Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 06:46 pm BST

PDB ID	:	8AGZ
EMDB ID	:	EMD-15428
Title	:	Yeast RQC complex in state with the RING domain of Ltn1 in the OUT position
Authors	:	Tesina, P.; Buschauer, R.; Beckmann, R.
Deposited on	:	2022-07-20
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

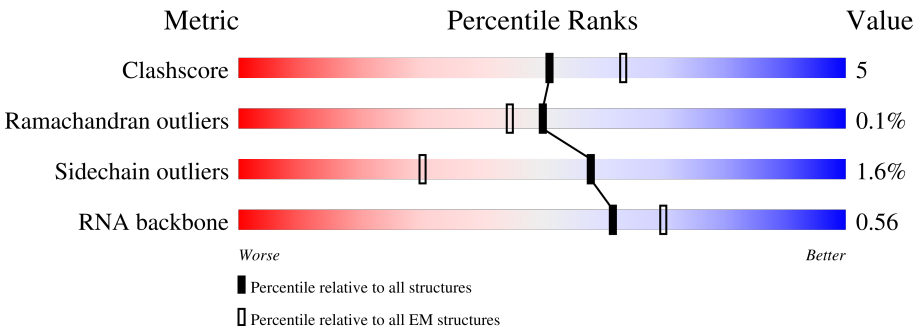
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	204	92% 8%
2	B	199	87% 12% ••
3	C	184	• 88% 12% •
4	D	186	92% 8% •
5	E	189	• 76% 7% 17%
6	F	172	88% 12% •
7	G	160	89% 11% •

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Mol	Chain	Length	Quality of chain
8	H	121	67% 15% 17%
9	I	137	88% 11%
10	J	155	37% 59%
11	K	142	84% 15%
12	L	127	92% 6%
13	M	136	92% 7%
14	N	149	92% 7%
15	O	59	83% 12%
16	P	105	86% 6% 9%
17	Q	113	80% 17%
18	R	130	92% 6%
19	S	107	93% 6%
20	T	121	88% 5% 7%
21	U	120	93% 6%
22	V	100	93% 6%
23	W	88	85% 7% 8%
24	X	78	88% 10%
25	Y	51	98%
26	Z	128	41% 59%
27	b	106	97%
28	c	92	99%
29	d	25	16% 88% 12%
30	f	3395	75% 18% 5%
31	h	121	85% 15%
32	i	158	78% 20%

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Mol	Chain	Length	Quality of chain
33	j	254	97%
34	k	387	99%
35	l	362	99%
36	m	297	98%
37	n	176	94% 5%
38	o	244	91% 9%
39	p	256	89% 9%
40	q	191	98%
41	r	221	98%
42	s	174	94%
43	t	199	96%
44	u	138	97%
45	a	1038	21% 81% 18%
46	e	1562	16% 92% 6%
47	g	245	91% 8%
48	v	157	39% 89% 10%
49	w	217	88% 99%
50	x	76	5% 66% 30%
50	y	76	67% 25%
51	z	165	89% 10%
52	0	312	30% 7% 61%
53	1	18	78% 22%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 151339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	203	1720	1077	361	281	1	0	0

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	197	1555	1003	289	262	1	197	0

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	183	1416	879	284	253	0	0

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	185	1441	908	290	241	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	156	1258	781	265	212	0	0

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	171	1437	925	266	243	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	159	1272	802	245	221	4	0	0

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	100	796	516	131	149	0	0

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	136	1003	628	189	179	7	0	0

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	63	518	333	102	82	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	121	964	620	169	173	2	0	0

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	125	984	620	191	173	0	0

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	135	1080	701	199	180	0	0

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	148	1169	747	231	188	3	0	0

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	58	462	289	100	73	0	0

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	96	737	476	123	137	1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	109	876	556	167	152	1	0	0

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	127	1013	642	205	165	1	0	0

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	106	850	540	165	144	1	0	0

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	112	880	545	179	152	4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	119	969	615	186	167	1	0	0

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	99	766	478	154	132	2	0	0

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	81	645	393	141	106	5	0	0

- Molecule 24 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	X	77	612	391	115	106	0	0

- Molecule 25 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	50	436	272	97	65	2	0	0

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	52	410	254	86	65	5	0	0

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	103	824	517	167	135	5	0	0

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	91	694	429	138	121	6	0	0

- Molecule 29 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	22	207	127	56	23	1	0	0

- Molecule 30 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	f	3216	68782	30723	12389	22454	3216	0	0

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	h	121	2579	1152	461	845	121	0	0

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	i	158	3353	1500	586	1109	158	0	0

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	246	1874	1168	380	325	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	386	3075	1950	584	533	8	0	0

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	361	2748	1729	522	494	3	0	0

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	294	2351	1484	410	455	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	n	167	1307	843	234	230	0	0

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	222	1784	1151	324	308	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	233	1804	1151	323	327	3	0	0

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	q	191	1508	957	274	273	4	0	0

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	r	218	1764	1117	334	306	7	0	0

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	s	169	1346	843	252	247	4	0	0

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	t	193	1543	962	315	266	0	0

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	u	136	1053	675	199	177	2	0	0

- Molecule 45 is a protein called RQC2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	a	848	6579	4194	1142	1226	17	0	0

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	e	1527	11506	7350	1937	2181	38	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	g	225	1651	1030	282	332	7	0	0

- Molecule 48 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	v	142	1085	676	183	217	9	0	0

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	w	216	1709	1092	298	310	9	0	0

- Molecule 50 is a RNA chain called Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	x	74	1579	702	277	526	74	0	0
50	y	73	1556	692	272	519	73	0	0

- Molecule 51 is a protein called 60S ribosomal protein L12-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	z	148	728	432	148	148	0	0

- Molecule 52 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	0	121	961	618	167	173	3	0	0

- Molecule 53 is a protein called CAT-tailed nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	1	18	90	54	18	18	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	A	1	1	1	0
54	C	1	1	1	0
54	E	1	1	1	0
54	I	1	1	1	0
54	R	1	1	1	0

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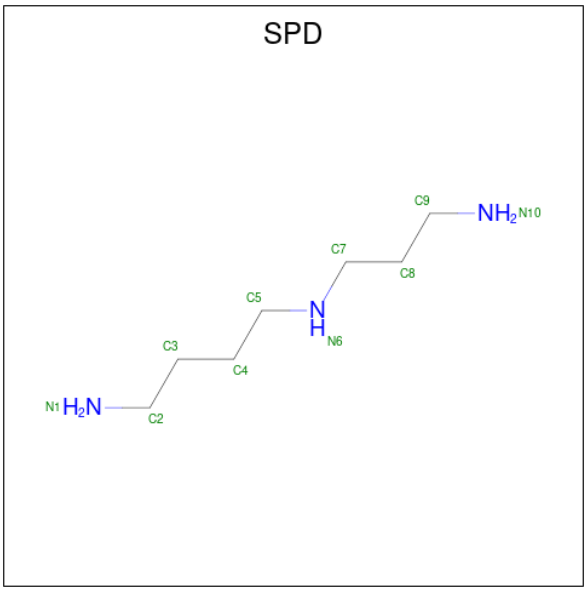
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	T	1	1	1	0
54	f	3	3	3	0
54	h	1	1	1	0
54	j	2	2	2	0
54	k	1	1	1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	T	1	1	1	0
55	W	1	1	1	0
55	Z	1	1	1	0
55	b	1	1	1	0
55	c	1	1	1	0
55	e	2	2	2	0

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

3 Residue-property plots (i)

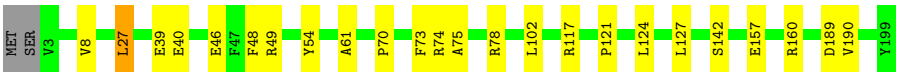
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 60S ribosomal protein L15-A

Chain A: 92% 8%

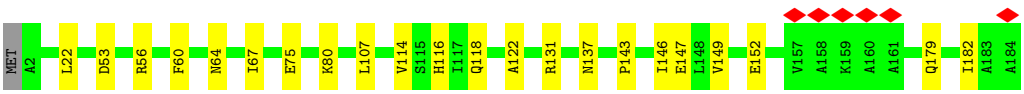
• Molecule 2: 60S ribosomal protein L16-A

Chain B: 87% 12%



• Molecule 3: 60S ribosomal protein L17-A

Chain C: 88% 12%

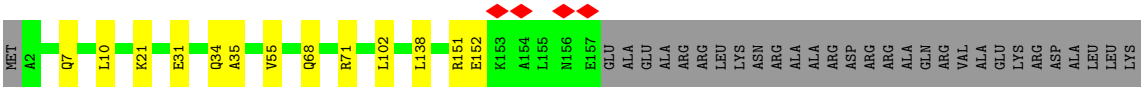


• Molecule 4: 60S ribosomal protein L18-A

Chain D: 92% 8%

• Molecule 5: 60S ribosomal protein L19-A

Chain E: 76% 7% 17%

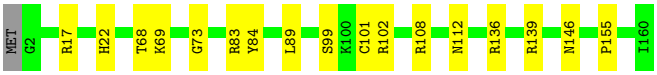


• Molecule 6: 60S ribosomal protein L20-A

Chain F:

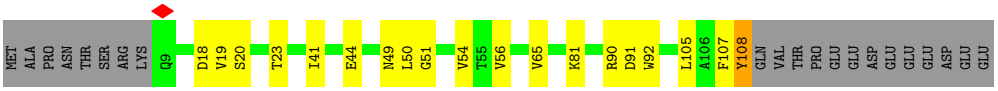
• Molecule 7: 60S ribosomal protein L21-A

Chain G:



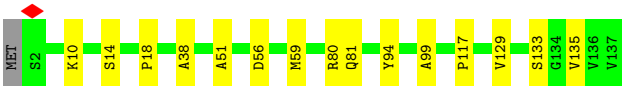
• Molecule 8: 60S ribosomal protein L22-A

Chain H:



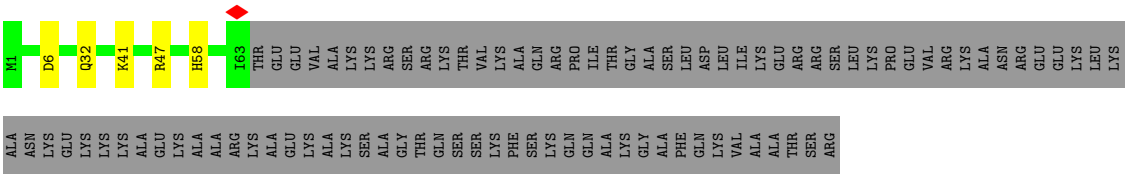
• Molecule 9: 60S ribosomal protein L23-A

Chain I:



• Molecule 10: 60S ribosomal protein L24-A

Chain J:

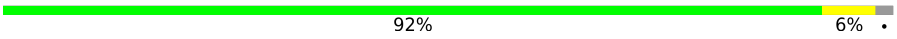


• Molecule 11: 60S ribosomal protein L25

Chain K:

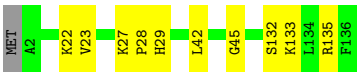
• Molecule 12: 60S ribosomal protein L26-A

Chain L:



• Molecule 13: 60S ribosomal protein L27-A

Chain M:

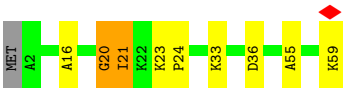


• Molecule 14: 60S ribosomal protein L28

Chain N:

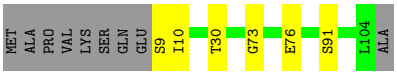
• Molecule 15: 60S ribosomal protein L29

Chain O:



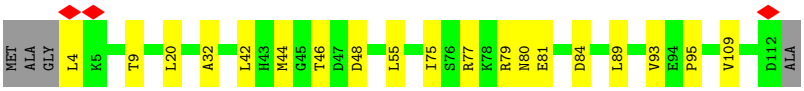
• Molecule 16: 60S ribosomal protein L30

Chain P:



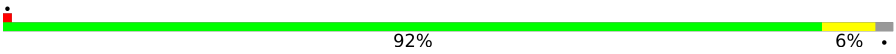
• Molecule 17: 60S ribosomal protein L31-A

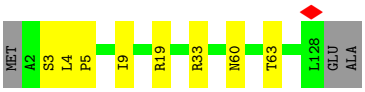
Chain Q:



• Molecule 18: 60S ribosomal protein L32

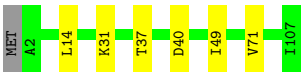
Chain R:





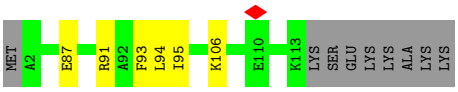
• Molecule 19: 60S ribosomal protein L33-A

Chain S: 93% 6%



• Molecule 20: 60S ribosomal protein L34-A

Chain T: 88% 5% 7%



• Molecule 21: 60S ribosomal protein L35-A

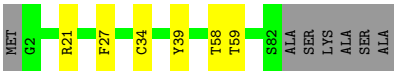
Chain U: 93% 6%

• Molecule 22: 60S ribosomal protein L36-A

Chain V: 93% 6%

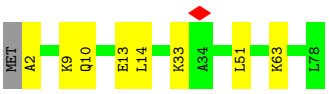
• Molecule 23: 60S ribosomal protein L37-A

Chain W: 85% 7% 8%



• Molecule 24: 60S ribosomal protein L38

Chain X: 88% 10%

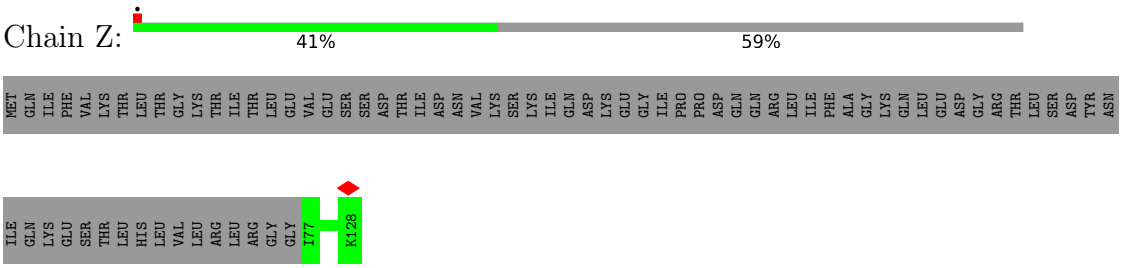


• Molecule 25: 60S ribosomal protein L39

Chain Y: 98%

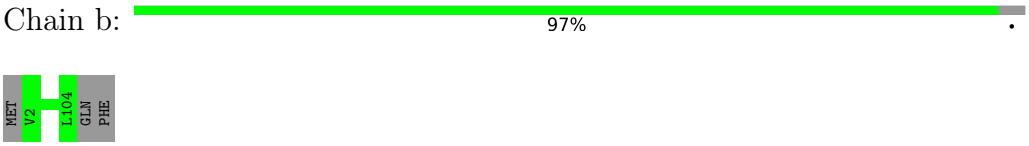
• Molecule 26: Ubiquitin-60S ribosomal protein L40

Chain Z:



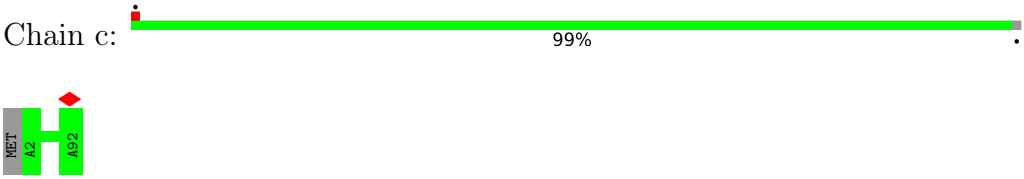
- Molecule 27: 60S ribosomal protein L42-A

Chain b:



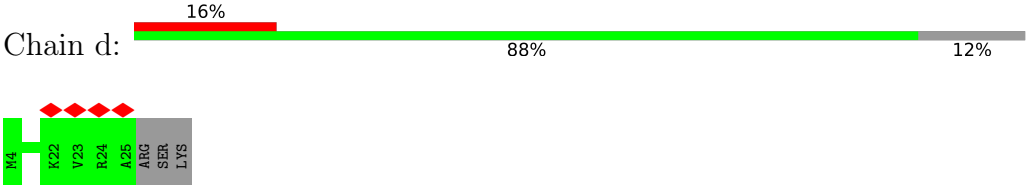
- Molecule 28: 60S ribosomal protein L43-A

Chain c:



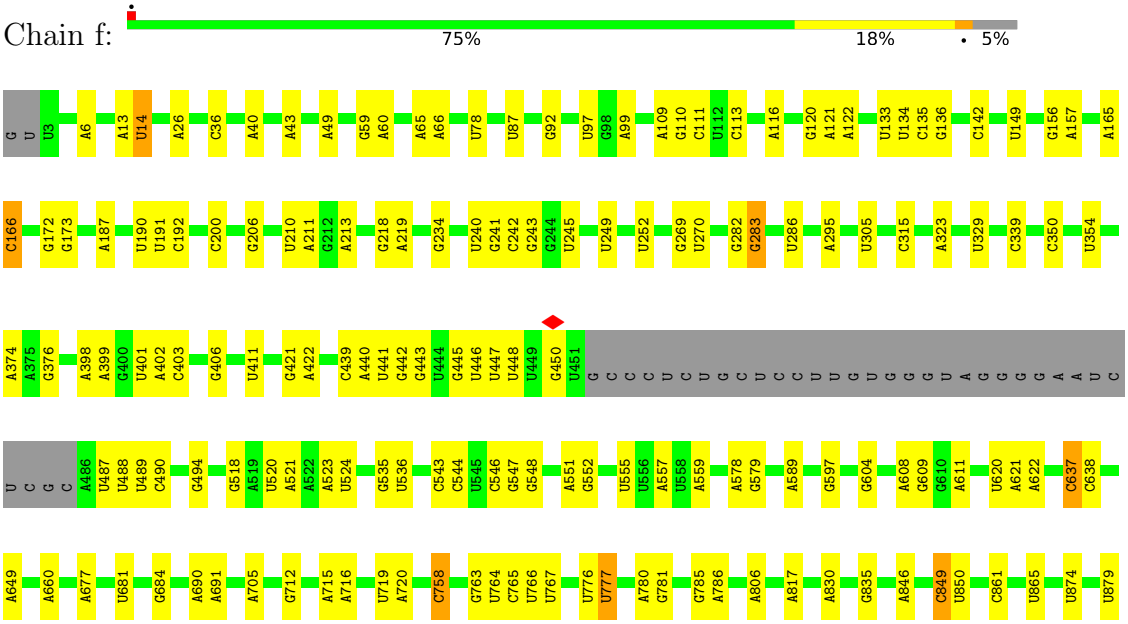
- Molecule 29: 60S ribosomal protein L41-A

