



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 02:07 PM EST

PDB ID : 4V75
EMDB ID : EMD-1721
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^{fMet} complex in classic post-translocation state (post1)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 12.00 Å (reported)
Based on initial models : 2HGP, 3I1O, 2K4C, 2WRI

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

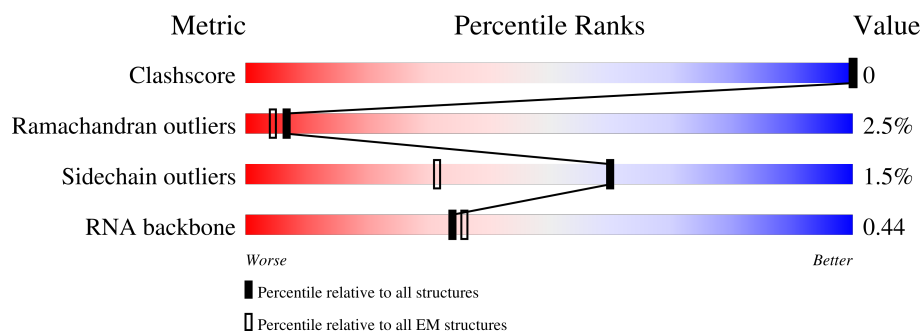
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	AB	220	<div> <div>34%</div> <div>97%</div> <div>.</div> </div>
2	AC	208	<div> <div>35%</div> <div>91%</div> <div>8%</div> </div>
3	AD	206	<div> <div>35%</div> <div>89%</div> <div>11%</div> </div>
4	AE	152	<div> <div>30%</div> <div>89%</div> <div>11%</div> </div>
5	AF	101	<div> <div>22%</div> <div>87%</div> <div>13%</div> </div>
6	AG	152	<div> <div>28%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
7	AH	130	<div> <div>30%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	AI	128	
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	

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Mol	Chain	Length	Quality of chain
33	BK	123	
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	amidation	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	acetylation	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	acetylation	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	amidation	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	amidation	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	57	Total	C	N	O		0	1
			459	290	87	82			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	acetylation	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	amidation	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	acetylation	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	amidation	UNP P60422

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BG	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	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	amidation	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	amidation	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	amidation	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	amidation	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	acetylation	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	acetylation	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	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	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

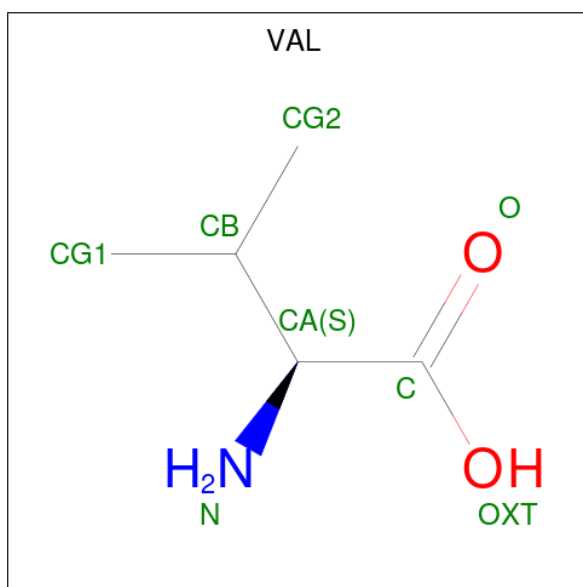
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

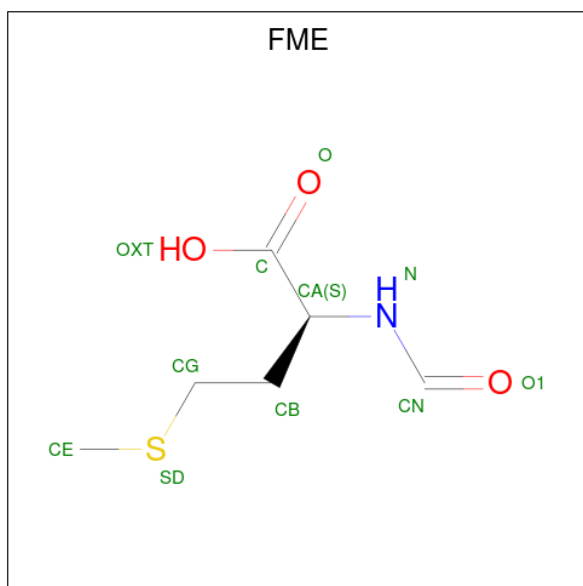
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

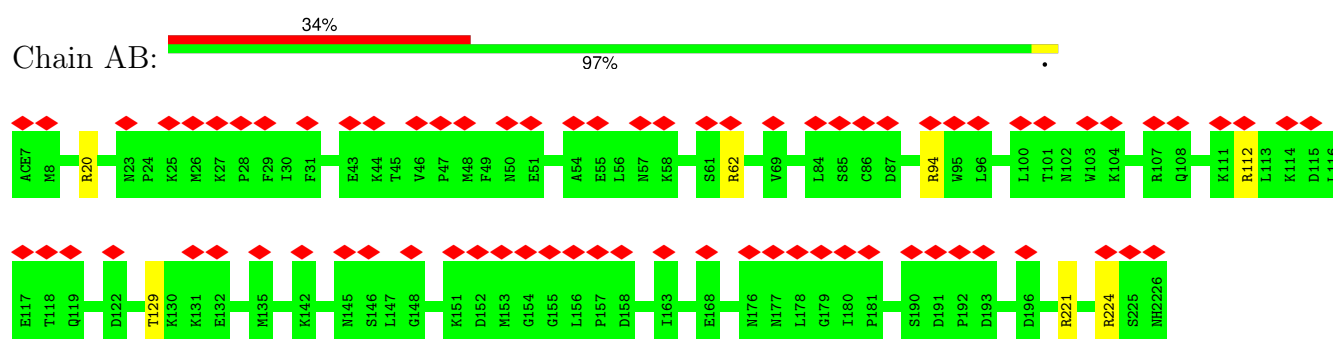


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

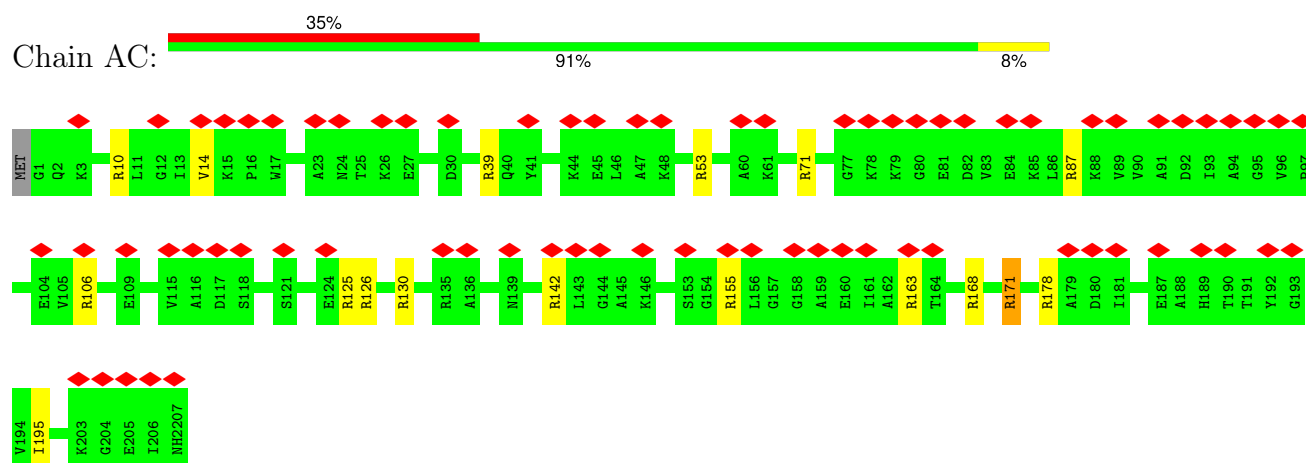
3 Residue-property plots

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.

