0	0

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	N	116	885	550	158	172	5	0	0

- Molecule 60 is a protein called Ribosomal 40S subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	O	150	1187	757	219	210	1	0	0

- Molecule 61 is a protein called Ribosomal 40S subunit protein S14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	P	127	942	579	186	174	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	119	IAS	ASP	modified residue	UNP A0A1D8PDT3

- Molecule 62 is a protein called Ribosomal 40S subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	Q	118	935	598	169	162	6	0	0

- Molecule 63 is a protein called Ribosomal 40S subunit protein S16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	R	140	1091	700	198	192	1	0	0

- Molecule 64 is a protein called Ribosomal 40S subunit protein S17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	S	125	1002	631	184	186	1	0	0

- Molecule 65 is a protein called Ribosomal 40S subunit protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	T	142	1169	733	228	205	3	0	0

- Molecule 66 is a protein called Ribosomal 40S subunit protein S19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	U	141	1100	689	210	200	1	0	0

- Molecule 67 is a protein called Ribosomal 40S subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	V	100	790	499	146	143	2	0	0

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	W	87	676	415	126	133	2	0	0

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	X	129	1032	655	191	183	3	0	0

- Molecule 70 is a protein called Ribosomal 40S subunit protein S23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Y	143	1110	701	219	188	2	0	0

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
71	Z	132	1072	670	216	186	0	0

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	a	72	578	369	103	106	0	0

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	b	100	799	494	169	130	6	0	0

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	c	81	614	383	110	114	7	0	0

- Molecule 75 is a protein called Ribosomal 40S subunit protein S28B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	d	62	487	299	98	88	2	0	0

- Molecule 76 is a protein called Ribosomal 40S subunit protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	e	55	454	281	94	75	4	0	0

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	f	56	444	278	89	75	2	0	0

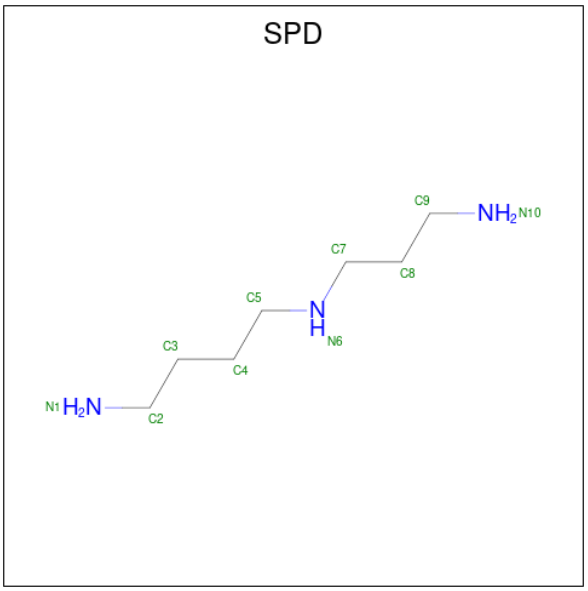
- Molecule 78 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	g	70	574	362	113	93	6	0	0

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

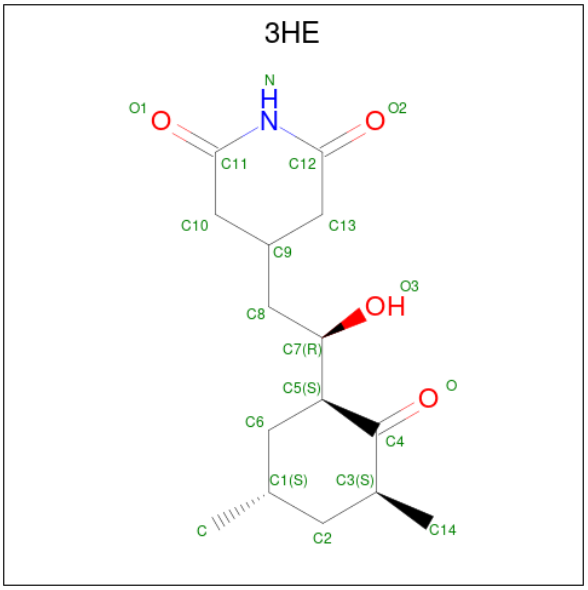
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	h	311	2398	1519	412	462	5	0	0

- Molecule 80 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
80	1	1	10	7	3	0

- Molecule 81 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
81	1	1	20	15	1	4	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

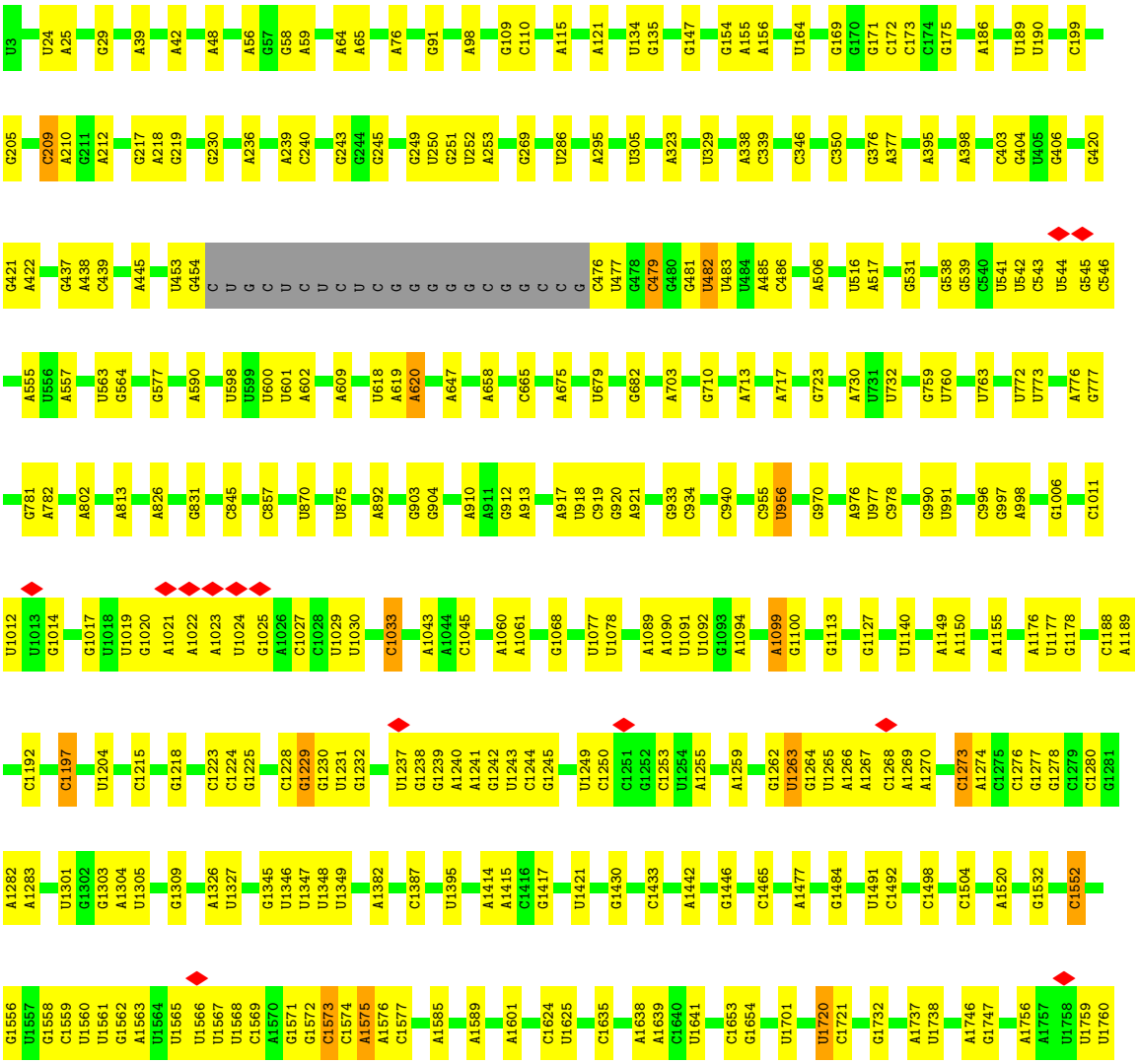
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	AK	1	1	1	0
82	AN	1	1	1	0
82	AP	1	1	1	0
82	AQ	1	1	1	0
82	b	1	1	1	0
82	c	1	1	1	0
82	e	1	1	1	0
82	g	1	1	1	0

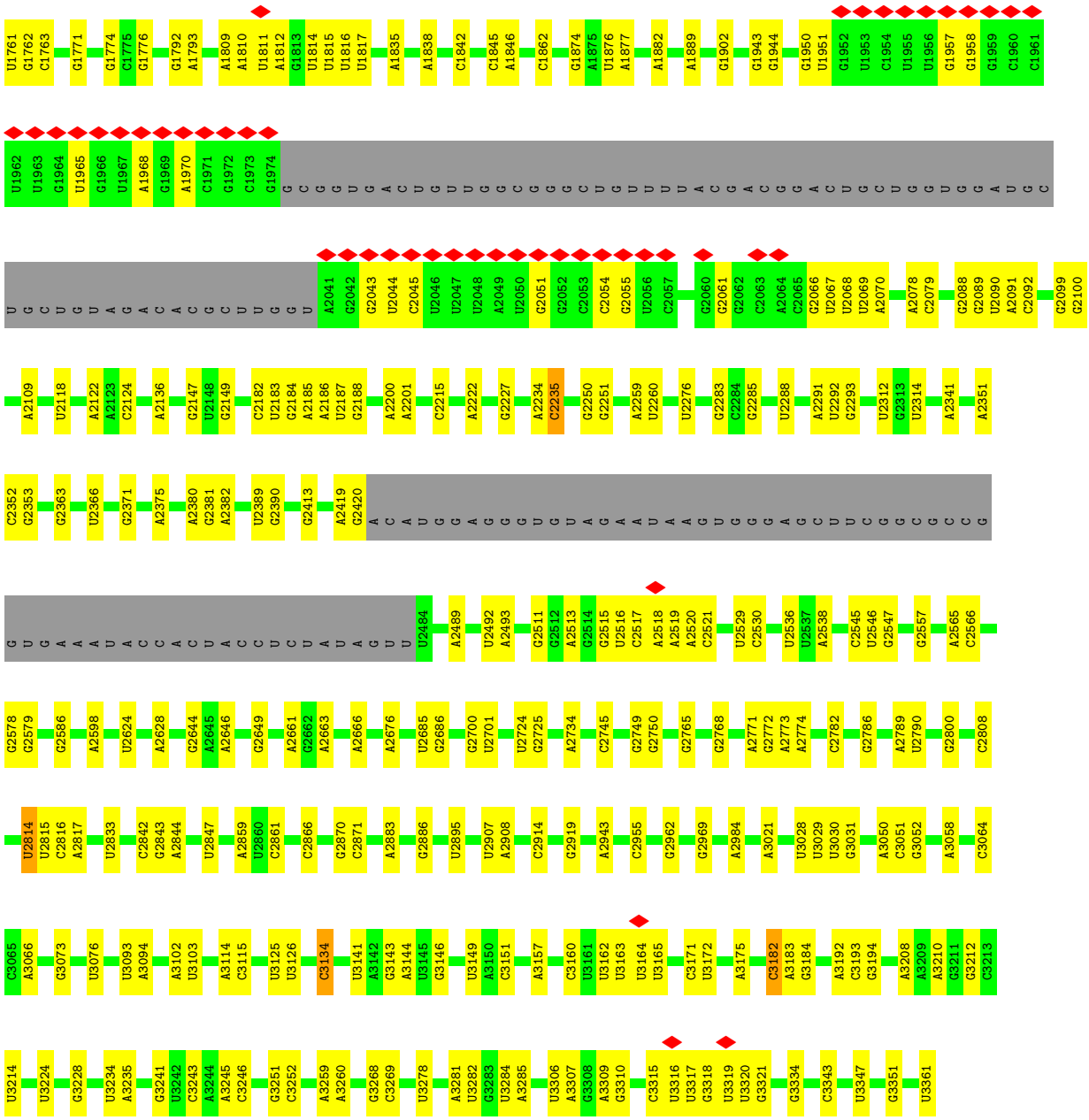
3 Residue-property plots (i)

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: 25S ribosomal RNA

Chain 1:



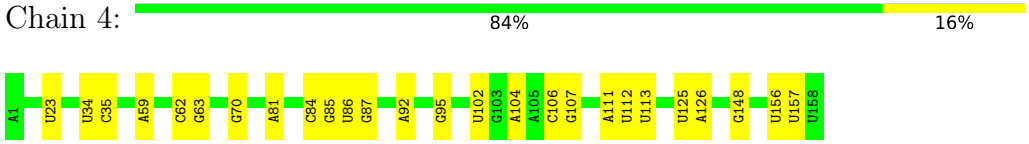


- Molecule 2: 5S ribosomal RNA

Chain 3:

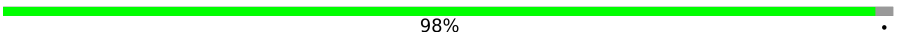
- Molecule 3: 5.8S ribosomal RNA

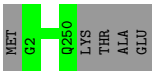
Chain 4:



• Molecule 4: Ribosomal 60S subunit protein L2A

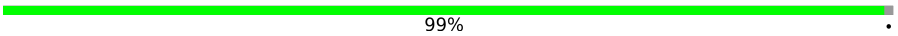
Chain j:

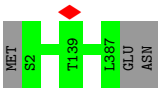




• Molecule 5: Ribosomal 60S subunit protein L3

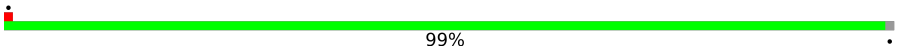
Chain k:

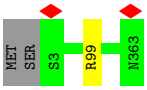




• Molecule 6: Ribosomal 60S subunit protein L4B

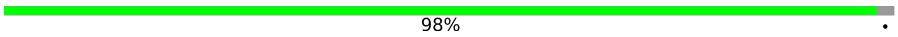
Chain l:

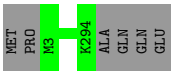




• Molecule 7: Ribosomal 60S subunit protein L5

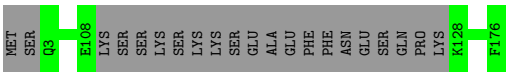
Chain m:





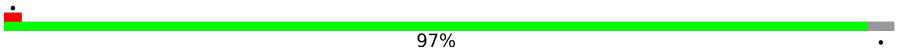
• Molecule 8: 60S ribosomal protein L6

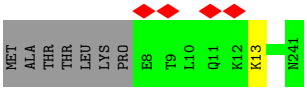
Chain n:



• Molecule 9: Ribosomal 60S subunit protein L7A

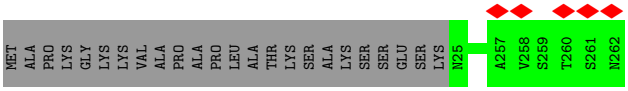
Chain o:





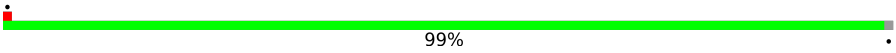
• Molecule 10: 60S ribosomal protein L8

Chain p:



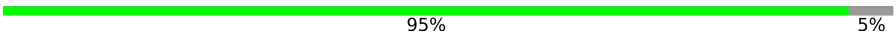
• Molecule 11: Ribosomal 60S subunit protein L9B

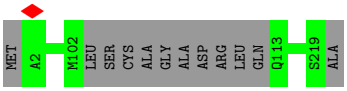
Chain q:



• Molecule 12: Ribosomal 60S subunit protein L10

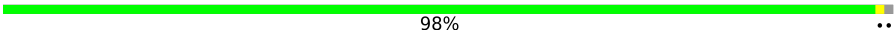
Chain r:





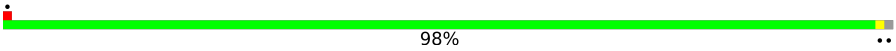
• Molecule 13: Ribosomal 60S subunit protein L11B

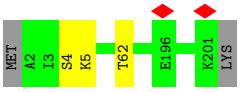
Chain s:



• Molecule 14: 60S ribosomal protein L13

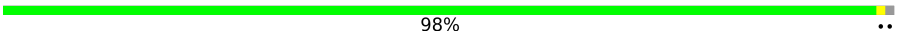
Chain t:





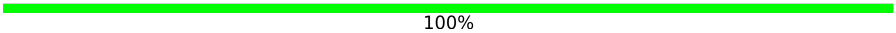
• Molecule 15: Ribosomal 60S subunit protein L14B

Chain u:



• Molecule 16: Ribosomal protein L15

Chain v:

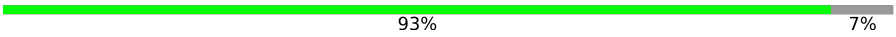


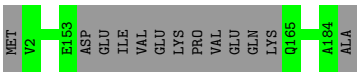
• Molecule 17: Ribosomal 60S subunit protein L16A

Chain w:

• Molecule 18: Ribosomal 60S subunit protein L17B

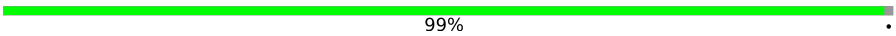
Chain x:





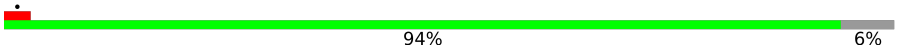
• Molecule 19: Ribosomal 60S subunit protein L18A

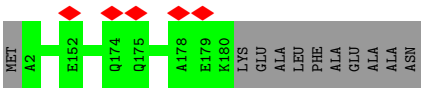
Chain y:



• Molecule 20: Ribosomal protein L19

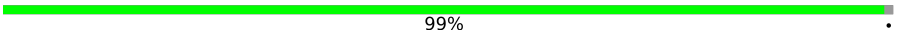
Chain z:





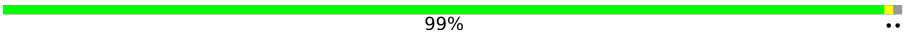
• Molecule 21: 60S ribosomal protein L20

Chain 0:



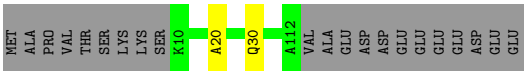
• Molecule 22: Ribosomal 60S subunit protein L21A

Chain 2:



• Molecule 23: Ribosomal 60S subunit protein L22B

Chain 5:

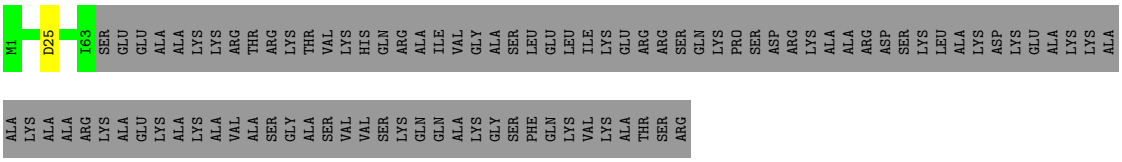


• Molecule 24: Ribosomal 60S subunit protein L23B

Chain 6: 96%

• Molecule 25: Ribosomal 60S subunit protein L24A

Chain 7: 40% 59%

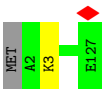


• Molecule 26: Ribosomal 60S subunit protein L25

Chain 8: 85% 15%

• Molecule 27: Ribosomal 60S subunit protein L26B

Chain 9: 98%



• Molecule 28: 60S ribosomal protein L27

Chain AA: 99%

• Molecule 29: Ribosomal 60S subunit protein L28

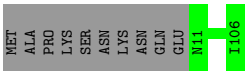
Chain AB: 99%

• Molecule 30: 60S ribosomal protein L29

Chain AC: 100%

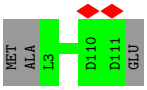
• Molecule 31: Ribosomal 60S subunit protein L30

Chain AD: 91% 9%



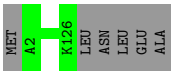
• Molecule 32: Ribosomal 60S subunit protein L31B

Chain AE: 97%



• Molecule 33: Ribosomal 60S subunit protein L32

Chain AF: 95% 5%

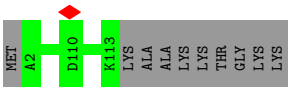


• Molecule 34: Ribosomal 60S subunit protein L33A

Chain AG: 99%

• Molecule 35: Ribosomal 60S subunit protein L34B

Chain AH: 92% 8%



• Molecule 36: Ribosomal 60S subunit protein L35A

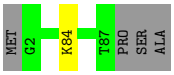
Chain AI: 99%

• Molecule 37: 60S ribosomal protein L36

Chain AJ: 98%

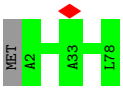
• Molecule 38: Ribosomal protein L37

Chain AK: 94%



• Molecule 39: Ribosomal 60S subunit protein L38

Chain AL: 99%



• Molecule 40: 60S ribosomal protein L39

Chain AM: 98%

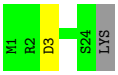
• Molecule 41: Rpl40bp

Chain AN: 100%

There are no outlier residues recorded for this chain.

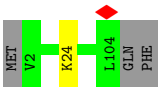
• Molecule 42: 60S ribosomal protein eL41

Chain AO: 92%



• Molecule 43: Ribosomal 60S subunit protein L42A

Chain AP: 96%

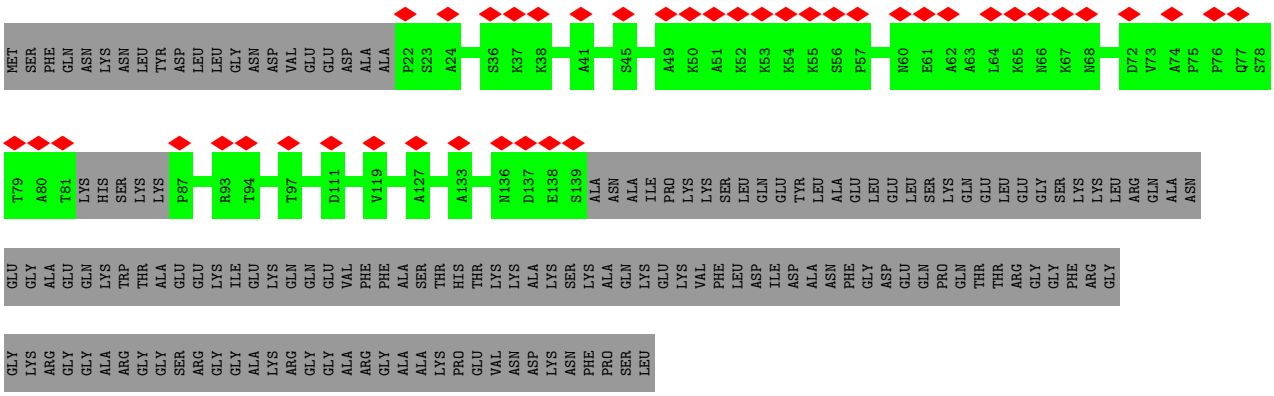


• Molecule 44: Ribosomal 60S subunit protein L43A

Chain AQ: 99%

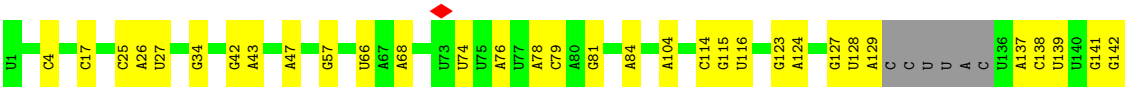
• Molecule 45: HABP4_PAI-RBP1 domain-containing protein

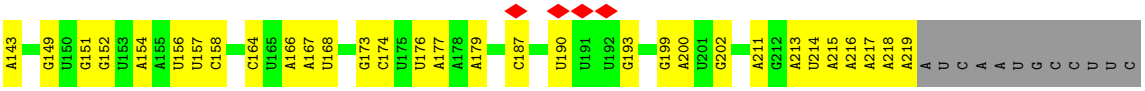
Chain i:

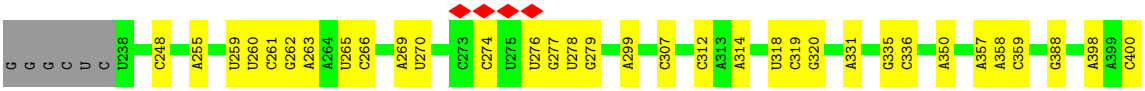


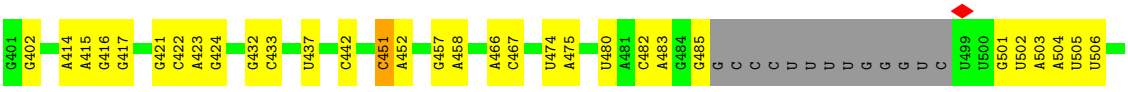
- Molecule 46: 18S ribosomal RNA

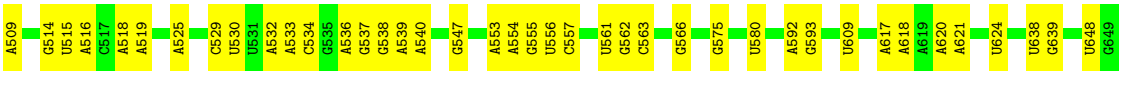
Chain A:

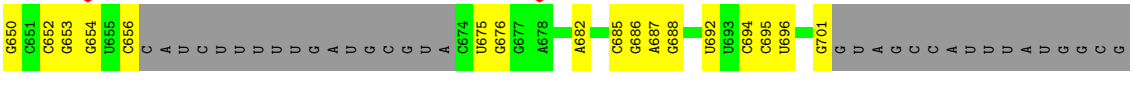


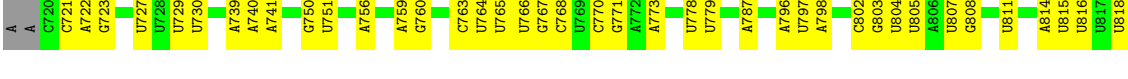


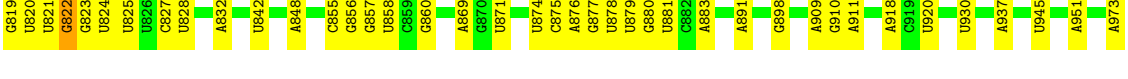


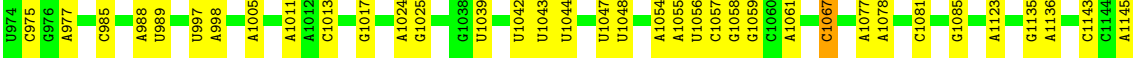


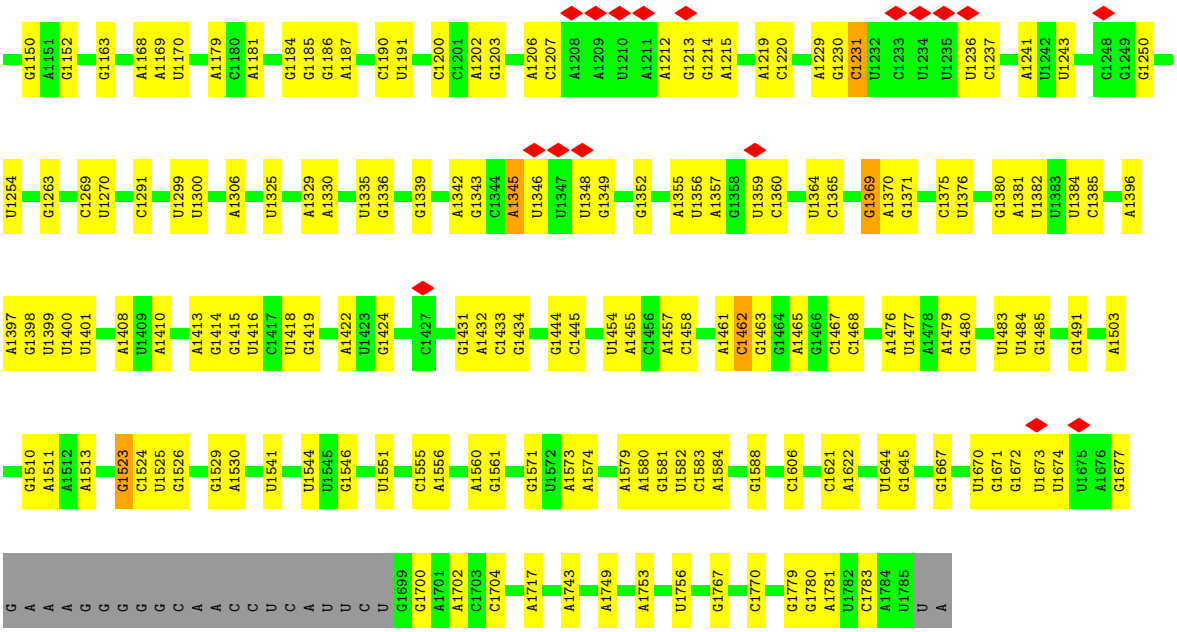






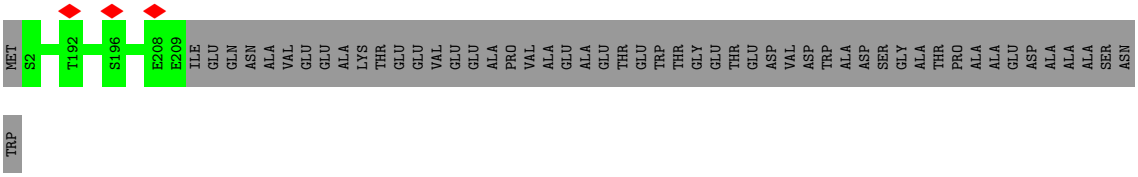






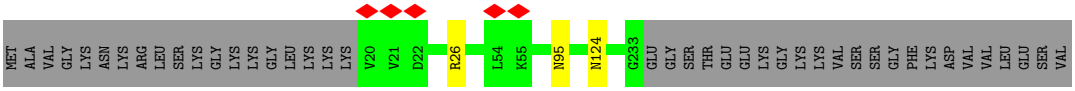
- Molecule 47: 40S ribosomal protein S0

Chain B:



- Molecule 48: 40S ribosomal protein S1

Chain C:

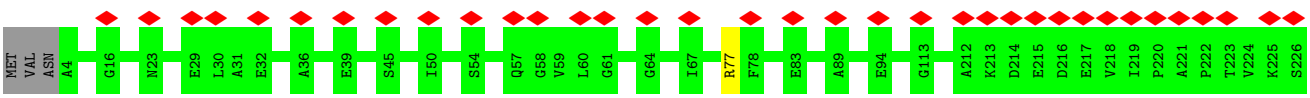


- Molecule 49: Ribosomal 40S subunit protein S2

Chain D:

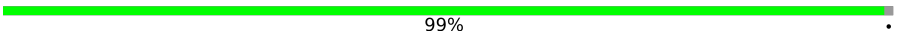
- Molecule 50: Ribosomal 40S subunit protein S3

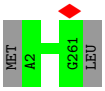
Chain E:



• Molecule 51: 40S ribosomal protein S4

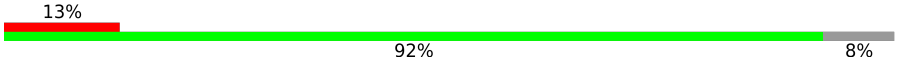
Chain F:

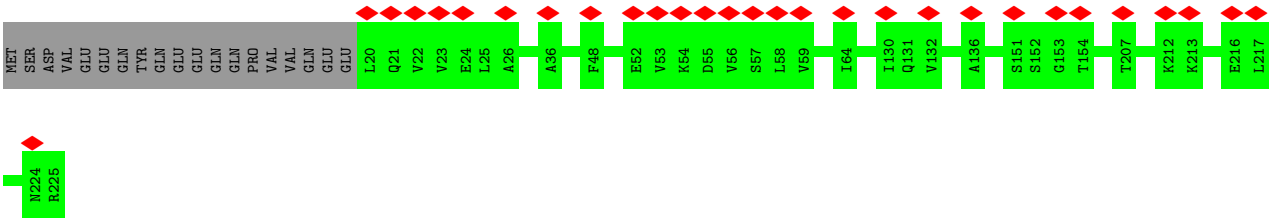




• Molecule 52: Ribosomal 40S subunit protein S5

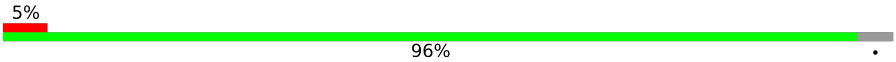
Chain G:

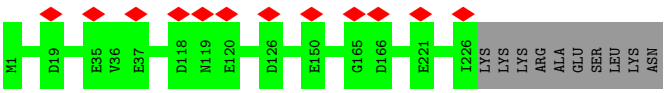




• Molecule 53: 40S ribosomal protein S6

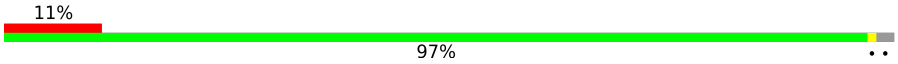
Chain H:

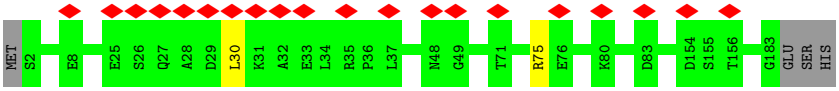




• Molecule 54: 40S ribosomal protein S7

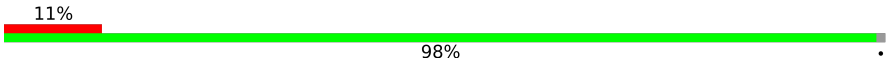
Chain I:

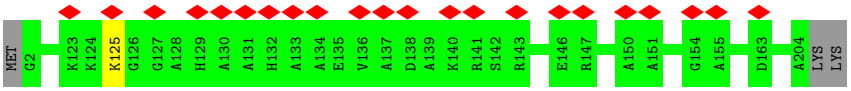




• Molecule 55: 40S ribosomal protein S8

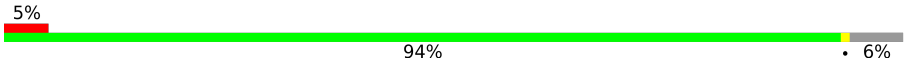
Chain J:

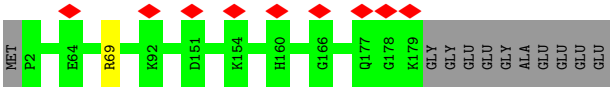




• Molecule 56: Ribosomal 40S subunit protein S9B

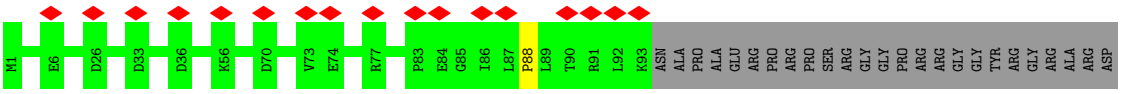
Chain K:





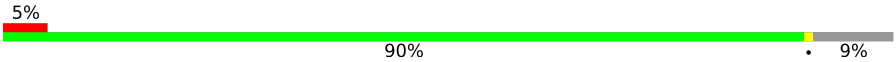
• Molecule 57: Ribosomal 40S subunit protein S10A

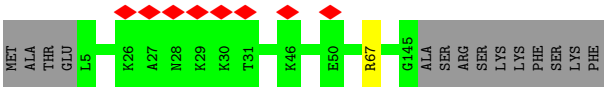
Chain L:



• Molecule 58: Ribosomal 40S subunit protein S11A

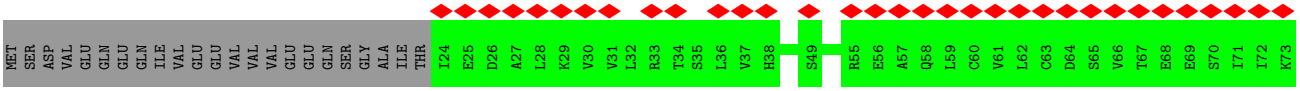
Chain M:

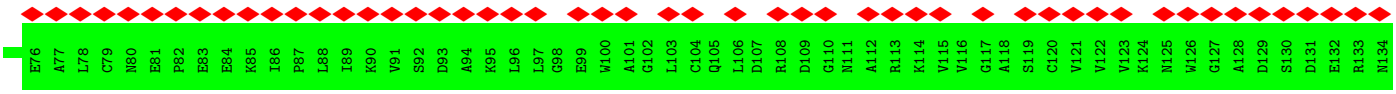


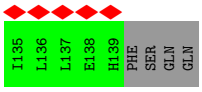


• Molecule 59: 40S ribosomal protein S12

Chain N:

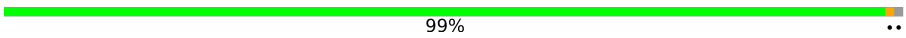






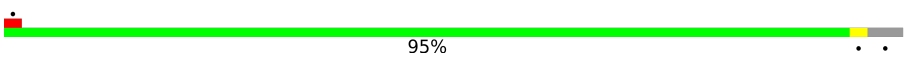
• Molecule 60: Ribosomal 40S subunit protein S13

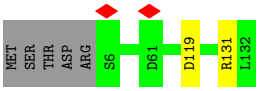
Chain O:



• Molecule 61: Ribosomal 40S subunit protein S14B

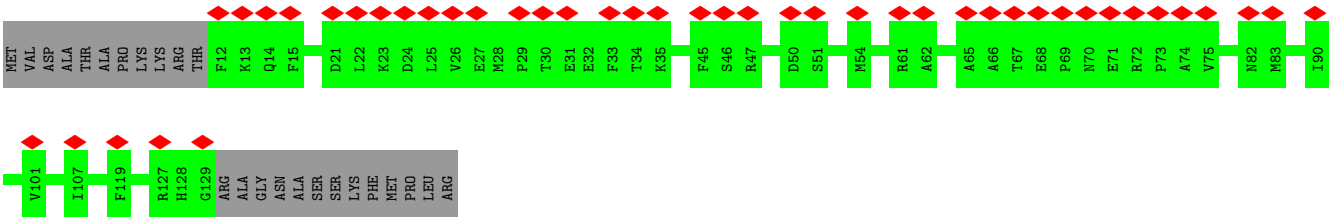
Chain P:





• Molecule 62: Ribosomal 40S subunit protein S15

Chain Q: 31% 83% 17%

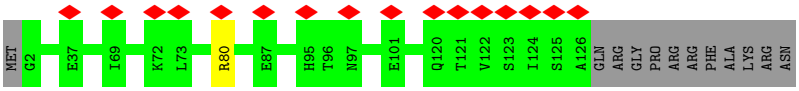


- Molecule 63: Ribosomal 40S subunit protein S16A

Chain R: 99%

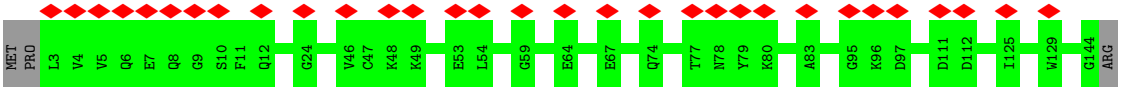
- Molecule 64: Ribosomal 40S subunit protein S17B

Chain S: 12% 91% 9%



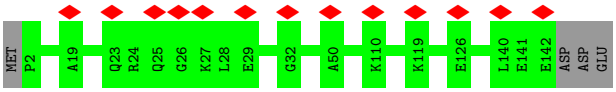
- Molecule 65: Ribosomal 40S subunit protein S18B

Chain T: 21% 98%



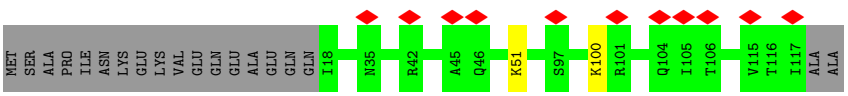
- Molecule 66: Ribosomal 40S subunit protein S19A

Chain U: 9% 97%



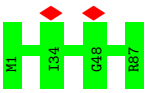
- Molecule 67: Ribosomal 40S subunit protein S20

Chain V: 9% 82% 16%

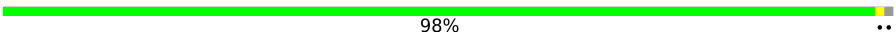


- Molecule 68: 40S ribosomal protein S21

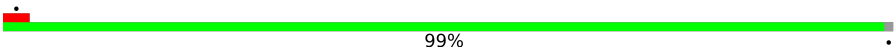
Chain W: 100%

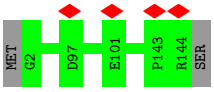


• Molecule 69: 40S ribosomal protein S22-A

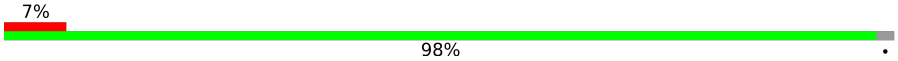
Chain X: 

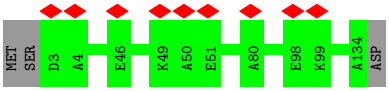
• Molecule 70: Ribosomal 40S subunit protein S23B

Chain Y: 



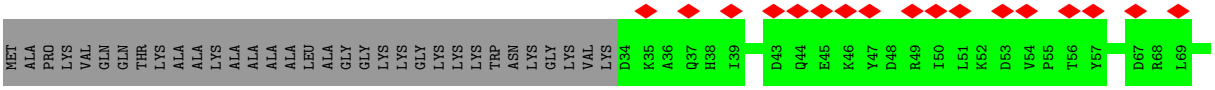
• Molecule 71: 40S ribosomal protein S24

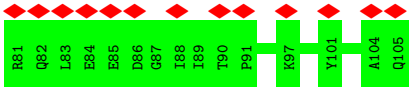
Chain Z: 



• Molecule 72: 40S ribosomal protein S25

Chain a:

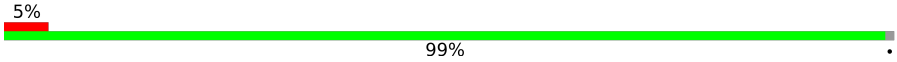


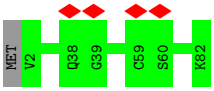


• Molecule 73: 40S ribosomal protein S26

Chain b:

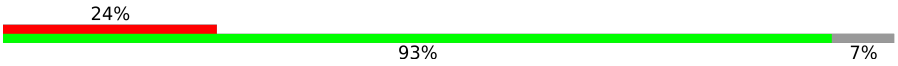
• Molecule 74: 40S ribosomal protein S27

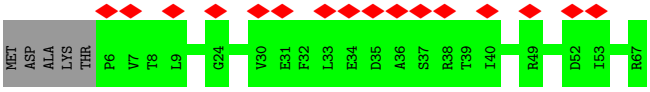
Chain c: 



• Molecule 75: Ribosomal 40S subunit protein S28B

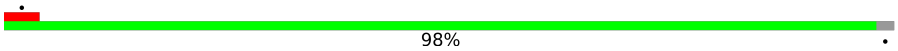
Chain d:

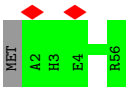




• Molecule 76: Ribosomal 40S subunit protein S29A

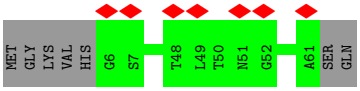
Chain e:





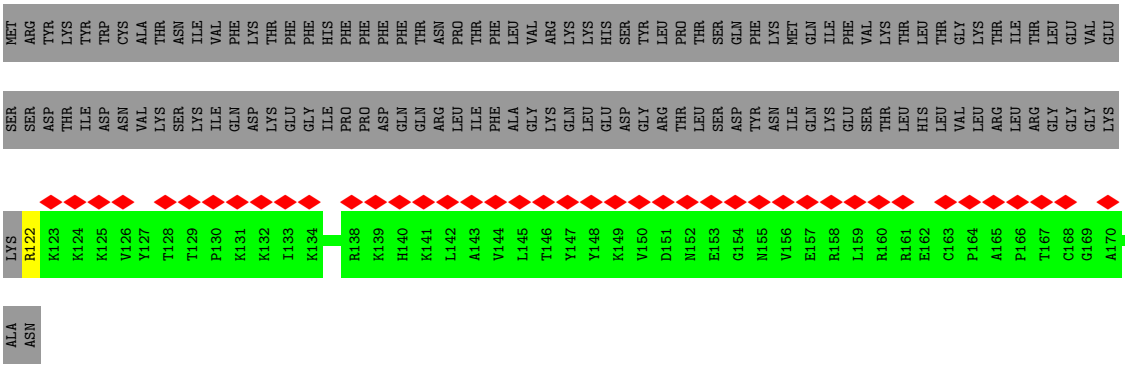
• Molecule 77: 40S ribosomal protein S30

Chain f:



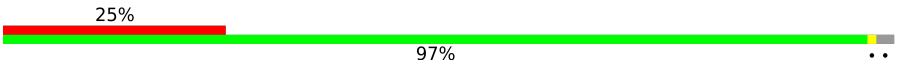
• Molecule 78: Ubiquitin-ribosomal 40S subunit protein S31 fusion protein

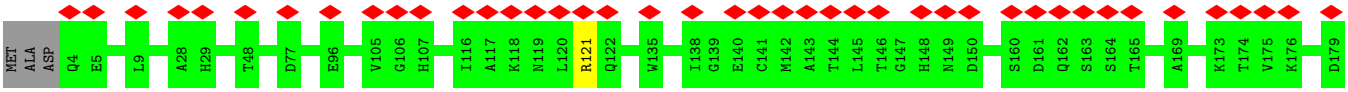
Chain g:

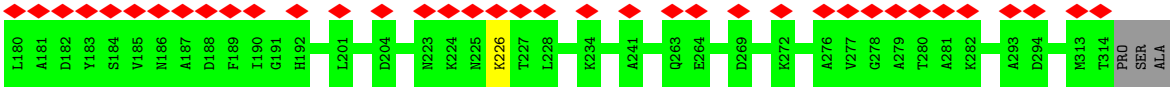


• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

Chain h:






L180
A181
D182
Y183
S184
V185
N186
A187
D188
F189
I190
G191
H192
L201
D204
N223
K224
N225
K226
T227
L228
K234
A241
Q263
E264
D269
K272
A276
V277
G278
A279
T280
A281
K282
A293
D294
M313
T314
PRO
SER
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.339	Depositor
Minimum map value	-1.298	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.122	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	426.36002, 426.36002, 426.36002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, IAS, OMG, ZN, OMC, 3HE, MLZ

