



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 02:34 AM EST

PDB ID : 8AGT
EMDB ID : EMD-15423
Title : Yeast RQC complex in state F
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

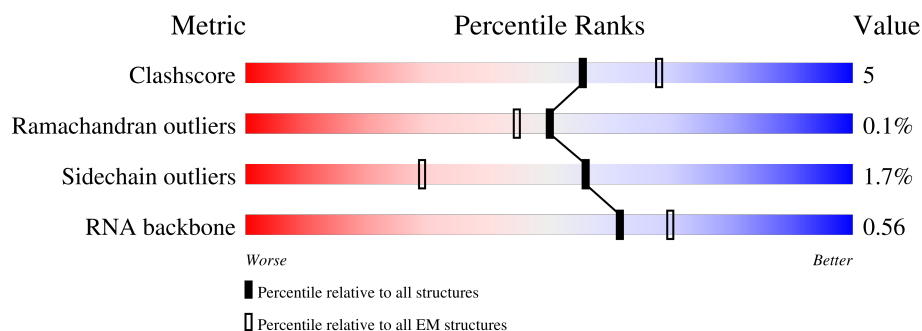
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.




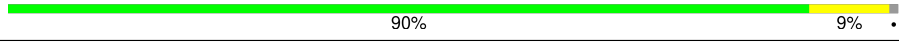
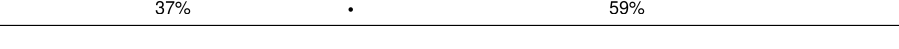
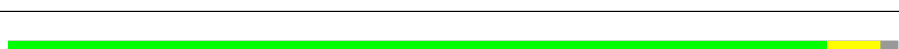

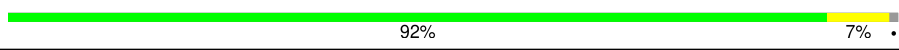

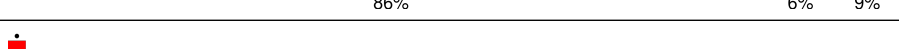
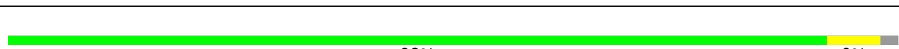
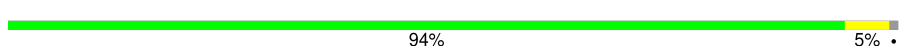

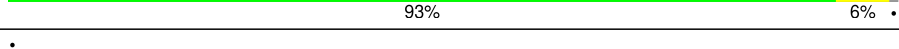
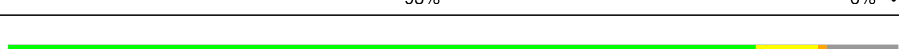
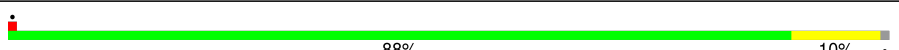
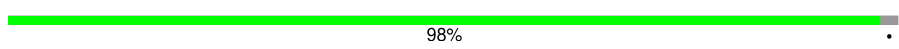

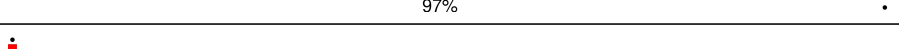







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	
2	B	199	
3	C	184	
4	D	186	
5	E	189	
6	F	172	
7	G	160	

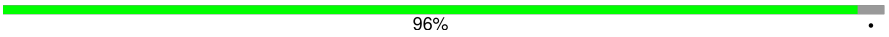
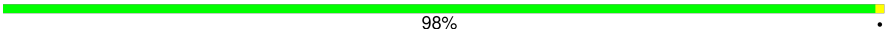
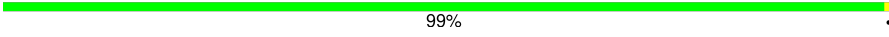
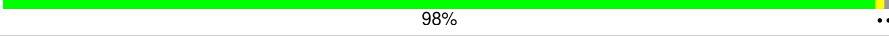
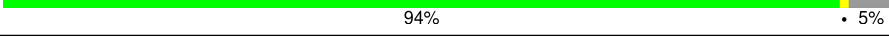


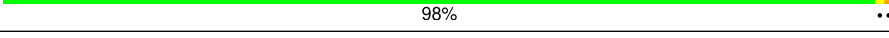
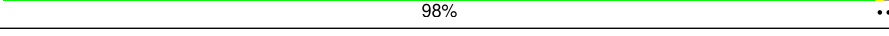
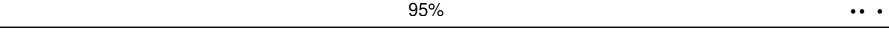
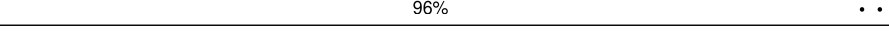
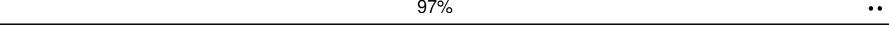

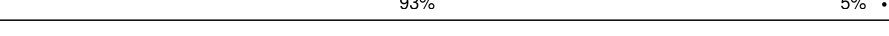

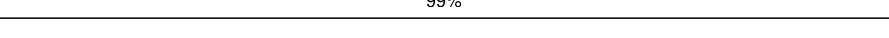
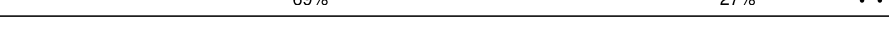

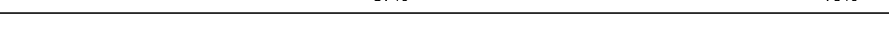



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Mol	Chain	Length	Quality of chain
8	H	121	
9	I	137	
10	J	155	
11	K	142	
12	L	127	
13	M	136	
14	N	149	
15	O	59	
16	P	105	
17	Q	113	
18	R	130	
19	S	107	
20	T	121	
21	U	120	
22	V	100	
23	W	88	
24	X	78	
25	Y	51	
26	Z	128	
27	b	106	
28	c	92	
29	d	25	
30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

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Mol	Chain	Length	Quality of chain
33	j	254	 96% .
34	k	387	 98% .
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	 95% .. .
43	t	199	 96% . .
44	u	138	 97% ..
45	a	1038	 78% . 18%
46	e	1562	 62% 93% 5% .
47	g	245	 91% 8%
48	w	217	 21% 99%
49	x	77	 69% 27% . .
50	y	76	 66% 30% .
51	z	165	 87% . 10%
52	0	312	 30% 7% . 61%
53	1	18	 94% 6%
54	v	157	 8% 87% . 10%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 151341 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
1	A	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	3216	Total	C	N	O	P	1	0
			68802	30732	12391	22462	3217		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	G	deletion	GB 2211412835

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Ribosome quality control complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	848	Total	C	N	O	S	0	0
			6569	4188	1138	1226	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	e	1527	Total	C	N	O	S	0	0
			11508	7354	1936	2180	38		

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

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

- Molecule 48 is a protein called 60S ribosomal protein L1-A.

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

- Molecule 49 is a RNA chain called A-site Ala aminoacyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	75	Total	C	N	O	P	0	0
			1584	705	279	526	74		

- Molecule 50 is a RNA chain called P-site petidyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	73	Total	C	N	O	P	0	0
			1556	692	273	518	73		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	72	C	-	insertion	GB 1554469083
y	73	G	-	insertion	GB 1554469083
y	75	C	A	conflict	GB 1554469083

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 5A-1.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	1	Total	Mg	0
			1	1	
55	C	1	Total	Mg	0
			1	1	
55	E	1	Total	Mg	0
			1	1	
55	I	1	Total	Mg	0
			1	1	
55	R	1	Total	Mg	0
			1	1	
55	T	1	Total	Mg	0
			1	1	
55	f	3	Total	Mg	0
			3	3	
55	h	1	Total	Mg	0
			1	1	
55	j	2	Total	Mg	0
			2	2	
55	k	1	Total	Mg	0
			1	1	

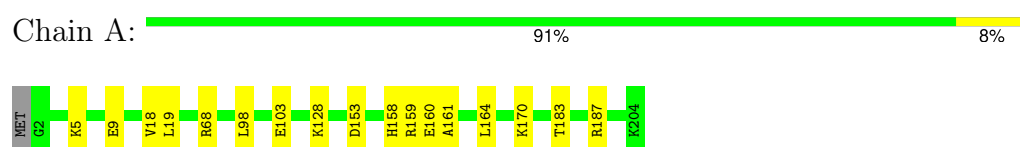
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

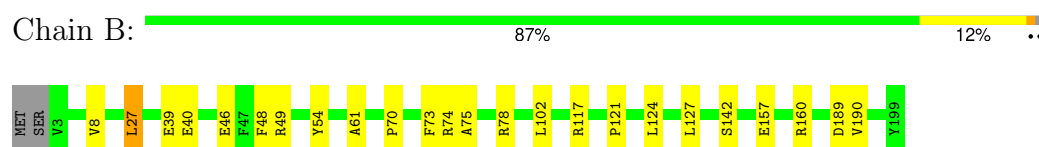
3 Residue-property plots [i](#)

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.

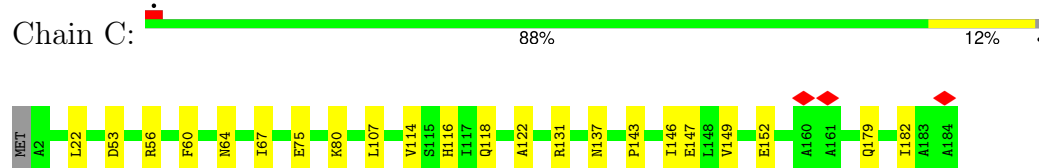
• Molecule 1: 60S ribosomal protein L15-A



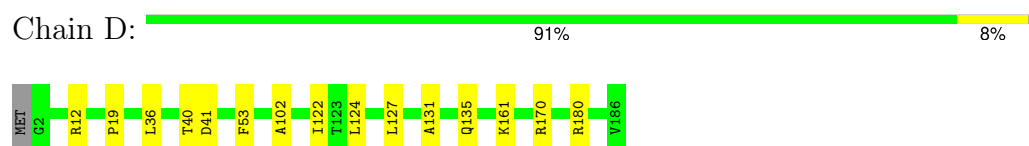
• Molecule 2: 60S ribosomal protein L16-A



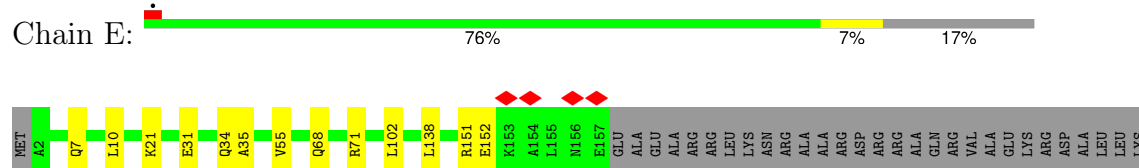
• Molecule 3: 60S ribosomal protein L17-A



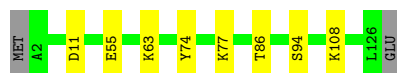
• Molecule 4: 60S ribosomal protein L18-A



• Molecule 5: 60S ribosomal protein L19-A



Chain L:  92% 6% .



- Molecule 13: 60S ribosomal protein L27-A

Chain M:  92% 7% .




- Molecule 14: 60S ribosomal protein L28

Chain N:  92% 7% .




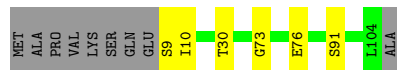
- Molecule 15: 60S ribosomal protein L29

Chain O:  83% 12% . . .




- Molecule 16: 60S ribosomal protein L30

Chain P:  86% 6% 9%



- Molecule 17: 60S ribosomal protein L31-A

Chain Q:  80% 17% .




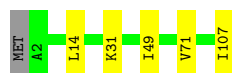
- Molecule 18: 60S ribosomal protein L32

Chain R:  92% 6% .




- Molecule 19: 60S ribosomal protein L33-A

Chain S:  94% 5%



- Molecule 20: 60S ribosomal protein L34-A

Chain T:  88% 5% 7%



- Molecule 21: 60S ribosomal protein L35-A

Chain U:  93% 6%



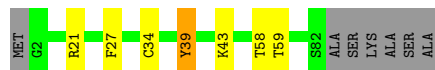
- Molecule 22: 60S ribosomal protein L36-A

Chain V:  93% 6%




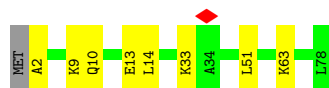
- Molecule 23: 60S ribosomal protein L37-A

