



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 09:11 am BST

PDB ID : 9TI6 / pdb_00009ti6
EMDB ID : EMD-55945
Title : Staphylococcus aureus 70S ribosome with p/E tRNA and RRF oriented towards the LSU (postTC-RRF-LSU)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2025-12-05
Resolution : 2.62 Å (reported)
Based on initial models : ., 9GHG

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

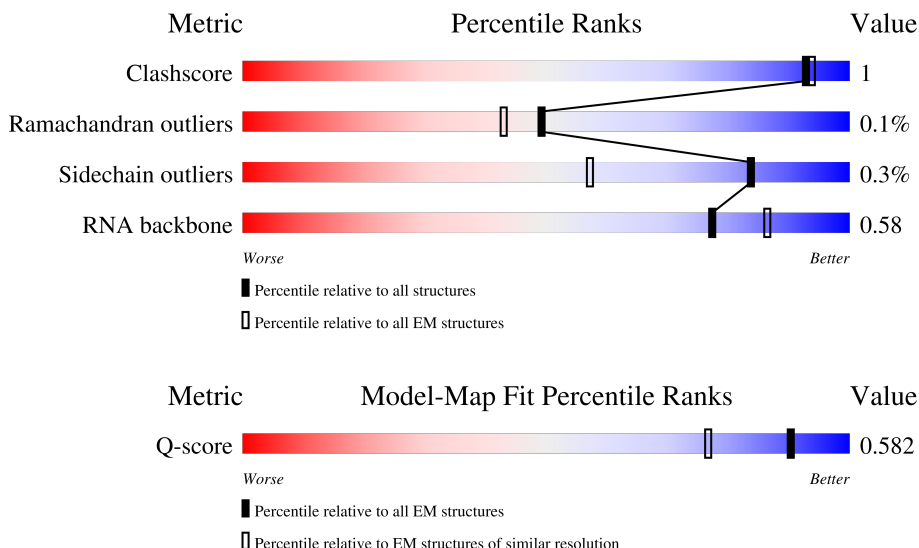
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

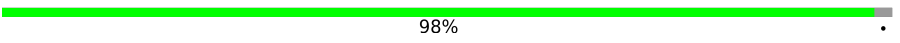
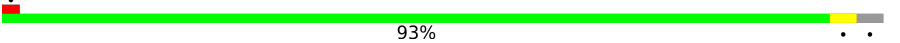
The reported resolution of this entry is 2.62 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8810 (2.12 - 3.12)

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	1	62	 98%
2	2	69	 88% 6% 6%
3	3	59	 93%

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Mol	Chain	Length	Quality of chain
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	
10	A	2923	
11	B	115	
12	C	186	
13	D	93	
14	G	277	
15	H	220	
16	I	207	
17	J	179	
18	K	178	
19	L	140	
20	M	145	
21	N	122	
22	O	146	
23	P	144	
24	Q	122	
25	R	119	
26	S	116	
27	T	118	
28	U	102	

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Mol	Chain	Length	Quality of chain
29	V	117	
30	W	91	
31	X	105	
32	Y	217	
33	Z	94	
34	a	1555	
35	b	24	
36	c	255	
37	d	217	
38	e	200	
39	f	166	
40	g	98	
41	h	156	
42	i	132	
43	j	132	
44	k	102	
45	l	129	
46	m	137	
47	n	121	
48	o	61	
49	p	89	
50	q	91	
51	r	87	
52	s	80	
53	t	92	

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Mol	Chain	Length	Quality of chain
54	u	83	 98%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142252 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 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			482	298	104	79	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	57	Total	C	N	O	0	0
			446	277	84	85		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	59	Total	C	N	O	S	0	0
			485	310	76	96	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	65	Total	C	N	O	S	0	0
			531	330	115	84	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2800	Total	C	N	O	P	0	0
			60048	26816	10994	19438	2800		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	183	Total	C	N	O	S	0	0
			1419	866	255	293	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q2FZ21
C	-1	HIS	-	expression tag	UNP Q2FZ21

- Molecule 13 is a RNA chain called tRNA(Ser3).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	D	93	Total	C	N	O	P	S	0	0
			2000	893	365	648	92	2		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	205	Total	C	N	O	S	0	0
			1569	983	287	297	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	177	Total	C	N	O	S	0	0
			1403	891	242	263	7		

- Molecule 18 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	175	Total	C	N	O	S	0	0
			1368	850	250	265	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	136	Total	C	N	O	S	0	0
			1010	635	175	195	5		

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	146	Total	C	N	O	S	0	0
			1099	680	215	203	1		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 26 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	S	114	Total	C	N	O		
			922	580	185	157	0	0

- Molecule 27 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	T	117	Total	C	N	O	S	
			953	599	191	159	4	0

- Molecule 28 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total	C	N	O	S	
			799	506	142	150	1	0

- Molecule 29 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	V	111	Total	C	N	O	S	
			853	532	163	155	3	0

- Molecule 30 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	90	Total	C	N	O	S	
			734	461	132	137	4	0

- Molecule 31 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	102	Total	C	N	O	S	
			787	497	144	144	2	0

- Molecule 32 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	94	Total	C	N	O	S	
			738	471	131	134	2	0

- Molecule 33 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	76	Total	C	N	O	0	0
			585	361	114	110		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1498	Total	C	N	O	P	0	0
			32104	14339	5863	10404	1498		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	18	Total	C	N	O	P	0	0
			396	177	82	119	18		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	204	Total	C	N	O	S	0	0
			1609	1012	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	157	Total	C	N	O	S	0	0
			1169	735	214	218	2		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	94	Total	C	N	O	S	0	0
			781	494	137	147	3		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	146	Total	C	N	O	S	0	0
			1165	727	222	212	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	98	Total	C	N	O	S	0	0
			783	494	143	145	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	118	Total	C	N	O	S	0	0
			877	542	166	166	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	114	Total	C	N	O	S	0	0
			909	559	180	169	1		

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	81	Total	C	N	O	S	0	0
			671	424	121	125	1		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	64	Total	C	N	O	S	0	0
			525	335	97	90	3		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	83	Total	C	N	O	S	0	0
			672	432	122	116	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	

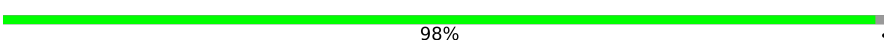
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	102	Total	Mg	0
			102	102	
56	G	1	Total	Mg	0
			1	1	
56	a	19	Total	Mg	0
			19	19	

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: 50S ribosomal protein L28

Chain 1:  98%

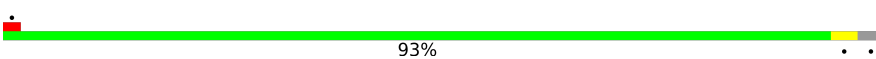


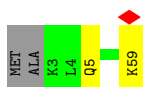
- Molecule 2: 50S ribosomal protein L29

Chain 2:  88% 6% 6%



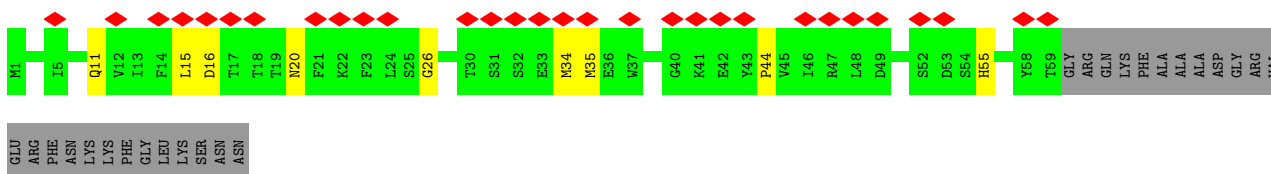
- Molecule 3: 50S ribosomal protein L30

Chain 3:  93%

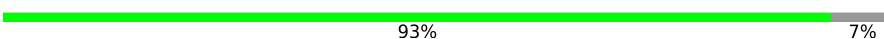


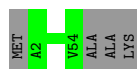
- Molecule 4: 50S ribosomal protein L31 type B

Chain 4:  36% 60% 11% 30%

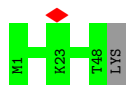


- Molecule 5: Large ribosomal subunit protein bL32

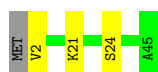
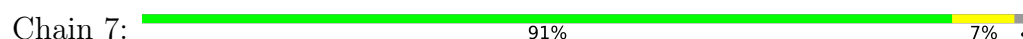
Chain 5:  93% 7%



- Molecule 6: Large ribosomal subunit protein bL33A



- Molecule 7: 50S ribosomal protein L34



- Molecule 8: 50S ribosomal protein L35

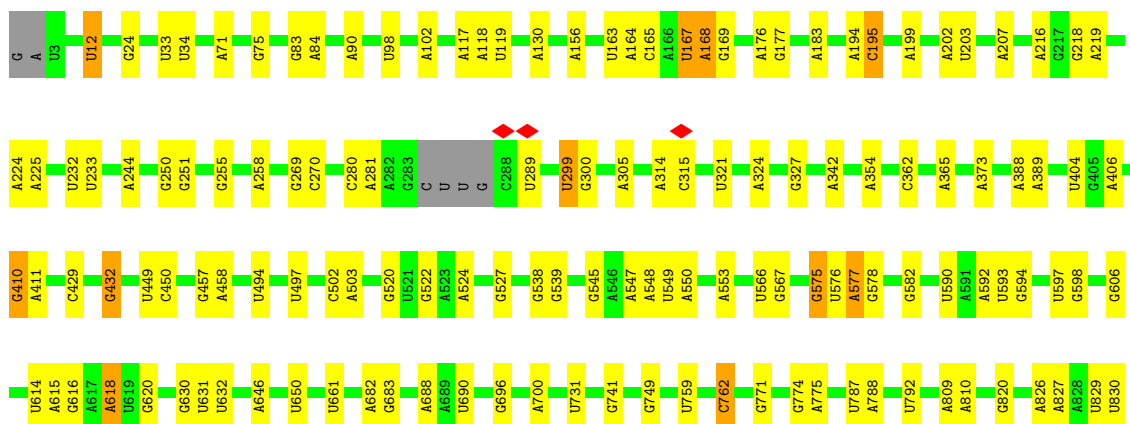
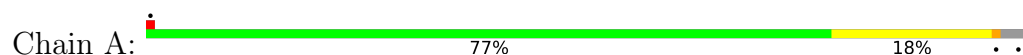


- Molecule 9: 50S ribosomal protein L36



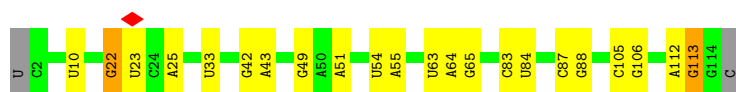
There are no outlier residues recorded for this chain.

- Molecule 10: 23S rRNA

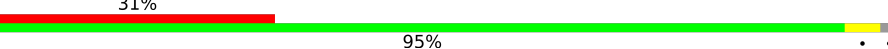


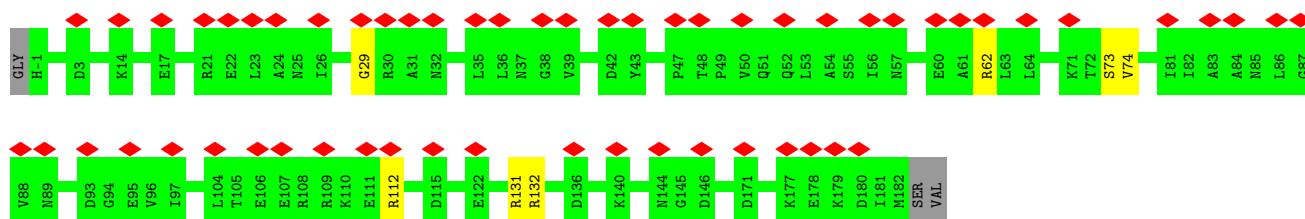


Chain B:  79% 17% ..



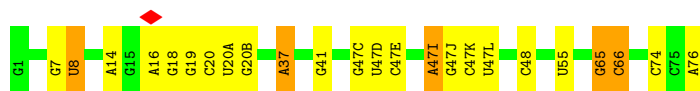
- Molecule 12: Ribosome-recycling factor

Chain C:  31% 95% ..

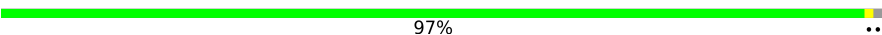


- Molecule 13: tRNA(Ser3)

Chain D:  74% 20% 5%

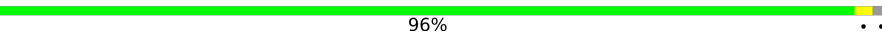


- Molecule 14: 50S ribosomal protein L2

Chain G:  97% ..



- Molecule 15: 50S ribosomal protein L3

Chain H:  96% ..



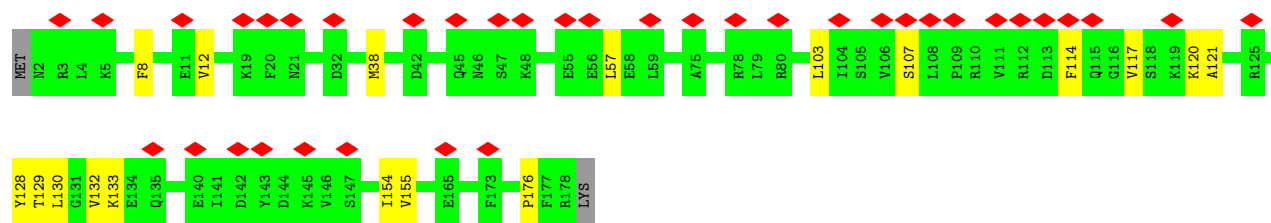
- Molecule 16: 50S ribosomal protein L4

Chain I:  96% ..

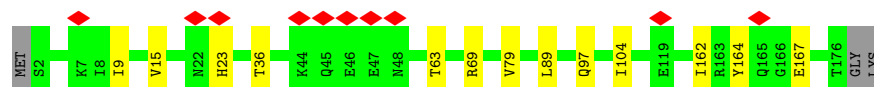
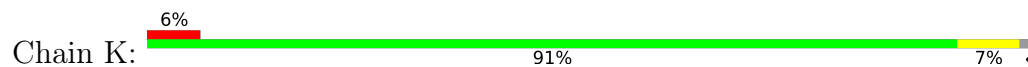


- Molecule 17: 50S ribosomal protein L5

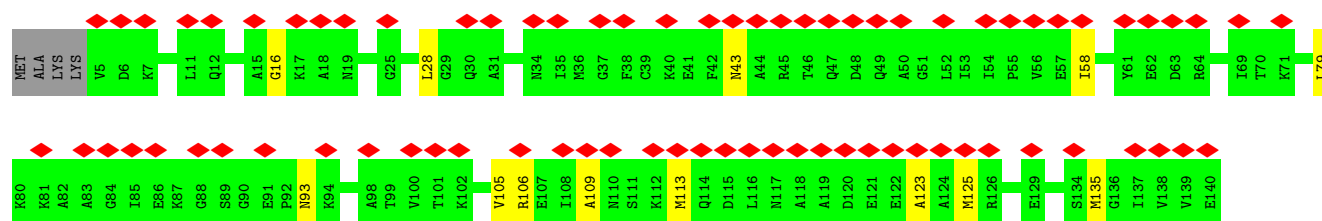
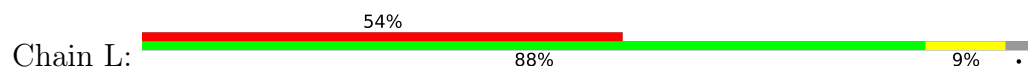
Chain J:  21% 89% 10% .



- Molecule 18: Large ribosomal subunit protein uL6



- Molecule 19: Large ribosomal subunit protein uL11



- Molecule 20: 50S ribosomal protein L13



- Molecule 21: 50S ribosomal protein L14

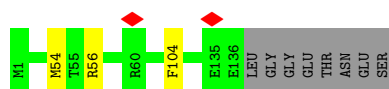


- Molecule 22: 50S ribosomal protein L15

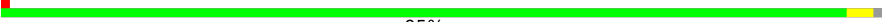


- Molecule 23: 50S ribosomal protein L16

Chain P:  92% • 6%

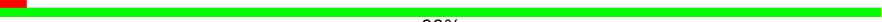


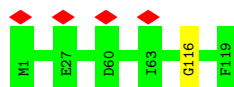
- Molecule 24: 50S ribosomal protein L17

Chain Q:  95% • •



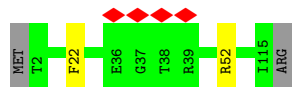
- Molecule 25: 50S ribosomal protein L18

Chain R:  99% •

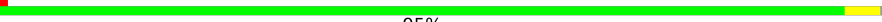


- Molecule 26: 50S ribosomal protein L19

Chain S:  97% • •



- Molecule 27: 50S ribosomal protein L20

Chain T:  95% • •



- Molecule 28: 50S ribosomal protein L21

Chain U:  100%

There are no outlier residues recorded for this chain.

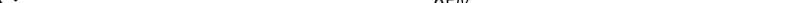
- Molecule 29: 50S ribosomal protein L22

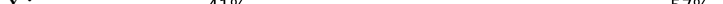
Chain V:  89% 6% 5%



- Molecule 30: 50S ribosomal protein L23

Diagram illustrating a protein structure with residues MET, E2, A3, R4, M56, and N91. A red diamond is positioned above the N91 residue.

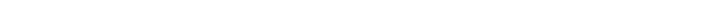
- Chain X:  7% 95% ...

