



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 08:19 pm BST

PDB ID : 8AGV
EMDB ID : EMD-15425
Title : Yeast RQC complex in state H
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 : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

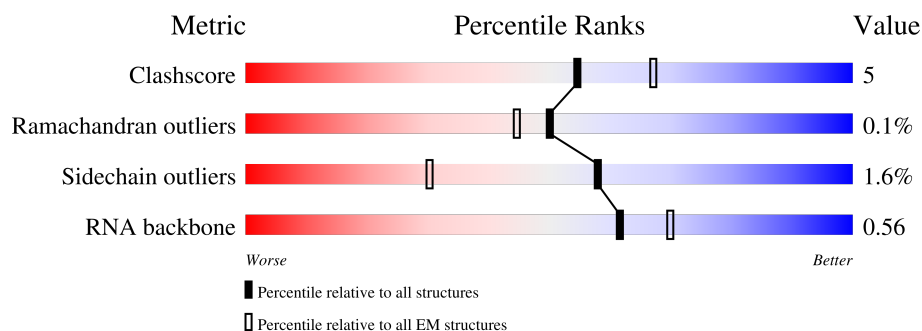
1 Overall quality at a glance

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.







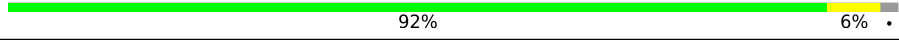
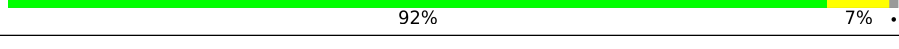
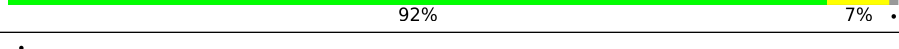
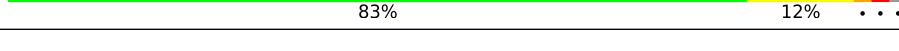
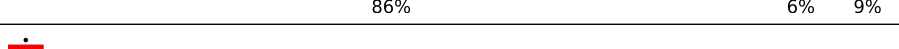
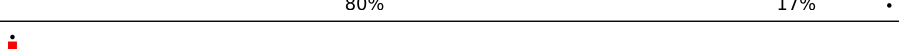
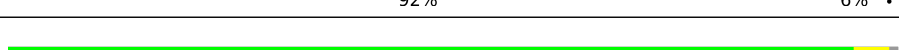
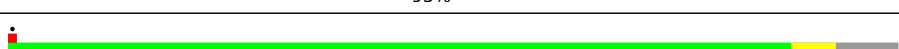
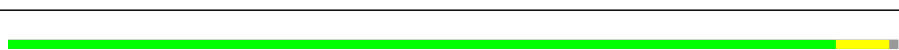
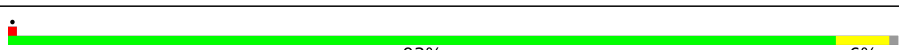
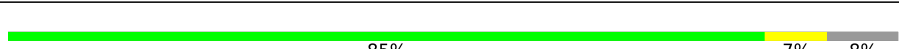

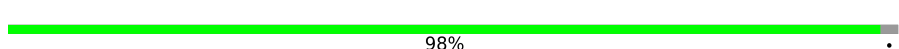

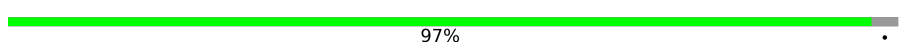
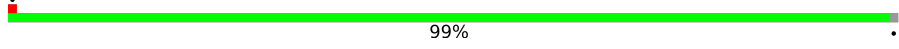
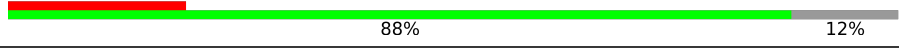
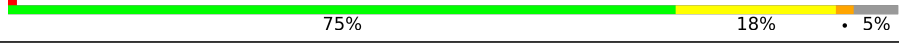



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	

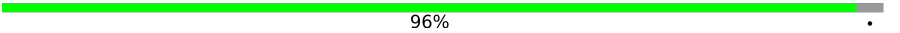
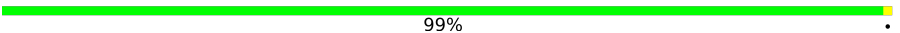
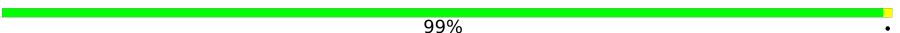
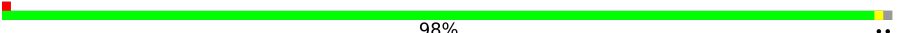












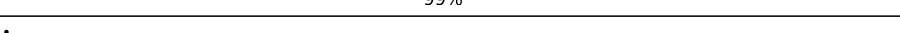




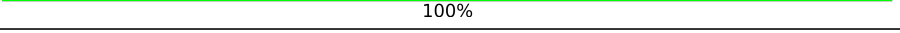
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Mol	Chain	Length	Quality of chain
8	H	121	
9	I	137	
10	J	155	
11	K	142	
12	L	127	
13	M	136	
14	N	149	
15	O	59	
16	P	105	
17	Q	113	
18	R	130	
19	S	107	
20	T	121	
21	U	120	
22	V	100	
23	W	88	
24	X	78	
25	Y	51	
26	Z	128	
27	b	106	
28	c	92	
29	d	25	
30	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	 99% .
35	l	362	 99% .
36	m	297	 98% ..
37	n	176	 94% . 5%
38	o	244	 91% 9%
39	p	256	 89% . 9%
40	q	191	 98% ..
41	r	221	 98% ..
42	s	174	 95% .. .
43	t	199	 96% . .
44	u	138	 97% ..
45	a	1038	 78% . 18%
46	e	1562	 66% 94% . .
47	g	245	 91% 8%
48	w	217	 99%
49	x	76	 67% 30% .
49	y	76	 57% 39% .
50	z	165	 89% . 10%
51	0	312	 31% 7% . 61%
52	1	18	 100%
53	v	157	 88% . 10%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 151349 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		

- 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 RQC2 isoform 1.

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
			11516	7358	1937	2183	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 Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	74	Total	C	N	O	P	0	0
			1579	702	278	525	74		
49	y	73	Total	C	N	O	P	0	0
			1556	692	273	518	73		

- Molecule 50 is a protein called 60S ribosomal protein L12-B.

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

- Molecule 51 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	121	Total	C	N	O	S	0	0
			961	618	167	173	3		

- Molecule 52 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 5A-1.

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

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

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

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

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

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

3 Residue-property plots [i](#)


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

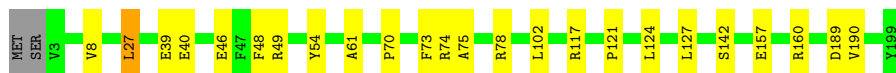
- Molecule 1: 60S ribosomal protein L15-A

Chain A: 




- Molecule 2: 60S ribosomal protein L16-A

Chain B: 



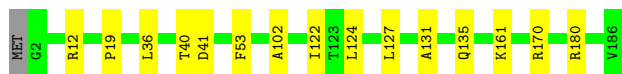
- Molecule 3: 60S ribosomal protein L17-A

Chain C: 



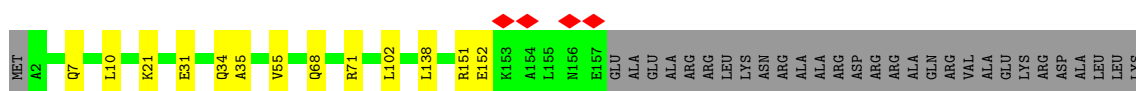
- Molecule 4: 60S ribosomal protein L18-A

Chain D: 




- Molecule 5: 60S ribosomal protein L19-A

Chain E: 



GLU
ASP
ALA

• Molecule 6: 60S ribosomal protein L20-A

Chain F:  87% 12%

MET A2 Q8 P22 S32 I36 R40 I64 V77 R80 T87 E93 I94 R95 D96 V97 L106 H122 I123 I124 R125 V126 V140 R155 V156 Y172

• Molecule 7: 60S ribosomal protein L21-A

Chain G:  90% 9%


MET G2 R17 H22 G73 R83 Y84 L89 S99 R100 C101 R102 R108 M112 R136 R139 M146 P155 I160

• Molecule 8: 60S ribosomal protein L22-A

Chain H:  74% 9% 17%

MET ALA PRO THR SER ARG LYS Q9 D18 V19 S20 T23 T41 E44 M49 L50 G51 V54 T55 V56 V65 Y108 G1N VAL THR PRO GLU GLU ASP GLU GLU ASP GLU GLU

• Molecule 9: 60S ribosomal protein L23-A

Chain I:  90% 9%


MET S2 S14 P18 A38 A51 M59 R80 Q81 Y94 A99 P117 V129 S133 G134 V135 V136 V137

• Molecule 10: 60S ribosomal protein L24-A

Chain J:  37% 59%

M1 D6 Q32 K41 R47 H58 I63 THR GLU GLU VAL ALA LYS ARG SER ARG LYS THR VAL LYS LYS ALA G1N ARG PRO ILE THR GLY ALA SER LEU ASP LEU ILE LYS ALA GLU ARG ARG SER LEU LYS PRO VAL ARG LYS ASN ARG ARG GLU LYS LYS

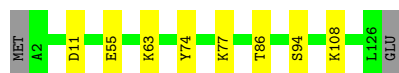
• Molecule 11: 60S ribosomal protein L25

Chain K:  84% 15%

MET ALA PRO SER LYS ALA THR ALA LYS VAL VAL GLY THR ASN GLY LYS K22 A50 D134 I142

• Molecule 12: 60S ribosomal protein L26-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% .




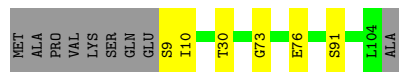
- Molecule 15: 60S ribosomal protein L29

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% .




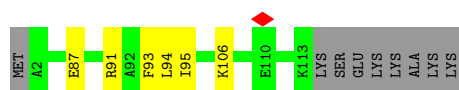
- Molecule 19: 60S ribosomal protein L33-A

Chain S:  95%



- Molecule 20: 60S ribosomal protein L34-A

Chain T:  88% 5% 7%



- Molecule 21: 60S ribosomal protein L35-A

Chain U:  93% 6%




- Molecule 22: 60S ribosomal protein L36-A

Chain V:  93% 6%




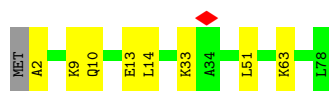
- Molecule 23: 60S ribosomal protein L37-A

Chain W:  85% 7% 8%



- Molecule 24: 60S ribosomal protein L38

Chain X:  88% 10%



- Molecule 25: 60S ribosomal protein L39

Chain Y:  98%



- Molecule 26: Ubiquitin-60S ribosomal protein L40

Chain Z:  41% 59%

MET GLN ILE PHE VAL LYS THR LEU THR GLY LYS THR ILE THR LEU VAL GLU SER SER ASP THR ILE ASP ASN VAL LYS SER LYS ILE GLN ASP LYS GLY ILE PRO PRO ASP ASP GLN ARG ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS SER THR LEU HIS VAL LEU ARG LEU ARG GLY I77 K128

- Molecule 27: 60S ribosomal protein L42-A

Chain b:  97%


MET V2 L104 GLN PHE

- Molecule 28: 60S ribosomal protein L43-A

Chain c:  99%


MET A2 A92

- Molecule 29: 60S ribosomal protein L41-A

Chain d:  20% 88% 12%

M4 R20 R21 K22 V23 R24 A25 ARG SER LYS

- Molecule 30: 25S rRNA

Chain f:  75% 18% 5%

G U U3 A6 A13 U14 A26 C36 A40 A43 A49 G59 A60 A65 A66 U78 U87 G92 U97 G98 A99 A109 G110 C111 U112 C113 A116 G120 A121 A122 U133 U134 C135 G136 C142 U149 G156 A157 A165

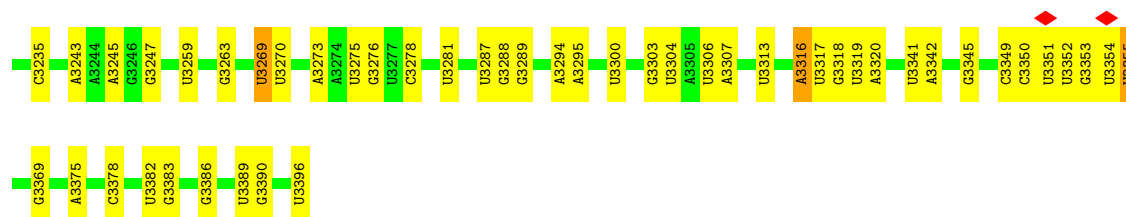
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A374 A375 G376 A398 A399 G400 U401 A402 C403 G406 U411 G421 A422 C439 A440 U441 G442 G443 G444 G445 U446 U447 U448 U449 G450 G451 G C C C U C C G C C C U U G C C U U G C G G U A C G G A A U C