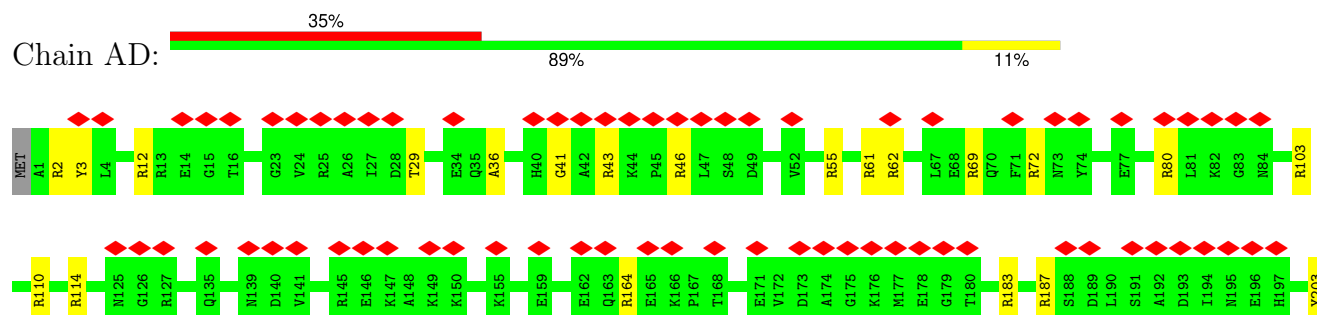
• Molecule 1: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S3



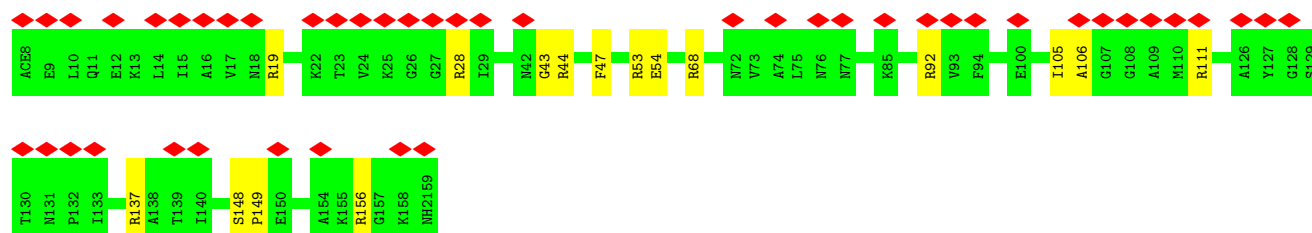
• Molecule 3: 30S ribosomal protein S4





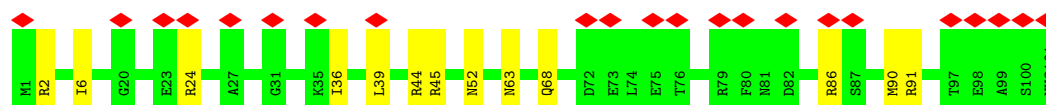
• Molecule 4: 30S ribosomal protein S5

Chain AE:



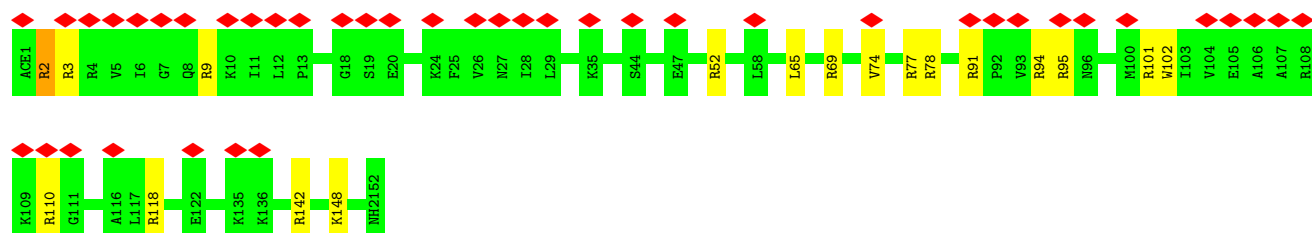
• Molecule 5: 30S ribosomal protein S6

Chain AF:



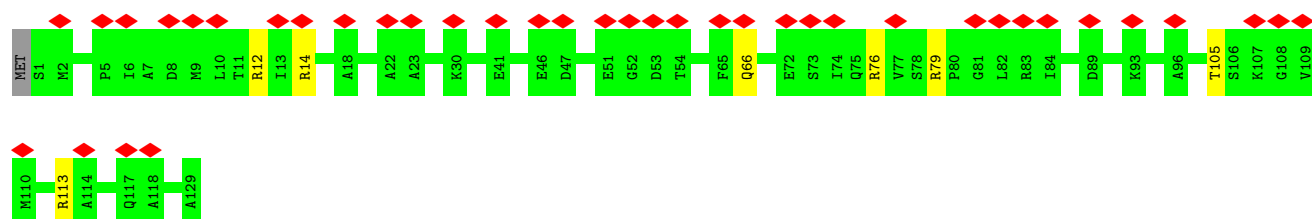
• Molecule 6: 30S ribosomal protein S7

Chain AG:



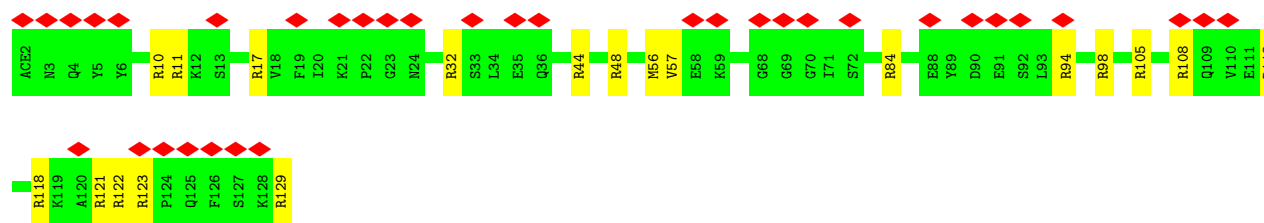
• Molecule 7: 30S ribosomal protein S8

Chain AH:

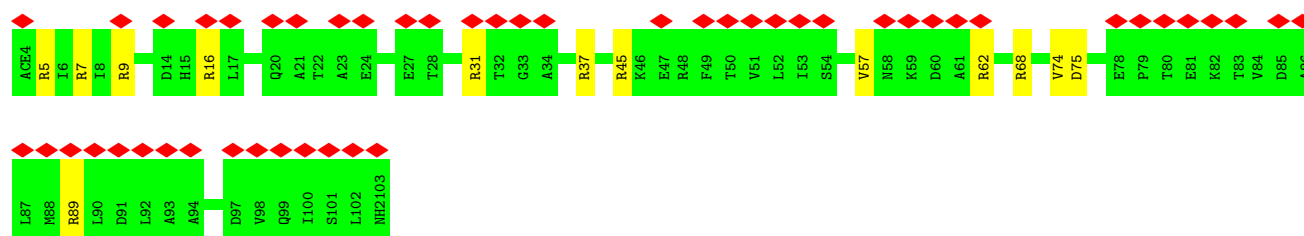
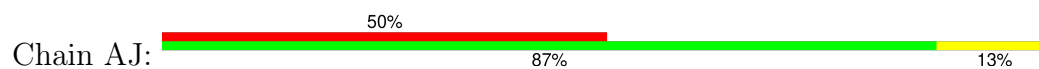