- Chain Y:  41% 57%

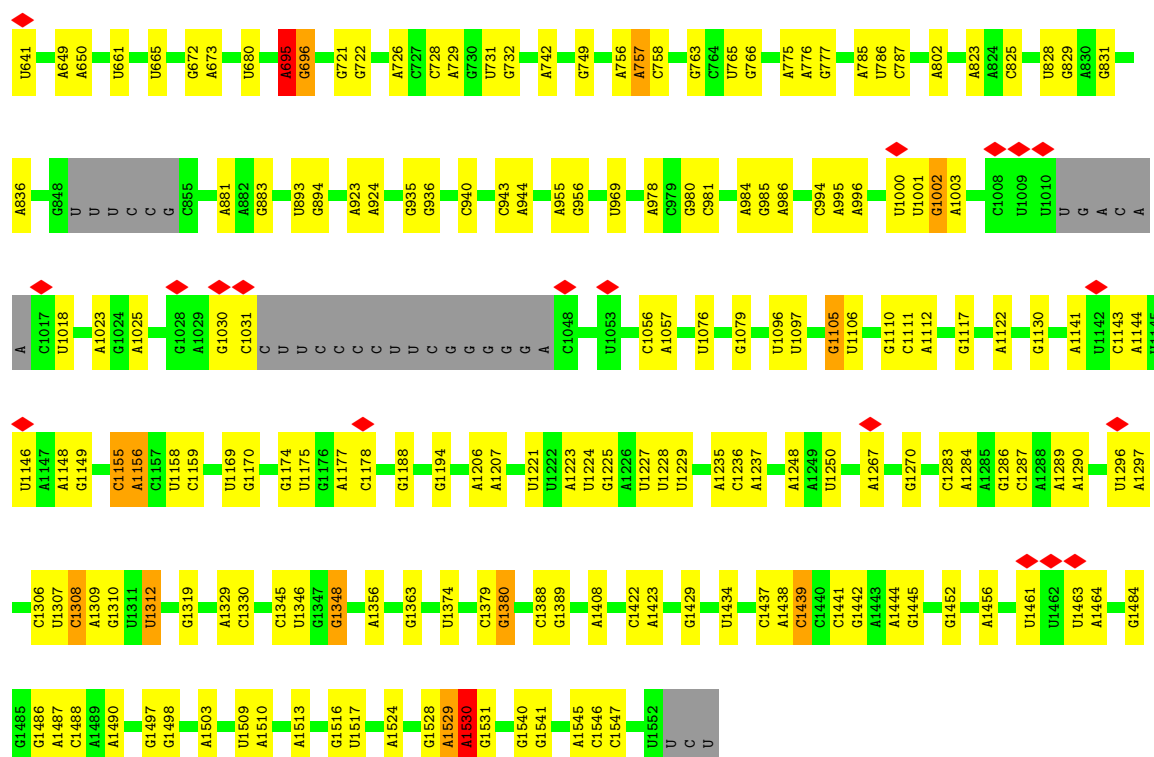
GLU	GLU	PRO	GLU	GLU	VAL	VAL	GLY	GLU	SER	LYS	GLU	ASP	GLU	GLU	LYS	THR	GLU	GLU	GLU	GLN	PRO	THR	GLU	ASN	LEU	GLU	VAL	THR	ALA	THR	GLY	GLN	ASP	ASN	ILE	THR	GLN	THR		
ALA	ILE	GLU	VAL	ASP	ILE	THR	GLU	LEU	ASN	ILE	ASN	ASP	SER	LEU	THR	VAL	ALA	ASP	VAL	LYS	ILE	GLU	ASN	ASP	VAL	VAL	THR	VAL	VAL	VAL	THR	GLU	PRO	THR	ALA	THR	GLN	THR		
MET	ALA	S3	I7	V43	V65	I70	M73	T94	N95	N96	SER	GLU	GLU	ARG	THR	GLU	VAL	VAL	PRO	GLN	LEU	VAL	GLY	GLY	VAL	GLU	GLN	PRO	LEU	PHE	ASN	LEU	GLU	VAL	THR	ALA	THR	GLN	PRO	GLU

- Chain Z:  81% 19%

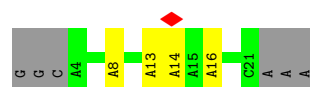
MET
LEU
LYS
LEU
ASN
LEU
GLN
PHE
PHE
ALA
SER
LYS
LYS
GLY
VAL
SER
SER
T18
A93
GLU

- Chain a:  76% 18% ..

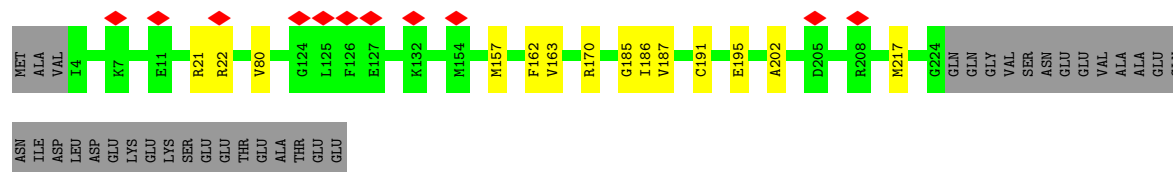
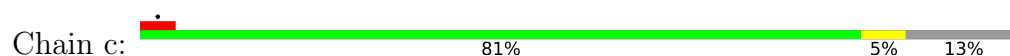
Category	Item	Value	Color
A	A456	100	Orange
	A457	100	Orange
	A458	100	Green
	A459	100	Green
	A460	100	Green
	A461	100	Yellow
	A462	100	Yellow
	A463	100	Yellow
	A464	100	Yellow
	A465	100	Yellow
B	B466	100	Yellow
	B467	100	Yellow
	B468	100	Yellow
	B469	100	Yellow
	B470	100	Yellow
	B471	100	Yellow
	B472	100	Yellow
	B473	100	Yellow
	B474	100	Yellow
	B475	100	Yellow
C	C476	100	Yellow
	C477	100	Yellow
	C478	100	Yellow
	C479	100	Yellow
	C480	100	Yellow
	C481	100	Yellow
	C482	100	Yellow
	C483	100	Yellow
	C484	100	Yellow
	C485	100	Yellow
D	D486	100	Yellow
	D487	100	Yellow
	D488	100	Yellow
	D489	100	Yellow
	D490	100	Yellow
	D491	100	Yellow
	D492	100	Yellow
	D493	100	Yellow
	D494	100	Yellow
	D495	100	Yellow
E	E496	100	Yellow
	E497	100	Yellow
	E498	100	Yellow
	E499	100	Yellow
	E500	100	Yellow
	E501	100	Yellow
	E502	100	Yellow
	E503	100	Yellow
	E504	100	Yellow
	E505	100	Yellow
F	F506	100	Yellow
	F507	100	Yellow
	F508	100	Yellow
	F509	100	Yellow
	F510	100	Yellow
	F511	100	Yellow
	F512	100	Yellow
	F513	100	Yellow
	F514	100	Yellow
	F515	100	Yellow
G	G516	100	Yellow
	G517	100	Yellow
	G518	100	Yellow
	G519	100	Yellow
	G520	100	Yellow
	G521	100	Yellow
	G522	100	Yellow
	G523	100	Yellow
	G524	100	Yellow
	G525	100	Yellow
H	H526	100	Yellow
	H527	100	Yellow
	H528	100	Yellow
	H529	100	Yellow
	H530	100	Yellow
	H531	100	Yellow
	H532	100	Yellow
	H533	100	Yellow
	H534	100	Yellow
	H535	100	Yellow
I	I536	100	Yellow
	I537	100	Yellow
	I538	100	Yellow
	I539	100	Yellow
	I540	100	Yellow
	I541	100	Yellow
	I542	100	Yellow
	I543	100	Yellow
	I544	100	Yellow
	I545	100	Yellow
J	J546	100	Yellow
	J547	100	Yellow
	J548	100	Yellow
	J549	100	Yellow
	J550	100	Yellow
	J551	100	Yellow
	J552	100	Yellow
	J553	100	Yellow
	J554	100	Yellow
	J555	100	Yellow
K	K556	100	Yellow
	K557	100	Yellow
	K558	100	Yellow
	K559	100	Yellow
	K560	100	Yellow
	K561	100	Yellow
	K562	100	Yellow
	K563	100	Yellow
	K564	100	Yellow
	K565	100	Yellow
L	L566	100	Yellow
	L567	100	Yellow
	L568	100	Yellow
	L569	100	Yellow
	L570	100	Yellow
	L571	100	Yellow
	L572	100	Yellow
	L573	100	Yellow
	L574	100	Yellow
	L575	100	Yellow
M	M576	100	Yellow
	M577	100	Yellow
	M578	100	Yellow
	M579	100	Yellow
	M580	100	Yellow
	M581	100	Yellow
	M582	100	Yellow
	M583	100	Yellow
	M584	100	Yellow
	M585	100	Yellow
N	N586	100	Yellow
	N587	100	Yellow
	N588	100	Yellow
	N589	100	Yellow
	N590	100	Yellow
	N591	100	Yellow
	N592	100	Yellow
	N593	100	Yellow
	N594	100	Yellow
	N595	100	Yellow
O	O596	100	Yellow
	O597	100	Yellow
	O598	100	Yellow
	O599	100	Yellow
	O600		



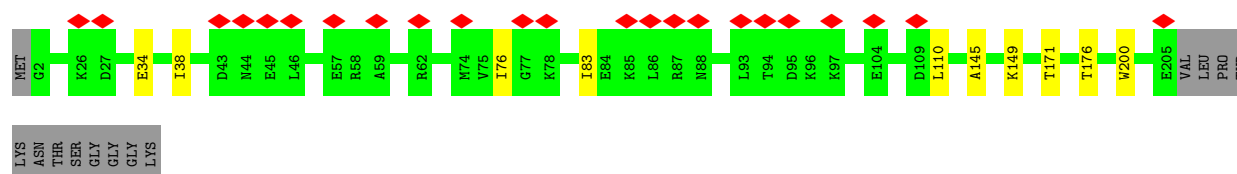
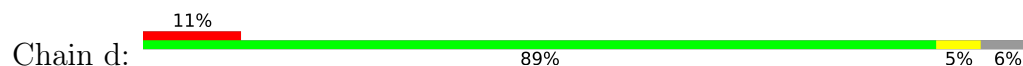
- Molecule 35: mRNA



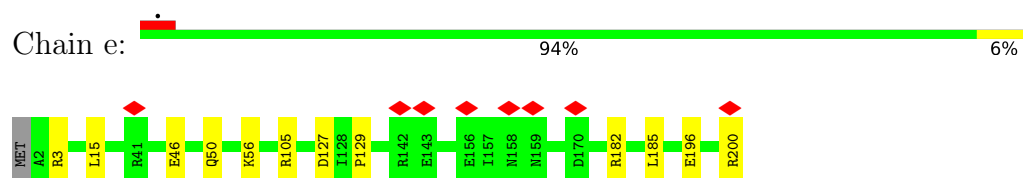
- Molecule 36: 30S ribosomal protein S2



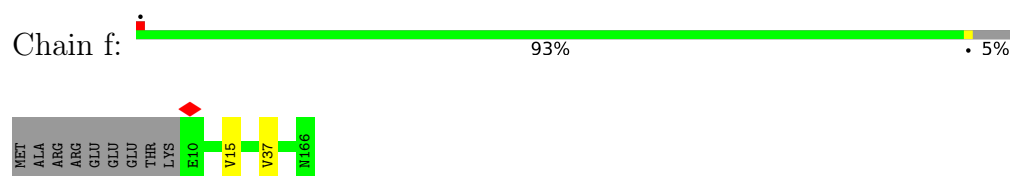
- Molecule 37: 30S ribosomal protein S3



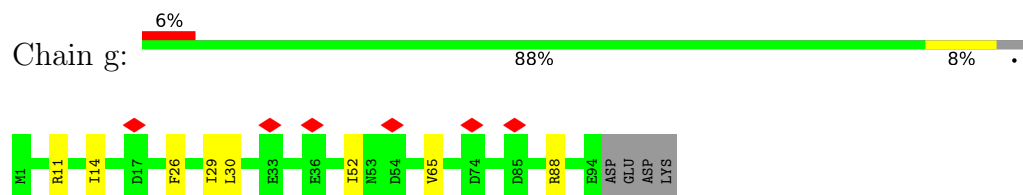
- Molecule 38: 30S ribosomal protein S4



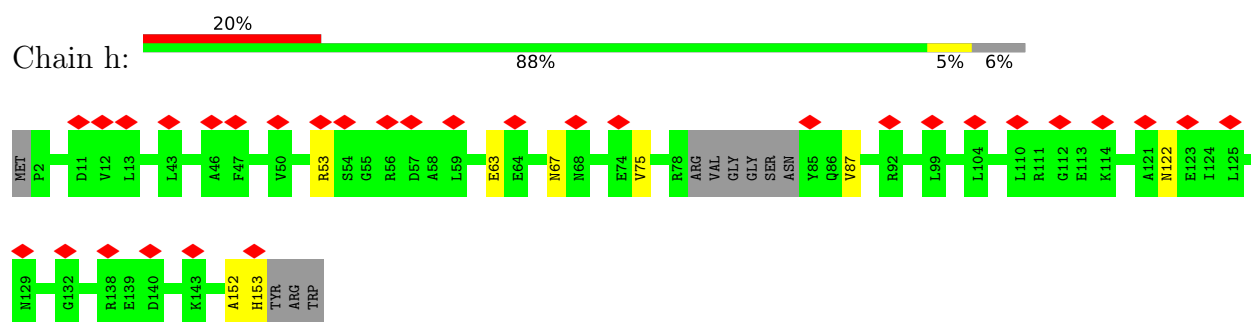
- Molecule 39: 30S ribosomal protein S5



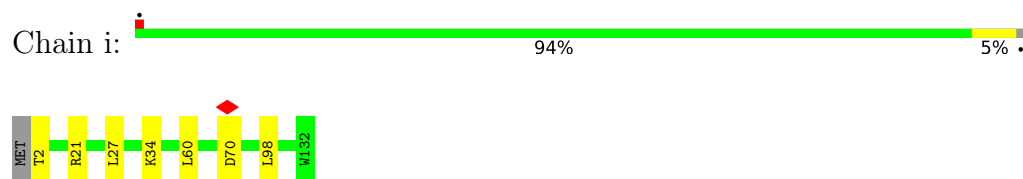
- Molecule 40: 30S ribosomal protein S6



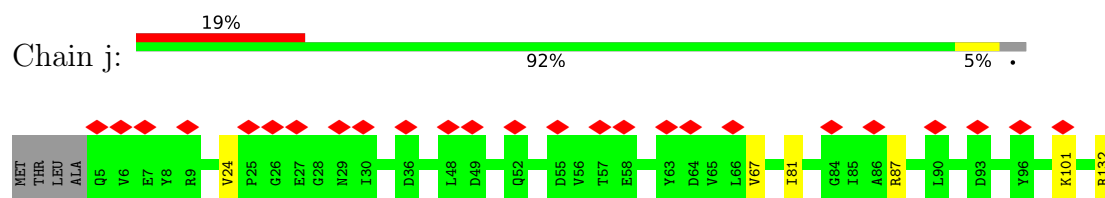
- Molecule 41: 30S ribosomal protein S7



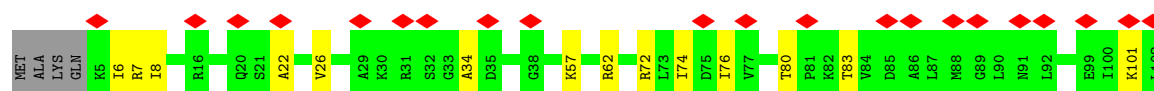
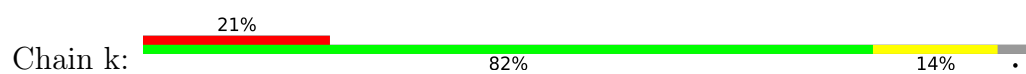
- Molecule 42: 30S ribosomal protein S8



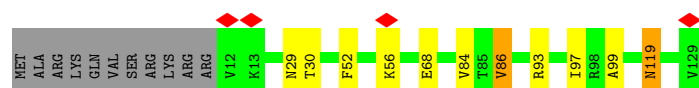
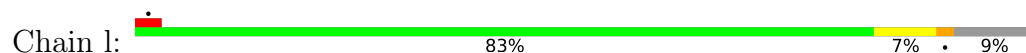
- Molecule 43: 30S ribosomal protein S9



- Molecule 44: Small ribosomal subunit protein uS10



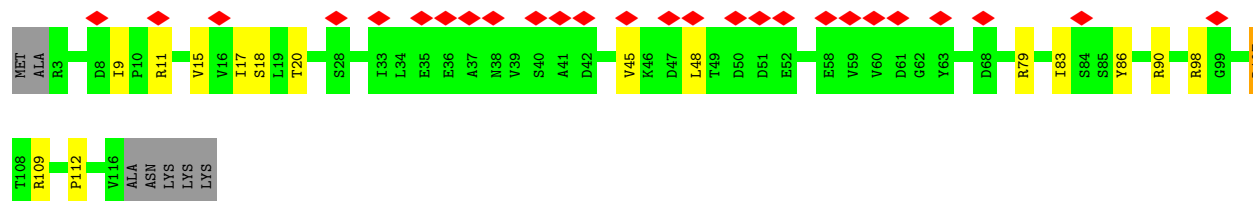
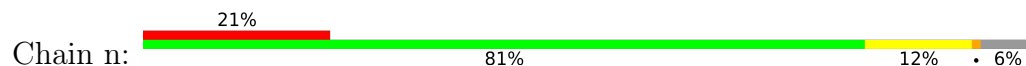
- Molecule 45: 30S ribosomal protein S11



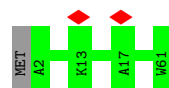
- Molecule 46: 30S ribosomal protein S12



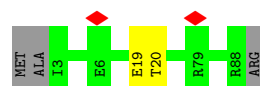
- Molecule 47: 30S ribosomal protein S13



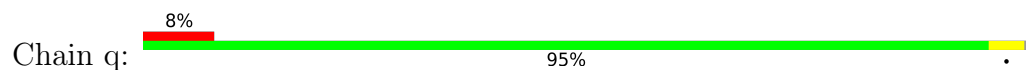
- Molecule 48: 30S ribosomal protein S14 type Z

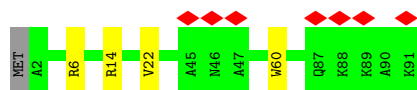


- Molecule 49: 30S ribosomal protein S15

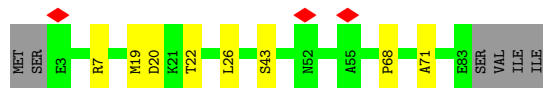
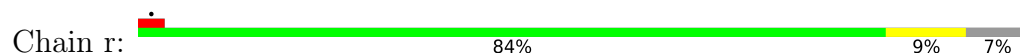


- Molecule 50: 30S ribosomal protein S16

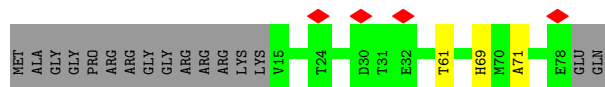
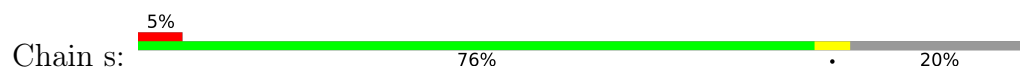