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C1219	A1352	U1041	U1041	C1219	A1352	U1569	U1763	A	A	A	C	A2404	A2404	C2537	A2689	C2844	U3079
G1222	G1353	A1047	U1047	G1222	G1353	U1572	U1765	G	G	G	U	A2405	C2405	U2537	A2690	A2845	G3080
A1225	A1355	A1048	A1048	A1225	A1355	U1573	G1766	C	C	C	C	U2411	U2411	U2538	A2691	U2846	A3086
G1226	U1356	C1049	C1049	G1226	U1356	C1574	G1770	C	C	C	U	U2416	U2416	C2539	A2695	C2849	C3092
C1227	G1357	U1063	U1063	C1227	G1357	A1575	G1775	A	A	A	A	A2419	A2419	U2540	A2696	U2860	U3104
U1235	A1386	A1064	A1064	U1235	A1386	G1576	G1776	C	C	C	C	A2437	A2437	U2541	A2704	C2867	A3113
G1236	A1065	A916	A916	G1236	A1065	A1580	G1780	A	A	A	A	G2444	G2444	U2542	G2714	G2871	A3122
U1237	A917	A917	A917	U1237	A917	A1581	A1797	U	U	U	U	A2445	A2445	U2543	U2719	A2872	A3130
C1238	G1072	U1081	U1081	C1238	G1072	C1582	A1814	C	C	C	C	U2446	U2446	U2544	C2726	U2873	A3131
C1239	U1081	U1081	U1081	C1239	U1081	A1583	A1815	A	A	A	A	A2447	A2447	U2545	U2727	C2876	U3142
A1240	U1081	U1081	U1081	A1240	U1081	G1590	A1816	C	C	C	C	U2448	U2448	U2546	A2728	A2887	C3143
G1242	U1081	U1081	U1081	G1242	U1081	A1597	U1820	C	C	C	C	U2449	U2449	U2547	U2729	U2888	U3148
G1243	U1081	U1081	U1081	G1243	U1081	C1597	U1821	C	C	C	C	G2450	G2450	U2548	A2752	G2898	U3151
A1244	U1081	U1081	U1081	A1244	U1081	G1604	U1835	C	C	C	C	A2461	A2461	U2549	G2753	C2899	U3152
A1245	U1081	U1081	U1081	A1245	U1081	A1605	A1839	C	C	C	C	A2462	A2462	U2550	G2754	G2911	U3153
A1251	U1081	U1081	U1081	A1251	U1081	U1606	U1840	C	C	C	C	U2463	U2463	U2551	G2755	G2914	U3154
U1252	U1081	U1081	U1081	U1252	U1081	U1607	U1841	C	C	C	C	U2464	U2464	U2552	C2764	U2923	U3155
C1254	U1081	U1081	U1081	C1254	U1081	C1608	U1842	C	C	C	C	U2465	U2465	U2553	U2772	U2935	U3156
U1258	U1081	U1081	U1081	U1258	U1081	U1620	C1846	C	C	C	C	A2468	A2468	U2554	C2773	U2936	U3157
A1263	U1081	U1081	U1081	A1263	U1081	U1629	C1849	C	C	C	C	G2479	G2479	U2555	G2777	A2941	A3165
G1264	U1081	U1081	U1081	G1264	U1081	C1639	U1850	C	C	C	C	A2480	A2480	U2556	G2778	C2942	A3170
U1265	U1081	U1081	U1081	U1265	U1081	A1642	C1866	C	C	C	C	A2481	A2481	U2557	U2783	G2947	G3173
U1269	U1081	U1081	U1081	U1269	U1081	A1643	U1867	C	C	C	C	A2482	A2482	U2558	U2784	A2971	A3174
C1272	U1081	U1081	U1081	C1272	U1081	U1644	A1872	C	C	C	C	A2483	A2483	U2559	U2785	C2983	U3175
G1277	U1081	U1081	U1081	G1277	U1081	U1645	C1878	C	C	C	C	A2484	A2484	U2560	U2786	U2990	U3176
A1278	U1081	U1081	U1081	A1278	U1081	C1657	G1879	C	C	C	C	A2485	A2485	U2561	U2796	G2991	A3180
C1279	U1081	U1081	U1081	C1279	U1081	A1683	U1880	C	C	C	C	A2486	A2486	U2562	G2800	A2991	A3181
G1282	U1081	U1081	U1081	G1282	U1081	U1688	A1881	C	C	C	C	A2487	A2487	U2563	A2802	U2992	A3186
U1285	U1081	U1081	U1081	U1285	U1081	U1716	A1883	C	C	C	C	A2488	A2488	U2564	A2803	U2996	A3187
A1286	U1081	U1081	U1081	A1286	U1081	U1717	G1906	C	C	C	C	A2489	A2489	U2565	C2810	A3006	U3196
A1287	U1081	U1081	U1081	A1287	U1081	C1725	C1907	C	C	C	C	A2490	A2490	U2566	U2814	A3012	U3207
G1289	U1081	U1081	U1081	G1289	U1081	U1732	G1943	C	C	C	C	A2491	A2491	U2567	U2815	G3208	A3209
U1285	U1081	U1081	U1081	U1285	U1081	U1736	G1951	C	C	C	C	A2492	A2492	U2568	U2816	A3034	U3214
A1286	U1081	U1081	U1081	A1286	U1081	A1741	G1952	C	C	C	C	A2493	A2493	U2569	U2817	A3048	U3217
A1287	U1081	U1081	U1081	A1287	U1081	A1750	G1954	C	C	C	C	A2494	A2494	U2570	U2818	U3056	C3218
G1295	U1081	U1081	U1081	G1295	U1081	G1751	U1955	C	C	C	C	A2495	A2495	U2571	U2819	U3057	G3219
U1295	U1081	U1081	U1081	U1295	U1081	A1760	U1956	C	C	C	C	A2496	A2496	U2572	U2820	U3058	C3220
A1295	U1081	U1081	U1081	A1295	U1081	A1761	U1957	C	C	C	C	A2497	A2497	U2573	U2821	U3059	G3221
G1295	U1081	U1081	U1081	G1295	U1081	A1762	U1958	C	C	C	C	A2498	A2498	U2574	U2822	U3060	G3222
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A1295	U1081	U1081	U1081	A1295	U1081	A1773	U1969	C	C	C	C	A2509	A2509	U2585	U2833	U3071	G3233
G1295	U1081	U1081	U1081	G1295	U1081	A1774	U1970	C	C	C	C	A2510	A2510	U2586	U2834	U3072	G3234
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A1295	U1081	U1081	U1081	A1295	U1081	A1785	U1981	C	C	C	C	A2521	A2521	U2597	U2845	U3083	G3245
G1295	U1081	U1081	U1081	G1295	U1081	A1786	U1982	C	C	C	C	A2522	A2522	U2598	U2846	U3084	G3246
U1295	U1081	U1081	U1081	U1295	U1081	A1787	U1983	C	C	C	C	A2523	A2523	U2599	U2847	U3085	G3247
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G1295	U1081	U1081	U1081	G1295	U1081	A1789	U1985	C	C	C	C	A2525	A2525	U2601	U2849	U3087	G3249
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G1295	U1081	U1081	U1081	G1295	U1081	A1798	U1994	C	C	C	C	A2534	A2534	U2610	U2858	U3096	G3258
U1295	U1081	U1081	U1081	U1295	U1081	A1799	U1995	C	C	C	C	A2535	A2535	U2611	U2859	U3097	G3259
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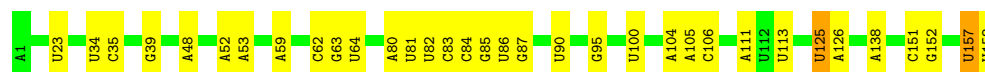
• Molecule 31: 5S rRNA

Chain h: 86% 14%



• 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: 99%



• Molecule 35: 60S ribosomal protein L4-A

Chain l: 99%



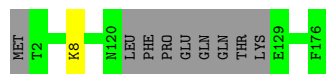
• Molecule 36: 60S ribosomal protein L5

Chain m: 98%



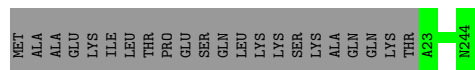
- Molecule 37: 60S ribosomal protein L6-B

Chain n:  94% • 5%




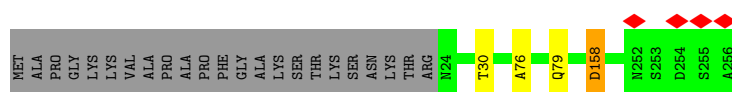
- Molecule 38: 60S ribosomal protein L7-A

Chain o:  91% 9%



- Molecule 39: 60S ribosomal protein L8-A

Chain p:  89% • 9%



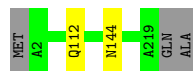
- Molecule 40: 60S ribosomal protein L9-A

Chain q:  98% ..



- Molecule 41: 60S ribosomal protein L10

Chain r:  98% ..



- Molecule 42: 60S ribosomal protein L11-A

Chain s:  95% ..

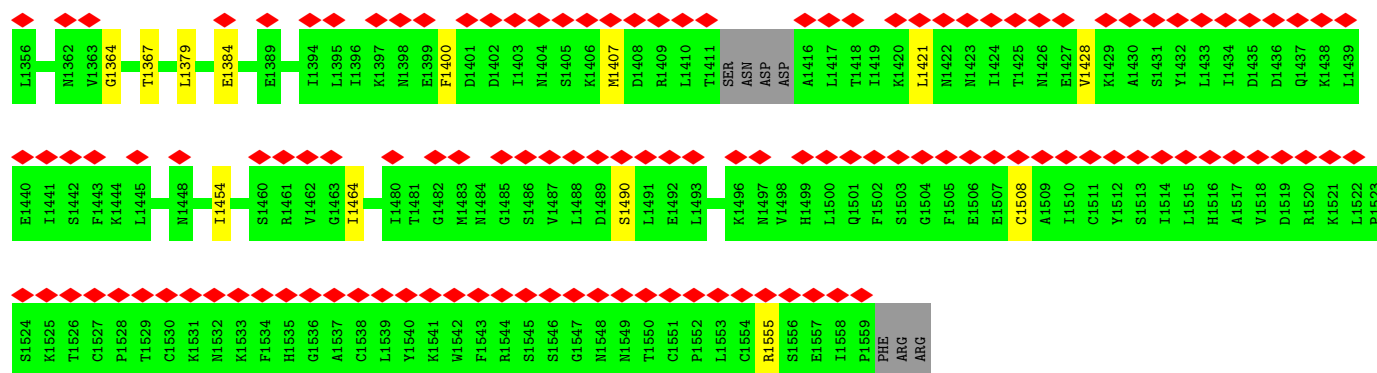


- Molecule 43: 60S ribosomal protein L13-A

Chain t:  96% ..



Q1293	L1294	K1295	E1296	A1297	Q1298	L1299	I1300	N1301	R1302	M1303	F1306	D1309	D1312	L1313	R1314	D1315	T1316	E1317	F1318	W1319	K1320	Q1321	V1322	D1323	T1324	K1325	E1326	I1327	S1328	E1329	Y1330	N1331	I1332	V1333	G1334	N1335	N1336	F1337	S1338	P1339	Y1340	K1341	E1342	D1343	I1344	F1345	E1346	E1347	C1348	K1349	K1350	L1351	L1352	C1353	H1354	T1355						
SER	ALA	SER	ASP	ASN	ASP	VAL	N1235	S1236	K1237	F1238	K1239	L1240	F1241	Q1242	K1243	L1244	L1245	Q1246	K1247	V1248	T1249	D1250	E1251	P1253	K1254	E1255	Y1256	L1257	E1258	Y1259	E1260	N1261	K1262	N1263	S1264	Y1268	L1269	W1270	Y1271	H1273	L1276	F1279	K1280	S1283	Y1284	N1285	M1286	R1287	Q1288	I1289	F1290	I1291	E1292									
T1108	L1109	S1110	Q1111	GLY	VAL	SER	ASN	GLY	GLU	GLU	ILE	SER	E1122	Y1123	G1124	D1125	E1126	I1127	Q1128	E1129	N1130	L1131	I1132	E1133	L1134	M1135	F1136	L1137	N1138	F1139	N1140	Q1141	E1142	R1143	N1144	M1145	Q1146	V1147	S1148	T1149	L1150	F1151	Y1152	Q1153	K1154	L1155	Y1156	K1157	V1158	I1159	S1160	S1161	M1162	E1163	L1164	K1165	L1166	L1167				
E1168	S1169	Q1170	Y1171	K1172	R1173	I1174	F1175	E1176	V1177	V1178	L1179	M1180	D1181	K1182	D1183	I1184	G1185	S1186	M1187	I1188	N1189	Q1190	S1191	L1192	L1193	L1194	T1195	L1196	L1197	L1198	G1199	S1200	L1201	V1202	V1203	K1204	T1205	Q1206	Q1207	D1208	I1209	I1210	I1211	E1212	E1214	L1213	E1214	L1215	L1216	I1217	GLN	LYS	GLN	THR	GLY	SER	ASP	VAL	GLY			
SER	ALA	SER	ASP	ASN	ASP	VAL	N1235	S1236	K1237	F1238	K1239	L1240	F1241	Q1242	K1243	L1244	L1245	Q1246	K1247	V1248	T1249	D1250	E1251	P1253	K1254	E1255	Y1256	L1257	E1258	Y1259	E1260	N1261	K1262	N1263	S1264	Y1268	L1269	W1270	Y1271	H1273	L1276	F1279	K1280	S1283	Y1284	N1285	M1286	R1287	Q1288	I1289	F1290	I1291	E1292									
N569	S570	K571	F572	F573	K574	M575	N576	T577	D578	A579	I580	T581	S582	L583	E584	D585	F586	F587	I588	V589	A590	L591	S592	F593	N594	L595	P596	K597	T598	I599	I600	L601	A602	A662	V663	A664	N605	E606	L607	D608	N609	D610	I611	Y612	Q613	Q614	L615	M616	K617	S618	D619	S620	L621	E622	E624	L625	Y626	I627				
E628	D629	F630	M631	F632	K633	Y634	K635	F636	D637	D638	S639	G640	E641	I642	F643	K644	G645	N646	M647	K648	F649	L650	N651	Q652	R653	T654	I655	T656	T657	L658	Y659	R660	S661	A662	V663	A664	N665	G666	Q667	V668	E669	Q670	I671	C672	C673	V674	L675	S676	K677	L678	D679	E680	T681	F682	F683	S684	T685	L686	L687			
L688	N689	T690	D691	F692	L693	S694	C695	A696	L697	Y698	E699	V700	S701	E702	D703	T704	N705	E706	K707	L708	F709	L710	L711	S712	L713	Q714	L715	A716	K717	T598	G718	N719	S720	E721	I722	T723	A723	N724	K725	L726	Q727	Q728	V729	I730	L731	Q732	H733	A734	Q735	L736	V737	Y737	F738	S739	P740	G741	A742	K743	I804	T745	Y746	V747
T748	H749	A750	V751	E752	L753	I754	N755	G756	T757	N758	D759	T760	S761	Q762	I763	F764	F765	F766	A767	N768	A769	I770	E771	V772	H773	A774	R775	Y776	M777	F778	T779	I780	D781	Y782	R783	S784	S785	L786	T787	S788	S789	L790	S791	T792	N793	T794	H795	L796	L797	L798	T799	D800	D801	K802	P803	I804	N805	L806	K807			
N808	M809	Q810	K811	L812	L813	R814	Y815	A816	L817	F818	L819	D820	A821	L822	L823	D824	A825	L826	P827	E828	R829	V830	N831	N832	H833	I834	V835	A836	F837	I838	T839	V840	N841	S842	R843	L844	V845	T846	D847	Y848	N849	C850	L851	S852	E853	E854	P855	N856	D857	L858	Y859	Y860	D861	F862	G863	H864	T865	F866	F867			
K868	H869	G870	K871	V872	N873	L874	N875	F876	S877	D878	I879	V880	G881	N882	V883	I884	Q885	P886	A887	N888	G889	S890	D891	A892	H893	L894	T895	F896	D897	I898	A899	E900	S901	N902	S903	V904	Y905	F906	F907	Y908	Y909	S910	R911	V912	L913	Y914	K915	V916	L917	L918	N919	S920	I921	D922	T923	V924	S925	S926	T927			
T928	L929	N930	G931	L932	L933	A934	S935	V936	E937	S938	F939	V940	T941	K942	T943	V944	D945	D946	Q947	K948	S949	T950	D951	K952	D953	Y954	L955	L956	C957	A958	I959	L960	L961	L962	N963	F964	N965	R966	S967	N968	S969	K970	D971	E972	L973	T974	K975	L976	R977	T978	L979	L980	A981	S982	Q983	L984	I985	G986	I987			
R988	E989	V990	E991	L992	V993	D994	Q995	E996	F997	K998	S999	L1000	A1001	L1002	L1003	N1004	N1005	L1006	L1007	D1008	I1009	P1010	Q1011	A1012	D1013	Y1014	Q1015	F1016	V1017	P1018	I1019	A1020	P1021	Q1022	R1023	L1024	N1025	M1026	I1027	F1028	R1029	S1030	I1031	L1032	K1033	W1034	L1035	D1036	S1037	D1038	L1039	A1040	Y1041	E1042	P1043	S1044	F1045	T1046	T1047			
V1048	R1049	L1050	L1051	L1052	L1053	D1054	F1055	F1056	T1057	K1058	L1059	M1060	R1061	F1062	E1063	G1064	V1065	R1066	D1067	M1068	G1069	I1070	T1071	A1072	F1073	E1074	L1075	S1076	E1077	R1078	L1079	L1080	A1081	D1082	S1083	L1084	S1085	M1086	C1087	Q1088	T1089	D1090	D1091	L1092	L1093	Y1094	L1095	L1096	E1097	L1098	R1099	S1100	C1102	L1103	N1104	Y1106	E1107					
T1108	L1109	S1110	Q1111	GLY	VAL	SER	ASN	GLY	GLU	GLU	ILE	SER	E1122	Y1123	G1124	D1125	E1126	I1127	Q1128	E1129	N1130	L1131	I1132	E1133	L1134	M1135	F1136	L1137	N1138	F1139	N1140	Q1141	E1142	R1143	N1144	M1145	Q1146	V1147	S1148	T1149	L1150	F1151	Y1152	Q1153	K1154	L1155	Y1156	K1157	V1158	I1159	S1160	S1161	M1162	E1163	L1164	K1165	L1166	L1167				
E1168	S1169	Q1170	Y1171	K1172	R1173	I1174	F1175	E1176	V1177	V1178	L1179	M1180	D1181	K1182	D1183	I1184	G1185	S1186	M1187	I1188	N1189	Q1190	S1191	L1192	L1193	L1194	T1195	L1196	L1197	L1198	G1199	S1200	L1201	V1202	V1203	K1204	T1205	Q1206	Q1207	D1208	I1209	I1210	I1211	E1212	E1214	L1213	E1214	L1215	L1216	I1217	GLN	LYS	GLN	THR	GLY	SER	ASP	VAL	GLY			
SER	ALA	SER	ASP	ASN	ASP	VAL	N1235	S1236	K1237	F1238	K1239	L1240	F1241	Q1242	K1243	L1244	L1245	Q1246	K1247	V1248	T1249	D1250	E1251	P1253	K1254	E1255	Y1256	L1257	E1258	Y1259	E1260	N1261	K1262	N1263	S1264	Y1268	L1269	W1270	Y1271	H1273	L1276	F1279	K1280	S1283	Y1284	N1285	M1286	R1287	Q1288	I1289	F1290	I1291	E1292									