Chain W:  84% 7% 8%



- Molecule 24: 60S ribosomal protein L38

Chain X:  88% 10%

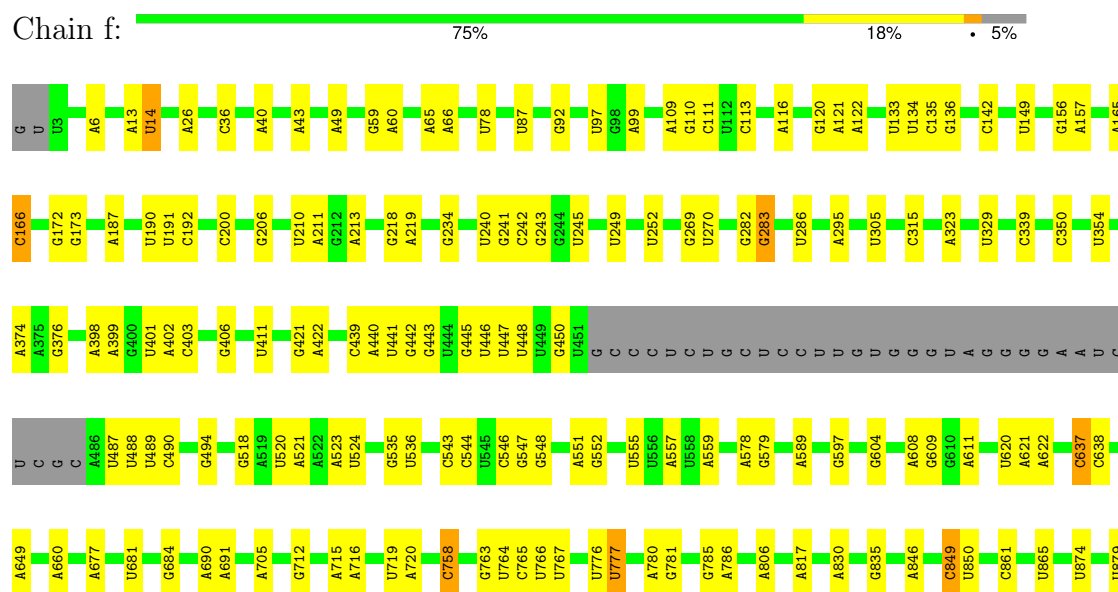


- Molecule 25: 60S ribosomal protein L39

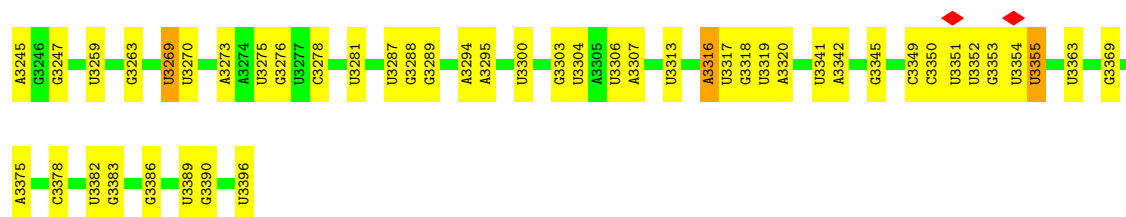
Chain Y:  98%



- Molecule 26: Ubiquitin-60S ribosomal protein L40



C3092	A2691	U2537	A2404	A2223	G	U	G	A1760	A1566	G1349	A1217	U1028	U885
U2860	A2694	U2538	C2405	A2224	C	A	A	C1761	U1567	A1350	A1218	A1036	C890
C2867	A2695	A2539	U2411	U2225	U	G	G	U1764	U1568	U1351	C1219	U1041	A896
G2871	A2696	A2540	U2419	A2226	G	C	C	U1765	U1569	G1352	G1222	A1047	G907
A2872	U2541	U2542	G2437	C2235	C	U	A	G1766	U1572	U1353	G1225	C1049	G908
A2887	U2543	U2544	G2444	G2249	U	G	C	G1770	G1573	A1355	A1226	G1063	A914
A2898	U2545	A2547	A2445	U2254	A	U	A	G1775	A1574	U1356	G1227	A1064	A915
C2899	U2550	U2551	A2446	A	A	C	U	G1780	G1576	G1357	A1065	A1065	G916
A2911	U2552	U2553	A2447	C	U	U	C	A1797	G1577	A1386	U1235	A1066	A917
G2914	U2554	U2555	G2450	U	U	U	C	A1814	A1580	G1392	U1236	A1067	A920
U2923	U2556	A2561	A2461	A	A	U	C	A1816	C1581	U1393	G1237	A1068	A921
U2935	U2557	C2568	G2463	G	G	G	C	U1819	C1582	A1399	C1238	U1081	U922
A2936	U2558	U2569	U2464	A2262	A2093	C	A	U1820	A1583	G1400	U1240	G1087	G924
A2941	G2728	U2570	G2471	A	C2094	U	C	U1821	G1578	A1419	A1241	A1083	A925
C2942	U2729	U2571	U2472	U2282	U2101	G	C	A1835	A1579	U1425	G1242	U1084	G937
G2947	A2740	U2572	C2473	G2288	U2102	U	C	U1839	G1597	U1434	G1243	U1085	C944
U2954	U2752	A2568	G2474	G2272	G2111	C	A	U1840	C1604	G1437	A1251	G1097	U954
A2971	G2753	U2569	A2468	U2273	U2112	C	C	A1841	A1605	U1446	U1252	A1103	C959
C2972	C2754	U2570	C2470	U2274	A2113	U	C	U1842	U1606	U1447	C1254	G1104	U960
A2941	C2755	U2571	U2471	A2281	C2114	G	C	G1846	U1607	A1481	A1263	G1115	C969
C2942	C2764	U2572	U2472	U2282	G2121	U	C	U1850	C1608	A1482	G1264	G1116	U981
G2972	C2772	U2573	G2473	G2288	G2122	G	C	A1866	C1608	G1487	U1265	G1131	C982
U2954	C2773	U2581	G2474	G2288	G2122	U	C	A1867	C1608	U1488	U1269	U1144	U985
A2971	G2777	U2582	C2479	G2307	A2131	G	C	C1872	U1620	C1496	C1272	A1153	U986
C2972	G2778	U2583	A2480	G2308	U2132	A	C	U1878	U1629	C1502	C1277	G991	
C2983	U2783	U2584	A2484	A2309	U2133	C	U	A1880	C1639	C1508	A1278	G994	
G2990	C2788	U2594	A2485	A2310	G2134	G	C	U1881	A1642	G1525	A1286	U1180	U995
A3180	G2796	U2606	U2487	A2313	U2140	C	C	A1889	A1643	G1536	A1287	G1177	G1001
C3181	G2796	U2607	A2488	G2315	U2140	U	C	U1906	C1644	A1539	G1295	A1190	A1002
A3186	G2800	U2614	A2494	U2334	A2144	U	C	G1907	U1645	U1554	G1307	A1191	G1010
A3187	A2801	U2617	C2495	G2335	A2158	G	C	A1893	U1716	U1555	A1308	U1181	U1015
U3196	A2802	U2622	U2496	U2336	U2159	U	C	U1907	U1717	C1556	A1309	G1192	C1016
U3207	A2803	U2622	U2498	C2366	G2169	G	C	U1907	U1724	A1557	U1309	G1193	G1017
G3208	U2804	U2622	U2499	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
A3209	U2805	U2622	U2500	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
U3214	U2806	U2622	U2501	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
C3217	U2807	U2622	U2502	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
A3218	U2808	U2622	U2503	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
G3219	U2809	U2622	U2504	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
C3228	U2810	U2622	U2505	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
G3229	U2811	U2622	U2506	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
C3235	U2812	U2622	U2507	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
A3243	U2813	U2622	U2508	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018
A3244	U2814	U2622	U2509	C2366	G2169	U	C	U1907	U1724	G1560	G1313	C1196	G1018



• Molecule 31: 5S rRNA

Chain h: 85% 15%



• Molecule 32: 5.8S rRNA

Chain i: 78% 20%



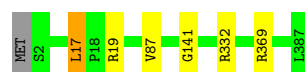
• Molecule 33: 60S ribosomal protein L2-A

Chain j: 96%



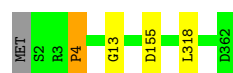
• Molecule 34: 60S ribosomal protein L3

Chain k: 98%



• Molecule 35: 60S ribosomal protein L4-A

Chain l: 99%



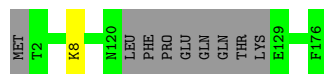
• Molecule 36: 60S ribosomal protein L5

Chain m: 98%



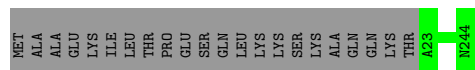
- Molecule 37: 60S ribosomal protein L6-B

Chain n:  94% • 5%




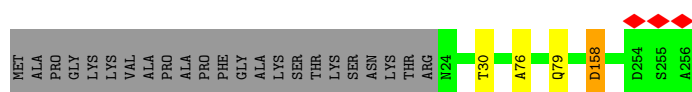
- Molecule 38: 60S ribosomal protein L7-A

Chain o:  91% 9%



- Molecule 39: 60S ribosomal protein L8-A

Chain p:  89% • 9%



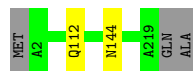
- Molecule 40: 60S ribosomal protein L9-A

Chain q:  98% ..



- Molecule 41: 60S ribosomal protein L10

Chain r:  98% ..



- Molecule 42: 60S ribosomal protein L11-A

Chain s:  95% ..



- Molecule 43: 60S ribosomal protein L13-A

Chain t:  96% ..



- MET
SER
T3
W12
D47
A138

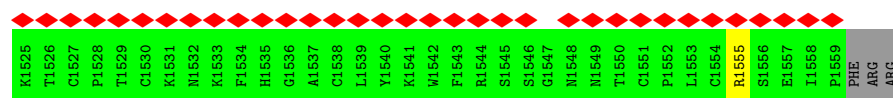
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ASN	R682	L409
GLU		
VAL	L697	V450
ASN		D453
GLY	W705	S456
LEU	K708	LYS
GLU	THR	LEU
LYS	GLY	GLY
GLY	GLN	ASN
ASP	ASN	THR
SER	ASN	SER
ASN	ASP	SER
ASP	ASP	SER
SER	THR	GLU
THR	GLY	ASP
LYS	ASP	GLU
ASN	ASP	ASN
ASN	ASP	GLU
SER	GLU	SER
PHE	GLU	GLY
GLU	GLU	GLY
HIS	GLU	ASN
ASP	GLU	THR
ASN	GLU	THR
LEU	GLU	ASP
LEU	GLU	SER
LYS	GLU	SER
ASP	GLU	SER
ILE	GLU	ASP
GLU	GLU	SER
LYS	GLU	ASP
HIS	GLU	SER
CYS	GLU	GLU
THR	GLU	ASP
ILE	GLU	MET
SER	GLU	GLU
SER	GLU	SER
ASP	GLU	SER
THR	GLU	LYS
ASP	GLU	GLU
SER	GLU	ARG
ASP	GLU	THR
SER	LYS	THR
GLY	GLU	LYS
ASN	GLU	SER
ALA	GLU	MET
LYS	GLU	LYS
ALA	LYS	ARG
LYS	GLU	LYS
ASN	GLU	SER
ASN	GLU	LYS
ASP	GLU	THR
ASN	GLN	H501
SER	GLN	H589
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ILE	ASP	V640
LEU	SER	

[illegible]

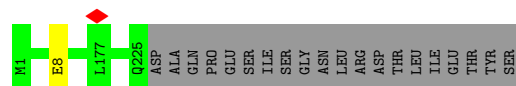
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| Y612 | F544 | S468 | H368 | T8 |
| Q613 | I545 | D469 | S369 | V23 |
| Q614 | N546 | E470 | F370 | F30 |
| L615 | E547 | D471 | L371 | I125 |
| M616 | I548 | I472 | D372 | L143 |
| K617 | P549 | R473 | Y373 | T166 |
| S618 | T550 | K474 | Y374 | L178 |
| D619 | L551 | I475 | L375 | S194 |
| S620 | V552 | K476 | | E206 |
| L621 | Q553 | V477 | F380 | S230 |
| E622 | E554 | | R387 | I240 |
| L623 | S555 | T489 | | W247 |
| E624 | T556 | S490 | | K248 |
| L625 | V557 | K491 | G392 | L249 |
| Y626 | Q558 | H492 | F393 | K253 |
| I627 | N559 | I493 | S394 | N254 |
| E628 | F560 | E494 | A395 | G255 |
| D629 | A561 | S495 | R396 | Q256 |
| F630 | S568 | A496 | N397 | Y276 |
| M631 | K571 | I497 | L410 | H297 |
| K632 | F572 | S498 | | I298 |
| N633 | F573 | R499 | A413 | T299 |
| Y634 | K574 | L500 | E414 | S300 |
| F636 | N575 | D502 | D415 | K301 |
| D637 | N576 | F503 | S416 | K305 |
| D638 | T577 | F504 | S417 | V309 |
| D639 | E578 | V505 | E418 | Y323 |
| S639 | S839 | Q506 | E419 | E324 |
| G640 | A579 | L507 | R420 | D325 |
| E641 | I580 | I508 | W421 | G326 |
| I642 | T581 | E509 | | S330 |
| F643 | S882 | T510 | K437 | Y331 |
| K644 | L583 | D511 | S438 | D332 |
| G645 | F587 | F512 | L439 | S334 |
| N646 | I588 | S513 | S440 | K338 |
| N647 | V589 | N514 | E441 | F342 |
| K648 | A590 | V515 | Y442 | |
| F649 | L591 | F516 | T443 | |
| L650 | S592 | N517 | | |
| N651 | F593 | K518 | S450 | |
| Q652 | N594 | Y519 | C451 | |
| R653 | L595 | D520 | V452 | |
| T654 | P596 | G521 | F453 | |
| I655 | K597 | L526 | P454 | |
| T656 | T598 | | P455 | |
| L658 | I599 | D531 | K457 | |
| Y659 | I600 | S532 | W458 | |
| R660 | L601 | D533 | E459 | |
| S661 | A602 | M534 | R460 | |
| A662 | T603 | T535 | E461 | |
| V663 | M604 | F536 | F465 | |
| A664 | N605 | L537 | E463 | |
| N665 | L607 | N538 | D464 | |
| G666 | D608 | O539 | Y465 | |
| Q667 | N609 | K540 | F466 | |
| V668 | D610 | T541 | | |
| E669 | | G542 | | |

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K1438	L1351	Q1153	L1093	K1033	T973	L913	E853	N793	A673
L1439	L1352	K1154	Y1094	W1034	T974	Y914	E854	T794	V674
L1440	G1353	L1155	L1095	D1035	K975	K915	P855	H795	L675
I1441	H1354	Y1156	L1096	D1036	L976	V916	N856	L796	S676
S1442	T1355	K1157	E1097	S1037	R977	L917	D857	L797	K677
F1443	L1356	Y1158	L1098	D1038	T978	L918	L958	L798	L678
Y1449	L1357	L1159	R1099	L1039	L979	N919	Y859	T799	D679
I1454	Q1358	K1295	S1100	A1040	L980	S920	Y860	D800	E680
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R1461	N1362	E1163	L1103	L1043	Q983	T923	G863	P803	F683
V1462	N1361	L1164	N1104	S1044	L984	V924	H864	I804	S684
G1463	L1299	K1165	L1105	F1045	L985	S925	T865	N805	T685
I1464	I1300	K1166	Y1106	S1046	Q866	S926	F866	L806	L686
T1367	M1301	L1167	E1107	T1047	R987	T927	F867	K807	L687
L1379	R1302	E1168	T1108	V1048	R988	T928	K868	N808	L688
K1385	M1303	S1169	L1109	R1049	E989	L929	H869	M809	N689
F1386	D1305	Q1170	S1110	L1050	V990	N930	G870	Q810	T690
F1386	D1309	Y1171	Q1111	L1051	E991	G931	K871	V751	D691
E1399	D1312	K1172	GLY	L1052	L992	L932	N872	L812	F692
F1400	L1313	R1173	VAL	L1053	V993	L933	N873	I813	L693
D1401	L1314	I1174	LYS	D1054	D994	A934	L874	R814	S694
D1402	R1315	F1175	ASN	F1055	Q995	S935	N875	Y815	C695
I1403	D1316	E1176	GLY	F1056	E996	V936	F876	A816	A696
N1404	T1317	V1177	GLU	T1057	F997	E937	S877	L817	L697
S1405	E1317	Y1178	GLU	T1058	K998	S938	D878	F818	L697
K1406	K1243	L1179	ILE	K1058	S999	S939	D879	N758	Y698
M1407	L1244	M1180	SER	M1059	E999	F939	I879	L819	E699
D1408	L1245	D1181	E1122	M1060	L1000	V940	V880	D820	V700
H1409	L1246	D1182	Y1123	R1061	A1001	T941	G881	A821	S701
L1410	K1247	K1183	G1124	F1062	L1002	K942	N882	L822	E702
L1411	V1248	D1184	D1125	E1063	L1003	T943	V883	L823	D703
SER	T1249	G1185	E1126	G1064	N1004	V944	I884	D824	T704
ASN	D1250	G1186	I1127	V1065	N1005	R945	Q885	A825	N705
ASP	E1251	S1187	Q1128	R1066	L1006	D946	P886	L826	E706
ASP	V1252	I1188	E1129	D1067	L1007	Q947	A887	P827	K707
A1416	P1253	N1189	M1130	M1068	D1008	K948	N888	E828	L708
L1417	K1254	Q1190	L1131	G1069	I1009	S949	G889	R829	F709
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N1423	E1258	L1194	M1135	F1073	D1013	D953	M893	H833	S712
I1424	Y1259	T1195	F1136	E1074	K1014	Y954	L894	I834	L713
T1425	E1260	T1196	L1137	L1075	Q1015	L955	T895	V835	Q714
N1426	N1261	L1197	M1138	S1076	F1016	L956	F896	A836	L715
E1427	K1262	L1198	F1139	E1077	V1017	C957	D897	F837	K717
L1428	N1263	G1199	M1140	R1078	P1018	A958	I898	I838	G718
K1429	S1264	S1200	Q1141	L1079	I1019	I959	A899	T839	L719
A1430	L1269	R1143	E1142	L1080	A1020	L960	E900	V840	N720
S1431	L1201	N1144	R1143	A1081	P1021	L961	S901	V841	E721
D1343	V1202	M1145	N1144	D1082	Q1022	L962	N902	S842	T722
I1344	V1203	Q1146	N1145	S1083	R1023	M963	S903	E843	A723
F1345	K1204	V1147	Q1146	L1084	L1024	F964	V904	L844	N724
E1346	T1205	V1147	S1085	S1085	N1025	N965	Y905	V845	K725
E1347	Q1206	S1148	M1086	M1086	M1026	R966	F906	L786	L726
C1348	Q1207	T1149	C1087	C1087	S967	N967	F907	D847	A727
	D1208	L1150	Q1087	I1089	R1029	S969	Y909	N849	G728
	I1209		I1089	D1090			S910		V729
	I1210								I730