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	1	0.79	12/76718 (0.0%)	0.83	53/119600 (0.0%)
2	3	0.67	0/2884	0.75	0/4492
3	4	0.80	0/3746	0.78	0/5832
4	j	0.41	0/1931	0.58	0/2592
5	k	0.39	0/3156	0.55	0/4246
6	l	0.36	0/2799	0.53	0/3777
7	m	0.34	0/2447	0.50	0/3294
8	n	0.35	0/1258	0.53	0/1696
9	o	0.37	0/1929	0.52	0/2589
10	p	0.34	0/1869	0.48	0/2519
11	q	0.33	0/1537	0.53	0/2067
12	r	0.36	0/1724	0.54	0/2314
13	s	0.32	0/1404	0.56	0/1880
14	t	0.37	0/1637	0.56	0/2195
15	u	0.35	0/1044	0.53	0/1407
16	v	0.46	0/1753	0.58	0/2347
17	w	0.39	0/1620	0.51	0/2167
18	x	0.38	0/1398	0.55	0/1879
19	y	0.37	0/1511	0.58	0/2022
20	z	0.34	0/1483	0.55	0/1972
21	0	0.40	0/1483	0.54	0/1997
22	2	0.39	0/1305	0.53	0/1749
23	5	0.35	0/871	0.48	0/1175
24	6	0.36	0/994	0.56	0/1339
25	7	0.40	0/536	0.66	1/712 (0.1%)
26	8	0.38	0/990	0.54	0/1337
27	9	0.36	0/999	0.53	0/1334
28	AA	0.37	0/1112	0.48	0/1488
29	AB	0.40	0/1199	0.53	0/1607
30	AC	0.32	0/522	0.51	0/692
31	AD	0.36	0/738	0.49	0/994
32	AE	0.36	0/902	0.53	0/1212

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	AF	0.40	0/1039	0.54	0/1390
34	AG	0.43	0/895	0.54	0/1201
35	AH	0.40	0/934	0.59	0/1242
36	AI	0.35	0/1004	0.57	0/1337
37	AJ	0.33	0/780	0.56	0/1033
38	AK	0.40	0/690	0.61	0/916
39	AL	0.33	0/632	0.52	0/842
40	AM	0.36	0/458	0.58	0/609
41	AN	0.33	0/436	0.55	0/577
42	AO	0.25	0/228	0.78	1/293 (0.3%)
43	AP	0.38	0/840	0.54	0/1108
44	AQ	0.38	0/705	0.59	0/940
45	i	0.25	0/864	0.49	0/1156
46	A	0.39	0/40362	0.84	17/62888 (0.0%)
47	B	0.28	0/1666	0.49	0/2273
48	C	0.26	0/1750	0.53	0/2354
49	D	0.30	0/1648	0.50	0/2237
50	E	0.28	0/1731	0.55	0/2324
51	F	0.27	0/2096	0.53	0/2822
52	G	0.25	0/1631	0.51	0/2199
53	H	0.26	0/1845	0.53	0/2464
54	I	0.27	0/1490	0.53	1/2004 (0.0%)
55	J	0.30	0/1606	0.58	0/2150
56	K	0.26	0/1478	0.54	0/1978
57	L	0.26	0/801	0.53	0/1081
58	M	0.31	0/1154	0.54	0/1553
59	N	0.25	0/892	0.59	0/1203
60	O	0.47	1/1210 (0.1%)	0.70	3/1631 (0.2%)
61	P	0.28	0/944	0.59	0/1265
62	Q	0.28	0/954	0.57	0/1282
63	R	0.27	0/1109	0.52	0/1486
64	S	0.25	0/1014	0.54	0/1361
65	T	0.26	0/1186	0.56	0/1590
66	U	0.26	0/1120	0.52	0/1508
67	V	0.26	0/800	0.53	0/1082
68	W	0.30	0/683	0.57	0/918
69	X	0.29	0/1049	0.55	1/1412 (0.1%)
70	Y	0.30	0/1128	0.57	0/1505
71	Z	0.27	0/1086	0.57	0/1447
72	a	0.24	0/585	0.50	0/789
73	b	0.29	0/811	0.59	0/1085
74	c	0.26	0/624	0.51	0/843
75	d	0.25	0/489	0.64	0/654

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	e	0.28	0/466	0.60	0/620
77	f	0.28	0/451	0.56	0/601
78	g	0.25	0/585	0.58	0/778
79	h	0.25	0/2451	0.52	0/3337
All	All	0.56	13/213899 (0.0%)	0.73	77/313891 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1737	A	O3'-P	-15.10	1.43	1.61
60	O	82	PRO	CG-CD	-12.21	1.10	1.50
1	1	209	C	O3'-P	11.48	1.75	1.61
1	1	1738	U	O3'-P	-7.21	1.52	1.61
1	1	1573	C	O3'-P	-6.63	1.53	1.61
1	1	1738	U	P-OP1	-6.39	1.38	1.49
1	1	482	U	C1'-N1	6.12	1.57	1.48
1	1	477	U	C1'-N1	6.11	1.57	1.48
1	1	1575	A	O3'-P	-5.96	1.53	1.61
1	1	483	U	C1'-N1	5.92	1.57	1.48
1	1	479	C	C1'-N1	5.46	1.56	1.48
1	1	476	C	C1'-N1	5.45	1.56	1.48
1	1	1738	U	P-OP2	-5.02	1.40	1.49

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1263	U	OP2-P-O3'	-18.84	63.74	105.20
46	A	822	G	P-O3'-C3'	15.77	138.62	119.70
60	O	82	PRO	N-CD-CG	-15.47	79.99	103.20
1	1	1017	G	P-O3'-C3'	13.46	135.85	119.70
46	A	822	G	O3'-P-O5'	11.90	126.60	104.00
1	1	1263	U	P-O3'-C3'	11.68	133.72	119.70
1	1	1263	U	OP1-P-O3'	10.21	127.65	105.20
1	1	1263	U	O3'-P-O5'	8.66	120.46	104.00
1	1	1276	C	N3-C2-O2	-8.64	115.86	121.90
60	O	82	PRO	CA-CB-CG	-8.56	87.74	104.00
46	A	1375	C	C2-N1-C1'	8.05	127.66	118.80
1	1	2215	C	N3-C2-O2	-8.00	116.30	121.90
1	1	3182	C	C2-N1-C1'	7.50	127.05	118.80
1	1	3126	U	C2-N1-C1'	7.36	126.53	117.70
1	1	918	U	C2-N1-C1'	7.10	126.22	117.70
60	O	82	PRO	CA-N-CD	-7.05	101.63	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3182	C	N1-C2-O2	6.73	122.94	118.90
1	1	1273	C	N1-C2-O2	6.58	122.85	118.90
1	1	620	A	N1-C6-N6	6.55	122.53	118.60
1	1	1017	G	OP1-P-O3'	6.50	119.49	105.20
1	1	1273	C	N3-C2-O2	-6.49	117.36	121.90
1	1	437	G	N3-C4-N9	-6.35	122.19	126.00
1	1	2215	C	N1-C2-O2	6.33	122.70	118.90
54	I	30	LEU	CA-CB-CG	6.13	129.40	115.30
1	1	437	G	N3-C4-C5	6.10	131.65	128.60
1	1	1099	A	OP2-P-O3'	6.06	118.53	105.20
1	1	2814	U	N1-C2-O2	6.05	127.04	122.80
46	A	1462	C	C2-N1-C1'	5.93	125.32	118.80
46	A	1067	C	C2-N1-C1'	5.92	125.31	118.80
1	1	2814	U	C2-N1-C1'	5.80	124.66	117.70
25	7	25	ASP	CB-CG-OD1	5.77	123.49	118.30
1	1	620	A	C6-C5-N7	-5.76	128.27	132.30
1	1	1276	C	N1-C2-O2	5.74	122.34	118.90
1	1	3029	U	N3-C2-O2	-5.74	118.18	122.20
1	1	1575	A	O4'-C4'-C3'	-5.73	98.27	104.00
1	1	3182	C	N3-C2-O2	-5.72	117.90	121.90
1	1	1738	U	O5'-P-OP1	-5.62	100.64	105.70
1	1	620	A	C5-C6-N6	-5.61	119.21	123.70
1	1	1552	C	N1-C2-O2	5.61	122.27	118.90
46	A	1375	C	C6-N1-C1'	-5.59	114.09	120.80
46	A	561	U	N3-C2-O2	-5.51	118.34	122.20
1	1	406	G	O4'-C1'-N9	5.48	112.59	108.20
1	1	2235	C	N1-C2-O2	5.48	122.19	118.90
1	1	3243	C	N1-C2-O2	5.47	122.18	118.90
46	A	1375	C	N1-C2-O2	5.41	122.15	118.90
1	1	3182	C	C6-N1-C1'	-5.39	114.33	120.80
1	1	1720	U	O4'-C1'-N1	5.34	112.48	108.20
1	1	1737	A	OP1-P-O3'	5.33	116.94	105.20
1	1	3030	U	C2-N1-C1'	5.33	124.09	117.70
1	1	3245	A	O4'-C1'-N9	5.33	112.46	108.20
1	1	3134	C	C2-N1-C1'	5.30	124.63	118.80
1	1	2814	U	N3-C2-O2	-5.25	118.52	122.20
1	1	1229	G	C4-N9-C1'	5.22	133.29	126.50
46	A	1345	A	N1-C2-N3	5.22	131.91	129.30
42	AO	3	ASP	CB-CG-OD2	5.20	122.98	118.30
1	1	2235	C	C2-N1-C1'	5.18	124.50	118.80
1	1	620	A	C4-C5-N7	5.17	113.29	110.70
46	A	985	C	C2-N1-C1'	5.16	124.47	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A	1375	C	C6-N1-C2	-5.16	118.24	120.30
1	1	1099	A	P-O3'-C3'	5.15	125.88	119.70
69	X	93	LEU	C-N-CA	-5.15	108.83	121.70
46	A	1523	G	N3-C4-C5	-5.13	126.04	128.60
1	1	918	U	N1-C2-O2	5.12	126.38	122.80
46	A	802	C	C2-N1-C1'	5.11	124.42	118.80
1	1	831	G	O4'-C1'-N9	5.11	112.28	108.20
1	1	3029	U	N1-C2-O2	5.10	126.37	122.80
1	1	1033	C	C2-N1-C1'	5.09	124.40	118.80
1	1	1492	C	C2-N1-C1'	5.09	124.40	118.80
1	1	1197	C	N1-C2-O2	5.09	121.95	118.90
1	1	2842	C	C6-N1-C1'	5.08	126.90	120.80
1	1	620	A	N9-C4-C5	-5.06	103.78	105.80
46	A	1369	G	P-O3'-C3'	5.05	125.76	119.70
46	A	822	G	OP2-P-O3'	-5.03	94.13	105.20
1	1	1276	C	C6-N1-C2	-5.02	118.29	120.30
46	A	451	C	N1-C2-O2	5.01	121.91	118.90
1	1	956	U	C2-N1-C1'	5.01	123.71	117.70
46	A	1231	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	j	248/254 (98%)	240 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	k	385/389 (99%)	374 (97%)	11 (3%)	0	100	100
6	l	359/363 (99%)	350 (98%)	9 (2%)	0	100	100
7	m	290/298 (97%)	280 (97%)	10 (3%)	0	100	100
8	n	152/176 (86%)	149 (98%)	3 (2%)	0	100	100
9	o	233/241 (97%)	227 (97%)	6 (3%)	0	100	100
10	p	236/262 (90%)	232 (98%)	4 (2%)	0	100	100
11	q	188/191 (98%)	181 (96%)	7 (4%)	0	100	100
12	r	204/220 (93%)	198 (97%)	6 (3%)	0	100	100
13	s	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
14	t	198/202 (98%)	193 (98%)	5 (2%)	0	100	100
15	u	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	x	168/185 (91%)	167 (99%)	1 (1%)	0	100	100
19	y	186/186 (100%)	183 (98%)	3 (2%)	0	100	100
20	z	178/190 (94%)	176 (99%)	2 (1%)	0	100	100
21	0	171/172 (99%)	170 (99%)	1 (1%)	0	100	100
22	2	159/160 (99%)	158 (99%)	1 (1%)	0	100	100
23	5	103/124 (83%)	89 (86%)	13 (13%)	1 (1%)	15	21
24	6	129/137 (94%)	128 (99%)	1 (1%)	0	100	100
25	7	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
26	8	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
27	9	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
28	AA	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	AB	146/149 (98%)	140 (96%)	6 (4%)	0	100	100
30	AC	62/63 (98%)	60 (97%)	2 (3%)	0	100	100
31	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
32	AE	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
33	AF	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
34	AG	107/107 (100%)	103 (96%)	4 (4%)	0	100	100
35	AH	114/122 (93%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AI	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
37	AJ	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
38	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
40	AM	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
41	AN	51/52 (98%)	51 (100%)	0	0	100	100
42	AO	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	i	109/267 (41%)	104 (95%)	5 (5%)	0	100	100
47	B	206/261 (79%)	196 (95%)	10 (5%)	0	100	100
48	C	212/256 (83%)	203 (96%)	9 (4%)	0	100	100
49	D	214/249 (86%)	209 (98%)	5 (2%)	0	100	100
50	E	221/251 (88%)	216 (98%)	5 (2%)	0	100	100
51	F	258/262 (98%)	251 (97%)	7 (3%)	0	100	100
52	G	204/225 (91%)	196 (96%)	8 (4%)	0	100	100
53	H	224/236 (95%)	220 (98%)	4 (2%)	0	100	100
54	I	180/186 (97%)	174 (97%)	6 (3%)	0	100	100
55	J	201/206 (98%)	197 (98%)	4 (2%)	0	100	100
56	K	176/189 (93%)	169 (96%)	7 (4%)	0	100	100
57	L	91/118 (77%)	84 (92%)	6 (7%)	1 (1%)	14	19
58	M	139/155 (90%)	133 (96%)	6 (4%)	0	100	100
59	N	114/143 (80%)	93 (82%)	21 (18%)	0	100	100
60	O	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
61	P	123/132 (93%)	120 (98%)	3 (2%)	0	100	100
62	Q	116/142 (82%)	107 (92%)	9 (8%)	0	100	100
63	R	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
64	S	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
65	T	140/145 (97%)	129 (92%)	11 (8%)	0	100	100
66	U	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
67	V	98/119 (82%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	W	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
69	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	Y	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
71	Z	130/135 (96%)	129 (99%)	1 (1%)	0	100	100
72	a	70/105 (67%)	68 (97%)	2 (3%)	0	100	100
73	b	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
74	c	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	d	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
76	e	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
77	f	54/63 (86%)	53 (98%)	1 (2%)	0	100	100
78	g	68/193 (35%)	62 (91%)	6 (9%)	0	100	100
79	h	309/317 (98%)	292 (94%)	17 (6%)	0	100	100
All	All	11010/12138 (91%)	10656 (97%)	352 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	5	20	ALA
57	L	88	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	191/194 (98%)	191 (100%)	0	100	100
5	k	326/328 (99%)	326 (100%)	0	100	100
6	l	290/292 (99%)	289 (100%)	1 (0%)	92	96
7	m	247/252 (98%)	247 (100%)	0	100	100
8	n	135/154 (88%)	135 (100%)	0	100	100
9	o	199/204 (98%)	198 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	p	198/216 (92%)	198 (100%)	0	100	100
11	q	169/170 (99%)	169 (100%)	0	100	100
12	r	178/186 (96%)	178 (100%)	0	100	100
13	s	148/149 (99%)	147 (99%)	1 (1%)	84	90
14	t	166/168 (99%)	163 (98%)	3 (2%)	59	73
15	u	108/109 (99%)	107 (99%)	1 (1%)	78	87
16	v	177/178 (99%)	177 (100%)	0	100	100
17	w	166/167 (99%)	166 (100%)	0	100	100
18	x	142/154 (92%)	142 (100%)	0	100	100
19	y	156/154 (101%)	156 (100%)	0	100	100
20	z	147/153 (96%)	147 (100%)	0	100	100
21	0	158/157 (101%)	158 (100%)	0	100	100
22	2	135/134 (101%)	134 (99%)	1 (1%)	84	90
23	5	95/112 (85%)	94 (99%)	1 (1%)	73	83
24	6	101/103 (98%)	101 (100%)	0	100	100
25	7	57/127 (45%)	57 (100%)	0	100	100
26	8	108/121 (89%)	108 (100%)	0	100	100
27	9	111/112 (99%)	110 (99%)	1 (1%)	78	87
28	AA	117/118 (99%)	117 (100%)	0	100	100
29	AB	120/121 (99%)	120 (100%)	0	100	100
30	AC	50/49 (102%)	50 (100%)	0	100	100
31	AD	81/90 (90%)	81 (100%)	0	100	100
32	AE	98/100 (98%)	98 (100%)	0	100	100
33	AF	111/115 (96%)	111 (100%)	0	100	100
34	AG	94/92 (102%)	94 (100%)	0	100	100
35	AH	99/102 (97%)	99 (100%)	0	100	100
36	AI	106/106 (100%)	106 (100%)	0	100	100
37	AJ	79/79 (100%)	78 (99%)	1 (1%)	69	80
38	AK	70/73 (96%)	69 (99%)	1 (1%)	67	78
39	AL	69/69 (100%)	69 (100%)	0	100	100
40	AM	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	AN	48/47 (102%)	48 (100%)	0	100	100
42	AO	23/24 (96%)	23 (100%)	0	100	100
43	AP	88/89 (99%)	86 (98%)	2 (2%)	50	64
44	AQ	72/73 (99%)	72 (100%)	0	100	100
45	i	92/212 (43%)	92 (100%)	0	100	100
47	B	176/215 (82%)	176 (100%)	0	100	100
48	C	194/229 (85%)	191 (98%)	3 (2%)	65	77
49	D	174/198 (88%)	173 (99%)	1 (1%)	86	92
50	E	174/196 (89%)	173 (99%)	1 (1%)	86	92
51	F	218/220 (99%)	218 (100%)	0	100	100
52	G	178/197 (90%)	178 (100%)	0	100	100
53	H	195/204 (96%)	195 (100%)	0	100	100
54	I	163/167 (98%)	162 (99%)	1 (1%)	86	92
55	J	157/160 (98%)	156 (99%)	1 (1%)	86	92
56	K	153/160 (96%)	152 (99%)	1 (1%)	84	90
57	L	87/104 (84%)	87 (100%)	0	100	100
58	M	122/134 (91%)	121 (99%)	1 (1%)	81	88
59	N	98/123 (80%)	98 (100%)	0	100	100
60	O	129/130 (99%)	128 (99%)	1 (1%)	81	88
61	P	96/101 (95%)	95 (99%)	1 (1%)	76	84
62	Q	102/121 (84%)	102 (100%)	0	100	100
63	R	114/116 (98%)	114 (100%)	0	100	100
64	S	112/122 (92%)	111 (99%)	1 (1%)	78	87
65	T	126/129 (98%)	126 (100%)	0	100	100
66	U	113/117 (97%)	113 (100%)	0	100	100
67	V	90/105 (86%)	88 (98%)	2 (2%)	52	66
68	W	71/71 (100%)	71 (100%)	0	100	100
69	X	112/113 (99%)	112 (100%)	0	100	100
70	Y	116/118 (98%)	116 (100%)	0	100	100
71	Z	109/112 (97%)	109 (100%)	0	100	100
72	a	64/85 (75%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	b	86/102 (84%)	86 (100%)	0	100	100
74	c	72/73 (99%)	72 (100%)	0	100	100
75	d	54/58 (93%)	54 (100%)	0	100	100
76	e	47/48 (98%)	47 (100%)	0	100	100
77	f	48/54 (89%)	48 (100%)	0	100	100
78	g	62/175 (35%)	61 (98%)	1 (2%)	62	76
79	h	259/263 (98%)	257 (99%)	2 (1%)	81	88
All	All	9443/10220 (92%)	9412 (100%)	31 (0%)	92	96