- Molecule 47: Eukaryotic translation initiation factor 6



- Molecule 48: 60S ribosomal protein L1-A



- Molecule 49: Ala tRNA



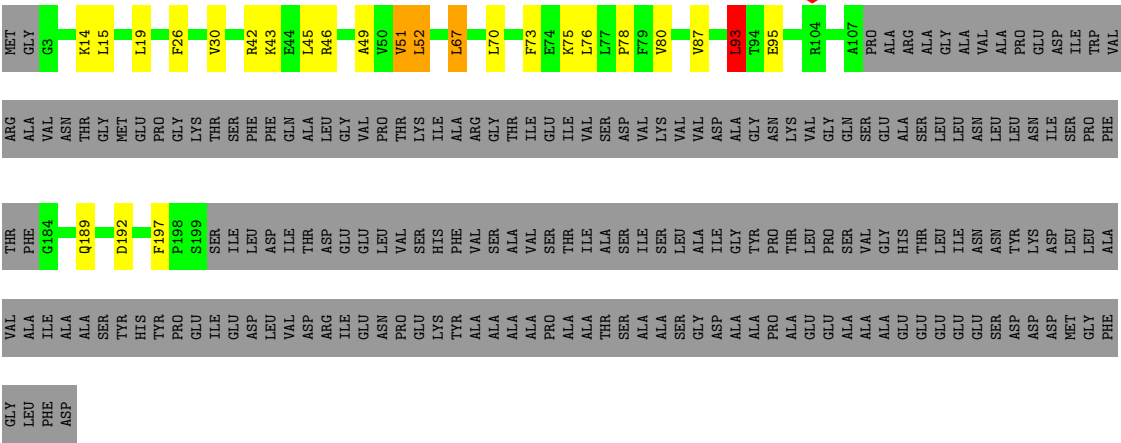
- Molecule 49: Ala tRNA



- Molecule 50: 60S ribosomal protein L12-B



- Molecule 51: 60S acidic ribosomal protein P0

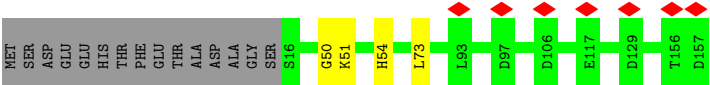
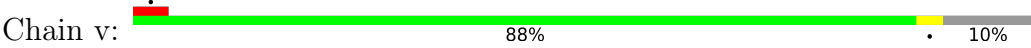


- Molecule 52: CAT-tailed nascent peptide



There are no outlier residues recorded for this chain.

- Molecule 53: Eukaryotic translation initiation factor 5A-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54175	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	3.799	Depositor
Minimum map value	-0.723	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

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	0.36	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	0.68	1/1329 (0.1%)
13	M	0.36	0/1106	0.61	0/1485
14	N	0.40	0/1200	0.62	0/1607
15	O	0.32	0/473	0.72	2/629 (0.3%)
16	P	0.35	0/745	0.68	0/1001
17	Q	0.39	0/890	0.77	2/1196 (0.2%)
18	R	0.32	0/1034	0.59	0/1385
19	S	0.38	0/868	0.61	0/1168
20	T	0.35	0/890	0.67	0/1189
21	U	0.34	0/978	0.65	1/1301 (0.1%)
22	V	0.34	0/772	0.66	0/1026
23	W	0.38	0/660	0.69	0/875
24	X	0.33	0/618	0.78	1/826 (0.1%)
25	Y	0.33	0/443	0.65	0/588
26	Z	0.33	0/416	0.70	0/553
27	b	0.36	0/836	0.66	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	1/77011 (0.0%)	1.03	297/120065 (0.2%)
31	h	0.53	0/2883	0.98	8/4491 (0.2%)
32	i	0.60	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.39	0/1908	0.68	0/2564
34	k	0.36	0/3146	0.64	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	0.64	0/2416
42	s	0.33	0/1367	0.70	3/1834 (0.2%)
43	t	0.36	0/1568	0.68	1/2106 (0.0%)
44	u	0.34	0/1068	0.66	1/1438 (0.1%)
45	a	0.30	0/6679	0.49	0/9012
46	e	0.38	0/11715	0.55	2/15908 (0.0%)
47	g	0.32	0/1672	0.63	0/2281
48	w	0.33	0/1736	0.65	0/2332
49	x	0.21	0/1761	0.64	0/2742
49	y	0.23	0/1735	0.65	0/2701
50	z	0.37	0/726	0.60	0/1006
51	0	0.33	0/976	0.55	0/1313
53	v	0.32	0/1084	0.63	1/1456 (0.1%)
All	All	0.50	1/161759 (0.0%)	0.87	348/236301 (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
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
47	g	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	2416	U	O3'-P	-5.92	1.54	1.61