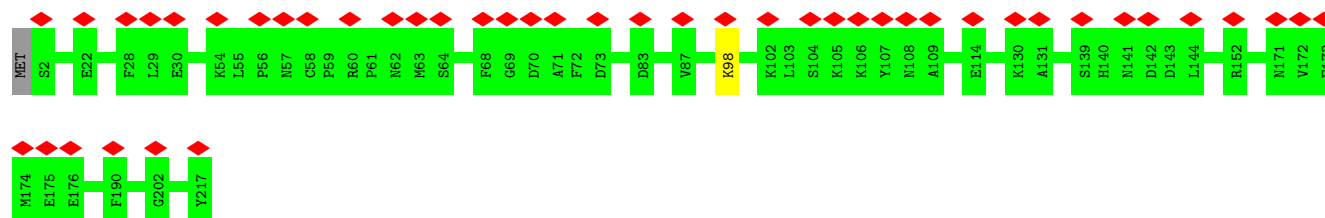
- Molecule 47: Eukaryotic translation initiation factor 6

Chain g: 91% 8%



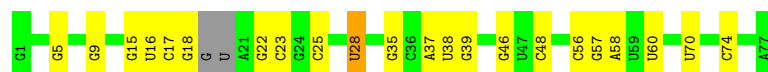
- Molecule 48: 60S ribosomal protein L1-A

Chain w: 21% 99%



- Molecule 49: A-site Ala aminoacyl-tRNA

Chain x: 69% 27%



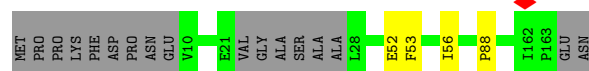
- Molecule 50: P-site petidyl-tRNA

Chain y: 66% 30%



- Molecule 51: 60S ribosomal protein L12-A

Chain z: 87% 10%



- Molecule 52: 60S acidic ribosomal protein P0

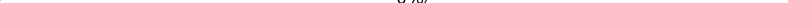
Chain 0: 30% 7% 61%

- Molecule 53: CAT tailed nascent peptide

Chain 1:  94% 6%



- Molecule 54: Eukaryotic translation initiation factor 5A-1

Chain v:  8% 87% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	3.681	Depositor
Minimum map value	-0.788	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CT, MG

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	0.38	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	0.37	0/812	0.73	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	0.50	0/868	0.64	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	0.67	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	0.34	0/416	0.70	0/553
27	b	0.36	0/836	0.66	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	0/77011	1.03	296/120065 (0.2%)
31	h	0.53	0/2883	0.98	9/4491 (0.2%)
32	i	0.61	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.38	0/1908	0.67	0/2564
34	k	0.36	0/3146	0.63	1/4228 (0.0%)
35	l	0.36	0/2800	0.64	2/3790 (0.1%)
36	m	0.34	0/2400	0.67	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	0.63	0/2416
42	s	0.33	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	0.29	0/6679	0.49	0/9012
46	e	0.28	0/11707	0.49	0/15897
47	g	0.32	0/1672	0.63	0/2281
48	w	0.33	0/1736	0.65	0/2332
49	x	0.33	0/1765	1.00	8/2746 (0.3%)
50	y	0.22	0/1735	0.65	0/2701
51	z	0.37	0/726	0.60	0/1006
52	0	0.33	0/976	0.55	0/1313
54	v	0.33	0/1084	0.63	1/1456 (0.1%)
All	All	0.50	0/161755	0.87	354/236294 (0.1%)

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
23	W	0	1
34	k	0	2
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	2
47	g	0	1
All	All	0	15

There are no bond length outliers.

