



## wwPDB EM Validation Summary Report ⓘ

Jun 11, 2026 – 12:46 PM JST

PDB ID : 9VVI / pdb\_00009vvi  
EMDB ID : EMD-65381  
Title : Cryo-EM structure of SecM-arrested 70S ribosome with YheS  
Authors : Iso, K.; Ando, Y.; Taguchi, H.; Nureki, O.; Chadani, Y.; Itoh, Y.  
Deposited on : 2025-07-15  
Resolution : 2.82 Å(reported)  
Based on initial models : 8B0X, 8QOA

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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) : 2.49

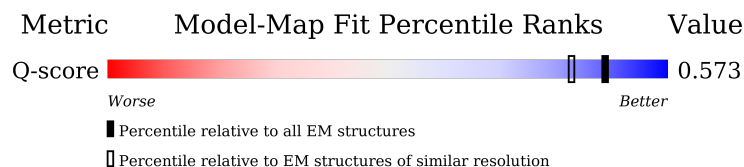
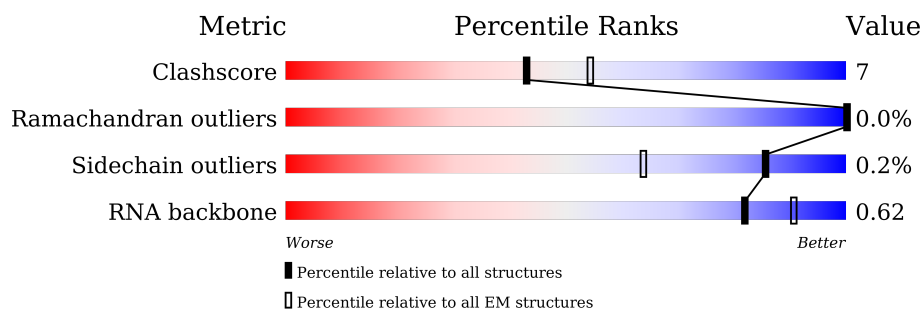
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.82 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.









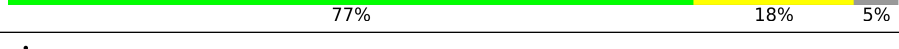
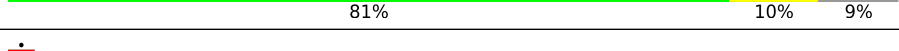
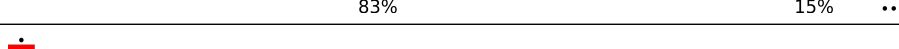
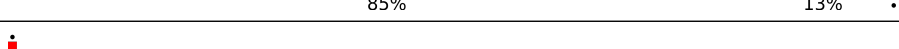
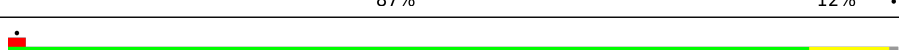
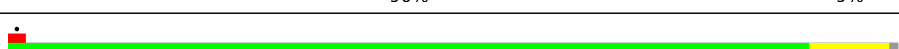
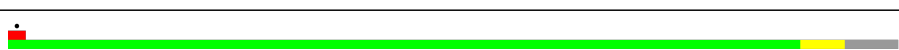

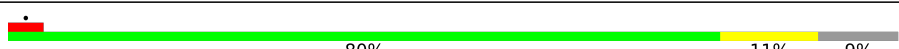
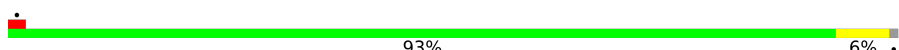
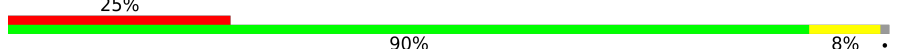



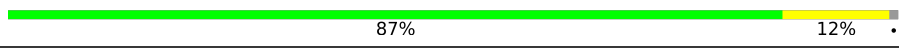
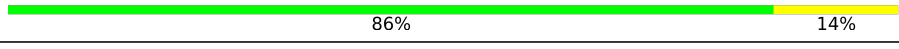



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11795 ( 2.32 - 3.32 )

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  $\geq 3$ , 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	1542	
2	B	241	
3	C	233	

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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	119	
24	7	234	
25	c	273	
26	d	209	
27	e	201	
28	f	179	


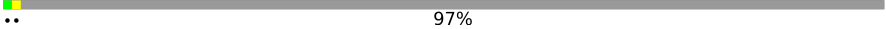


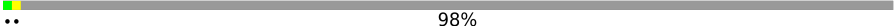
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Mol	Chain	Length	Quality of chain
29	g	177	
30	h	149	
31	i	142	
32	j	123	
33	k	144	
34	l	136	
35	m	127	
36	n	117	
37	o	115	
38	p	118	
39	q	103	
40	r	110	
41	s	100	
42	t	104	
43	u	94	
44	v	85	
45	w	78	
46	x	63	
47	y	59	
48	4	70	
49	z	57	
50	0	55	
51	1	46	
52	2	65	
53	3	38	

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Mol	Chain	Length	Quality of chain
54	W	647	
55	X	629	
56	Y	77	
57	Z	76	
58	6	165	

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 150953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1525	Total	C	N	O	P	0	0
			32741	14609	6009	10598	1525		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2845	Total	C	N	O	P	0	0
			61098	27261	11245	19747	2845		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2550	1135	466	830	119		

- Molecule 24 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7	230	Total	C	N	O	S	0	0
			1702	1063	309	324	6		

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	136	Total	C	N	O	S	1	0
			1083	691	208	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 49 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 50 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	51	Total	C	N	O	S	0	0
			417	269	76	72			

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a protein called Probable ATP-binding protein YheS.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	531	Total	C	N	O	S	3	0
			4241	2678	768	786	9		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-9	MET	-	initiating methionine	UNP P63390
W	-8	ARG	-	expression tag	UNP P63390
W	-7	GLY	-	expression tag	UNP P63390
W	-6	HIS	-	expression tag	UNP P63390
W	-5	HIS	-	expression tag	UNP P63390
W	-4	HIS	-	expression tag	UNP P63390
W	-3	HIS	-	expression tag	UNP P63390
W	-2	HIS	-	expression tag	UNP P63390
W	-1	HIS	-	expression tag	UNP P63390
W	0	GLY	-	expression tag	UNP P63390
W	1	SER	-	expression tag	UNP P63390
W	175	GLN	GLU	engineered mutation	UNP P63390
W	456	GLN	GLU	engineered mutation	UNP P63390

- Molecule 55 is a RNA chain called SecM mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X	16	Total	C	N	O	P	0	0
			336	150	58	112	16		

- Molecule 56 is a RNA chain called A-site tRNA (prolyl-tRNA<sup>Pro</sup>).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Y	77	Total	C	N	O	P	0	0
			1651	736	295	543	77		

- Molecule 57 is a RNA chain called P-site tRNA (tRNA<sup>Gly</sup>).

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Z	76	Total	C	N	O	P	S	0	0
			1624	724	287	536	76	1		

- Molecule 58 is a protein called Secretion monitor.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	6	3	Total	C	N	O	0	0
			20	11	6	3		

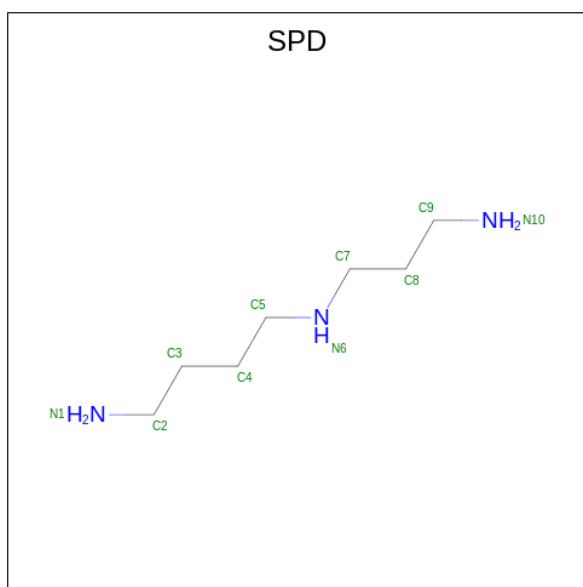
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	A	34	Total 34	K 34	0
59	a	84	Total 84	K 84	0
59	c	4	Total 4	K 4	0
59	e	1	Total 1	K 1	0
59	t	1	Total 1	K 1	0
59	Z	1	Total 1	K 1	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	70	Total 70	Mg 70	0
60	B	1	Total 1	Mg 1	0
60	a	186	Total 186	Mg 186	0
60	b	4	Total 4	Mg 4	0
60	c	2	Total 2	Mg 2	0
60	d	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	z	1	Total 1	Mg 1	0
60	W	2	Total 2	Mg 2	0
60	X	1	Total 1	Mg 1	0

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



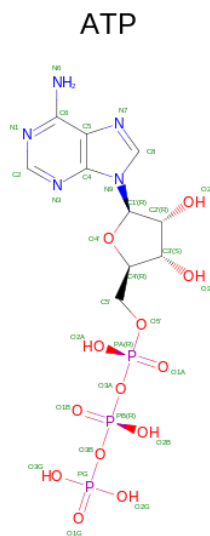
Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	4	1	Total	Zn	0
			1	1	
62	3	1	Total	Zn	0
			1	1	

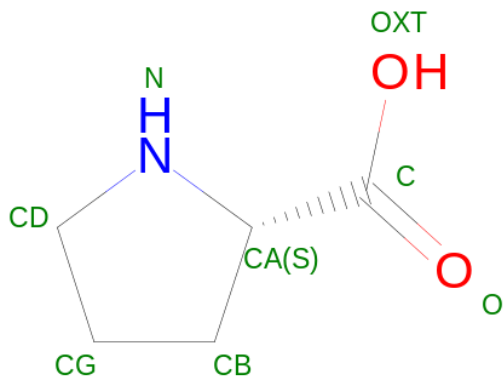
- Molecule 63 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
63	W	1	Total 31	C 10	N 5	O 13	P 3	0
63	W	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 64 is PROLINE (CCD ID: PRO) (formula:  $\text{C}_5\text{H}_9\text{NO}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
64	Y	1	Total	C	N	O	0
			7	5	1	1	

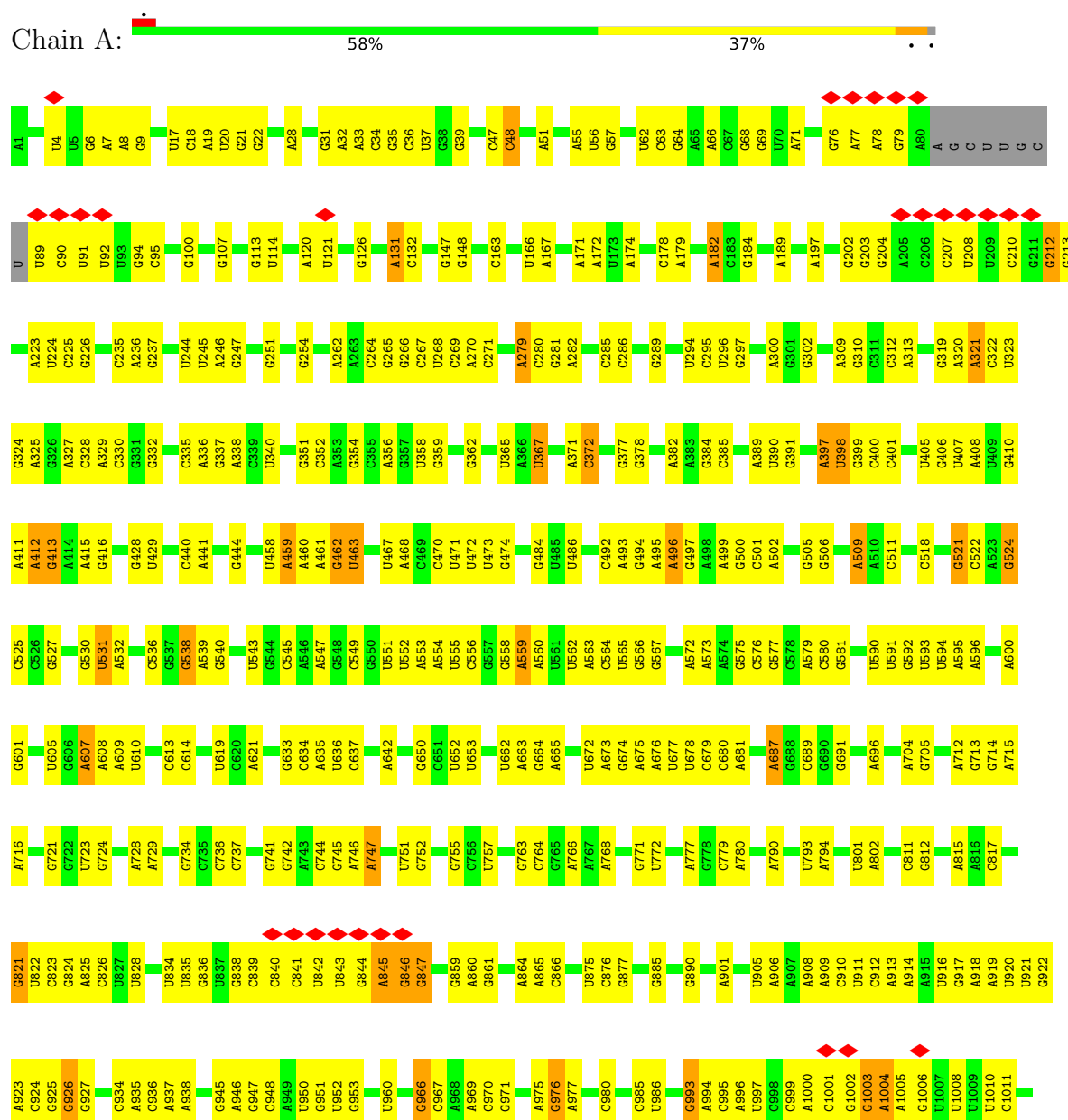
- Molecule 65 is water.