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3217	C	N1-C2-O2	12.13	126.18	118.90
30	f	3217	C	C2-N1-C1'	11.32	131.25	118.80
30	f	3217	C	N3-C2-O2	-9.75	115.08	121.90
11	K	134	ASP	CB-CG-OD1	9.69	127.02	118.30
30	f	922	U	C2-N1-C1'	9.30	128.86	117.70
17	Q	84	ASP	CB-CG-OD1	9.23	126.60	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	3278	C	N1-C2-O2	8.73	124.14	118.90
30	f	3181	C	N1-C2-O2	8.71	124.12	118.90
30	f	3181	C	C2-N1-C1'	8.46	128.11	118.80
30	f	1279	C	C5-C6-N1	8.39	125.19	121.00
30	f	2836	C	N3-C2-O2	-8.38	116.04	121.90
30	f	2836	C	C2-N1-C1'	8.18	127.80	118.80
30	f	1496	C	C2-N1-C1'	8.12	127.73	118.80
36	m	230	ASP	CB-CG-OD1	8.08	125.57	118.30
30	f	1645	U	N3-C2-O2	-7.95	116.64	122.20
30	f	922	U	N3-C2-O2	-7.93	116.65	122.20
30	f	406	G	O4'-C1'-N9	7.92	114.54	108.20
30	f	3217	C	C6-N1-C2	-7.87	117.15	120.30
30	f	2205	U	N1-C2-O2	7.85	128.30	122.80
4	D	41	ASP	CB-CG-OD1	7.80	125.32	118.30
30	f	2983	C	C2-N1-C1'	7.79	127.37	118.80
30	f	2444	C	C2-N1-C1'	7.77	127.35	118.80
30	f	3217	C	C6-N1-C1'	-7.74	111.52	120.80
30	f	1208	U	N1-C2-O2	7.73	128.21	122.80
30	f	2652	U	N3-C2-O2	-7.67	116.83	122.20
30	f	3306	U	N3-C2-O2	-7.60	116.88	122.20
30	f	3278	C	N3-C2-O2	-7.58	116.59	121.90
30	f	2541	U	P-O3'-C3'	7.57	128.78	119.70
30	f	3306	U	C2-N1-C1'	7.55	126.75	117.70
30	f	3278	C	C2-N1-C1'	7.52	127.08	118.80
30	f	2836	C	N1-C2-O2	7.49	123.39	118.90
30	f	2205	U	N3-C2-O2	-7.48	116.97	122.20
30	f	758	C	C2-N1-C1'	7.47	127.02	118.80
30	f	1645	U	N1-C2-O2	7.45	128.02	122.80
30	f	1277	C	C2-N1-C1'	7.43	126.97	118.80
30	f	2502	A	OP2-P-O3'	7.41	121.50	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3181	C	N3-C2-O2	-7.34	116.77	121.90
30	f	2235	C	C2-N1-C1'	7.30	126.83	118.80
15	O	36	ASP	CB-CG-OD1	7.29	124.86	118.30
30	f	1239	C	C2-N1-C1'	7.23	126.75	118.80
30	f	1556	C	N1-C2-O2	7.22	123.23	118.90
30	f	2531	C	C2-N1-C1'	7.17	126.68	118.80
42	s	170	ASP	CB-CG-OD1	7.16	124.74	118.30
30	f	2923	U	N1-C2-O2	7.15	127.80	122.80
39	p	158	ASP	CB-CG-OD1	7.15	124.73	118.30
30	f	36	C	N1-C2-O2	7.15	123.19	118.90
30	f	1349	G	N3-C4-C5	-7.14	125.03	128.60
30	f	2502	A	P-O3'-C3'	7.14	128.27	119.70
30	f	1277	C	N1-C2-O2	7.12	123.17	118.90
30	f	1227	C	N1-C2-O2	7.12	123.17	118.90
30	f	1227	C	C2-N1-C1'	7.11	126.62	118.80
30	f	2205	U	C2-N1-C1'	7.09	126.21	117.70
30	f	1815	U	P-O3'-C3'	7.08	128.20	119.70
30	f	1307	G	P-O3'-C3'	7.08	128.19	119.70
30	f	78	U	N3-C2-O2	-7.04	117.27	122.20
30	f	982	C	C2-N1-C1'	7.04	126.54	118.80
30	f	1645	U	C2-N1-C1'	7.02	126.12	117.70
30	f	1604	G	C4-N9-C1'	7.01	135.61	126.50
30	f	1872	C	N1-C2-O2	7.00	123.10	118.90
30	f	14	U	O5'-P-OP2	-6.99	99.41	105.70
30	f	1272	C	N1-C2-O2	6.98	123.09	118.90
30	f	3217	C	C5-C6-N1	6.96	124.48	121.00
30	f	1208	U	C2-N1-C1'	6.95	126.04	117.70
30	f	1349	G	C4-N9-C1'	6.95	135.53	126.50
30	f	2405	C	C6-N1-C2	-6.90	117.54	120.30
30	f	3275	U	OP1-P-O3'	6.86	120.28	105.20
30	f	3306	U	N1-C2-O2	6.83	127.58	122.80
30	f	3235	C	C2-N1-C1'	6.81	126.29	118.80
30	f	2846	U	N3-C2-O2	-6.79	117.44	122.20
30	f	2846	U	C2-N1-C1'	6.75	125.81	117.70
30	f	2923	U	N3-C2-O2	-6.75	117.47	122.20
30	f	1227	C	C5-C6-N1	6.72	124.36	121.00
12	L	11	ASP	CB-CG-OD1	6.72	124.35	118.30
30	f	270	U	N1-C2-O2	6.70	127.49	122.80
30	f	2983	C	N3-C2-O2	-6.68	117.22	121.90
31	h	26	C	N1-C2-O2	6.66	122.90	118.90
30	f	1227	C	C6-N1-C2	-6.65	117.64	120.30
30	f	2537	U	P-O3'-C3'	6.64	127.67	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2836	C	C6-N1-C2	-6.60	117.66	120.30
30	f	2531	C	N3-C2-O2	-6.60	117.28	121.90
30	f	2112	U	OP2-P-O3'	6.60	119.71	105.20
30	f	270	U	N3-C2-O2	-6.59	117.58	122.20
30	f	1208	U	N3-C2-O2	-6.59	117.59	122.20
30	f	3058	U	C2-N1-C1'	6.57	125.58	117.70
30	f	1239	C	N1-C2-O2	6.56	122.84	118.90
30	f	3214	U	C2-N1-C1'	6.53	125.53	117.70
2	B	27[A]	LEU	CB-CG-CD2	-6.52	99.91	111.00
30	f	2189	U	N1-C2-O2	6.52	127.37	122.80
30	f	2189	U	N3-C2-O2	-6.47	117.67	122.20
32	i	64	U	N3-C2-O2	-6.47	117.67	122.20
30	f	2235	C	C6-N1-C2	-6.46	117.71	120.30
30	f	2101	C	P-O3'-C3'	6.46	127.45	119.70
30	f	3034	C	N1-C2-O2	6.46	122.78	118.90
31	h	105	C	N1-C2-O2	6.46	122.78	118.90
30	f	2112	U	P-O3'-C3'	6.46	127.45	119.70
30	f	2550	U	N3-C2-O2	-6.43	117.70	122.20
30	f	524	U	N1-C2-O2	6.41	127.29	122.80
30	f	1269	U	N1-C2-O2	6.39	127.28	122.80
35	l	155	ASP	CB-CG-OD1	6.37	124.04	118.30
30	f	524	U	N3-C2-O2	-6.34	117.76	122.20
30	f	1269	U	C2-N1-C1'	6.34	125.31	117.70
30	f	3058	U	N1-C2-O2	6.34	127.24	122.80
30	f	865	U	N3-C2-O2	-6.33	117.77	122.20
21	U	79	ASP	CB-CG-OD1	6.33	124.00	118.30
44	u	47	ASP	CB-CG-OD1	6.33	124.00	118.30
30	f	1556	C	N3-C2-O2	-6.33	117.47	121.90
30	f	2274	U	N1-C2-O2	6.32	127.23	122.80
30	f	2983	C	N1-C2-O2	6.32	122.69	118.90
30	f	986	U	N3-C2-O2	-6.32	117.78	122.20
30	f	36	C	N3-C2-O2	-6.29	117.50	121.90
30	f	2464	U	C2-N1-C1'	6.29	125.25	117.70
1	A	153	ASP	CB-CG-OD1	6.27	123.94	118.30
30	f	2617	U	N3-C2-O2	-6.26	117.82	122.20
30	f	922	U	C6-N1-C1'	-6.26	112.44	121.20
36	m	137	ASP	CB-CG-OD1	6.24	123.92	118.30
30	f	1716	U	P-O3'-C3'	6.24	127.18	119.70
30	f	192	C	C2-N1-C1'	6.23	125.65	118.80
30	f	2726	C	N3-C2-O2	-6.23	117.54	121.90
40	q	42	ASP	CB-CG-OD1	6.23	123.90	118.30
30	f	1496	C	C6-N1-C2	-6.23	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3104	U	N1-C2-O2	6.21	127.15	122.80
30	f	2444	C	C6-N1-C2	-6.21	117.82	120.30
30	f	2726	C	C2-N1-C1'	6.21	125.63	118.80
30	f	1269	U	N3-C2-O2	-6.20	117.86	122.20
46	e	437	LYS	N-CA-C	-6.20	94.26	111.00
30	f	1097	G	P-O3'-C3'	6.20	127.13	119.70
30	f	1878	G	C4-N9-C1'	6.19	134.54	126.50
30	f	2846	U	N1-C2-O2	6.18	127.13	122.80
30	f	637	C	P-O3'-C3'	6.18	127.11	119.70
30	f	2550	U	C2-N1-C1'	6.14	125.07	117.70
30	f	1349	G	N3-C4-N9	6.13	129.68	126.00
30	f	915	A	C2-N3-C4	6.12	113.66	110.60
30	f	3104	U	N3-C2-O2	-6.11	117.93	122.20
30	f	2132	C	N3-C2-O2	-6.09	117.64	121.90
30	f	1115	G	C4-N9-C1'	6.09	134.41	126.50
30	f	995	U	N1-C2-O2	6.06	127.04	122.80
30	f	1907	C	N1-C2-O2	6.05	122.53	118.90
30	f	1064	A	P-O3'-C3'	6.05	126.96	119.70
30	f	1279	C	C6-N1-C2	-6.05	117.88	120.30
30	f	2553	U	C2-N1-C1'	6.05	124.96	117.70
30	f	2388	U	N3-C2-O2	-6.05	117.97	122.20
30	f	2923	U	C2-N1-C1'	6.04	124.95	117.70
30	f	1604	G	N3-C4-N9	6.04	129.62	126.00
30	f	2842	U	N1-C2-O2	6.03	127.02	122.80
30	f	2132	C	C6-N1-C2	-6.03	117.89	120.30
30	f	3300	U	N3-C2-O2	-6.03	117.98	122.20
30	f	985	U	N3-C2-O2	-6.01	117.99	122.20
30	f	3131	U	C2-N1-C1'	6.01	124.91	117.70
30	f	2405	C	N3-C2-O2	-6.00	117.70	121.90
30	f	2274	U	C2-N1-C1'	6.00	124.89	117.70
30	f	3181	C	C6-N1-C1'	-5.99	113.61	120.80
30	f	1556	C	C2-N1-C1'	5.99	125.39	118.80
30	f	1872	C	N3-C2-O2	-5.97	117.72	121.90
30	f	1604	G	C8-N9-C1'	-5.97	119.24	127.00
30	f	969	C	C6-N1-C2	-5.96	117.92	120.30
8	H	18	ASP	CB-CG-OD1	5.94	123.65	118.30
8	H	51	GLY	C-N-CA	5.94	136.55	121.70
30	f	1355	A	P-O3'-C3'	5.94	126.82	119.70
34	k	87	VAL	CG1-CB-CG2	-5.93	101.42	110.90
30	f	2652	U	N1-C2-O2	5.93	126.95	122.80
31	h	26	C	C6-N1-C2	-5.93	117.93	120.30
30	f	865	U	N1-C2-O2	5.92	126.95	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1604	G	N3-C4-C5	-5.92	125.64	128.60
30	f	1425	U	N3-C2-O2	-5.92	118.06	122.20
32	i	100	U	C2-N1-C1'	5.92	124.80	117.70
30	f	2585	G	N3-C4-C5	-5.91	125.65	128.60
30	f	1272	C	N3-C2-O2	-5.90	117.77	121.90
30	f	2204	C	C6-N1-C2	-5.89	117.94	120.30
30	f	2622	C	N1-C2-O2	5.87	122.42	118.90
30	f	1525	G	C4-N9-C1'	5.86	134.11	126.50
30	f	1562	C	P-O3'-C3'	5.86	126.73	119.70
30	f	1820	U	P-O3'-C3'	5.86	126.73	119.70
30	f	2638	C	N1-C2-O2	5.86	122.41	118.90
30	f	835	G	O4'-C1'-N9	5.84	112.87	108.20
30	f	3350	C	C6-N1-C2	-5.84	117.97	120.30
30	f	3214	U	N3-C2-O2	-5.82	118.13	122.20
30	f	3048	A	O4'-C1'-N9	5.82	112.85	108.20
30	f	1577	G	N1-C6-O6	-5.81	116.41	119.90
30	f	2531	C	C6-N1-C2	-5.81	117.98	120.30
30	f	1437	C	C2-N1-C1'	5.80	125.18	118.80
30	f	3316	A	P-O3'-C3'	5.79	126.65	119.70
30	f	97	U	N3-C2-O2	-5.79	118.15	122.20
30	f	758	C	C6-N1-C2	-5.76	118.00	120.30
30	f	270	U	C2-N1-C1'	5.75	124.60	117.70
42	s	9	MET	CA-CB-CG	5.75	123.07	113.30
30	f	2204	C	C5-C6-N1	5.74	123.87	121.00
30	f	2274	U	N3-C2-O2	-5.74	118.18	122.20
30	f	142	C	N1-C2-O2	5.74	122.34	118.90
30	f	2992	U	N3-C2-O2	-5.73	118.19	122.20
30	f	3228	C	P-O3'-C3'	5.72	126.57	119.70
30	f	2132	C	N1-C2-O2	5.71	122.33	118.90
30	f	2531	C	C5-C6-N1	5.71	123.86	121.00
30	f	2899	C	C2-N1-C1'	5.70	125.07	118.80
32	i	64	U	N1-C2-O2	5.70	126.79	122.80
30	f	3034	C	N3-C2-O2	-5.69	117.92	121.90
30	f	354	U	N1-C2-O2	5.68	126.78	122.80
30	f	1448	U	N3-C2-O2	-5.68	118.22	122.20
30	f	1190	A	C4-N9-C1'	5.68	136.52	126.30
30	f	2899	C	N3-C2-O2	-5.68	117.93	121.90
30	f	3058	U	N3-C2-O2	-5.67	118.23	122.20
30	f	3218	A	P-O3'-C3'	5.67	126.51	119.70
46	e	1364	GLY	N-CA-C	5.67	127.29	113.10
30	f	282	G	P-O3'-C3'	5.67	126.50	119.70
30	f	916	G	P-O3'-C3'	5.66	126.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	50	LEU	CA-CB-CG	5.65	128.30	115.30
30	f	2553	U	C6-N1-C1'	-5.65	113.29	121.20
30	f	1277	C	N3-C2-O2	-5.64	117.95	121.90
30	f	3057	U	N3-C2-O2	-5.63	118.26	122.20
30	f	142	C	C6-N1-C2	-5.62	118.05	120.30
30	f	2983	C	C6-N1-C2	-5.61	118.06	120.30
30	f	1349	G	C8-N9-C1'	-5.60	119.72	127.00
30	f	2366	C	C2-N1-C1'	5.59	124.95	118.80
30	f	113	C	C2-N1-C1'	5.59	124.95	118.80
31	h	26	C	N3-C2-O2	-5.58	117.99	121.90
30	f	777	U	N3-C2-O2	-5.58	118.30	122.20
30	f	2378	C	C2-N1-C1'	5.58	124.94	118.80
30	f	2137	U	C2-N1-C1'	5.58	124.39	117.70
3	C	53	ASP	CB-CG-OD1	5.55	123.30	118.30
30	f	3269	U	P-O3'-C3'	5.55	126.36	119.70
31	h	35	C	N1-C2-O2	5.54	122.23	118.90
30	f	1496	C	C5-C6-N1	5.54	123.77	121.00
30	f	2842	U	N3-C2-O2	-5.53	118.33	122.20
30	f	2764	C	N1-C2-O2	5.53	122.22	118.90
32	i	125	U	C2-N1-C1'	5.53	124.33	117.70
30	f	1688	U	N3-C2-O2	-5.52	118.33	122.20
30	f	2366	C	C5-C6-N1	5.51	123.76	121.00
30	f	2726	C	N1-C2-O2	5.51	122.21	118.90
30	f	995	U	N3-C2-O2	-5.51	118.34	122.20
30	f	1554	U	P-O3'-C3'	5.51	126.31	119.70
40	q	107	ASP	CB-CG-OD1	5.51	123.26	118.30
30	f	2444	C	N1-C2-O2	5.50	122.20	118.90
30	f	982	C	N1-C2-O2	5.48	122.19	118.90
30	f	283	G	N3-C4-N9	5.48	129.29	126.00
30	f	2552	C	N1-C2-O2	5.48	122.19	118.90
24	X	14	LEU	CA-CB-CG	5.47	127.89	115.30
30	f	315	C	C2-N1-C1'	5.46	124.81	118.80
30	f	1496	C	N1-C2-O2	5.46	122.18	118.90
30	f	982	C	C6-N1-C2	-5.46	118.12	120.30
30	f	1190	A	C2-N3-C4	5.46	113.33	110.60
31	h	52	G	P-O3'-C3'	5.46	126.25	119.70
30	f	1878	G	C8-N9-C1'	-5.44	119.93	127.00
30	f	2552	C	C2-N1-C1'	5.44	124.79	118.80
30	f	3057	U	N1-C2-O2	5.44	126.61	122.80
30	f	3355	U	C2-N1-C1'	5.44	124.22	117.70
30	f	283	G	C4-N9-C1'	5.43	133.56	126.50
30	f	3214	U	N1-C2-O2	5.43	126.60	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1277	C	C6-N1-C2	-5.42	118.13	120.30
30	f	2585	G	N3-C4-N9	5.42	129.25	126.00
30	f	2622	C	N3-C2-O2	-5.42	118.10	121.90
30	f	2783	U	N3-C2-O2	-5.41	118.41	122.20
30	f	3350	C	P-O3'-C3'	5.41	126.19	119.70
30	f	2210	G	N3-C4-C5	-5.41	125.89	128.60
30	f	3153	U	C2-N1-C1'	5.40	124.18	117.70
30	f	986	U	N1-C2-O2	5.39	126.58	122.80
30	f	982	C	C5-C6-N1	5.39	123.70	121.00
30	f	1496	C	C6-N1-C1'	-5.39	114.33	120.80
30	f	78	U	N1-C2-O2	5.38	126.57	122.80
30	f	411	U	N3-C2-O2	-5.38	118.43	122.20
30	f	1349	G	C2-N3-C4	5.38	114.59	111.90
3	C	114	VAL	CG1-CB-CG2	-5.38	102.30	110.90
30	f	1425	U	N1-C2-O2	5.36	126.55	122.80
30	f	915	A	C4-N9-C1'	5.36	135.95	126.30
30	f	1732	U	N1-C2-O2	5.36	126.55	122.80
30	f	3278	C	C6-N1-C1'	-5.36	114.37	120.80
30	f	2497	U	N3-C2-O2	-5.35	118.46	122.20
30	f	3235	C	N1-C2-O2	5.33	122.10	118.90
30	f	890	C	N1-C2-O2	5.32	122.09	118.90
30	f	2500	A	P-O3'-C3'	5.32	126.08	119.70
30	f	2336	U	N3-C2-O2	-5.32	118.48	122.20
30	f	2444	C	C5-C6-N1	5.32	123.66	121.00
30	f	2836	C	C6-N1-C1'	-5.31	114.42	120.80
32	i	125	U	N1-C2-O2	5.31	126.51	122.80
30	f	1907	C	N3-C2-O2	-5.30	118.19	121.90
30	f	2235	C	N1-C2-O2	5.29	122.08	118.90
30	f	142	C	N3-C2-O2	-5.29	118.20	121.90
43	t	136	GLU	CA-CB-CG	5.29	125.04	113.40
30	f	1560	G	N3-C4-N9	-5.29	122.83	126.00
30	f	3349	C	C6-N1-C2	-5.29	118.19	120.30
30	f	2726	C	C6-N1-C2	-5.28	118.19	120.30
30	f	192	C	C6-N1-C2	-5.28	118.19	120.30
30	f	1115	G	C8-N9-C1'	-5.28	120.14	127.00
30	f	1732	U	N3-C2-O2	-5.28	118.50	122.20
30	f	1525	G	C8-N9-C1'	-5.28	120.14	127.00
30	f	2568	C	O4'-C1'-N1	5.27	112.42	108.20
30	f	1608	C	C2-N1-C1'	5.26	124.59	118.80
31	h	105	C	N3-C2-O2	-5.26	118.22	121.90
53	v	50	GLY	N-CA-C	-5.26	99.95	113.10
30	f	915	A	C8-N9-C4	-5.25	103.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1608	C	C5-C6-N1	5.25	123.63	121.00
42	s	108	GLU	CA-CB-CG	5.24	124.93	113.40
30	f	2622	C	C6-N1-C2	-5.24	118.21	120.30
30	f	1237	G	N3-C4-N9	5.23	129.14	126.00
30	f	1608	C	C6-N1-C2	-5.22	118.21	120.30
30	f	2366	C	C6-N1-C2	-5.22	118.21	120.30
30	f	3148	U	N3-C2-O2	-5.22	118.55	122.20
30	f	149	U	N3-C2-O2	-5.21	118.55	122.20
30	f	2114	C	C6-N1-C2	-5.21	118.22	120.30
30	f	1437	C	C6-N1-C2	-5.21	118.22	120.30
30	f	2496	C	C2-N1-C1'	5.21	124.53	118.80
30	f	2405	C	N1-C2-O2	5.20	122.02	118.90
30	f	2983	C	C6-N1-C1'	-5.20	114.56	120.80
30	f	1239	C	C6-N1-C1'	-5.19	114.58	120.80
30	f	969	C	N3-C2-O2	-5.18	118.27	121.90
30	f	2585	G	C4-N9-C1'	5.18	133.24	126.50
30	f	2772	C	N1-C2-O2	5.18	122.00	118.90
30	f	890	C	N3-C2-O2	-5.17	118.28	121.90
30	f	849	C	P-O3'-C3'	5.16	125.90	119.70
30	f	954	U	N3-C2-O2	-5.16	118.59	122.20
31	h	18	C	C2-N1-C1'	5.16	124.48	118.80
30	f	2446	U	O4'-C1'-N1	5.15	112.32	108.20
30	f	637	C	OP1-P-O3'	5.15	116.53	105.20
30	f	1563	C	C6-N1-C1'	5.15	126.97	120.80
30	f	166	C	C2-N1-C1'	5.14	124.45	118.80
30	f	2235	C	C5-C6-N1	5.14	123.57	121.00
30	f	1951	C	C2-N1-C1'	5.13	124.45	118.80
30	f	2405	C	C2-N1-C1'	5.13	124.44	118.80
30	f	2638	C	N3-C2-O2	-5.12	118.31	121.90
30	f	3181	C	C6-N1-C2	-5.12	118.25	120.30
30	f	2899	C	N1-C2-O2	5.11	121.97	118.90
30	f	2873	U	C2-N1-C1'	5.09	123.81	117.70
30	f	1597	C	C5-C6-N1	5.09	123.55	121.00
36	m	222	LEU	CA-CB-CG	5.09	127.00	115.30
32	i	100	U	N1-C2-O2	5.08	126.36	122.80
35	l	4	PRO	C-N-CA	5.08	134.41	121.70
30	f	87	U	N1-C2-O2	5.08	126.36	122.80
32	i	157	U	N1-C2-O2	5.07	126.35	122.80
17	Q	42	LEU	CA-CB-CG	5.07	126.95	115.30
30	f	1097	G	OP2-P-O3'	5.06	116.34	105.20
30	f	2899	C	C6-N1-C2	-5.06	118.28	120.30
30	f	3355	U	N1-C2-O2	5.06	126.34	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2550	U	N1-C2-O2	5.05	126.34	122.80
30	f	758	C	N1-C2-O2	5.05	121.93	118.90
39	p	79	GLN	CA-CB-CG	5.04	124.50	113.40
30	f	1820	U	OP2-P-O3'	5.04	116.28	105.20
30	f	2444	C	C6-N1-C1'	-5.03	114.76	120.80
30	f	1272	C	C6-N1-C2	-5.03	118.29	120.30
30	f	354	U	N3-C2-O2	-5.03	118.68	122.20
15	O	21	ILE	CG1-CB-CG2	-5.03	100.34	111.40
30	f	969	C	N1-C2-O2	5.03	121.92	118.90
30	f	2497	U	N1-C2-O2	5.02	126.31	122.80
30	f	777	U	N1-C2-O2	5.02	126.31	122.80
5	E	10	LEU	CB-CG-CD1	5.02	119.53	111.00
36	m	146	LEU	CB-CG-CD1	-5.02	102.47	111.00
30	f	1355	A	OP2-P-O3'	5.01	116.22	105.20
30	f	1688	U	N1-C2-O2	5.01	126.30	122.80
30	f	282	G	C2'-C3'-O3'	5.00	121.71	113.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
47	g	8	GLU	Peptide
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	Peptide