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3217	C	N1-C2-O2	12.17	126.20	118.90
30	f	3217	C	C2-N1-C1'	11.30	131.23	118.80
30	f	3217	C	N3-C2-O2	-9.78	115.05	121.90
11	K	134	ASP	CB-CG-OD1	9.65	126.99	118.30
30	f	922	U	C2-N1-C1'	9.29	128.84	117.70
17	Q	84	ASP	CB-CG-OD1	9.28	126.65	118.30
30	f	2531	C	N1-C2-O2	8.88	124.23	118.90
30	f	922	U	N1-C2-O2	8.82	128.97	122.80
30	f	3181	C	N1-C2-O2	8.72	124.13	118.90
30	f	3278	C	N1-C2-O2	8.70	124.12	118.90
30	f	3181	C	C2-N1-C1'	8.48	128.13	118.80
30	f	2836	C	N3-C2-O2	-8.29	116.09	121.90
30	f	1279	C	C5-C6-N1	8.28	125.14	121.00
30	f	2836	C	C2-N1-C1'	8.20	127.81	118.80
36	m	230	ASP	CB-CG-OD1	8.15	125.64	118.30
30	f	1496	C	C2-N1-C1'	8.05	127.66	118.80
30	f	922	U	N3-C2-O2	-7.99	116.61	122.20
30	f	1645	U	N3-C2-O2	-7.94	116.64	122.20
30	f	406	G	O4'-C1'-N9	7.91	114.53	108.20
30	f	2205	U	N1-C2-O2	7.88	128.32	122.80
30	f	1208	U	N1-C2-O2	7.81	128.27	122.80
30	f	2444	C	C2-N1-C1'	7.80	127.38	118.80
30	f	2983	C	C2-N1-C1'	7.78	127.36	118.80
30	f	3217	C	C6-N1-C2	-7.76	117.19	120.30
30	f	3217	C	C6-N1-C1'	-7.75	111.50	120.80
30	f	3306	U	N3-C2-O2	-7.75	116.78	122.20
4	D	41	ASP	CB-CG-OD1	7.73	125.25	118.30
30	f	2652	U	N3-C2-O2	-7.66	116.84	122.20
30	f	2205	U	N3-C2-O2	-7.57	116.90	122.20
30	f	3278	C	N3-C2-O2	-7.57	116.60	121.90
30	f	3306	U	C2-N1-C1'	7.56	126.78	117.70
30	f	2541	U	P-O3'-C3'	7.55	128.75	119.70
30	f	3278	C	C2-N1-C1'	7.53	127.09	118.80
30	f	758	C	C2-N1-C1'	7.48	127.03	118.80
30	f	1645	U	N1-C2-O2	7.47	128.03	122.80
30	f	3181	C	N3-C2-O2	-7.39	116.73	121.90
30	f	2502	A	OP2-P-O3'	7.38	121.43	105.20
30	f	1277	C	C2-N1-C1'	7.37	126.91	118.80
30	f	2836	C	N1-C2-O2	7.35	123.31	118.90
30	f	2235	C	C2-N1-C1'	7.31	126.84	118.80
30	f	1239	C	C2-N1-C1'	7.24	126.76	118.80
30	f	2531	C	C2-N1-C1'	7.21	126.73	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	36	ASP	CB-CG-OD1	7.21	124.79	118.30
30	f	1556	C	N1-C2-O2	7.21	123.22	118.90
42	s	170	ASP	CB-CG-OD1	7.19	124.77	118.30
30	f	2502	A	P-O3'-C3'	7.15	128.28	119.70
30	f	2923	U	N1-C2-O2	7.15	127.80	122.80
30	f	78	U	N3-C2-O2	-7.14	117.20	122.20
30	f	1227	C	N1-C2-O2	7.13	123.18	118.90
30	f	2205	U	C2-N1-C1'	7.11	126.23	117.70
30	f	36	C	N1-C2-O2	7.10	123.16	118.90
30	f	1349	G	N3-C4-C5	-7.10	125.05	128.60
30	f	1277	C	N1-C2-O2	7.08	123.15	118.90
30	f	1815	U	P-O3'-C3'	7.08	128.19	119.70
30	f	1227	C	C2-N1-C1'	7.07	126.58	118.80
39	p	158	ASP	CB-CG-OD1	7.06	124.66	118.30
30	f	982	C	C2-N1-C1'	7.06	126.56	118.80
30	f	14	U	O5'-P-OP2	-7.05	99.35	105.70
30	f	1604	G	C4-N9-C1'	7.03	135.63	126.50
30	f	1307	G	P-O3'-C3'	7.02	128.13	119.70
30	f	1645	U	C2-N1-C1'	7.02	126.12	117.70
30	f	1349	G	C4-N9-C1'	6.98	135.57	126.50
49	x	25	C	N3-C2-O2	-6.97	117.02	121.90
30	f	1272	C	N1-C2-O2	6.93	123.06	118.90
30	f	3306	U	N1-C2-O2	6.92	127.64	122.80
30	f	1872	C	N1-C2-O2	6.92	123.05	118.90
30	f	3217	C	C5-C6-N1	6.92	124.46	121.00
30	f	1208	U	C2-N1-C1'	6.89	125.97	117.70
30	f	2405	C	C6-N1-C2	-6.88	117.55	120.30
30	f	3275	U	OP1-P-O3'	6.87	120.32	105.20
30	f	3235	C	C2-N1-C1'	6.85	126.33	118.80
30	f	2836	C	C6-N1-C2	-6.84	117.56	120.30
30	f	2846	U	C2-N1-C1'	6.80	125.86	117.70
30	f	2846	U	N3-C2-O2	-6.80	117.44	122.20
30	f	1227	C	C5-C6-N1	6.78	124.39	121.00
30	f	2923	U	N3-C2-O2	-6.76	117.47	122.20
30	f	2983	C	N3-C2-O2	-6.72	117.20	121.90
30	f	270	U	N1-C2-O2	6.71	127.50	122.80
12	L	11	ASP	CB-CG-OD1	6.70	124.33	118.30
30	f	1227	C	C6-N1-C2	-6.70	117.62	120.30
30	f	270	U	N3-C2-O2	-6.68	117.52	122.20
30	f	1239	C	N1-C2-O2	6.67	122.91	118.90
30	f	2537	U	P-O3'-C3'	6.67	127.70	119.70
30	f	2531	C	N3-C2-O2	-6.66	117.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	26	C	N1-C2-O2	6.63	122.88	118.90
30	f	2112	U	OP2-P-O3'	6.62	119.76	105.20
30	f	2189	U	N1-C2-O2	6.61	127.43	122.80
30	f	3058	U	C2-N1-C1'	6.59	125.61	117.70
49	x	28	U	N3-C4-O4	6.58	124.01	119.40
30	f	3214	U	C2-N1-C1'	6.57	125.58	117.70
30	f	1208	U	N3-C2-O2	-6.55	117.61	122.20
31	h	105	C	N1-C2-O2	6.53	122.81	118.90
2	B	27[A]	LEU	CB-CG-CD2	-6.52	99.91	111.00
30	f	2189	U	N3-C2-O2	-6.52	117.64	122.20
30	f	2235	C	C6-N1-C2	-6.48	117.71	120.30
30	f	2550	U	N3-C2-O2	-6.48	117.67	122.20
32	i	64	U	N3-C2-O2	-6.47	117.67	122.20
30	f	2112	U	P-O3'-C3'	6.45	127.43	119.70
30	f	3034	C	N1-C2-O2	6.44	122.76	118.90
30	f	2101	C	P-O3'-C3'	6.43	127.42	119.70
30	f	524	U	N1-C2-O2	6.42	127.29	122.80
35	l	155	ASP	CB-CG-OD1	6.42	124.08	118.30
30	f	1269	U	C2-N1-C1'	6.42	125.40	117.70
30	f	2274	U	N1-C2-O2	6.40	127.28	122.80
30	f	2983	C	N1-C2-O2	6.37	122.72	118.90
44	u	47	ASP	CB-CG-OD1	6.36	124.02	118.30
30	f	986	U	N3-C2-O2	-6.34	117.76	122.20
1	A	153	ASP	CB-CG-OD1	6.34	124.01	118.30
30	f	865	U	N3-C2-O2	-6.34	117.76	122.20
30	f	36	C	N3-C2-O2	-6.33	117.47	121.90
30	f	2726	C	N3-C2-O2	-6.33	117.47	121.90
30	f	3058	U	N1-C2-O2	6.33	127.23	122.80
30	f	1556	C	N3-C2-O2	-6.33	117.47	121.90
30	f	2617	U	N3-C2-O2	-6.33	117.77	122.20
36	m	137	ASP	CB-CG-OD1	6.33	123.99	118.30
30	f	1269	U	N1-C2-O2	6.32	127.22	122.80
30	f	2464	U	C2-N1-C1'	6.31	125.27	117.70
21	U	79	ASP	CB-CG-OD1	6.27	123.95	118.30
30	f	524	U	N3-C2-O2	-6.25	117.82	122.20
30	f	922	U	C6-N1-C1'	-6.25	112.45	121.20
30	f	1269	U	N3-C2-O2	-6.25	117.82	122.20
40	q	42	ASP	CB-CG-OD1	6.25	123.92	118.30
30	f	2444	C	C6-N1-C2	-6.25	117.80	120.30
30	f	1716	U	P-O3'-C3'	6.23	127.18	119.70
30	f	1097	G	P-O3'-C3'	6.23	127.17	119.70
30	f	192	C	C2-N1-C1'	6.20	125.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2726	C	C2-N1-C1'	6.20	125.62	118.80
30	f	1878	G	C4-N9-C1'	6.19	134.55	126.50
30	f	3104	U	N1-C2-O2	6.17	127.12	122.80
30	f	1496	C	C6-N1-C2	-6.17	117.83	120.30
30	f	3104	U	N3-C2-O2	-6.14	117.90	122.20
30	f	637	C	P-O3'-C3'	6.13	127.06	119.70
30	f	2553	U	C2-N1-C1'	6.12	125.04	117.70
30	f	915	A	C2-N3-C4	6.12	113.66	110.60
30	f	2846	U	N1-C2-O2	6.11	127.08	122.80
30	f	2132	C	C6-N1-C2	-6.11	117.86	120.30
30	f	2550	U	C2-N1-C1'	6.10	125.02	117.70
30	f	1064	A	P-O3'-C3'	6.09	127.01	119.70
30	f	1115	G	C4-N9-C1'	6.08	134.41	126.50
30	f	2923	U	C2-N1-C1'	6.08	125.00	117.70
30	f	2388	U	N3-C2-O2	-6.08	117.95	122.20
30	f	1349	G	N3-C4-N9	6.07	129.64	126.00
30	f	2842	U	N1-C2-O2	6.07	127.05	122.80
30	f	2132	C	N3-C2-O2	-6.06	117.66	121.90
30	f	2405	C	N3-C2-O2	-6.05	117.66	121.90
30	f	969	C	C6-N1-C2	-6.04	117.88	120.30
30	f	995	U	N1-C2-O2	6.03	127.02	122.80
30	f	1604	G	N3-C4-N9	6.03	129.62	126.00
30	f	3131	U	C2-N1-C1'	6.03	124.94	117.70
30	f	1907	C	N1-C2-O2	6.02	122.51	118.90
30	f	1604	G	C8-N9-C1'	-6.01	119.19	127.00
30	f	2274	U	C2-N1-C1'	6.00	124.89	117.70
30	f	1279	C	C6-N1-C2	-5.99	117.91	120.30
30	f	1425	U	N3-C2-O2	-5.98	118.01	122.20
30	f	1604	G	N3-C4-C5	-5.98	125.61	128.60
30	f	985	U	N3-C2-O2	-5.97	118.02	122.20
30	f	1556	C	C2-N1-C1'	5.96	125.36	118.80
30	f	2204	C	C6-N1-C2	-5.96	117.92	120.30
30	f	3300	U	N3-C2-O2	-5.96	118.03	122.20
30	f	3181	C	C6-N1-C1'	-5.96	113.65	120.80
31	h	26	C	C6-N1-C2	-5.95	117.92	120.30
8	H	51	GLY	C-N-CA	5.94	136.55	121.70
34	k	87	VAL	CG1-CB-CG2	-5.94	101.40	110.90
8	H	18	ASP	CB-CG-OD1	5.93	123.64	118.30
30	f	1872	C	N3-C2-O2	-5.93	117.75	121.90
30	f	2652	U	N1-C2-O2	5.91	126.94	122.80
30	f	1355	A	P-O3'-C3'	5.91	126.79	119.70
30	f	865	U	N1-C2-O2	5.90	126.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1272	C	N3-C2-O2	-5.89	117.78	121.90
30	f	3048	A	O4'-C1'-N9	5.89	112.91	108.20
32	i	100	U	C2-N1-C1'	5.89	124.77	117.70
30	f	1820	U	P-O3'-C3'	5.88	126.76	119.70
30	f	2585	G	N3-C4-C5	-5.87	125.66	128.60
30	f	3350	C	C6-N1-C2	-5.87	117.95	120.30
30	f	1562	C	P-O3'-C3'	5.86	126.73	119.70
30	f	1437	C	C2-N1-C1'	5.85	125.23	118.80
30	f	3214	U	N3-C2-O2	-5.84	118.11	122.20
30	f	1525	G	C4-N9-C1'	5.84	134.09	126.50
30	f	835	G	O4'-C1'-N9	5.82	112.85	108.20
30	f	2274	U	N3-C2-O2	-5.80	118.14	122.20
30	f	2531	C	C6-N1-C2	-5.80	117.98	120.30
42	s	9	MET	CA-CB-CG	5.79	123.15	113.30
30	f	2638	C	N1-C2-O2	5.79	122.37	118.90
30	f	3316	A	P-O3'-C3'	5.77	126.62	119.70
30	f	270	U	C2-N1-C1'	5.77	124.62	117.70
30	f	142	C	N1-C2-O2	5.76	122.36	118.90
30	f	2622	C	N1-C2-O2	5.76	122.35	118.90
30	f	2531	C	C5-C6-N1	5.75	123.88	121.00
30	f	3228	C	P-O3'-C3'	5.74	126.59	119.70
30	f	142	C	C6-N1-C2	-5.74	118.00	120.30
30	f	758	C	C6-N1-C2	-5.74	118.01	120.30
30	f	1577	G	N1-C6-O6	-5.73	116.46	119.90
30	f	2899	C	C2-N1-C1'	5.72	125.09	118.80
30	f	354	U	N1-C2-O2	5.71	126.80	122.80
30	f	2553	U	C6-N1-C1'	-5.71	113.21	121.20
30	f	3218	A	P-O3'-C3'	5.71	126.55	119.70
30	f	1190	A	C4-N9-C1'	5.71	136.57	126.30
30	f	3058	U	N3-C2-O2	-5.70	118.21	122.20
30	f	2204	C	C5-C6-N1	5.70	123.85	121.00
30	f	2366	C	C2-N1-C1'	5.69	125.06	118.80
32	i	64	U	N1-C2-O2	5.68	126.78	122.80
30	f	97	U	N3-C2-O2	-5.68	118.22	122.20
30	f	2899	C	N3-C2-O2	-5.67	117.93	121.90
30	f	916	G	P-O3'-C3'	5.66	126.49	119.70
8	H	50	LEU	CA-CB-CG	5.66	128.31	115.30
30	f	2992	U	N3-C2-O2	-5.65	118.24	122.20
30	f	1448	U	N3-C2-O2	-5.65	118.25	122.20
30	f	282	G	P-O3'-C3'	5.65	126.47	119.70
30	f	3034	C	N3-C2-O2	-5.63	117.96	121.90
30	f	2842	U	N3-C2-O2	-5.63	118.26	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2378	C	C2-N1-C1'	5.62	124.99	118.80
30	f	1349	G	C8-N9-C1'	-5.62	119.69	127.00
30	f	2132	C	N1-C2-O2	5.62	122.27	118.90
30	f	1277	C	N3-C2-O2	-5.61	117.97	121.90
30	f	113	C	C2-N1-C1'	5.61	124.97	118.80
30	f	777	U	N3-C2-O2	-5.61	118.28	122.20
30	f	2983	C	C6-N1-C2	-5.60	118.06	120.30
30	f	2137	U	C2-N1-C1'	5.60	124.42	117.70
30	f	3057	U	N3-C2-O2	-5.59	118.28	122.20
30	f	2726	C	N1-C2-O2	5.59	122.25	118.90
30	f	1496	C	N1-C2-O2	5.59	122.25	118.90
31	h	26	C	N3-C2-O2	-5.57	118.00	121.90
30	f	982	C	N1-C2-O2	5.56	122.24	118.90
49	x	25	C	N1-C2-O2	5.56	122.24	118.90
30	f	2552	C	N1-C2-O2	5.56	122.24	118.90
40	q	107	ASP	CB-CG-OD1	5.56	123.30	118.30
30	f	2764	C	N1-C2-O2	5.55	122.23	118.90
30	f	3269	U	P-O3'-C3'	5.55	126.36	119.70
49	x	25	C	C6-N1-C2	-5.55	118.08	120.30
30	f	995	U	N3-C2-O2	-5.54	118.32	122.20
32	i	125	U	C2-N1-C1'	5.54	124.35	117.70
30	f	1496	C	C5-C6-N1	5.53	123.77	121.00
30	f	2366	C	C5-C6-N1	5.53	123.76	121.00
49	x	70	U	N1-C2-O2	5.53	126.67	122.80
30	f	2210	G	N3-C4-C5	-5.52	125.84	128.60
31	h	35	C	N1-C2-O2	5.50	122.20	118.90
30	f	1554	U	P-O3'-C3'	5.50	126.30	119.70
3	C	53	ASP	CB-CG-OD1	5.50	123.25	118.30
31	h	52	G	P-O3'-C3'	5.49	126.28	119.70
49	x	28	U	C5-C4-O4	-5.48	122.61	125.90
30	f	283	G	C4-N9-C1'	5.47	133.61	126.50
30	f	986	U	N1-C2-O2	5.47	126.63	122.80
24	X	14	LEU	CA-CB-CG	5.46	127.87	115.30
30	f	3214	U	N1-C2-O2	5.46	126.62	122.80
30	f	2444	C	N1-C2-O2	5.45	122.17	118.90
30	f	283	G	N3-C4-N9	5.45	129.27	126.00
30	f	315	C	C2-N1-C1'	5.45	124.79	118.80
30	f	3355	U	C2-N1-C1'	5.44	124.23	117.70
30	f	411	U	N3-C2-O2	-5.43	118.40	122.20
30	f	3350	C	P-O3'-C3'	5.42	126.20	119.70
30	f	1878	G	C8-N9-C1'	-5.41	119.97	127.00
30	f	1732	U	N1-C2-O2	5.41	126.58	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1688	U	N3-C2-O2	-5.40	118.42	122.20
30	f	3153	U	C2-N1-C1'	5.40	124.18	117.70
30	f	2552	C	C2-N1-C1'	5.39	124.73	118.80
30	f	3057	U	N1-C2-O2	5.38	126.57	122.80
30	f	2585	G	N3-C4-N9	5.38	129.23	126.00
30	f	78	U	N1-C2-O2	5.37	126.56	122.80
30	f	982	C	C6-N1-C2	-5.37	118.15	120.30
30	f	915	A	C4-N9-C1'	5.37	135.96	126.30
30	f	2500	A	P-O3'-C3'	5.36	126.14	119.70
30	f	3235	C	N1-C2-O2	5.36	122.12	118.90
30	f	2114	C	C6-N1-C2	-5.36	118.16	120.30
30	f	890	C	N1-C2-O2	5.35	122.11	118.90
3	C	114	VAL	CG1-CB-CG2	-5.35	102.34	110.90
30	f	1496	C	C6-N1-C1'	-5.35	114.38	120.80
30	f	1425	U	N1-C2-O2	5.35	126.54	122.80
30	f	3278	C	C6-N1-C1'	-5.34	114.39	120.80
30	f	1732	U	N3-C2-O2	-5.33	118.47	122.20
30	f	1277	C	C6-N1-C2	-5.33	118.17	120.30
30	f	142	C	N3-C2-O2	-5.32	118.17	121.90
30	f	1525	G	C8-N9-C1'	-5.32	120.08	127.00
30	f	2622	C	N3-C2-O2	-5.32	118.18	121.90
30	f	2726	C	C6-N1-C2	-5.32	118.17	120.30
30	f	2783	U	N3-C2-O2	-5.32	118.48	122.20
30	f	2497	U	N3-C2-O2	-5.31	118.48	122.20
30	f	192	C	C6-N1-C2	-5.31	118.18	120.30
30	f	2444	C	C5-C6-N1	5.31	123.65	121.00
30	f	1115	G	C8-N9-C1'	-5.30	120.11	127.00
43	t	136	GLU	CA-CB-CG	5.29	125.05	113.40
31	h	105	C	N3-C2-O2	-5.29	118.20	121.90
30	f	915	A	C8-N9-C4	-5.28	103.69	105.80
30	f	1560	G	N3-C4-N9	-5.28	122.83	126.00
30	f	1349	G	C2-N3-C4	5.28	114.54	111.90
30	f	3181	C	C6-N1-C2	-5.28	118.19	120.30
30	f	982	C	C5-C6-N1	5.28	123.64	121.00
30	f	2366	C	C6-N1-C2	-5.28	118.19	120.30
30	f	2405	C	N1-C2-O2	5.28	122.07	118.90
32	i	125	U	N1-C2-O2	5.28	126.49	122.80
30	f	2772	C	N1-C2-O2	5.27	122.06	118.90
30	f	1437	C	C6-N1-C2	-5.27	118.19	120.30
30	f	1608	C	C2-N1-C1'	5.27	124.59	118.80
30	f	1907	C	N3-C2-O2	-5.27	118.21	121.90
54	v	50	GLY	N-CA-C	-5.26	99.95	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2235	C	C5-C6-N1	5.26	123.63	121.00
30	f	2336	U	N3-C2-O2	-5.25	118.53	122.20
30	f	2836	C	C6-N1-C1'	-5.25	114.50	120.80
30	f	2568	C	O4'-C1'-N1	5.25	112.40	108.20
30	f	2235	C	N1-C2-O2	5.24	122.05	118.90
42	s	108	GLU	CA-CB-CG	5.24	124.92	113.40
30	f	1608	C	C5-C6-N1	5.23	123.62	121.00
30	f	2585	G	C4-N9-C1'	5.23	133.30	126.50
30	f	1239	C	C6-N1-C1'	-5.23	114.53	120.80
30	f	2496	C	C2-N1-C1'	5.22	124.54	118.80
30	f	890	C	N3-C2-O2	-5.22	118.25	121.90
30	f	2622	C	C6-N1-C2	-5.20	118.22	120.30
30	f	954	U	N3-C2-O2	-5.20	118.56	122.20
30	f	1237	G	N3-C4-N9	5.19	129.12	126.00
31	h	18	C	C2-N1-C1'	5.19	124.51	118.80
30	f	2983	C	C6-N1-C1'	-5.19	114.57	120.80
30	f	849	C	P-O3'-C3'	5.17	125.91	119.70
30	f	2446	U	O4'-C1'-N1	5.17	112.34	108.20
30	f	3148	U	N3-C2-O2	-5.16	118.59	122.20
30	f	637	C	OP1-P-O3'	5.16	116.54	105.20
30	f	1190	A	C2-N3-C4	5.15	113.18	110.60
30	f	1608	C	C6-N1-C2	-5.15	118.24	120.30
30	f	2405	C	C2-N1-C1'	5.15	124.47	118.80
30	f	2550	U	N1-C2-O2	5.15	126.41	122.80
32	i	100	U	N1-C2-O2	5.15	126.41	122.80
49	x	70	U	N3-C2-O2	-5.15	118.60	122.20
30	f	87	U	N1-C2-O2	5.15	126.40	122.80
30	f	166	C	C2-N1-C1'	5.15	124.46	118.80
49	x	23	C	C6-N1-C2	-5.14	118.24	120.30
30	f	1563	C	C6-N1-C1'	5.13	126.96	120.80
30	f	1951	C	C2-N1-C1'	5.13	124.44	118.80
30	f	969	C	N3-C2-O2	-5.12	118.31	121.90
30	f	1272	C	C6-N1-C2	-5.12	118.25	120.30
30	f	3349	C	C6-N1-C2	-5.12	118.25	120.30
36	m	222	LEU	CA-CB-CG	5.09	127.00	115.30
30	f	149	U	N3-C2-O2	-5.09	118.64	122.20
32	i	157	U	N1-C2-O2	5.08	126.36	122.80
30	f	1597	C	C5-C6-N1	5.08	123.54	121.00
30	f	1097	G	OP2-P-O3'	5.07	116.35	105.20
35	l	4	PRO	C-N-CA	5.07	134.38	121.70
17	Q	42	LEU	CA-CB-CG	5.07	126.95	115.30
30	f	2836	C	O4'-C1'-N1	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2899	C	N1-C2-O2	5.07	121.94	118.90
30	f	885	U	N3-C2-O2	-5.06	118.66	122.20
30	f	2638	C	N3-C2-O2	-5.06	118.36	121.90
30	f	1820	U	OP2-P-O3'	5.05	116.31	105.20
15	O	21	ILE	CG1-CB-CG2	-5.05	100.29	111.40
39	p	79	GLN	CA-CB-CG	5.05	124.51	113.40
30	f	758	C	N1-C2-O2	5.04	121.93	118.90
30	f	2444	C	C6-N1-C1'	-5.04	114.75	120.80
30	f	87	U	N3-C2-O2	-5.04	118.67	122.20
36	m	146	LEU	CB-CG-CD1	-5.04	102.43	111.00
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	969	C	N1-C2-O2	5.02	121.91	118.90
30	f	777	U	N1-C2-O2	5.01	126.31	122.80
5	E	10	LEU	CB-CG-CD1	5.01	119.52	111.00
30	f	282	G	C2'-C3'-O3'	5.00	121.70	113.70
30	f	2497	U	N1-C2-O2	5.00	126.30	122.80
30	f	3363	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
23	W	39	TYR	Peptide
46	e	392	GLY	Peptide
46	e	396	ARG	Peptide
47	g	8	GLU	Peptide
34	k	141	GLY	Peptide
34	k	17	LEU	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 ⓘ