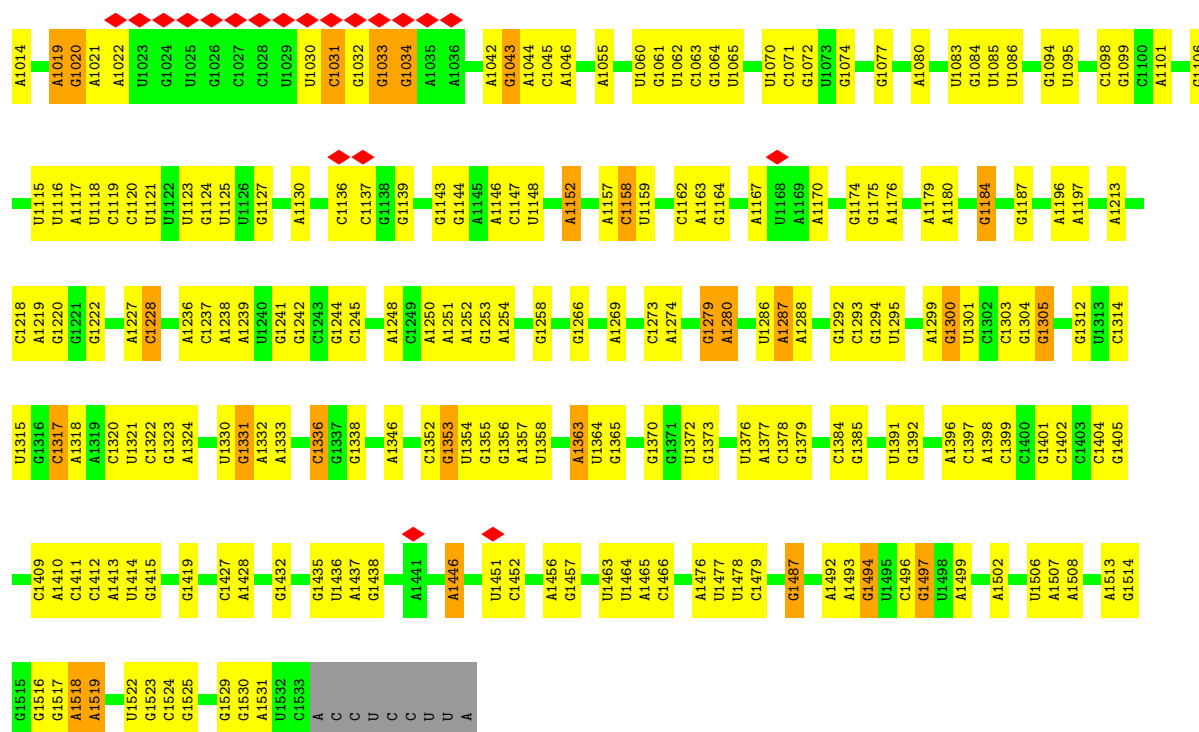
Mol	Chain	Residues	Atoms		AltConf
65	a	18	Total 18	O 18	0

### 3 Residue-property plots

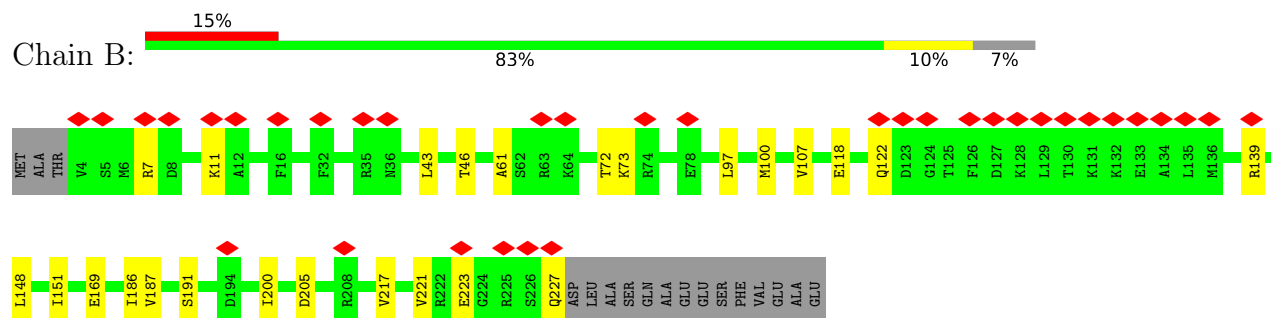
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

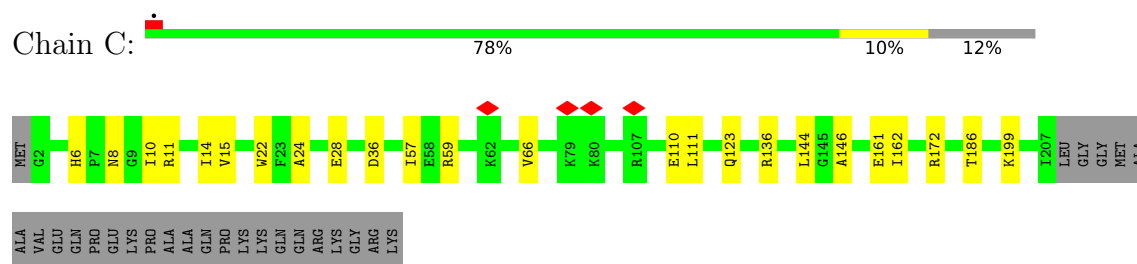




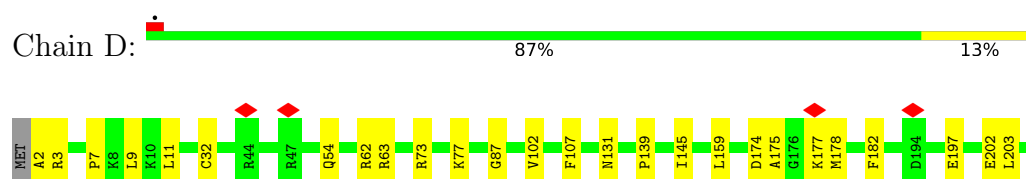
• Molecule 2: 30S ribosomal protein S2



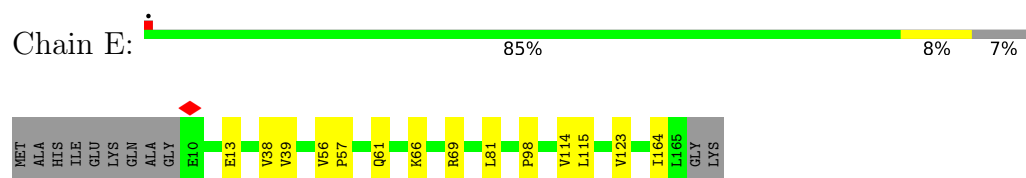
• Molecule 3: Small ribosomal subunit protein uS3



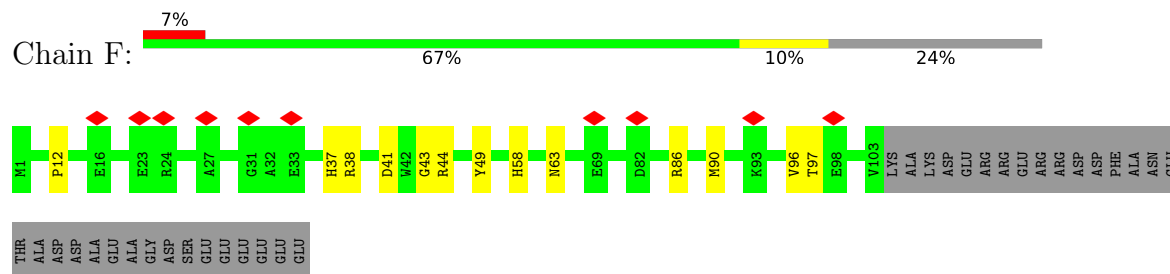
• Molecule 4: Small ribosomal subunit protein uS4



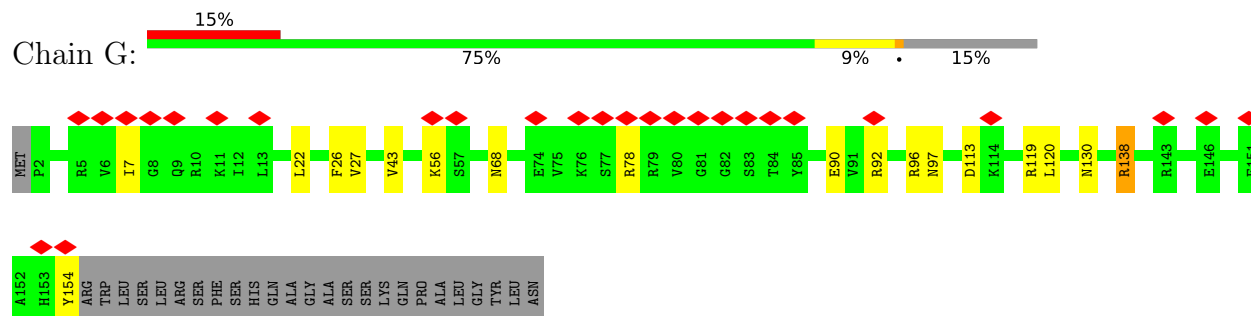
- Molecule 5: Small ribosomal subunit protein uS5



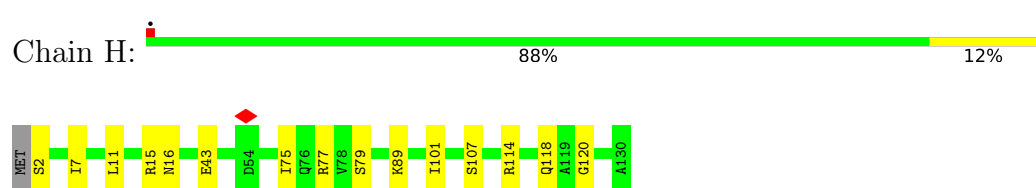
- Molecule 6: 30S ribosomal protein S6, fully modified isoform



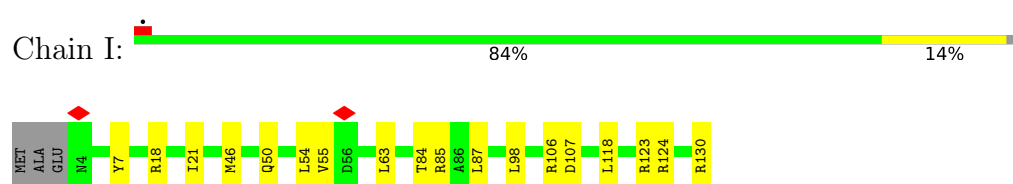
- Molecule 7: Small ribosomal subunit protein uS7



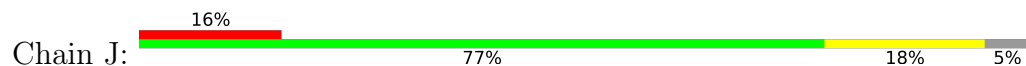
- Molecule 8: Small ribosomal subunit protein uS8

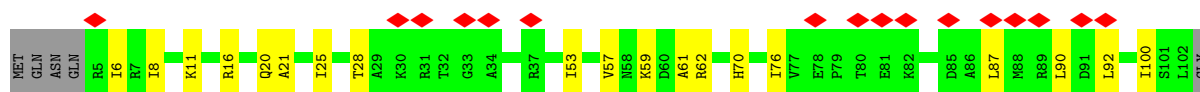


- Molecule 9: Small ribosomal subunit protein uS9

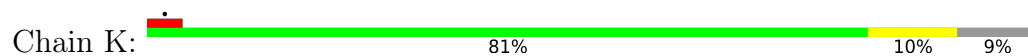


- Molecule 10: Small ribosomal subunit protein uS10

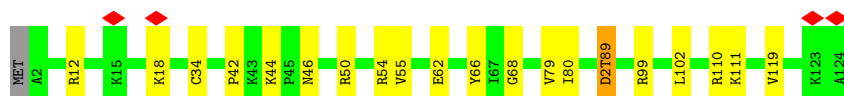
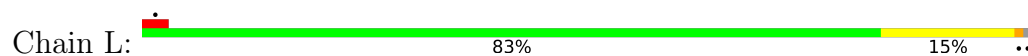




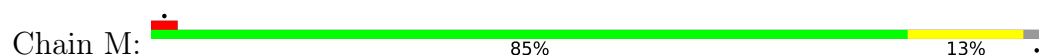
- Molecule 11: Small ribosomal subunit protein uS11



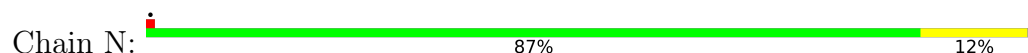
- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13



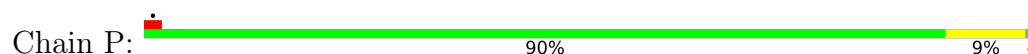
- Molecule 14: Small ribosomal subunit protein uS14




- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16




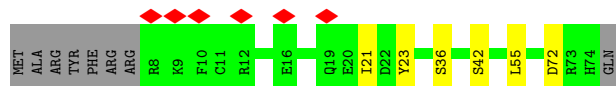
- Molecule 17: Small ribosomal subunit protein uS17

Chain Q:  89% 5% 6%




- Molecule 18: Small ribosomal subunit protein bS18

Chain R:  8% 81% 8% 11%



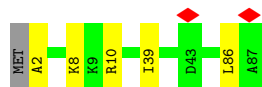
- Molecule 19: Small ribosomal subunit protein uS19

Chain S:  80% 11% 9%




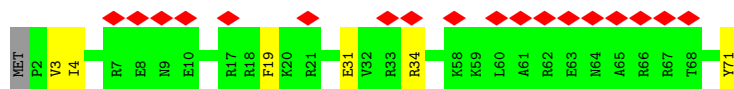
- Molecule 20: Small ribosomal subunit protein bS20

Chain T:  93% 6%



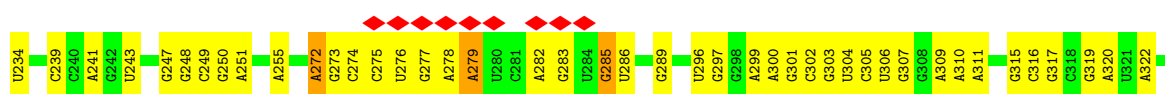
- Molecule 21: 30S ribosomal protein S21