5.2 Too-close contacts ⓘ

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	3	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	u	1053	0	1149	0	0
45	a	6569	0	6460	0	0
46	e	11516	0	10776	0	0
47	g	1651	0	1613	0	0
48	w	1709	0	1799	0	0
49	x	1579	0	799	0	0
49	y	1556	0	789	0	0
50	z	728	0	337	0	0
51	0	961	0	979	11	0
52	1	90	0	21	0	0
53	v	1085	0	1086	0	0
54	A	1	0	0	0	0
54	C	1	0	0	0	0
54	E	1	0	0	0	0
54	I	1	0	0	0	0
54	R	1	0	0	0	0
54	T	1	0	0	0	0
54	f	3	0	0	0	0
54	h	1	0	0	0	0
54	j	2	0	0	0	0
54	k	1	0	0	0	0
55	T	1	0	0	0	0
55	W	1	0	0	0	0
55	Z	1	0	0	0	0
55	b	1	0	0	0	0
55	c	1	0	0	0	0
55	e	2	0	0	0	0
All	All	151349	0	113598	146	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 (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.90
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
51:O:26:PHE:HB2	51: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.84	0.59
51:O:192:ASP:HB2	51:O:197:PHE:HE2	1.67	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
51:O:43:LYS:HA	51: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
51:O:42:ARG:HG2	51: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
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	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	0.53
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
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	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
7:G:99:SER:HG	7:G:101:CYS:HG	1.59	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.51
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2.38	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
4:D:131:ALA:HB1	4:D:135:GLN:H	1.78	0.48
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
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.96	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
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
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
51:O:26:PHE:HZ	51:O:93:LEU:HA	1.80	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	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
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.47
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.97	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.46
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.46
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
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
4:D:161:LYS:HD3	4:D:161:LYS:HA	1.82	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.44
15:O:21:ILE:HD12	15:O:21:ILE:HG23	1.83	0.43
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.43
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.43
51:O:45:LEU:HB3	51:O:49:ALA:HB3	1.99	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
51:O:15:LEU:O	51:O:19:LEU:HG	2.18	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
51:O:75:LYS:O	51:O:78:PRO:HD2	2.19	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.52	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
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	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	0.43
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	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
51:O:70:LEU:HB3	51:O:73:PHE:CD1	2.55	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42
51:O:14:LYS:HE3	51:O:52:LEU:HD11	2.00	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.01	0.42
51:O:67:LEU:HD22	51:O:67:LEU:HA	1.85	0.42
16:P:73:GLY:N	16:P:76:GLU:OE2	2.42	0.42
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
20:T:95:ILE:HD13	20:T:95:ILE:HG21	1.81	0.41
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	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	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	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
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.41
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.02	0.40
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.40
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.40
4:D:180:ARG:HE	4:D:180:ARG:HB2	1.61	0.40
6:F:40:ARG:HA	6:F:40:ARG:HD2	1.84	0.40
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.40
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	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
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	61 (100%)	0	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	14
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
34	k	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	37	59
36	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
37	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	25	47
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	830 (99%)	12 (1%)	0	100	100
46	e	1519/1562 (97%)	1495 (98%)	22 (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
50	z	144/165 (87%)	135 (94%)	8 (6%)	1 (1%)	19	38
51	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	31
53	v	139/157 (88%)	139 (100%)	0	0	100	100
All	All	9314/10279 (91%)	8956 (96%)	349 (4%)	9 (0%)	50	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
50	z	88	PRO
46	e	437	LYS
46	e	855	PRO
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
51	0	93	LEU
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	90 (100%)	0	100	100
20	T	95/103 (92%)	94 (99%)	1 (1%)	70	86
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	X	68/69 (99%)	66 (97%)	2 (3%)	37	64
25	Y	45/46 (98%)	45 (100%)	0	100	100
26	Z	45/116 (39%)	45 (100%)	0	100	100
27	b	87/91 (96%)	87 (100%)	0	100	100
28	c	71/72 (99%)	71 (100%)	0	100	100
29	d	20/23 (87%)	20 (100%)	0	100	100
33	j	189/196 (96%)	188 (100%)	1 (0%)	86	95
34	k	321/323 (99%)	319 (99%)	2 (1%)	84	94
35	l	288/289 (100%)	288 (100%)	0	100	100
36	m	241/245 (98%)	241 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	638 (94%)	38 (6%)	17	38
46	e	1152/1451 (79%)	1092 (95%)	60 (5%)	19	41
47	g	180/211 (85%)	180 (100%)	0	100	100
48	w	197/198 (100%)	196 (100%)	1 (0%)	86	95
51	0	104/254 (41%)	95 (91%)	9 (9%)	8	17
53	v	119/132 (90%)	117 (98%)	2 (2%)	56	78
All	All	7564/8690 (87%)	7442 (98%)	122 (2%)	58	79

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

Mol	Chain	Res	Type
4	D	12	ARG
7	G	83	ARG
15	O	33	LYS
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
33	j	221	LYS
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
45	a	74	SER
45	a	89	LEU
45	a	114	LEU
45	a	121	ASN
45	a	139	LEU
45	a	157	PHE

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Mol	Chain	Res	Type
45	a	255	LEU
45	a	261	LEU
45	a	285	ILE
45	a	293	TYR
45	a	308	THR
45	a	309	PHE
45	a	316	ILE
45	a	541	LYS
45	a	580	PHE
45	a	589	MET
45	a	605	ILE
45	a	609	ASP
45	a	612	MET
45	a	627	LYS
45	a	649	TRP
45	a	665	VAL
45	a	675	ILE
45	a	696	GLN
45	a	697	LEU
45	a	705	TRP
45	a	837	VAL
45	a	855	ASP
45	a	868	THR
45	a	881	GLU
45	a	896	ARG
45	a	924	LEU
45	a	947	LEU
45	a	973	TYR
45	a	979	LEU
45	a	994	HIS
45	a	1003	GLN
45	a	1014	LEU
46	e	8	THR
46	e	30	PHE
46	e	105	VAL
46	e	125	ILE
46	e	169	LEU
46	e	205	GLU
46	e	254	ASN
46	e	271	LEU
46	e	277	MET
46	e	299	THR

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Mol	Chain	Res	Type
46	e	309	VAL
46	e	319	THR
46	e	327	THR
46	e	364	SER
46	e	400	GLU
46	e	707	LYS
46	e	710	LYS
46	e	731	LEU
46	e	733	HIS
46	e	754	ILE
46	e	770	ILE
46	e	780	ILE
46	e	797	LEU
46	e	799	THR
46	e	807	LYS
46	e	826	LEU
46	e	867	PHE
46	e	904	VAL
46	e	910	SER
46	e	924	VAL
46	e	933	LEU
46	e	978	THR
46	e	989	GLU
46	e	1032	LEU
46	e	1059	LEU
46	e	1102	CYS
46	e	1149	THR
46	e	1164	LEU
46	e	1175	PHE
46	e	1179	LEU
46	e	1189	ASN
46	e	1239	LYS
46	e	1269	LEU
46	e	1286	MET
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	1384	GLU
46	e	1400	PHE

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Mol	Chain	Res	Type
46	e	1407	MET
46	e	1421	LEU
46	e	1428	VAL
46	e	1454	ILE
46	e	1464	ILE
46	e	1490	SER
46	e	1508	CYS
46	e	1555	ARG
48	w	98	LYS
51	0	30	VAL
51	0	51	VAL
51	0	52	LEU
51	0	67	LEU
51	0	76	LEU
51	0	80	VAL
51	0	93	LEU
51	0	95	GLU
51	0	189	GLN
53	v	54	HIS
53	v	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	141	HIS
45	a	143	ASN
45	a	382	GLN
45	a	413	GLN
45	a	532	GLN
45	a	599	GLN
45	a	696	GLN
45	a	957	GLN
45	a	1003	GLN
46	e	79	ASN
46	e	160	ASN
46	e	189	ASN
46	e	226	ASN
46	e	233	ASN
46	e	251	ASN
46	e	805	ASN
46	e	902	ASN
46	e	1141	GLN

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Mol	Chain	Res	Type
46	e	1288	GLN
46	e	1455	GLN
46	e	1457	ASN
46	e	1477	GLN
46	e	1499	HIS
46	e	1501	GLN
47	g	9	ASN
51	0	36	GLN
53	v	52	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3211/3395 (94%)	591 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
49	x	72/76 (94%)	23 (31%)	0
49	y	71/76 (93%)	30 (42%)	0
All	All	3631/3826 (94%)	688 (18%)	0

All (688) RNA backbone outliers are listed below:

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type
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	2270	A
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A
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

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

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

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Mol	Chain	Res	Type
30	f	2814	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2834	G
30	f	2842	U
30	f	2844	C
30	f	2845	A
30	f	2849	C
30	f	2860	U
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2876	C
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2941	A
30	f	2942	C
30	f	2947	G
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A
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

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

Continued on next page...