• Molecule 8: 30S ribosomal protein S9

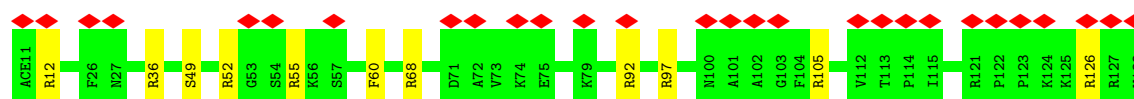
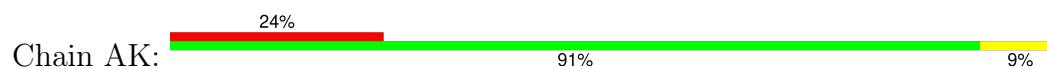
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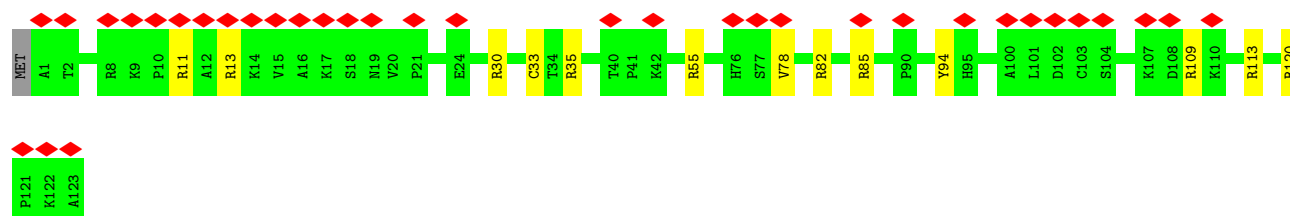
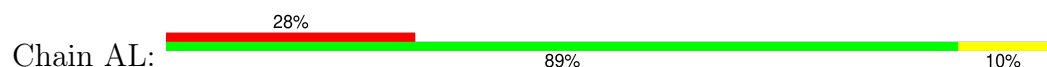
• Molecule 9: 30S ribosomal protein S10



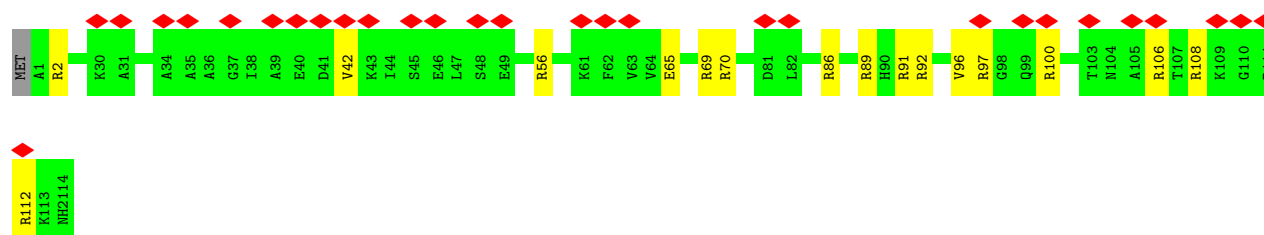
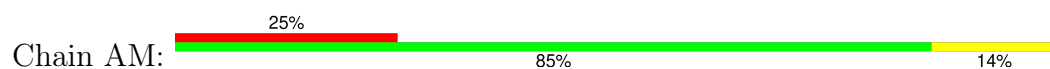
• Molecule 10: 30S ribosomal protein S11




• Molecule 11: 30S ribosomal protein S12

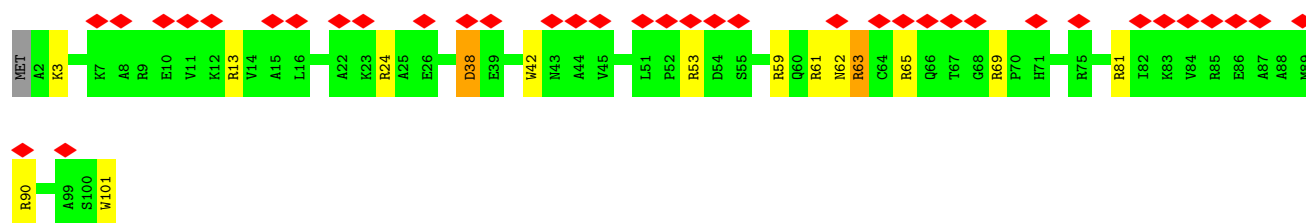


• Molecule 12: 30S ribosomal protein S13




• Molecule 13: 30S ribosomal protein S14

Chain AN: 




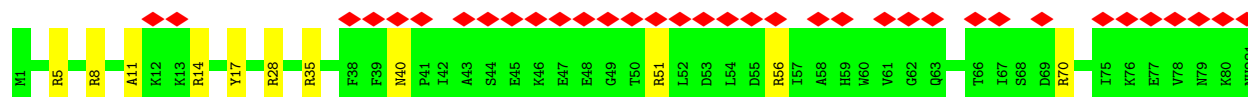
- Molecule 14: 30S ribosomal protein S15

Chain AO: 




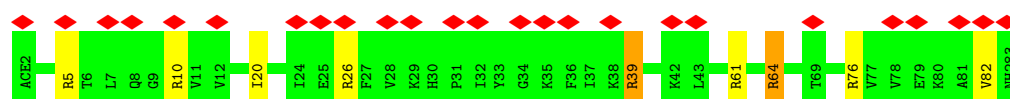
- Molecule 15: 30S ribosomal protein S16

Chain AP: 




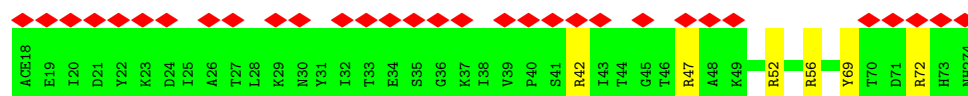
- Molecule 16: 30S ribosomal protein S17

Chain AQ: 



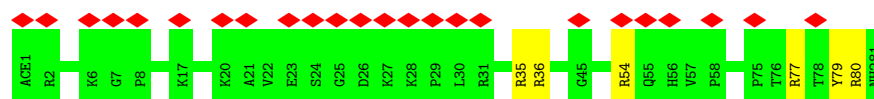
- Molecule 17: 30S ribosomal protein S18

Chain AR: 

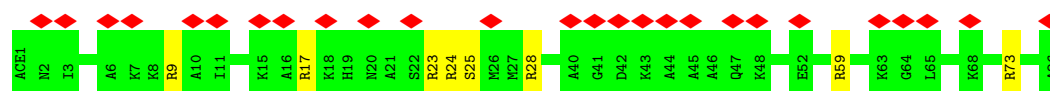
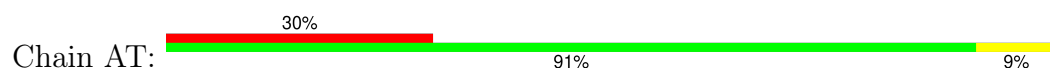