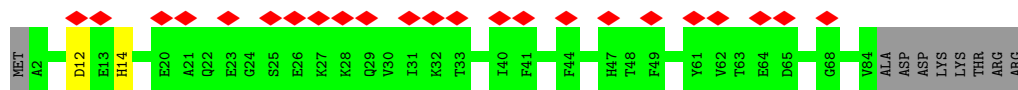
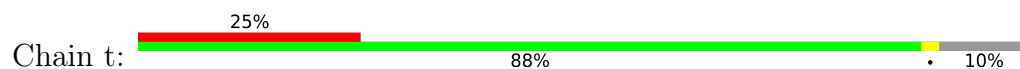
- Molecule 51: 30S ribosomal protein S17



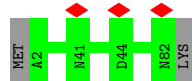
- Molecule 52: 30S ribosomal protein S18



- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	28.403	Depositor
Minimum map value	-16.229	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.953	Depositor
Recommended contour level	2.2	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.672, 0.672, 0.672	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, 5MC, OMG, G7M, 5MU, 2MG, 2MA, MA6, 4SU, 3TD, H2U, ZN, MG, PSU, 4OC, RSP, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.49	0/488	0.82	0/649
2	2	0.45	0/536	1.06	0/713
3	3	0.49	0/448	0.96	0/601
4	4	0.52	0/499	0.92	0/674
5	5	0.51	0/429	0.87	0/571
6	6	0.46	0/407	0.87	0/545
7	7	0.51	0/377	0.98	0/491
8	8	0.50	0/536	0.91	0/701
9	9	0.53	0/300	0.85	0/393
10	A	0.54	1/67024 (0.0%)	0.79	10/104521 (0.0%)
11	B	0.56	0/2692	0.76	0/4193
12	C	0.48	0/1428	1.05	0/1922
13	D	0.58	1/2088 (0.0%)	0.78	0/3255
14	G	0.51	0/2120	0.88	0/2847
15	H	0.49	0/1652	0.88	0/2216
16	I	0.49	0/1592	0.93	0/2148
17	J	0.48	0/1421	0.98	0/1907
18	K	0.50	0/1386	0.93	0/1865
19	L	0.53	0/1024	1.01	0/1384
20	M	0.49	0/1173	0.87	0/1578
21	N	0.49	0/927	0.89	0/1243
22	O	0.50	0/1113	0.91	0/1482
23	P	0.49	0/1113	0.89	0/1493
24	Q	0.46	0/956	0.96	0/1277
25	R	0.48	0/931	0.96	0/1244
26	S	0.50	0/934	0.86	0/1249
27	T	0.47	0/965	1.02	0/1276
28	U	0.49	0/809	0.82	0/1080
29	V	0.51	0/861	0.90	0/1159
30	W	0.47	0/742	0.91	0/989
31	X	0.51	0/796	0.91	0/1063

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.48	0/746	0.89	0/1000
33	Z	0.49	0/591	0.89	0/785
34	a	0.55	2/35762 (0.0%)	0.77	2/55757 (0.0%)
35	b	0.57	0/446	0.76	0/695
36	c	0.48	0/1808	1.00	0/2426
37	d	0.48	0/1631	0.94	0/2190
38	e	0.49	0/1647	0.96	0/2211
39	f	0.51	0/1183	0.93	0/1595
40	g	0.46	0/792	0.92	0/1062
41	h	0.50	0/1181	1.04	0/1587
42	i	0.48	0/1044	0.92	0/1401
43	j	0.50	0/1033	0.95	0/1386
44	k	0.52	0/795	0.97	0/1071
45	l	0.55	0/892	0.94	0/1203
46	m	0.52	0/1075	0.87	0/1439
47	n	0.49	0/916	1.07	0/1228
48	o	0.48	0/512	0.92	0/678
49	p	0.48	0/730	1.02	0/975
50	q	0.49	0/723	0.95	0/971
51	r	0.47	0/679	0.90	0/907
52	s	0.48	0/534	0.98	0/716
53	t	0.51	0/690	0.96	0/926
54	u	0.47	0/611	1.09	0/817
All	All	0.53	4/153788 (0.0%)	0.83	12/229755 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	I	0	1
29	V	0	1
31	X	0	1
38	e	0	1
40	g	0	1
43	j	0	1
44	k	0	1
46	m	0	1
47	n	0	1
51	r	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	535	G7M	O3'-P	5.16	1.61	1.56
13	D	37	T6A	O3'-P	5.14	1.61	1.56
10	A	2601	G7M	O3'-P	5.02	1.61	1.56
34	a	1509	UR3	O3'-P	5.00	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2673	C	O3'-P-O5'	-7.15	93.28	104.00
10	A	1962	G	O3'-P-O5'	-6.12	94.81	104.00
10	A	1275	A	O3'-P-O5'	-5.86	95.21	104.00
10	A	1812	A	O3'-P-O5'	-5.62	95.58	104.00
10	A	244	A	O3'-P-O5'	-5.57	95.65	104.00
10	A	207	A	O3'-P-O5'	-5.54	95.68	104.00
10	A	2077	C	O3'-P-O5'	-5.54	95.68	104.00
10	A	826	A	O3'-P-O5'	-5.53	95.71	104.00
34	a	1488	C	O3'-P-O5'	-5.23	96.16	104.00
10	A	299	U	O3'-P-O5'	-5.14	96.29	104.00
10	A	2851	G	O3'-P-O5'	-5.06	96.41	104.00
34	a	695	A	C2'-C3'-O3'	5.04	117.06	109.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	I	168	ARG	Sidechain
29	V	92	ARG	Sidechain
31	X	92	ARG	Sidechain
38	e	105	ARG	Sidechain
40	g	88	ARG	Sidechain
43	j	132	ARG	Sidechain
44	k	62	ARG	Sidechain
46	m	12	ARG	Sidechain
47	n	107	ARG	Sidechain
51	r	7	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	482	0	523	0	0
2	2	535	0	566	2	0
3	3	446	0	486	1	0
4	4	485	0	458	5	0
5	5	422	0	426	0	0
6	6	402	0	413	0	0
7	7	373	0	420	2	0
8	8	531	0	599	2	0
9	9	297	0	339	0	0
10	A	60048	0	30201	122	0
11	B	2408	0	1218	3	0
12	C	1419	0	1450	5	0
13	D	2000	0	1020	9	0
14	G	2085	0	2192	3	0
15	H	1628	0	1667	3	0
16	I	1569	0	1614	3	0
17	J	1403	0	1457	8	0
18	K	1368	0	1399	7	0
19	L	1010	0	1047	7	0
20	M	1151	0	1145	4	0
21	N	920	0	981	2	0
22	O	1099	0	1142	4	0
23	P	1089	0	1155	2	0
24	Q	952	0	999	2	0
25	R	922	0	968	0	0
26	S	922	0	994	1	0
27	T	953	0	1027	4	0
28	U	799	0	836	0	0
29	V	853	0	914	4	0
30	W	734	0	767	2	0
31	X	787	0	853	1	0
32	Y	738	0	787	5	0
33	Z	585	0	597	0	0
34	a	32104	0	16179	90	0
35	b	396	0	197	1	0
36	c	1781	0	1844	7	0
37	d	1609	0	1668	6	0
38	e	1617	0	1646	8	0
39	f	1169	0	1229	1	0
40	g	781	0	784	4	0
41	h	1165	0	1204	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	i	1032	0	1082	3	0
43	j	1017	0	1039	3	0
44	k	783	0	825	6	0
45	l	877	0	895	7	0
46	m	1058	0	1130	6	0
47	n	909	0	959	10	0
48	o	502	0	523	0	0
49	p	721	0	751	1	0
50	q	712	0	744	3	0
51	r	671	0	708	6	0
52	s	525	0	554	3	0
53	t	672	0	677	2	0
54	u	611	0	655	0	0
55	5	1	0	0	0	0
55	9	1	0	0	0	0
55	o	1	0	0	0	0
56	A	102	0	0	0	0
56	G	1	0	0	0	0
56	a	19	0	0	0	0
All	All	142252	0	95953	329	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 1.