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

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Mol	Chain	Res	Type
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	7	G
49	x	10	G
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	33	U
49	x	35	G
49	x	37	A
49	x	38	U
49	x	42	A

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Mol	Chain	Res	Type
49	x	43	G
49	x	46	G
49	x	48	C
49	x	49	U
49	x	56	C
49	x	57	G
49	x	59	U
49	x	60	U
49	x	61	C
49	x	74	C
49	y	7	G
49	y	8	U
49	y	9	G
49	y	13	U
49	y	16	U
49	y	17	C
49	y	22	G
49	y	23	C
49	y	25	C
49	y	26	G
49	y	28	U
49	y	34	A
49	y	35	G
49	y	36	C
49	y	38	U
49	y	42	A
49	y	43	G
49	y	44	A
49	y	46	G
49	y	47	U
49	y	48	C
49	y	56	C
49	y	58	A
49	y	59	U
49	y	60	U
49	y	61	C
49	y	68	C
49	y	71	C
49	y	75	C
49	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	$\# Z > 2$
53	5CT	v	51	53	13,14,15	0.76	0	9,15,17	1.29	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	5CT	v	51	53	-	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(°)
53	v	51	5CT	C4-C3-C2	-2.20	108.84	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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.

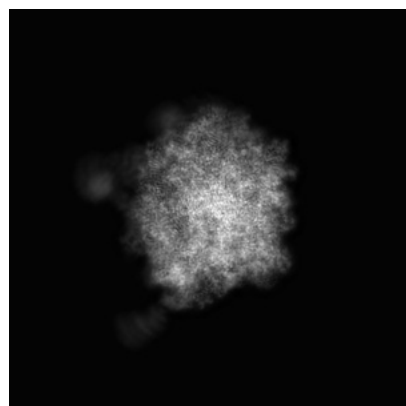
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15425. These allow visual inspection of the internal detail of the map and identification of artifacts.

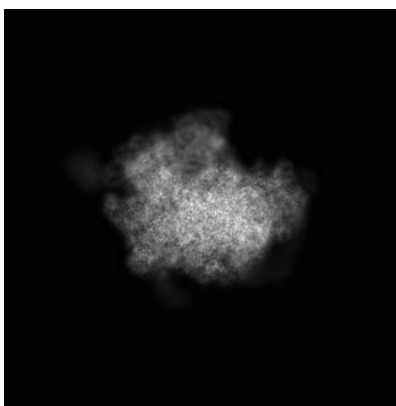
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

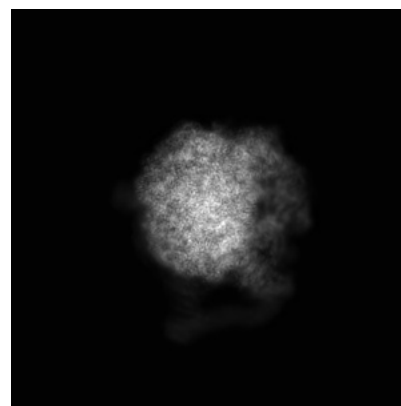
6.1.1 Primary map



X

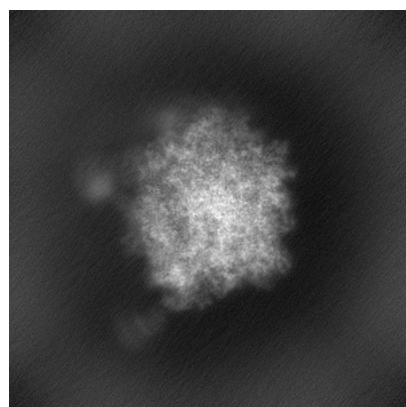


Y

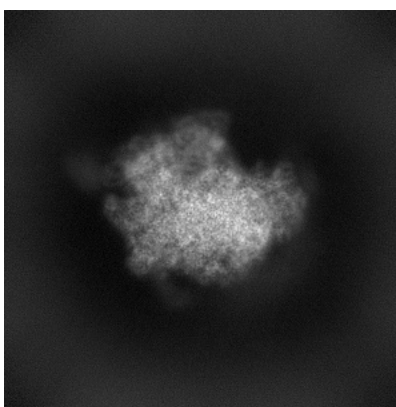


Z

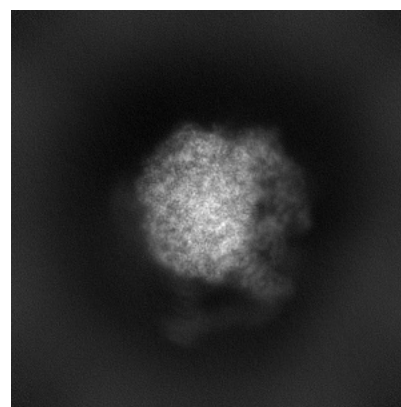
6.1.2 Raw map



X



Y

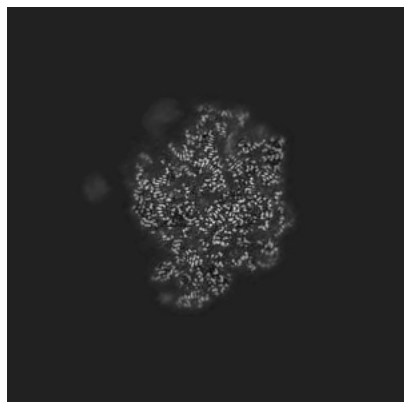


Z

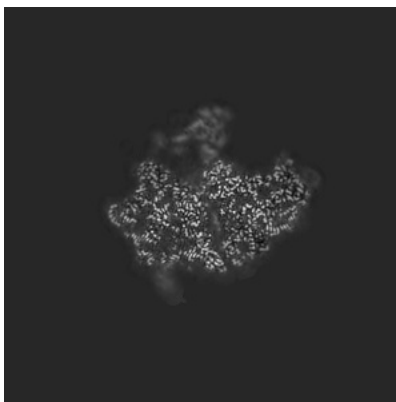
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

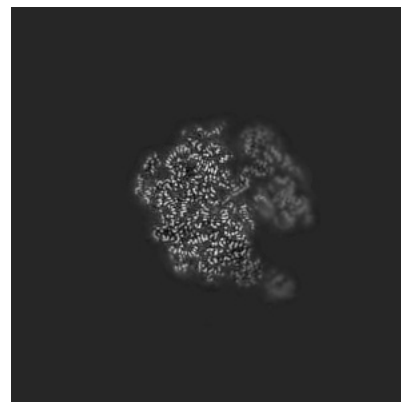
6.2.1 Primary map



X Index: 225

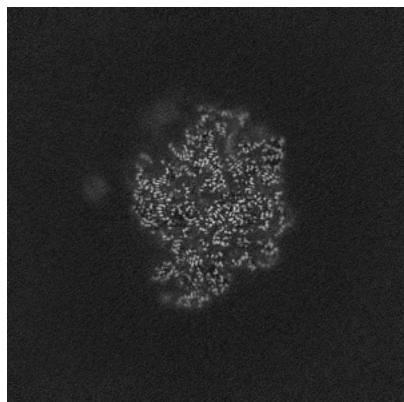


Y Index: 225

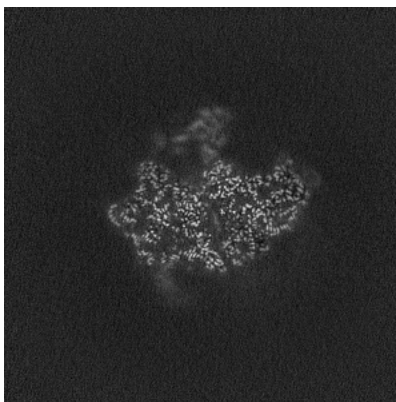


Z Index: 225

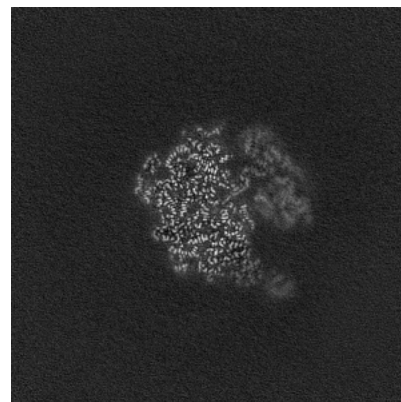
6.2.2 Raw map



X Index: 225



Y Index: 225

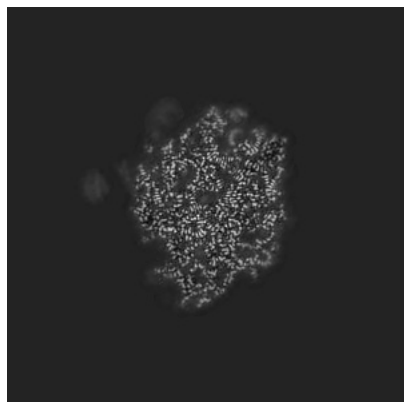


Z Index: 225

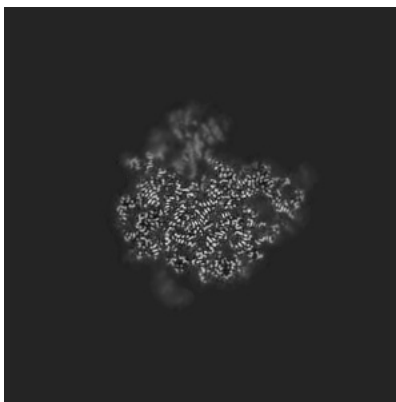
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

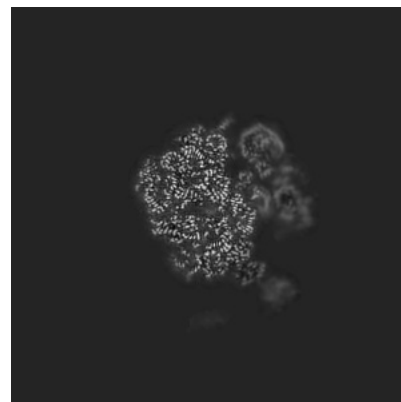
6.3.1 Primary map



X Index: 219

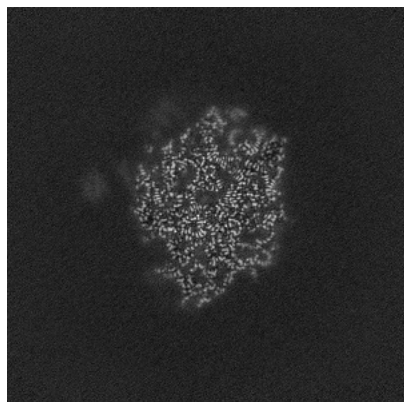


Y Index: 242

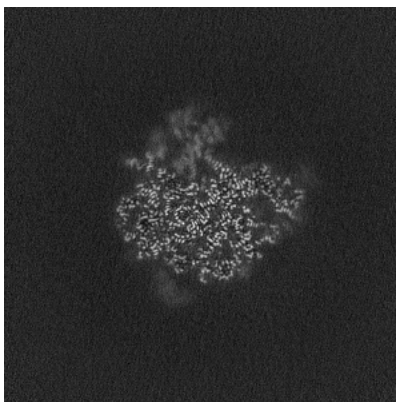


Z Index: 231

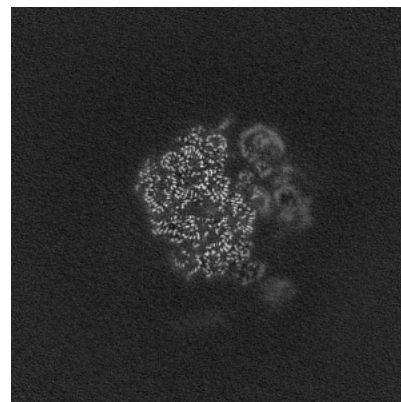
6.3.2 Raw map



X Index: 219



Y Index: 241

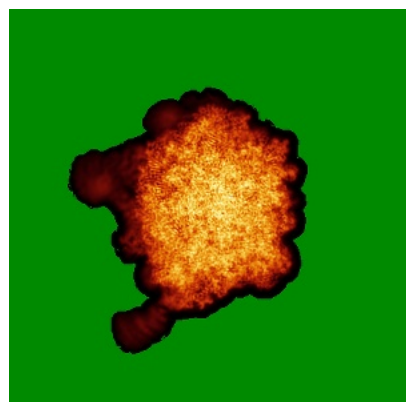


Z Index: 231

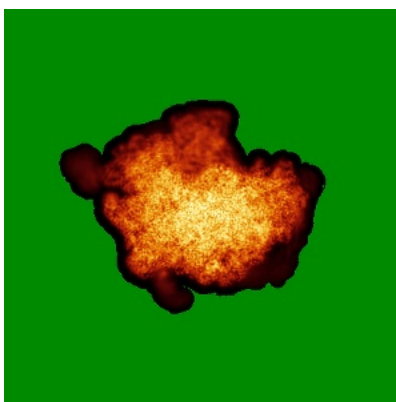
The images above show the largest variance slices of the map in three orthogonal directions.