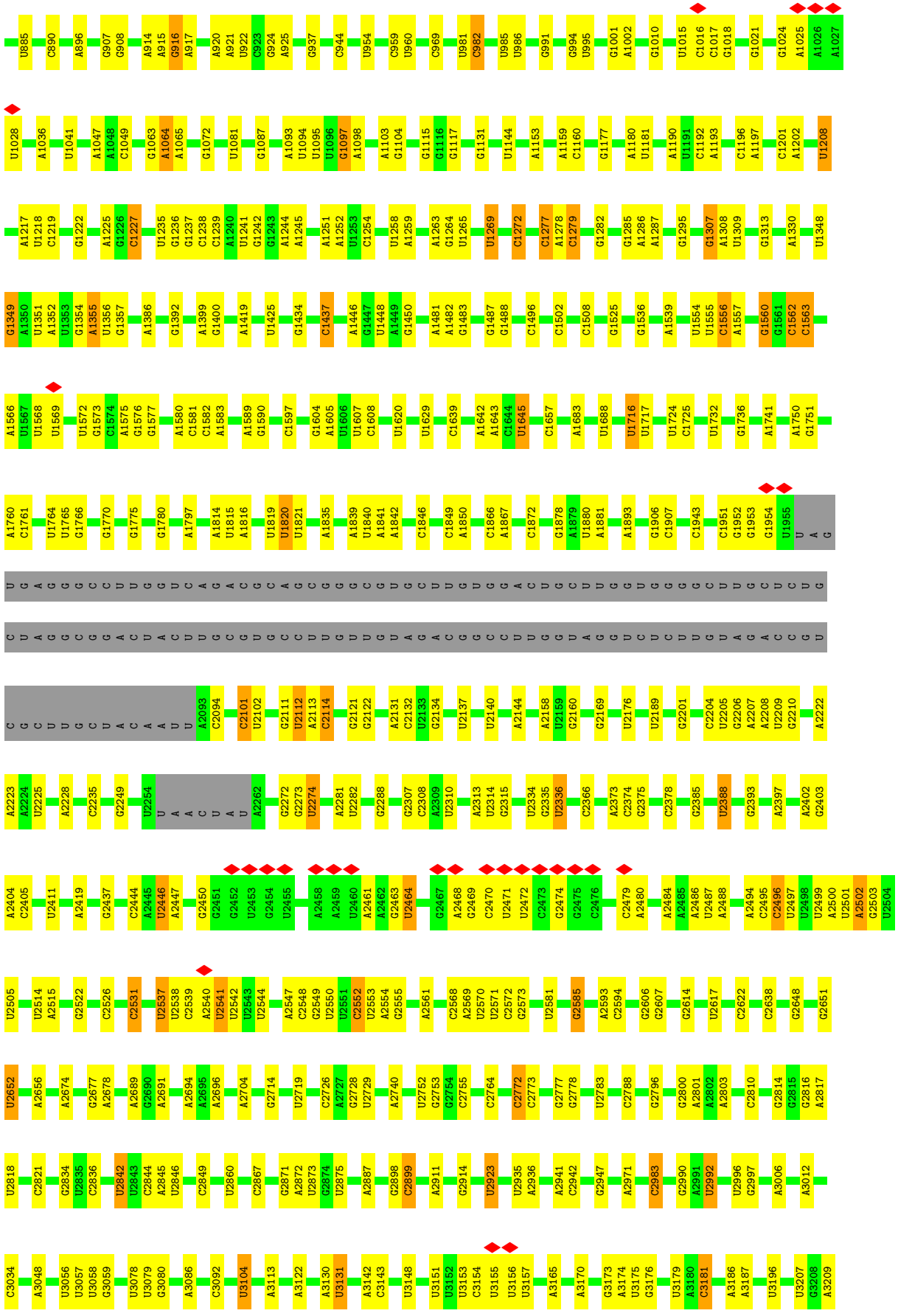
Chain d:



- Molecule 30: 25S rRNA

Chain f:

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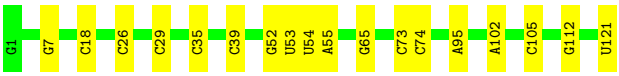
U1028 A1036 U1041 A1047 A1048 C1049 G1063 A1064 A1065 G1072 U1081 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 G1115 G1116 G1117 G1131 U1144 A1153 A1159 C1160 G1177 A1180 U1181 A1190 U1191 C1192 A1193 C1196 A1197 C1201 A1202 U1208
A1217 U1218 C1219 G1222 A1225 G1226 C1227 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 A1251 A1252 U1253 C1254 U1258 A1259 A1263 G1264 U1265 U1269 C1272 C1277 A1278 C1279 G1282 G1285 A1286 A1287 G1295 G1307 A1308 U1309 G1313 A1330 U1348
G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 A1386 G1392 A1399 G1400 A1419 U1425 G1434 C1437 A1446 G1447 U1448 A1449 G1450 A1481 A1482 G1483 G1487 G1488 C1496 C1502 C1508 G1525 G1536 A1539 U1554 U1555 C1556 A1557 G1560 G1561 C1562 C1563
A1566 U1567 U1568 U1569 U1572 G1573 C1574 A1575 G1576 G1577 A1580 C1581 C1582 A1583 A1589 G1590 C1597 G1604 A1605 U1606 U1607 C1608 U1620 U1629 C1639 A1642 A1643 C1644 U1645 C1657 A1683 U1688 U1716 U1717 U1724 C1725 U1732 G1736 A1741 A1750 G1751
A1760 C1761 U1764 U1765 G1766 G1770 G1775 G1780 A1797 A1814 U1815 A1816 U1819 U1820 U1821 A1835 A1839 U1840 A1841 A1842 C1846 C1849 A1850 C1866 A1867 C1872 G1878 A1879 U1880 A1881 A1893 G1906 C1907 C1943 C1951 G1952 G1953 G1954 U1955 U A G
U G A G G C C G U U G G G U C A G A C G G C A G C C U G G G C U G C U U G C C U U G C C U A G G U C U U G U C C U G
C U A G G C G G A C U A A C U U U G C C G U G C C C U G G U U C G U U G A G C U U G C G G C U U U G C C U U G G G U A G G U C U U G C C U G G G U C C U U G
C G C U U G C U A C A A U U A2093 C2094 C2101 U2102 G2111 U2112 A2113 C2114 G2121 G2122 A2131 C2132 U2133 G2134 U2137 U2140 A2144 A2158 U2159 G2160 G2169 U2176 U2189 G2201 C2204 U2205 G2206 A2207 A2208 U2209 G2210 A2222
A2223 A2224 U2225 A2228 C2235 G2249 U2254 U A A C U A U A2262 G2272 G2273 U2274 A2281 U2282 G2288 G2307 C2308 A2309 U2310 A2313 U2314 G2315 U2334 G2335 U2336 C2366 A2373 C2374 G2375 C2378 G2385 U2388 G2393 A2397 A2402 G2403
A2404 C2405 U2411 A2419 G2437 C2444 A2445 U2446 A2447 G2450 G2451 G2452 U2453 G2454 U2455 A2458 A2459 U2460 A2461 A2462 G2463 U2464 G2467 A2468 G2469 C2470 U2471 U2472 C2473 G2474 G2475 C2476 C2479 A2480 A2484 A2485 A2486 U2487 A2488 A2494 C2495 C2496 U2497 U2498 U2499 A2500 U2501 A2502 G2503 U2504
U2505 U2514 A2515 G2522 C2526 C2531 U2537 U2538 C2539 A2540 U2541 U2542 U2543 U2544 A2547 C2548 G2549 U2550 U2551 C2552 U2553 A2554 G2555 A2561 C2568 A2569 U2570 U2571 C2572 G2573 U2581 G2585 A2593 C2594 G2606 G2607 G2614 U2617 C2622 C2638 G2648 G2651
U2652 A2656 A2674 G2677 A2678 A2689 G2690 A2691 A2694 A2695 A2696 A2704 G2714 U2719 C2726 A2727 G2728 U2729 A2740 U2752 G2753 G2754 C2755 C2764 C2772 C2773 G2777 G2778 U2783 C2788 G2796 G2800 A2801 A2802 A2803 C2810 G2814 G2815 G2816 A2817
U2818 C2821 G2834 U2835 C2836 U2842 U2843 C2844 A2845 U2846 C2849 U2860 C2867 G2871 A2872 U2873 G2874 U2875 A2887 G2898 C2899 A2911 G2914 U2923 U2935 A2936 A2941 C2942 G2947 A2971 C2983 G2990 A2991 U2992 U2996 G2997 A3006 A3012
C3034 A3048 U3056 U3057 U3058 G3059 U3078 U3079 G3080 A3086 C3092 U3104 A3113 A3122 A3130 U3131 A3142 C3143 U3148 U3151 U3152 U3153 C3154 U3155 U3156 U3157 A3165 A3170 G3173 A3174 U3175 G3176 U3179 A3180 C3181 A3186 A3187 U3196 U3207 G3208 A3209

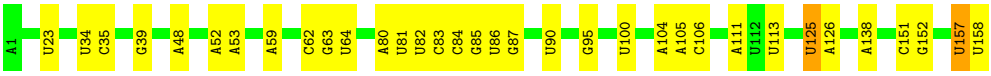
- Molecule 31: 5S rRNA

Chain h: 85% 15%



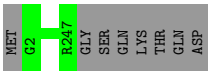
- Molecule 32: 5.8S rRNA

Chain i: 78% 20%



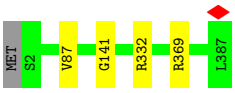
- Molecule 33: 60S ribosomal protein L2-A

Chain j: 97%



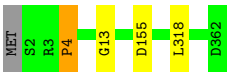
- Molecule 34: 60S ribosomal protein L3

Chain k: 99%



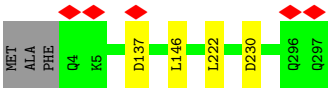
- Molecule 35: 60S ribosomal protein L4-A

Chain l: 99%



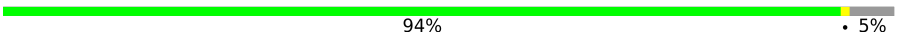
- Molecule 36: 60S ribosomal protein L5

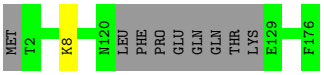
Chain m: 98%



- Molecule 37: 60S ribosomal protein L6-B

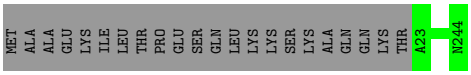
Chain n:





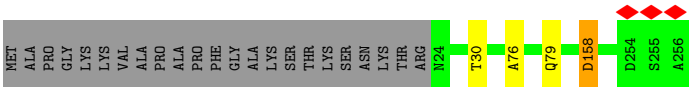
- Molecule 38: 60S ribosomal protein L7-A

Chain o:



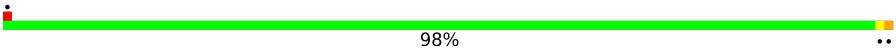
- Molecule 39: 60S ribosomal protein L8-A

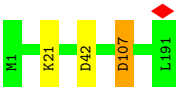
Chain p:



- Molecule 40: 60S ribosomal protein L9-A

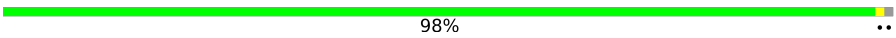
Chain q:

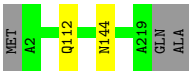




- Molecule 41: 60S ribosomal protein L10

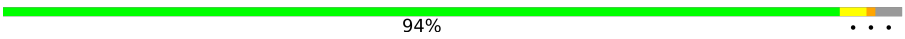
Chain r:

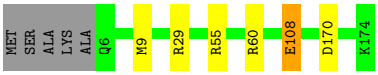




- Molecule 42: 60S ribosomal protein L11-A

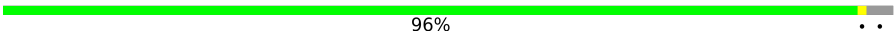
Chain s:

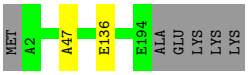




- Molecule 43: 60S ribosomal protein L13-A

Chain t:





• Molecule 44: 60S ribosomal protein L14-A

Chain u: 97%

MET SER T3 W12 D47 A138

• Molecule 45: RQC2 isoform 1

Chain a: 21% 81% 18%

M1 I5 K82 H83 V95 D96 Q97 D98 R99 I100 D107 F117 E127 N128 M132 R136 L139 E140 V145 G146 E150 M151 F152 D153 E154 S155 L156 F157 T158 T159 N160 N161 E162 S163 A164 D165 E166 S167 I168 E169 K170 N171 R172 K173 A174 E175 Y176 T177 S178

E179 L180 V181 N182 E183 W184 I185 K186 A187 V188 Q189 A190 K191 Y192 E193 S194 D195 I196 T197 V198 I199 K200 Q201 L202 N203 I204 Q205 G206 K207 E208 G209 A210 K211 K212 K213 K214 V215 K216 V217 P218 S219 I220 H221 K222 L223 L224 L225 S226 K227 V228 P229 H230 L231 S232 S233 D234 L240 F243

N244 I245 D246 P247 S248 E249 S250 C251 L252 N253 L254 L255 E256 E257 T258 D259 S260 L261 A262 E263 N266 L275 L276 T277 T278 T279 D280 R281 R289 N290 E291 N292 Y293 I294 S295 E296 K297 D298 T299 A300 D301 L302 E303 F304 I305 Y306 F309 I316 N317 G318 G319 D320 T321 D322 S323

S324 N334 A360 K363 D366 A367 L439 S456 LYS GLU LEU ASN THR SER SER ASP GLU ASP ASN GLU SER GLU GLY ASN THR THR ASP SER SER SER ASP SER ASP SER GLU ASP MET GLU SER SER LYS GLU ARG SER THR LYS SER MET LYS ARG LYS SER N501

K559 D560 S561 D607 S615 K627 T628 E629 V630 K651 S656 G670 S671 D672 N673 P677 A680 E686 H691 L697 F701 V707 K708 THR SER GLY ASN GLU ASP ASN GLY ASP ASP ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU

GLU GLU GLU GLU GLU GLU GLU GLU GLU LYS GLU GLU GLU LYS GLU GLU GLN GLN GLN ASP GLU ASP ASP SER ASN GLU VAL ASN GLY LEU GLU LYS GLY GLY ASP SER ASN ASP SER THR LYS ASN ASN SER PHE GLU HIS ASP ASN LEU GLU LYS ASP ILE GLU LYS

HIS CYS THR ILE SER SER ASP THR ASP SER ASP SER GLY ASN ALA LYS ALA LYS ASN ASP ASN SER SER THR GLN ARG ILE LEU ASP GLU PRO GLY VAL PRO ILE SER LEU ILE GLU ASN ILE ASN S835 E882 R889 E890 D891 R892 K893 R896 F907 T908 K909 K910 E911 K912

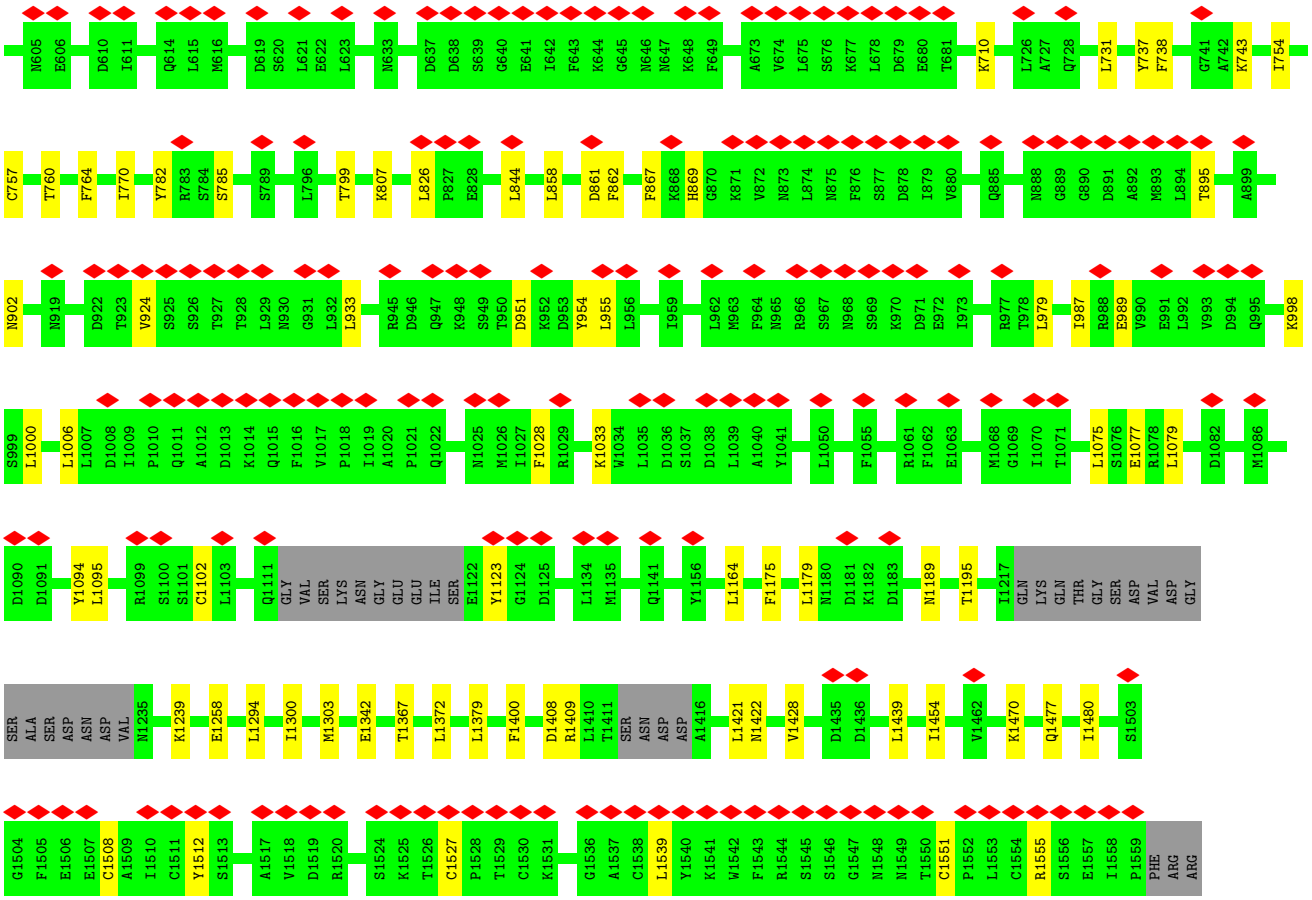
A913 R914 H920 L928 D929 K930 G931 D932 V933 V934 D935 D936 I937 I938 S960 S976 R977 P978 L979 D980 G981 S982 S983 T984 D985 N986 E987 H994 L1009 T1017 I1018 ALA GLY GLN LYS SER THR LYS ASN GLY GLY ASN SER SER LYS LYS GLY LYS LYS LYS ARG