All (329) 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)
10:A:1968:C:O2	12:C:131:ARG:NH2	2.21	0.74
32:Y:7:ILE:HD11	32:Y:65:VAL:HA	1.69	0.72
34:a:695:A:O2'	34:a:696:G:OP2	2.11	0.68
51:r:26:LEU:HD11	51:r:43:SER:HB3	1.78	0.66
34:a:384:G:H5''	50:q:6:ARG:HB2	1.82	0.62
10:A:2715:G:OP1	10:A:2740:A:N6	2.32	0.62
34:a:831:G:HO2'	42:i:2:THR:N	1.98	0.61
10:A:575:G:O2'	10:A:577:A:N7	2.32	0.60
40:g:30:LEU:HB3	40:g:65:VAL:HG11	1.82	0.60
46:m:135:PRO:O	46:m:136:LYS:C	2.44	0.59
10:A:788:A:OP1	15:H:144:GLY:HA2	2.01	0.59
7:7:2:VAL:N	10:A:1663:G:HO2'	2.00	0.59
47:n:11:ARG:HA	47:n:45:VAL:HB	1.84	0.58
34:a:1117:G:H5''	37:d:171:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:37:T6A:N1	13:D:37:T6A:N11	2.46	0.58
34:a:728:C:O2'	52:s:61:THR:HG21	2.04	0.57
17:J:117:VAL:HG22	17:J:176:PRO:O	2.03	0.57
34:a:777:G:H4'	34:a:1524:A:H4'	1.85	0.57
13:D:65:G:O2'	13:D:66:C:OP1	2.23	0.57
34:a:411:C:H5''	38:e:129:PRO:HD2	1.87	0.57
42:i:21:ARG:NH1	42:i:70:ASP:O	2.38	0.57
10:A:83:G:H21	10:A:102:A:H2	1.53	0.56
13:D:74:C:O4'	13:D:74:C:O2	2.24	0.56
10:A:1756:U:H2'	10:A:1757:U:O4'	2.05	0.56
4:4:55:HIS:NE2	17:J:114:PHE:HB3	2.21	0.56
34:a:995:A:H2'	34:a:996:A:O4'	2.06	0.55
44:k:6:ILE:HB	44:k:76:ILE:HB	1.88	0.55
10:A:12:U:H2'	10:A:12:U:O2	2.06	0.55
10:A:1109:U:H2'	10:A:1110:U:O4'	2.07	0.55
10:A:2040:A:OP1	29:V:97:ASN:N	2.35	0.55
34:a:1306:C:H4'	34:a:1312:U:O4	2.06	0.55
43:j:67:VAL:HG11	43:j:81:ILE:HG12	1.88	0.54
47:n:9:ILE:HG23	47:n:18:SER:HB3	1.89	0.54
10:A:922:G:H22	10:A:944:G:P	2.30	0.54
20:M:1:MET:O	27:T:93:LYS:NZ	2.31	0.54
41:h:152:ALA:O	41:h:153:HIS:C	2.51	0.54
10:A:2774:G:O6	10:A:2782:C:H5''	2.07	0.53
10:A:1111:A:H4'	10:A:1112:G:OP1	2.08	0.53
32:Y:73:MET:HB2	32:Y:94:ILE:HD11	1.91	0.53
10:A:1149:U:H2'	10:A:1150:A:C8	2.43	0.53
10:A:923:A:H1'	10:A:924:G:O5'	2.08	0.53
13:D:47(K):C:H2'	13:D:47(L):U:O4'	2.09	0.53
34:a:726:A:H5'	45:l:119:ASN:HB2	1.91	0.53
10:A:1648:C:O2'	10:A:1654:A:N1	2.39	0.53
10:A:167:U:H2'	10:A:168:A:O4'	2.09	0.52
34:a:491:C:O2'	50:q:14:ARG:NH2	2.42	0.52
34:a:756:A:H1'	34:a:757:A:H2	1.74	0.52
10:A:1828:U:OP2	14:G:150:LYS:NZ	2.39	0.52
10:A:1357:G:C2	10:A:1366:U:H5''	2.45	0.51
19:L:79:LEU:HD23	19:L:135:MET:SD	2.51	0.51
34:a:665:U:H3	34:a:757:A:H62	1.58	0.51
10:A:2355:A:H2'	10:A:2356:A:C8	2.46	0.51
44:k:7:ARG:HB2	44:k:101:LYS:HB2	1.91	0.51
10:A:620:G:O2'	10:A:1292:A:OP1	2.28	0.51
10:A:1513:A:H2'	10:A:1514:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:26:C:H5'	34:a:532:G:H1'	1.92	0.50
10:A:2687:A:H2'	10:A:2688:G:O4'	2.11	0.50
32:Y:7:ILE:C	32:Y:7:ILE:HD12	2.36	0.50
32:Y:65:VAL:HB	32:Y:70:ILE:HD13	1.93	0.50
34:a:1158:U:H2'	34:a:1159:C:O4'	2.11	0.50
3:3:5:GLN:HB2	3:3:59:LYS:HD2	1.93	0.50
34:a:1079:G:N7	34:a:1105:G:H2'	2.27	0.50
10:A:788:A:O2'	10:A:1703:U:OP1	2.29	0.50
34:a:627:U:H5	38:e:127:ASP:HB3	1.77	0.50
10:A:892:U:H5	10:A:977:A:N1	2.10	0.50
40:g:26:PHE:HA	40:g:29:ILE:HD12	1.94	0.50
44:k:8:ILE:N	44:k:74:ILE:O	2.45	0.50
34:a:786:U:H2'	34:a:787:C:O4'	2.12	0.49
10:A:1959:A:H2'	10:A:1960:G:O4'	2.13	0.49
10:A:1806:U:H5	10:A:1811:A:N7	2.11	0.49
35:b:13:A:H2'	35:b:14:A:C8	2.48	0.49
14:G:107:PRO:HD2	14:G:110:LEU:HD22	1.95	0.49
34:a:756:A:H1'	34:a:757:A:C2	2.48	0.49
34:a:1002:G:O2'	34:a:1003:A:N7	2.45	0.49
10:A:631:U:H2'	10:A:632:U:C6	2.48	0.49
10:A:903:G:N3	10:A:2295:A:H2'	2.28	0.49
10:A:1996:A:O2'	10:A:1999:G:N3	2.40	0.49
34:a:1545:A:H2'	34:a:1546:C:O4'	2.11	0.49
34:a:1422:C:H2'	34:a:1423:A:C8	2.48	0.49
10:A:582:G:OP1	10:A:1039:C:N4	2.46	0.48
34:a:1025:A:HO2'	34:a:1227:U:HO2'	1.60	0.48
10:A:84:A:N1	10:A:98:U:O2'	2.39	0.48
10:A:852:U:O2	16:I:74:ARG:NH2	2.47	0.48
10:A:902:A:N6	10:A:903:G:C6	2.81	0.48
10:A:955:A:H2'	10:A:956:A:C8	2.48	0.48
10:A:2335:G:N3	10:A:2335:G:H2'	2.28	0.48
10:A:2776:A:H1'	18:K:63:THR:HG22	1.94	0.48
13:D:47(D):U:H2'	13:D:47(E):C:O4'	2.14	0.48
10:A:1572:G:N2	10:A:1593:G:O6	2.46	0.48
34:a:9:A:C5	38:e:200:ARG:HB3	2.48	0.48
34:a:9:A:N6	38:e:196:GLU:O	2.46	0.48
34:a:1486:G:H2'	34:a:1487:A:O4'	2.13	0.48
45:l:84:VAL:HG11	45:l:97:ILE:HG12	1.96	0.48
34:a:1497:G:H2'	34:a:1498:G:C8	2.49	0.48
20:M:18:VAL:HG23	20:M:138:PRO:HB2	1.96	0.48
34:a:1155:C:H4'	34:a:1156:A:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:18:U:H2'	34:a:19:C:C6	2.49	0.47
10:A:2672:G:H4'	10:A:2759:G:O2'	2.14	0.47
34:a:100:A:O5'	34:a:100:A:H8	1.97	0.47
34:a:5:A:O2'	34:a:7:G:N7	2.42	0.47
34:a:641:U:H2'	34:a:641:U:O2	2.15	0.47
8:8:54:ASP:OD1	8:8:57:ARG:NH2	2.45	0.47
10:A:1038:C:OP1	27:T:53:ARG:NH2	2.48	0.47
10:A:2053:U:H2'	10:A:2054:G:O4'	2.14	0.47
34:a:317:G:O2'	34:a:615:A:N1	2.45	0.47
10:A:164:A:H2'	10:A:165:C:O4'	2.14	0.47
34:a:757:A:H2'	34:a:758:C:O4'	2.13	0.47
47:n:45:VAL:HA	47:n:48:LEU:HG	1.96	0.47
10:A:1125:U:H4'	19:L:123:ALA:HB1	1.95	0.47
10:A:1757:U:H2'	10:A:1758:A:H5''	1.97	0.47
36:c:157:MET:HE2	36:c:157:MET:HA	1.96	0.47
49:p:19:GLU:O	49:p:20:THR:OG1	2.26	0.47
21:N:35:ILE:HG21	21:N:103:ALA:HB3	1.97	0.47
44:k:34:ALA:HB2	44:k:83:THR:HG21	1.97	0.47
34:a:68:C:H2'	34:a:69:G:C8	2.49	0.47
34:a:262:G:O2'	51:r:20:ASP:O	2.33	0.47
10:A:856:U:H2'	22:O:21:ARG:HA	1.97	0.47
34:a:1130:G:OP1	43:j:87:ARG:NH1	2.48	0.47
10:A:2037:G:H5''	29:V:42:ALA:HB2	1.97	0.46
47:n:17:ILE:O	47:n:20:THR:OG1	2.28	0.46
34:a:108:A:C6	34:a:334:G:C6	3.03	0.46
34:a:1286:G:H2'	34:a:1287:C:O4'	2.15	0.46
10:A:1112:G:O2'	10:A:1113:A:P	2.73	0.46
10:A:2654:G:O2'	10:A:2808:A:N1	2.44	0.46
34:a:456:A:H2'	34:a:457:A:O4'	2.16	0.46
13:D:19:G:OP2	13:D:20:C:N4	2.48	0.46
17:J:103:LEU:HA	17:J:107:SER:HB3	1.97	0.46
46:m:26:LYS:O	46:m:43:LYS:NZ	2.48	0.46
10:A:194:A:H2'	10:A:195:C:C6	2.50	0.46
10:A:688:A:N1	10:A:2396:A:O2'	2.43	0.46
10:A:830:U:H2'	10:A:831:C:C6	2.51	0.46
10:A:1990:C:O2'	12:C:132:ARG:NH1	2.49	0.46
10:A:2872:G:H2'	10:A:2873:C:O4'	2.16	0.46
24:Q:24:LEU:HD23	24:Q:44:VAL:HG21	1.98	0.46
10:A:195:C:O2'	10:A:847:A:N3	2.45	0.46
34:a:615:A:OP1	34:a:639:G:N2	2.46	0.46
10:A:522:G:H4'	10:A:547:A:N1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1766:C:H2'	10:A:1767:G:O4'	2.16	0.46
10:A:2372:G:N3	10:A:2408:C:H2'	2.30	0.46
34:a:588:C:H2'	34:a:589:G:O4'	2.15	0.46
34:a:955:A:H2'	34:a:956:G:C8	2.50	0.46
40:g:11:ARG:HG3	40:g:14:ILE:HB	1.97	0.46
10:A:12:U:O2	10:A:12:U:C2'	2.63	0.46
10:A:1817:C:H2'	10:A:1818:A:C5	2.52	0.45
10:A:2251:G:H4'	10:A:2253:C:C2	2.51	0.45
34:a:221:U:H4'	34:a:222:G:O5'	2.16	0.45
34:a:1307:U:H1'	34:a:1308:C:H5	1.81	0.45
10:A:1068:G:C6	10:A:1069:G:C6	3.04	0.45
10:A:1112:G:O2'	10:A:1113:A:O5'	2.32	0.45
26:S:22:PHE:O	26:S:52:ARG:NH1	2.48	0.45
18:K:23:HIS:HA	18:K:36:THR:HA	1.98	0.45
10:A:250:G:H4'	10:A:432:G:C5	2.52	0.45
10:A:945:A:H2'	10:A:946:A:O4'	2.17	0.45
10:A:1675:G:H1'	10:A:1679:A:N6	2.32	0.45
10:A:1880:A:H2'	10:A:1881:A:C8	2.52	0.45
17:J:129:THR:HG23	17:J:155:VAL:HG22	1.99	0.45
42:i:34:LYS:HG2	42:i:60:LEU:HD21	1.99	0.45
50:q:22:VAL:HG21	50:q:60:TRP:CD1	2.52	0.45
10:A:538:G:H2'	10:A:539:G:O4'	2.17	0.45
10:A:597:U:H2'	10:A:598:G:O4'	2.17	0.45
32:Y:7:ILE:HG22	32:Y:43:VAL:HB	1.99	0.45
40:g:52:ILE:HD11	52:s:71:ALA:HB2	1.99	0.45
34:a:1188:G:N7	43:j:101:LYS:NZ	2.57	0.45
10:A:342:A:N3	10:A:362:C:O2'	2.49	0.45
10:A:774:G:C6	14:G:207:LYS:HB2	2.51	0.45
10:A:2917:U:O2'	20:M:135:ALA:O	2.31	0.45
34:a:529:G:H4'	46:m:83:ILE:HG12	1.97	0.45
10:A:787:U:H2'	10:A:788:A:C8	2.52	0.44
10:A:2325:A:H2'	10:A:2326:G:O4'	2.17	0.44
10:A:2599:A:N7	15:H:158:SER:OG	2.43	0.44
4:4:16:ASP:O	4:4:20:ASN:N	2.50	0.44
34:a:489:G:O2'	34:a:491:C:N4	2.49	0.44
34:a:1122:A:N1	37:d:176:THR:HG22	2.31	0.44
34:a:1529:MA6:H103	34:a:1530:MA6:H102	1.99	0.44
11:B:83:C:H2'	11:B:84:U:O4'	2.18	0.44
24:Q:26:ILE:HD11	24:Q:69:VAL:HG21	1.99	0.44
17:J:130:LEU:O	17:J:154:ILE:N	2.50	0.44
34:a:994:C:H2'	34:a:995:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1146:U:O2'	34:a:1148:A:N7	2.45	0.44
10:A:1966:5MU:OP1	10:A:2631:U:O2'	2.36	0.44
10:A:2601:G7M:O5'	10:A:2601:G7M:H8	2.17	0.44
10:A:2654:G:N2	10:A:2804:G:OP2	2.48	0.44
36:c:162:PHE:CE1	36:c:217:MET:HG3	2.52	0.44
44:k:22:ALA:O	44:k:26:VAL:HG23	2.17	0.44
10:A:2692:A:H2'	10:A:2693:C:O4'	2.18	0.44
34:a:390:A:H2'	34:a:391:A:C8	2.53	0.44
34:a:1143:C:H2'	34:a:1144:A:C8	2.53	0.44
10:A:1111:A:O4'	10:A:1112:G:H8	2.01	0.44
12:C:29:GLY:O	12:C:62:ARG:NH1	2.49	0.44
29:V:36:LEU:HD13	29:V:48:GLU:HA	1.99	0.44
47:n:9:ILE:HG21	47:n:45:VAL:HG11	2.00	0.44
10:A:858:U:H2'	10:A:859:C:C6	2.53	0.43
10:A:2439:A:H2'	10:A:2440:G:O4'	2.18	0.43
34:a:52:A:N7	34:a:113:U:O2'	2.51	0.43
12:C:112:ARG:HD3	12:C:112:ARG:HA	1.93	0.43
34:a:1283:C:H2'	34:a:1284:A:O4'	2.18	0.43
37:d:34:GLU:O	37:d:38:ILE:HG12	2.18	0.43
38:e:182:ARG:HA	38:e:185:LEU:HD12	2.00	0.43
10:A:566:U:H2'	10:A:567:G:C8	2.53	0.43
10:A:1113:A:H4'	10:A:1114:A:C8	2.52	0.43
10:A:759:U:H1'	10:A:762:C:H5	1.82	0.43
10:A:1897:U:H2'	10:A:1898:C:C6	2.54	0.43
45:l:93:ARG:O	45:l:97:ILE:HG13	2.17	0.43
4:4:11:GLN:HA	4:4:26:GLY:HA2	1.99	0.43
10:A:2253:C:H2'	10:A:2254:A:O4'	2.19	0.43
34:a:242:C:H4'	51:r:68:PRO:HG3	2.01	0.43
34:a:583:G:O2'	34:a:829:G:H5'	2.19	0.43
34:a:728:C:H2'	34:a:729:A:C8	2.54	0.43
53:t:12:ASP:HB3	53:t:14:HIS:CE1	2.53	0.43
10:A:2403:A:H2'	10:A:2404:A:O4'	2.18	0.43
17:J:121:ALA:HB3	17:J:128:TYR:CE1	2.54	0.43
27:T:31:LEU:HB2	27:T:34:VAL:HG12	2.00	0.43
34:a:63:U:OP1	34:a:393:C:O2'	2.37	0.43
10:A:749:G:N3	10:A:771:G:C2	2.87	0.43
34:a:509:C:P	46:m:127:ARG:HH22	2.42	0.43
36:c:187:VAL:HG13	36:c:191:CYS:HB2	2.00	0.43
47:n:86:TYR:CZ	47:n:90:ARG:HD2	2.54	0.43
10:A:1121:A:H4'	19:L:93:ASN:HB3	2.01	0.43
10:A:1572:G:C6	10:A:1591:G:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:680:U:HO2'	52:s:69:HIS:HE2	1.62	0.43
34:a:765:U:H2'	34:a:766:G:O4'	2.19	0.43
10:A:2318:U:H2'	10:A:2319:U:C6	2.54	0.43
45:l:68:GLU:HG3	45:l:99:ALA:HB1	2.01	0.43
10:A:877:G:N3	22:O:52:GLY:HA3	2.34	0.42
34:a:134:A:H2'	34:a:135:C:O4'	2.19	0.42
34:a:381:A:O2'	34:a:459:A:N7	2.52	0.42
37:d:149:LYS:HB3	37:d:200:TRP:HB2	2.01	0.42
10:A:280:C:H2'	10:A:281:A:C8	2.54	0.42
10:A:2793:G:N3	10:A:2793:G:H2'	2.34	0.42
13:D:47(I):A:H2'	13:D:47(J):G:O4'	2.20	0.42
44:k:80:THR:HB	44:k:83:THR:HG23	2.01	0.42
10:A:1065:A:H3'	10:A:1065:A:N3	2.35	0.42
34:a:1023:A:H4'	53:t:14:HIS:CE1	2.55	0.42
34:a:1444:A:H2'	34:a:1445:G:O4'	2.20	0.42
10:A:1940:A:N6	34:a:1503:A:O2'	2.52	0.42
18:K:9:ILE:HD11	18:K:69:ARG:HG2	2.01	0.42
18:K:89:LEU:HG	18:K:162:ILE:HG12	2.00	0.42
19:L:16:GLY:HA2	19:L:43:ASN:HA	2.02	0.42
36:c:170:ARG:NH1	36:c:195:GLU:OE1	2.53	0.42
41:h:53:ARG:NH1	41:h:122:ASN:OD1	2.52	0.42
10:A:1875:A:H2'	10:A:1876:G:O4'	2.19	0.42
10:A:2227:C:O2	10:A:2253:C:N4	2.50	0.42
23:P:54:MET:HE1	23:P:104:PHE:CG	2.55	0.42
2:2:26:PHE:CG	30:W:4:ARG:HD2	2.55	0.42
10:A:1312:A:N3	10:A:1313:G:H1'	2.34	0.42
31:X:70:LEU:HD11	31:X:92:ARG:NH2	2.35	0.42
34:a:160:A:H2'	34:a:161:A:O4'	2.19	0.42
47:n:79:ARG:O	47:n:83:ILE:HG12	2.20	0.42
4:4:34:MET:HA	4:4:44:PRO:HA	2.00	0.42
10:A:365:A:OP2	16:I:169:ASN:HB2	2.20	0.42
10:A:1394:U:H2'	10:A:1395:G:O4'	2.20	0.42
34:a:1228:U:H2'	34:a:1229:U:C6	2.54	0.42
37:d:110:LEU:HD22	37:d:145:ALA:HB2	2.01	0.42
17:J:8:PHE:HA	17:J:12:VAL:HB	2.01	0.42
36:c:163:VAL:O	36:c:185:GLY:HA2	2.20	0.42
38:e:46:GLU:OE2	38:e:50:GLN:NE2	2.52	0.42
45:l:52:PHE:HD2	45:l:56:LYS:HB3	1.85	0.42
10:A:1110:U:H2'	10:A:1112:G:H1'	2.01	0.42
13:D:65:G:O2'	13:D:66:C:P	2.78	0.42
34:a:272:C:O2'	51:r:68:PRO:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:15:LEU:HD13	38:e:56:LYS:HA	2.01	0.42
11:B:22:G:O2'	11:B:25:A:N6	2.53	0.41
12:C:73:SER:O	12:C:74:VAL:C	2.63	0.41
34:a:274:G:H3'	51:r:71:ALA:HB2	2.02	0.41
10:A:2869:G:O2'	10:A:2886:G:N2	2.53	0.41
34:a:721:G:H2'	34:a:722:G:C8	2.55	0.41
36:c:186:ILE:HG23	36:c:202:ALA:HB3	2.02	0.41
45:l:29:ASN:OD1	45:l:30:THR:N	2.53	0.41
10:A:1238:U:H1'	27:T:4:VAL:HG22	2.03	0.41
19:L:109:ALA:O	19:L:113:MET:N	2.53	0.41
34:a:122:C:H5''	34:a:319:C:O2'	2.20	0.41
34:a:413:U:H1'	34:a:506:A:H2'	2.03	0.41
46:m:23:ALA:O	46:m:72:ASN:ND2	2.53	0.41
2:2:1:MET:HE1	2:2:17:GLN:HG2	2.03	0.41
10:A:923:A:H2'	10:A:923:A:N3	2.35	0.41
10:A:1051:C:OP1	20:M:38:ARG:NH1	2.54	0.41
10:A:1748:G:H5'	34:a:1439:C:H5'	2.03	0.41
10:A:2496:A:H4'	23:P:56:ARG:CD	2.50	0.41
22:O:118:ASP:HA	22:O:139:LYS:HE2	2.02	0.41
41:h:63:GLU:O	41:h:67:ASN:ND2	2.54	0.41
10:A:524:A:N1	10:A:545:G:H4'	2.36	0.41
10:A:1378:U:O4'	30:W:56:MET:HE2	2.21	0.41
34:a:51:A:O2'	34:a:368:G:N2	2.53	0.41
34:a:99:U:H2'	34:a:100:A:C8	2.56	0.41
34:a:775:A:H2'	34:a:776:A:O4'	2.21	0.41
17:J:38:MET:HE2	17:J:57:LEU:HD22	2.03	0.41
21:N:97:ARG:HH12	34:a:345:G:P	2.44	0.41
34:a:112:G:N3	34:a:361:A:O2'	2.50	0.41
46:m:79:TYR:HB2	46:m:106:VAL:HG11	2.02	0.41
10:A:618:A:OP2	10:A:2526:C:O2'	2.33	0.41
10:A:2318:U:OP1	10:A:2407:A:O2'	2.38	0.41
37:d:76:ILE:HA	37:d:83:ILE:HB	2.03	0.41
8:8:42:ARG:O	8:8:45:ARG:HG2	2.21	0.41
10:A:168:A:H3'	10:A:169:G:H8	1.86	0.41
10:A:1072:A:N6	10:A:1169:G:H2'	2.35	0.41
10:A:2007:G:O2'	10:A:2009:U:OP2	2.33	0.41
10:A:2016:A:H2'	10:A:2017:C:O4'	2.21	0.41
10:A:2714:U:H2'	10:A:2715:G:O4'	2.21	0.41
11:B:112:A:H2'	11:B:113:G:O4'	2.21	0.41
18:K:97:GLN:HG3	18:K:104:ILE:HB	2.03	0.41
19:L:106:ARG:HA	19:L:125:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1097:U:H3	34:a:1110:G:H22	1.67	0.41
34:a:1319:G:N7	47:n:98:ARG:NH2	2.68	0.41
39:f:15:VAL:HG12	39:f:37:VAL:HG22	2.01	0.41
47:n:15:VAL:HA	47:n:45:VAL:HG23	2.03	0.41
47:n:107:ARG:NH2	47:n:112:PRO:HA	2.36	0.41
51:r:19:MET:HB2	51:r:22:THR:HB	2.03	0.41
4:4:15:LEU:HD13	4:4:35:MET:HE1	2.03	0.41
10:A:305:A:N6	10:A:410:G:H22	2.19	0.41
15:H:159:ASP:HA	15:H:160:ALA:HA	1.89	0.41
22:O:91:VAL:HA	22:O:95:LEU:HD23	2.03	0.41
34:a:1379:C:H2'	34:a:1380:G:C8	2.56	0.41
10:A:1252:A:H4'	10:A:1277:C:H4'	2.04	0.40
16:I:148:GLN:HB3	16:I:152:VAL:HG21	2.01	0.40
18:K:15:VAL:HG22	18:K:79:VAL:HG23	2.04	0.40
34:a:476:C:O2	34:a:476:C:O4'	2.38	0.40
34:a:1441:C:H2'	34:a:1442:G:O4'	2.22	0.40
13:D:41:G:O2'	34:a:1348:G:N3	2.53	0.40
19:L:28:LEU:HD21	19:L:58:ILE:HD13	2.03	0.40
34:a:412:G:N7	38:e:3:ARG:NH2	2.69	0.40
34:a:828:U:H4'	34:a:829:G:OP2	2.21	0.40
45:l:86:VAL:HG11	45:l:93:ARG:HG3	2.02	0.40
10:A:24:G:O2'	29:V:78:GLU:O	2.39	0.40
10:A:971:U:H2'	10:A:972:A:C8	2.56	0.40
10:A:2341:A:H2'	10:A:2342:U:C6	2.56	0.40
34:a:672:G:H22	34:a:749:G:H1	1.69	0.40
7:7:21:LYS:O	7:7:24:SER:OG	2.38	0.40
18:K:164:TYR:HB2	18:K:167:GLU:HB2	2.03	0.40
36:c:21:ARG:HG3	36:c:22:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	4	57/84 (68%)	56 (98%)	1 (2%)	0	100	100
5	5	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
6	6	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
7	7	42/45 (93%)	42 (100%)	0	0	100	100
8	8	63/66 (96%)	63 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	181/186 (97%)	175 (97%)	6 (3%)	0	100	100
14	G	271/277 (98%)	267 (98%)	4 (2%)	0	100	100
15	H	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
16	I	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
17	J	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
18	K	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
19	L	134/140 (96%)	129 (96%)	5 (4%)	0	100	100
20	M	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
21	N	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
22	O	144/146 (99%)	140 (97%)	3 (2%)	1 (1%)	18	35
23	P	134/144 (93%)	131 (98%)	3 (2%)	0	100	100
24	Q	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
25	R	117/119 (98%)	114 (97%)	2 (2%)	1 (1%)	14	28
26	S	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
27	T	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
28	U	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
29	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
30	W	88/91 (97%)	87 (99%)	1 (1%)	0	100	100
31	X	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	Y	92/217 (42%)	89 (97%)	3 (3%)	0	100	100
33	Z	74/94 (79%)	70 (95%)	4 (5%)	0	100	100
36	c	219/255 (86%)	211 (96%)	8 (4%)	0	100	100
37	d	202/217 (93%)	196 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	e	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
39	f	155/166 (93%)	148 (96%)	7 (4%)	0	100	100
40	g	92/98 (94%)	90 (98%)	2 (2%)	0	100	100
41	h	142/156 (91%)	140 (99%)	2 (1%)	0	100	100
42	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
43	j	126/132 (96%)	120 (95%)	6 (5%)	0	100	100
44	k	96/102 (94%)	93 (97%)	2 (2%)	1 (1%)	12	26
45	l	116/129 (90%)	110 (95%)	5 (4%)	1 (1%)	14	28
46	m	133/137 (97%)	131 (98%)	2 (2%)	0	100	100
47	n	112/121 (93%)	108 (96%)	4 (4%)	0	100	100
48	o	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
49	p	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
50	q	88/91 (97%)	85 (97%)	3 (3%)	0	100	100
51	r	79/87 (91%)	75 (95%)	4 (5%)	0	100	100
52	s	62/80 (78%)	62 (100%)	0	0	100	100
53	t	81/92 (88%)	81 (100%)	0	0	100	100
54	u	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5637/6101 (92%)	5486 (97%)	147 (3%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	O	29	LYS
44	k	57	LYS
45	l	119	ASN
25	R	116	GLY