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

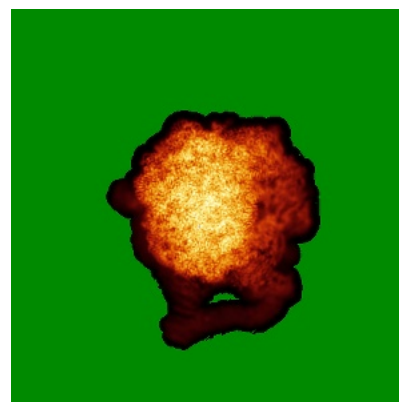
6.4.1 Primary map



X

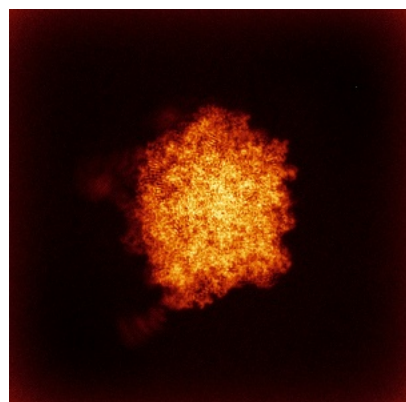


Y

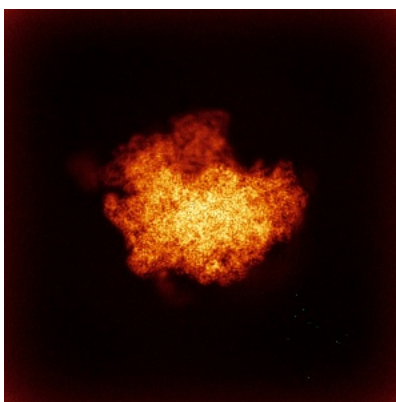


Z

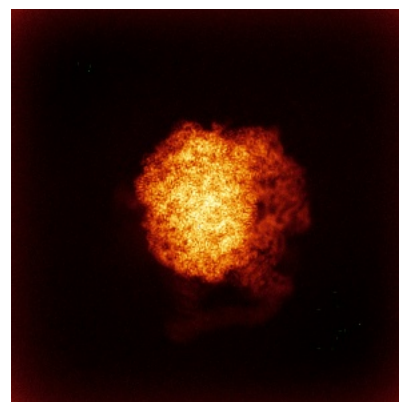
6.4.2 Raw map



X



Y



Z

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

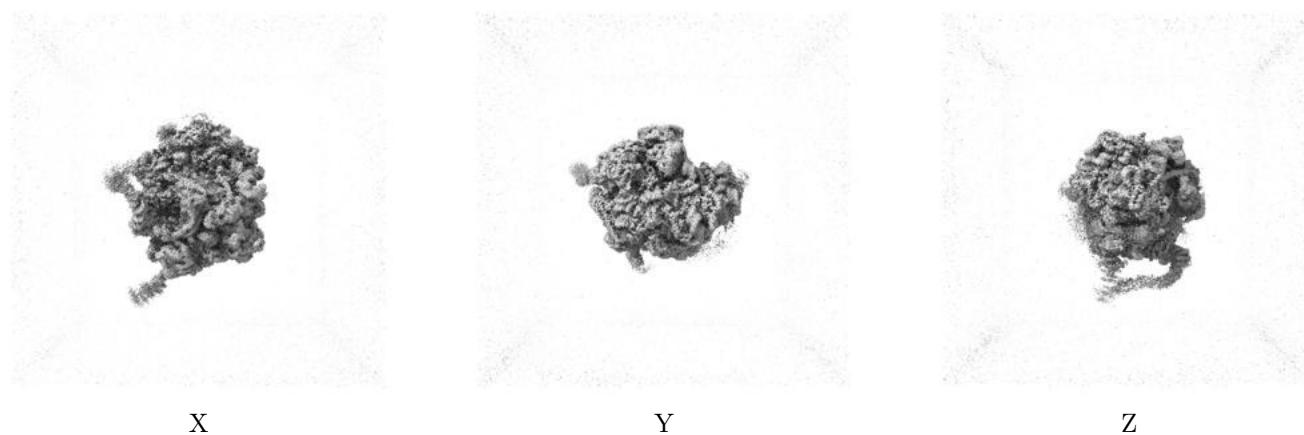
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

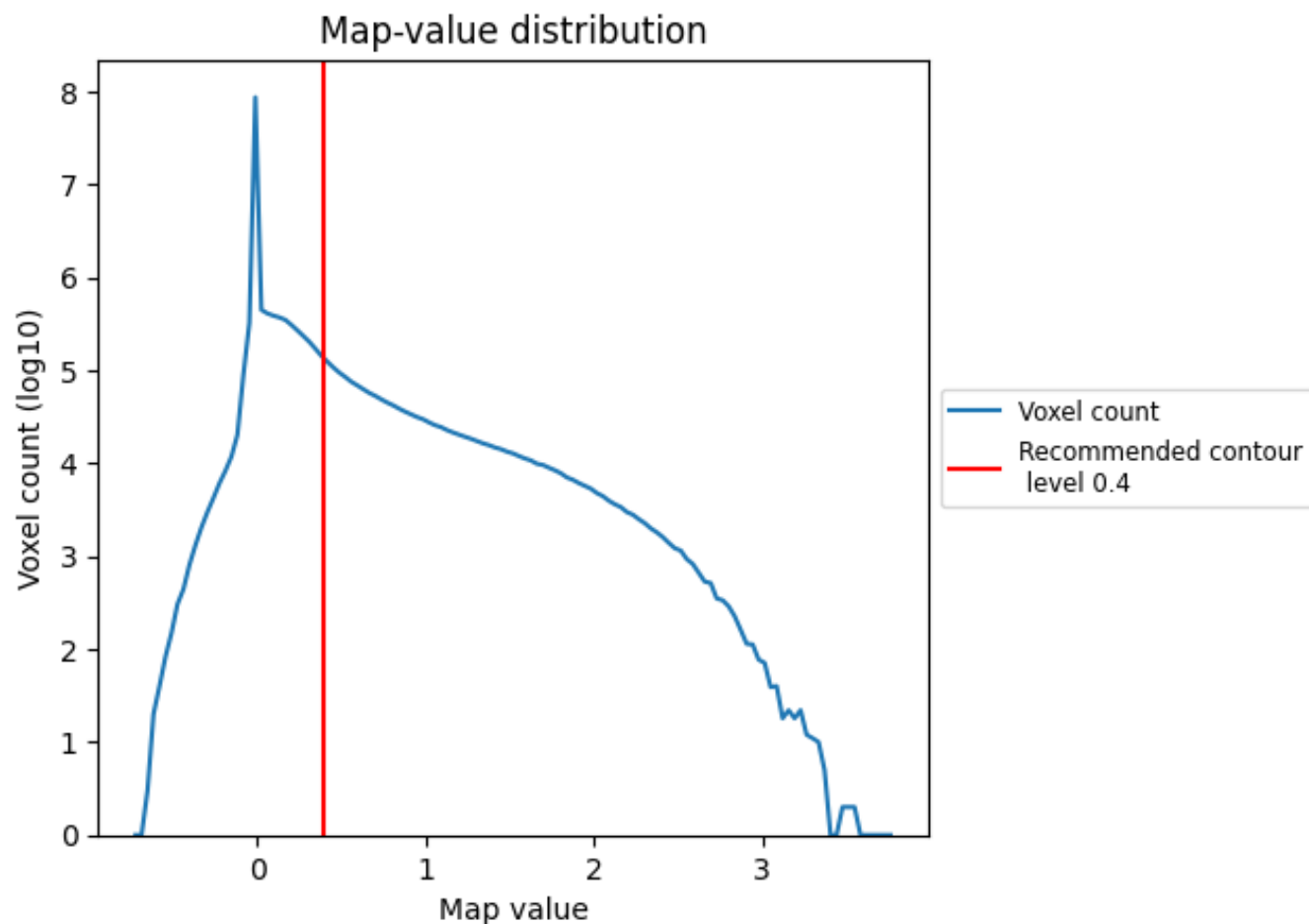
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

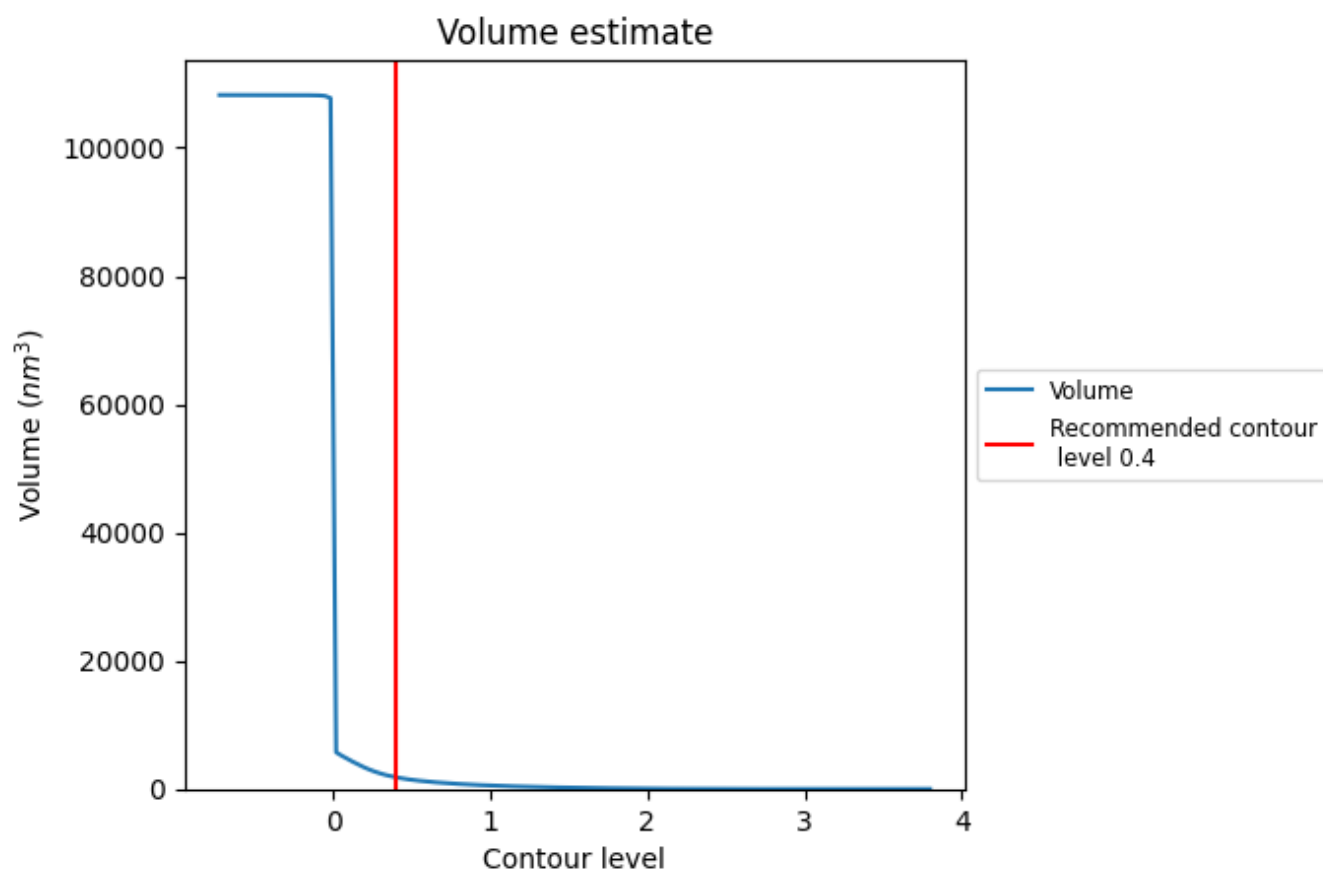
This section contains the results of statistical analysis of the map.

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.

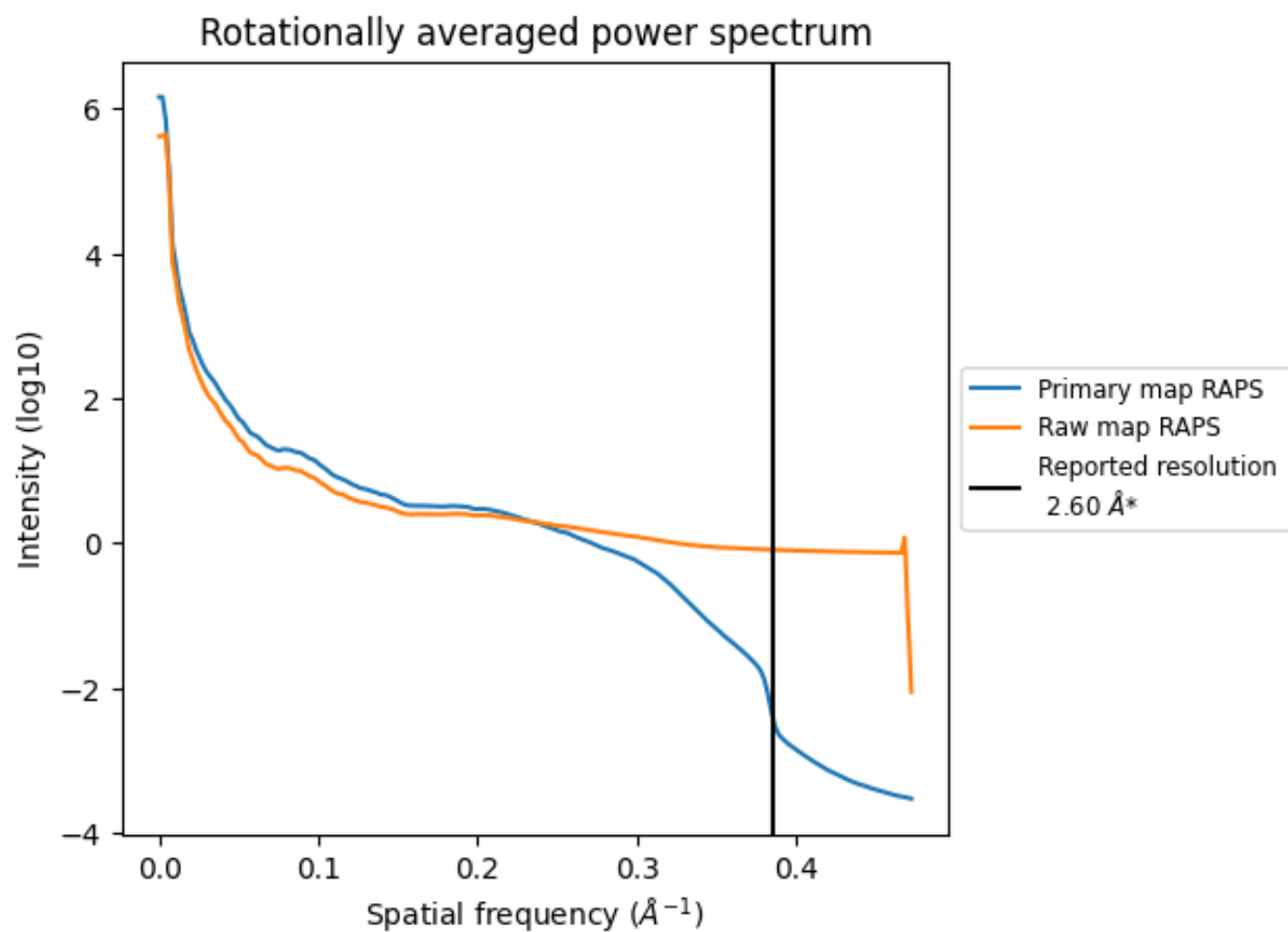
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1819 nm³; this corresponds to an approximate mass of 1643 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 ⓘ