Chain U:  25% 90% 8%



- Molecule 22: 23S rRNA

Chain a:  60% 35%

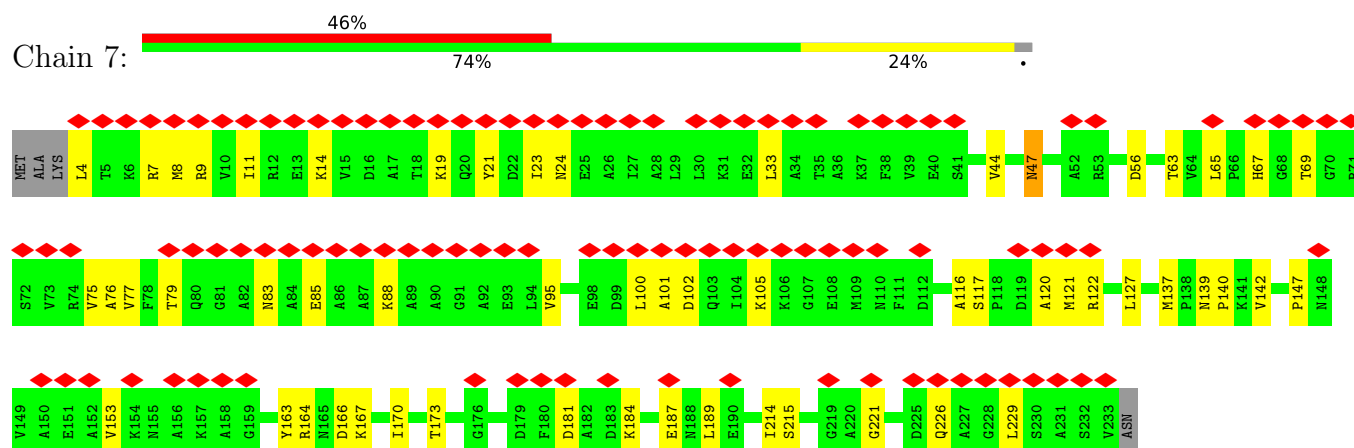




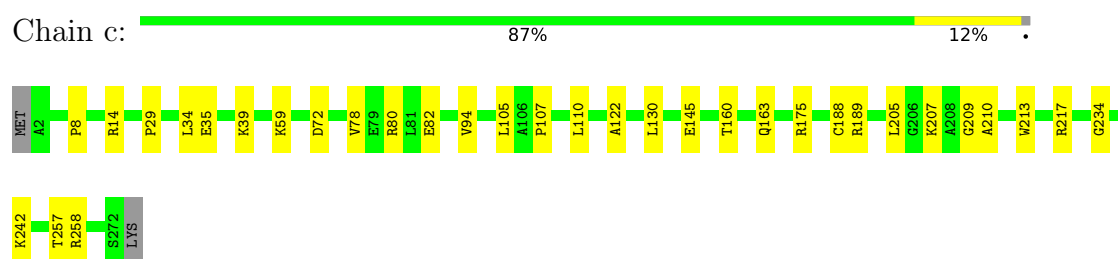




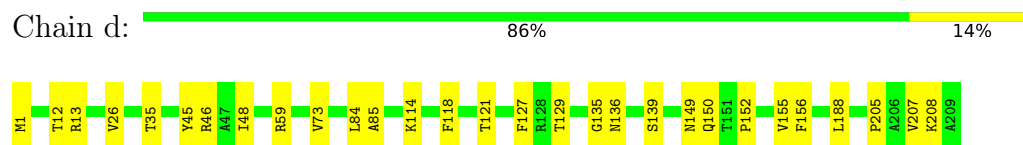
- Molecule 24: Large ribosomal subunit protein uL1



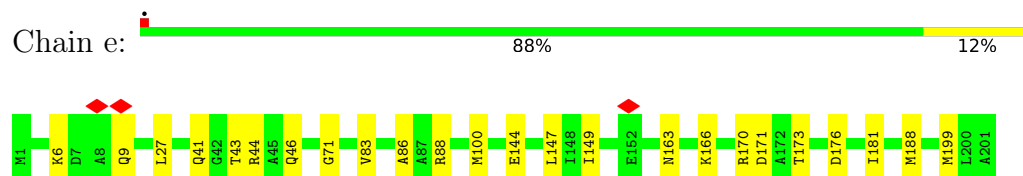
- Molecule 25: Large ribosomal subunit protein uL2



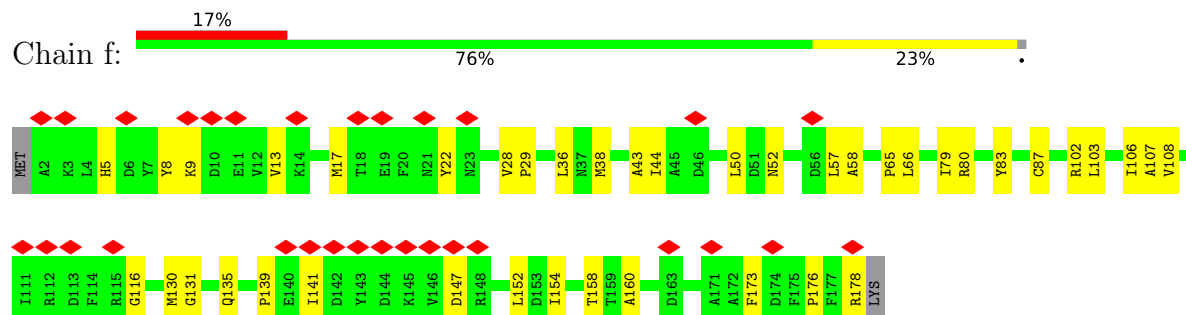
- Molecule 26: 50S ribosomal protein L3



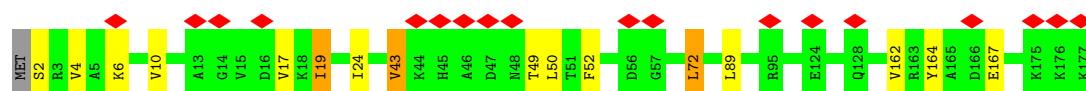
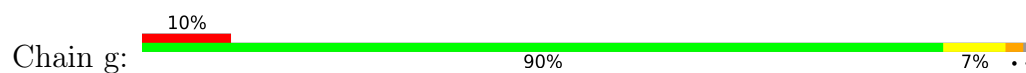
- Molecule 27: 50S ribosomal protein L4



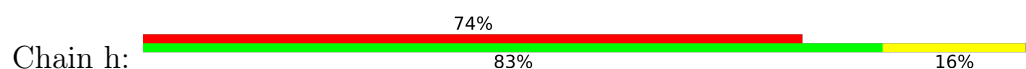
- Molecule 28: Large ribosomal subunit protein uL5



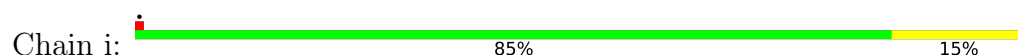
- Molecule 29: Large ribosomal subunit protein uL6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L13



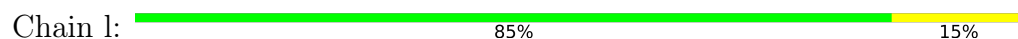
- Molecule 32: 50S ribosomal protein L14




- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16




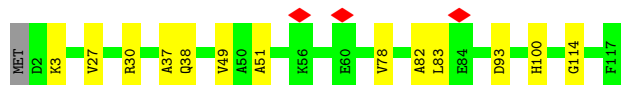
- Molecule 35: Large ribosomal subunit protein bL17

Chain m:  82% 11% 7%



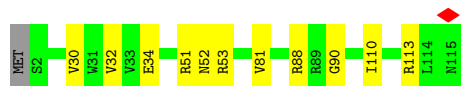
- Molecule 36: Large ribosomal subunit protein uL18

Chain n:  88% 11% .

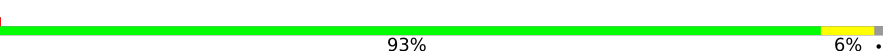


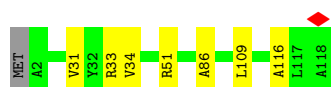
- Molecule 37: Large ribosomal subunit protein bL19

Chain o:  90% 10% .




- Molecule 38: Large ribosomal subunit protein bL20

Chain p:  93% 6% .




- Molecule 39: 50S ribosomal protein L21

Chain q:  89% 11%




- Molecule 40: 50S ribosomal protein L22

Chain r:  89% 11%

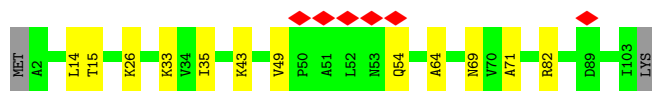
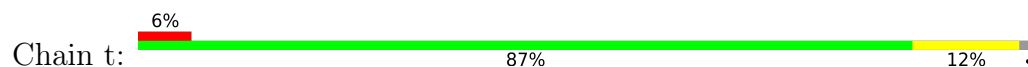


- Molecule 41: Large ribosomal subunit protein uL23

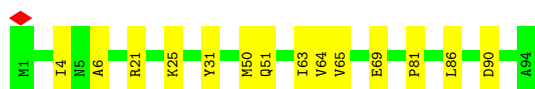
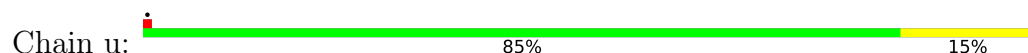
Chain s:  88% 5% 7%



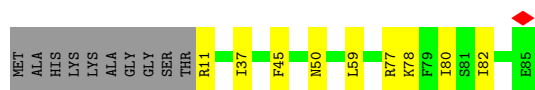
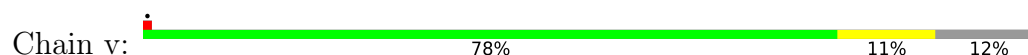
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



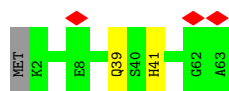
- Molecule 44: Large ribosomal subunit protein bL27



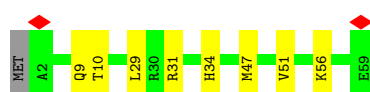
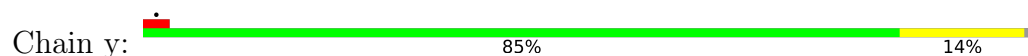
- Molecule 45: Large ribosomal subunit protein bL28



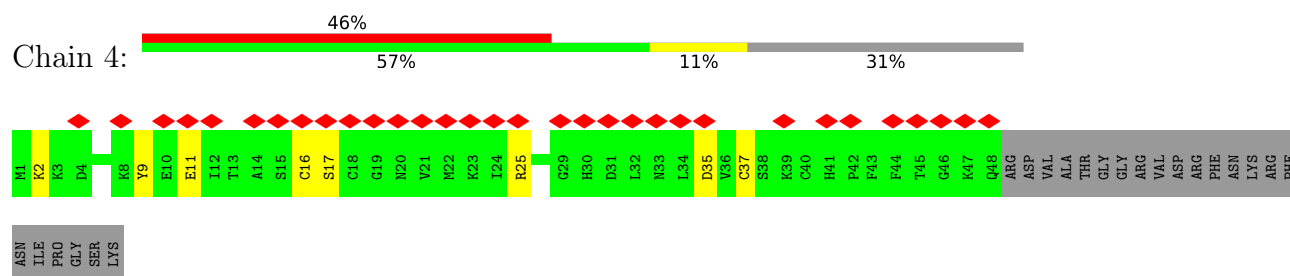
- Molecule 46: Large ribosomal subunit protein uL29



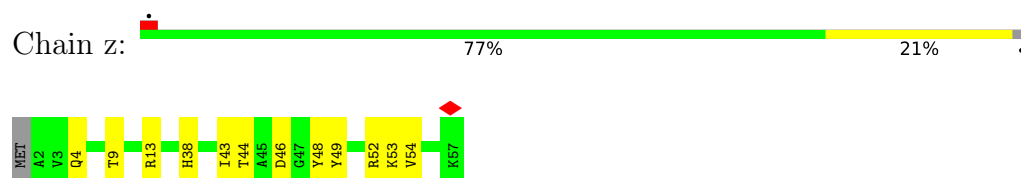
- Molecule 47: Large ribosomal subunit protein uL30



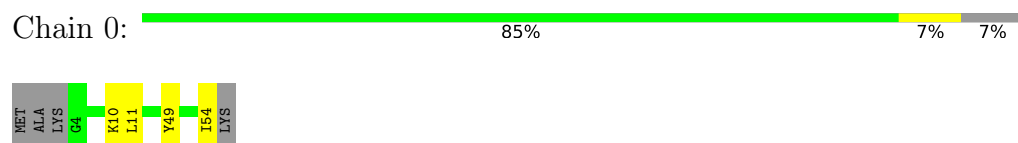
- Molecule 48: 50S ribosomal protein L31



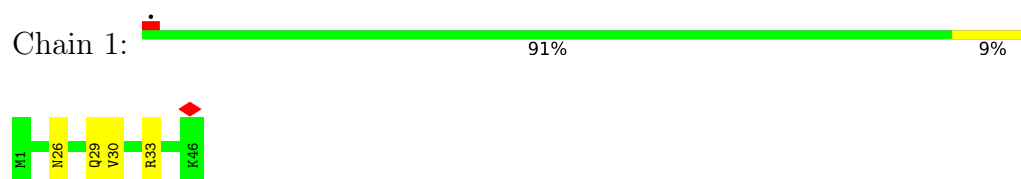
- Molecule 49: Large ribosomal subunit protein bL32



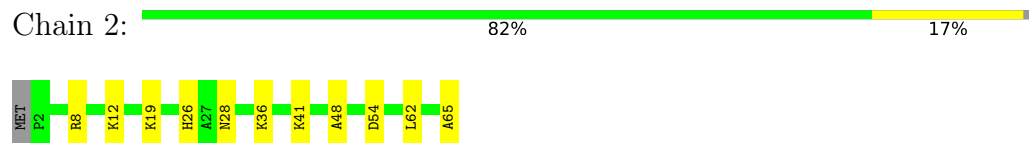
- Molecule 50: Large ribosomal subunit protein bL33