• Molecule 46: E3 ubiquitin-protein ligase listerin

Chain e: 16% 92% 6%

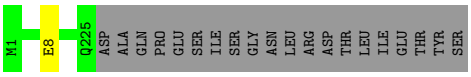
MET S2 Y12 F30 N77 V105 I125 T156 L178 V229 N254 V264 M277 T299 K305 V309 T327 P350 F354 D372 F380 R387 G392 F393 S394 A395 R396 F412 A413 E414 D415 S416 S417 E418 E419 R420 V421

K437 S440 E441 G451 V452 T467 D471 I472 R473 K474 I475 K476 T489 S490 P491 N492 N493 E494 I508 E509 T510 D511 P512 S513 N514 V515 D520 D533 M534 I535 F536 L537 I541 S555 K574 M575 N576 T577 D578 A579 I580 S592 F593 N594 L595 P596 K597 T598



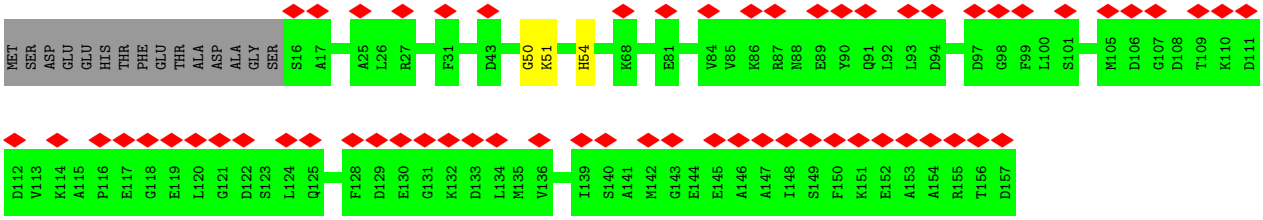
- Molecule 47: Eukaryotic translation initiation factor 6

Chain g:



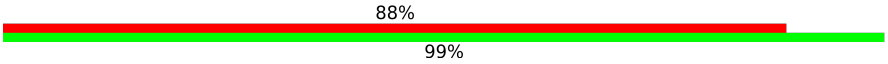
- Molecule 48: Eukaryotic translation initiation factor 5A-1

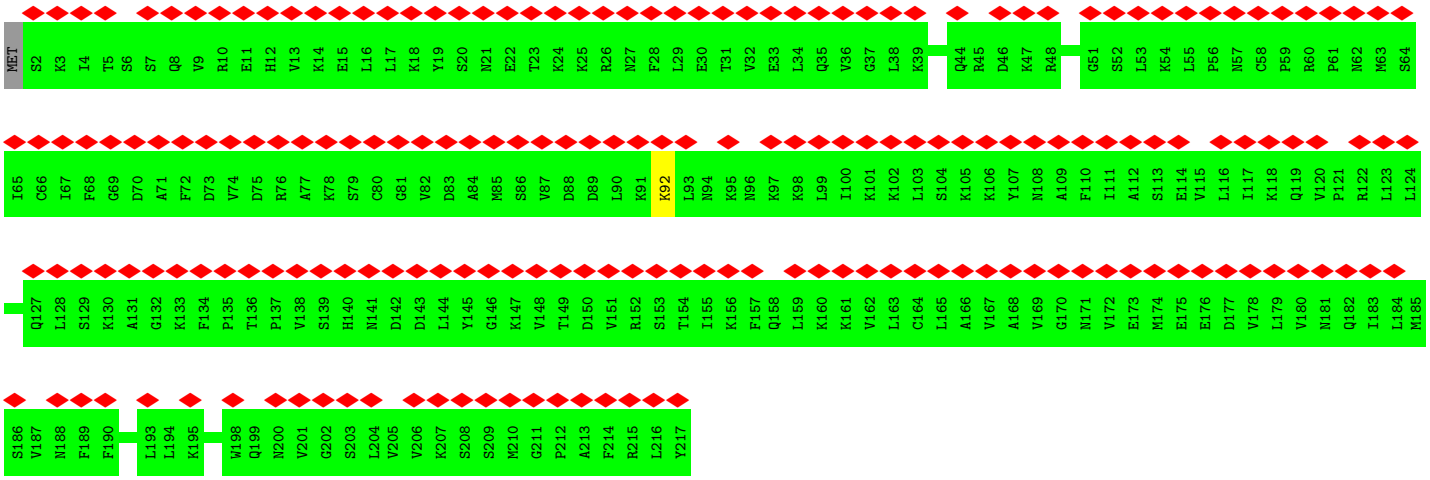
Chain v:



- Molecule 49: 60S ribosomal protein L1-A

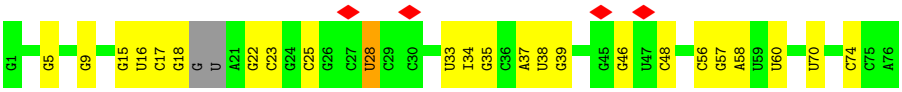
Chain w:





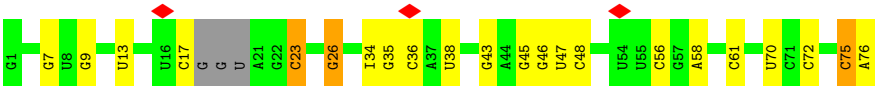
- Molecule 50: Ala tRNA

Chain x:



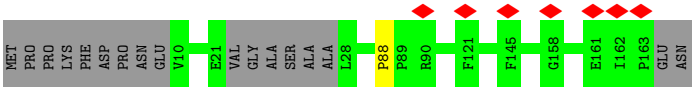
- Molecule 50: Ala tRNA

Chain y:



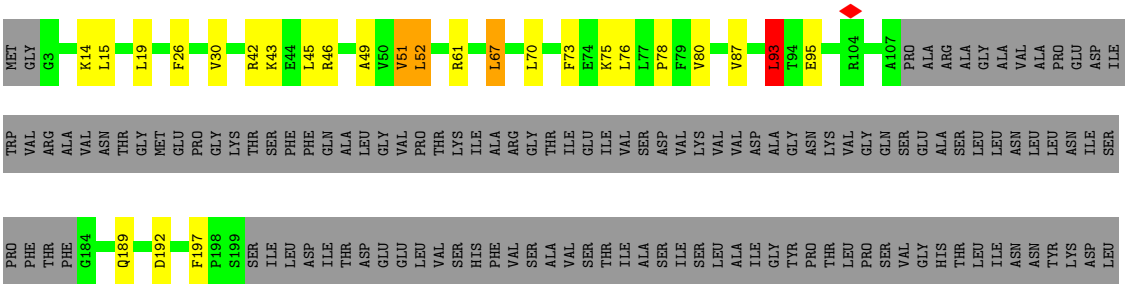
- Molecule 51: 60S ribosomal protein L12-B

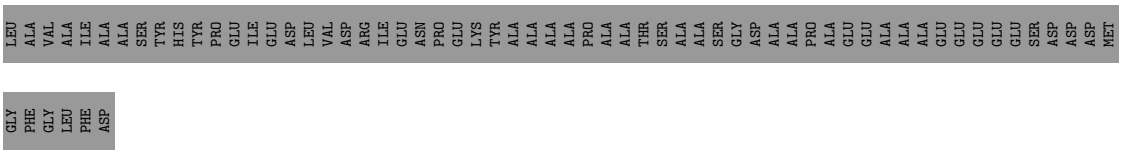
Chain z:



- Molecule 52: 60S acidic ribosomal protein P0

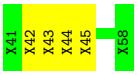
Chain 0:





• Molecule 53: CAT-tailed nascent chain

Chain 1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.680	Depositor
Minimum map value	-0.672	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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, ZN, MG, 5CT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/1757	0.70	1/2354 (0.0%)
2	B	0.39	0/1585	0.64	1/2128 (0.0%)
3	C	0.37	0/1439	0.71	2/1938 (0.1%)
4	D	0.34	0/1465	0.67	1/1965 (0.1%)
5	E	0.37	0/1275	0.67	1/1702 (0.1%)
6	F	0.38	0/1473	0.65	0/1980
7	G	0.36	0/1296	0.62	0/1739
8	H	0.39	0/812	0.69	3/1099 (0.3%)
9	I	0.35	0/1018	0.64	0/1369
10	J	0.36	0/530	0.63	0/703
11	K	0.41	0/979	0.69	1/1321 (0.1%)
12	L	0.35	0/995	0.67	1/1329 (0.1%)
13	M	0.36	0/1106	0.61	0/1485
14	N	0.40	0/1200	0.62	0/1607
15	O	0.32	0/473	0.72	2/629 (0.3%)
16	P	0.35	0/745	0.68	0/1001
17	Q	0.39	0/890	0.77	2/1196 (0.2%)
18	R	0.32	0/1034	0.59	0/1385
19	S	0.38	0/868	0.61	0/1168
20	T	0.35	0/890	0.67	0/1189
21	U	0.34	0/978	0.65	1/1301 (0.1%)
22	V	0.34	0/772	0.66	0/1026
23	W	0.39	0/660	0.69	0/875
24	X	0.33	0/618	0.78	1/826 (0.1%)
25	Y	0.33	0/443	0.65	0/588
26	Z	0.33	0/416	0.70	0/553
27	b	0.36	0/836	0.65	0/1104
28	c	0.36	0/701	0.66	0/934
29	d	0.26	0/208	0.84	0/267
30	f	0.61	0/76989	1.03	301/120031 (0.3%)
31	h	0.53	0/2883	0.98	9/4491 (0.2%)
32	i	0.60	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	j	0.37	0/1908	0.67	0/2564
34	k	0.37	0/3146	0.64	1/4228 (0.0%)
35	l	0.36	0/2800	0.65	2/3790 (0.1%)
36	m	0.34	0/2400	0.66	4/3239 (0.1%)
37	n	0.36	0/1329	0.67	0/1794
38	o	0.37	0/1821	0.61	0/2451
39	p	0.34	0/1836	0.62	2/2481 (0.1%)
40	q	0.37	0/1529	0.68	2/2060 (0.1%)
41	r	0.33	0/1801	0.64	0/2416
42	s	0.36	0/1367	0.70	3/1834 (0.2%)
43	t	0.36	0/1568	0.69	1/2106 (0.0%)
44	u	0.34	0/1068	0.66	1/1438 (0.1%)
45	a	0.31	0/6689	0.57	3/9023 (0.0%)
46	e	0.37	0/11705	0.57	1/15895 (0.0%)
47	g	0.32	0/1672	0.63	0/2281
48	v	0.31	0/1084	0.62	1/1456 (0.1%)
49	w	0.33	0/1736	0.65	0/2332
50	x	0.36	0/1760	1.02	8/2738 (0.3%)
50	y	0.40	0/1734	1.10	7/2697 (0.3%)
51	z	0.37	0/726	0.60	0/1006
52	0	0.33	0/976	0.55	0/1313
All	All	0.50	0/161735	0.88	370/236257 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	O	0	1
21	U	0	1
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	1
47	g	0	1
All	All	0	12

There are no bond length outliers.