- Molecule 18: 30S ribosomal protein S19

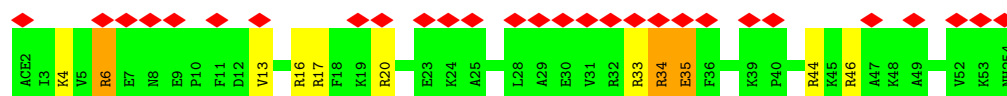
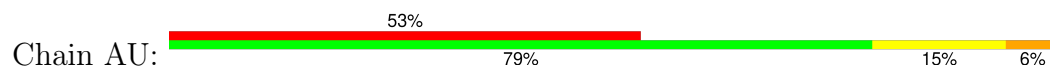
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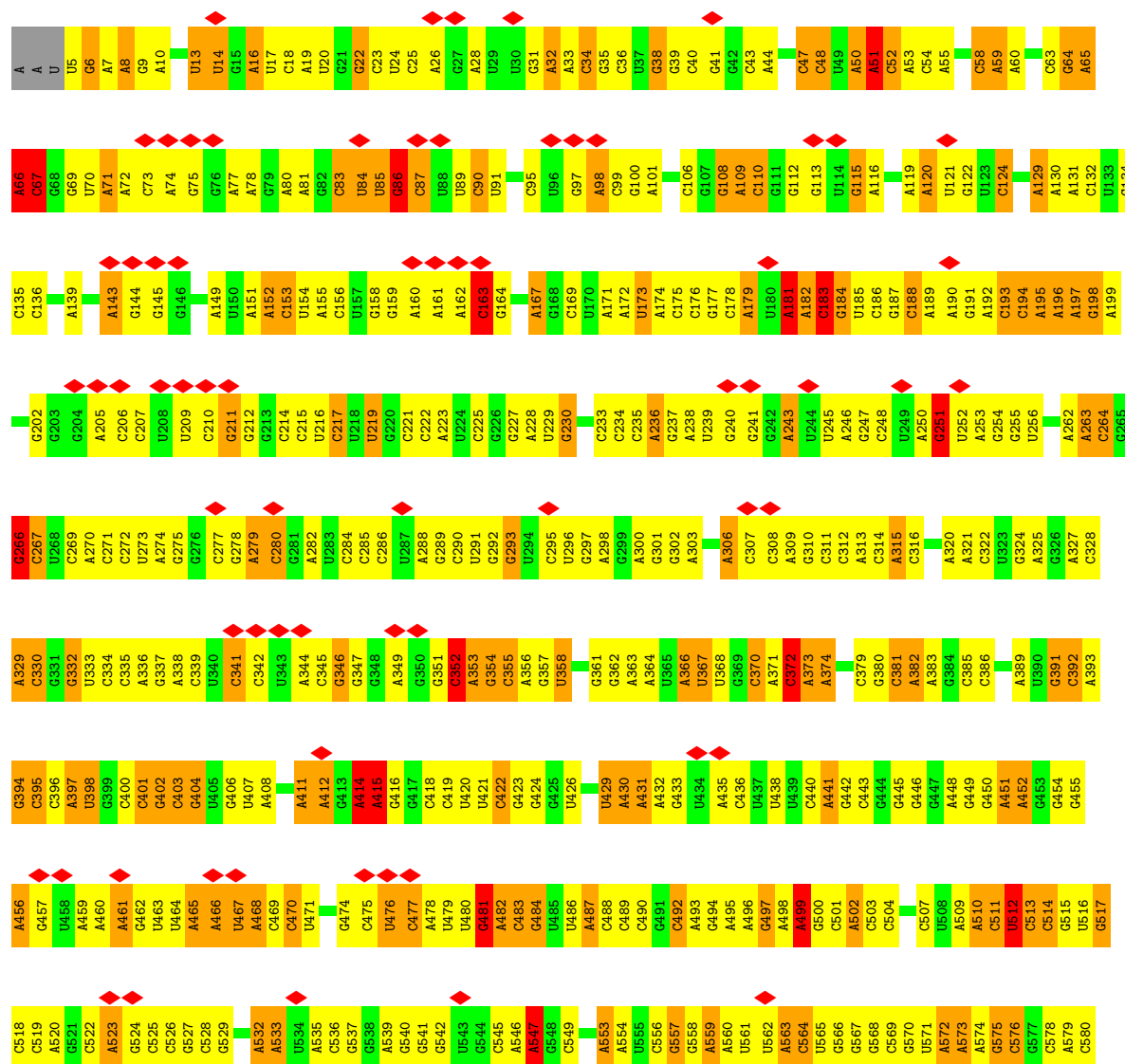
- Molecule 19: 30S ribosomal protein S20



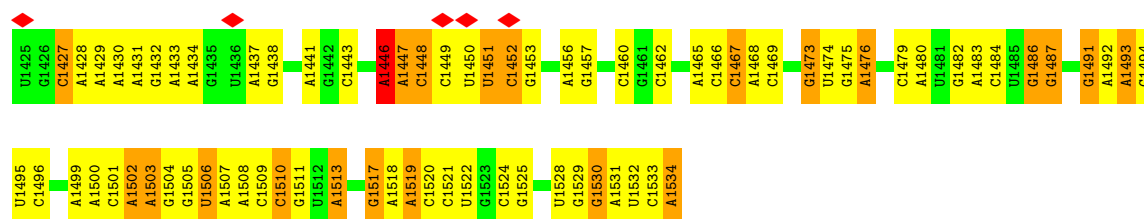
- Molecule 20: 30S ribosomal protein S21



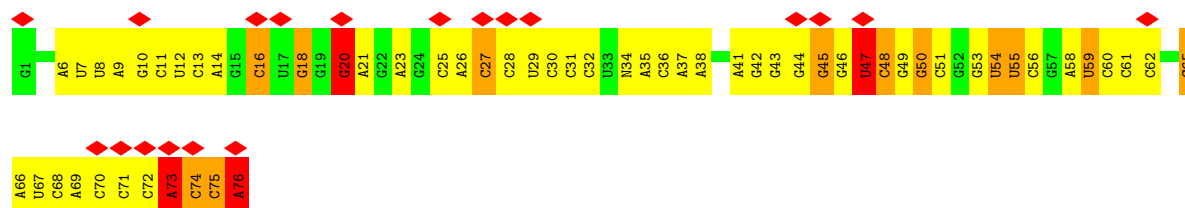
- Molecule 21: 16S ribosomal RNA



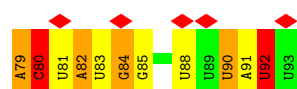
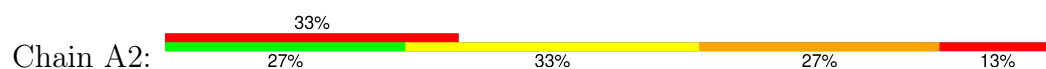




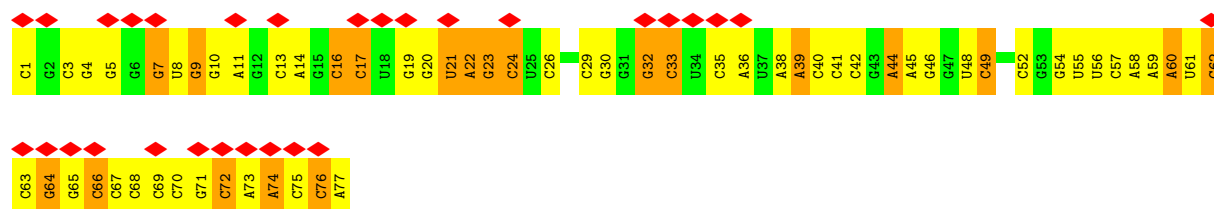
• Molecule 22: fMet-Val-tRNA-Val



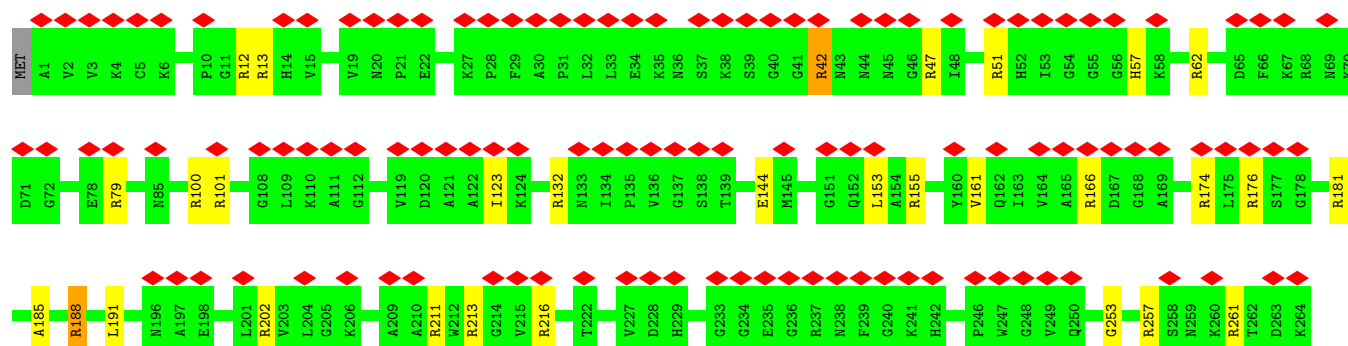
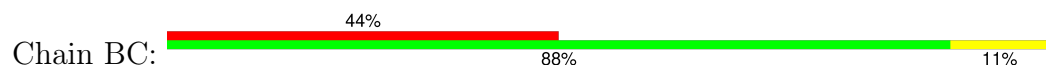
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