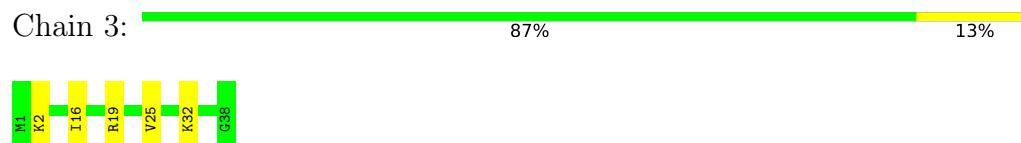
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: Large ribosomal subunit protein bL35

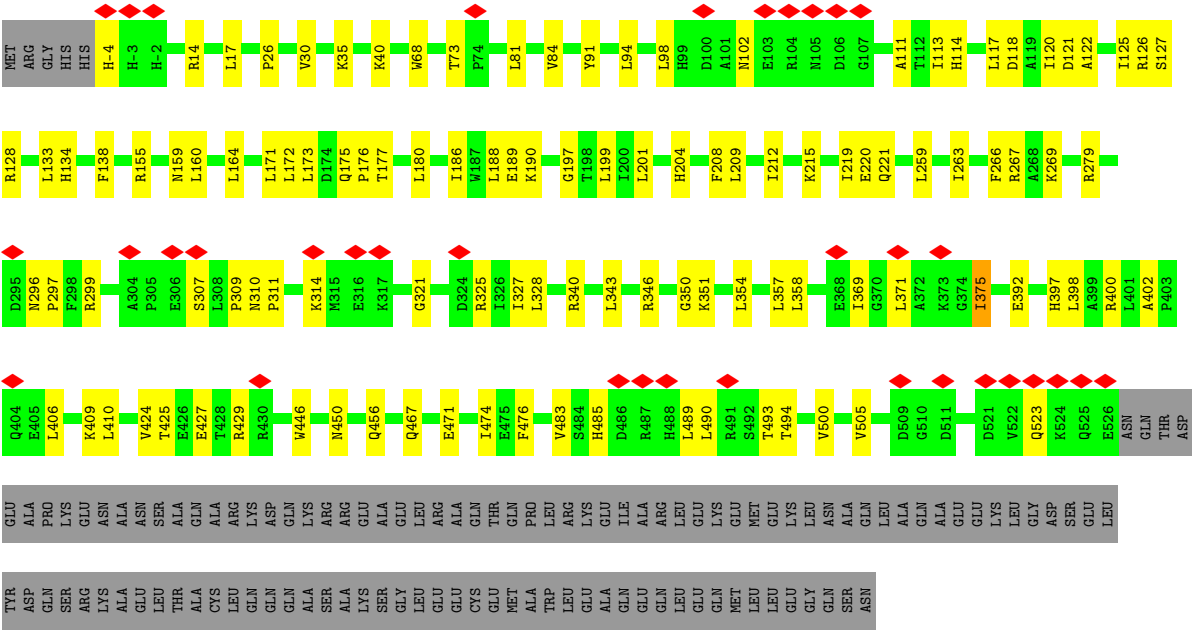


- Molecule 53: 50S ribosomal protein L36

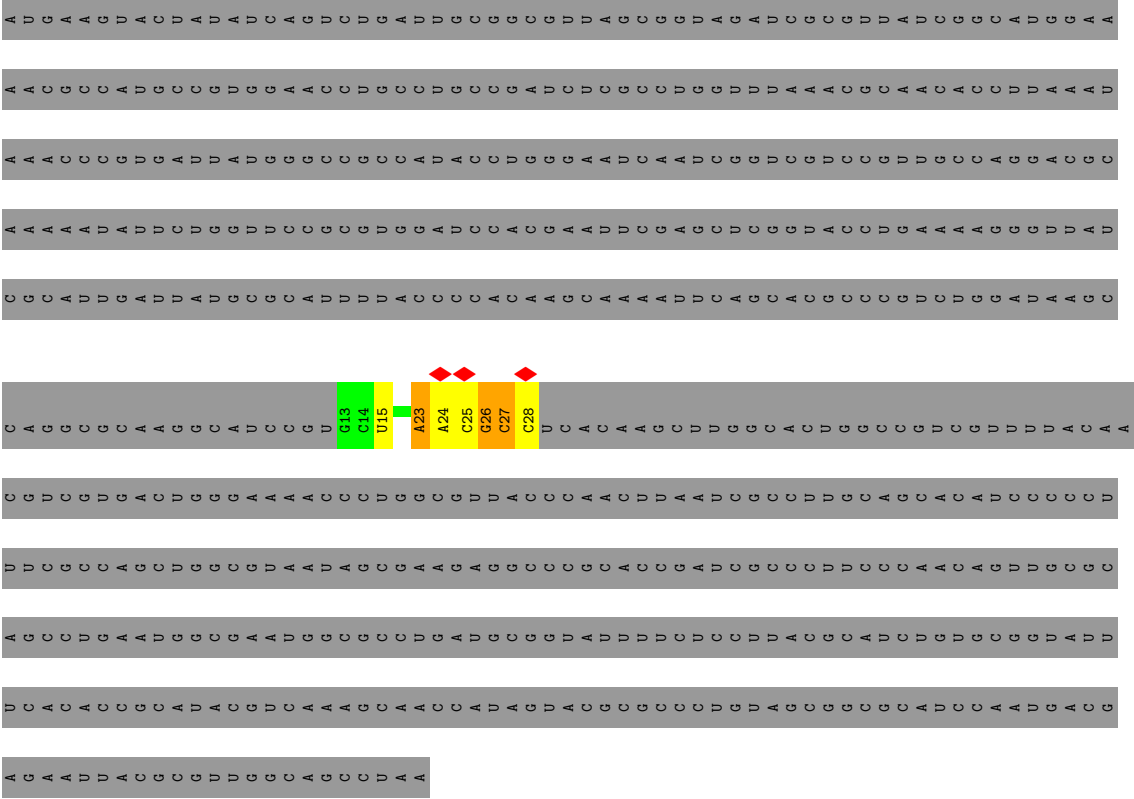


- Molecule 54: Probable ATP-binding protein YheS



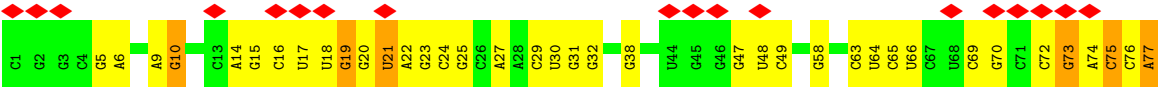


• Molecule 55: SecM mRNA

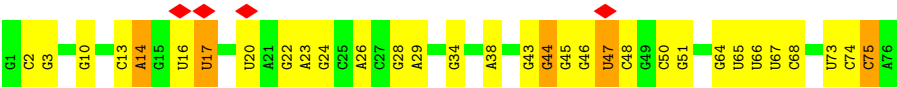


• Molecule 56: A-site tRNA (prolyl-tRNAPro)

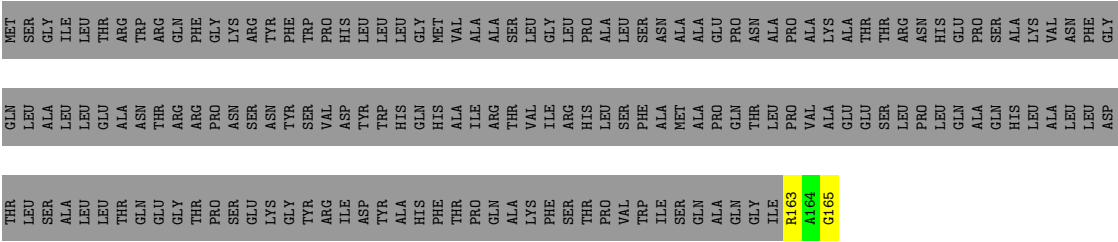




• Molecule 57: P-site tRNA (tRNA<sup>Gly</sup>)



• Molecule 58: Secretion monitor





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50797	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)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.356	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	431.60004, 431.60004, 431.60004	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6660494, 0.6660494, 0.6660494	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, MA6, IAS, 2MG, K, G7M, D2T, 5MU, OMG, 1MG, SPD, OMC, 2MA, MG, PSU, UR3, 5MC, 3TD, ZN, ATP, 4D4, H2U, 6MZ, 4SU, OMU, MEQ, MS6

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	0.11	0/36381	0.24	0/56747
2	B	0.11	0/1784	0.29	0/2403
3	C	0.12	0/1651	0.28	0/2225
4	D	0.10	0/1665	0.25	0/2227
5	E	0.13	0/1165	0.29	0/1568
6	F	0.12	0/858	0.29	0/1160
7	G	0.11	0/1219	0.29	0/1635
8	H	0.11	0/989	0.30	0/1326
9	I	0.12	0/1034	0.29	0/1375
10	J	0.12	0/796	0.31	0/1077
11	K	0.11	0/884	0.25	0/1191
12	L	0.12	0/960	0.30	0/1286
13	M	0.11	0/900	0.32	1/1204 (0.1%)
14	N	0.10	0/817	0.24	0/1088
15	O	0.10	0/722	0.26	0/964
16	P	0.11	0/653	0.32	0/877
17	Q	0.11	0/650	0.27	0/871
18	R	0.11	0/564	0.25	0/756
19	S	0.10	0/685	0.25	0/922
20	T	0.14	0/676	0.25	0/895
21	U	0.11	0/597	0.25	0/792
22	a	0.11	0/67853	0.25	0/105848
23	b	0.10	0/2851	0.25	0/4444
24	7	0.13	0/1717	0.31	0/2316
25	c	0.13	0/2121	0.31	0/2852
26	d	0.14	0/1576	0.32	0/2119
27	e	0.11	0/1571	0.28	0/2113
28	f	0.12	0/1434	0.33	0/1926
29	g	0.12	0/1343	0.31	0/1816
30	h	0.13	0/1112	0.32	0/1503
31	i	0.10	0/1152	0.24	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	j	0.12	0/955	0.30	0/1279
33	k	0.11	0/1062	0.28	0/1413
34	l	0.12	0/1084	0.28	0/1447
35	m	0.13	0/958	0.32	0/1281
36	n	0.11	0/902	0.27	0/1209
37	o	0.12	0/929	0.29	0/1242
38	p	0.11	0/960	0.25	0/1278
39	q	0.12	0/829	0.31	0/1107
40	r	0.13	0/864	0.31	0/1156
41	s	0.10	0/744	0.26	0/994
42	t	0.11	0/787	0.26	0/1051
43	u	0.12	0/766	0.29	0/1025
44	v	0.10	0/582	0.28	0/769
45	w	0.11	0/635	0.25	0/848
46	x	0.09	0/502	0.21	0/667
47	y	0.11	0/453	0.29	0/605
48	4	0.09	0/380	0.28	0/508
49	z	0.10	0/450	0.25	0/599
50	0	0.10	0/424	0.26	0/565
51	1	0.11	0/380	0.28	0/498
52	2	0.13	0/513	0.29	0/676
53	3	0.11	0/303	0.28	0/397
54	W	0.13	0/4334	0.31	0/5860
55	X	0.09	0/373	0.22	0/578
56	Y	0.19	0/1723	0.24	0/2684
57	Z	0.19	0/1653	0.23	0/2575
58	6	0.22	0/19	0.79	0/23
All	All	0.11	0/161944	0.26	1/241411 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	66	GLU	CB-CA-C	-5.68	110.00	116.54

There are no chirality outliers.

There are no planarity outliers.

## 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	32741	0	16491	411	0
2	B	1753	0	1780	14	0
3	C	1624	0	1696	14	0
4	D	1643	0	1707	18	0
5	E	1152	0	1196	9	0
6	F	839	0	833	8	0
7	G	1203	0	1254	13	0
8	H	979	0	1031	11	0
9	I	1022	0	1070	12	0
10	J	786	0	828	11	0
11	K	877	0	884	10	0
12	L	957	0	1017	15	0
13	M	891	0	952	9	0
14	N	805	0	844	7	0
15	O	714	0	734	5	0
16	P	643	0	661	4	0
17	Q	641	0	682	3	0
18	R	555	0	578	4	0
19	S	668	0	693	8	0
20	T	670	0	719	3	0
21	U	589	0	629	4	0
22	a	61098	0	30740	736	0
23	b	2550	0	1291	28	0
24	7	1702	0	1788	43	0
25	c	2082	0	2154	23	0
26	d	1566	0	1618	18	0
27	e	1552	0	1619	16	0
28	f	1410	0	1444	23	0
29	g	1323	0	1371	10	0
30	h	1101	0	1142	16	0
31	i	1129	0	1162	15	0
32	j	946	0	1023	4	0
33	k	1053	0	1129	6	0
34	l	1083	0	1158	12	0
35	m	945	0	989	9	0
36	n	892	0	923	9	0
37	o	917	0	962	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	p	947	0	1019	5	0
39	q	816	0	839	6	0
40	r	857	0	922	7	0
41	s	738	0	807	3	0
42	t	779	0	830	9	0
43	u	753	0	780	9	0
44	v	575	0	592	6	0
45	w	625	0	652	4	0
46	x	501	0	531	1	0
47	y	449	0	488	4	0
48	4	373	0	370	6	0
49	z	444	0	458	9	0
50	0	417	0	451	2	0
51	1	377	0	418	3	0
52	2	504	0	572	8	0
53	3	302	0	340	3	0
54	W	4241	0	4245	76	0
55	X	336	0	175	6	0
56	Y	1651	0	840	28	0
57	Z	1624	0	830	24	0
58	6	20	0	20	2	0
59	A	34	0	0	0	0
59	Z	1	0	0	0	0
59	a	84	0	0	0	0
59	c	4	0	0	0	0
59	e	1	0	0	0	0
59	t	1	0	0	0	0
60	A	70	0	0	0	0
60	B	1	0	0	0	0
60	W	2	0	0	0	0
60	X	1	0	0	0	0
60	a	186	0	0	0	0
60	b	4	0	0	0	0
60	c	2	0	0	0	0
60	d	1	0	0	0	0
60	m	1	0	0	0	0
60	z	1	0	0	0	0
61	a	40	0	76	3	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
63	W	62	0	24	2	0
64	Y	7	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	a	18	0	0	0	0
All	All	150953	0	103078	1646	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 7.