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3217	C	N1-C2-O2	12.11	126.17	118.90
30	f	3217	C	C2-N1-C1'	11.31	131.25	118.80
50	y	75	C	C6-N1-C2	-10.30	116.18	120.30
30	f	3217	C	N3-C2-O2	-9.73	115.09	121.90
11	K	134	ASP	CB-CG-OD1	9.72	127.05	118.30
30	f	922	U	C2-N1-C1'	9.30	128.86	117.70
17	Q	84	ASP	CB-CG-OD1	9.26	126.64	118.30
50	y	75	C	C5-C6-N1	9.09	125.55	121.00
30	f	2531	C	N1-C2-O2	8.89	124.23	118.90
30	f	922	U	N1-C2-O2	8.84	128.99	122.80
30	f	3278	C	N1-C2-O2	8.70	124.12	118.90
30	f	3181	C	N1-C2-O2	8.69	124.11	118.90
30	f	3181	C	C2-N1-C1'	8.47	128.12	118.80
30	f	2836	C	N3-C2-O2	-8.26	116.12	121.90
30	f	1279	C	C5-C6-N1	8.24	125.12	121.00
30	f	2836	C	C2-N1-C1'	8.19	127.81	118.80
36	m	230	ASP	CB-CG-OD1	8.12	125.61	118.30
30	f	1496	C	C2-N1-C1'	8.10	127.71	118.80
30	f	922	U	N3-C2-O2	-8.00	116.60	122.20
30	f	406	G	O4'-C1'-N9	7.98	114.58	108.20
30	f	1645	U	N3-C2-O2	-7.86	116.70	122.20
4	D	41	ASP	CB-CG-OD1	7.84	125.36	118.30
30	f	2205	U	N1-C2-O2	7.84	128.29	122.80
30	f	2444	C	C2-N1-C1'	7.82	127.40	118.80
30	f	3217	C	C6-N1-C2	-7.79	117.18	120.30
30	f	3217	C	C6-N1-C1'	-7.76	111.48	120.80
30	f	2983	C	C2-N1-C1'	7.74	127.31	118.80
30	f	1208	U	N1-C2-O2	7.73	128.21	122.80
30	f	3306	U	N3-C2-O2	-7.71	116.80	122.20
30	f	2652	U	N3-C2-O2	-7.66	116.84	122.20
30	f	3278	C	N3-C2-O2	-7.58	116.60	121.90
30	f	2541	U	P-O3'-C3'	7.53	128.74	119.70
30	f	3278	C	C2-N1-C1'	7.53	127.09	118.80
30	f	3306	U	C2-N1-C1'	7.53	126.74	117.70
30	f	2205	U	N3-C2-O2	-7.51	116.94	122.20
30	f	758	C	C2-N1-C1'	7.42	126.97	118.80
30	f	1277	C	C2-N1-C1'	7.41	126.95	118.80
30	f	1645	U	N1-C2-O2	7.41	127.98	122.80
30	f	2836	C	N1-C2-O2	7.40	123.34	118.90
30	f	2502	A	OP2-P-O3'	7.39	121.46	105.20
30	f	2235	C	C2-N1-C1'	7.38	126.92	118.80
30	f	3181	C	N3-C2-O2	-7.31	116.78	121.90
30	f	1556	C	N1-C2-O2	7.31	123.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	1239	C	C2-N1-C1'	7.26	126.78	118.80
30	f	1349	G	N3-C4-C5	-7.22	124.99	128.60
15	O	36	ASP	CB-CG-OD1	7.22	124.80	118.30
30	f	2531	C	C2-N1-C1'	7.18	126.70	118.80
42	s	170	ASP	CB-CG-OD1	7.18	124.76	118.30
30	f	2923	U	N1-C2-O2	7.15	127.81	122.80
39	p	158	ASP	CB-CG-OD1	7.13	124.72	118.30
30	f	2502	A	P-O3'-C3'	7.13	128.25	119.70
30	f	1227	C	C2-N1-C1'	7.12	126.64	118.80
30	f	1277	C	N1-C2-O2	7.11	123.17	118.90
30	f	2205	U	C2-N1-C1'	7.11	126.24	117.70
30	f	78	U	N3-C2-O2	-7.11	117.22	122.20
30	f	1227	C	N1-C2-O2	7.09	123.15	118.90
30	f	1307	G	P-O3'-C3'	7.07	128.19	119.70
30	f	1604	G	C4-N9-C1'	7.07	135.69	126.50
30	f	982	C	C2-N1-C1'	7.06	126.57	118.80
30	f	1815	U	P-O3'-C3'	7.06	128.17	119.70
30	f	14	U	O5'-P-OP2	-7.03	99.37	105.70
30	f	1645	U	C2-N1-C1'	7.01	126.11	117.70
30	f	36	C	N1-C2-O2	7.01	123.11	118.90
30	f	1872	C	N1-C2-O2	6.97	123.08	118.90
30	f	2405	C	C6-N1-C2	-6.97	117.51	120.30
30	f	1272	C	N1-C2-O2	6.96	123.07	118.90
30	f	1208	U	C2-N1-C1'	6.93	126.02	117.70
30	f	1349	G	C4-N9-C1'	6.93	135.51	126.50
50	x	25	C	N3-C2-O2	-6.92	117.05	121.90
30	f	3306	U	N1-C2-O2	6.90	127.63	122.80
30	f	1227	C	C5-C6-N1	6.86	124.43	121.00
30	f	3217	C	C5-C6-N1	6.86	124.43	121.00
30	f	3275	U	OP1-P-O3'	6.84	120.26	105.20
30	f	3235	C	C2-N1-C1'	6.83	126.32	118.80
30	f	2923	U	N3-C2-O2	-6.81	117.43	122.20
30	f	2846	U	C2-N1-C1'	6.80	125.86	117.70
30	f	2846	U	N3-C2-O2	-6.78	117.45	122.20
30	f	1227	C	C6-N1-C2	-6.78	117.59	120.30
30	f	270	U	N1-C2-O2	6.76	127.53	122.80
12	L	11	ASP	CB-CG-OD1	6.76	124.38	118.30
30	f	2537	U	P-O3'-C3'	6.67	127.71	119.70
50	x	28	U	N3-C4-O4	6.67	124.07	119.40
30	f	2983	C	N3-C2-O2	-6.66	117.23	121.90
30	f	2189	U	N1-C2-O2	6.66	127.46	122.80
30	f	2836	C	C6-N1-C2	-6.65	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	h	26	C	N1-C2-O2	6.65	122.89	118.90
30	f	270	U	N3-C2-O2	-6.64	117.55	122.20
30	f	2531	C	N3-C2-O2	-6.64	117.25	121.90
30	f	3058	U	C2-N1-C1'	6.61	125.63	117.70
30	f	2112	U	OP2-P-O3'	6.60	119.72	105.20
30	f	1239	C	N1-C2-O2	6.54	122.83	118.90
2	B	27[A]	LEU	CB-CG-CD2	-6.54	99.88	111.00
30	f	2189	U	N3-C2-O2	-6.52	117.64	122.20
30	f	2235	C	C6-N1-C2	-6.51	117.70	120.30
30	f	3214	U	C2-N1-C1'	6.51	125.51	117.70
32	i	64	U	N3-C2-O2	-6.49	117.66	122.20
30	f	1208	U	N3-C2-O2	-6.49	117.66	122.20
30	f	2101	C	P-O3'-C3'	6.47	127.46	119.70
30	f	3034	C	N1-C2-O2	6.46	122.78	118.90
30	f	2112	U	P-O3'-C3'	6.46	127.45	119.70
30	f	524	U	N1-C2-O2	6.40	127.28	122.80
44	u	47	ASP	CB-CG-OD1	6.40	124.06	118.30
30	f	2550	U	N3-C2-O2	-6.38	117.73	122.20
35	l	155	ASP	CB-CG-OD1	6.38	124.04	118.30
30	f	1556	C	N3-C2-O2	-6.38	117.44	121.90
30	f	1269	U	C2-N1-C1'	6.37	125.34	117.70
30	f	1269	U	N1-C2-O2	6.34	127.24	122.80
30	f	2983	C	N1-C2-O2	6.34	122.70	118.90
31	h	105	C	N1-C2-O2	6.33	122.70	118.90
30	f	865	U	N3-C2-O2	-6.33	117.77	122.20
21	U	79	ASP	CB-CG-OD1	6.32	123.99	118.30
30	f	986	U	N3-C2-O2	-6.32	117.78	122.20
30	f	2274	U	N1-C2-O2	6.31	127.22	122.80
30	f	3058	U	N1-C2-O2	6.31	127.22	122.80
30	f	524	U	N3-C2-O2	-6.29	117.80	122.20
30	f	2617	U	N3-C2-O2	-6.29	117.80	122.20
36	m	137	ASP	CB-CG-OD1	6.28	123.95	118.30
30	f	922	U	C6-N1-C1'	-6.27	112.42	121.20
30	f	2726	C	N3-C2-O2	-6.27	117.51	121.90
30	f	2464	U	C2-N1-C1'	6.26	125.21	117.70
30	f	1496	C	C6-N1-C2	-6.26	117.80	120.30
1	A	153	ASP	CB-CG-OD1	6.25	123.92	118.30
45	a	697	LEU	CA-CB-CG	6.25	129.67	115.30
30	f	36	C	N3-C2-O2	-6.22	117.54	121.90
30	f	1097	G	P-O3'-C3'	6.22	127.17	119.70
30	f	1269	U	N3-C2-O2	-6.22	117.85	122.20
30	f	2444	C	C6-N1-C2	-6.21	117.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	2726	C	C2-N1-C1'	6.21	125.62	118.80
30	f	1349	G	N3-C4-N9	6.20	129.72	126.00
30	f	192	C	C2-N1-C1'	6.19	125.61	118.80
30	f	1716	U	P-O3'-C3'	6.18	127.11	119.70
30	f	1878	G	C4-N9-C1'	6.18	134.53	126.50
40	q	42	ASP	CB-CG-OD1	6.18	123.86	118.30
30	f	3104	U	N1-C2-O2	6.17	127.12	122.80
30	f	637	C	P-O3'-C3'	6.14	127.07	119.70
30	f	915	A	C2-N3-C4	6.14	113.67	110.60
30	f	2846	U	N1-C2-O2	6.13	127.09	122.80
30	f	2550	U	C2-N1-C1'	6.13	125.05	117.70
30	f	2388	U	N3-C2-O2	-6.12	117.92	122.20
30	f	1115	G	C4-N9-C1'	6.09	134.41	126.50
30	f	2842	U	N1-C2-O2	6.08	127.06	122.80
30	f	2923	U	C2-N1-C1'	6.07	124.98	117.70
30	f	3104	U	N3-C2-O2	-6.06	117.96	122.20
30	f	995	U	N1-C2-O2	6.06	127.04	122.80
30	f	1064	A	P-O3'-C3'	6.04	126.95	119.70
30	f	2553	U	C2-N1-C1'	6.04	124.95	117.70
30	f	1872	C	N3-C2-O2	-6.04	117.67	121.90
30	f	3300	U	N3-C2-O2	-6.03	117.98	122.20
30	f	1604	G	C8-N9-C1'	-6.03	119.17	127.00
30	f	2274	U	C2-N1-C1'	6.03	124.93	117.70
30	f	2132	C	N3-C2-O2	-6.02	117.69	121.90
31	h	26	C	C6-N1-C2	-6.02	117.89	120.30
30	f	2204	C	C6-N1-C2	-6.01	117.90	120.30
30	f	3131	U	C2-N1-C1'	5.98	124.87	117.70
30	f	1907	C	N1-C2-O2	5.97	122.48	118.90
30	f	2585	G	N3-C4-C5	-5.97	125.61	128.60
30	f	2405	C	N3-C2-O2	-5.96	117.72	121.90
30	f	985	U	N3-C2-O2	-5.96	118.03	122.20
8	H	51	GLY	C-N-CA	5.95	136.59	121.70
30	f	1604	G	N3-C4-N9	5.95	129.57	126.00
8	H	18	ASP	CB-CG-OD1	5.94	123.65	118.30
34	k	87	VAL	CG1-CB-CG2	-5.94	101.39	110.90
30	f	969	C	C6-N1-C2	-5.94	117.92	120.30
30	f	2132	C	C6-N1-C2	-5.94	117.92	120.30
30	f	2652	U	N1-C2-O2	5.94	126.96	122.80
30	f	1355	A	P-O3'-C3'	5.94	126.82	119.70
30	f	3181	C	C6-N1-C1'	-5.93	113.68	120.80
30	f	1556	C	C2-N1-C1'	5.93	125.32	118.80
32	i	100	U	C2-N1-C1'	5.91	124.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	3048	A	O4'-C1'-N9	5.91	112.92	108.20
30	f	1425	U	N3-C2-O2	-5.90	118.07	122.20
30	f	865	U	N1-C2-O2	5.90	126.93	122.80
30	f	1279	C	C6-N1-C2	-5.88	117.95	120.30
30	f	1820	U	P-O3'-C3'	5.87	126.75	119.70
30	f	1562	C	P-O3'-C3'	5.87	126.74	119.70
30	f	3214	U	N3-C2-O2	-5.86	118.10	122.20
30	f	1525	G	C4-N9-C1'	5.86	134.11	126.50
30	f	1272	C	N3-C2-O2	-5.84	117.81	121.90
30	f	1437	C	C2-N1-C1'	5.83	125.21	118.80
30	f	1604	G	N3-C4-C5	-5.82	125.69	128.60
30	f	3316	A	P-O3'-C3'	5.82	126.68	119.70
30	f	2531	C	C6-N1-C2	-5.81	117.97	120.30
30	f	142	C	N1-C2-O2	5.80	122.38	118.90
30	f	835	G	O4'-C1'-N9	5.79	112.83	108.20
30	f	1577	G	N1-C6-O6	-5.79	116.42	119.90
30	f	2204	C	C5-C6-N1	5.79	123.90	121.00
42	s	9	MET	CA-CB-CG	5.79	123.14	113.30
30	f	2638	C	N1-C2-O2	5.78	122.37	118.90
30	f	3350	C	C6-N1-C2	-5.78	117.99	120.30
30	f	2274	U	N3-C2-O2	-5.75	118.18	122.20
30	f	2531	C	C5-C6-N1	5.74	123.87	121.00
30	f	3228	C	P-O3'-C3'	5.74	126.58	119.70
45	a	117	PHE	N-CA-CB	-5.73	100.29	110.60
30	f	270	U	C2-N1-C1'	5.72	124.57	117.70
30	f	2132	C	N1-C2-O2	5.71	122.32	118.90
30	f	2622	C	N1-C2-O2	5.71	122.32	118.90
30	f	3218	A	P-O3'-C3'	5.70	126.54	119.70
30	f	1190	A	C4-N9-C1'	5.70	136.56	126.30
30	f	282	G	P-O3'-C3'	5.69	126.53	119.70
30	f	354	U	N1-C2-O2	5.68	126.78	122.80
30	f	2992	U	N3-C2-O2	-5.68	118.22	122.20
8	H	50	LEU	CA-CB-CG	5.67	128.33	115.30
30	f	916	G	P-O3'-C3'	5.66	126.50	119.70
30	f	2899	C	N3-C2-O2	-5.66	117.94	121.90
30	f	97	U	N3-C2-O2	-5.65	118.24	122.20
30	f	3034	C	N3-C2-O2	-5.65	117.94	121.90
30	f	142	C	C6-N1-C2	-5.65	118.04	120.30
30	f	2899	C	C2-N1-C1'	5.65	125.02	118.80
30	f	1277	C	N3-C2-O2	-5.65	117.95	121.90
30	f	2366	C	C2-N1-C1'	5.65	125.01	118.80
30	f	2553	U	C6-N1-C1'	-5.64	113.30	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	2842	U	N3-C2-O2	-5.62	118.27	122.20
30	f	113	C	C2-N1-C1'	5.62	124.98	118.80
30	f	3058	U	N3-C2-O2	-5.61	118.27	122.20
31	h	26	C	N3-C2-O2	-5.61	117.98	121.90
30	f	1448	U	N3-C2-O2	-5.60	118.28	122.20
30	f	2378	C	C2-N1-C1'	5.60	124.96	118.80
30	f	1349	G	C8-N9-C1'	-5.60	119.72	127.00
50	x	25	C	N1-C2-O2	5.59	122.25	118.90
30	f	2137	U	C2-N1-C1'	5.59	124.40	117.70
32	i	64	U	N1-C2-O2	5.58	126.71	122.80
30	f	1496	C	C5-C6-N1	5.58	123.79	121.00
30	f	2726	C	N1-C2-O2	5.58	122.25	118.90
3	C	53	ASP	CB-CG-OD1	5.58	123.32	118.30
50	y	70	U	N1-C2-O2	5.56	126.69	122.80
40	q	107	ASP	CB-CG-OD1	5.56	123.30	118.30
32	i	125	U	C2-N1-C1'	5.55	124.37	117.70
50	x	70	U	N1-C2-O2	5.55	126.69	122.80
30	f	2552	C	N1-C2-O2	5.55	122.23	118.90
30	f	2983	C	C6-N1-C2	-5.55	118.08	120.30
30	f	758	C	C6-N1-C2	-5.55	118.08	120.30
30	f	1496	C	N1-C2-O2	5.54	122.22	118.90
30	f	3269	U	P-O3'-C3'	5.54	126.34	119.70
30	f	2764	C	N1-C2-O2	5.53	122.22	118.90
30	f	3057	U	N3-C2-O2	-5.53	118.33	122.20
50	x	28	U	C5-C4-O4	-5.53	122.58	125.90
30	f	3214	U	N1-C2-O2	5.53	126.67	122.80
30	f	777	U	N3-C2-O2	-5.53	118.33	122.20
30	f	982	C	N1-C2-O2	5.51	122.20	118.90
30	f	995	U	N3-C2-O2	-5.50	118.35	122.20
30	f	1554	U	P-O3'-C3'	5.49	126.29	119.70
30	f	1688	U	N3-C2-O2	-5.49	118.36	122.20
30	f	2366	C	C5-C6-N1	5.49	123.74	121.00
31	h	35	C	N1-C2-O2	5.48	122.19	118.90
31	h	52	G	P-O3'-C3'	5.48	126.28	119.70
30	f	283	G	C4-N9-C1'	5.47	133.62	126.50
24	X	14	LEU	CA-CB-CG	5.46	127.86	115.30
50	x	25	C	C6-N1-C2	-5.46	118.12	120.30
30	f	3355	U	C2-N1-C1'	5.46	124.25	117.70
30	f	315	C	C2-N1-C1'	5.44	124.79	118.80
30	f	986	U	N1-C2-O2	5.44	126.61	122.80
30	f	982	C	C6-N1-C2	-5.44	118.12	120.30
30	f	2585	G	N3-C4-N9	5.43	129.26	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	411	U	N3-C2-O2	-5.43	118.40	122.20
30	f	3153	U	C2-N1-C1'	5.43	124.21	117.70
50	y	72	C	C2-N1-C1'	5.43	124.77	118.80
30	f	283	G	N3-C4-N9	5.42	129.25	126.00
45	a	439	LEU	CA-CB-CG	-5.42	102.83	115.30
30	f	2783	U	N3-C2-O2	-5.42	118.41	122.20
30	f	1732	U	N1-C2-O2	5.42	126.59	122.80
30	f	1878	G	C8-N9-C1'	-5.41	119.96	127.00
30	f	3350	C	P-O3'-C3'	5.41	126.20	119.70
30	f	2210	G	N3-C4-C5	-5.41	125.89	128.60
30	f	1349	G	C2-N3-C4	5.40	114.60	111.90
30	f	2552	C	C2-N1-C1'	5.40	124.74	118.80
30	f	78	U	N1-C2-O2	5.40	126.58	122.80
30	f	1425	U	N1-C2-O2	5.40	126.58	122.80
30	f	2444	C	N1-C2-O2	5.40	122.14	118.90
3	C	114	VAL	CG1-CB-CG2	-5.39	102.27	110.90
30	f	2500	A	P-O3'-C3'	5.39	126.17	119.70
30	f	142	C	N3-C2-O2	-5.37	118.14	121.90
30	f	1437	C	C6-N1-C2	-5.37	118.15	120.30
30	f	890	C	N1-C2-O2	5.36	122.11	118.90
30	f	1277	C	C6-N1-C2	-5.36	118.16	120.30
30	f	1496	C	C6-N1-C1'	-5.36	114.37	120.80
30	f	2336	U	N3-C2-O2	-5.36	118.45	122.20
30	f	2366	C	C6-N1-C2	-5.35	118.16	120.30
30	f	1525	G	C8-N9-C1'	-5.35	120.05	127.00
30	f	2497	U	N3-C2-O2	-5.34	118.46	122.20
30	f	3057	U	N1-C2-O2	5.33	126.53	122.80
30	f	915	A	C4-N9-C1'	5.33	135.90	126.30
30	f	1190	A	C2-N3-C4	5.33	113.26	110.60
30	f	3181	C	C6-N1-C2	-5.33	118.17	120.30
30	f	3278	C	C6-N1-C1'	-5.33	114.41	120.80
50	y	26	G	N3-C4-N9	5.32	129.19	126.00
30	f	3235	C	N1-C2-O2	5.32	122.09	118.90
30	f	2114	C	C6-N1-C2	-5.31	118.17	120.30
30	f	1608	C	C2-N1-C1'	5.31	124.64	118.80
30	f	2836	C	C6-N1-C1'	-5.31	114.43	120.80
30	f	982	C	C5-C6-N1	5.30	123.65	121.00
30	f	1115	G	C8-N9-C1'	-5.30	120.11	127.00
30	f	2622	C	N3-C2-O2	-5.30	118.19	121.90
30	f	2726	C	C6-N1-C2	-5.30	118.18	120.30
30	f	1732	U	N3-C2-O2	-5.29	118.50	122.20
43	t	136	GLU	CA-CB-CG	5.28	125.02	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	1907	C	N3-C2-O2	-5.28	118.20	121.90
30	f	2622	C	C6-N1-C2	-5.27	118.19	120.30
30	f	1560	G	N3-C4-N9	-5.27	122.84	126.00
30	f	3148	U	N3-C2-O2	-5.26	118.52	122.20
31	h	105	C	N3-C2-O2	-5.25	118.22	121.90
30	f	2444	C	C5-C6-N1	5.24	123.62	121.00
30	f	2568	C	O4'-C1'-N1	5.24	112.40	108.20
48	v	50	GLY	N-CA-C	-5.24	99.99	113.10
32	i	125	U	N1-C2-O2	5.24	126.47	122.80
46	e	437	LYS	N-CA-C	-5.24	96.85	111.00
30	f	2496	C	C2-N1-C1'	5.24	124.56	118.80
30	f	2585	G	C4-N9-C1'	5.24	133.31	126.50
30	f	890	C	N3-C2-O2	-5.23	118.24	121.90
42	s	108	GLU	CA-CB-CG	5.22	124.89	113.40
30	f	1239	C	C6-N1-C1'	-5.21	114.54	120.80
30	f	1608	C	C5-C6-N1	5.21	123.60	121.00
30	f	2235	C	N1-C2-O2	5.21	122.02	118.90
30	f	192	C	C6-N1-C2	-5.19	118.22	120.30
30	f	2405	C	N1-C2-O2	5.18	122.01	118.90
30	f	758	C	N1-C2-O2	5.18	122.01	118.90
30	f	3349	C	C6-N1-C2	-5.18	118.23	120.30
30	f	1563	C	C6-N1-C1'	5.18	127.01	120.80
50	x	70	U	N3-C2-O2	-5.17	118.58	122.20
30	f	149	U	N3-C2-O2	-5.17	118.58	122.20
30	f	2983	C	C6-N1-C1'	-5.17	114.60	120.80
50	y	23	C	C6-N1-C2	-5.17	118.23	120.30
30	f	1237	G	N3-C4-N9	5.17	129.10	126.00
30	f	915	A	C8-N9-C4	-5.16	103.73	105.80
30	f	1597	C	C5-C6-N1	5.16	123.58	121.00
30	f	969	C	N3-C2-O2	-5.16	118.29	121.90
30	f	637	C	OP1-P-O3'	5.16	116.55	105.20
30	f	1608	C	C6-N1-C2	-5.16	118.24	120.30
30	f	2446	U	O4'-C1'-N1	5.16	112.33	108.20
30	f	2405	C	C2-N1-C1'	5.15	124.47	118.80
30	f	2772	C	N1-C2-O2	5.15	121.99	118.90
30	f	1951	C	C2-N1-C1'	5.15	124.47	118.80
31	h	18	C	C2-N1-C1'	5.15	124.46	118.80
30	f	2899	C	N1-C2-O2	5.14	121.99	118.90
30	f	166	C	C2-N1-C1'	5.12	124.44	118.80
50	x	23	C	C6-N1-C2	-5.12	118.25	120.30
30	f	849	C	P-O3'-C3'	5.10	125.83	119.70
50	y	70	U	N3-C2-O2	-5.10	118.63	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	2235	C	C5-C6-N1	5.10	123.55	121.00
30	f	87	U	N1-C2-O2	5.09	126.37	122.80
30	f	954	U	N3-C2-O2	-5.09	118.64	122.20
32	i	157	U	N1-C2-O2	5.09	126.36	122.80
35	l	4	PRO	C-N-CA	5.08	134.41	121.70
30	f	2638	C	N3-C2-O2	-5.08	118.34	121.90
30	f	2873	U	C2-N1-C1'	5.08	123.79	117.70
17	Q	42	LEU	CA-CB-CG	5.07	126.96	115.30
30	f	1097	G	OP2-P-O3'	5.07	116.35	105.20
30	f	2444	C	C6-N1-C1'	-5.07	114.72	120.80
36	m	222	LEU	CA-CB-CG	5.07	126.95	115.30
30	f	2550	U	N1-C2-O2	5.06	126.34	122.80
32	i	100	U	N1-C2-O2	5.06	126.34	122.80
30	f	1562	C	N3-C2-O2	-5.06	118.36	121.90
30	f	885	U	N3-C2-O2	-5.05	118.66	122.20
30	f	969	C	N1-C2-O2	5.05	121.93	118.90
15	O	21	ILE	CG1-CB-CG2	-5.04	100.30	111.40
39	p	79	GLN	CA-CB-CG	5.04	124.49	113.40
30	f	3355	U	N1-C2-O2	5.04	126.33	122.80
30	f	2873	U	N3-C2-O2	-5.03	118.68	122.20
30	f	2836	C	O4'-C1'-N1	5.03	112.22	108.20
30	f	354	U	N3-C2-O2	-5.03	118.68	122.20
31	h	39	C	N1-C2-O2	5.03	121.92	118.90
30	f	1820	U	OP2-P-O3'	5.02	116.25	105.20
30	f	1272	C	C6-N1-C2	-5.02	118.29	120.30
30	f	2497	U	N1-C2-O2	5.02	126.31	122.80
30	f	3306	U	O4'-C1'-N1	5.01	112.21	108.20
5	E	10	LEU	CB-CG-CD1	5.01	119.52	111.00
30	f	283	G	C8-N9-C1'	-5.01	120.48	127.00
36	m	146	LEU	CB-CG-CD1	-5.01	102.48	111.00
30	f	1355	A	OP2-P-O3'	5.01	116.21	105.20
30	f	2899	C	C6-N1-C2	-5.00	118.30	120.30
30	f	282	G	C2'-C3'-O3'	5.00	121.71	113.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
46	e	392	GLY	Peptide
47	g	8	GLU	Peptide