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	10	0
2	B	1555	0	1659	13	0
3	C	1416	0	1433	11	0
4	D	1441	0	1543	8	0
5	E	1258	0	1342	6	0
6	F	1437	0	1475	15	0
7	G	1272	0	1312	9	0
8	H	796	0	812	4	0
9	I	1003	0	1048	7	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	6	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	2	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	5	0
24	X	612	0	682	3	0
25	Y	436	0	475	0	0
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	68802	0	34573	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6569	0	6460	0	0
46	e	11508	0	10762	0	0
47	g	1651	0	1613	0	0
48	w	1709	0	1799	0	0
49	x	1584	0	803	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	85	0	20	0	0
54	v	1085	0	1086	0	0
55	A	1	0	0	0	0
55	C	1	0	0	0	0
55	E	1	0	0	0	0
55	I	1	0	0	0	0
55	R	1	0	0	0	0
55	T	1	0	0	0	0
55	f	3	0	0	0	0
55	h	1	0	0	0	0
55	j	2	0	0	0	0
55	k	1	0	0	0	0
56	T	1	0	0	0	0
56	W	1	0	0	0	0
56	Z	1	0	0	0	0
56	b	1	0	0	0	0
56	c	1	0	0	0	0
56	e	2	0	0	0	0
All	All	151341	0	113586	149	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 (149) 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	1.68	0.90
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
52:O:26:PHE:HB2	52:O:87:VAL:HB	1.73	0.68
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.64
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.62	0.63
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
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.60
52:O:192:ASP:HB2	52:O:197:PHE:HE2	1.67	0.59
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.85	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	1.85	0.58
52:O:43:LYS:HA	52:O: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:OE1	20:T:91:ARG:NH1	2.39	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
52:O:42:ARG:HG2	52:O:51:VAL:HG11	1.88	0.55
2:B:157[A]:GLU:OE1	2:B:160[A]:ARG:NH2	2.40	0.54
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.53
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.90	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.51
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.93	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
7:G:99:SER:HG	7:G:101:CYS:HG	1.59	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
23:W:21:ARG:HH21	23:W:39:TYR:N	2.10	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
16:P:9:SER:OG	16:P:10:ILE:N	2.39	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
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.49
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.48
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
4:D:131:ALA:HB1	4:D:135:GLN:H	1.79	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.95	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	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
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47
52:O:26:PHE:HZ	52:O:93:LEU:HA	1.80	0.47
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	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
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
23:W:43:LYS:HB2	23:W:43:LYS:HE3	1.66	0.46
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.98	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	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
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	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
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
15:O:21:ILE:HD12	15:O:21:ILE:HG23	1.83	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
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.43
4:D:161:LYS:HD3	4:D:161:LYS:HA	1.82	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
52:0:45:LEU:HB3	52:0:49:ALA:HB3	1.99	0.43
20:T:95:ILE:HG21	20:T:95:ILE:HD13	1.81	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
52:0:15:LEU:O	52:0:19:LEU:HG	2.18	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
52:0:75:LYS:O	52:0:78:PRO:HD2	2.19	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.01	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.52	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
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
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
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42
52:0:70:LEU:HB3	52:0:73:PHE:CD1	2.55	0.42
52:0:67:LEU:HD22	52:0:67:LEU:HA	1.85	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.00	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
52:0:61:ARG:HA	52:0:61:ARG:HD2	1.92	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:0:14:LYS:HE3	52:0:52:LEU:HD11	2.00	0.42
16:P:73:GLY:N	16:P:76:GLU:OE2	2.42	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
1:A:170:LYS:HE3	1:A:170:LYS:HB3	4.56	0.41
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.77	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	0.41
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
5:E:7:GLN:NE2	5:E:35:ALA:O	2.53	0.41
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.41
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.40
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.40
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.01	0.40
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
5:E:31:GLU:HA	5:E:34:GLN:HB2	2.03	0.40
6:F:40:ARG:HA	6:F:40:ARG:HD2	1.84	0.40
4:D:180:ARG:HE	4:D:180:ARG:HB2	1.62	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/204 (98%)	190 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	100 (96%)	4 (4%)	0	100	100
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%)	74 (94%)	5 (6%)	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%)	364 (95%)	20 (5%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	37	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	m	292/297 (98%)	278 (95%)	14 (5%)	0	100	100
37	n	163/176 (93%)	153 (94%)	10 (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%)	832 (99%)	10 (1%)	0	100	100
46	e	1519/1562 (97%)	1503 (99%)	14 (1%)	2 (0%)	48	71
47	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
48	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
51	z	144/165 (87%)	135 (94%)	5 (4%)	4 (3%)	4	7
52	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	31
54	v	139/157 (88%)	139 (100%)	0	0	100	100
All	All	9314/10279 (91%)	8965 (96%)	337 (4%)	12 (0%)	50	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	e	437	LYS
51	z	88	PRO
51	z	52	GLU
51	z	53	PHE
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
51	z	56	ILE
52	0	93	LEU
46	e	855	PRO
15	O	21	ILE
43	t	47	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	87 (100%)	0	100	100
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
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	89 (99%)	1 (1%)	70	86
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	188 (100%)	1 (0%)	86	95
34	k	320/323 (99%)	316 (99%)	4 (1%)	65	84
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%)	145 (100%)	0	100	100
43	t	154/159 (97%)	154 (100%)	0	100	100
44	u	107/109 (98%)	107 (100%)	0	100	100
45	a	676/949 (71%)	642 (95%)	34 (5%)	20	43
46	e	1150/1451 (79%)	1080 (94%)	70 (6%)	15	34
47	g	180/211 (85%)	180 (100%)	0	100	100
48	w	197/198 (100%)	196 (100%)	1 (0%)	86	95
52	0	104/254 (41%)	95 (91%)	9 (9%)	8	17
54	v	119/132 (90%)	116 (98%)	3 (2%)	42	68
All	All	7561/8690 (87%)	7429 (98%)	132 (2%)	56	78

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
7	G	83	ARG
15	O	33	LYS
19	S	107	ILE
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
33	j	198	LYS
34	k	17	LEU

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Mol	Chain	Res	Type
34	k	19	ARG
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
45	a	21	LEU
45	a	74	SER
45	a	89	LEU
45	a	124	LEU
45	a	139	LEU
45	a	157	PHE
45	a	179	GLU
45	a	180	LEU
45	a	199	ILE
45	a	255	LEU
45	a	293	TYR
45	a	308	THR
45	a	309	PHE
45	a	316	ILE
45	a	337	LEU
45	a	409	LEU
45	a	450	VAL
45	a	453	ASP
45	a	589	MET
45	a	606	GLU
45	a	630	VAL
45	a	649	TRP
45	a	682	ARG
45	a	697	LEU
45	a	705	TRP
45	a	837	VAL
45	a	854	GLN
45	a	855	ASP
45	a	868	THR
45	a	884	MET
45	a	896	ARG
45	a	947	LEU
45	a	1003	GLN
45	a	1014	LEU
46	e	8	THR
46	e	23	VAL

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Mol	Chain	Res	Type
46	e	30	PHE
46	e	125	ILE
46	e	143	LEU
46	e	156	THR
46	e	178	LEU
46	e	194	SER
46	e	205	GLU
46	e	230	SER
46	e	249	LEU
46	e	299	THR
46	e	309	VAL
46	e	698	TYR
46	e	707	LYS
46	e	710	LYS
46	e	731	LEU
46	e	733	HIS
46	e	754	ILE
46	e	763	ILE
46	e	770	ILE
46	e	780	ILE
46	e	799	THR
46	e	807	LYS
46	e	826	LEU
46	e	844	LEU
46	e	853	GLU
46	e	867	PHE
46	e	904	VAL
46	e	910	SER
46	e	924	VAL
46	e	933	LEU
46	e	967	SER
46	e	989	GLU
46	e	1017	VAL
46	e	1046	SER
46	e	1050	LEU
46	e	1059	LEU
46	e	1079	LEU
46	e	1094	TYR
46	e	1095	LEU
46	e	1102	CYS
46	e	1123	TYR
46	e	1151	PHE

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Mol	Chain	Res	Type
46	e	1175	PHE
46	e	1179	LEU
46	e	1184	ILE
46	e	1189	ASN
46	e	1193	LEU
46	e	1195	THR
46	e	1239	LYS
46	e	1240	LEU
46	e	1269	LEU
46	e	1294	LEU
46	e	1300	ILE
46	e	1303	MET
46	e	1341	LYS
46	e	1342	GLU
46	e	1367	THR
46	e	1379	LEU
46	e	1407	MET
46	e	1417	LEU
46	e	1421	LEU
46	e	1439	LEU
46	e	1441	ILE
46	e	1464	ILE
46	e	1480	ILE
46	e	1488	LEU
46	e	1508	CYS
46	e	1555	ARG
48	w	98	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
54	v	54	HIS
54	v	71	GLU
54	v	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	141	HIS
45	a	143	ASN
45	a	413	GLN
45	a	445	GLN
45	a	599	GLN
45	a	664	ASN
45	a	696	GLN
45	a	957	GLN
45	a	1003	GLN
46	e	10	GLN
46	e	84	ASN
46	e	160	ASN
46	e	189	ASN
46	e	251	ASN
46	e	805	ASN
46	e	902	ASN
46	e	1111	GLN
46	e	1288	GLN
46	e	1499	HIS
47	g	9	ASN
52	0	36	GLN
54	v	52	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3211/3395 (94%)	590 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
49	x	72/77 (93%)	19 (26%)	0
50	y	71/76 (93%)	23 (32%)	0
All	All	3631/3827 (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

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Mol	Chain	Res	Type
30	f	49	A
30	f	59	G
30	f	60	A
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

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Mol	Chain	Res	Type
30	f	269	G
30	f	283	G
30	f	286	U
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

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Mol	Chain	Res	Type
30	f	547	G
30	f	548	G
30	f	551	A
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

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Mol	Chain	Res	Type
30	f	781	G
30	f	785	G
30	f	786	A
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

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Mol	Chain	Res	Type
30	f	1041	U
30	f	1047	A
30	f	1049	C
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

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Mol	Chain	Res	Type
30	f	1242	G
30	f	1244	A
30	f	1245	A
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

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Mol	Chain	Res	Type
30	f	1450	G
30	f	1481	A
30	f	1482	A
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

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Mol	Chain	Res	Type
30	f	1725	C
30	f	1736	G
30	f	1741	A
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

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Mol	Chain	Res	Type
30	f	2113	A
30	f	2114	C
30	f	2121	G
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

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Mol	Chain	Res	Type
30	f	2393	G
30	f	2397	A
30	f	2402	A
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

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Mol	Chain	Res	Type
30	f	2540	A
30	f	2541	U
30	f	2542	U
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

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Mol	Chain	Res	Type
30	f	2755	C
30	f	2772	C
30	f	2773	C
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	2817	A
30	f	2818	U
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	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	2954	U
30	f	2971	A
30	f	2972	G
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G

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Mol	Chain	Res	Type
30	f	3006	A
30	f	3012	A
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

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Mol	Chain	Res	Type
30	f	3259	U
30	f	3263	G
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

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Mol	Chain	Res	Type
31	h	55	A
31	h	65	G
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
49	x	5	G
49	x	9	G

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Mol	Chain	Res	Type
49	x	15	G
49	x	16	U
49	x	17	C
49	x	18	G
49	x	22	G
49	x	28	U
49	x	35	G
49	x	37	A
49	x	38	U
49	x	39	G
49	x	46	G
49	x	48	C
49	x	56	C
49	x	57	G
49	x	58	A
49	x	60	U
49	x	74	C
50	y	5	G
50	y	7	G
50	y	9	G
50	y	13	U
50	y	16	U
50	y	17	C
50	y	22	G
50	y	34	A
50	y	35	G
50	y	36	C
50	y	38	U
50	y	42	A
50	y	43	G
50	y	44	A
50	y	46	G
50	y	47	U
50	y	48	C
50	y	54	U
50	y	56	C
50	y	58	A
50	y	61	C
50	y	65	A
50	y	76	A

There are no RNA pucker outliers to report.