The worst 5 of 1646 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)
56:Y:23:G:O6	56:Y:47:G7M:N2	2.02	0.91
1:A:1086:U:H3	1:A:1099:G:H22	1.27	0.81
1:A:664:G:H22	1:A:741:G:H1	1.32	0.77
1:A:673:A:H2'	1:A:674:G:C8	2.19	0.77
22:a:2305:U:H5''	28:f:131:GLY:HA3	1.69	0.75

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	
2	B	222/241 (92%)	218 (98%)	4 (2%)	0	100	100
3	C	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
4	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
6	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
7	G	151/179 (84%)	151 (100%)	0	0	100	100
8	H	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	96/103 (93%)	95 (99%)	0	1 (1%)	12	36
11	K	113/129 (88%)	112 (99%)	1 (1%)	0	100	100
12	L	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
13	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	N	98/101 (97%)	98 (100%)	0	0	100	100
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	65/75 (87%)	65 (100%)	0	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	7	228/234 (97%)	222 (97%)	6 (3%)	0	100	100
25	c	269/273 (98%)	268 (100%)	1 (0%)	0	100	100
26	d	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	24	53
27	e	199/201 (99%)	199 (100%)	0	0	100	100
28	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
29	g	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
30	h	146/149 (98%)	145 (99%)	1 (1%)	0	100	100
31	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	j	121/123 (98%)	121 (100%)	0	0	100	100
33	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	l	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
36	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
37	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
38	p	115/118 (98%)	115 (100%)	0	0	100	100
39	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
40	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	s	91/100 (91%)	91 (100%)	0	0	100	100
42	t	100/104 (96%)	99 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	u	92/94 (98%)	92 (100%)	0	0	100	100
44	v	73/85 (86%)	73 (100%)	0	0	100	100
45	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	x	60/63 (95%)	60 (100%)	0	0	100	100
47	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	4	46/70 (66%)	46 (100%)	0	0	100	100
49	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
50	0	49/55 (89%)	49 (100%)	0	0	100	100
51	1	44/46 (96%)	44 (100%)	0	0	100	100
52	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
53	3	36/38 (95%)	36 (100%)	0	0	100	100
54	W	532/647 (82%)	526 (99%)	6 (1%)	0	100	100
58	6	1/165 (1%)	1 (100%)	0	0	100	100
All	All	6338/6959 (91%)	6259 (99%)	77 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	d	149	ASN
10	J	57	VAL

### 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	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	126/147 (86%)	125 (99%)	1 (1%)	73	90
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	58/65 (89%)	58 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	7	178/181 (98%)	177 (99%)	1 (1%)	78	92
25	c	216/218 (99%)	216 (100%)	0	100	100
26	d	163/163 (100%)	162 (99%)	1 (1%)	78	92
27	e	165/165 (100%)	165 (100%)	0	100	100
28	f	148/150 (99%)	147 (99%)	1 (1%)	76	91
29	g	137/138 (99%)	134 (98%)	3 (2%)	45	77
30	h	113/114 (99%)	113 (100%)	0	100	100
31	i	116/116 (100%)	116 (100%)	0	100	100
32	j	104/104 (100%)	104 (100%)	0	100	100
33	k	103/103 (100%)	102 (99%)	1 (1%)	68	88
34	l	108/107 (101%)	108 (100%)	0	100	100
35	m	98/103 (95%)	98 (100%)	0	100	100
36	n	86/87 (99%)	86 (100%)	0	100	100
37	o	99/100 (99%)	99 (100%)	0	100	100
38	p	89/90 (99%)	89 (100%)	0	100	100
39	q	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	r	93/93 (100%)	93 (100%)	0	100	100
41	s	80/84 (95%)	80 (100%)	0	100	100
42	t	83/85 (98%)	83 (100%)	0	100	100
43	u	78/78 (100%)	78 (100%)	0	100	100
44	v	57/63 (90%)	57 (100%)	0	100	100
45	w	67/68 (98%)	67 (100%)	0	100	100
46	x	54/55 (98%)	54 (100%)	0	100	100
47	y	48/49 (98%)	48 (100%)	0	100	100
48	4	44/62 (71%)	44 (100%)	0	100	100
49	z	47/48 (98%)	47 (100%)	0	100	100
50	0	46/49 (94%)	46 (100%)	0	100	100
51	1	38/38 (100%)	38 (100%)	0	100	100
52	2	51/52 (98%)	51 (100%)	0	100	100
53	3	34/34 (100%)	34 (100%)	0	100	100
54	W	451/544 (83%)	450 (100%)	1 (0%)	87	96
58	6	1/134 (1%)	1 (100%)	0	100	100
All	All	5273/5684 (93%)	5264 (100%)	9 (0%)	85	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	k	116	VAL
54	W	375	ILE
28	f	152	LEU
29	g	19	ILE
29	g	43	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
34	l	13	HIS
46	x	58	ASN
36	n	38	GLN
40	r	9	HIS
53	3	13	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1523/1542 (98%)	198 (13%)	0
22	a	2842/2904 (97%)	309 (10%)	0
23	b	118/119 (99%)	13 (11%)	0
55	X	15/629 (2%)	4 (26%)	0
56	Y	76/77 (98%)	12 (15%)	0
57	Z	75/76 (98%)	6 (8%)	0
All	All	4649/5347 (86%)	542 (11%)	0

5 of 542 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	32	A

There are no RNA pucker outliers to report.

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

52 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	$\# Z  > 2$
22	6MZ	a	2030	22	22,25,26	0.26	0	30,36,39	0.40	0
1	5MC	A	1407	1	18,22,23	0.33	0	26,32,35	0.45	0
57	H2U	Z	20	57	18,21,22	0.30	0	21,30,33	1.02	1 (4%)
12	D2T	L	89	12	7,9,10	0.88	0	6,11,13	1.69	2 (33%)
22	2MG	a	1835	22	23,26,27	0.29	0	32,38,41	0.33	0
57	H2U	Z	17	57	18,21,22	0.29	0	21,30,33	0.73	1 (4%)
1	MA6	A	1519	1	23,26,27	0.32	0	34,38,41	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	PSU	a	2605	22	18,21,22	0.46	0	22,30,33	0.60	0
22	3TD	a	1915	22	18,22,23	0.15	0	22,32,35	0.32	0
22	2MG	a	2445	22	23,26,27	0.32	0	32,38,41	0.34	0
22	OMC	a	2498	22,60	19,22,23	0.28	0	26,31,34	0.42	0
22	PSU	a	746	22,60	18,21,22	0.53	0	22,30,33	0.39	0
57	5MU	Z	54	57	19,22,23	0.30	0	28,32,35	0.31	0
22	5MU	a	1939	22,59	19,22,23	0.29	0	28,32,35	0.38	0
56	1MG	Y	38	56	22,26,27	0.41	0	33,39,42	0.47	0
22	PSU	a	1917	22	18,21,22	0.51	0	22,30,33	0.55	0
1	UR3	A	1498	1	19,22,23	0.28	0	26,32,35	0.35	0
1	4OC	A	1402	1	20,23,24	0.33	0	26,32,35	0.48	0
1	5MC	A	967	1	18,22,23	0.31	0	26,32,35	0.45	0
22	OMU	a	2552	22	19,22,23	0.28	0	26,31,34	0.43	0
56	H2U	Y	21	56	18,21,22	0.30	0	21,30,33	0.55	0
22	PSU	a	2580	22	18,21,22	0.51	0	22,30,33	0.65	1 (4%)
22	5MU	a	747	22	19,22,23	0.31	0	28,32,35	0.34	0
22	G7M	a	2069	22,59	23,26,27	0.37	0	35,39,42	0.51	0
22	PSU	a	955	22,59	18,21,22	0.46	0	22,30,33	0.58	0
22	OMG	a	2251	57,22,59	23,26,27	0.28	0	33,38,41	0.38	0
22	PSU	a	2457	22	18,21,22	0.49	0	22,30,33	0.61	0
22	PSU	a	2604	22	18,21,22	0.50	0	22,30,33	0.57	0
56	G7M	Y	47	56	23,26,27	0.32	0	35,39,42	0.46	0
11	IAS	K	119	11	6,7,8	0.80	0	6,8,10	0.94	0
1	PSU	A	516	1,60	18,21,22	0.50	0	22,30,33	0.59	0
22	2MA	a	2503	22,59,60	22,25,26	0.97	1 (4%)	33,37,40	1.38	3 (9%)
57	H2U	Z	16	57	18,21,22	0.42	0	21,30,33	0.56	0
57	G7M	Z	46	57	23,26,27	0.33	0	35,39,42	0.48	0
1	2MG	A	1207	59,1	23,26,27	0.29	0	32,38,41	0.34	0
34	4D4	l	81	34	9,11,12	0.91	1 (11%)	8,13,15	1.97	3 (37%)
22	6MZ	a	1618	22	22,25,26	0.25	0	30,36,39	0.42	0
22	1MG	a	745	22	22,26,27	0.43	0	33,39,42	0.47	0
22	PSU	a	1911	22	18,21,22	0.48	0	22,30,33	0.57	0
22	H2U	a	2449	22	18,21,22	0.28	0	21,30,33	0.45	0
57	4SU	Z	8	57	18,21,22	0.30	0	26,30,33	0.36	0
22	5MC	a	1962	22,59	18,22,23	0.30	0	26,32,35	0.46	0
57	PSU	Z	55	57	18,21,22	0.49	0	22,30,33	0.58	0
22	PSU	a	2504	22,59	18,21,22	0.49	0	22,30,33	0.56	0
34	MS6	l	82	34	5,7,8	0.30	0	2,7,9	0.07	0
1	G7M	A	527	1	23,26,27	0.33	0	35,39,42	0.49	0
56	PSU	Y	56	56	18,21,22	0.48	0	22,30,33	0.58	0
1	2MG	A	1516	1	23,26,27	0.31	0	32,38,41	0.37	0
26	MEQ	d	150	26	8,9,10	0.51	0	5,10,12	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	5MU	Y	55	56	19,22,23	0.30	0	28,32,35	0.30	0
1	MA6	A	1518	1	23,26,27	0.36	0	34,38,41	0.66	1 (2%)
1	2MG	A	966	1	23,26,27	0.30	0	32,38,41	0.45	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
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
57	H2U	Z	20	57	-	0/7/38/39	0/2/2/2
12	D2T	L	89	12	-	1/7/12/14	-
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
57	H2U	Z	17	57	-	2/7/38/39	0/2/2/2
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	0/9/27/28	0/3/3/3
22	OMC	a	2498	22,60	-	0/9/27/28	0/2/2/2
22	PSU	a	746	22,60	-	4/7/25/26	0/2/2/2
57	5MU	Z	54	57	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22,59	-	0/7/25/26	0/2/2/2
56	1MG	Y	38	56	-	0/7/25/26	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
56	H2U	Y	21	56	-	4/7/38/39	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22,59	-	1/7/25/26	0/3/3/3
22	PSU	a	955	22,59	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	57,22,59	-	0/9/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
56	G7M	Y	47	56	-	0/7/25/26	0/3/3/3
11	IAS	K	119	11	-	4/7/7/8	-
1	PSU	A	516	1,60	-	0/7/25/26	0/2/2/2

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	2MA	a	2503	22,59,60	-	1/7/25/26	0/3/3/3
57	H2U	Z	16	57	-	2/7/38/39	0/2/2/2
57	G7M	Z	46	57	-	0/7/25/26	0/3/3/3
1	2MG	A	1207	59,1	-	0/9/27/28	0/3/3/3
34	4D4	l	81	34	-	1/11/12/14	-
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
57	4SU	Z	8	57	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22,59	-	0/7/25/26	0/2/2/2
57	PSU	Z	55	57	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22,59	-	2/7/25/26	0/2/2/2
34	MS6	l	82	34	-	1/4/6/8	-
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
56	PSU	Y	56	56	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
26	MEQ	d	150	26	-	2/8/9/11	-
56	5MU	Y	55	56	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2503	2MA	C6-N6	-3.18	1.26	1.34
34	l	81	4D4	CZ-NE	2.10	1.37	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2503	2MA	N6-C6-N1	4.73	123.71	117.03
57	Z	20	H2U	C4-N3-C2	-4.14	122.36	125.79
34	l	81	4D4	NE-CZ-NH2	4.07	127.85	120.70
22	a	2503	2MA	C2-N1-C6	3.93	124.21	118.08
22	a	2503	2MA	C5-C6-N1	-3.81	112.44	119.01

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	a	746	PSU	C2'-C1'-C5-C4
22	a	746	PSU	C2'-C1'-C5-C6
56	Y	21	H2U	O4'-C1'-N1-C6
56	Y	21	H2U	C2'-C1'-N1-C2
56	Y	21	H2U	C2'-C1'-N1-C6

There are no ring outliers.