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	l	99	ARG
9	o	13	LYS
13	s	13	ARG
14	t	4	SER
14	t	5	LYS
14	t	62	THR
15	u	23	ASN
22	2	83	ARG
23	5	30	GLN
27	9	3	LYS
37	AJ	98	ARG
38	AK	84	LYS
43	AP	24[A]	LYS
43	AP	24[B]	LYS
48	C	26	ARG
48	C	95	ASN
48	C	124	ASN
49	D	136	ARG
50	E	77	ARG
54	I	75	ARG
55	J	125	LYS
56	K	69	ARG
58	M	67	ARG
60	O	82	PRO
61	P	131	ARG
64	S	80	ARG
67	V	51	LYS
67	V	100	LYS

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Mol	Chain	Res	Type
78	g	122	ARG
79	h	121	ARG
79	h	226	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
7	m	94	ASN
18	x	118	GLN
18	x	120	ASN
21	0	8	GLN
47	B	30	GLN
47	B	33	ASN
52	G	63	GLN
52	G	116	HIS
54	I	19	GLN
54	I	48	ASN
54	I	167	GLN
62	Q	79	HIS
62	Q	103	ASN
68	W	74	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3205/3359 (95%)	567 (17%)	38 (1%)
2	3	120/121 (99%)	7 (5%)	0
3	4	157/158 (99%)	26 (16%)	2 (1%)
46	A	1685/1787 (94%)	439 (26%)	44 (2%)
All	All	5167/5425 (95%)	1039 (20%)	84 (1%)

All (1039) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A
1	1	42	A
1	1	48	A

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Mol	Chain	Res	Type
1	1	56	A
1	1	58	G
1	1	59	A
1	1	64	A
1	1	65	A
1	1	76	A
1	1	91	G
1	1	98	A
1	1	109	G
1	1	110	C
1	1	115	A
1	1	121	A
1	1	134	U
1	1	135	G
1	1	147	G
1	1	154	G
1	1	155	A
1	1	156	A
1	1	164	U
1	1	169	G
1	1	171	G
1	1	172	C
1	1	173	C
1	1	175	G
1	1	186	A
1	1	189	U
1	1	190	U
1	1	199	C
1	1	205	G
1	1	209	C
1	1	210	A
1	1	212	A
1	1	217	G
1	1	218	A
1	1	219	G
1	1	230	G
1	1	236	A
1	1	239	A
1	1	240	C
1	1	243	G
1	1	245	G
1	1	249	G

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Mol	Chain	Res	Type
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	269	G
1	1	286	U
1	1	295	A
1	1	305	U
1	1	323	A
1	1	329	U
1	1	338	A
1	1	339	C
1	1	346	C
1	1	350	C
1	1	376	G
1	1	377	A
1	1	395	A
1	1	398	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	445	A
1	1	453	U
1	1	454	G
1	1	479	C
1	1	481	G
1	1	482	U
1	1	485	A
1	1	486	C
1	1	506	A
1	1	516	U
1	1	517	A
1	1	531	G
1	1	538	G
1	1	539	G
1	1	541	U
1	1	542	U
1	1	543	C

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Mol	Chain	Res	Type
1	1	544	U
1	1	545	G
1	1	546	C
1	1	555	A
1	1	557	A
1	1	564	G
1	1	577	G
1	1	590	A
1	1	598	U
1	1	600	U
1	1	602	A
1	1	609	A
1	1	618	U
1	1	619	A
1	1	620	A
1	1	647	A
1	1	658	A
1	1	665	C
1	1	675	A
1	1	679	U
1	1	682	G
1	1	703	A
1	1	710	G
1	1	713	A
1	1	717	A
1	1	723	G
1	1	730	A
1	1	732	U
1	1	760	U
1	1	763	U
1	1	772	U
1	1	773	U
1	1	776	A
1	1	777	G
1	1	781	G
1	1	782	A
1	1	802	A
1	1	813	A
1	1	826	A
1	1	845	C
1	1	857	C
1	1	870	U

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Mol	Chain	Res	Type
1	1	875	U
1	1	892	A
1	1	903	G
1	1	904	G
1	1	910	A
1	1	912	G
1	1	913	A
1	1	917	A
1	1	919	C
1	1	920	G
1	1	921	A
1	1	933	G
1	1	934	C
1	1	940	C
1	1	955	C
1	1	956	U
1	1	970	G
1	1	976	A
1	1	977	U
1	1	978	C
1	1	990	G
1	1	991	U
1	1	996	C
1	1	997	G
1	1	998	A
1	1	1006	G
1	1	1011	C
1	1	1012	U
1	1	1014	G
1	1	1019	U
1	1	1020	G
1	1	1021	A
1	1	1022	A
1	1	1023	A
1	1	1024	U
1	1	1025	G
1	1	1027	C
1	1	1030	U
1	1	1033	C
1	1	1043	A
1	1	1045	C
1	1	1060	A

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Mol	Chain	Res	Type
1	1	1061	A
1	1	1068	G
1	1	1077	U
1	1	1078	U
1	1	1089	A
1	1	1090	A
1	1	1091	U
1	1	1092	U
1	1	1094	A
1	1	1099	A
1	1	1100	G
1	1	1113	G
1	1	1127	G
1	1	1140	U
1	1	1149	A
1	1	1150	A
1	1	1155	A
1	1	1176	A
1	1	1177	U
1	1	1178	G
1	1	1188	C
1	1	1189	A
1	1	1192	C
1	1	1197	C
1	1	1204	U
1	1	1215	C
1	1	1218	G
1	1	1223	C
1	1	1224	C
1	1	1225	G
1	1	1228	C
1	1	1229	G
1	1	1230	G
1	1	1231	U
1	1	1232	G
1	1	1237	U
1	1	1238	G
1	1	1239	G
1	1	1240	A
1	1	1241	A
1	1	1242	G
1	1	1243	U

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Mol	Chain	Res	Type
1	1	1244	C
1	1	1245	G
1	1	1249	U
1	1	1250	C
1	1	1253	C
1	1	1255	A
1	1	1259	A
1	1	1262	G
1	1	1263	U
1	1	1264	G
1	1	1265	U
1	1	1266	A
1	1	1267	A
1	1	1268	C
1	1	1269	A
1	1	1270	A
1	1	1273	C
1	1	1274	A
1	1	1277	G
1	1	1278	G
1	1	1280	C
1	1	1282	A
1	1	1283	A
1	1	1301	U
1	1	1303	G
1	1	1304	A
1	1	1305	U
1	1	1309	G
1	1	1326	A
1	1	1327	U
1	1	1345	G
1	1	1346	U
1	1	1347	U
1	1	1348	U
1	1	1349	U
1	1	1382	A
1	1	1387	C
1	1	1395	U
1	1	1414	A
1	1	1415	A
1	1	1417	G
1	1	1421	U

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Mol	Chain	Res	Type
1	1	1430	G
1	1	1433	C
1	1	1442	A
1	1	1446	G
1	1	1465	C
1	1	1477	A
1	1	1484	G
1	1	1491	U
1	1	1498	C
1	1	1504	C
1	1	1520	A
1	1	1532	G
1	1	1552	C
1	1	1556	G
1	1	1558	G
1	1	1559	C
1	1	1560	U
1	1	1561	U
1	1	1562	G
1	1	1563	A
1	1	1565	U
1	1	1566	U
1	1	1567	U
1	1	1568	U
1	1	1569	C
1	1	1571	G
1	1	1572	G
1	1	1573	C
1	1	1574	C
1	1	1575	A
1	1	1576	A
1	1	1577	C
1	1	1585	A
1	1	1589	A
1	1	1601	A
1	1	1624	C
1	1	1625	U
1	1	1635	C
1	1	1638	A
1	1	1639	A
1	1	1641	U
1	1	1653	C

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Mol	Chain	Res	Type
1	1	1654	G
1	1	1701	U
1	1	1720	U
1	1	1721	C
1	1	1732	G
1	1	1746	A
1	1	1747	G
1	1	1756	A
1	1	1759	U
1	1	1760	U
1	1	1761	U
1	1	1762	G
1	1	1763	C
1	1	1771	G
1	1	1774	G
1	1	1776	G
1	1	1792	G
1	1	1793	A
1	1	1809	A
1	1	1810	A
1	1	1811	U
1	1	1812	A
1	1	1814	U
1	1	1815	U
1	1	1816	U
1	1	1817	U
1	1	1835	A
1	1	1838	A
1	1	1842	C
1	1	1845	C
1	1	1846	A
1	1	1862	C
1	1	1874	G
1	1	1876	U
1	1	1877	A
1	1	1882	A
1	1	1889	A
1	1	1902	G
1	1	1944	G
1	1	1950	G
1	1	1951	U
1	1	1958	G

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Mol	Chain	Res	Type
1	1	1965	U
1	1	1968	A
1	1	1970	A
1	1	2043	G
1	1	2045	C
1	1	2051	G
1	1	2054	C
1	1	2055	G
1	1	2061	G
1	1	2066	G
1	1	2067	U
1	1	2068	U
1	1	2069	U
1	1	2070	A
1	1	2078	A
1	1	2079	C
1	1	2088	G
1	1	2089	G
1	1	2090	U
1	1	2091	A
1	1	2092	C
1	1	2099	G
1	1	2100	G
1	1	2109	A
1	1	2118	U
1	1	2122	A
1	1	2124	C
1	1	2136	A
1	1	2147	G
1	1	2149	G
1	1	2182	C
1	1	2183	U
1	1	2184	G
1	1	2185	A
1	1	2186	A
1	1	2187	U
1	1	2188	G
1	1	2200	A
1	1	2201	A
1	1	2222	A
1	1	2227	G
1	1	2234	A

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Mol	Chain	Res	Type
1	1	2235	C
1	1	2250	G
1	1	2251	G
1	1	2259	A
1	1	2260	U
1	1	2276	U
1	1	2283	G
1	1	2285	G
1	1	2288	U
1	1	2291	A
1	1	2292	U
1	1	2293	G
1	1	2312	U
1	1	2314	U
1	1	2341	A
1	1	2351	A
1	1	2352	C
1	1	2353	G
1	1	2363	G
1	1	2366	U
1	1	2371	G
1	1	2375	A
1	1	2380	A
1	1	2381	G
1	1	2382	A
1	1	2389	U
1	1	2390	G
1	1	2413	G
1	1	2419	A
1	1	2420	G
1	1	2489	A
1	1	2492	U
1	1	2493	A
1	1	2511	G
1	1	2513	A
1	1	2515	G
1	1	2516	U
1	1	2517	C
1	1	2518	A
1	1	2519	A
1	1	2520	A
1	1	2521	C

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Mol	Chain	Res	Type
1	1	2529	U
1	1	2530	C
1	1	2536	U
1	1	2538	A
1	1	2545	C
1	1	2546	U
1	1	2547	G
1	1	2557	G
1	1	2565	A
1	1	2566	C
1	1	2578	G
1	1	2579	G
1	1	2586	G
1	1	2598	A
1	1	2624	U
1	1	2628	A
1	1	2644	G
1	1	2646	A
1	1	2649	G
1	1	2661	A
1	1	2663	A
1	1	2666	A
1	1	2676	A
1	1	2685	U
1	1	2686	G
1	1	2700	G
1	1	2701	U
1	1	2724	U
1	1	2725	G
1	1	2734	A
1	1	2745	C
1	1	2749	G
1	1	2750	G
1	1	2768	G
1	1	2771	A
1	1	2772	G
1	1	2773	A
1	1	2774	A
1	1	2782	C
1	1	2786	G
1	1	2789	A
1	1	2790	U