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Mol	Chain	Res	Type	Group
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1779	9	0
2	B	1555	0	1659	13	0
3	C	1416	0	1433	11	0
4	D	1441	0	1543	7	0
5	E	1258	0	1342	6	0
6	F	1437	0	1475	14	0
7	G	1272	0	1312	10	0
8	H	796	0	812	8	0
9	I	1003	0	1048	8	0
10	J	518	0	542	3	0
11	K	964	0	1025	1	0
12	L	984	0	1075	4	0
13	M	1080	0	1122	5	0
14	N	1169	0	1211	7	0
15	O	462	0	491	5	0
16	P	737	0	792	3	0
17	Q	876	0	912	9	0
18	R	1013	0	1077	5	0
19	S	850	0	880	3	0
20	T	880	0	942	3	0
21	U	969	0	1078	3	0
22	V	766	0	844	4	0
23	W	645	0	645	3	0
24	X	612	0	682	3	0
25	Y	436	0	475	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	410	0	442	0	0
27	b	824	0	888	0	0
28	c	694	0	734	0	0
29	d	207	0	250	0	0
30	f	68782	0	34563	0	0
31	h	2579	0	1304	0	0
32	i	3353	0	1695	0	0
33	j	1874	0	1943	0	0
34	k	3075	0	3142	0	0
35	l	2748	0	2859	0	0
36	m	2351	0	2294	0	0
37	n	1307	0	1377	0	0
38	o	1784	0	1862	0	0
39	p	1804	0	1877	0	0
40	q	1508	0	1572	0	0
41	r	1764	0	1804	0	0
42	s	1346	0	1370	0	0
43	t	1543	0	1608	0	0
44	u	1053	0	1149	0	0
45	a	6579	0	6482	0	0
46	e	11506	0	10754	0	0
47	g	1651	0	1613	0	0
48	v	1085	0	1086	0	0
49	w	1709	0	1799	0	0
50	x	1579	0	798	0	0
50	y	1556	0	788	0	0
51	z	728	0	337	0	0
52	0	961	0	979	12	0
53	1	90	0	23	3	0
54	A	1	0	0	0	0
54	C	1	0	0	0	0
54	E	1	0	0	0	0
54	I	1	0	0	0	0
54	R	1	0	0	0	0
54	T	1	0	0	0	0
54	f	3	0	0	0	0
54	h	1	0	0	0	0
54	j	2	0	0	0	0
54	k	1	0	0	0	0
55	T	1	0	0	0	0
55	W	1	0	0	0	0
55	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	b	1	0	0	0	0
55	c	1	0	0	0	0
55	e	2	0	0	0	0
56	f	10	0	19	0	0
All	All	151339	0	113607	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.90
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
52:0:26:PHE:HB2	52:0:87:VAL:HB	1.73	0.69
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
53:1:44:UNK:O	53:1:45:UNK:C	2.43	0.67
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.65
2:B:27[A]:LEU:HD21	2:B:102[A]:LEU:HB2	1.80	0.63
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
9:I:14:SER:O	9:I:81:GLN:NE2	2.33	0.62
52:0:192:ASP:HB2	52:0:197:PHE:HE2	1.67	0.60
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.59
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.84	0.59
1:A:183:THR:HG22	1:A:187:ARG:HB2	1.85	0.59
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.58
6:F:77:VAL:HG22	6:F:126:VAL:HG23	1.86	0.58
52:0:43:LYS:HA	52:0:46:ARG:HG2	1.87	0.57
11:K:50:ALA:HB1	21:U:66:VAL:HG11	1.86	0.57
17:Q:4:LEU:O	17:Q:79:ARG:NH2	2.38	0.56
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.56
20:T:87:GLU:OE2	20:T:91:ARG:NH1	2.39	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
52:0:42:ARG:HG2	52:0:51:VAL:HG11	1.89	0.55
8:H:19:VAL:HG12	8:H:105:LEU:HD22	1.89	0.55
2:B:157[A]:GLU:OE2	2:B:160[A]:ARG:NH2	2.40	0.55
53:1:43:UNK:C	53:1:45:UNK:H2	2.20	0.54
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.54
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.54
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.90	0.53
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.53
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.52
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.93	0.51
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.49
2:B:46[A]:GLU:HG3	2:B:48[A]:PHE:H	1.77	0.49
7:G:99:SER:HG	7:G:101:CYS:HG	1.59	0.49
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.49
6:F:155:ARG:HB2	6:F:172:TYR:HD1	1.77	0.49
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.49
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.49
16:P:9:SER:OG	16:P:10:ILE:N	2.38	0.49
4:D:131:ALA:HB1	4:D:135:GLN:H	1.78	0.48
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.95	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.47
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
52:0:26:PHE:HZ	52:0:93:LEU:HA	1.80	0.47
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.44	0.47
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.97	0.46
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
8:H:90:ARG:O	8:H:91:ASP:HB2	2.16	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
9:I:38:ALA:HB3	9:I:59:MET:HB2	1.99	0.44
9:I:10:LYS:NZ	9:I:56:ASP:OD1	2.41	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.43
7:G:68:THR:OG1	7:G:69:LYS:N	2.51	0.43
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
52:0:15:LEU:O	52:0:19:LEU:HG	2.18	0.43
52:0:45:LEU:HB3	52:0:49:ALA:HB3	1.99	0.43
53:1:42:UNK:O	53:1:43:UNK:C	2.66	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
20:T:95:ILE:HG21	20:T:95:ILE:HD13	1.81	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.00	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
4:D:161:LYS:HA	4:D:161:LYS:HD3	1.82	0.43
52:0:75:LYS:O	52:0:78:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:0:67:LEU:HD22	52:0:67:LEU:HA	1.85	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.52	0.43
3:C:179:GLN:HA	3:C:182:ILE:HG22	2.00	0.42
6:F:95:ARG:HB2	6:F:140:VAL:HG23	2.00	0.42
8:H:81:LYS:HD2	8:H:90:ARG:NH1	2.33	0.42
52:0:14:LYS:HE3	52:0:52:LEU:HD11	2.00	0.42
2:B:54[A]:TYR:OH	2:B:73[A]:PHE:O	2.37	0.42
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	0.42
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.01	0.42
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
52:0:70:LEU:HB3	52:0:73:PHE:CD1	2.55	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
52:0:61:ARG:HA	52:0:61:ARG:HD2	1.92	0.42
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.77	0.42
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.41
16:P:73:GLY:N	16:P:76:GLU:OE1	2.42	0.41
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
8:H:107:PHE:O	8:H:108:TYR:C	2.58	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.02	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.01	0.41
5:E:7:GLN:NE2	5:E:35:ALA:O	2.53	0.41
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	0.41
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.02	0.40
5:E:31:GLU:HA	5:E:34:GLN:HB2	2.03	0.40
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:37:THR:HG23	19:S:40:ASP:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
2	B	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
3	C	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
4	D	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	E	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
6	F	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
7	G	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
8	H	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	61 (100%)	0	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	14
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
34	k	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	37	59
36	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
37	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	25	47
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
42	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	22	43
43	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	25	47
44	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
45	a	842/1038 (81%)	827 (98%)	15 (2%)	0	100	100
46	e	1519/1562 (97%)	1501 (99%)	16 (1%)	2 (0%)	48	71
47	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
48	v	139/157 (88%)	139 (100%)	0	0	100	100
49	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
51	z	144/165 (87%)	134 (93%)	9 (6%)	1 (1%)	19	38
52	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	31
All	All	9314/10279 (91%)	8958 (96%)	347 (4%)	9 (0%)	50	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	z	88	PRO
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
46	e	437	LYS
52	0	93	LEU
46	e	350	PRO
15	O	21	ILE
43	t	47	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/176 (99%)	175 (100%)	0	100	100
2	B	160/162 (99%)	160 (100%)	0	100	100
3	C	138/146 (94%)	138 (100%)	0	100	100
4	D	150/151 (99%)	149 (99%)	1 (1%)	81	93
5	E	129/154 (84%)	129 (100%)	0	100	100
6	F	155/156 (99%)	155 (100%)	0	100	100
7	G	135/137 (98%)	134 (99%)	1 (1%)	81	93
8	H	87/107 (81%)	85 (98%)	2 (2%)	45	71
9	I	104/105 (99%)	104 (100%)	0	100	100
10	J	54/129 (42%)	54 (100%)	0	100	100
11	K	104/118 (88%)	104 (100%)	0	100	100
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	45 (98%)	1 (2%)	47	72
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	94 (99%)	1 (1%)	70	86
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	X	68/69 (99%)	66 (97%)	2 (3%)	37	64
25	Y	45/46 (98%)	45 (100%)	0	100	100
26	Z	45/116 (39%)	45 (100%)	0	100	100
27	b	87/91 (96%)	87 (100%)	0	100	100
28	c	71/72 (99%)	71 (100%)	0	100	100
29	d	20/23 (87%)	20 (100%)	0	100	100
33	j	189/196 (96%)	189 (100%)	0	100	100
34	k	321/323 (99%)	319 (99%)	2 (1%)	84	94
35	l	288/289 (100%)	288 (100%)	0	100	100
36	m	241/245 (98%)	241 (100%)	0	100	100
37	n	139/155 (90%)	138 (99%)	1 (1%)	81	93
38	o	186/205 (91%)	186 (100%)	0	100	100
39	p	187/208 (90%)	187 (100%)	0	100	100
40	q	168/171 (98%)	168 (100%)	0	100	100
41	r	185/187 (99%)	183 (99%)	2 (1%)	70	86
42	s	145/150 (97%)	142 (98%)	3 (2%)	48	73
43	t	154/159 (97%)	154 (100%)	0	100	100
44	u	107/109 (98%)	107 (100%)	0	100	100
45	a	678/949 (71%)	675 (100%)	3 (0%)	89	96
46	e	1149/1451 (79%)	1057 (92%)	92 (8%)	10	21
47	g	180/211 (85%)	180 (100%)	0	100	100
48	v	119/132 (90%)	118 (99%)	1 (1%)	79	91
49	w	197/198 (100%)	196 (100%)	1 (0%)	86	95
52	0	104/254 (41%)	95 (91%)	9 (9%)	8	17
All	All	7563/8690 (87%)	7441 (98%)	122 (2%)	58	79

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
7	G	83	ARG
8	H	92	TRP
8	H	108	TYR
15	O	33	LYS
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
42	s	29	ARG
42	s	55	ARG
42	s	60	ARG
45	a	98	ASP
45	a	136	ARG
45	a	893	LYS
46	e	30	PHE
46	e	77	ASN
46	e	105	VAL
46	e	125	ILE
46	e	156	THR
46	e	178	LEU
46	e	229	VAL
46	e	254	ASN
46	e	264	VAL
46	e	277	MET
46	e	299	THR
46	e	309	VAL
46	e	327	THR
46	e	354	PHE
46	e	372	ASP
46	e	380	PHE
46	e	387	ARG
46	e	412	PHE
46	e	710	LYS
46	e	731	LEU
46	e	737	TYR
46	e	738	PHE
46	e	743	LYS

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Mol	Chain	Res	Type
46	e	754	ILE
46	e	757	CYS
46	e	760	THR
46	e	764	PHE
46	e	770	ILE
46	e	782	TYR
46	e	785	SER
46	e	799	THR
46	e	807	LYS
46	e	826	LEU
46	e	844	LEU
46	e	858	LEU
46	e	861	ASP
46	e	862	PHE
46	e	867	PHE
46	e	869	HIS
46	e	895	THR
46	e	902	ASN
46	e	924	VAL
46	e	933	LEU
46	e	951	ASP
46	e	954	TYR
46	e	955	LEU
46	e	979	LEU
46	e	987	ILE
46	e	989	GLU
46	e	998	LYS
46	e	1000	LEU
46	e	1006	LEU
46	e	1028	PHE
46	e	1033	LYS
46	e	1075	LEU
46	e	1077	GLU
46	e	1079	LEU
46	e	1094	TYR
46	e	1095	LEU
46	e	1102	CYS
46	e	1123	TYR
46	e	1164	LEU
46	e	1175	PHE
46	e	1179	LEU
46	e	1189	ASN

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Mol	Chain	Res	Type
46	e	1195	THR
46	e	1239	LYS
46	e	1258	GLU
46	e	1294	LEU
46	e	1300	ILE
46	e	1303	MET
46	e	1342	GLU
46	e	1367	THR
46	e	1372	LEU
46	e	1379	LEU
46	e	1400	PHE
46	e	1408	ASP
46	e	1409	ARG
46	e	1421	LEU
46	e	1422	ASN
46	e	1428	VAL
46	e	1439	LEU
46	e	1454	ILE
46	e	1470	LYS
46	e	1477	GLN
46	e	1480	ILE
46	e	1508	CYS
46	e	1512	TYR
46	e	1527	CYS
46	e	1539	LEU
46	e	1551	CYS
46	e	1555	ARG
48	v	54	HIS
49	w	92	LYS
52	0	30	VAL
52	0	51	VAL
52	0	52	LEU
52	0	67	LEU
52	0	76	LEU
52	0	80	VAL
52	0	93	LEU
52	0	95	GLU
52	0	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	121	ASN
46	e	13	ASN
46	e	174	GLN
46	e	189	ASN
46	e	254	ASN
46	e	368	HIS
46	e	397	ASN
46	e	795	HIS
46	e	805	ASN
46	e	810	GLN
46	e	832	ASN
46	e	902	ASN
46	e	1141	GLN
46	e	1189	ASN
46	e	1288	GLN
46	e	1457	ASN
47	g	9	ASN
48	v	52	HIS
52	0	36	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3212/3395 (94%)	591 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
50	x	72/76 (94%)	21 (29%)	0
50	y	71/76 (93%)	20 (28%)	0
All	All	3632/3826 (94%)	676 (18%)	0

All (676) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	f	6	A
30	f	13	A
30	f	14	U
30	f	26	A
30	f	40	A
30	f	43	A
30	f	49	A
30	f	59	G
30	f	60	A

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Mol	Chain	Res	Type
30	f	65	A
30	f	66	A
30	f	92	G
30	f	99	A
30	f	109	A
30	f	110	G
30	f	111	C
30	f	116	A
30	f	120	G
30	f	121	A
30	f	122	A
30	f	133	U
30	f	134	U
30	f	135	C
30	f	136	G
30	f	156	G
30	f	157	A
30	f	165	A
30	f	166	C
30	f	172	G
30	f	173	G
30	f	187	A
30	f	190	U
30	f	191	U
30	f	200	C
30	f	206	G
30	f	210	U
30	f	211	A
30	f	213	A
30	f	218	G
30	f	219	A
30	f	234	G
30	f	240	U
30	f	241	G
30	f	242	C
30	f	243	G
30	f	245	U
30	f	249	U
30	f	252	U
30	f	269	G
30	f	283	G
30	f	286	U