15 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	2030	6MZ	2	0
12	L	89	D2T	2	0
1	A	1519	MA6	1	0
56	Y	38	1MG	1	0
1	A	1402	4OC	1	0
1	A	967	5MC	1	0
56	Y	21	H2U	2	0
22	a	2251	OMG	1	0
56	Y	47	G7M	1	0
57	Z	16	H2U	1	0
57	Z	46	G7M	1	0
1	A	1516	2MG	2	0
26	d	150	MEQ	1	0
1	A	1518	MA6	2	0
1	A	966	2MG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 403 ligands modelled in this entry, 396 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	SPD	a	3243	-	9,9,9	0.27	0	8,8,8	0.86	0
61	SPD	a	3241	-	9,9,9	0.24	0	8,8,8	0.84	0
61	SPD	a	3240	-	9,9,9	0.25	0	8,8,8	0.83	0
61	SPD	a	3242	-	9,9,9	0.24	0	8,8,8	0.90	0
63	ATP	W	701	60	29,33,33	0.49	0	44,52,52	0.50	0
63	ATP	W	702	60	29,33,33	0.48	0	44,52,52	0.50	0
64	PRO	Y	101	56	5,7,8	0.54	0	7,8,10	1.34	1 (14%)

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
61	SPD	a	3243	-	-	0/7/7/7	-
61	SPD	a	3241	-	-	0/7/7/7	-
61	SPD	a	3240	-	-	0/7/7/7	-
61	SPD	a	3242	-	-	0/7/7/7	-
63	ATP	W	701	60	-	2/22/38/38	0/3/3/3
63	ATP	W	702	60	-	2/22/38/38	0/3/3/3
64	PRO	Y	101	56	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	Y	101	PRO	O-C-CA	-2.11	119.24	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	W	701	ATP	PA-O3A-PB-O1B
63	W	702	ATP	PG-O3B-PB-O2B
63	W	701	ATP	PA-O3A-PB-O2B
63	W	702	ATP	PG-O3B-PB-O1B

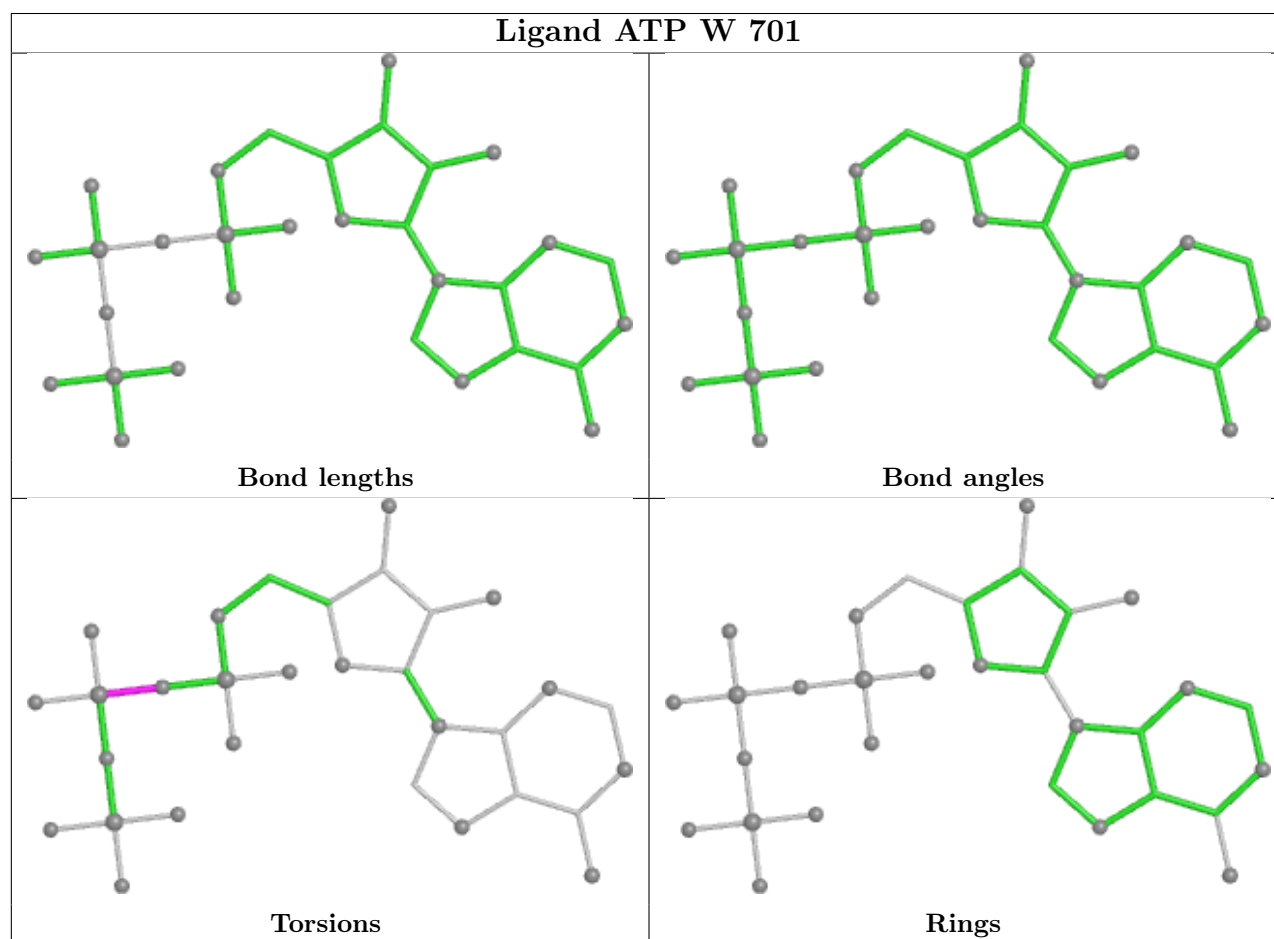
There are no ring outliers.

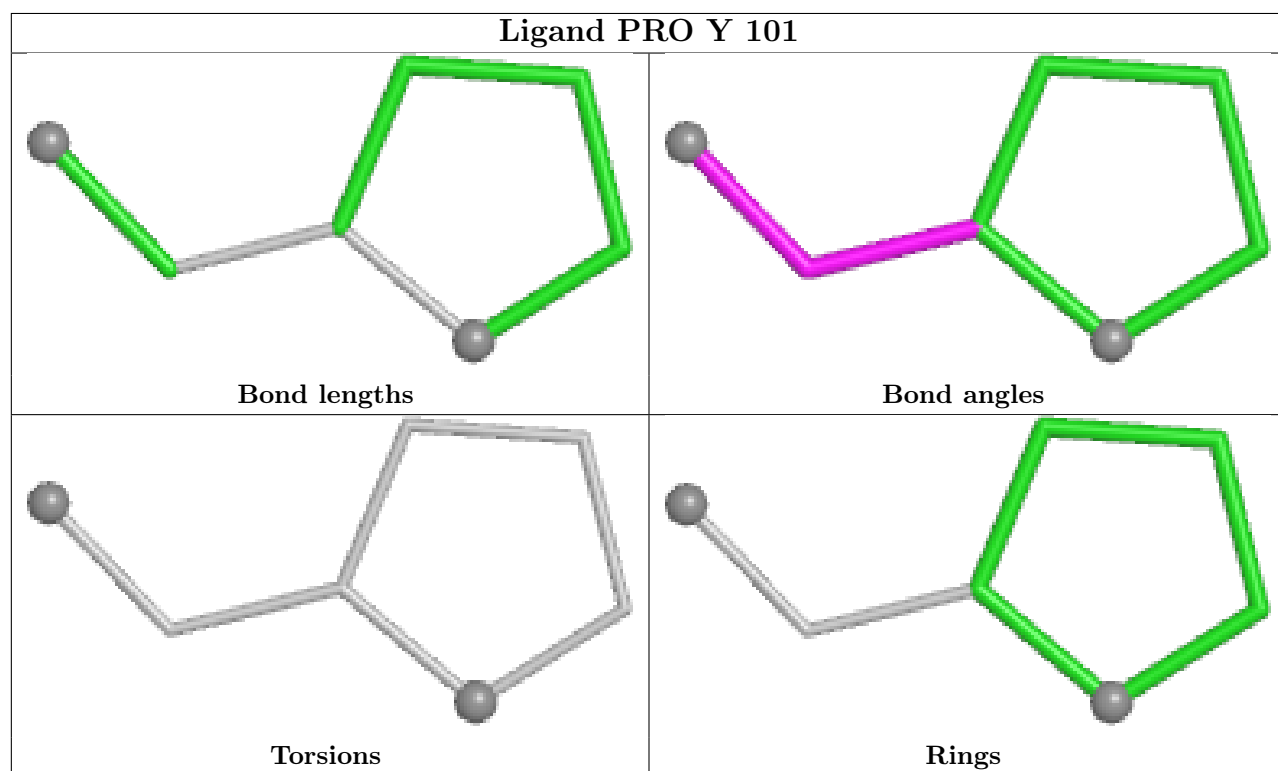
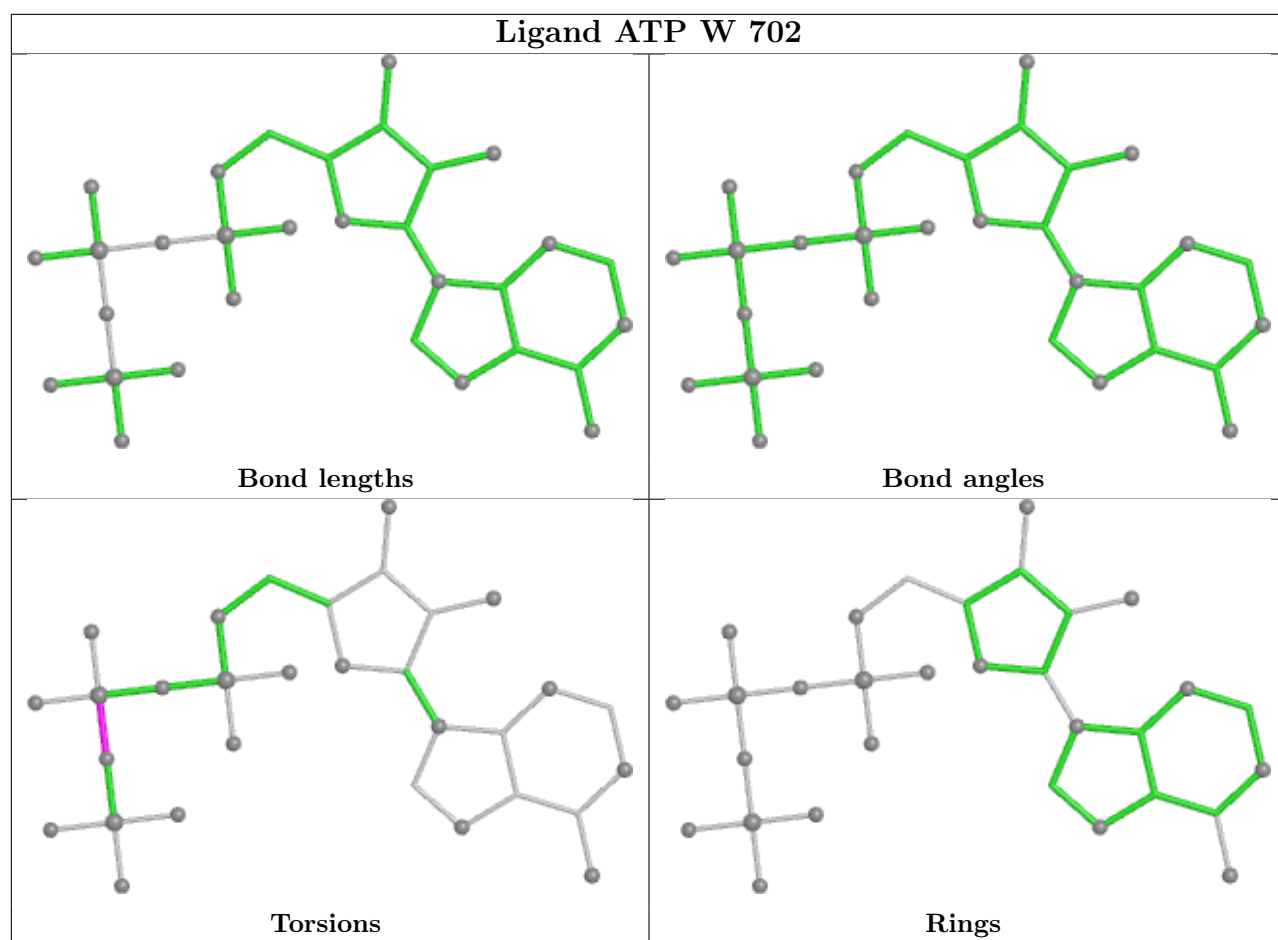
5 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	3243	SPD	2	0
61	a	3242	SPD	1	0
63	W	701	ATP	1	0
63	W	702	ATP	1	0
64	Y	101	PRO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

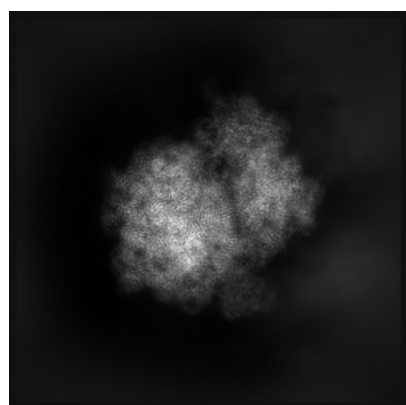
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65381. These allow visual inspection of the internal detail of the map and identification of artifacts.

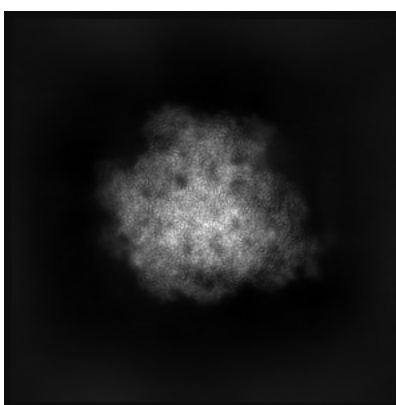
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

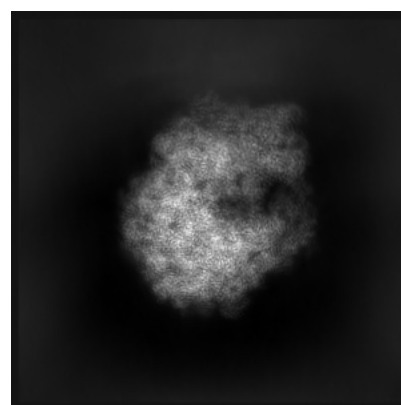
#### 6.1.1 Primary map



X



Y

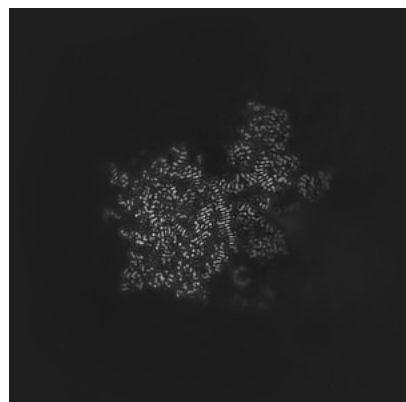


Z

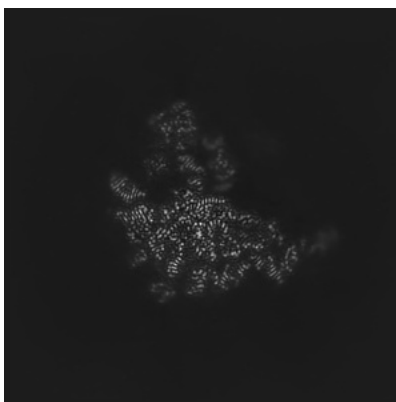
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