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	1	51/52 (98%)	51 (100%)	0	100	100
2	2	59/62 (95%)	58 (98%)	1 (2%)	53	76
3	3	52/53 (98%)	52 (100%)	0	100	100
4	4	56/75 (75%)	56 (100%)	0	100	100
5	5	48/50 (96%)	48 (100%)	0	100	100
6	6	46/47 (98%)	46 (100%)	0	100	100
7	7	39/40 (98%)	39 (100%)	0	100	100
8	8	56/57 (98%)	56 (100%)	0	100	100
9	9	35/35 (100%)	35 (100%)	0	100	100
12	C	160/162 (99%)	160 (100%)	0	100	100
14	G	220/224 (98%)	220 (100%)	0	100	100
15	H	173/177 (98%)	173 (100%)	0	100	100
16	I	168/169 (99%)	167 (99%)	1 (1%)	78	90
17	J	156/158 (99%)	153 (98%)	3 (2%)	50	74
18	K	153/155 (99%)	153 (100%)	0	100	100
19	L	108/111 (97%)	107 (99%)	1 (1%)	70	86
20	M	123/123 (100%)	123 (100%)	0	100	100
21	N	100/100 (100%)	100 (100%)	0	100	100
22	O	112/112 (100%)	111 (99%)	1 (1%)	70	86
23	P	113/119 (95%)	113 (100%)	0	100	100
24	Q	101/102 (99%)	101 (100%)	0	100	100
25	R	95/95 (100%)	95 (100%)	0	100	100
26	S	100/102 (98%)	100 (100%)	0	100	100
27	T	97/98 (99%)	97 (100%)	0	100	100
28	U	86/86 (100%)	86 (100%)	0	100	100
29	V	90/94 (96%)	89 (99%)	1 (1%)	65	83
30	W	81/82 (99%)	81 (100%)	0	100	100
31	X	87/90 (97%)	87 (100%)	0	100	100
32	Y	83/190 (44%)	83 (100%)	0	100	100
33	Z	59/75 (79%)	59 (100%)	0	100	100
36	c	192/221 (87%)	191 (100%)	1 (0%)	81	91
37	d	165/175 (94%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	e	174/175 (99%)	174 (100%)	0	100	100
39	f	123/131 (94%)	123 (100%)	0	100	100
40	g	82/86 (95%)	82 (100%)	0	100	100
41	h	124/132 (94%)	122 (98%)	2 (2%)	55	78
42	i	112/113 (99%)	110 (98%)	2 (2%)	51	75
43	j	106/109 (97%)	105 (99%)	1 (1%)	70	86
44	k	88/91 (97%)	87 (99%)	1 (1%)	65	83
45	l	94/104 (90%)	93 (99%)	1 (1%)	65	83
46	m	117/119 (98%)	117 (100%)	0	100	100
47	n	99/104 (95%)	98 (99%)	1 (1%)	68	85
48	o	52/53 (98%)	52 (100%)	0	100	100
49	p	79/81 (98%)	79 (100%)	0	100	100
50	q	76/77 (99%)	76 (100%)	0	100	100
51	r	76/82 (93%)	76 (100%)	0	100	100
52	s	57/68 (84%)	57 (100%)	0	100	100
53	t	72/80 (90%)	72 (100%)	0	100	100
54	u	67/69 (97%)	67 (100%)	0	100	100
All	All	4862/5165 (94%)	4845 (100%)	17 (0%)	84	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	42	ARG
16	I	49	HIS
17	J	120	LYS
17	J	132	VAL
17	J	133	LYS
19	L	105	VAL
22	O	59	ARG
29	V	11	ARG
36	c	80	VAL
41	h	75	VAL
41	h	87	VAL
42	i	27	LEU
42	i	98	LEU
43	j	24	VAL

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Mol	Chain	Res	Type
44	k	72	ARG
45	l	86	VAL
47	n	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	GLN
1	1	20	HIS
5	5	14	ASN
6	6	4	ASN
7	7	27	ASN
8	8	60	GLN
12	C	165	ASN
14	G	134	ASN
14	G	199	GLN
15	H	14	GLN
15	H	136	GLN
15	H	200	ASN
16	I	188	ASN
17	J	161	ASN
20	M	119	GLN
23	P	13	HIS
24	Q	79	GLN
25	R	48	ASN
27	T	52	GLN
28	U	101	ASN
29	V	90	GLN
32	Y	38	ASN
32	Y	85	GLN
36	c	55	ASN
37	d	3	GLN
37	d	53	HIS
37	d	61	ASN
37	d	118	ASN
38	e	158	ASN
39	f	146	ASN
41	h	40	GLN
41	h	148	ASN
42	i	48	ASN
45	l	18	ASN
45	l	64	GLN

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Mol	Chain	Res	Type
46	m	39	ASN
46	m	90	HIS
47	n	31	GLN
47	n	76	ASN
50	q	73	ASN
53	t	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2795/2923 (95%)	365 (13%)	70 (2%)
11	B	112/115 (97%)	16 (14%)	4 (3%)
13	D	92/93 (98%)	11 (11%)	2 (2%)
34	a	1493/1555 (96%)	190 (12%)	0
35	b	17/24 (70%)	2 (11%)	0
All	All	4509/4710 (95%)	584 (12%)	76 (1%)

All (584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	12	U
10	A	33	U
10	A	34	U
10	A	71	A
10	A	75	G
10	A	90	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	156	A
10	A	163	U
10	A	167	U
10	A	168	A
10	A	177	G
10	A	183	A
10	A	199	A
10	A	202	A
10	A	203	U
10	A	216	A
10	A	218	G
10	A	219	A

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Mol	Chain	Res	Type
10	A	224	A
10	A	225	A
10	A	232	U
10	A	233	U
10	A	251	G
10	A	255	G
10	A	269	G
10	A	270	C
10	A	289	U
10	A	299	U
10	A	300	G
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A
10	A	327	G
10	A	354	A
10	A	373	A
10	A	388	A
10	A	389	A
10	A	404	U
10	A	406	A
10	A	410	G
10	A	411	A
10	A	429	C
10	A	432	G
10	A	449	U
10	A	450	C
10	A	457	G
10	A	458	A
10	A	494	U
10	A	497	U
10	A	502	C
10	A	503	A
10	A	527	G
10	A	548	A
10	A	549	U
10	A	550	A
10	A	553	A
10	A	575	G
10	A	576	U
10	A	577	A

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Mol	Chain	Res	Type
10	A	578	G
10	A	590	U
10	A	592	A
10	A	593	U
10	A	594	G
10	A	606	G
10	A	614	U
10	A	615	A
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	682	A
10	A	683	G
10	A	690	U
10	A	696	G
10	A	700	A
10	A	731	U
10	A	762	C
10	A	775	A
10	A	792	5MU
10	A	809	A
10	A	810	A
10	A	820	G
10	A	827	A
10	A	829	U
10	A	835	U
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	903	G
10	A	904	G
10	A	910	C
10	A	911	A
10	A	919	G
10	A	920	A
10	A	923	A
10	A	924	G
10	A	943	C
10	A	944	G

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Mol	Chain	Res	Type
10	A	945	A
10	A	955	A
10	A	969	A
10	A	970	U
10	A	985	A
10	A	988	C
10	A	989	A
10	A	990	G
10	A	1001	A
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1028	G
10	A	1029	C
10	A	1040	A
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1098	A
10	A	1102	U
10	A	1104	U
10	A	1105	U
10	A	1111	A
10	A	1112	G
10	A	1113	A
10	A	1114	A
10	A	1115	G
10	A	1117	A
10	A	1119	C
10	A	1123	C
10	A	1124	A
10	A	1128	A
10	A	1129	A
10	A	1131	G
10	A	1132	A
10	A	1134	U
10	A	1139	A
10	A	1140	A

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Mol	Chain	Res	Type
10	A	1151	G
10	A	1155	A
10	A	1156	G
10	A	1174	U
10	A	1176	U
10	A	1177	A
10	A	1179	C
10	A	1186	A
10	A	1199	A
10	A	1216	U
10	A	1217	U
10	A	1258	A
10	A	1276	G
10	A	1291	A
10	A	1292	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1326	C
10	A	1337	A
10	A	1357	G
10	A	1358	A
10	A	1382	C
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1421	A
10	A	1449	A
10	A	1450	A
10	A	1455	U
10	A	1457	U
10	A	1458	A
10	A	1459	A
10	A	1463	A
10	A	1471	A
10	A	1472	C
10	A	1490	G
10	A	1496	G
10	A	1497	A
10	A	1504	U
10	A	1505	G

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Mol	Chain	Res	Type
10	A	1511	C
10	A	1526	G
10	A	1533	A
10	A	1536	C
10	A	1537	A
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1574	G
10	A	1578	A
10	A	1606	C
10	A	1616	A
10	A	1625	U
10	A	1630	A
10	A	1631	G
10	A	1634	A
10	A	1651	C
10	A	1652	A
10	A	1657	G
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1708	A
10	A	1718	G
10	A	1740	G
10	A	1758	A
10	A	1759	G
10	A	1772	G
10	A	1783	G
10	A	1790	G
10	A	1791	G
10	A	1800	A
10	A	1809	C
10	A	1818	A
10	A	1827	C
10	A	1828	U
10	A	1829	A
10	A	1839	G
10	A	1843	U
10	A	1856	A
10	A	1874	A
10	A	1875	A

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Mol	Chain	Res	Type
10	A	1899	U
10	A	1909	C
10	A	1933	G
10	A	1934	G
10	A	1939	A
10	A	1940	A
10	A	1941	C
10	A	1942	3TD
10	A	1943	A
10	A	1946	A
10	A	1949	G
10	A	1951	C
10	A	1952	C
10	A	1957	G
10	A	1958	U
10	A	1963	A
10	A	1964	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G
10	A	2018	U
10	A	2020	U
10	A	2040	A
10	A	2047	A
10	A	2050	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2062	G
10	A	2063	C
10	A	2070	C
10	A	2076	A
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A
10	A	2090	C
10	A	2096	G

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Mol	Chain	Res	Type
10	A	2120	G
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2266	G
10	A	2295	A
10	A	2305	A
10	A	2309	G
10	A	2310	C
10	A	2313	A
10	A	2314	A
10	A	2316	G
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2339	U
10	A	2349	A
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2406	G
10	A	2410	G
10	A	2412	C
10	A	2429	U
10	A	2430	C
10	A	2433	C
10	A	2436	G
10	A	2450	U
10	A	2451	C
10	A	2452	A
10	A	2456	G
10	A	2457	A
10	A	2458	U
10	A	2462	A
10	A	2468	C
10	A	2475	A
10	A	2492	C
10	A	2495	A
10	A	2496	A
10	A	2502	C

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Mol	Chain	Res	Type
10	A	2529	G
10	A	2532	G
10	A	2545	A
10	A	2556	G
10	A	2557	U
10	A	2561	C
10	A	2581	U
10	A	2593	A
10	A	2594	G
10	A	2600	C
10	A	2605	G
10	A	2613	C
10	A	2629	A
10	A	2637	C
10	A	2640	U
10	A	2659	A
10	A	2666	A
10	A	2681	A
10	A	2690	G
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2762	G
10	A	2769	G
10	A	2771	G
10	A	2775	A
10	A	2778	G
10	A	2784	A
10	A	2788	A
10	A	2792	A
10	A	2805	A
10	A	2806	U
10	A	2817	A
10	A	2818	A
10	A	2824	G
10	A	2825	U
10	A	2827	A
10	A	2828	U
10	A	2843	A

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Mol	Chain	Res	Type
10	A	2852	U
10	A	2887	G
10	A	2888	A
10	A	2892	G
10	A	2893	A
10	A	2894	C
10	A	2903	A
10	A	2913	G
11	B	10	U
11	B	22	G
11	B	23	U
11	B	33	U
11	B	43	A
11	B	49	G
11	B	51	A
11	B	54	U
11	B	55	A
11	B	63	U
11	B	64	A
11	B	65	G
11	B	87	C
11	B	88	G
11	B	106	G
11	B	113	G
13	D	7	G
13	D	8	4SU
13	D	16	A
13	D	18	G
13	D	20(B)	G
13	D	47(C)	G
13	D	47(I)	A
13	D	48	C
13	D	65	G
13	D	66	C
13	D	76	A
34	a	7	G
34	a	9	A
34	a	10	G
34	a	33	A
34	a	40	G
34	a	48	C
34	a	49	C

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Mol	Chain	Res	Type
34	a	51	A
34	a	52	A
34	a	53	U
34	a	119	A
34	a	120	C
34	a	131	C
34	a	142	G
34	a	159	G
34	a	163	C
34	a	173	U
34	a	183	U
34	a	190	A
34	a	198	G
34	a	205	A
34	a	212	A
34	a	220	U
34	a	221	U
34	a	222	G
34	a	223	C
34	a	248	U
34	a	249	G
34	a	253	U
34	a	255	G
34	a	258	A
34	a	259	G
34	a	274	G
34	a	275	C
34	a	297	G
34	a	313	G
34	a	314	A
34	a	329	A
34	a	336	C
34	a	338	C
34	a	340	G
34	a	355	G
34	a	360	C
34	a	362	G
34	a	364	A
34	a	375	U
34	a	380	C
34	a	392	G
34	a	400	G

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Mol	Chain	Res	Type
34	a	414	G
34	a	419	A
34	a	420	U
34	a	421	G
34	a	429	U
34	a	432	G
34	a	437	U
34	a	447	U
34	a	456	A
34	a	461	C
34	a	492	G
34	a	493	G
34	a	505	A
34	a	513	G
34	a	519	C
34	a	526	C
34	a	529	G
34	a	540	A
34	a	544	C
34	a	555	A
34	a	567	A
34	a	580	A
34	a	581	A
34	a	584	C
34	a	585	G
34	a	604	A
34	a	626	C
34	a	649	A
34	a	650	A
34	a	661	U
34	a	673	A
34	a	695	A
34	a	696	G
34	a	731	U
34	a	732	G
34	a	742	A
34	a	757	A
34	a	763	G
34	a	785	A
34	a	802	A
34	a	823	A
34	a	825	C

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Mol	Chain	Res	Type
34	a	836	A
34	a	881	A
34	a	883	G
34	a	893	U
34	a	894	G
34	a	923	A
34	a	924	A
34	a	935	G
34	a	936	G
34	a	940	C
34	a	943	C
34	a	944	A
34	a	969	U
34	a	978	A
34	a	980	G
34	a	981	C
34	a	984	A
34	a	985	G
34	a	986	A
34	a	1000	U
34	a	1001	U
34	a	1002	G
34	a	1018	U
34	a	1030	G
34	a	1031	C
34	a	1056	C
34	a	1057	A
34	a	1076	U
34	a	1096	U
34	a	1105	G
34	a	1106	U
34	a	1111	C
34	a	1112	A
34	a	1141	A
34	a	1149	G
34	a	1155	C
34	a	1156	A
34	a	1169	U
34	a	1170	G
34	a	1174	G
34	a	1175	U
34	a	1177	A

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Mol	Chain	Res	Type
34	a	1178	C
34	a	1194	G
34	a	1206	A
34	a	1207	A
34	a	1221	U
34	a	1223	A
34	a	1224	U
34	a	1225	G
34	a	1235	A
34	a	1236	C
34	a	1237	A
34	a	1248	A
34	a	1250	U
34	a	1267	A
34	a	1270	G
34	a	1289	A
34	a	1290	A
34	a	1296	U
34	a	1297	A
34	a	1308	C
34	a	1309	A
34	a	1310	G
34	a	1312	U
34	a	1329	A
34	a	1330	C
34	a	1345	C
34	a	1346	U
34	a	1348	G
34	a	1356	A
34	a	1363	G
34	a	1374	U
34	a	1380	G
34	a	1388	C
34	a	1389	G
34	a	1408	A
34	a	1429	G
34	a	1434	U
34	a	1437	C
34	a	1438	A
34	a	1439	C
34	a	1452	G
34	a	1456	A

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Mol	Chain	Res	Type
34	a	1461	U
34	a	1463	U
34	a	1464	A
34	a	1484	G
34	a	1490	A
34	a	1510	A
34	a	1513	A
34	a	1516	G
34	a	1517	U
34	a	1528	G
34	a	1530	MA6
34	a	1531	G
34	a	1540	G
34	a	1541	G
34	a	1547	C
35	b	8	A
35	b	16	A

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	33	U
10	A	130	A
10	A	176	A
10	A	183	A
10	A	195	C
10	A	202	A
10	A	232	U
10	A	258	A
10	A	388	A
10	A	449	U
10	A	520	G
10	A	548	A
10	A	614	U
10	A	661	U
10	A	700	A
10	A	741	G
10	A	809	A
10	A	903	G
10	A	910	C
10	A	923	A
10	A	969	A

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Mol	Chain	Res	Type
10	A	988	C
10	A	1017	A
10	A	1028	G
10	A	1097	U
10	A	1105	U
10	A	1111	A
10	A	1112	G
10	A	1114	A
10	A	1128	A
10	A	1131	G
10	A	1135	G
10	A	1139	A
10	A	1176	U
10	A	1185	U
10	A	1224	U
10	A	1291	A
10	A	1347	G
10	A	1357	G
10	A	1433	U
10	A	1496	G
10	A	1504	U
10	A	1540	U
10	A	1630	A
10	A	1651	C
10	A	1691	G
10	A	1789	A
10	A	1845	U
10	A	1874	A
10	A	1951	C
10	A	2049	U
10	A	2062	G
10	A	2094	G
10	A	2240	U
10	A	2309	G
10	A	2313	A
10	A	2347	A
10	A	2373	A
10	A	2409	G
10	A	2429	U
10	A	2449	C
10	A	2450	U
10	A	2457	A

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Mol	Chain	Res	Type
10	A	2495	A
10	A	2608	G
10	A	2783	U
10	A	2805	A
10	A	2816	C
10	A	2887	G
10	A	2893	A
11	B	22	G
11	B	42	G
11	B	64	A
11	B	105	C
13	D	14	A
13	D	65	G