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Mol	Chain	Res	Type
30	f	295	A
30	f	305	U
30	f	323	A
30	f	329	U
30	f	339	C
30	f	350	C
30	f	374	A
30	f	376	G
30	f	398	A
30	f	399	A
30	f	401	U
30	f	402	A
30	f	403	C
30	f	421	G
30	f	422	A
30	f	439	C
30	f	440	A
30	f	441	U
30	f	442	G
30	f	443	G
30	f	445	G
30	f	446	U
30	f	447	U
30	f	448	U
30	f	450	G
30	f	487	U
30	f	488	U
30	f	489	U
30	f	490	C
30	f	494	G
30	f	518	G
30	f	520	U
30	f	521	A
30	f	523	A
30	f	535	G
30	f	536	U
30	f	543	C
30	f	544	C
30	f	546	C
30	f	547	G
30	f	548	G
30	f	551	A

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Mol	Chain	Res	Type
30	f	552	G
30	f	555	U
30	f	557	A
30	f	559	A
30	f	578	A
30	f	579	G
30	f	589	A
30	f	597	G
30	f	604	G
30	f	608	A
30	f	609	G
30	f	611	A
30	f	620	U
30	f	621	A
30	f	622	A
30	f	637	C
30	f	638	C
30	f	649	A
30	f	660	A
30	f	677	A
30	f	681	U
30	f	684	G
30	f	690	A
30	f	691	A
30	f	705	A
30	f	712	G
30	f	715	A
30	f	716	A
30	f	719	U
30	f	720	A
30	f	758	C
30	f	763	G
30	f	764	U
30	f	765	C
30	f	766	U
30	f	767	U
30	f	776	U
30	f	777	U
30	f	780	A
30	f	781	G
30	f	785	G
30	f	786	A

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Mol	Chain	Res	Type
30	f	806	A
30	f	817	A
30	f	830	A
30	f	846	A
30	f	849	C
30	f	850	U
30	f	861	C
30	f	874	U
30	f	879	U
30	f	896	A
30	f	907	G
30	f	908	G
30	f	914	A
30	f	916	G
30	f	917	A
30	f	920	A
30	f	921	A
30	f	924	G
30	f	925	A
30	f	937	G
30	f	944	C
30	f	959	C
30	f	960	U
30	f	981	U
30	f	982	C
30	f	991	G
30	f	994	G
30	f	1001	G
30	f	1002	A
30	f	1010	G
30	f	1015	U
30	f	1016	C
30	f	1017	C
30	f	1018	G
30	f	1021	G
30	f	1024	G
30	f	1025	A
30	f	1028	U
30	f	1036	A
30	f	1041	U
30	f	1047	A
30	f	1049	C

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Mol	Chain	Res	Type
30	f	1063	G
30	f	1064	A
30	f	1065	A
30	f	1072	G
30	f	1081	U
30	f	1087	G
30	f	1093	A
30	f	1094	U
30	f	1095	U
30	f	1097	G
30	f	1098	A
30	f	1103	A
30	f	1104	G
30	f	1117	G
30	f	1131	G
30	f	1144	U
30	f	1153	A
30	f	1159	A
30	f	1160	C
30	f	1177	G
30	f	1180	A
30	f	1181	U
30	f	1192	C
30	f	1193	A
30	f	1196	C
30	f	1197	A
30	f	1201	C
30	f	1202	A
30	f	1208	U
30	f	1217	A
30	f	1218	U
30	f	1219	C
30	f	1222	G
30	f	1225	A
30	f	1227	C
30	f	1235	U
30	f	1236	G
30	f	1238	C
30	f	1241	U
30	f	1242	G
30	f	1244	A
30	f	1245	A

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Mol	Chain	Res	Type
30	f	1251	A
30	f	1252	A
30	f	1254	C
30	f	1258	U
30	f	1259	A
30	f	1263	A
30	f	1264	G
30	f	1265	U
30	f	1269	U
30	f	1272	C
30	f	1277	C
30	f	1278	A
30	f	1279	C
30	f	1282	G
30	f	1285	G
30	f	1286	A
30	f	1287	A
30	f	1295	G
30	f	1307	G
30	f	1308	A
30	f	1309	U
30	f	1313	G
30	f	1330	A
30	f	1348	U
30	f	1349	G
30	f	1351	U
30	f	1352	A
30	f	1354	G
30	f	1355	A
30	f	1356	U
30	f	1357	G
30	f	1386	A
30	f	1392	G
30	f	1399	A
30	f	1400	G
30	f	1419	A
30	f	1434	G
30	f	1437	C
30	f	1446	A
30	f	1450	G
30	f	1481	A
30	f	1482	A

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Mol	Chain	Res	Type
30	f	1483	G
30	f	1487	G
30	f	1488	G
30	f	1502	C
30	f	1508	C
30	f	1536	G
30	f	1539	A
30	f	1555	U
30	f	1556	C
30	f	1557	A
30	f	1560	G
30	f	1562	C
30	f	1563	C
30	f	1566	A
30	f	1568	U
30	f	1569	U
30	f	1572	U
30	f	1573	G
30	f	1575	A
30	f	1576	G
30	f	1580	A
30	f	1581	C
30	f	1582	C
30	f	1583	A
30	f	1589	A
30	f	1590	G
30	f	1605	A
30	f	1607	U
30	f	1620	U
30	f	1629	U
30	f	1639	C
30	f	1642	A
30	f	1643	A
30	f	1645	U
30	f	1657	C
30	f	1683	A
30	f	1716	U
30	f	1717	U
30	f	1724	U
30	f	1725	C
30	f	1736	G
30	f	1741	A

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Mol	Chain	Res	Type
30	f	1750	A
30	f	1751	G
30	f	1760	A
30	f	1761	C
30	f	1764	U
30	f	1765	U
30	f	1766	G
30	f	1770	G
30	f	1775	G
30	f	1780	G
30	f	1797	A
30	f	1814	A
30	f	1816	A
30	f	1819	U
30	f	1820	U
30	f	1821	U
30	f	1835	A
30	f	1839	A
30	f	1840	U
30	f	1841	A
30	f	1842	A
30	f	1846	C
30	f	1849	C
30	f	1850	A
30	f	1866	C
30	f	1867	A
30	f	1880	U
30	f	1881	A
30	f	1893	A
30	f	1906	G
30	f	1943	C
30	f	1952	G
30	f	1953	G
30	f	1954	G
30	f	2094	C
30	f	2101	C
30	f	2102	U
30	f	2111	G
30	f	2112	U
30	f	2113	A
30	f	2114	C
30	f	2121	G

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Mol	Chain	Res	Type
30	f	2122	G
30	f	2131	A
30	f	2134	G
30	f	2140	U
30	f	2144	A
30	f	2158	A
30	f	2160	G
30	f	2169	G
30	f	2176	U
30	f	2201	G
30	f	2206	G
30	f	2207	A
30	f	2208	A
30	f	2209	U
30	f	2222	A
30	f	2223	A
30	f	2225	U
30	f	2228	A
30	f	2249	G
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A

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Mol	Chain	Res	Type
30	f	2403	G
30	f	2404	A
30	f	2411	U
30	f	2419	A
30	f	2437	G
30	f	2446	U
30	f	2447	A
30	f	2450	G
30	f	2461	A
30	f	2463	G
30	f	2464	U
30	f	2468	A
30	f	2469	G
30	f	2470	C
30	f	2471	U
30	f	2472	U
30	f	2474	G
30	f	2479	C
30	f	2480	A
30	f	2484	A
30	f	2486	A
30	f	2487	U
30	f	2488	A
30	f	2494	A
30	f	2495	C
30	f	2496	C
30	f	2499	U
30	f	2501	U
30	f	2502	A
30	f	2503	G
30	f	2505	U
30	f	2514	U
30	f	2515	A
30	f	2522	G
30	f	2526	C
30	f	2531	C
30	f	2537	U
30	f	2538	U
30	f	2539	C
30	f	2540	A
30	f	2541	U
30	f	2542	U

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Mol	Chain	Res	Type
30	f	2544	U
30	f	2547	A
30	f	2548	C
30	f	2549	G
30	f	2552	C
30	f	2554	A
30	f	2555	G
30	f	2561	A
30	f	2569	A
30	f	2570	U
30	f	2571	U
30	f	2572	C
30	f	2573	G
30	f	2581	U
30	f	2585	G
30	f	2593	A
30	f	2594	C
30	f	2606	G
30	f	2607	G
30	f	2614	G
30	f	2648	G
30	f	2651	G
30	f	2652	U
30	f	2656	A
30	f	2674	A
30	f	2677	G
30	f	2678	A
30	f	2689	A
30	f	2691	A
30	f	2694	A
30	f	2696	A
30	f	2704	A
30	f	2714	G
30	f	2719	U
30	f	2728	G
30	f	2729	U
30	f	2740	A
30	f	2752	U
30	f	2753	G
30	f	2755	C
30	f	2772	C
30	f	2773	C

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Mol	Chain	Res	Type
30	f	2777	G
30	f	2778	G
30	f	2788	C
30	f	2796	G
30	f	2800	G
30	f	2801	A
30	f	2803	A
30	f	2810	C
30	f	2814	G
30	f	2816	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2834	G
30	f	2842	U
30	f	2844	C
30	f	2845	A
30	f	2849	C
30	f	2860	U
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2875	U
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2941	A
30	f	2942	C
30	f	2947	G
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A

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Mol	Chain	Res	Type
30	f	3056	U
30	f	3059	G
30	f	3078	U
30	f	3079	U
30	f	3080	G
30	f	3086	A
30	f	3092	C
30	f	3104	U
30	f	3113	A
30	f	3122	A
30	f	3130	A
30	f	3131	U
30	f	3142	A
30	f	3143	C
30	f	3151	U
30	f	3154	C
30	f	3155	U
30	f	3156	U
30	f	3157	U
30	f	3165	A
30	f	3170	A
30	f	3173	G
30	f	3174	A
30	f	3175	U
30	f	3176	G
30	f	3179	U
30	f	3181	C
30	f	3186	A
30	f	3187	A
30	f	3196	U
30	f	3207	U
30	f	3209	A
30	f	3217	C
30	f	3218	A
30	f	3219	G
30	f	3228	C
30	f	3229	G
30	f	3243	A
30	f	3245	A
30	f	3247	G
30	f	3259	U
30	f	3263	G

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Mol	Chain	Res	Type
30	f	3269	U
30	f	3270	U
30	f	3273	A
30	f	3276	G
30	f	3281	U
30	f	3287	U
30	f	3288	G
30	f	3289	G
30	f	3294	A
30	f	3295	A
30	f	3303	G
30	f	3304	U
30	f	3307	A
30	f	3313	U
30	f	3316	A
30	f	3317	U
30	f	3318	G
30	f	3319	U
30	f	3320	A
30	f	3341	U
30	f	3342	A
30	f	3345	G
30	f	3351	U
30	f	3352	U
30	f	3353	G
30	f	3354	U
30	f	3355	U
30	f	3369	G
30	f	3375	A
30	f	3378	C
30	f	3382	U
30	f	3383	G
30	f	3386	G
30	f	3389	U
30	f	3390	G
30	f	3396	U
31	h	7	G
31	h	29	C
31	h	53	U
31	h	54	U
31	h	55	A
31	h	65	G

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Mol	Chain	Res	Type
31	h	73	C
31	h	74	C
31	h	95	A
31	h	102	A
31	h	112	G
31	h	121	U
32	i	23	U
32	i	34	U
32	i	35	C
32	i	39	G
32	i	48	A
32	i	52	A
32	i	53	A
32	i	59	A
32	i	62	C
32	i	63	G
32	i	80	A
32	i	81	U
32	i	82	U
32	i	83	C
32	i	84	C
32	i	85	G
32	i	86	U
32	i	87	G
32	i	90	U
32	i	95	G
32	i	104	A
32	i	105	A
32	i	106	C
32	i	111	A
32	i	113	U
32	i	125	U
32	i	126	A
32	i	138	A
32	i	151	C
32	i	152	G
32	i	157	U
32	i	158	U
50	x	5	G
50	x	9	G
50	x	15	G
50	x	16	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	x	17	C
50	x	18	G
50	x	22	G
50	x	28	U
50	x	33	U
50	x	34	I
50	x	35	G
50	x	37	A
50	x	38	U
50	x	39	G
50	x	46	G
50	x	48	C
50	x	56	C
50	x	57	G
50	x	58	A
50	x	60	U
50	x	74	C
50	y	7	G
50	y	9	G
50	y	13	U
50	y	17	C
50	y	23	C
50	y	26	G
50	y	34	I
50	y	35	G
50	y	36	C
50	y	38	U
50	y	43	G
50	y	45	G
50	y	46	G
50	y	47	U
50	y	48	C
50	y	56	C
50	y	58	A
50	y	61	C
50	y	75	C
50	y	76	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	5CT	v	51	48	13,14,15	0.76	0	9,15,17	1.28	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	5CT	v	51	48	-	9/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	v	51	5CT	C4-C3-C2	-2.20	108.84	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	v	51	5CT	NZ-C1-C2-C3
48	v	51	5CT	O1-C2-C3-C4
48	v	51	5CT	C2-C3-C4-N1
48	v	51	5CT	C-CA-CB-CG
48	v	51	5CT	N-CA-CB-CG
48	v	51	5CT	NZ-C1-C2-O1
48	v	51	5CT	C1-C2-C3-C4
48	v	51	5CT	CE-CD-CG-CB
48	v	51	5CT	C2-C1-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SPD	f	3401	-	9,9,9	0.32	0	8,8,8	0.86	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
56	SPD	f	3401	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	f	3401	SPD	C3-C4-C5-N6
56	f	3401	SPD	N6-C7-C8-C9
56	f	3401	SPD	C2-C3-C4-C5
56	f	3401	SPD	C8-C7-N6-C5
56	f	3401	SPD	C4-C5-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

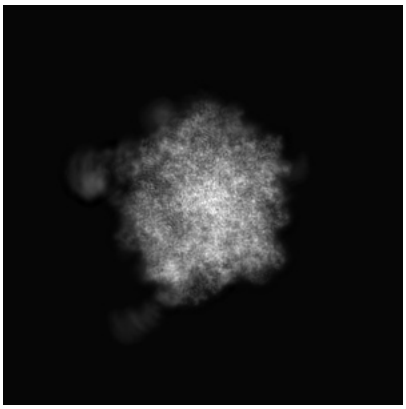
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15428. These allow visual inspection of the internal detail of the map and identification of artifacts.

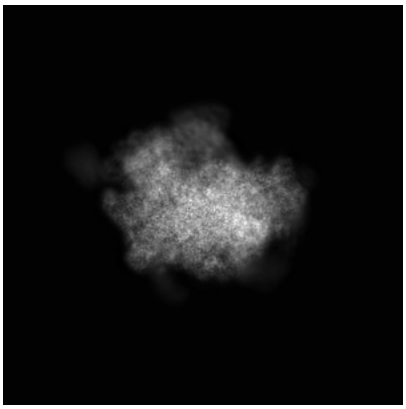
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

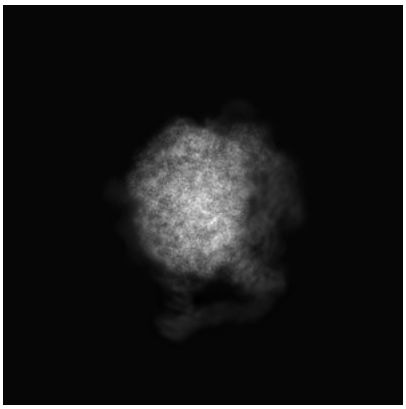
6.1.1 Primary map



X

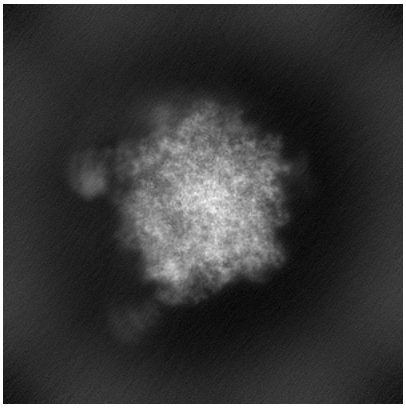


Y

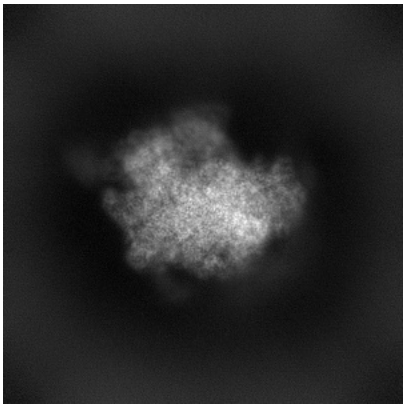


Z

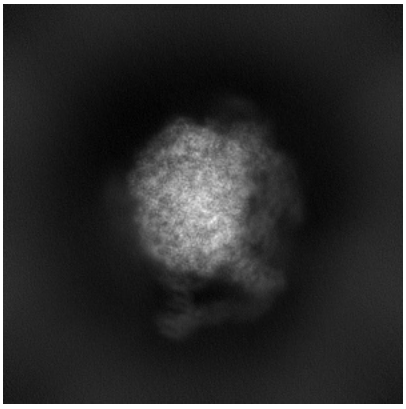
6.1.2 Raw map



X



Y

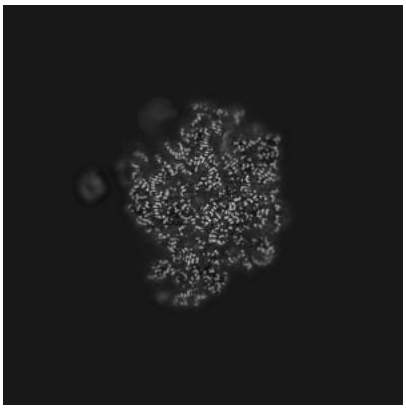


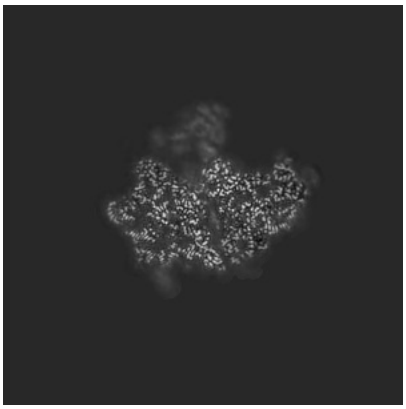
Z

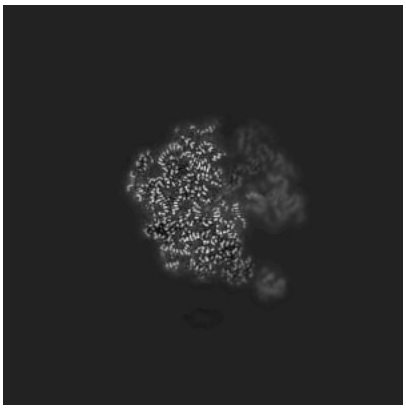
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