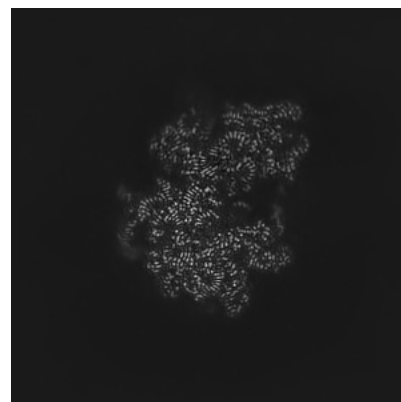
#### 6.2.1 Primary map



X Index: 324



Y Index: 324

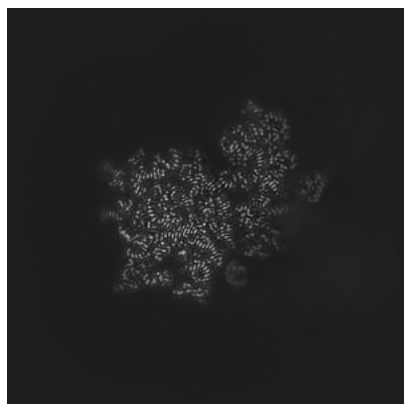


Z Index: 324

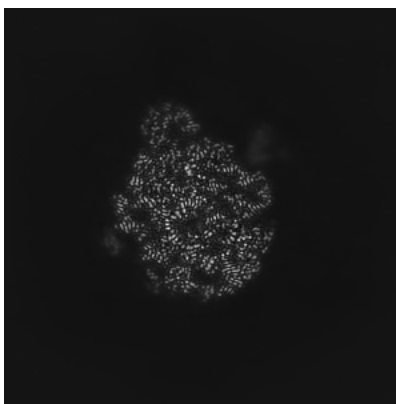
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

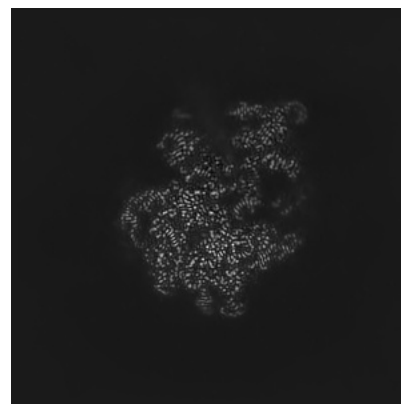
### 6.3.1 Primary map



X Index: 317



Y Index: 280

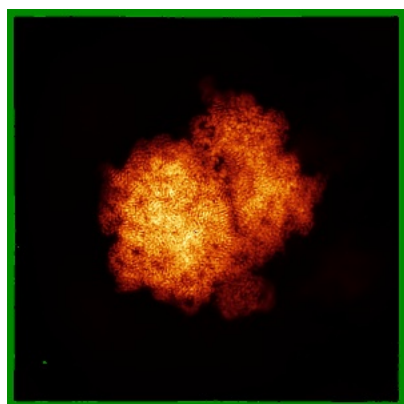


Z Index: 310

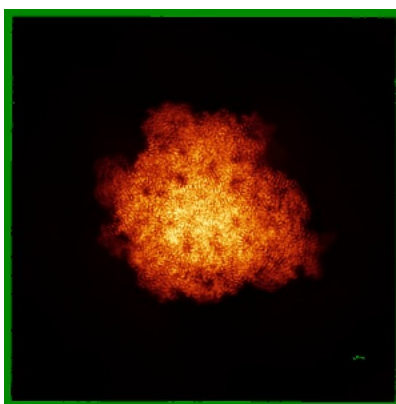
The images above show the largest variance slices of the map in three orthogonal directions.

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

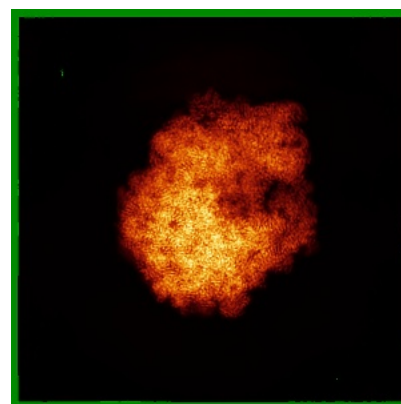
### 6.4.1 Primary map



X



Y

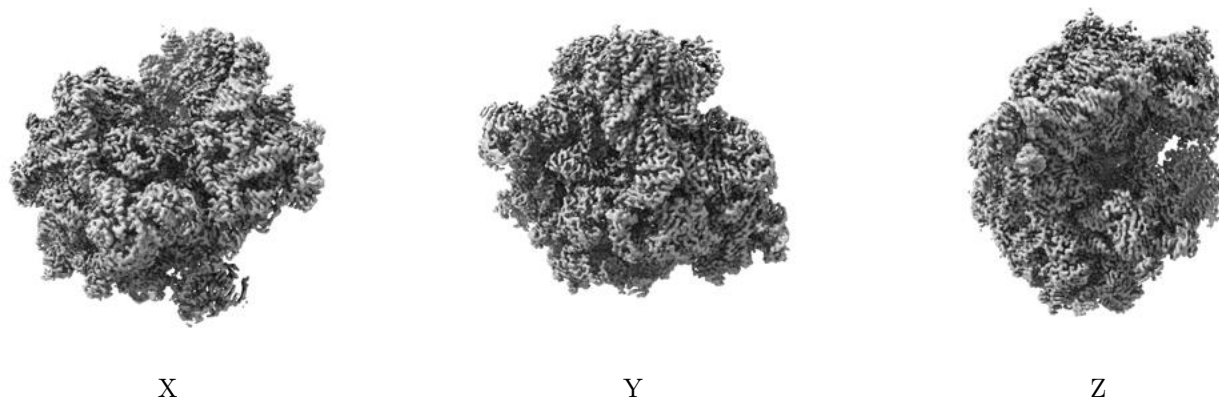


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

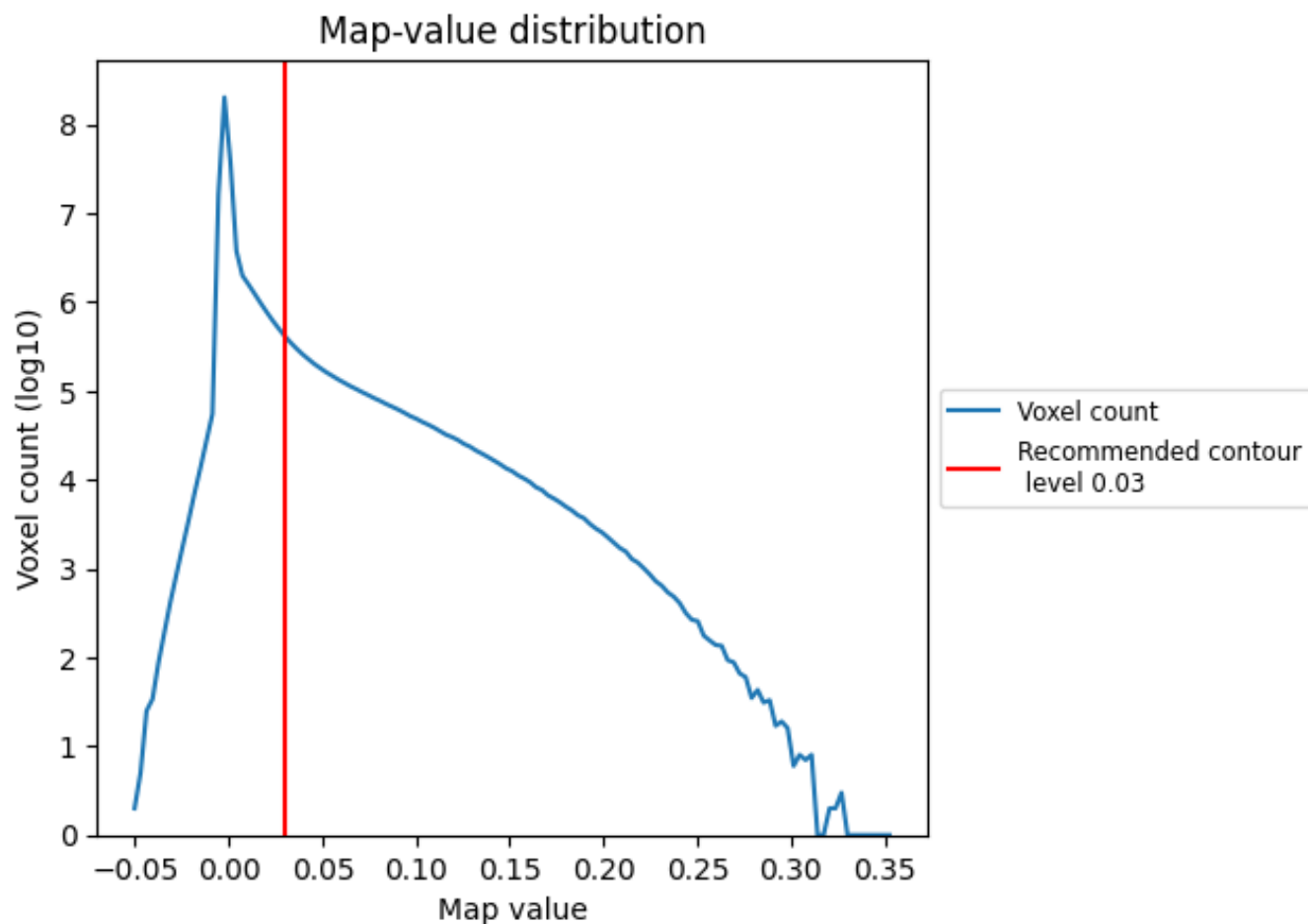
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

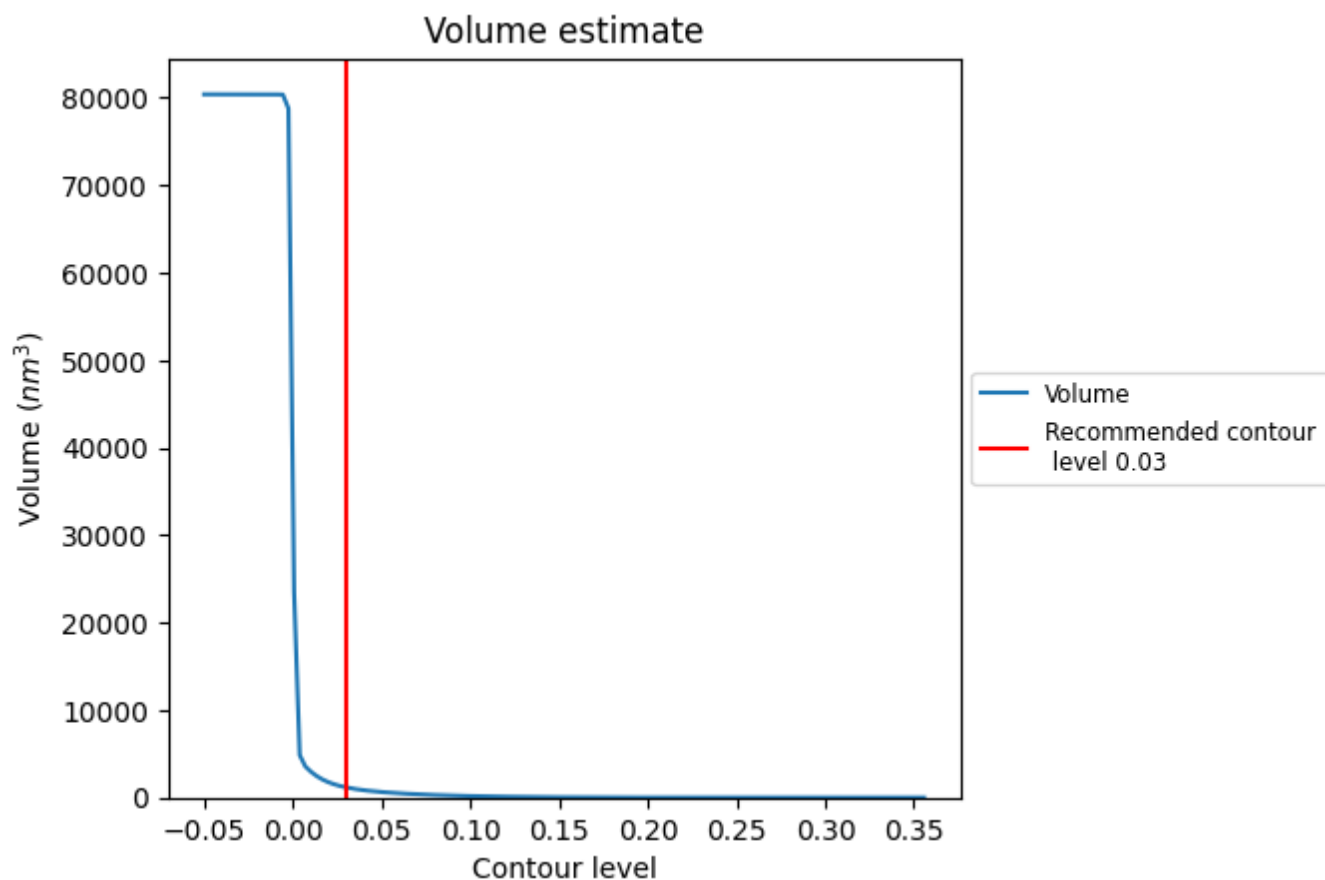
This section contains the results of statistical analysis of the map.