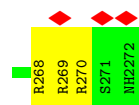


• Molecule 24: tRNA-fMet

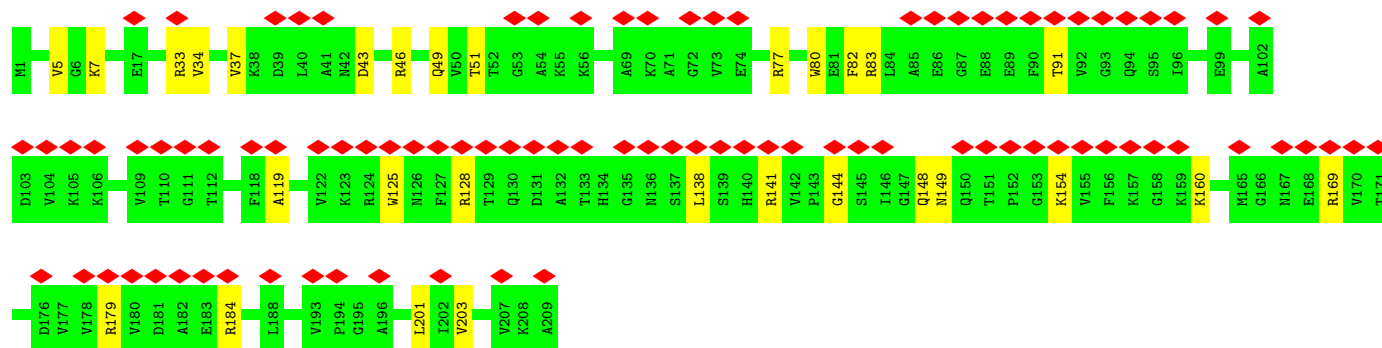
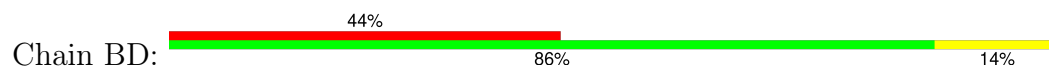


• Molecule 25: 50S ribosomal protein L2

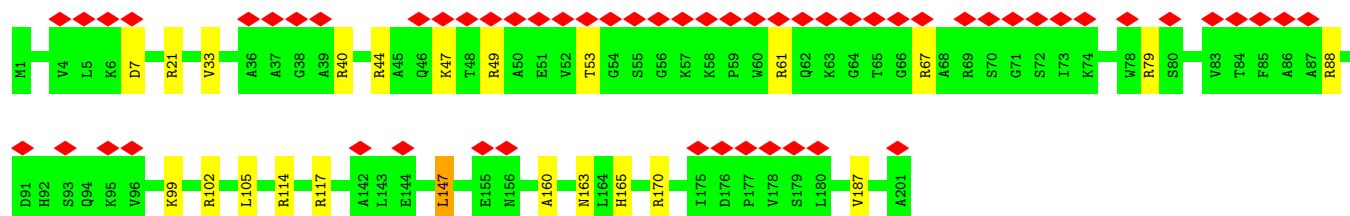
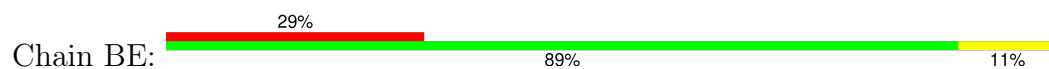




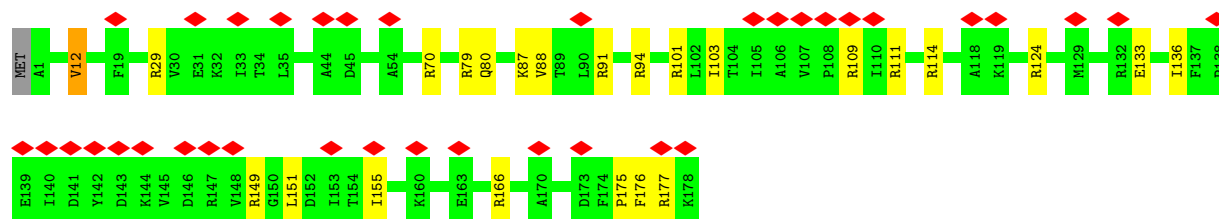
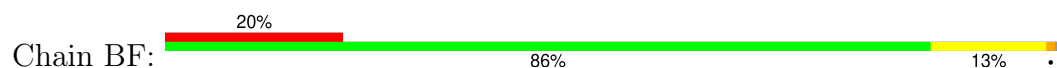
- Molecule 26: 50S ribosomal protein L3



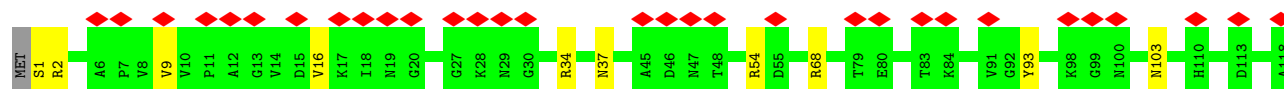
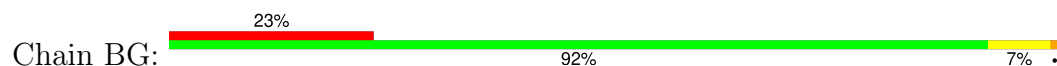
- Molecule 27: 50S ribosomal protein L4

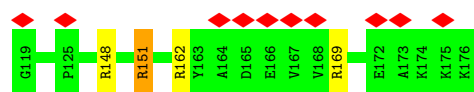


- Molecule 28: 50S ribosomal protein L5

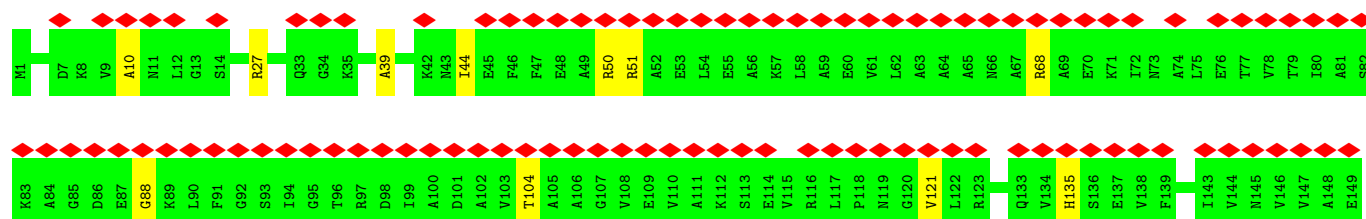


- Molecule 29: 50S ribosomal protein L6

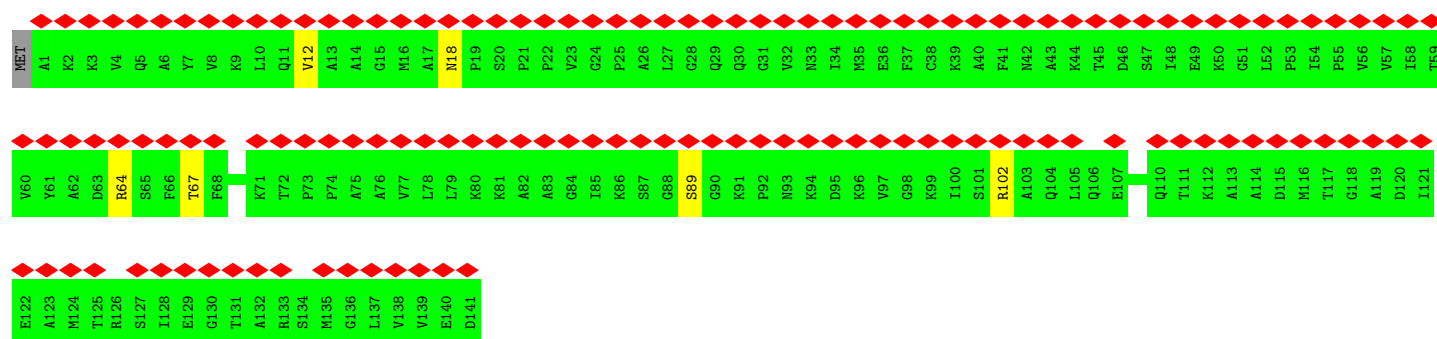




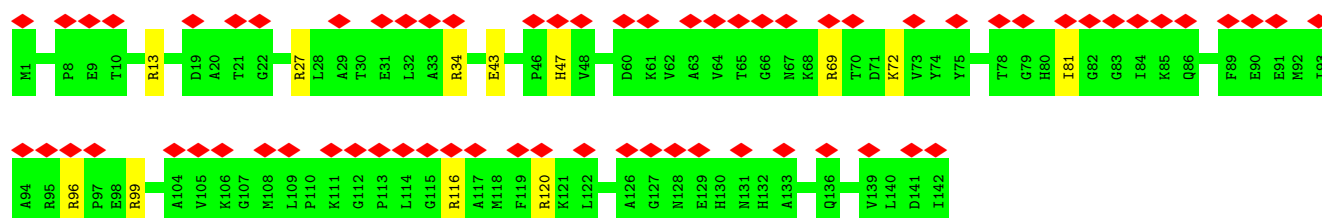
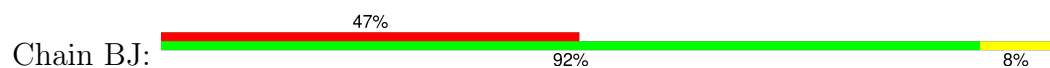
- Molecule 30: 50S ribosomal protein L9