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

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
54	5CT	v	51	54	13,14,15	0.79	0	8,15,17	1.29	1 (12%)

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
54	5CT	v	51	54	-	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(°)	Ideal(°)
54	v	51	5CT	C4-C3-C2	-2.19	108.86	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

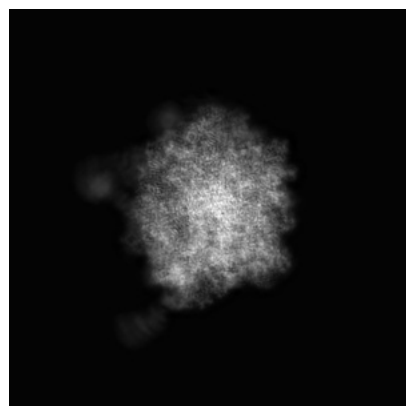
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15423. These allow visual inspection of the internal detail of the map and identification of artifacts.

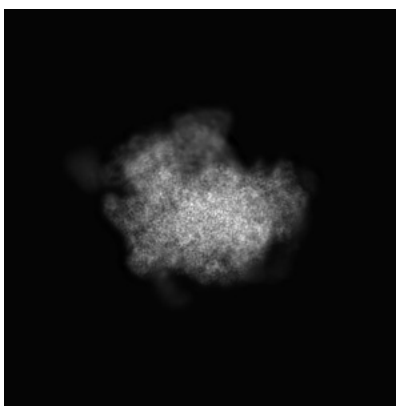
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

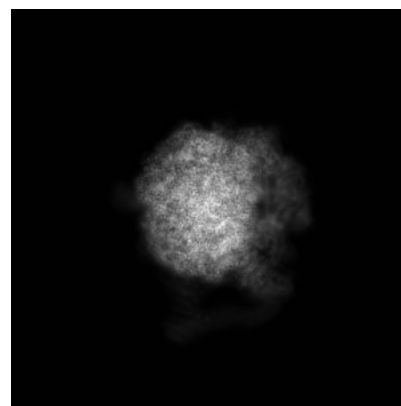
6.1.1 Primary map



X

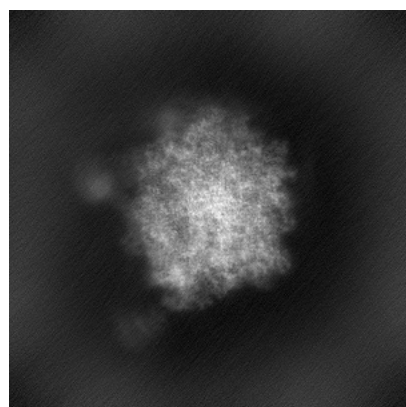


Y

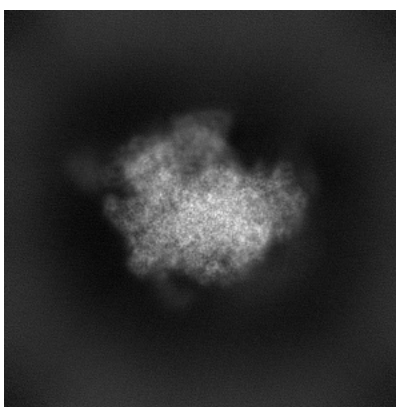


Z

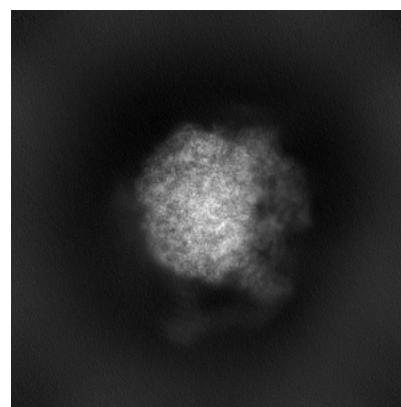
6.1.2 Raw map



X



Y

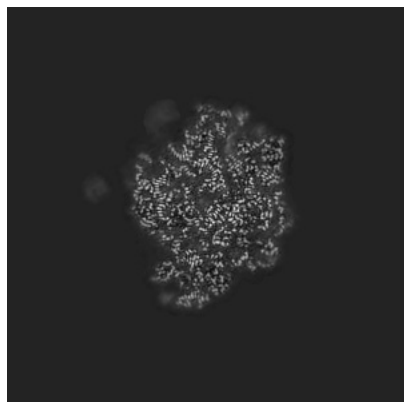


Z

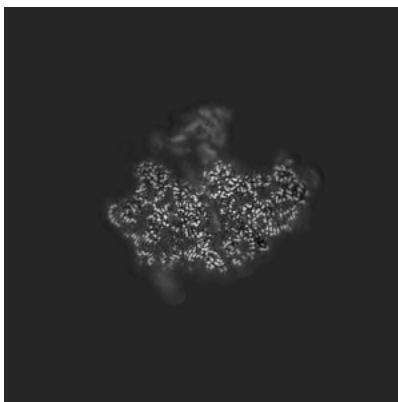
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

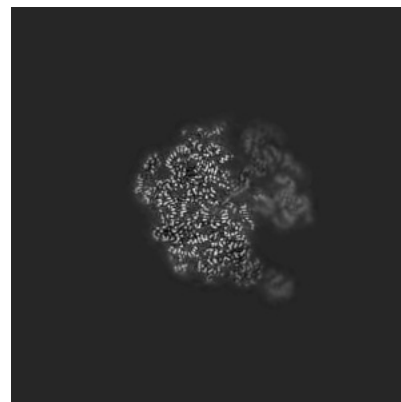
6.2.1 Primary map



X Index: 225

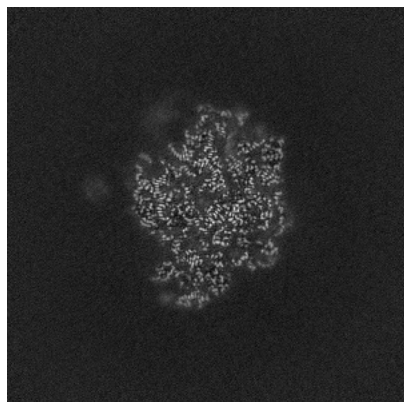


Y Index: 225

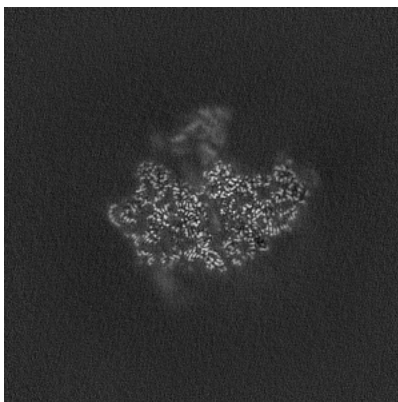


Z Index: 225

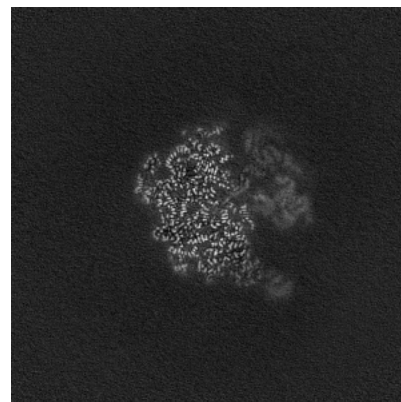
6.2.2 Raw map



X Index: 225



Y Index: 225

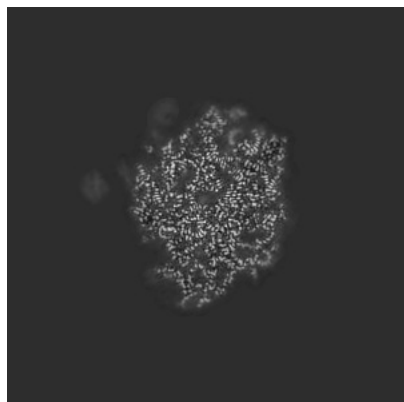


Z Index: 225

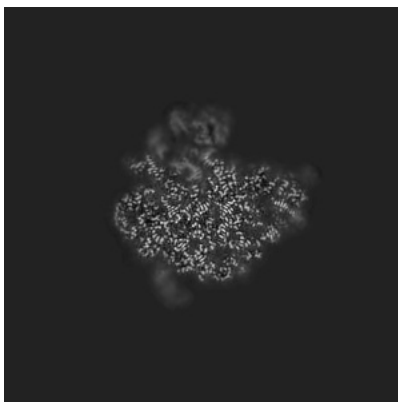
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

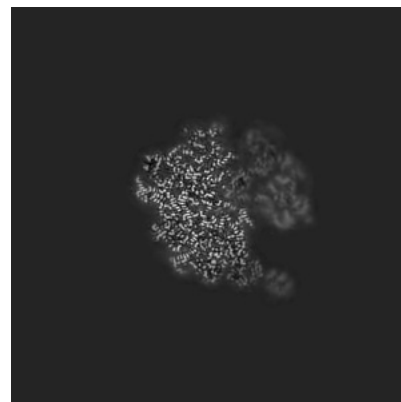
6.3.1 Primary map



X Index: 219

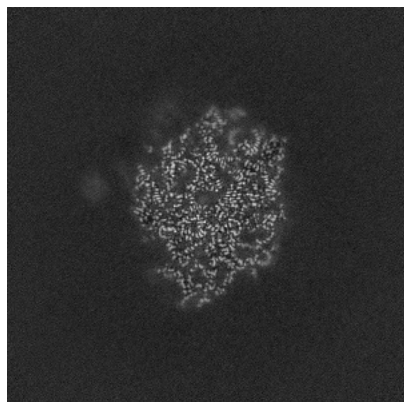


Y Index: 237

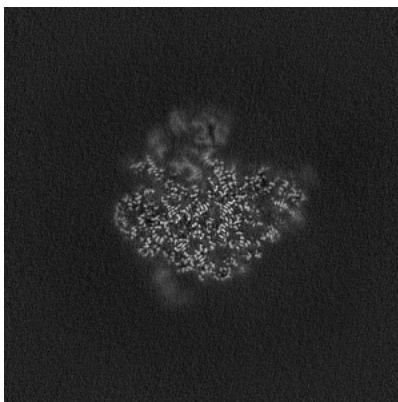


Z Index: 222

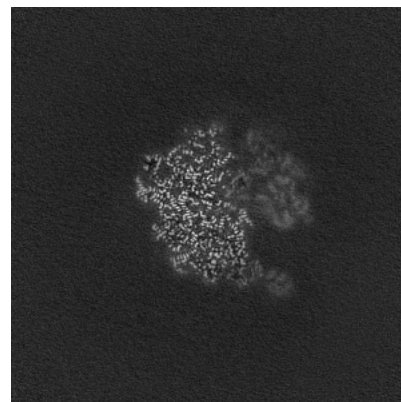
6.3.2 Raw map



X Index: 219



Y Index: 237

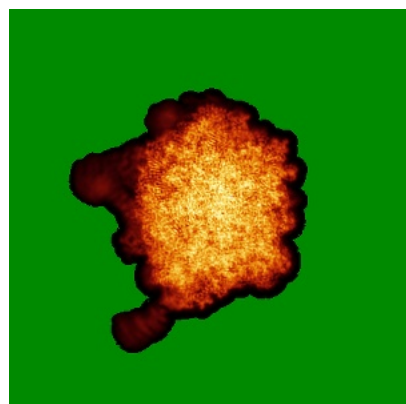


Z Index: 222

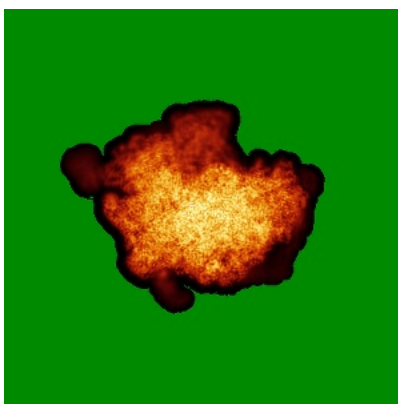
The images above show the largest variance slices of the map in three orthogonal directions.

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

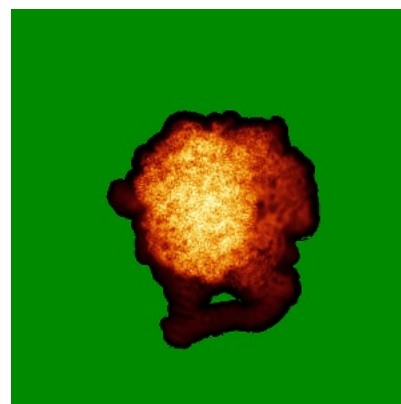
6.4.1 Primary map



X

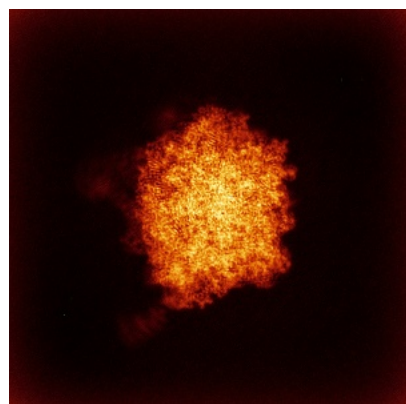


Y

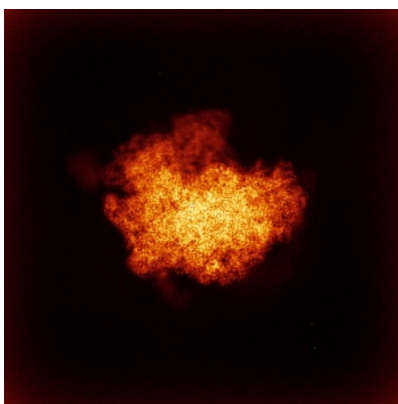


Z

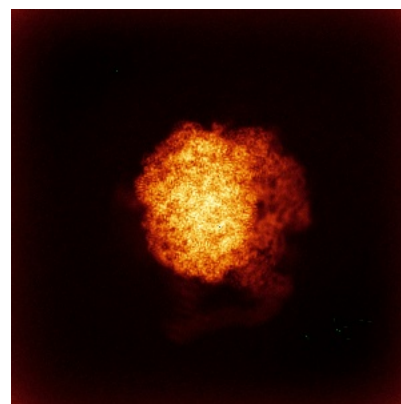
6.4.2 Raw map



X



Y

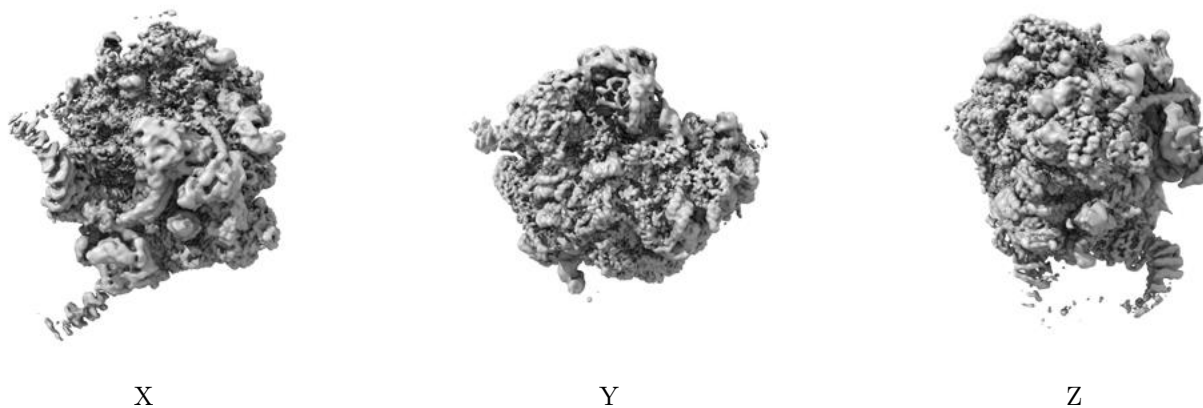


Z

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.