### 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](#)

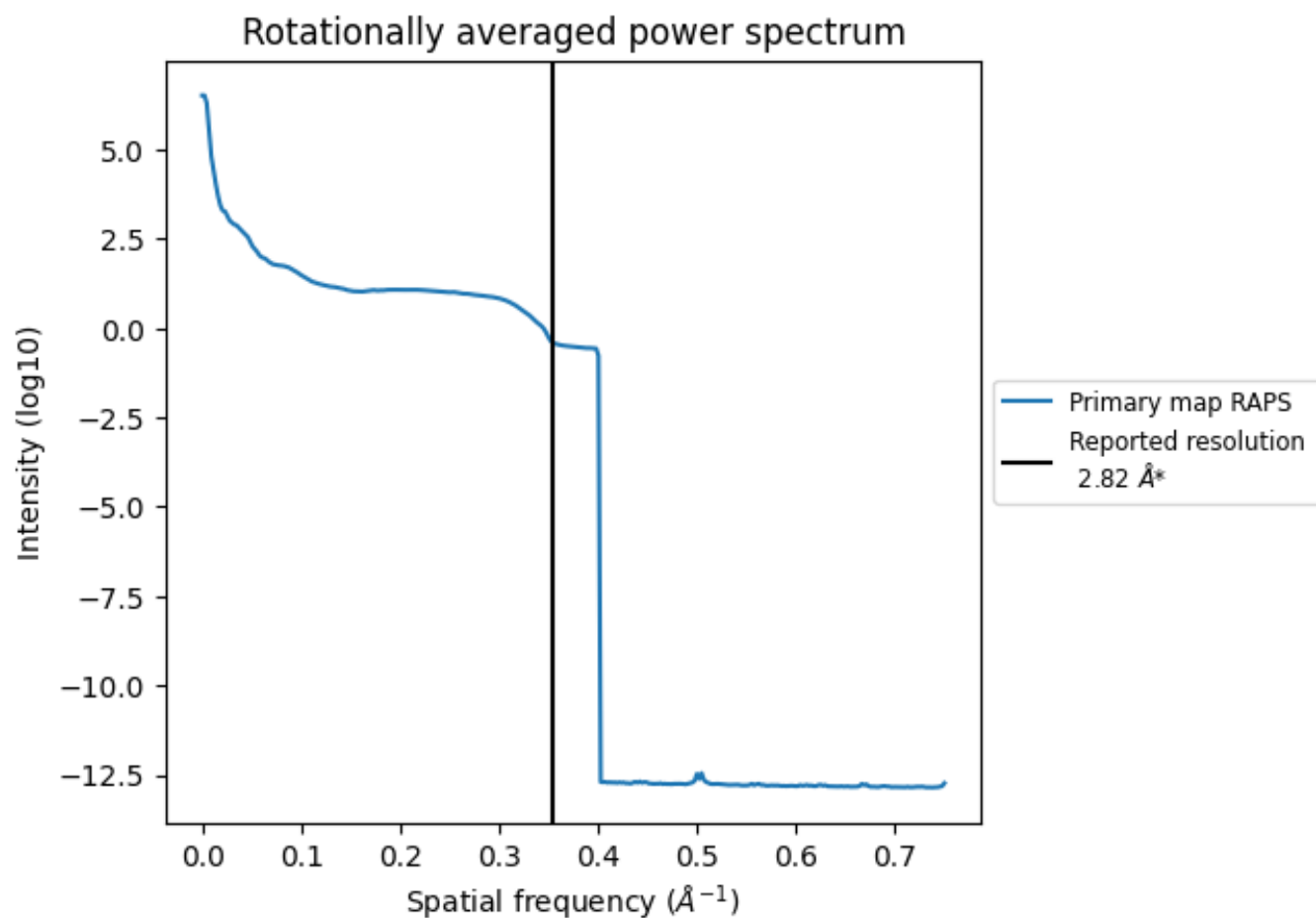


The volume at the recommended contour level is 1161 nm<sup>3</sup>; this corresponds to an approximate mass of 1048 kDa.

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

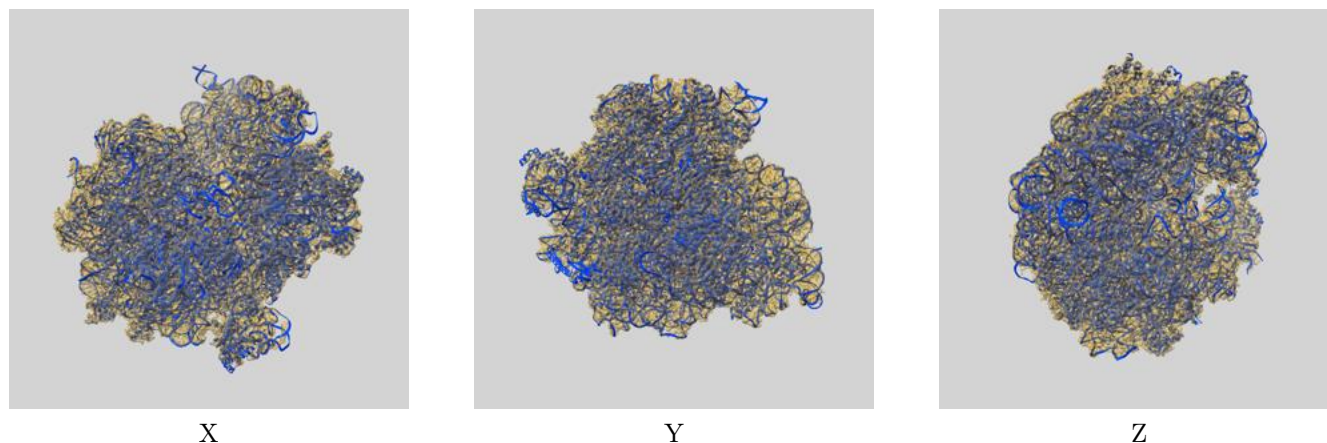
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

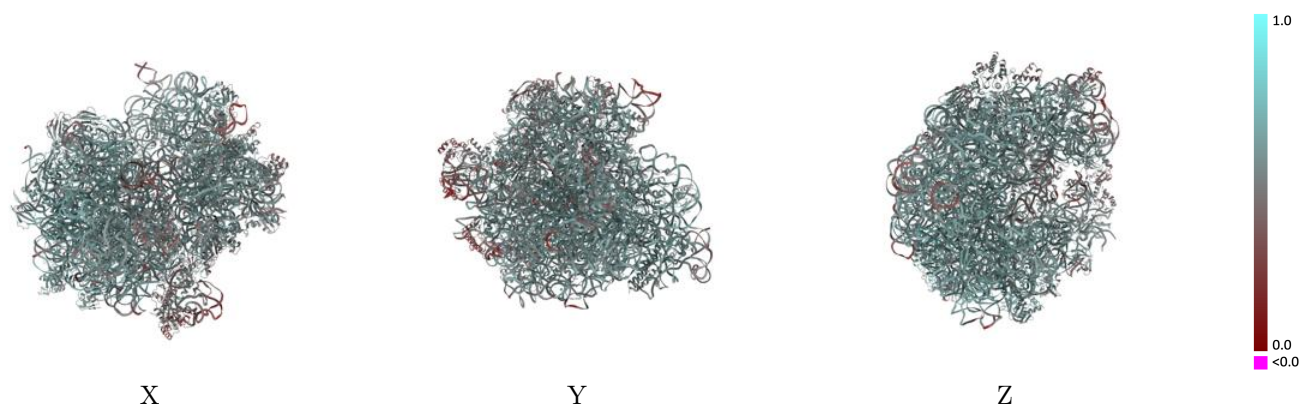
This section contains information regarding the fit between EMDB map EMD-65381 and PDB model 9VVI. Per-residue inclusion information can be found in section [3](#) on page [19](#).

### 9.1 Map-model overlay [i](#)



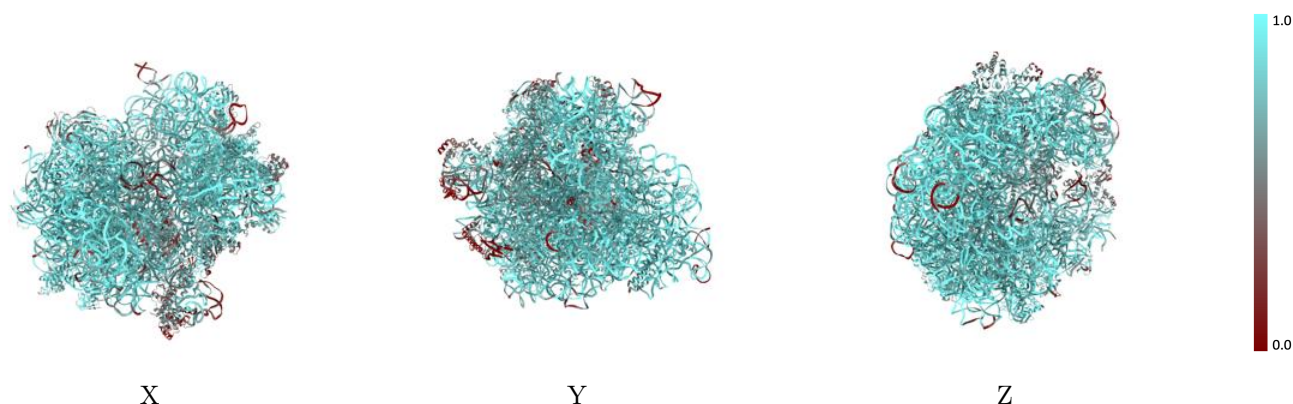
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



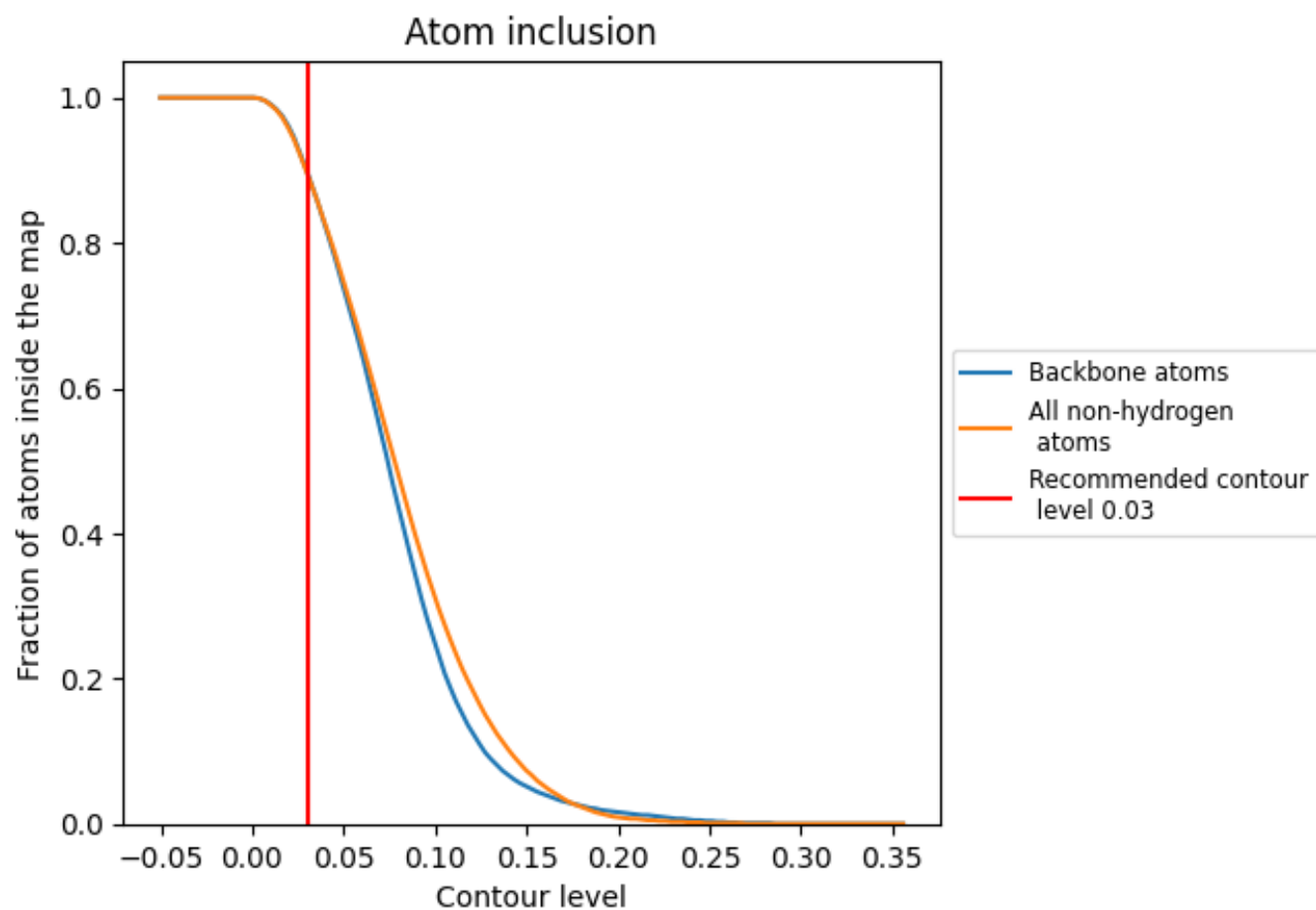
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5730
0	 0.9000	 0.5890
1	 0.9830	 0.6360
2	 0.9840	 0.6300
3	 0.9250	 0.5800
4	 0.3320	 0.3880
6	 0.7780	 0.4650
7	 0.3960	 0.4010
A	 0.9410	 0.5730
B	 0.6600	 0.4960
C	 0.8720	 0.5550
D	 0.8550	 0.5560
E	 0.9080	 0.5780
F	 0.7080	 0.5090
G	 0.6470	 0.4880
H	 0.9070	 0.5780
I	 0.8290	 0.5390
J	 0.7140	 0.5000
K	 0.7730	 0.5340
L	 0.8850	 0.5770
M	 0.7930	 0.5390
N	 0.8730	 0.5570
O	 0.8320	 0.5500
P	 0.9110	 0.5810
Q	 0.8460	 0.5490
R	 0.7820	 0.5340
S	 0.8360	 0.5530
T	 0.8760	 0.5560
U	 0.5580	 0.4510
W	 0.7660	 0.5340
X	 0.6620	 0.4480
Y	 0.6400	 0.4320
Z	 0.9120	 0.5700
a	 0.9480	 0.5960
b	 0.9210	 0.5580



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Chain	Atom inclusion	Q-score
c	 0.9610	 0.6180
d	 0.9400	 0.6090
e	 0.8970	 0.5870
f	 0.6240	 0.4670
g	 0.7190	 0.5180
h	 0.2090	 0.3510
i	 0.9490	 0.6080
j	 0.9360	 0.6080
k	 0.9360	 0.6010
l	 0.9400	 0.6100
m	 0.9770	 0.6220
n	 0.8440	 0.5400
o	 0.9020	 0.5960
p	 0.9730	 0.6220
q	 0.9120	 0.6030
r	 0.9400	 0.6050
s	 0.8790	 0.5700
t	 0.8520	 0.5680
u	 0.8400	 0.5630
v	 0.9480	 0.6040
w	 0.9400	 0.6110
x	 0.8280	 0.5420
y	 0.9040	 0.5990
z	 0.9160	 0.5930