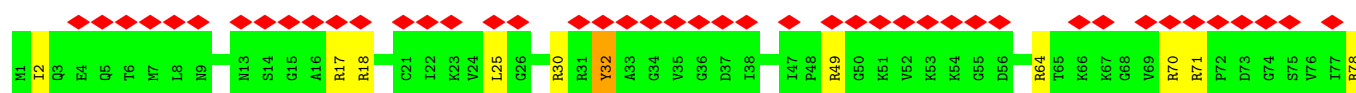
- Molecule 31: 50S ribosomal protein L11

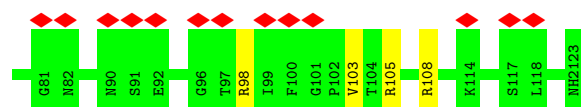


- Molecule 32: 50S ribosomal protein L13

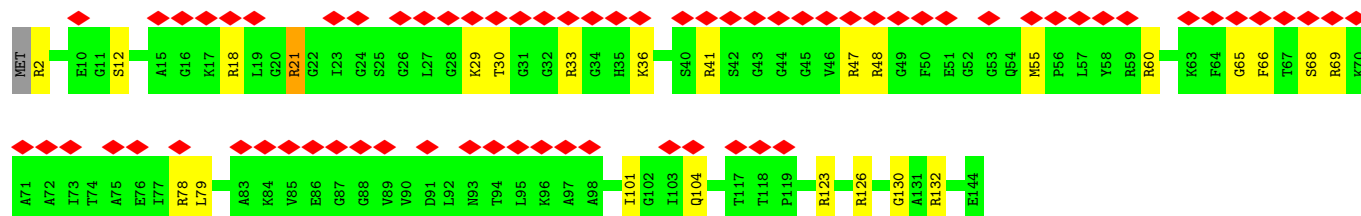
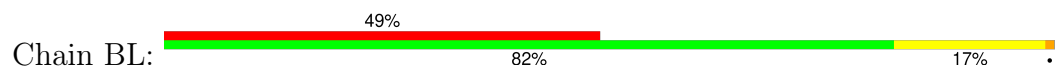


- Molecule 33: 50S ribosomal protein L14

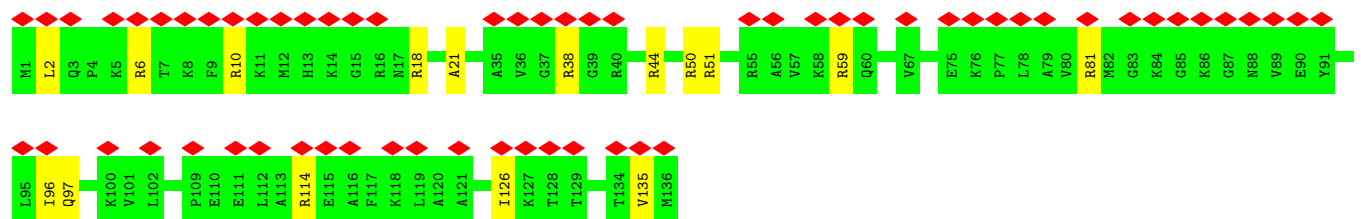
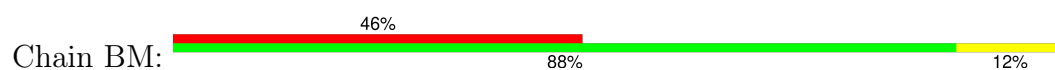




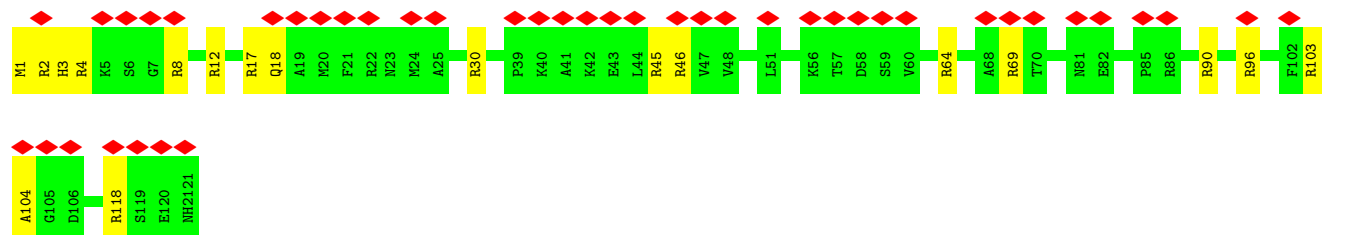
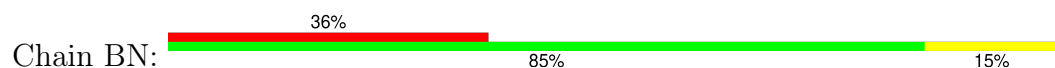
- Molecule 34: 50S ribosomal protein L15



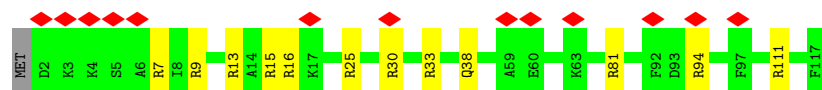
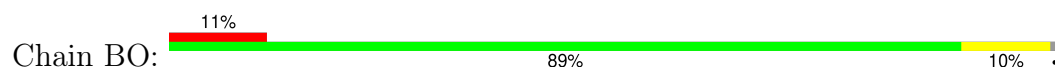
- Molecule 35: 50S ribosomal protein L16



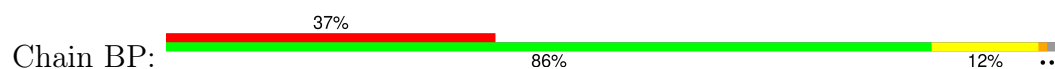
- Molecule 36: 50S ribosomal protein L17

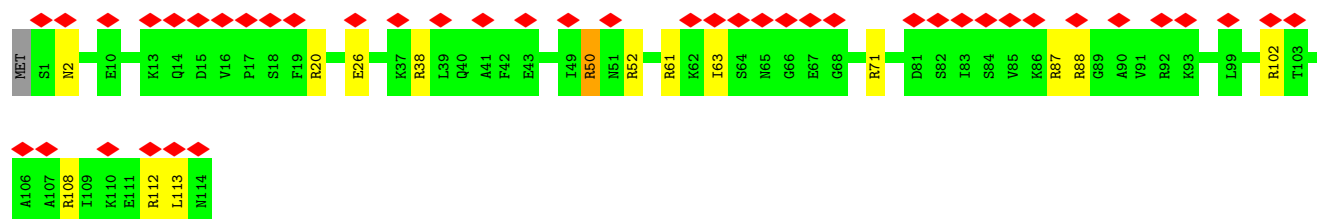


- Molecule 37: 50S ribosomal protein L18

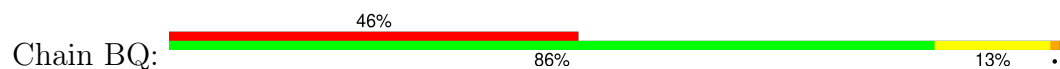


- Molecule 38: 50S ribosomal protein L19

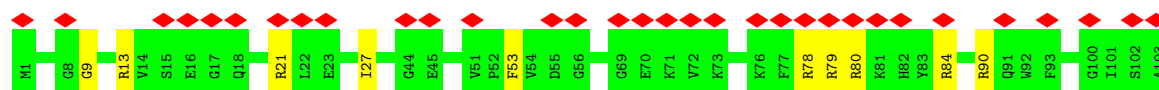
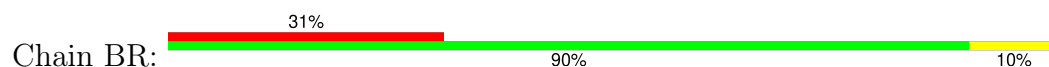