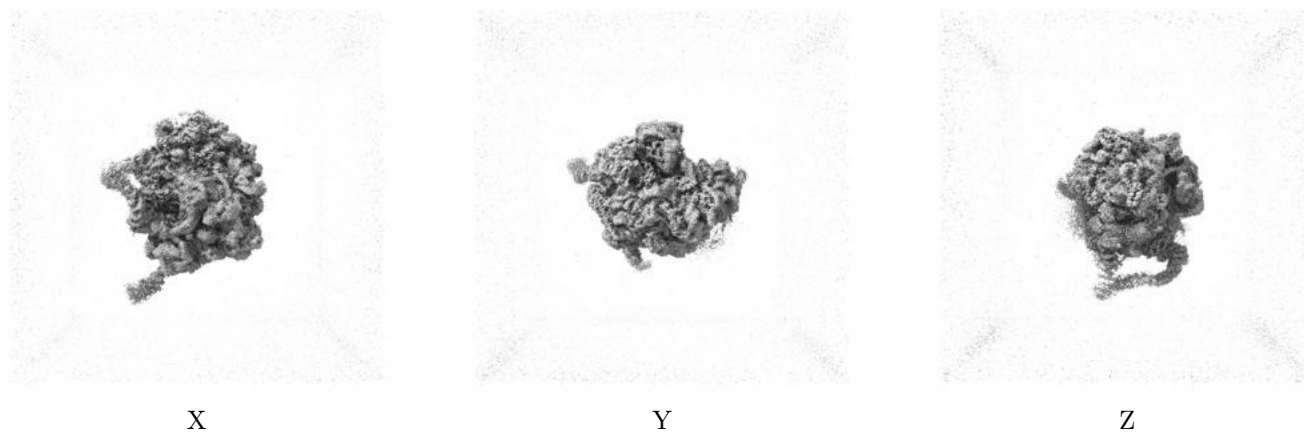
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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



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.

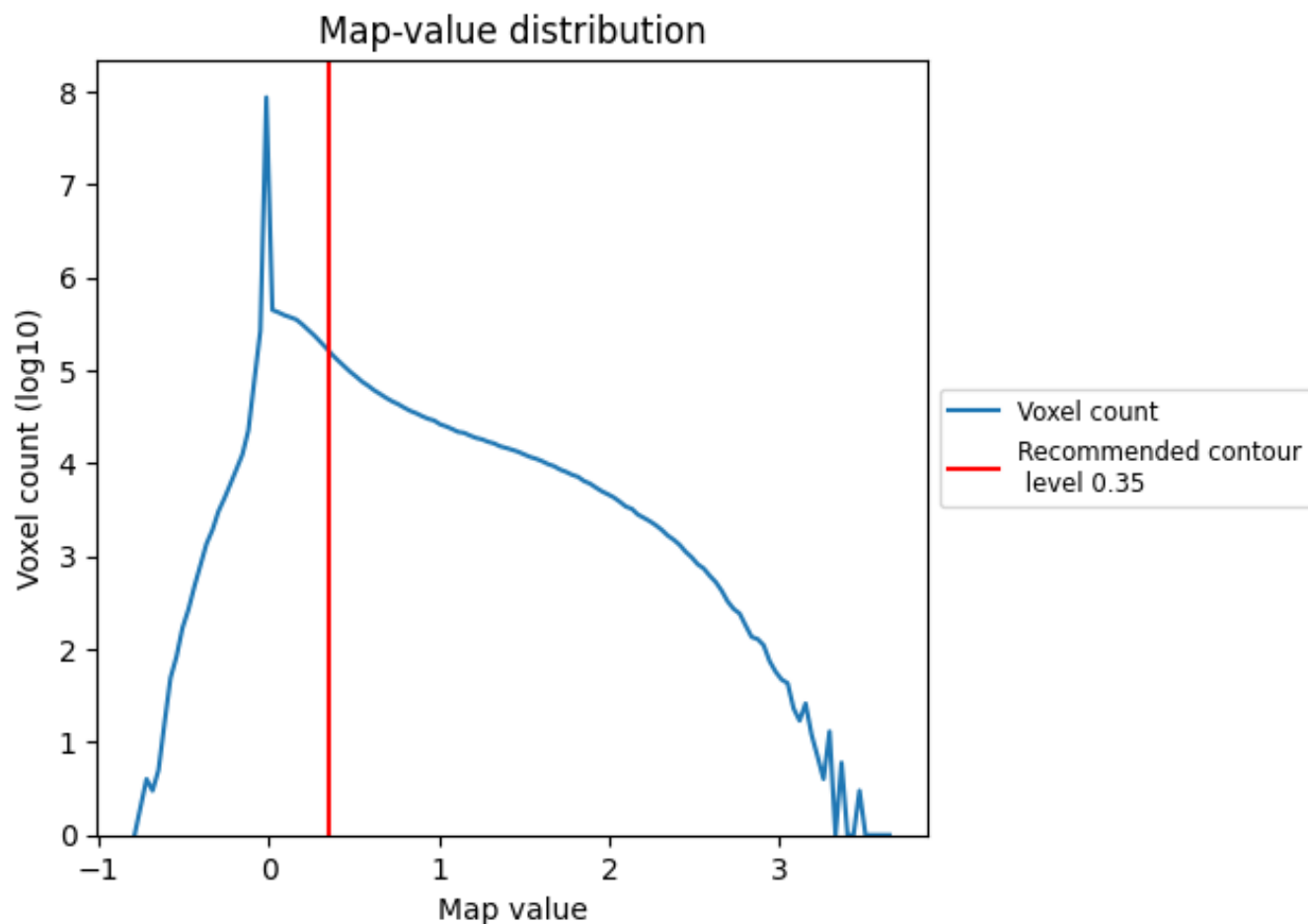
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

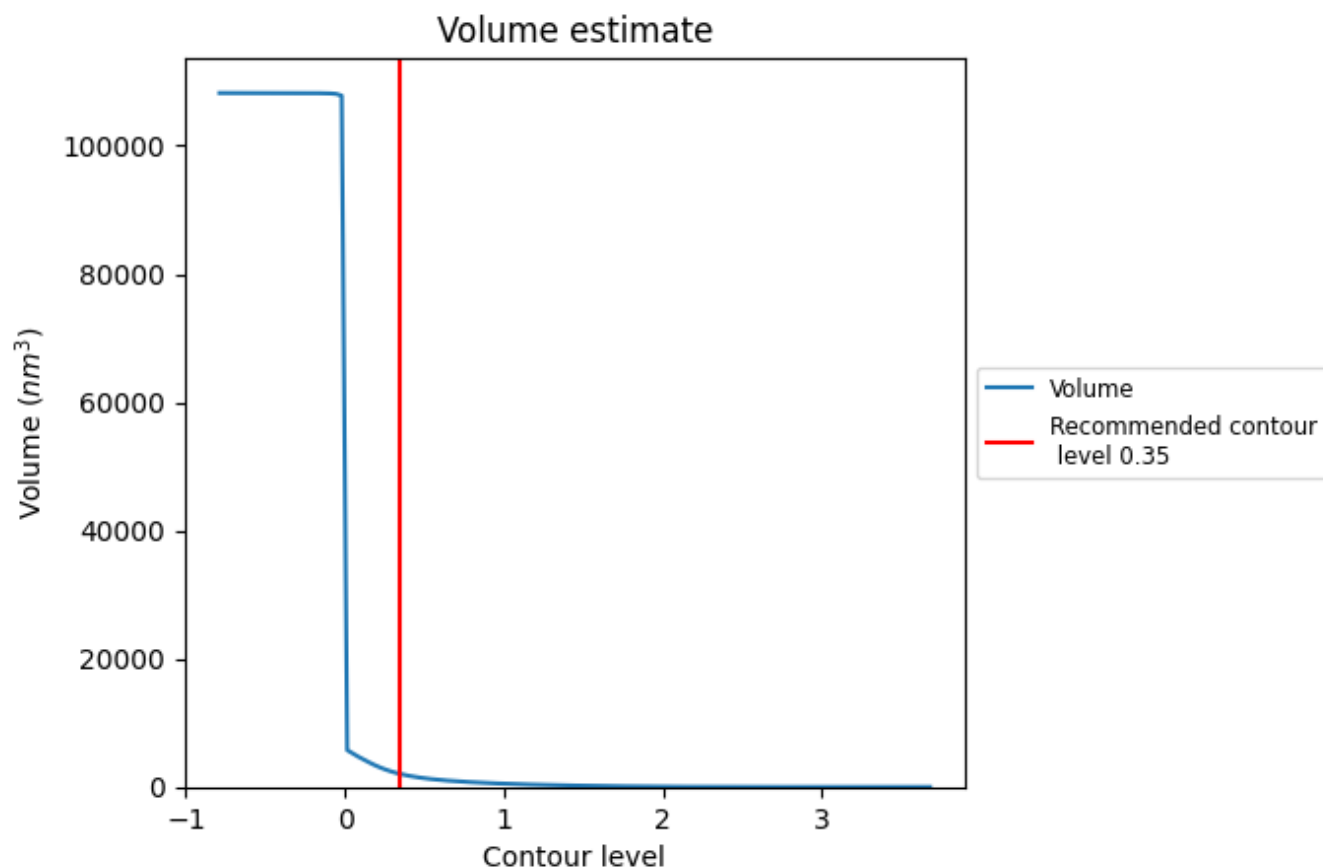
This section contains the results of statistical analysis of the map.

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.

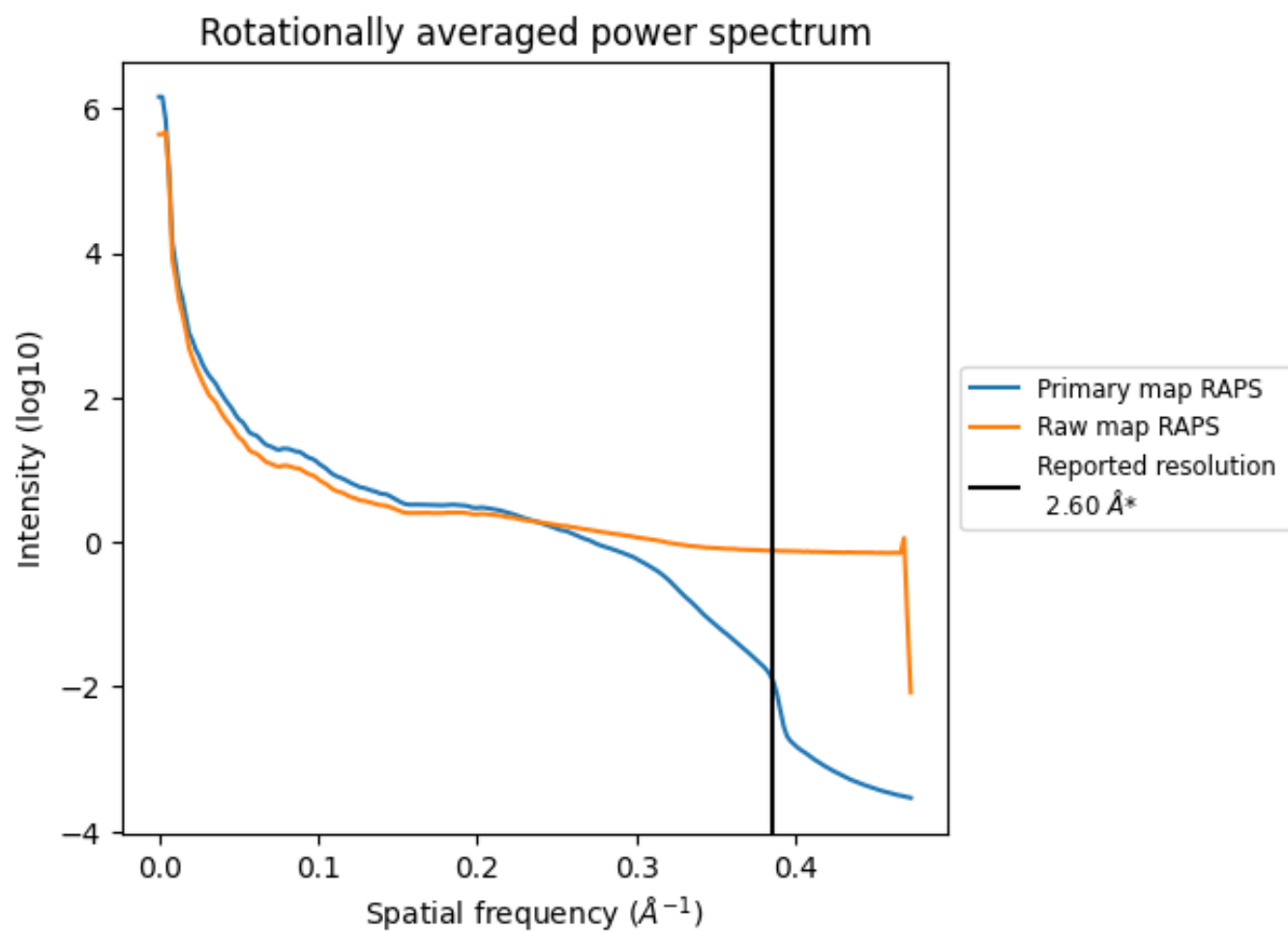
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2020 nm^3 ; this corresponds to an approximate mass of 1824 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