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	4SU	D	8	13	18,21,22	0.39	0	26,30,33	1.20	3 (11%)
10	2MG	A	2472	10	23,26,27	0.36	0	32,38,41	0.39	0
10	5MU	A	1966	10	19,22,23	0.31	0	28,32,35	0.35	0
34	MA6	a	1529	34	23,26,27	0.25	0	34,38,41	0.70	1 (2%)
10	2MA	A	2530	10	22,25,26	0.25	0	33,37,40	0.64	1 (3%)
13	T6A	D	37	13	31,34,35	0.47	0	44,49,52	0.61	1 (2%)
34	2MG	a	975	34	23,26,27	0.39	0	32,38,41	0.36	0
10	OMG	A	2580	10	23,26,27	0.33	0	33,38,41	0.42	0
10	H2U	A	2476	10	18,21,22	0.65	0	21,30,33	0.78	2 (9%)
34	MA6	a	1530	34	23,26,27	0.25	0	34,38,41	0.69	1 (2%)
13	RSP	D	32	13	17,21,22	0.38	0	22,30,33	0.64	0
10	5MU	A	792	10	19,22,23	0.26	0	28,32,35	0.34	0
10	3TD	A	1942	10	18,22,23	0.96	1 (5%)	22,32,35	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PSU	D	55	13	18,21,22	0.91	1 (5%)	22,30,33	0.56	0
34	G7M	a	535	34	23,26,27	0.71	1 (4%)	35,39,42	0.60	0
10	OMG	A	2278	10	23,26,27	0.32	0	33,38,41	0.54	1 (3%)
13	H2U	D	20(A)	13	18,21,22	0.66	1 (5%)	21,30,33	0.71	0
34	4OC	a	1412	56,34	20,23,24	0.38	0	26,32,35	0.51	0
13	5MU	D	54	13	19,22,23	0.28	0	28,32,35	0.26	0
10	G7M	A	2601	56,10	23,26,27	0.69	1 (4%)	35,39,42	0.53	0
34	UR3	a	1509	34	19,22,23	0.30	0	26,32,35	0.67	0
34	5MC	a	976	34	18,22,23	0.33	0	26,32,35	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	4SU	D	8	13	-	0/7/25/26	0/2/2/2
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
34	MA6	a	1529	34	-	0/11/29/30	0/3/3/3
10	2MA	A	2530	10	-	2/7/25/26	0/3/3/3
13	T6A	D	37	13	-	0/23/41/42	0/3/3/3
34	2MG	a	975	34	-	0/9/27/28	0/3/3/3
10	OMG	A	2580	10	-	1/9/27/28	0/3/3/3
10	H2U	A	2476	10	-	0/7/38/39	0/2/2/2
34	MA6	a	1530	34	-	3/11/29/30	0/3/3/3
13	RSP	D	32	13	-	0/7/25/26	0/2/2/2
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
10	3TD	A	1942	10	-	2/7/25/26	0/2/2/2
13	PSU	D	55	13	-	0/7/25/26	0/2/2/2
34	G7M	a	535	34	-	1/7/25/26	0/3/3/3
10	OMG	A	2278	10	-	1/9/27/28	0/3/3/3
13	H2U	D	20(A)	13	-	4/7/38/39	0/2/2/2
34	4OC	a	1412	56,34	-	2/9/29/30	0/2/2/2
13	5MU	D	54	13	-	0/7/25/26	0/2/2/2
10	G7M	A	2601	56,10	-	0/7/25/26	0/3/3/3
34	UR3	a	1509	34	-	0/7/25/26	0/2/2/2
34	5MC	a	976	34	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1942	3TD	C6-C5	3.64	1.39	1.35
13	D	55	PSU	C6-C5	3.58	1.39	1.35
34	a	535	G7M	C8-N7	2.51	1.37	1.33
10	A	2601	G7M	C8-N7	2.31	1.37	1.33
13	D	20(A)	H2U	C1'-N1	2.10	1.50	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	8	4SU	C4-N3-C2	-4.36	123.11	127.34
34	a	1530	MA6	C2-N1-C6	2.91	118.63	111.75
34	a	1529	MA6	C2-N1-C6	2.88	118.56	111.75
13	D	8	4SU	C5-C4-N3	2.76	117.25	114.69
10	A	2278	OMG	O2'-C2'-C1'	2.46	113.88	109.08
10	A	2530	2MA	C5-C4-N3	-2.34	124.56	127.19
10	A	1942	3TD	O3'-C3'-C2'	2.26	119.15	111.82
13	D	8	4SU	N3-C2-N1	2.23	117.85	114.89
13	D	37	T6A	C5-C6-N6	2.19	124.51	118.71
10	A	2476	H2U	N3-C2-N1	2.14	118.92	116.65
10	A	2476	H2U	O2-C2-N1	-2.10	120.47	123.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1530	MA6	O4'-C4'-C5'-O5'
34	a	1530	MA6	C3'-C4'-C5'-O5'
10	A	1942	3TD	C3'-C4'-C5'-O5'
10	A	1942	3TD	O4'-C4'-C5'-O5'
10	A	2278	OMG	C1'-C2'-O2'-CM2
13	D	20(A)	H2U	C2'-C1'-N1-C6
34	a	1412	4OC	O4'-C4'-C5'-O5'
13	D	20(A)	H2U	O4'-C1'-N1-C2
13	D	20(A)	H2U	C2'-C1'-N1-C2
34	a	1412	4OC	C3'-C4'-C5'-O5'
34	a	1530	MA6	C4'-C5'-O5'-P
10	A	2530	2MA	C4'-C5'-O5'-P
34	a	535	G7M	C3'-C4'-C5'-O5'
10	A	2530	2MA	O4'-C4'-C5'-O5'
10	A	2580	OMG	C3'-C2'-O2'-CM2
13	D	20(A)	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1966	5MU	1	0
34	a	1529	MA6	1	0
13	D	37	T6A	1	0
34	a	1530	MA6	1	0
10	A	2601	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 125 ligands modelled in this entry, 125 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.

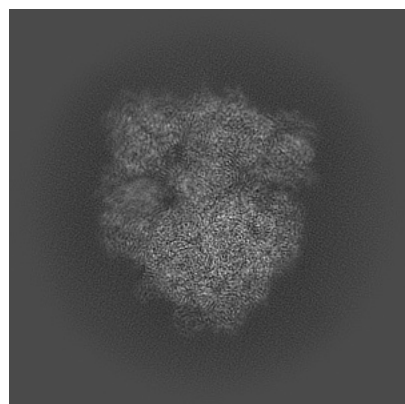
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55945. These allow visual inspection of the internal detail of the map and identification of artifacts.

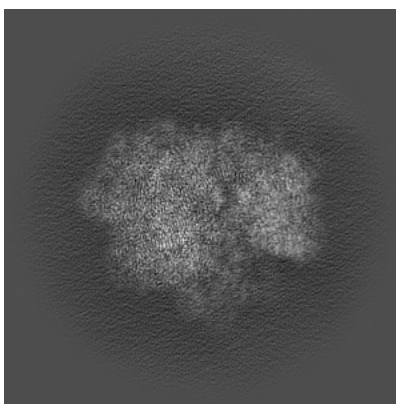
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

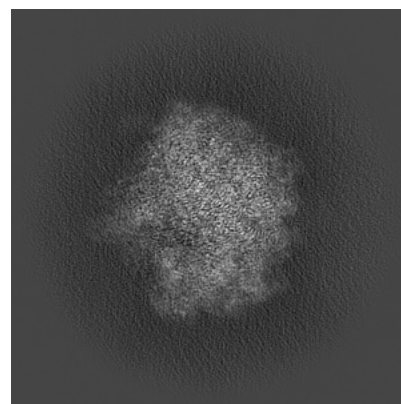
6.1.1 Primary map



X

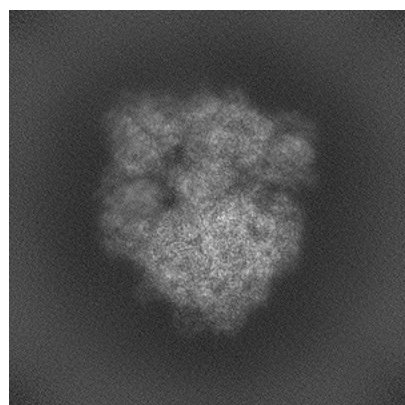


Y

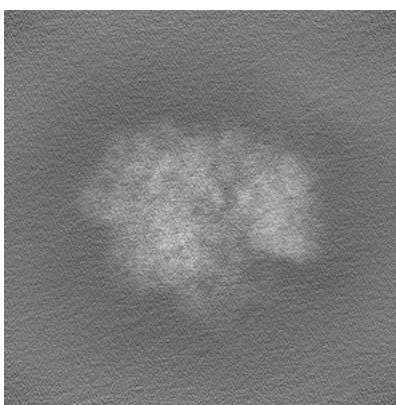


Z

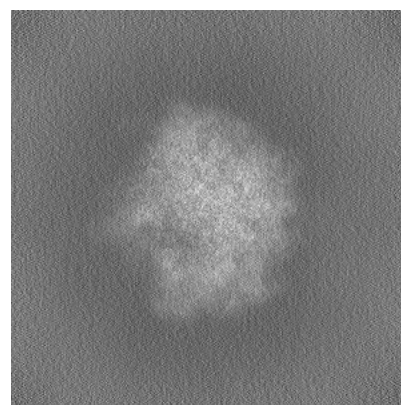
6.1.2 Raw map



X



Y

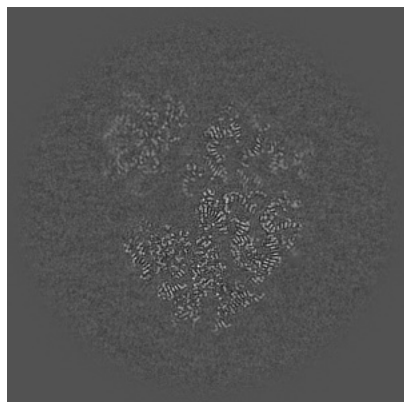


Z

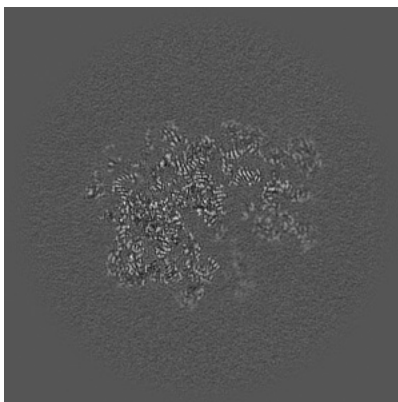
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

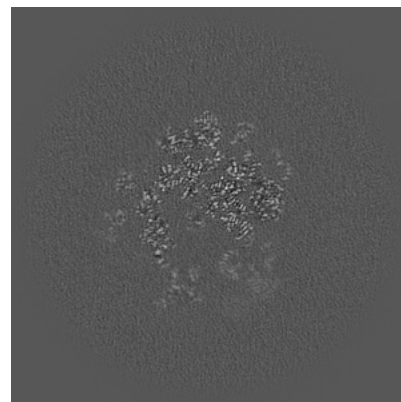
6.2.1 Primary map



X Index: 300

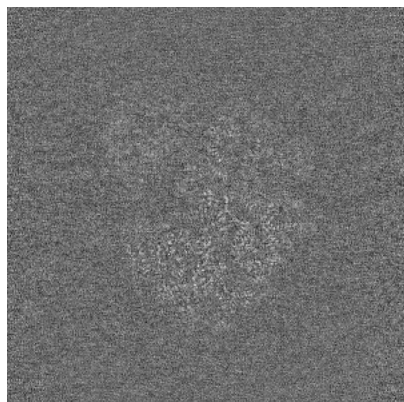


Y Index: 300

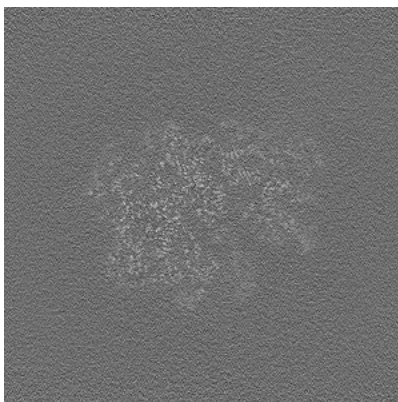


Z Index: 300

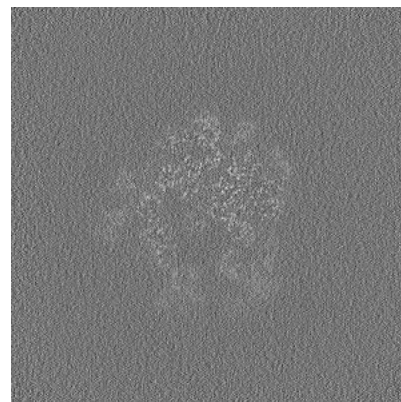
6.2.2 Raw map



X Index: 300



Y Index: 300

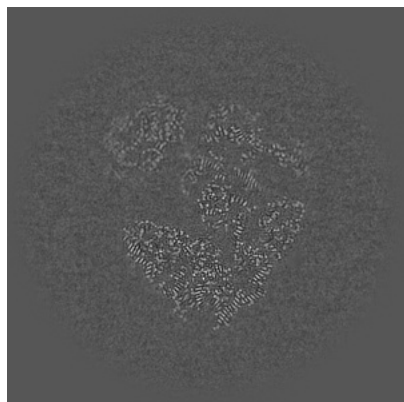


Z Index: 300

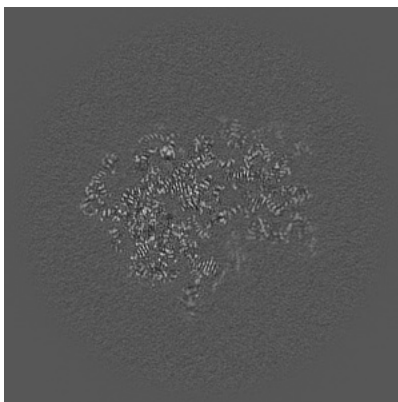
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

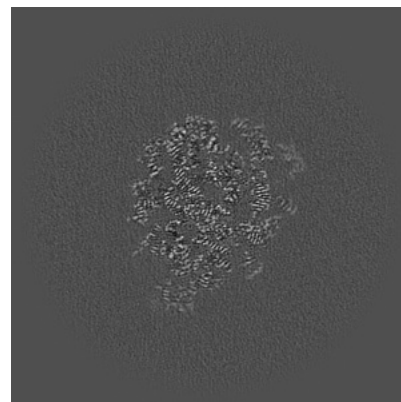
6.3.1 Primary map



X Index: 294

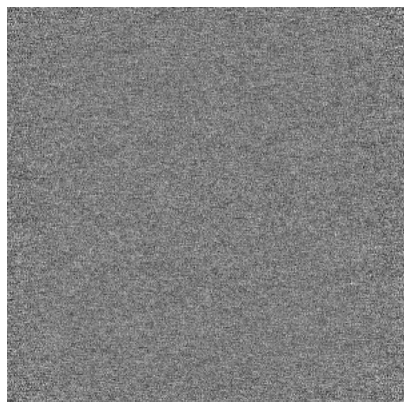


Y Index: 314

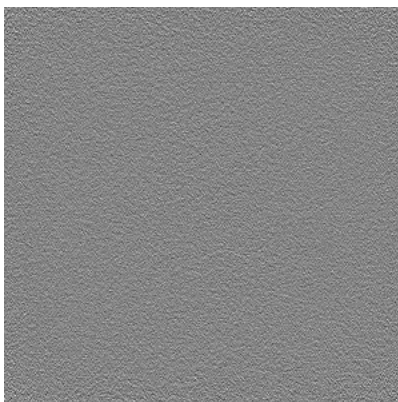


Z Index: 244

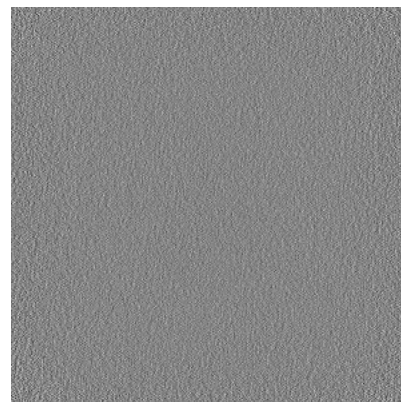
6.3.2 Raw map



X Index: 0



Y Index: 0

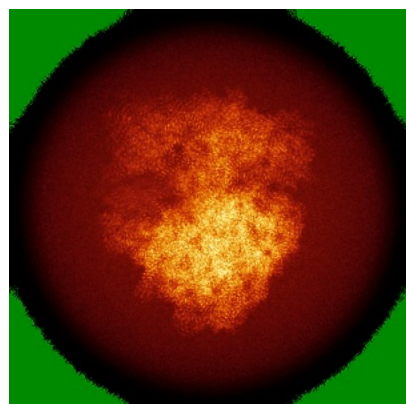


Z Index: 0

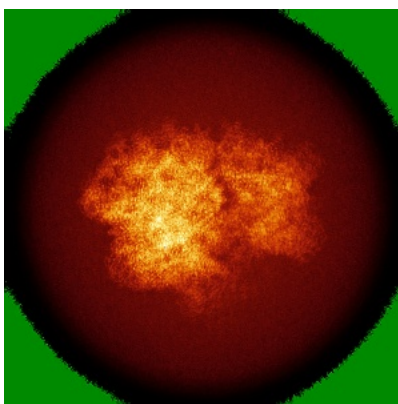
The images above show the largest variance slices of the map in three orthogonal directions.