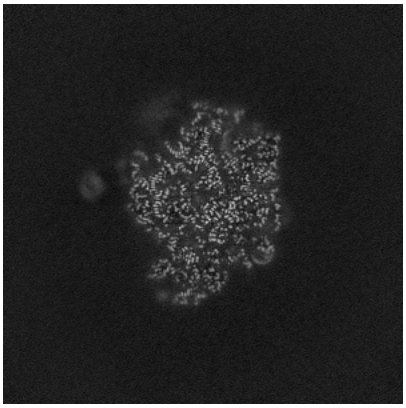
6.2.1 Primary map

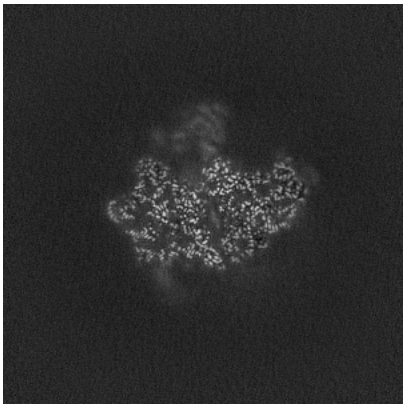

X Index: 225

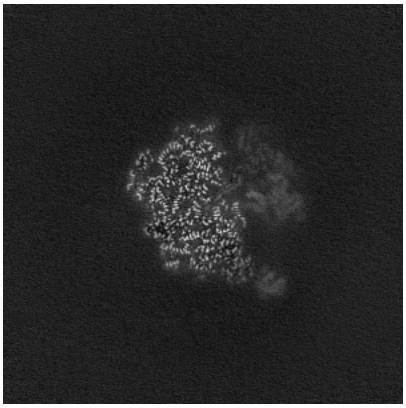

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

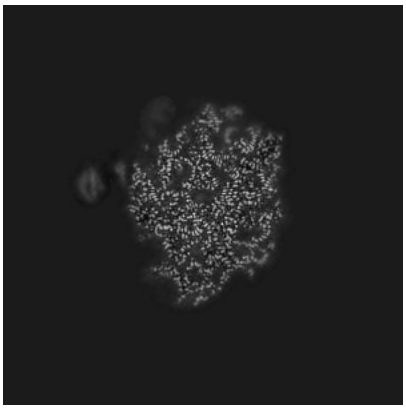

Y Index: 225


Z Index: 225

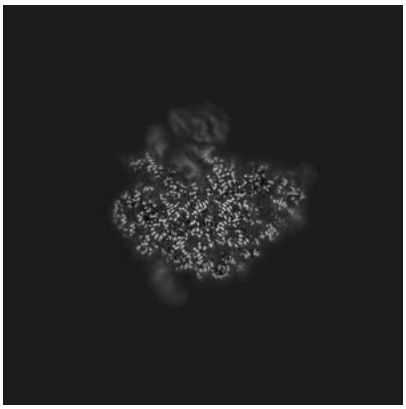
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

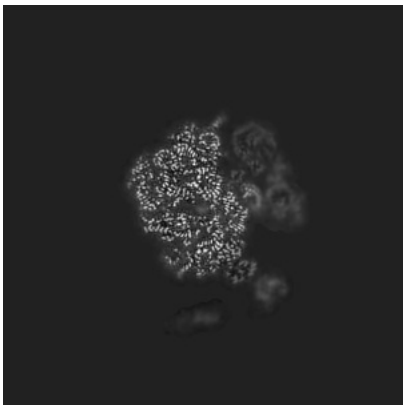
6.3.1 Primary map



X Index: 219

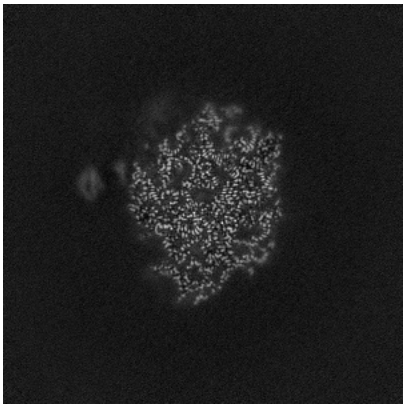


Y Index: 237

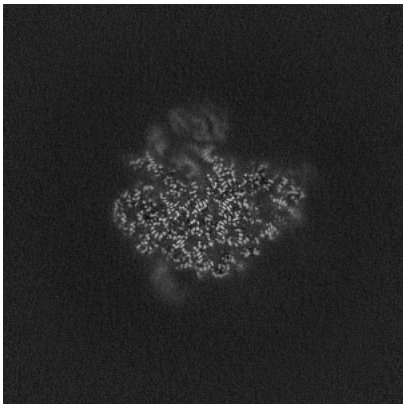


Z Index: 231

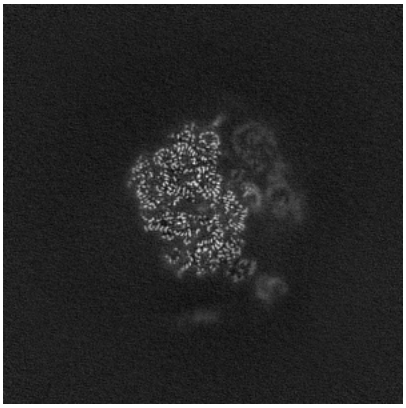
6.3.2 Raw map



X Index: 219



Y Index: 237

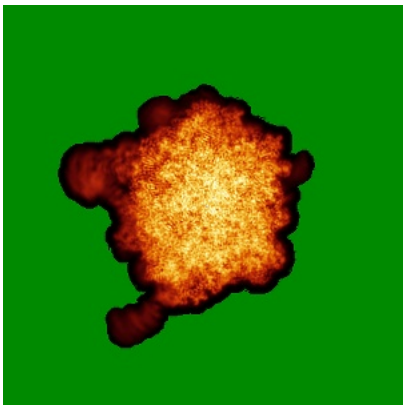


Z Index: 231

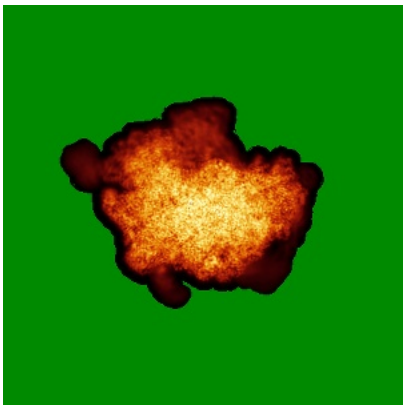
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

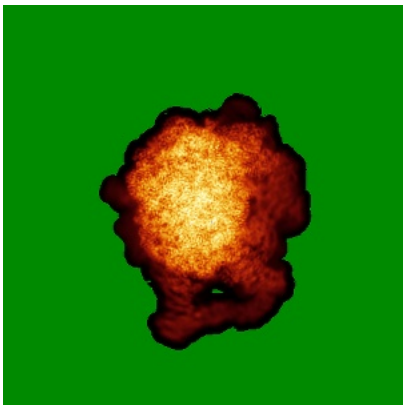
6.4.1 Primary map



X

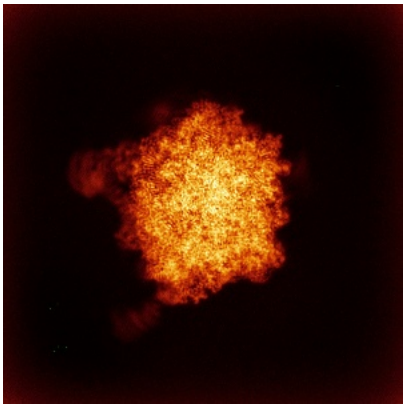


Y

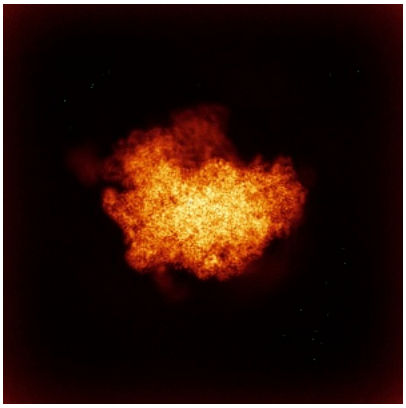


Z

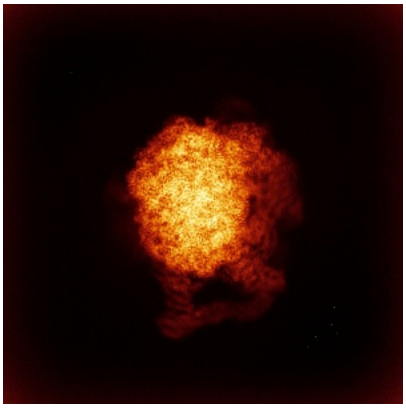
6.4.2 Raw map



X



Y

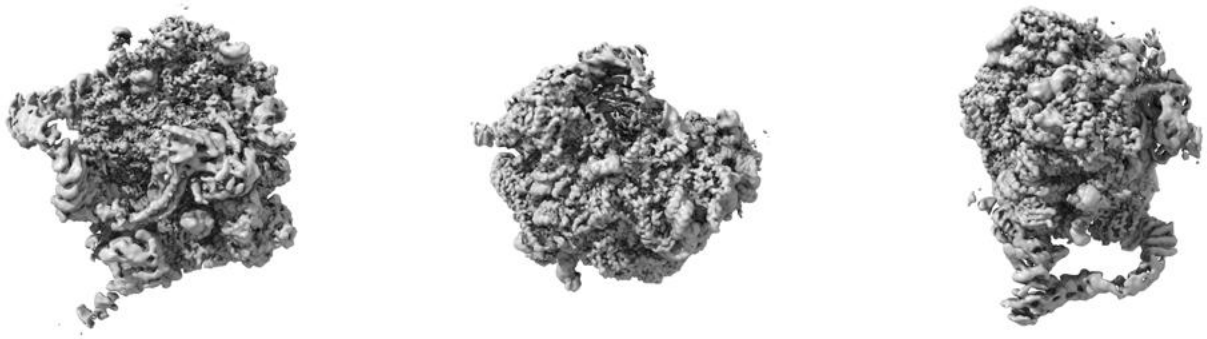


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

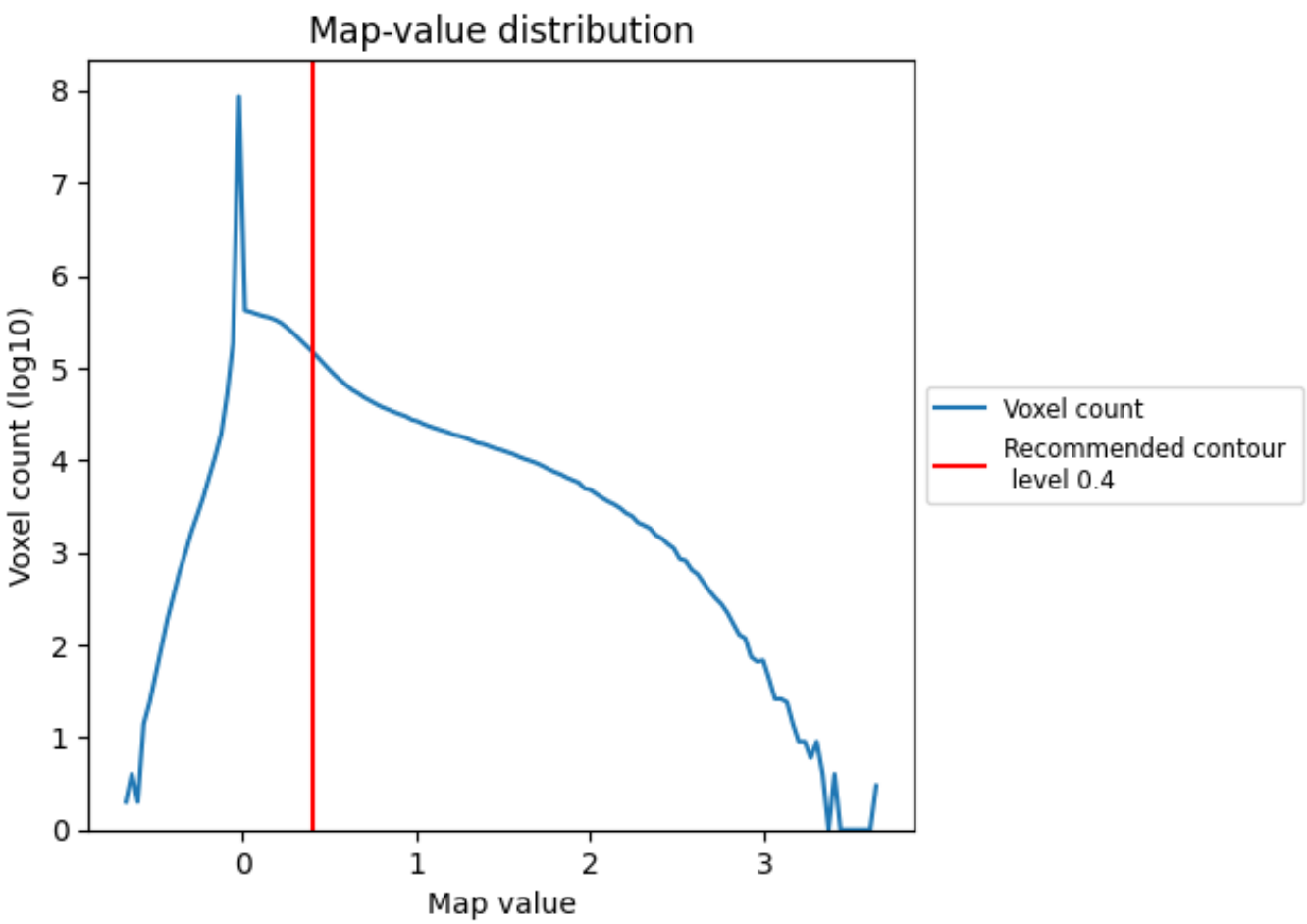
6.6 Mask visualisation (i)

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

7 Map analysis (i)

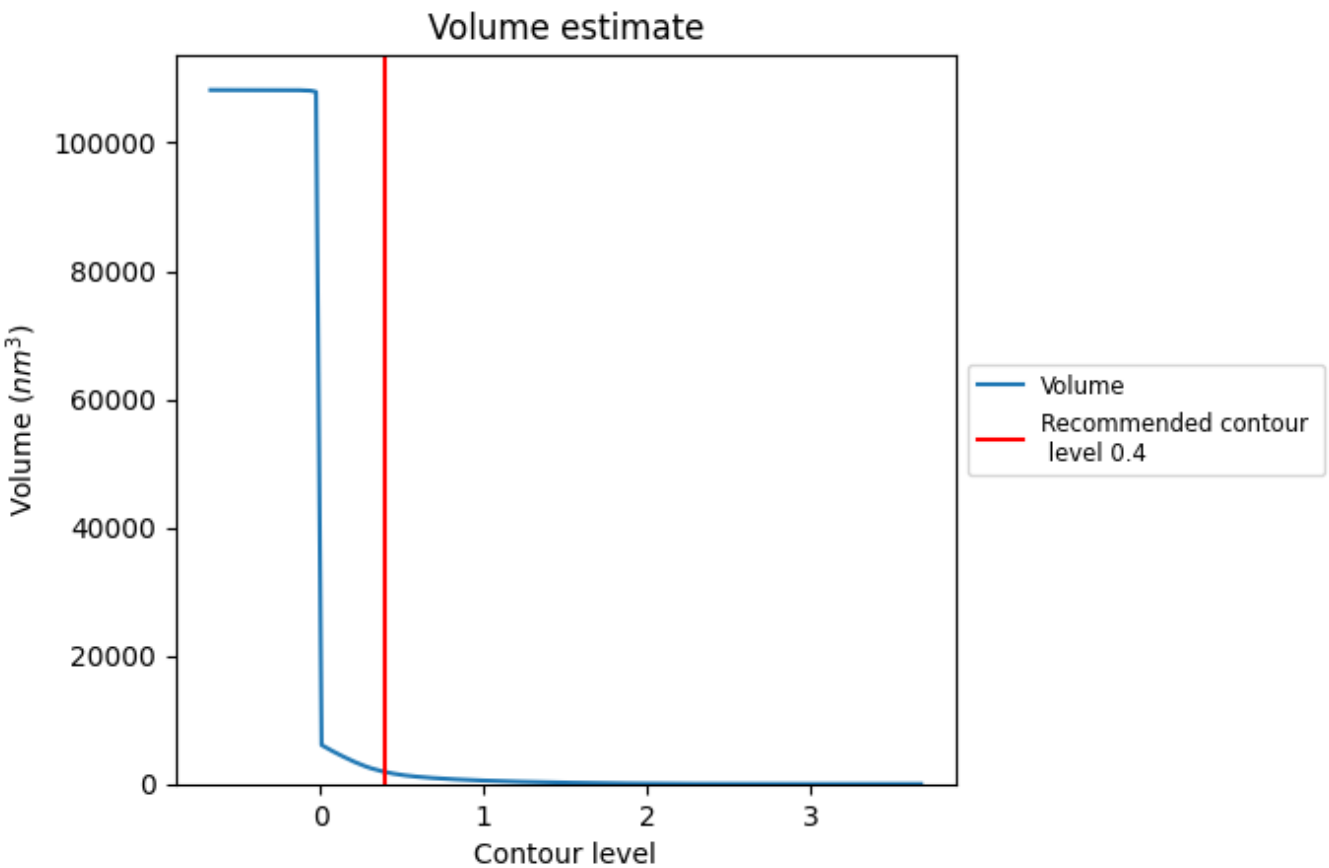
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