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Mol	Chain	Res	Type
1	1	2800	G
1	1	2814	U
1	1	2815	U
1	1	2816	C
1	1	2817	A
1	1	2833	U
1	1	2843	G
1	1	2844	A
1	1	2847	U
1	1	2859	A
1	1	2861	C
1	1	2866	C
1	1	2870	G
1	1	2871	C
1	1	2883	A
1	1	2886	G
1	1	2895	U
1	1	2907	U
1	1	2908	A
1	1	2914	C
1	1	2919	G
1	1	2943	A
1	1	2955	C
1	1	2962	G
1	1	2969	G
1	1	2984	A
1	1	3021	A
1	1	3028	U
1	1	3031	G
1	1	3050	A
1	1	3051	C
1	1	3052	G
1	1	3058	A
1	1	3064	C
1	1	3066	A
1	1	3073	G
1	1	3076	U
1	1	3094	A
1	1	3102	A
1	1	3103	U
1	1	3114	A
1	1	3115	C

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Mol	Chain	Res	Type
1	1	3125	U
1	1	3134	C
1	1	3141	U
1	1	3143	G
1	1	3144	A
1	1	3146	G
1	1	3149	U
1	1	3151	C
1	1	3157	A
1	1	3160	C
1	1	3162	U
1	1	3163	U
1	1	3164	U
1	1	3165	U
1	1	3171	C
1	1	3172	U
1	1	3175	A
1	1	3182	C
1	1	3183	A
1	1	3184	G
1	1	3192	A
1	1	3194	G
1	1	3208	A
1	1	3210	A
1	1	3212	G
1	1	3214	U
1	1	3224	U
1	1	3228	G
1	1	3235	A
1	1	3241	G
1	1	3246	C
1	1	3251	G
1	1	3252	C
1	1	3259	A
1	1	3260	A
1	1	3268	G
1	1	3269	C
1	1	3278	U
1	1	3281	A
1	1	3282	U
1	1	3284	U
1	1	3285	A

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Mol	Chain	Res	Type
1	1	3306	U
1	1	3307	A
1	1	3309	A
1	1	3310	G
1	1	3316	U
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	U
1	1	3321	G
1	1	3334	G
1	1	3343	C
1	1	3347	U
1	1	3351	G
1	1	3361	U
2	3	22	A
2	3	54	U
2	3	65	G
2	3	73	C
2	3	76	A
2	3	102	A
2	3	112	G
3	4	23	U
3	4	34	U
3	4	35	C
3	4	59	A
3	4	62	C
3	4	63	G
3	4	70	G
3	4	81	A
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	92	A
3	4	95	G
3	4	102	U
3	4	104	A
3	4	106	C
3	4	107	G
3	4	111	A
3	4	112	U

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Mol	Chain	Res	Type
3	4	113	U
3	4	125	U
3	4	126	A
3	4	148	G
3	4	156	U
3	4	157	U
46	A	4	C
46	A	17	C
46	A	25	C
46	A	26	A
46	A	27	U
46	A	34	G
46	A	42	G
46	A	43	A
46	A	47	A
46	A	57	G
46	A	66	U
46	A	68	A
46	A	74	U
46	A	76	A
46	A	78	A
46	A	79	C
46	A	81	G
46	A	84	A
46	A	104	A
46	A	114	C
46	A	115	G
46	A	116	U
46	A	123	G
46	A	124	A
46	A	127	G
46	A	128	U
46	A	129	A
46	A	138	C
46	A	139	U
46	A	141	G
46	A	142	G
46	A	143	A
46	A	149	G
46	A	151	G
46	A	152	G
46	A	154	A

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Mol	Chain	Res	Type
46	A	156	U
46	A	157	U
46	A	158	C
46	A	164	C
46	A	166	A
46	A	167	A
46	A	168	U
46	A	173	G
46	A	174	C
46	A	176	U
46	A	177	A
46	A	179	A
46	A	187	C
46	A	190	U
46	A	193	G
46	A	199	G
46	A	200	A
46	A	202	G
46	A	211	A
46	A	213	A
46	A	215	A
46	A	216	A
46	A	217	A
46	A	218	A
46	A	219	A
46	A	248	C
46	A	255	A
46	A	259	U
46	A	260	U
46	A	261	C
46	A	262	G
46	A	263	A
46	A	266	C
46	A	269	A
46	A	270	U
46	A	274	C
46	A	276	U
46	A	277	G
46	A	278	U
46	A	279	G
46	A	299	A
46	A	307	C

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Mol	Chain	Res	Type
46	A	312	C
46	A	314	A
46	A	318	U
46	A	319	C
46	A	320	G
46	A	331	A
46	A	335	G
46	A	336	C
46	A	350	A
46	A	357	A
46	A	358	A
46	A	359	C
46	A	388	G
46	A	398	A
46	A	400	C
46	A	402	G
46	A	414	A
46	A	416	G
46	A	417	G
46	A	421	G
46	A	422	C
46	A	423	A
46	A	424	G
46	A	432	G
46	A	433	C
46	A	437	U
46	A	442	C
46	A	452	A
46	A	457	G
46	A	458	A
46	A	466	A
46	A	467	C
46	A	474	U
46	A	475	A
46	A	480	U
46	A	482	C
46	A	483	A
46	A	485	G
46	A	501	G
46	A	502	U
46	A	503	A
46	A	504	A

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Mol	Chain	Res	Type
46	A	505	U
46	A	506	U
46	A	509	A
46	A	515	U
46	A	516	A
46	A	518	A
46	A	519	A
46	A	525	A
46	A	530	U
46	A	532	A
46	A	534	C
46	A	536	A
46	A	537	G
46	A	538	G
46	A	539	A
46	A	540	A
46	A	547	G
46	A	553	A
46	A	554	A
46	A	555	G
46	A	556	U
46	A	557	C
46	A	562	G
46	A	563	C
46	A	566	G
46	A	575	G
46	A	580	U
46	A	592	A
46	A	593	G
46	A	609	U
46	A	617	A
46	A	618	A
46	A	620	A
46	A	621	A
46	A	624	U
46	A	639	G
46	A	648	U
46	A	650	G
46	A	652	C
46	A	653	G
46	A	654	G
46	A	656	C

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Mol	Chain	Res	Type
46	A	675	U
46	A	676	G
46	A	682	A
46	A	686	G
46	A	687	A
46	A	688	G
46	A	692	U
46	A	694	C
46	A	695	C
46	A	696	U
46	A	701	G
46	A	721	C
46	A	722	A
46	A	723	G
46	A	727	U
46	A	729	U
46	A	730	U
46	A	739	A
46	A	740	A
46	A	741	A
46	A	750	G
46	A	751	U
46	A	756	A
46	A	759	A
46	A	760	G
46	A	764	U
46	A	765	U
46	A	766	U
46	A	767	G
46	A	768	C
46	A	770	C
46	A	771	G
46	A	773	A
46	A	778	U
46	A	779	U
46	A	787	A
46	A	796	A
46	A	797	U
46	A	798	A
46	A	803	G
46	A	804	U
46	A	805	U

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Mol	Chain	Res	Type
46	A	807	U
46	A	808	G
46	A	811	U
46	A	814	A
46	A	815	U
46	A	816	U
46	A	818	U
46	A	819	G
46	A	820	U
46	A	821	U
46	A	822	G
46	A	823	G
46	A	824	U
46	A	825	U
46	A	827	C
46	A	828	U
46	A	832	A
46	A	842	U
46	A	848	A
46	A	856	G
46	A	857	G
46	A	858	U
46	A	860	G
46	A	869	A
46	A	871	U
46	A	875	C
46	A	877	G
46	A	878	U
46	A	879	U
46	A	880	G
46	A	881	U
46	A	883	A
46	A	891	A
46	A	898	G
46	A	909	A
46	A	910	G
46	A	911	A
46	A	918	A
46	A	920	U
46	A	930	U
46	A	937	A
46	A	945	U

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Mol	Chain	Res	Type
46	A	951	A
46	A	973	A
46	A	975	C
46	A	977	A
46	A	988	A
46	A	989	U
46	A	997	U
46	A	998	A
46	A	1005	A
46	A	1011	A
46	A	1013	C
46	A	1017	G
46	A	1024	A
46	A	1025	G
46	A	1039	U
46	A	1042	U
46	A	1043	U
46	A	1044	U
46	A	1047	U
46	A	1048	U
46	A	1054	A
46	A	1055	A
46	A	1056	U
46	A	1057	C
46	A	1058	G
46	A	1059	G
46	A	1061	A
46	A	1067	C
46	A	1077	A
46	A	1078	A
46	A	1081	C
46	A	1085	G
46	A	1123	A
46	A	1135	G
46	A	1136	A
46	A	1143	C
46	A	1145	A
46	A	1150	G
46	A	1152	G
46	A	1163	G
46	A	1168	A
46	A	1169	A

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Mol	Chain	Res	Type
46	A	1170	U
46	A	1179	A
46	A	1181	A
46	A	1184	G
46	A	1185	G
46	A	1186	G
46	A	1187	A
46	A	1190	C
46	A	1191	U
46	A	1200	C
46	A	1202	A
46	A	1203	G
46	A	1206	A
46	A	1207	C
46	A	1212	A
46	A	1213	G
46	A	1214	G
46	A	1215	A
46	A	1219	A
46	A	1220	C
46	A	1229	A
46	A	1230	G
46	A	1231	C
46	A	1236	U
46	A	1237	C
46	A	1241	A
46	A	1243	U
46	A	1250	G
46	A	1254	U
46	A	1263	G
46	A	1269	C
46	A	1270	U
46	A	1291	C
46	A	1299	U
46	A	1300	U
46	A	1306	A
46	A	1325	U
46	A	1329	A
46	A	1330	A
46	A	1336	G
46	A	1339	G
46	A	1342	A

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Mol	Chain	Res	Type
46	A	1343	G
46	A	1345	A
46	A	1346	U
46	A	1348	U
46	A	1349	G
46	A	1352	G
46	A	1355	A
46	A	1356	U
46	A	1357	A
46	A	1359	U
46	A	1360	C
46	A	1364	U
46	A	1365	C
46	A	1369	G
46	A	1370	A
46	A	1371	G
46	A	1376	U
46	A	1380	G
46	A	1381	A
46	A	1382	U
46	A	1384	U
46	A	1385	C
46	A	1396	A
46	A	1397	A
46	A	1398	G
46	A	1399	U
46	A	1400	U
46	A	1401	U
46	A	1408	A
46	A	1410	A
46	A	1413	A
46	A	1414	G
46	A	1415	G
46	A	1416	U
46	A	1418	U
46	A	1419	G
46	A	1422	A
46	A	1424	G
46	A	1431	G
46	A	1432	A
46	A	1433	C
46	A	1434	G

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Mol	Chain	Res	Type
46	A	1444	G
46	A	1445	C
46	A	1454	U
46	A	1455	A
46	A	1457	A
46	A	1458	C
46	A	1461	A
46	A	1462	C
46	A	1463	G
46	A	1465	A
46	A	1468	C
46	A	1476	A
46	A	1477	U
46	A	1480	G
46	A	1483	U
46	A	1485	G
46	A	1491	G
46	A	1503	A
46	A	1510	G
46	A	1511	A
46	A	1513	A
46	A	1523	G
46	A	1524	C
46	A	1525	U
46	A	1526	G
46	A	1529	G
46	A	1530	A
46	A	1541	U
46	A	1544	U
46	A	1546	G
46	A	1551	U
46	A	1556	A
46	A	1560	A
46	A	1561	G
46	A	1571	G
46	A	1574	A
46	A	1580	A
46	A	1582	U
46	A	1583	C
46	A	1584	A
46	A	1588	G
46	A	1606	C

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Mol	Chain	Res	Type
46	A	1621	C
46	A	1622	A
46	A	1644	U
46	A	1645	G
46	A	1667	G
46	A	1670	U
46	A	1671	G
46	A	1672	G
46	A	1673	U
46	A	1674	U
46	A	1677	G
46	A	1700	G
46	A	1702	A
46	A	1704	C
46	A	1717	A
46	A	1743	A
46	A	1749	A
46	A	1753	A
46	A	1756	U
46	A	1767	G
46	A	1770	C
46	A	1779	G
46	A	1780	G
46	A	1781	A
46	A	1783	C

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	172	C
1	1	403	C
1	1	538	G
1	1	563	U
1	1	601	U
1	1	759	G
1	1	912	G
1	1	1029	U
1	1	1060	A
1	1	1099	A
1	1	1346	U
1	1	1347	U
1	1	1559	C

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Mol	Chain	Res	Type
1	1	1561	U
1	1	1574	C
1	1	1576	A
1	1	1762	G
1	1	1815	U
1	1	1943	G
1	1	1957	G
1	1	2044	U
1	1	2078	A
1	1	2090	U
1	1	2182	C
1	1	2183	U
1	1	2515	G
1	1	2519	A
1	1	2520	A
1	1	2545	C
1	1	2790	U
1	1	3093	U
1	1	3163	U
1	1	3193	C
1	1	3234	U
1	1	3284	U
1	1	3309	A
1	1	3315	C
1	1	3317	U
3	4	85	G
3	4	156	U
46	A	25	C
46	A	78	A
46	A	137	A
46	A	151	G
46	A	176	U
46	A	214	U
46	A	259	U
46	A	265	U
46	A	278	U
46	A	415	A
46	A	451	C
46	A	502	U
46	A	504	A
46	A	505	U
46	A	514	G

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Mol	Chain	Res	Type
46	A	518	A
46	A	529	C
46	A	533	A
46	A	553	A
46	A	638	U
46	A	685	C
46	A	740	A
46	A	763	C
46	A	820	U
46	A	824	U
46	A	855	C
46	A	874	U
46	A	876	A
46	A	1168	A
46	A	1335	U
46	A	1355	A
46	A	1359	U
46	A	1369	G
46	A	1396	A
46	A	1398	G
46	A	1457	A
46	A	1467	C
46	A	1479	A
46	A	1484	U
46	A	1523	G
46	A	1555	C
46	A	1573	A
46	A	1579	A
46	A	1581	G

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

6 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	$\#\|Z\| > 2$
24	MLZ	6	110	24	8,9,10	0.74	0	4,9,11	1.04	0
1	OMC	1	2808	1	15,22,23	3.16	6 (40%)	17,31,34	1.24	2 (11%)
43	MLZ	AP	40	43	8,9,10	0.70	0	4,9,11	1.00	0
43	MLZ	AP	55	43	8,9,10	0.66	0	4,9,11	0.92	0
61	IAS	P	119	61	4,7,8	0.90	0	2,8,10	1.77	1 (50%)
1	OMG	1	2765	1	18,26,27	3.32	8 (44%)	20,38,41	1.84	4 (20%)