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

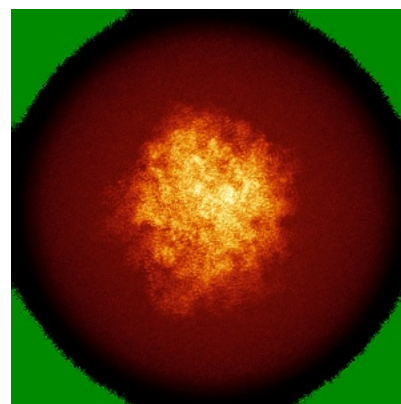
6.4.1 Primary map



X

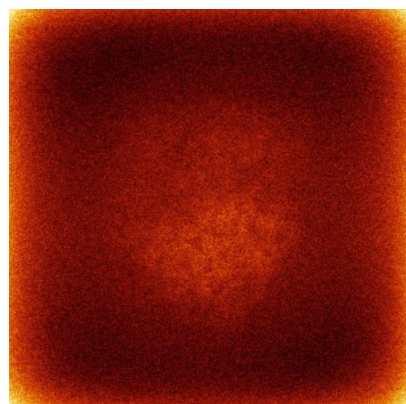


Y

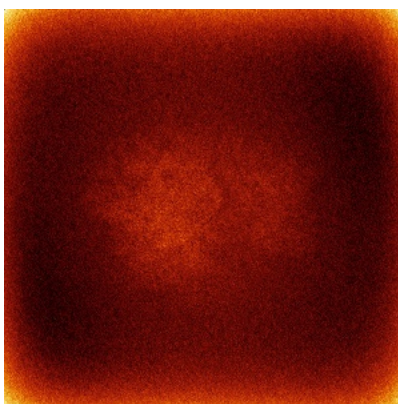


Z

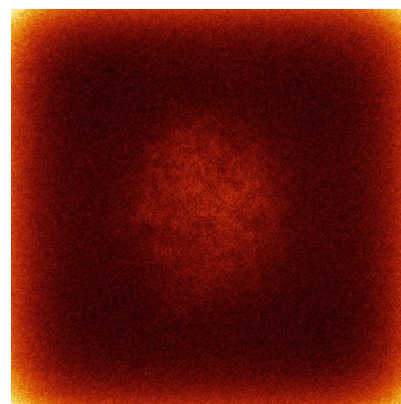
6.4.2 Raw map



X



Y

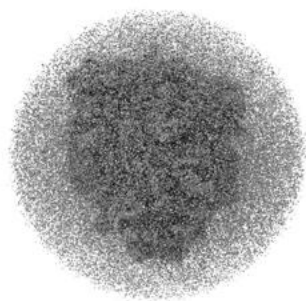


Z

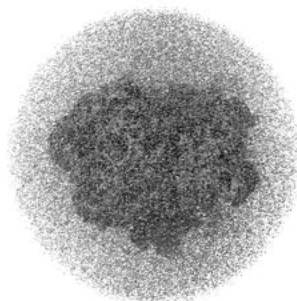
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

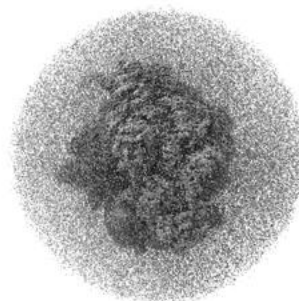
6.5.1 Primary map



X



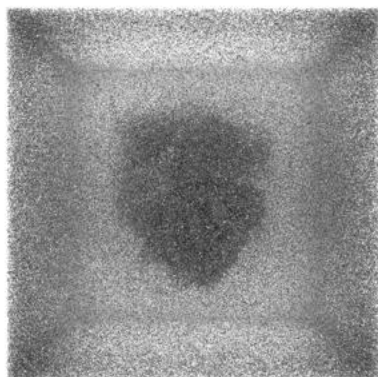
Y



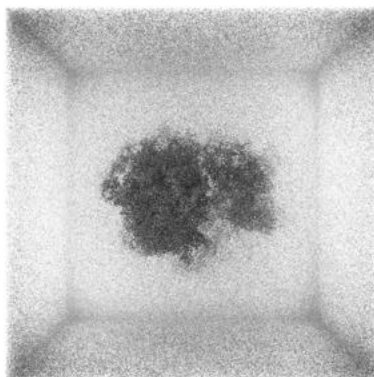
Z

The images above show the 3D surface view of the map at the recommended contour level 2.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

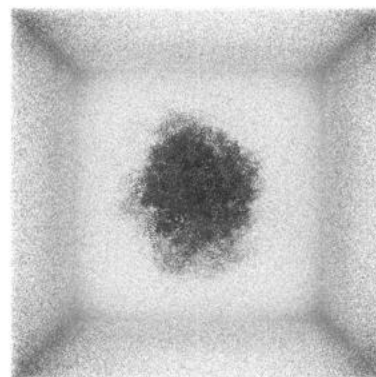
6.5.2 Raw map



X



Y



Z

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

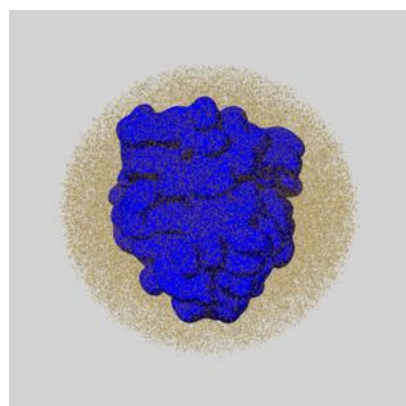
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

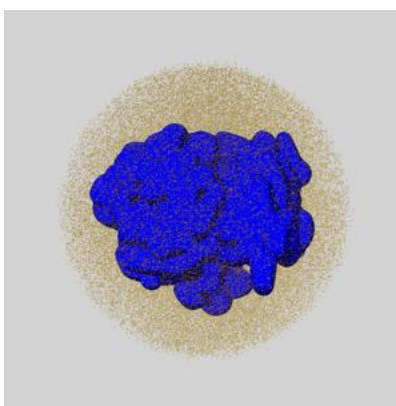
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

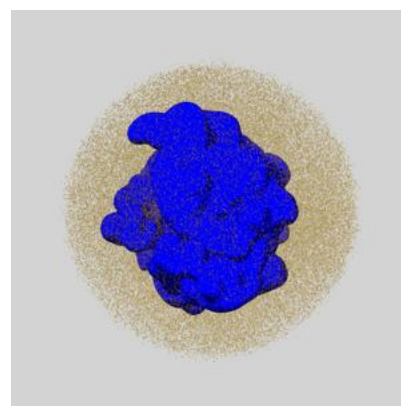
6.6.1 emd_55945_msk_1.map [i](#)



X

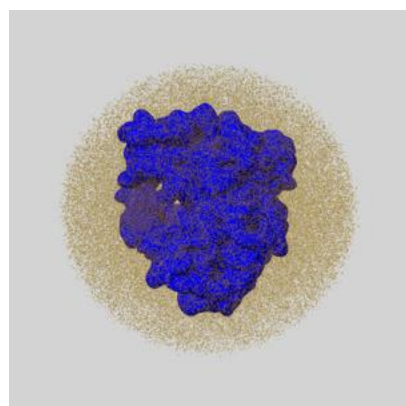


Y

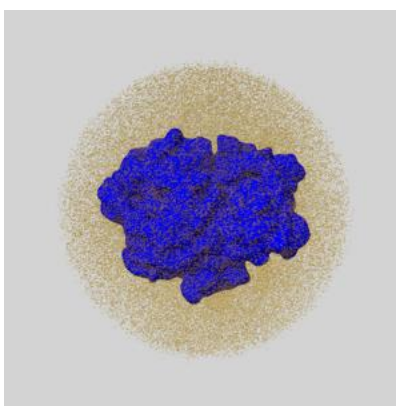


Z

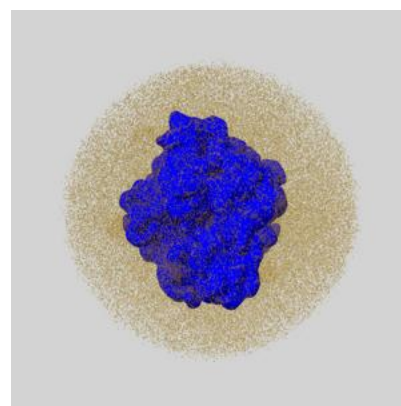
6.6.2 emd_55945_msk_2.map [i](#)



X

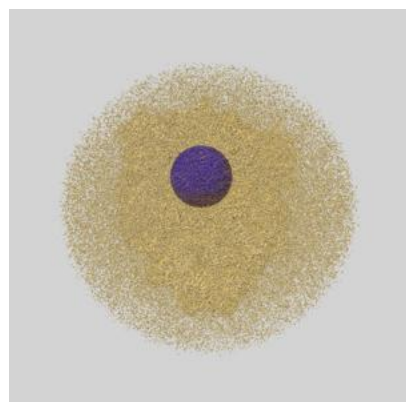


Y

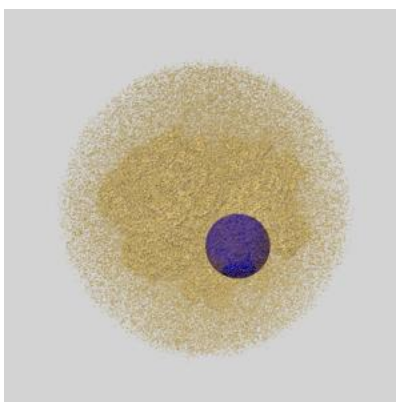


Z

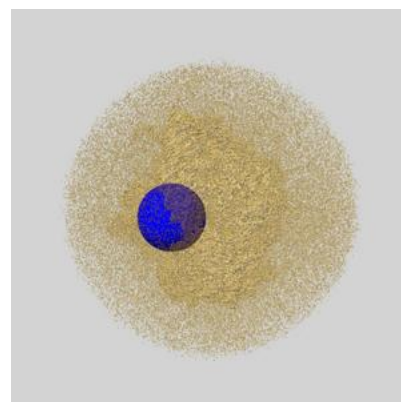
6.6.3 emd_55945_msk_3.map [i](#)



X

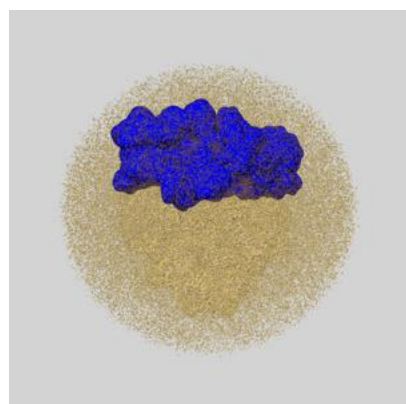


Y

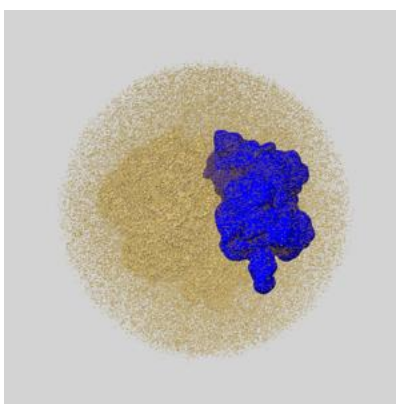


Z

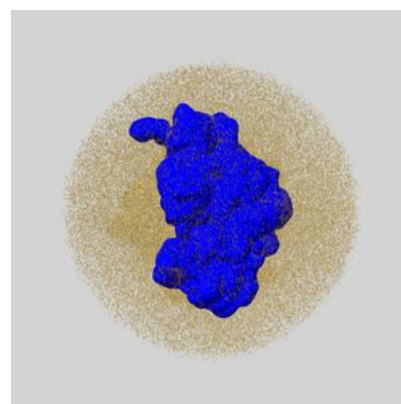
6.6.4 emd_55945_msk_4.map [i](#)



X

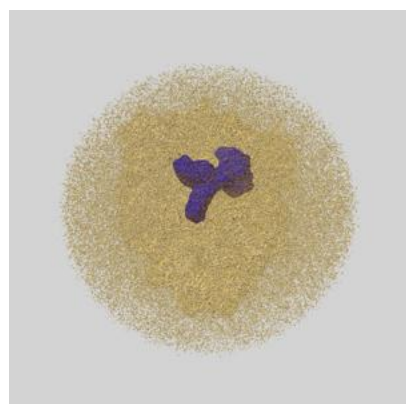


Y

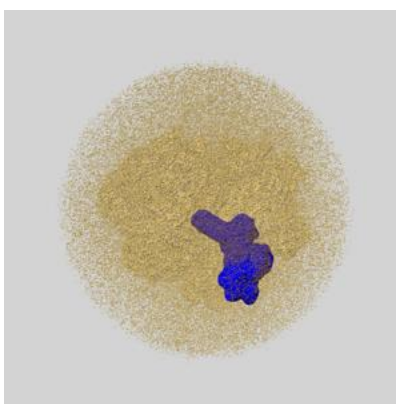


Z

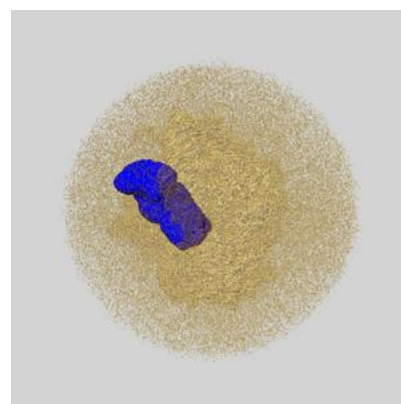
6.6.5 emd_55945_msk_5.map [i](#)



X



Y

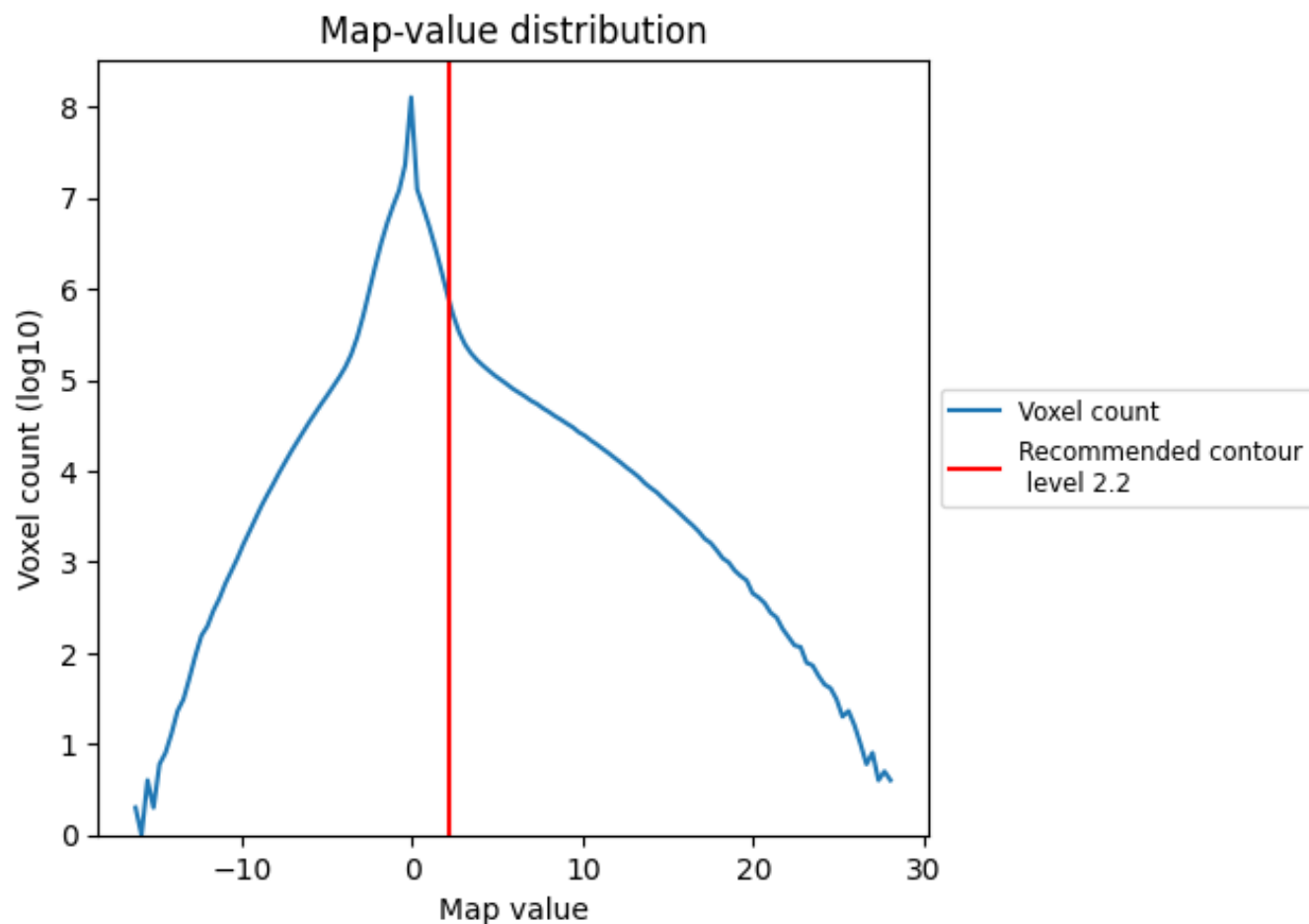


Z

7 Map analysis [i](#)

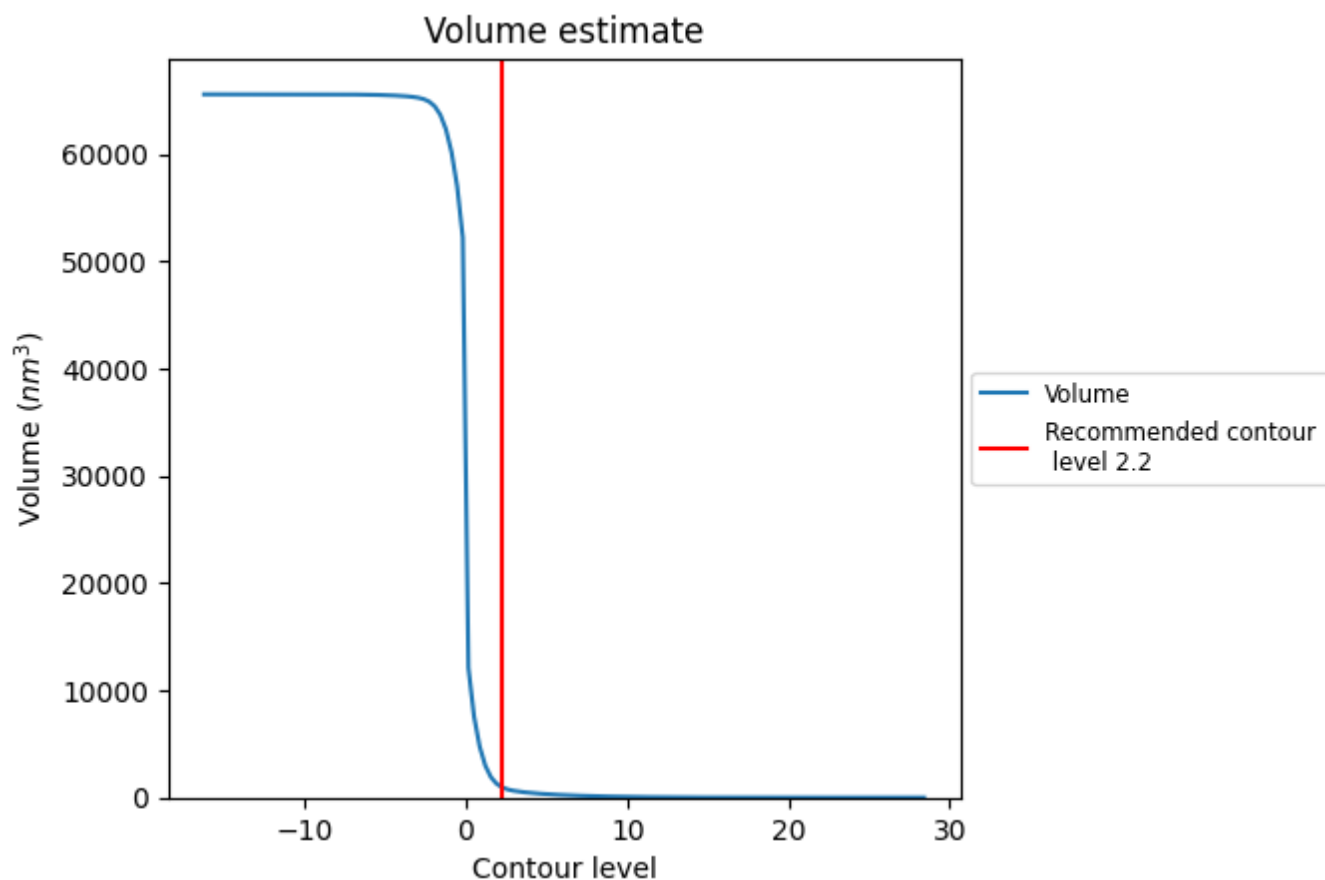
This section contains the results of statistical analysis of the map.

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.