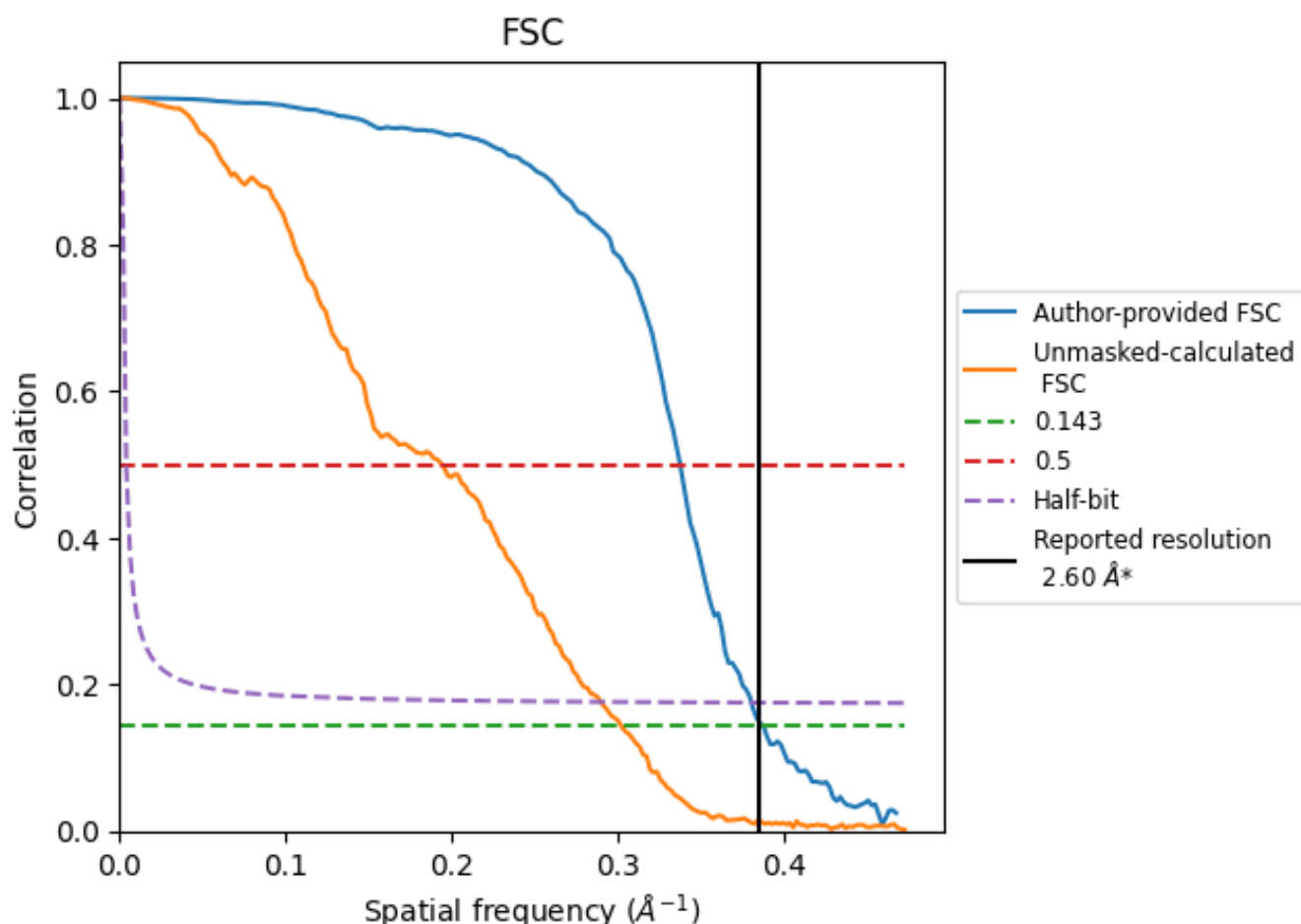


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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](#)

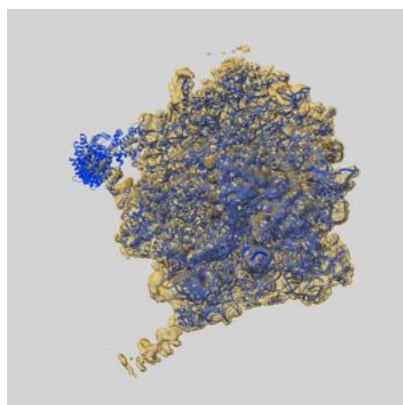
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.58	2.97	2.63
Unmasked-calculated*	3.32	5.16	3.46

*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 3.32 differs from the reported value 2.6 by more than 10 %

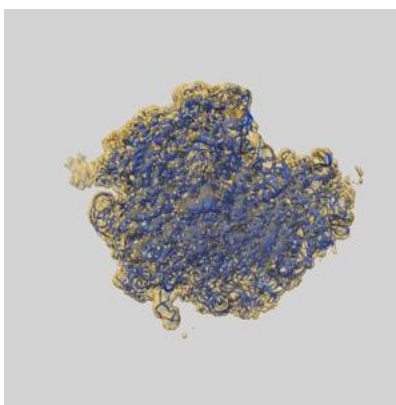
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15423 and PDB model 8AGT. Per-residue inclusion information can be found in section [3](#) on page [14](#).

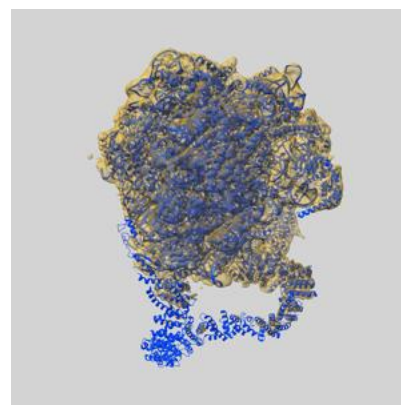
9.1 Map-model overlay [i](#)



X



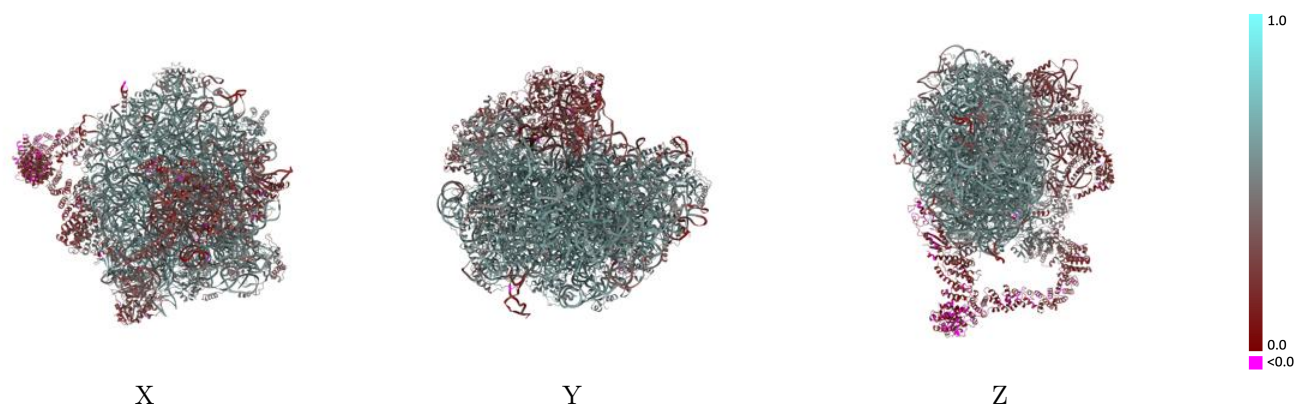
Y



Z

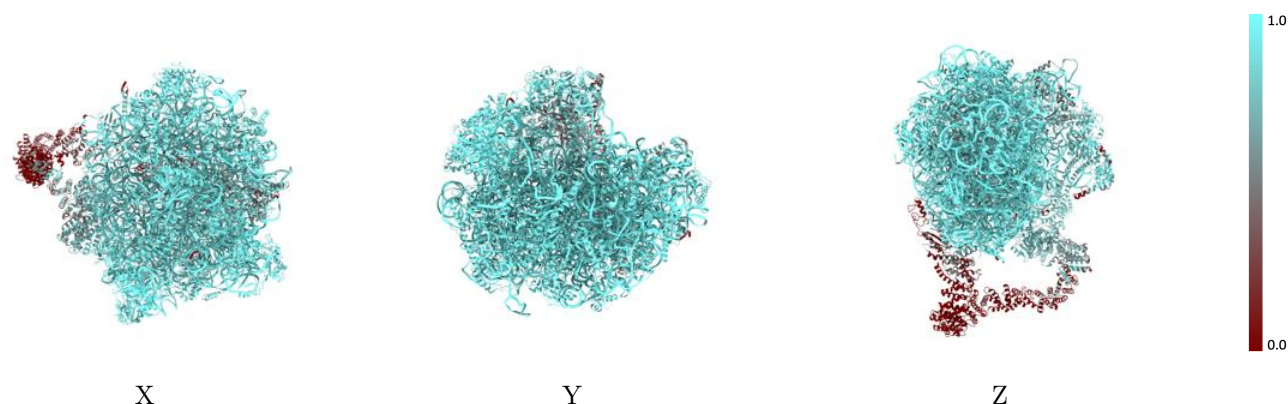
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



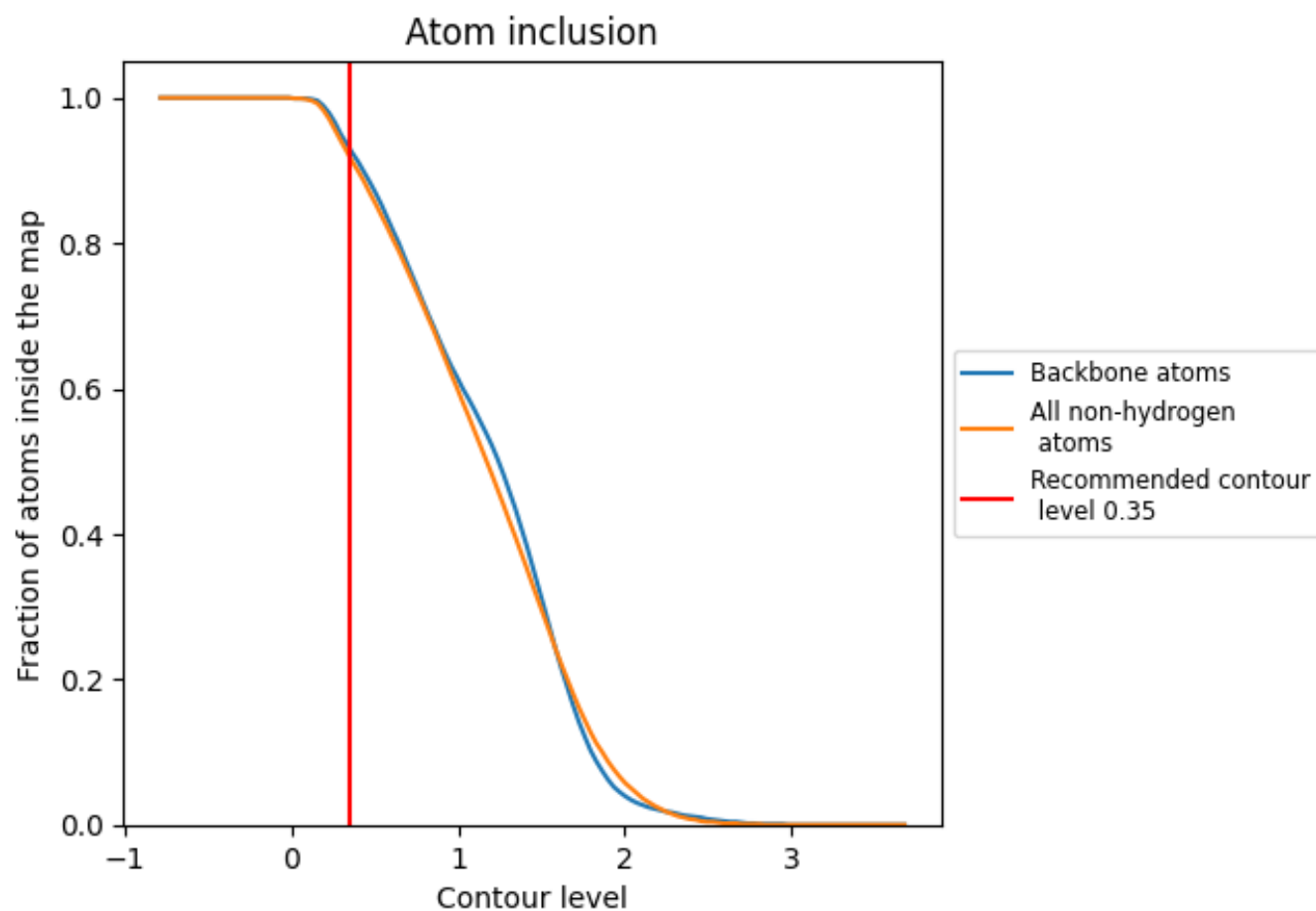
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5070
0	 0.8760	 0.3000
1	 0.9880	 0.4320
A	 0.9950	 0.6100
B	 0.9810	 0.5840
C	 0.9790	 0.5850
D	 0.9850	 0.5840
E	 0.9460	 0.5440
F	 0.9840	 0.5760
G	 0.9730	 0.5550
H	 0.9410	 0.4710
I	 0.9750	 0.5750
J	 0.9760	 0.5720
K	 0.9760	 0.5630
L	 0.9850	 0.5620
M	 0.9620	 0.5170
N	 0.9820	 0.5900
O	 0.9740	 0.5390
P	 0.9420	 0.5160
Q	 0.9440	 0.5440
R	 0.9900	 0.6000
S	 0.9940	 0.6160
T	 0.9800	 0.5730
U	 0.9720	 0.5520
V	 0.9690	 0.5230
W	 1.0000	 0.6240
X	 0.9420	 0.4940
Y	 1.0000	 0.5980
Z	 0.9650	 0.5730
a	 0.8550	 0.2670
b	 0.9630	 0.5730
c	 0.9780	 0.5680
d	 0.7870	 0.4160
e	 0.2940	 0.1860
f	 0.9920	 0.5680



Continued on next page...

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Chain	Atom inclusion	Q-score
g	 0.8200	 0.4650
h	 0.9990	 0.5650
i	 0.9970	 0.5950
j	 0.9910	 0.6000
k	 0.9850	 0.5850
l	 0.9820	 0.5720
m	 0.9520	 0.4800
n	 0.9600	 0.5210
o	 0.9760	 0.5650
p	 0.9590	 0.5220
q	 0.9660	 0.5450
r	 0.9730	 0.5430
s	 0.9460	 0.4360
t	 0.9790	 0.5600
u	 0.9790	 0.5430
v	 0.7620	 0.3880
w	 0.5790	 0.2430
x	 0.9850	 0.2700
y	 0.9920	 0.2810
z	 0.9790	 0.3160