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
24	MLZ	6	110	24	-	3/7/8/10	-
1	OMC	1	2808	1	-	1/7/27/28	0/2/2/2
43	MLZ	AP	40	43	-	1/7/8/10	-
43	MLZ	AP	55	43	-	3/7/8/10	-
61	IAS	P	119	61	-	3/3/7/8	-
1	OMG	1	2765	1	-	0/5/27/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2765	OMG	C4-N3	7.99	1.48	1.35
1	1	2808	OMC	C6-N1	7.44	1.45	1.35
1	1	2765	OMG	C5-C6	6.62	1.52	1.41
1	1	2765	OMG	C6-N1	5.65	1.42	1.33
1	1	2808	OMC	C2-N3	5.21	1.48	1.38
1	1	2808	OMC	C4-N3	4.89	1.43	1.35
1	1	2808	OMC	C6-C5	4.66	1.48	1.38
1	1	2765	OMG	C2-N2	4.65	1.43	1.33
1	1	2765	OMG	C2-N1	4.32	1.43	1.35
1	1	2808	OMC	C4-N4	3.36	1.45	1.35
1	1	2808	OMC	C5-C4	2.81	1.48	1.41
1	1	2765	OMG	O6-C6	-2.72	1.17	1.24
1	1	2765	OMG	C2-N3	2.37	1.45	1.34
1	1	2765	OMG	C5-C4	-2.03	1.35	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2765	OMG	N3-C2-N1	-5.29	120.16	127.22
1	1	2765	OMG	C2-N3-C4	3.99	119.92	115.36
1	1	2808	OMC	C4-N3-C2	3.47	119.86	116.34
1	1	2765	OMG	C5-C6-N1	-2.29	120.30	123.43
1	1	2765	OMG	C2-N1-C6	2.19	119.41	115.93
61	P	119	IAS	OD1-CG-CB	-2.18	119.07	125.43
1	1	2808	OMC	N4-C4-N3	2.05	119.73	116.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2808	OMC	C1'-C2'-O2'-CM2
24	6	110	MLZ	N-CA-CB-CG
61	P	119	IAS	N-CA-CB-CG
61	P	119	IAS	C-CA-CB-CG
43	AP	55	MLZ	CG-CD-CE-NZ
24	6	110	MLZ	CD-CE-NZ-CM
43	AP	55	MLZ	CE-CD-CG-CB
43	AP	55	MLZ	CA-CB-CG-CD
24	6	110	MLZ	C-CA-CB-CG
43	AP	40	MLZ	CG-CD-CE-NZ
61	P	119	IAS	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
80	SPD	1	3401	-	9,9,9	0.32	0	8,8,8	0.93	0
81	3HE	1	3402	-	21,21,21	0.54	0	19,30,30	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	SPD	1	3401	-	-	2/7/7/7	-
81	3HE	1	3402	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

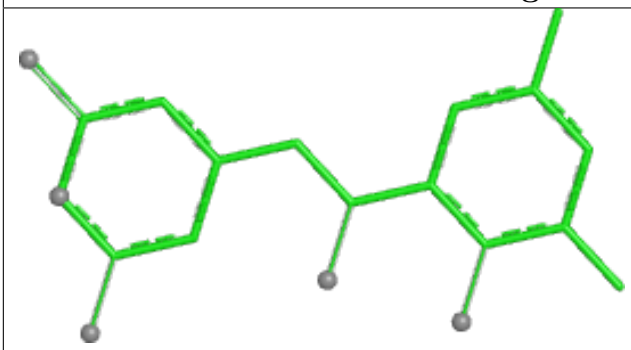
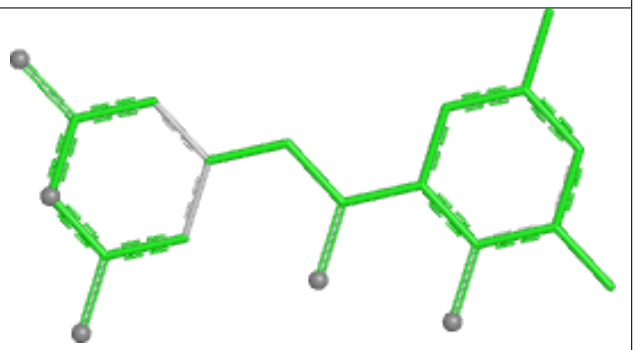
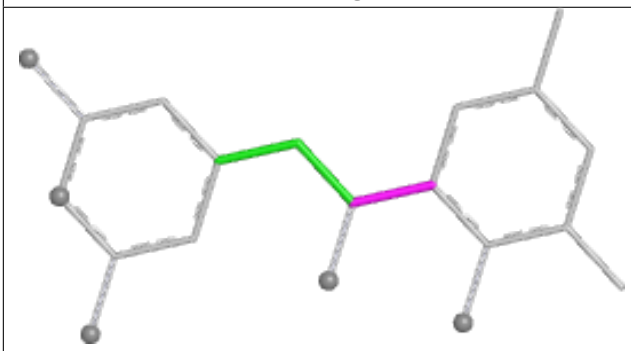
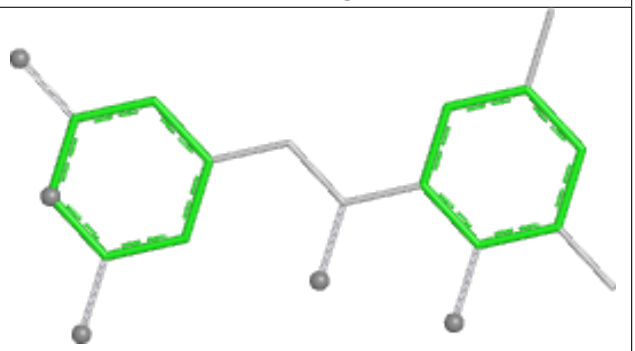
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1	3402	3HE	C6-C5-C7-C8
80	1	3401	SPD	N6-C7-C8-C9
80	1	3401	SPD	C7-C8-C9-N10
81	1	3402	3HE	C6-C5-C7-O3

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 then 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.

Ligand 3HE 1 3402	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

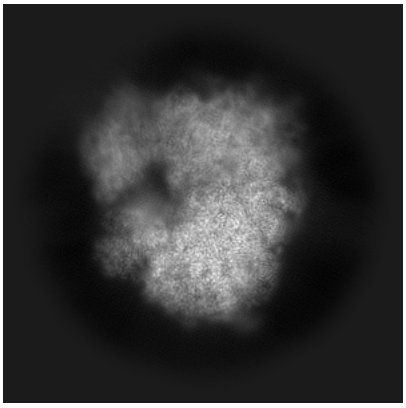
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13741. These allow visual inspection of the internal detail of the map and identification of artifacts.

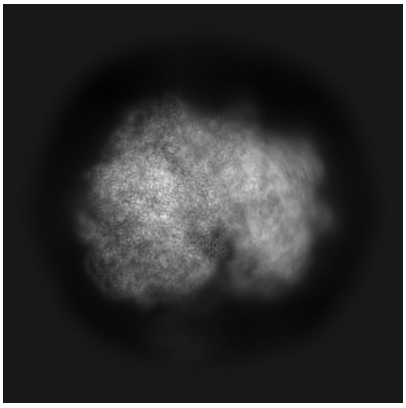
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

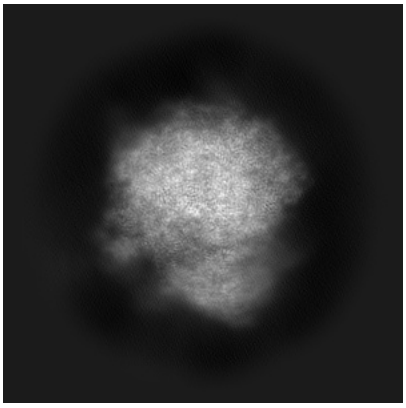
6.1.1 Primary map



X



Y

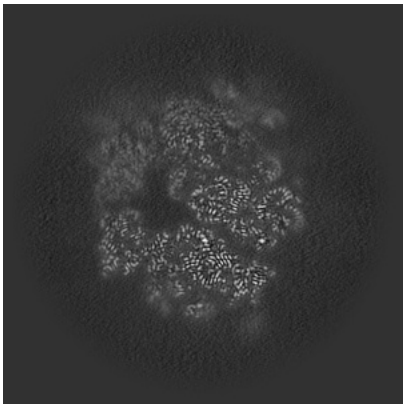


Z

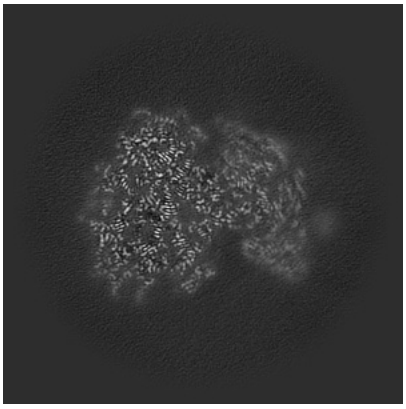
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

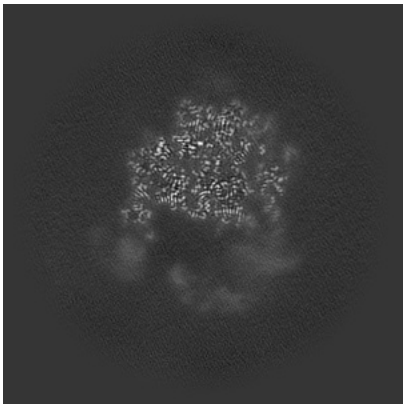
6.2.1 Primary map



X Index: 255



Y Index: 255

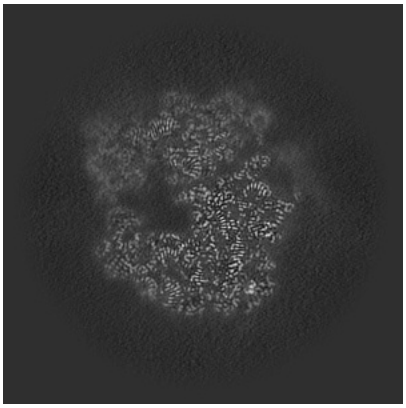


Z Index: 255

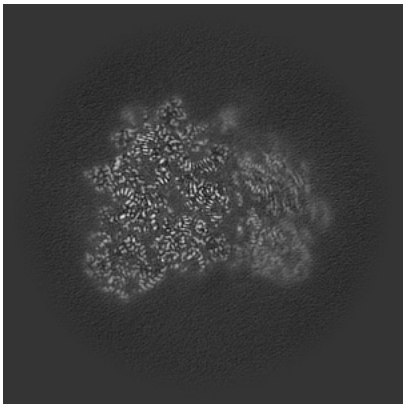
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

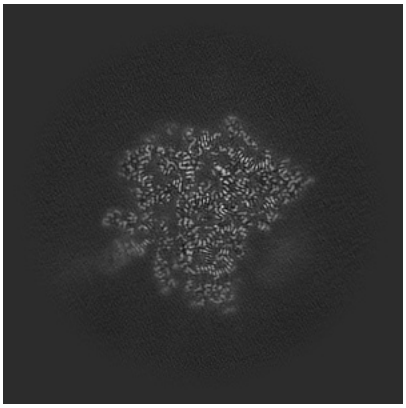
6.3.1 Primary map



X Index: 275



Y Index: 274

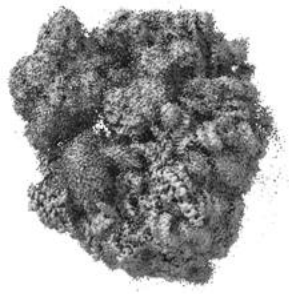


Z Index: 206

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

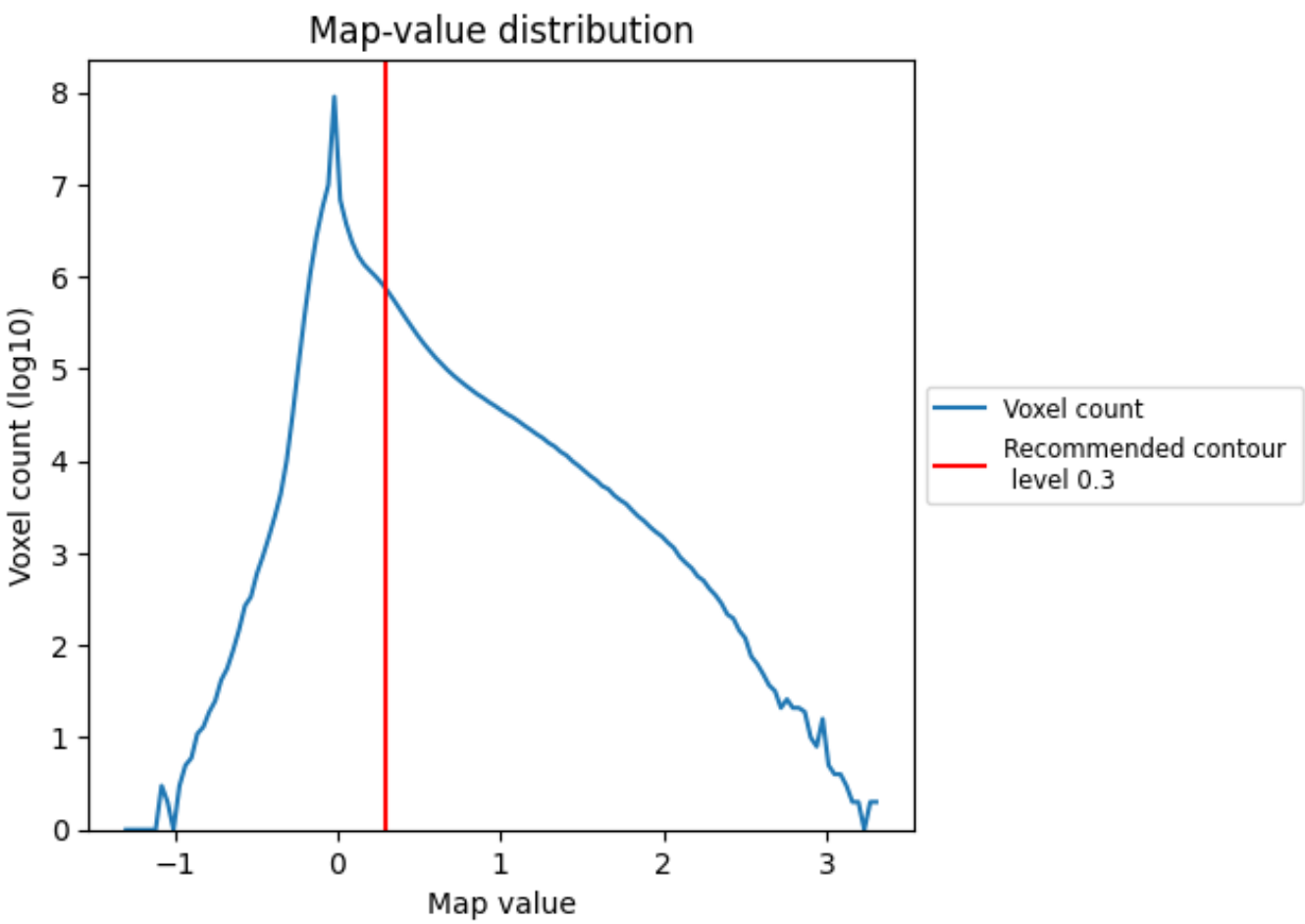
6.5 Mask visualisation (i)

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

7 Map analysis (i)

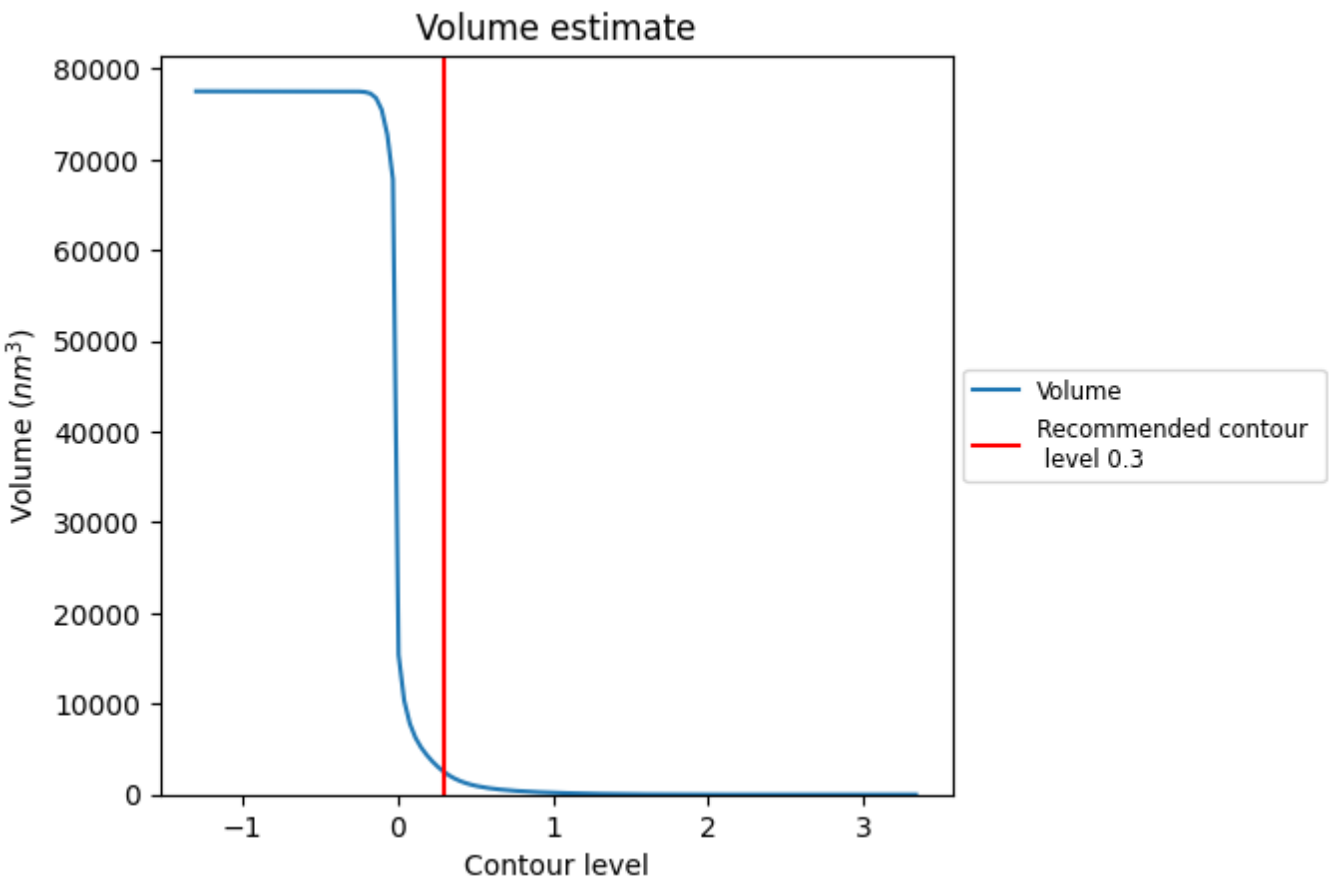
This section contains the results of statistical analysis of the map.