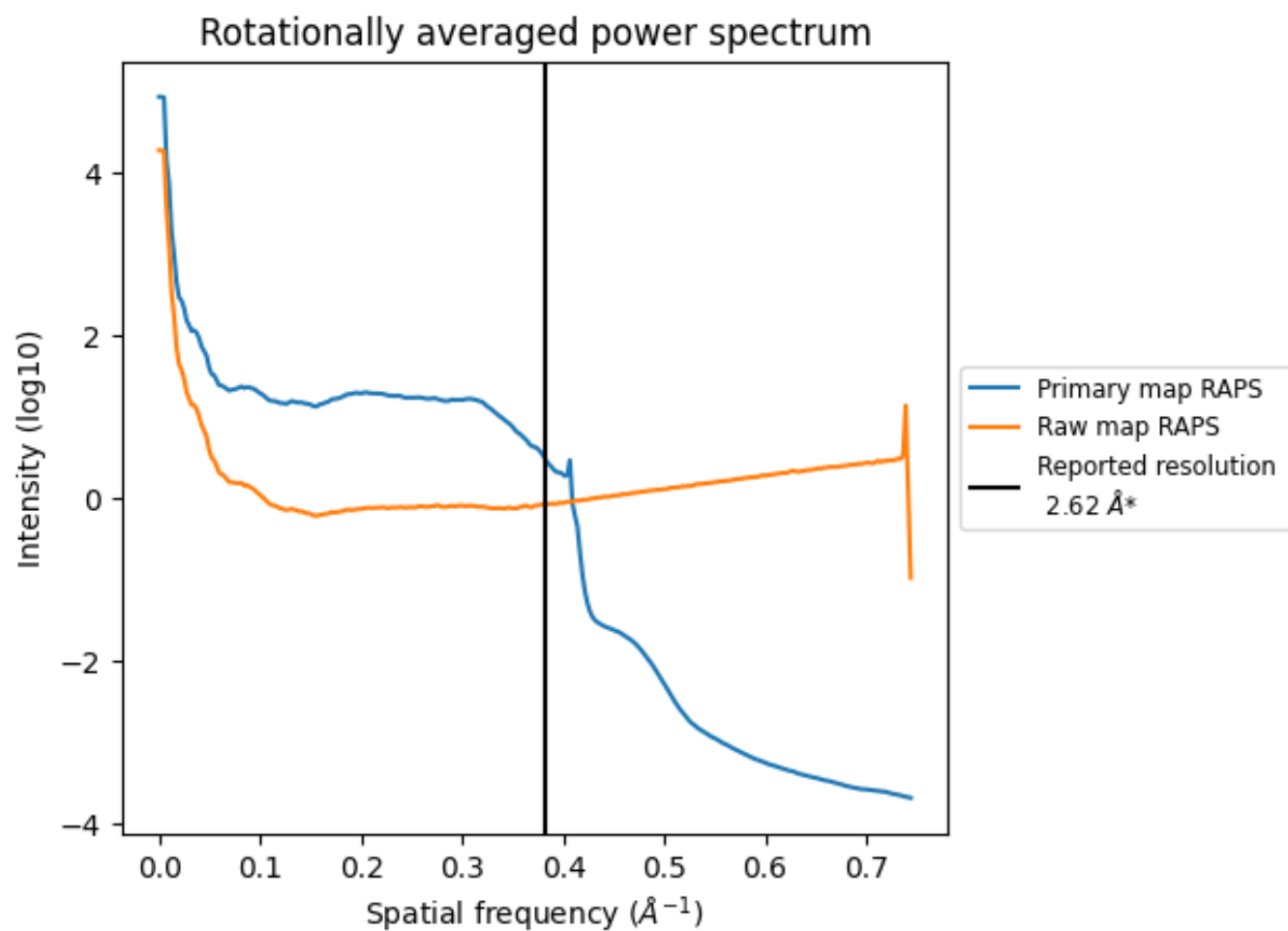
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1000 nm³; this corresponds to an approximate mass of 903 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

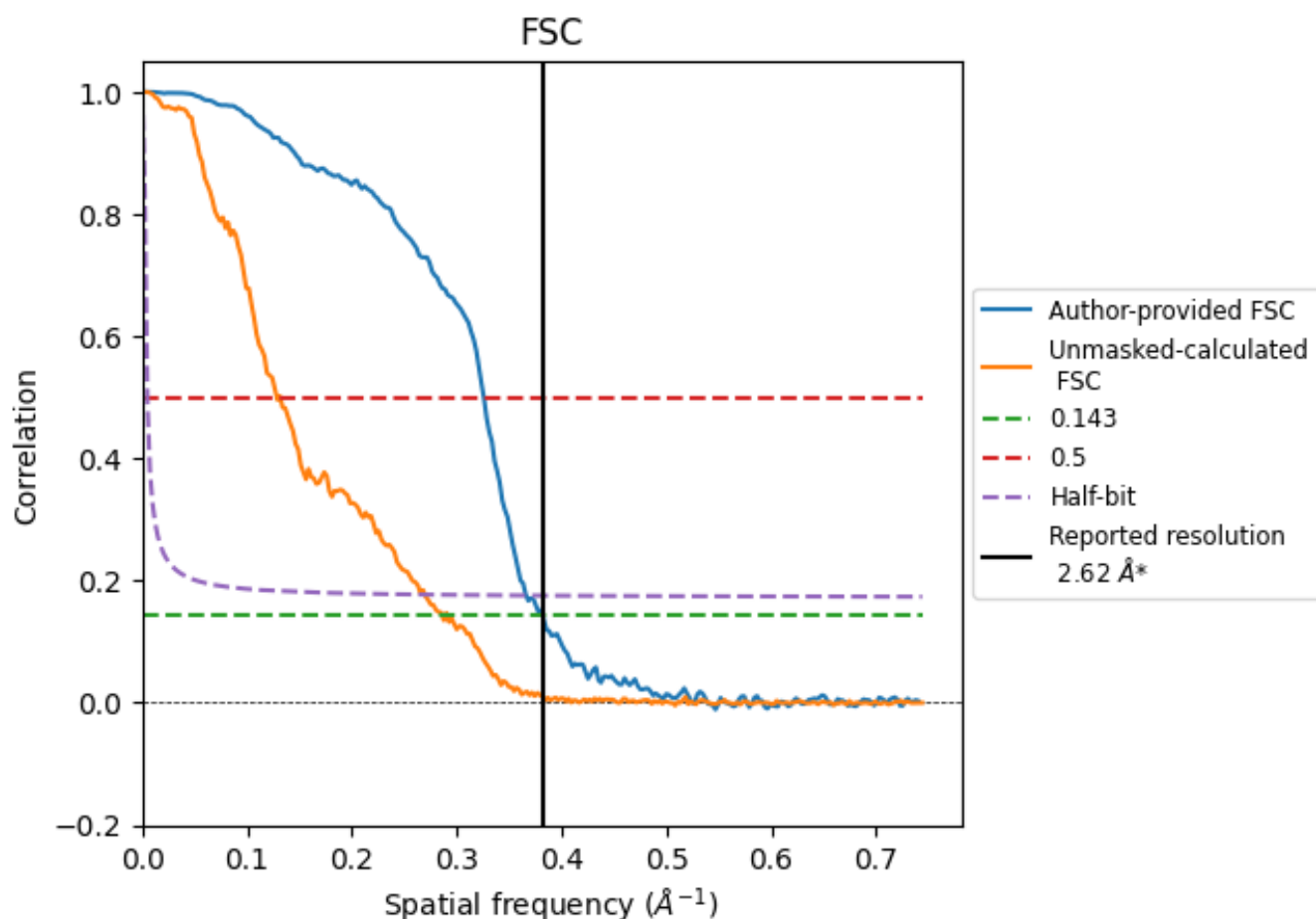


*Reported resolution corresponds to spatial frequency of 0.382 $\text{\AA}^{-1}$

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 0.382 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

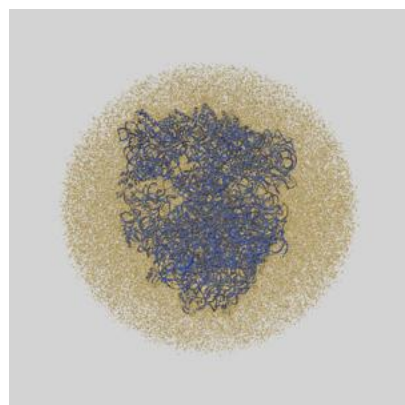
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.07	2.73
Unmasked-calculated*	3.50	7.79	3.71

*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 3.50 differs from the reported value 2.62 by more than 10 %

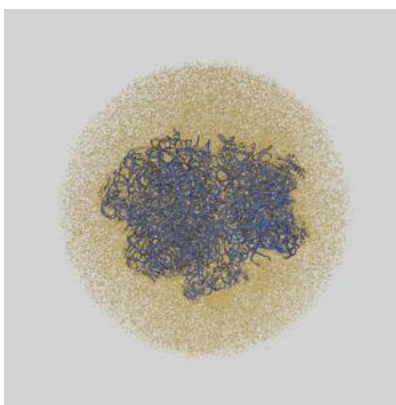
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55945 and PDB model 9TI6. Per-residue inclusion information can be found in section 3 on page 15.

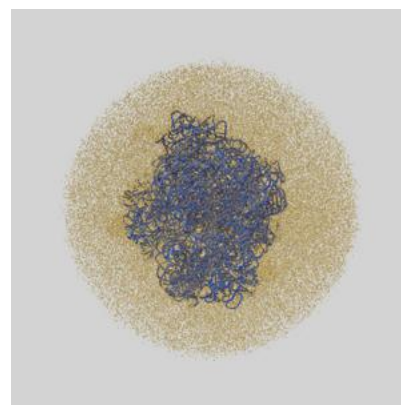
9.1 Map-model overlay [i](#)



X



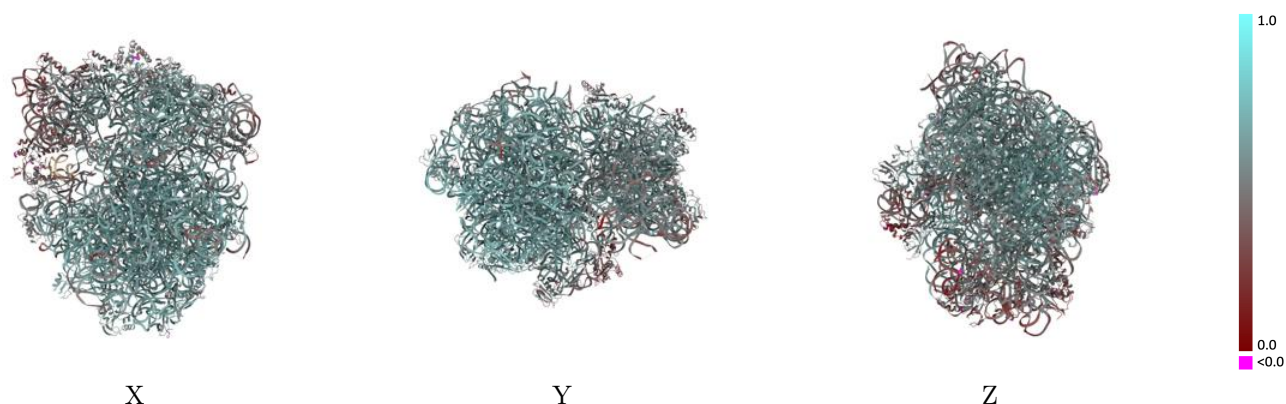
Y



Z

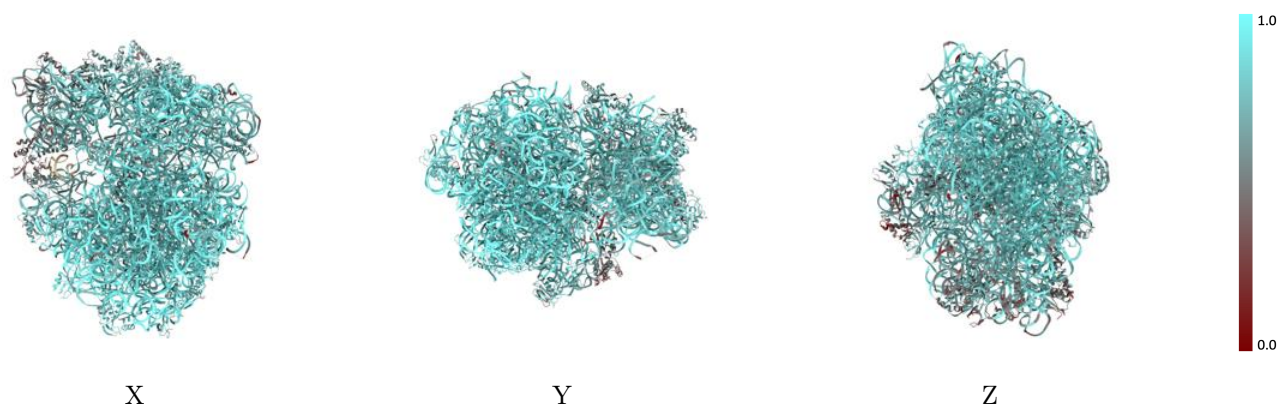
The images above show the 3D surface view of the map at the recommended contour level 2.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



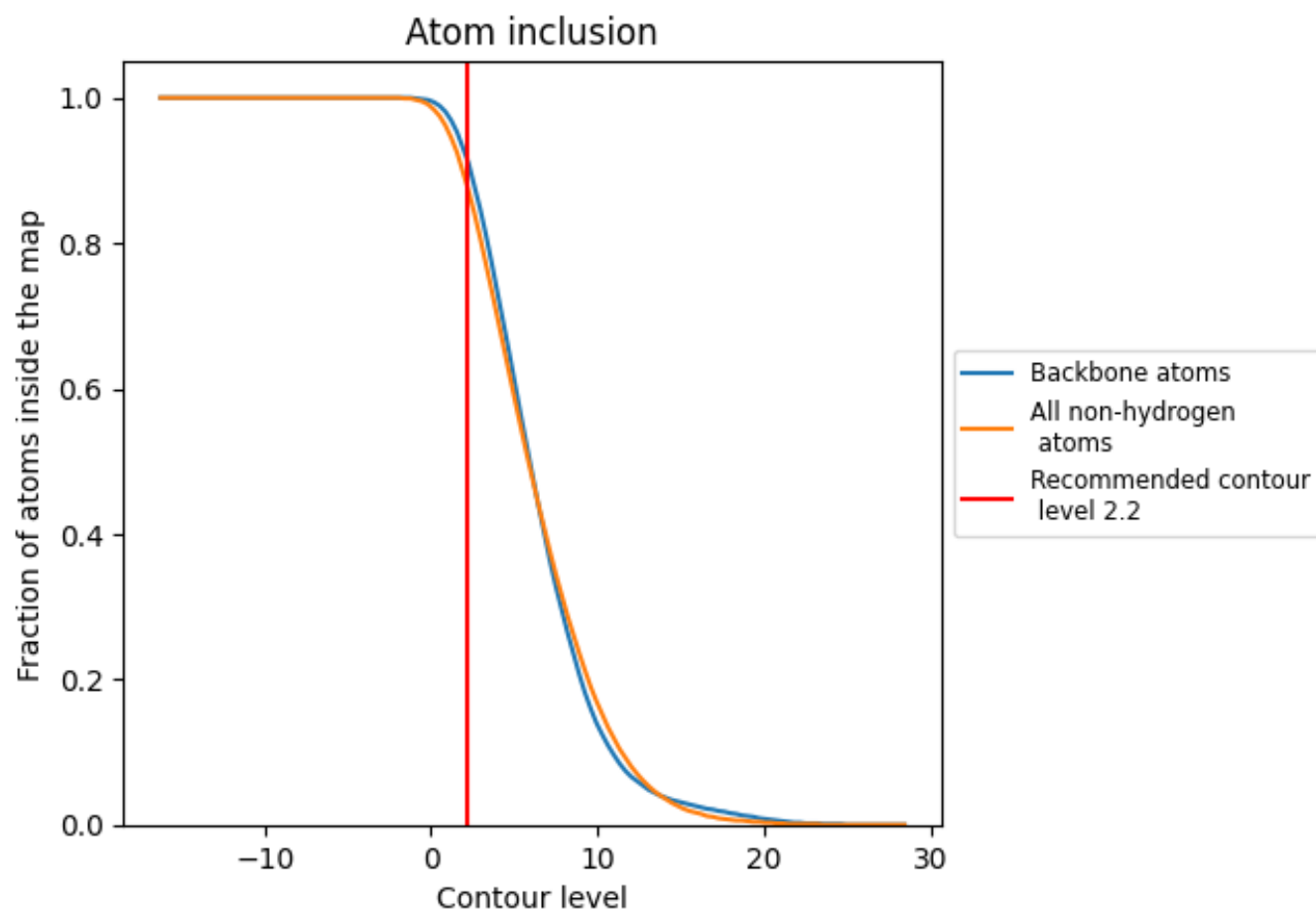
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (2.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5820
1	 0.8810	 0.6130
2	 0.8090	 0.5570
3	 0.9110	 0.6390
4	 0.4110	 0.3180
5	 0.9170	 0.6420
6	 0.7880	 0.5580
7	 0.9660	 0.6790
8	 0.9570	 0.6650
9	 0.9310	 0.6350
A	 0.9550	 0.6370
B	 0.8960	 0.5650
C	 0.5320	 0.3840
D	 0.7330	 0.4760
G	 0.9470	 0.6650
H	 0.9320	 0.6470
I	 0.8960	 0.6240
J	 0.5400	 0.3950
K	 0.7210	 0.4970
L	 0.3630	 0.2840
M	 0.9300	 0.6420
N	 0.9210	 0.6390
O	 0.9070	 0.6270
P	 0.9220	 0.6270
Q	 0.9150	 0.6340
R	 0.7390	 0.4990
S	 0.8660	 0.5920
T	 0.9370	 0.6630
U	 0.9170	 0.6280
V	 0.9280	 0.6470
W	 0.8910	 0.6200
X	 0.7810	 0.5410
Y	 0.7570	 0.5280
Z	 0.9240	 0.6310
a	 0.8760	 0.5510



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Chain	Atom inclusion	Q-score
b	 0.6970	 0.4880
c	 0.6870	 0.4870
d	 0.6630	 0.4590
e	 0.7450	 0.5090
f	 0.8790	 0.5920
g	 0.6940	 0.4660
h	 0.5670	 0.3860
i	 0.8440	 0.5800
j	 0.5920	 0.4010
k	 0.5980	 0.4210
l	 0.7220	 0.5140
m	 0.8220	 0.5710
n	 0.5790	 0.3810
o	 0.7550	 0.5010
p	 0.8160	 0.5630
q	 0.7380	 0.5070
r	 0.7360	 0.5060
s	 0.7950	 0.5520
t	 0.5250	 0.3750
u	 0.7780	 0.5310