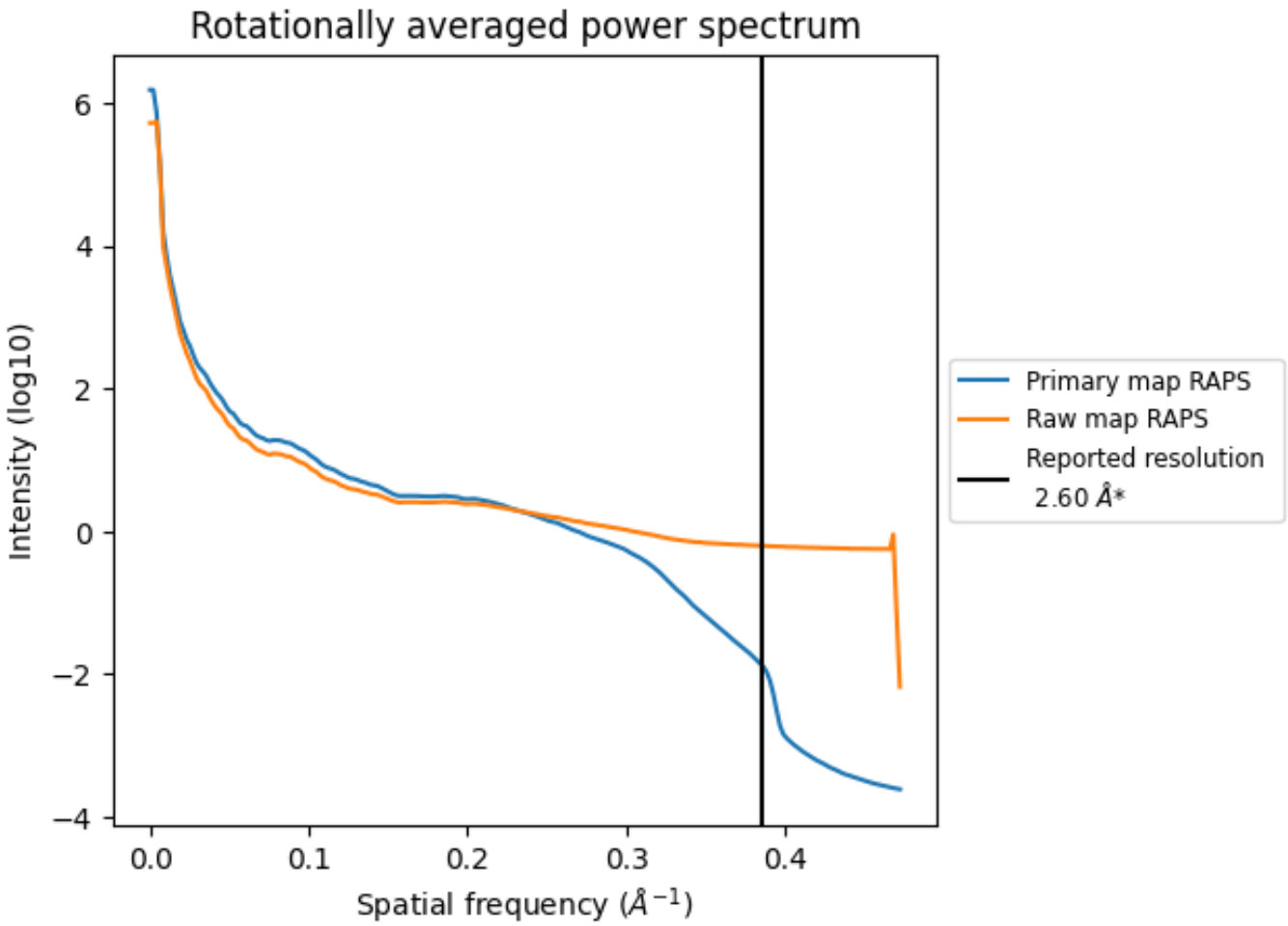
7.2 Volume estimate (i)



The volume at the recommended contour level is 1851 nm^3; this corresponds to an approximate mass of 1672 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)

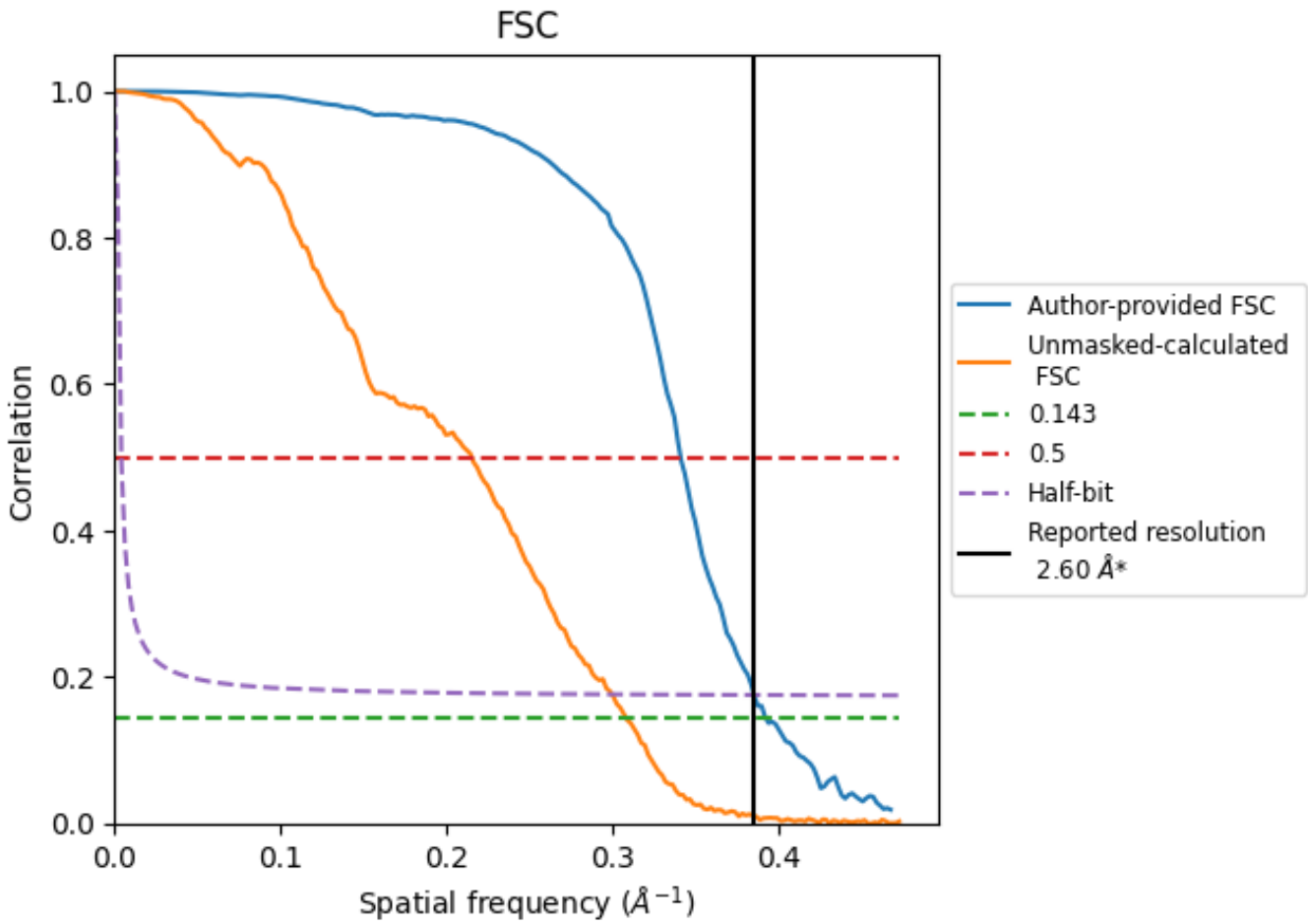


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

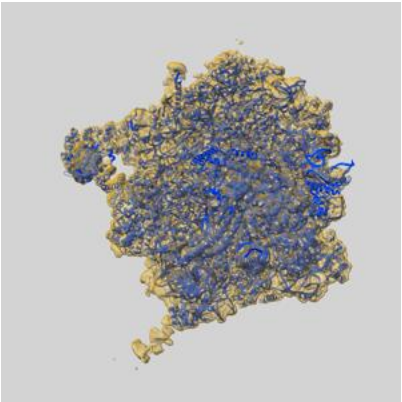
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.55	2.94	2.60
Unmasked-calculated*	3.25	4.65	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.6 by more than 10 %

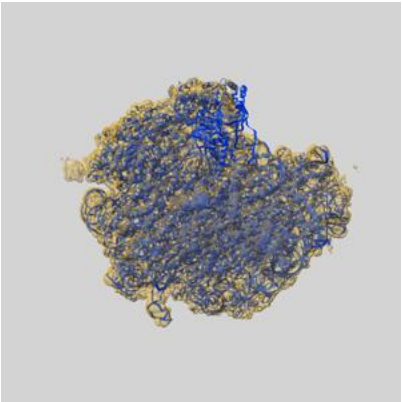
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15428 and PDB model 8AGZ. Per-residue inclusion information can be found in section 3 on page 15.

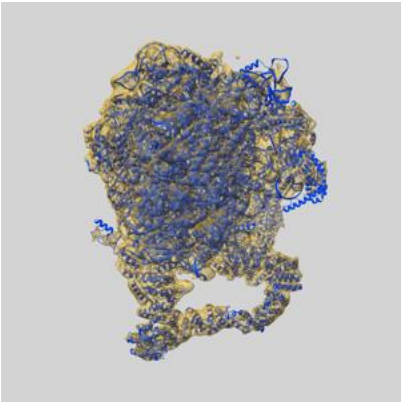
9.1 Map-model overlay (i)



X



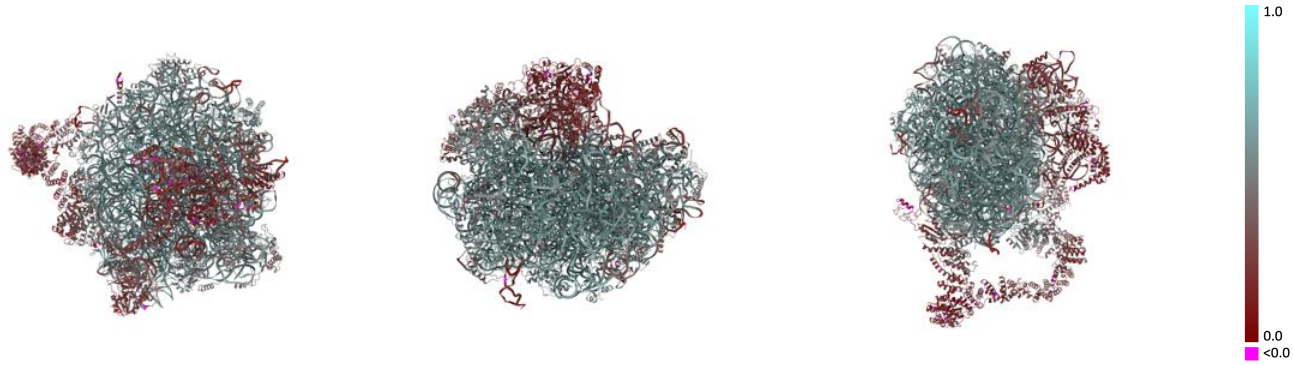
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

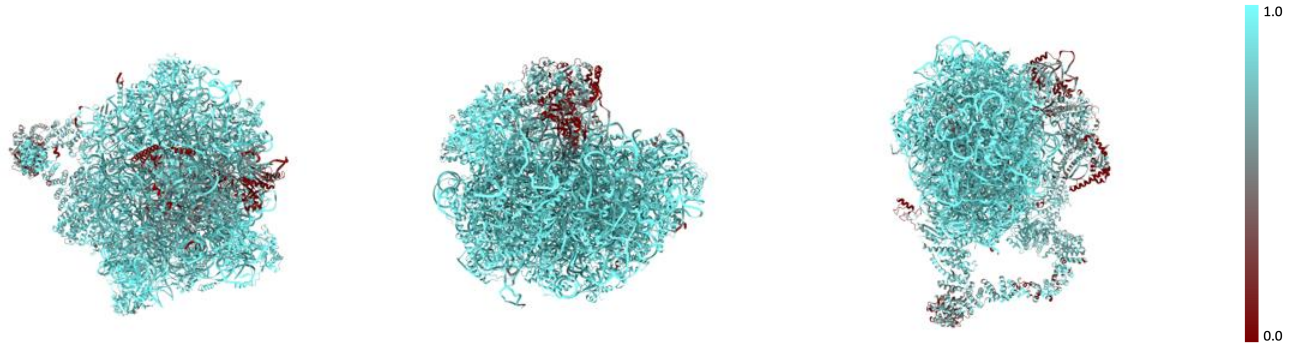
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

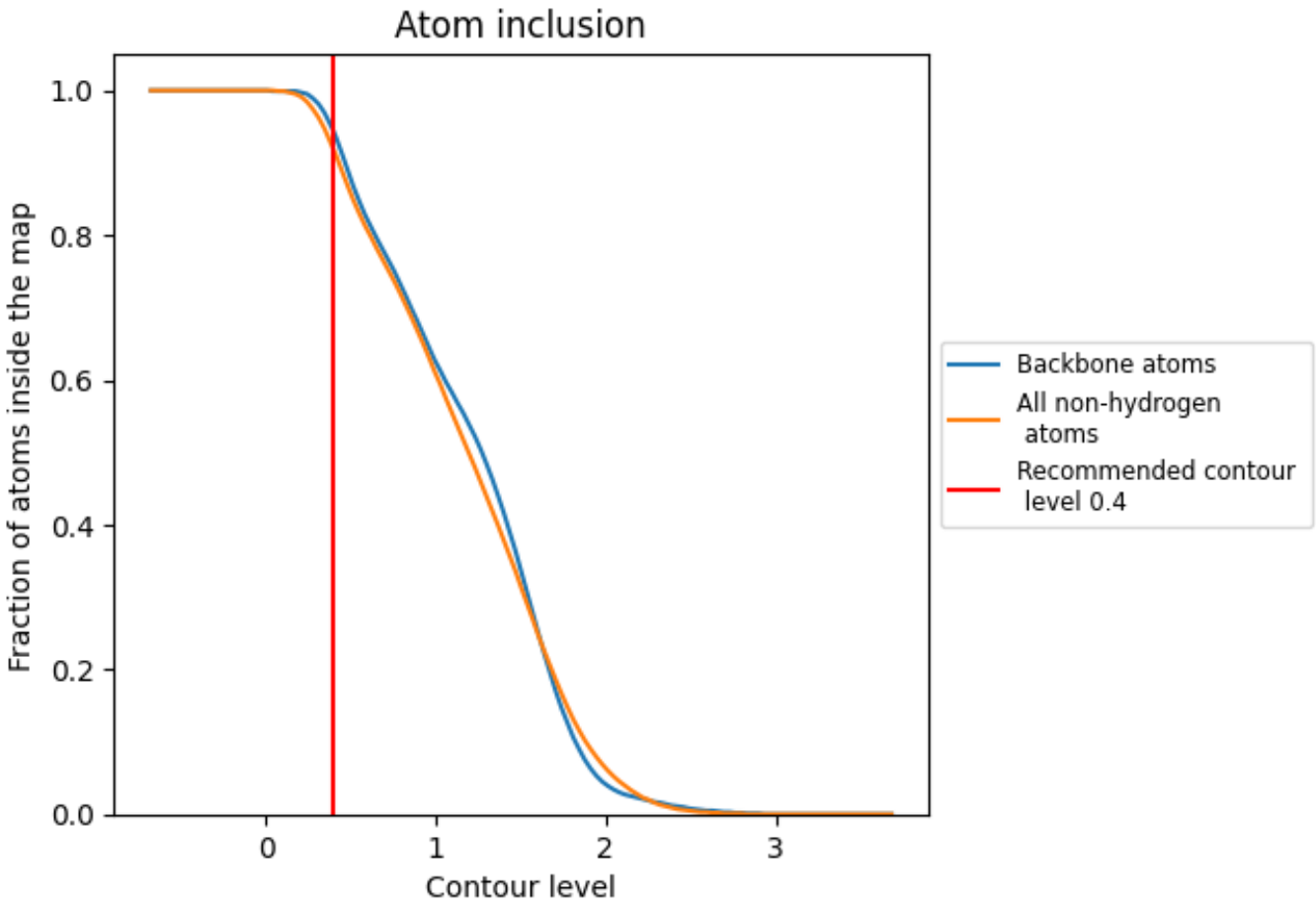
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9190	0.5120
0	0.8470	0.2900
1	1.0000	0.4020
A	0.9930	0.6120
B	0.9790	0.5890
C	0.9640	0.5890
D	0.9820	0.5850
E	0.9390	0.5500
F	0.9810	0.5800
G	0.9680	0.5650
H	0.9220	0.4640
I	0.9680	0.5780
J	0.9660	0.5780
K	0.9660	0.5740
L	0.9770	0.5700
M	0.9560	0.5210
N	0.9810	0.5940
O	0.9580	0.5420
P	0.9390	0.5230
Q	0.9260	0.5490
R	0.9820	0.5990
S	0.9920	0.6150
T	0.9770	0.5760
U	0.9670	0.5580
V	0.9600	0.5300
W	1.0000	0.6280
X	0.9210	0.4970
Y	1.0000	0.6020
Z	0.9700	0.5760
a	0.5850	0.2180
b	0.9640	0.5730
c	0.9720	0.5700
d	0.7610	0.4030
e	0.6980	0.2570
f	0.9820	0.5700

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Chain	Atom inclusion	Q-score
g	0.8440	0.4880
h	0.9990	0.5720
i	0.9970	0.5980
j	0.9910	0.6050
k	0.9790	0.5880
l	0.9780	0.5770
m	0.9400	0.4870
n	0.9500	0.5290
o	0.9690	0.5710
p	0.9460	0.5210
q	0.9610	0.5500
r	0.9610	0.5470
s	0.9300	0.4480
t	0.9710	0.5610
u	0.9700	0.5500
v	0.4610	0.3610
w	0.1230	0.2290
x	0.7470	0.2550
y	0.8690	0.2310
z	0.9090	0.2990