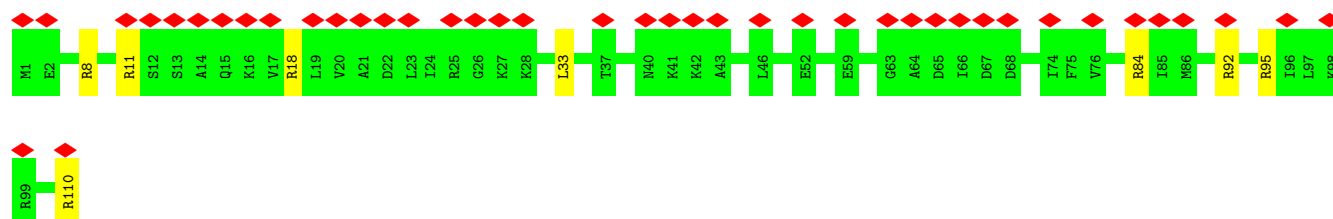
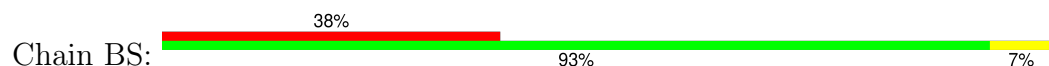
- Molecule 39: 50S ribosomal protein L20



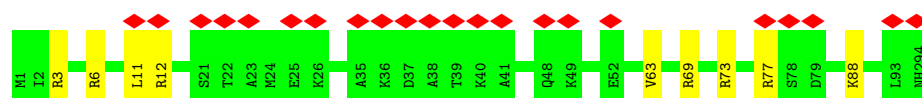
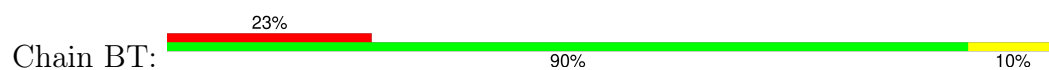
- Molecule 40: 50S ribosomal protein L21



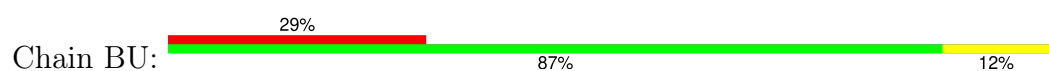
- Molecule 41: 50S ribosomal protein L22

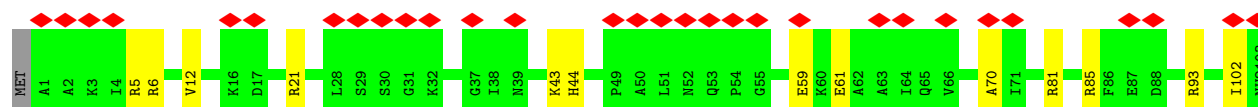


- Molecule 42: 50S ribosomal protein L23

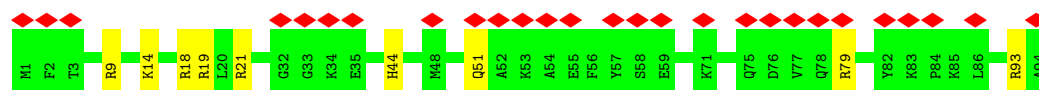
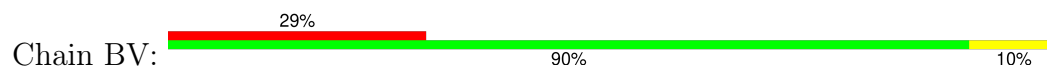


- Molecule 43: 50S ribosomal protein L24

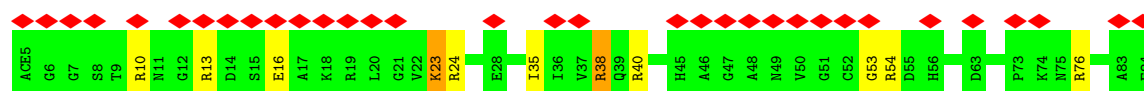
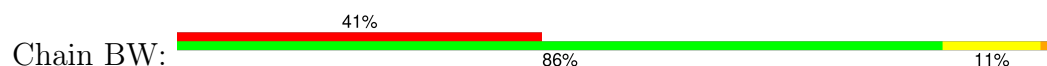




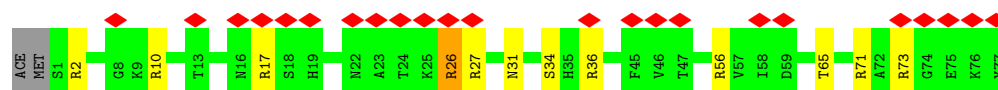
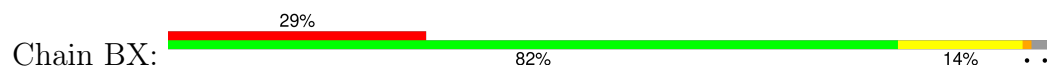
- Molecule 44: 50S ribosomal protein L25



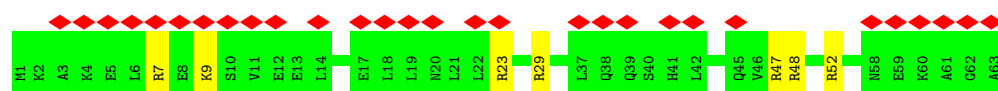
- Molecule 45: 50S ribosomal protein L27



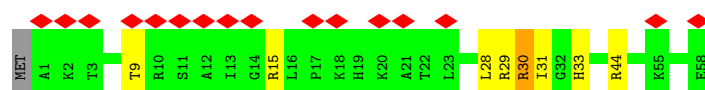
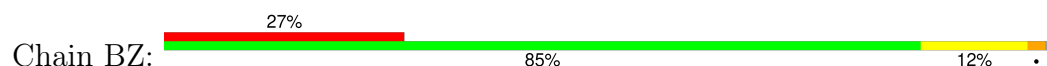
- Molecule 46: 50S ribosomal protein L28



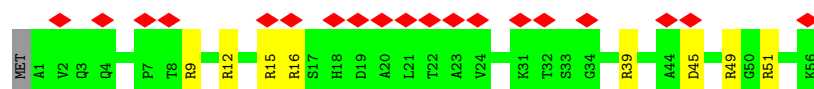
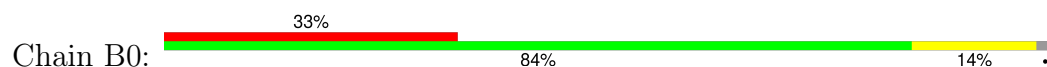
- Molecule 47: 50S ribosomal protein L29



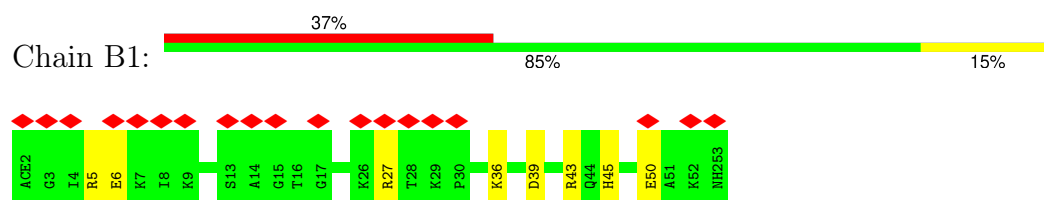
- Molecule 48: 50S ribosomal protein L30