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.

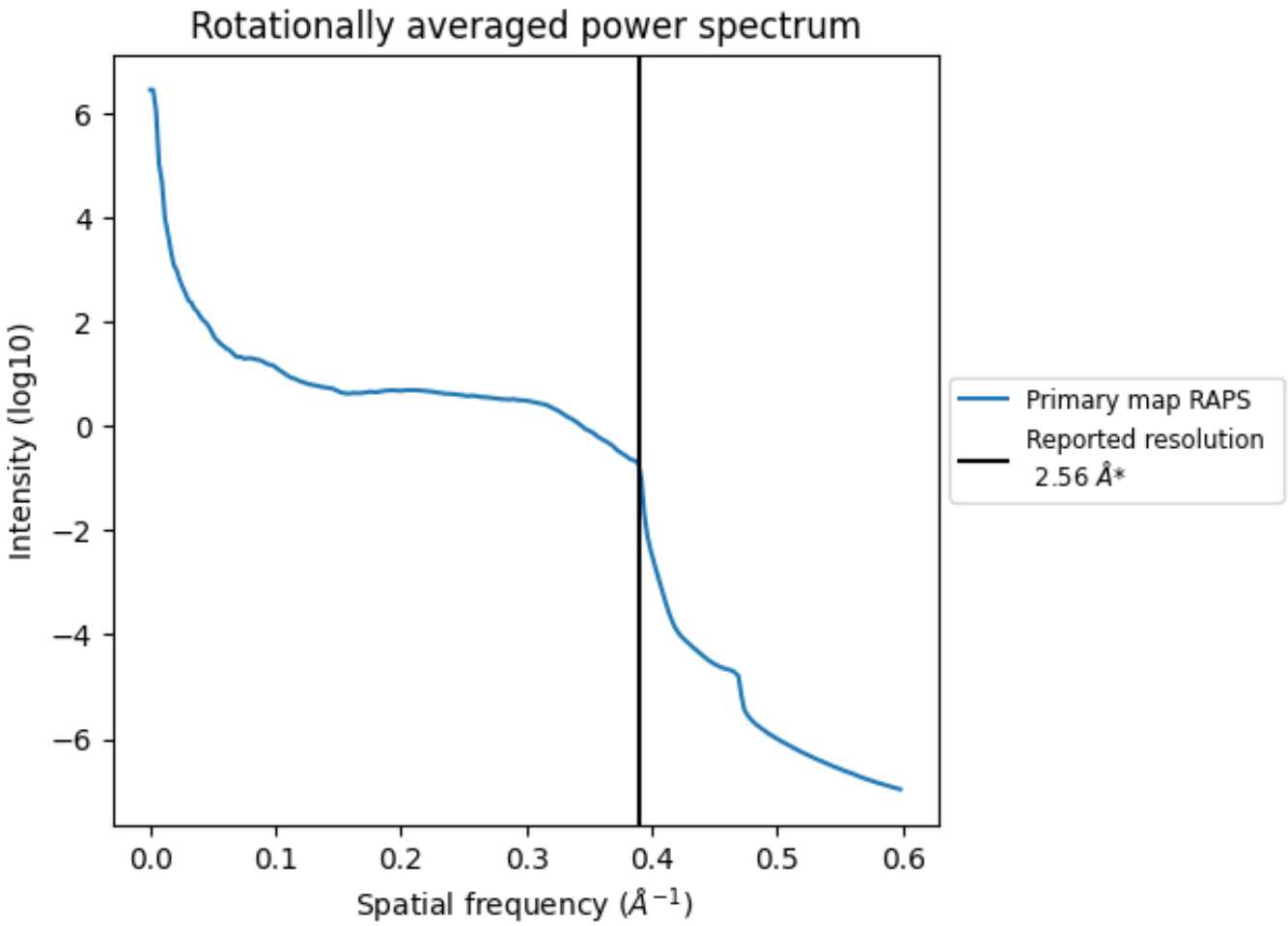
7.2 Volume estimate (i)



The volume at the recommended contour level is 2491 nm^3; this corresponds to an approximate mass of 2251 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

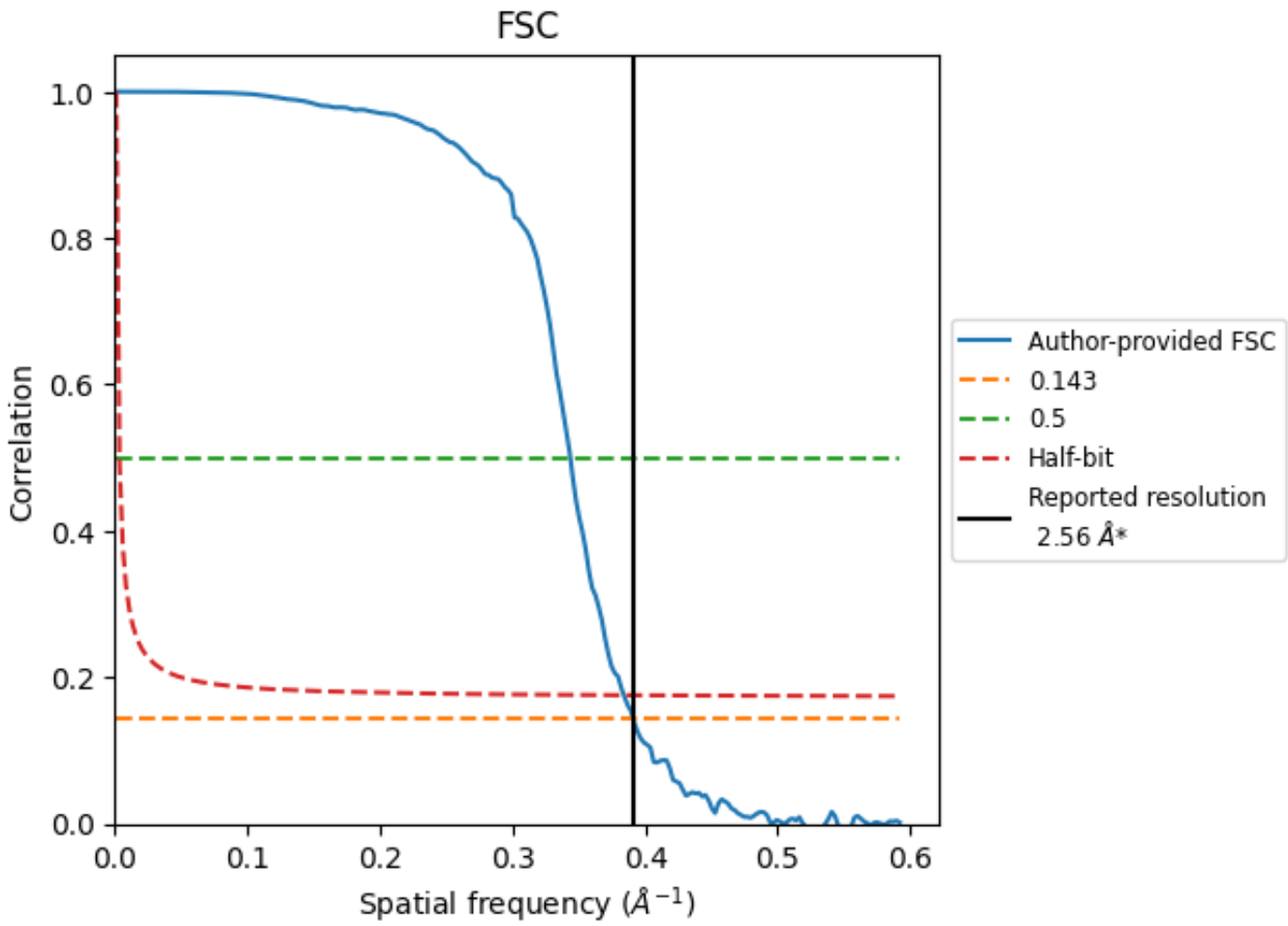


*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8.2 Resolution estimates (i)

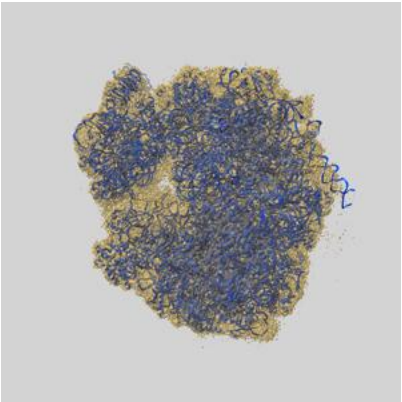
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	2.91	2.60
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

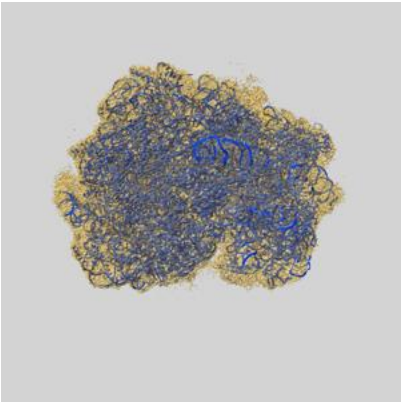
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13741 and PDB model 7Q08. Per-residue inclusion information can be found in section 3 on page 19.

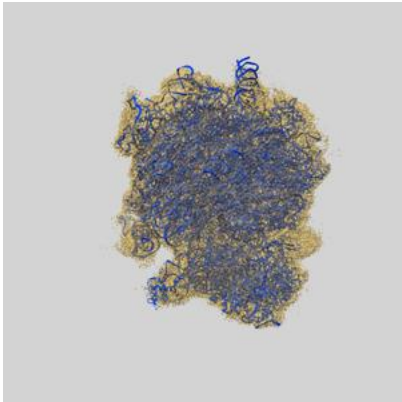
9.1 Map-model overlay (i)



X



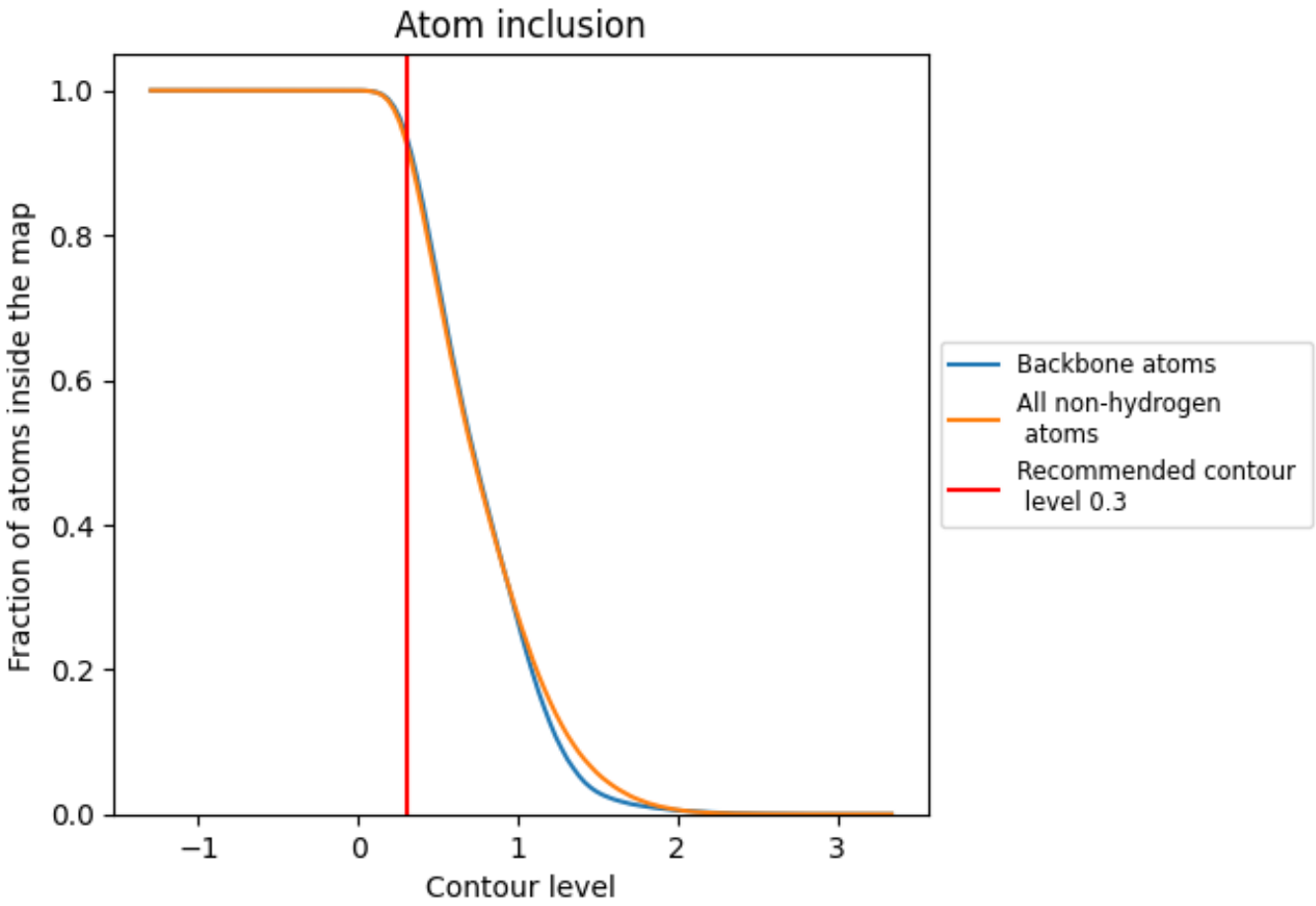
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.