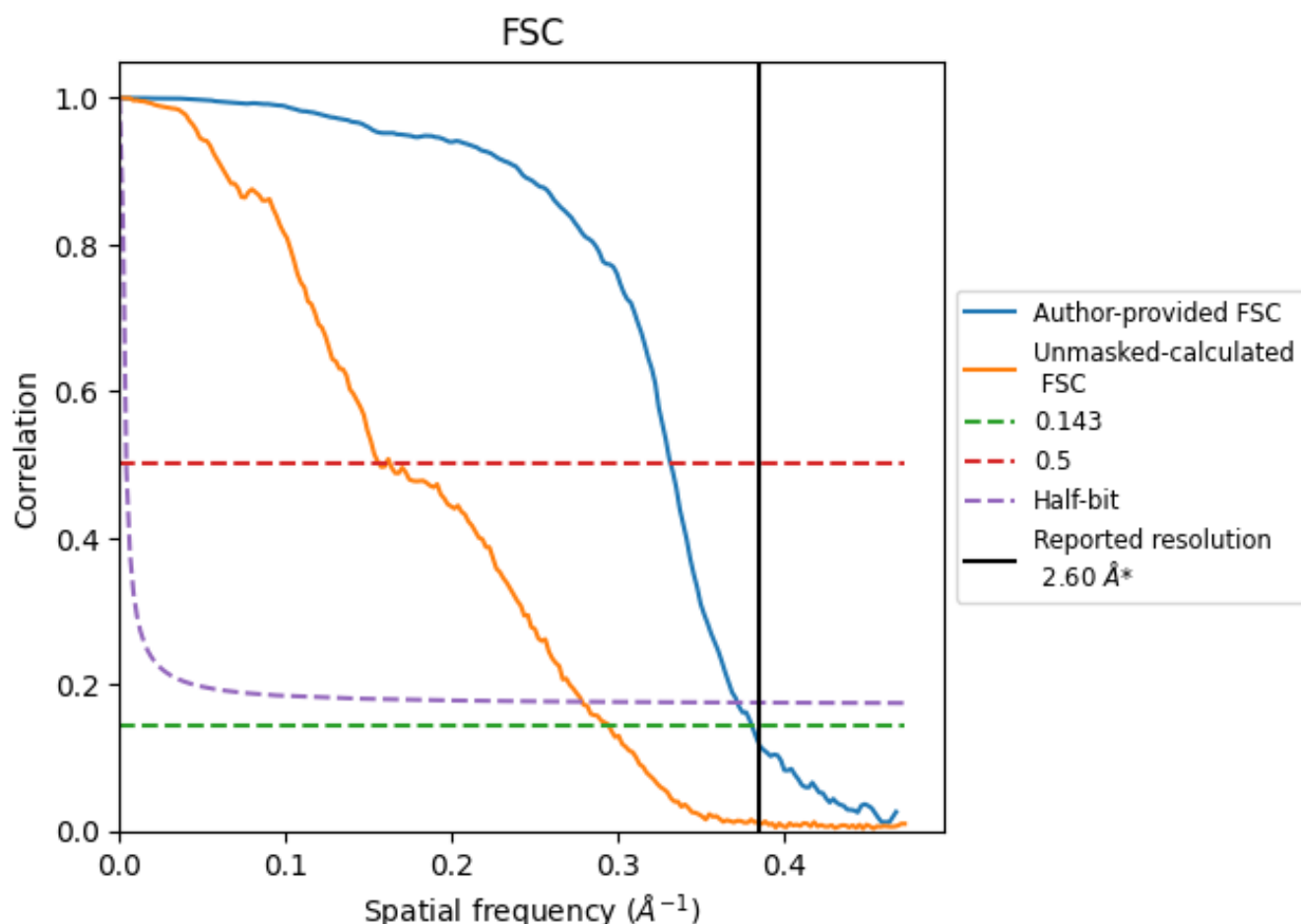


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

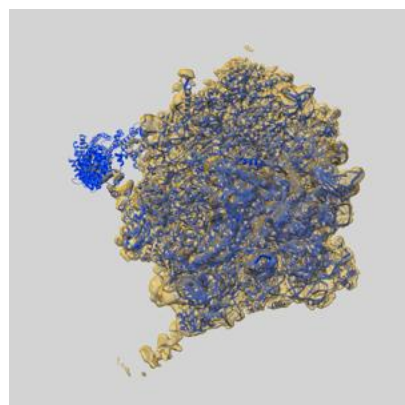
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.63	3.02	2.69
Unmasked-calculated*	3.40	6.40	3.59

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

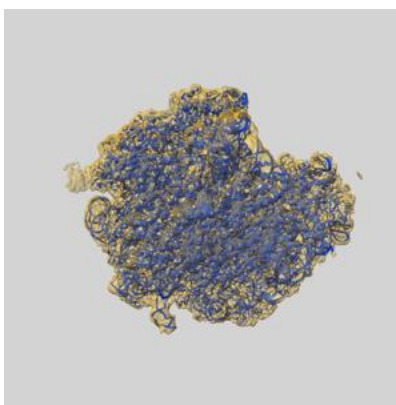
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15425 and PDB model 8AGV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

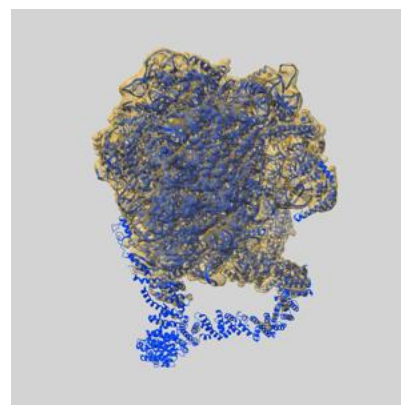
9.1 Map-model overlay [i](#)



X



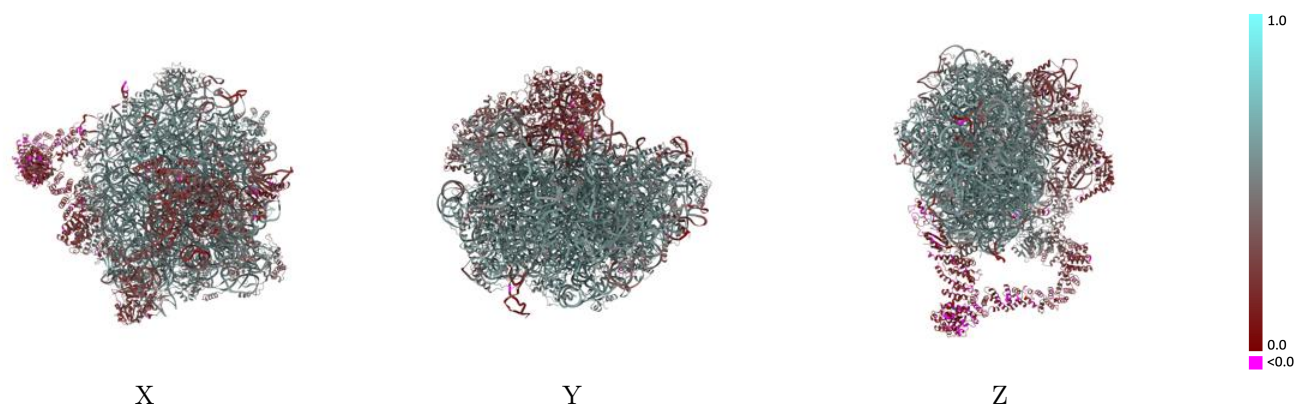
Y



Z

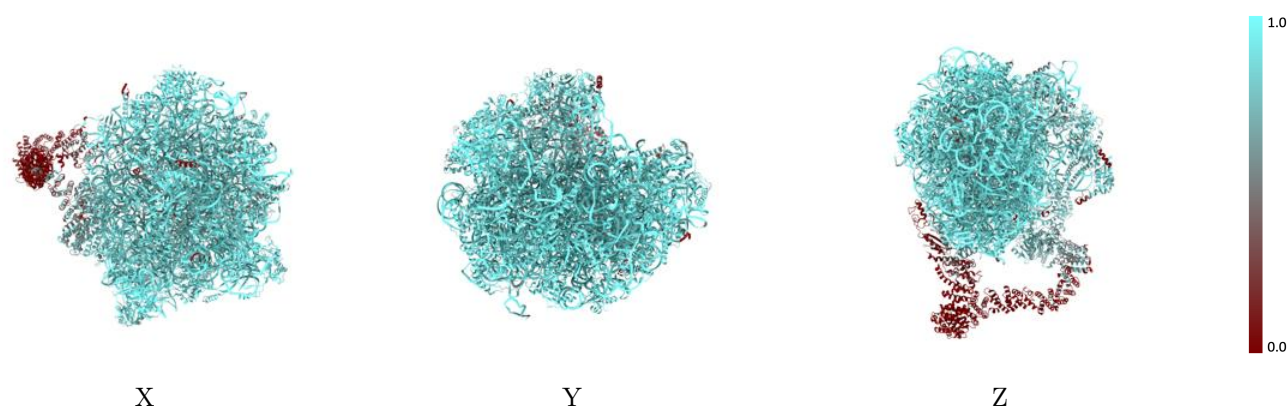
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



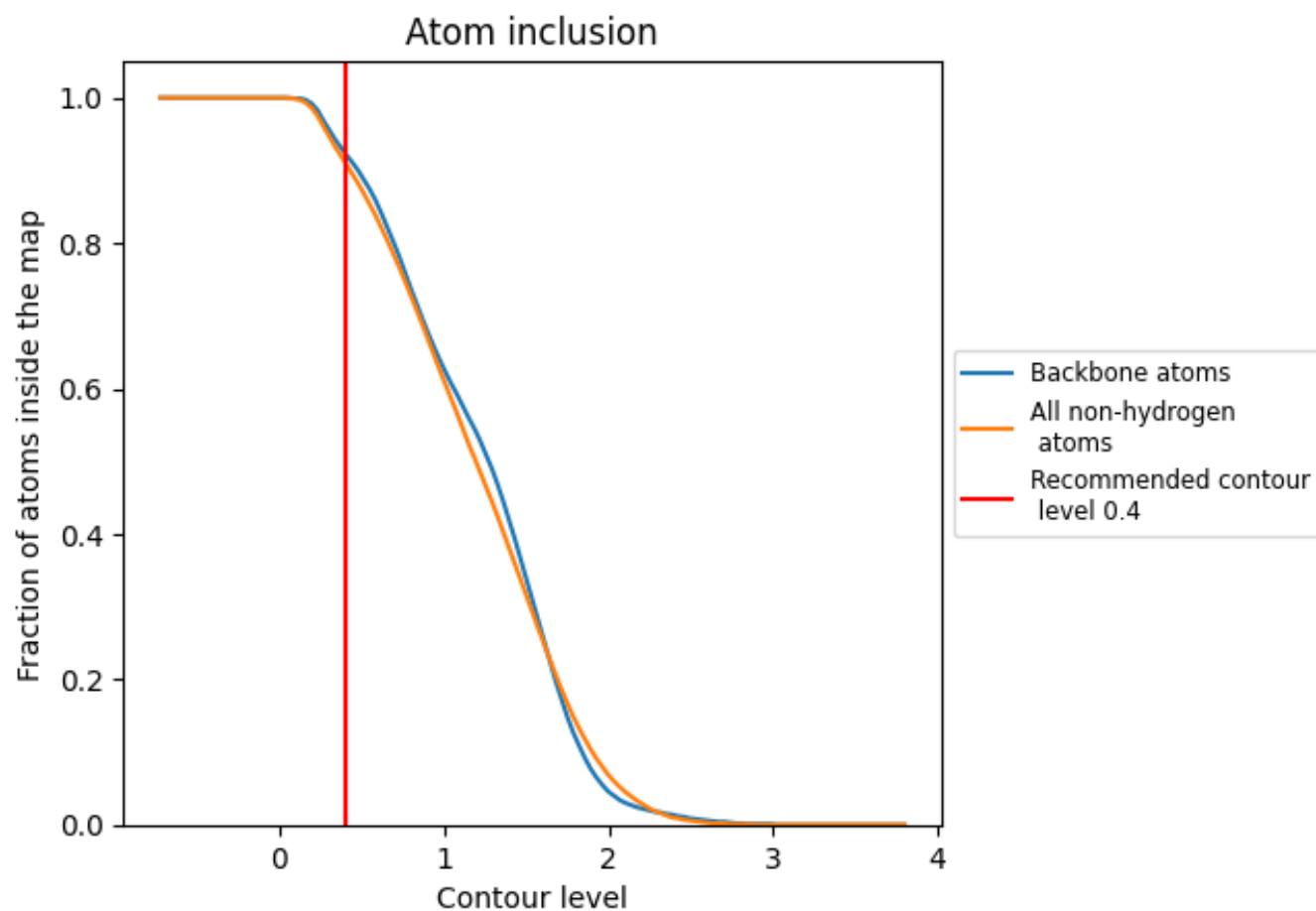
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5030
0	 0.8290	 0.2900
1	 1.0000	 0.4570
A	 0.9930	 0.6050
B	 0.9760	 0.5790
C	 0.9670	 0.5860
D	 0.9790	 0.5790
E	 0.9420	 0.5390
F	 0.9770	 0.5730
G	 0.9690	 0.5580
H	 0.9310	 0.4750
I	 0.9640	 0.5630
J	 0.9600	 0.5600
K	 0.9660	 0.5650
L	 0.9730	 0.5580
M	 0.9550	 0.5190
N	 0.9800	 0.5870
O	 0.9560	 0.5330
P	 0.9420	 0.5100
Q	 0.9250	 0.5480
R	 0.9810	 0.5950
S	 0.9900	 0.6120
T	 0.9660	 0.5690
U	 0.9670	 0.5480
V	 0.9570	 0.5200
W	 1.0000	 0.6200
X	 0.9200	 0.4970
Y	 0.9950	 0.5950
Z	 0.9670	 0.5650
a	 0.8080	 0.2780
b	 0.9640	 0.5640
c	 0.9720	 0.5620
d	 0.7130	 0.3910
e	 0.2590	 0.1800
f	 0.9910	 0.5650



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Chain	Atom inclusion	Q-score
g	 0.7570	 0.4630
h	 0.9990	 0.5600
i	 0.9950	 0.5920
j	 0.9860	 0.5960
k	 0.9790	 0.5810
l	 0.9760	 0.5680
m	 0.9350	 0.4780
n	 0.9450	 0.5190
o	 0.9690	 0.5640
p	 0.9410	 0.5120
q	 0.9590	 0.5410
r	 0.9530	 0.5300
s	 0.9250	 0.4200
t	 0.9670	 0.5540
u	 0.9680	 0.5400
v	 0.8470	 0.3530
w	 0.7890	 0.2020
x	 0.9770	 0.2800
y	 0.9760	 0.2610
z	 0.9130	 0.2760