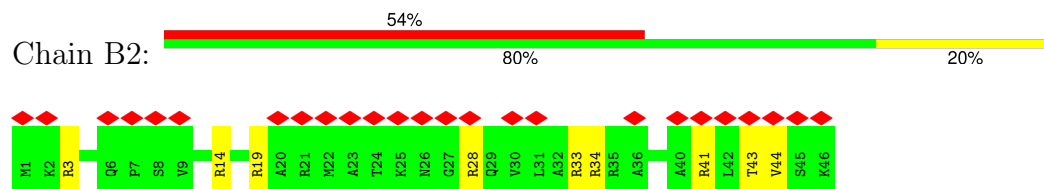
- Molecule 49: 50S ribosomal protein L32



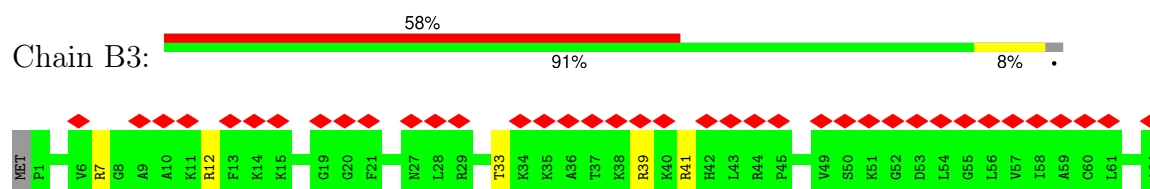
- Molecule 50: 50S ribosomal protein L33



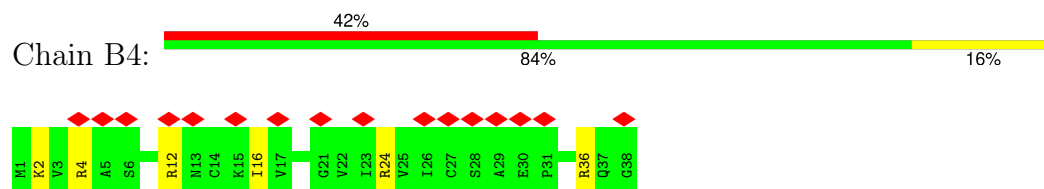
- Molecule 51: 50S ribosomal protein L34



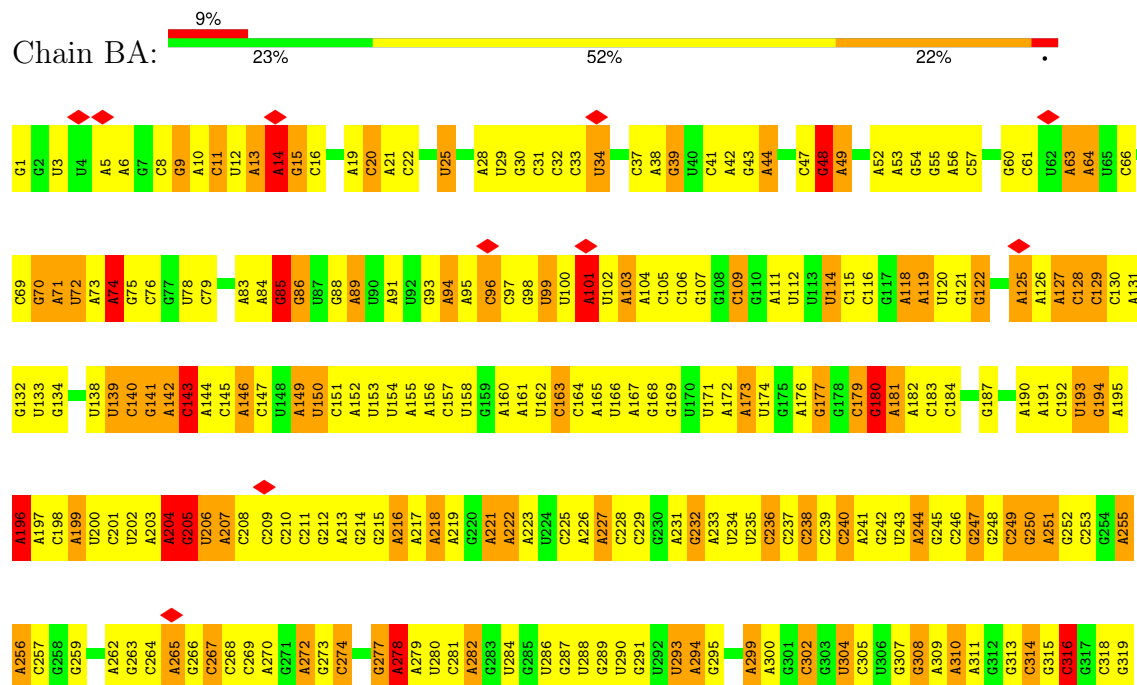
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



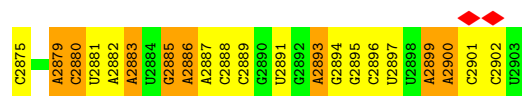
- Molecule 54: 23S ribosomal RNA



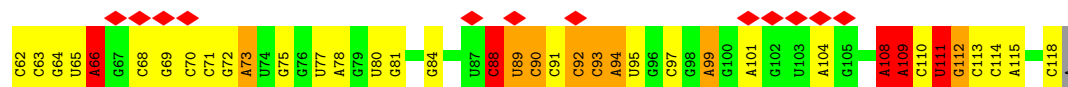
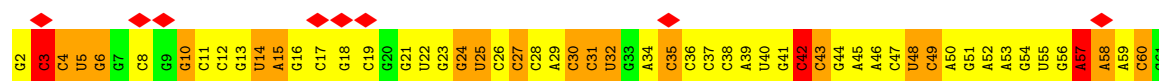
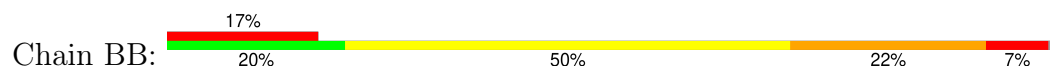


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G1922	U1923	C1924	C1925	U1926	A1927	U1928	U1929	U1930	U1931	U1932	U1933	C1934	U1935	U1936	A1937	A1938	U1939	U1940	U1941	C1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	A1951	A1952	C1953	U1954	U1955	U1956	C1957	U1958	U1959	C2002	C2003	C2004	C2005	U2026	C2027	U2028	C2029	U1966	C1967	U1968	A1969	U1970	U1971	C1972	C2036	C2035	A2037		C2040	U2041	A2042	C2043	C2044
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U1734	A1735	U1736	G1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765		U1768		U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795			
G1797	U1798	G1799	C1800	A1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833		U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856				
U1859	G1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	A1900	A1901	C1902	U1963	U1964	C1905	C1906	U1907	C1908	C1909		A1912	U1913	C1914	U1915	U1916	U1917	U1918	A1919	C1920	U1921	
U1982	U1983	G1984	C1985	C1986	A1987			C1990	C1993	U1993	U1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	U2007	U2008	C2009	U2010	U2011	C2012	C2013	A2014	U2015	U2016	U2017	C2018	A2019	A2020	C2021	U2022	C2023	C2024	C2025	U2026	C2027	U2028	C2029	C2030	A2031	C2032	A2033	U2034	C2035	C2036	A2037	C2040	U2041	A2042	C2043	C2044			
G1922	U1923	C1924	C1925	U1926	A1927	U1928	U1929	U1930	U1931	U1932	U1933	C1934	U1935	U1936	A1937	A1938	U1939	U1940	U1941	C1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	A1951	A1952	C1953	U1954	U1955	U1956	C1957	U1958	U1959	C2002	C2003	C2004	C2005	U2026	C2027	U2028	C2029	U1966	C1967	U1968	A1969	U1970	U1971	C1972	C2036	C2035	A2037		C2040	U2041	A2042	C2043	C2044
U1224	G1225	A1226	G1227	U1228	G1229	U1230	C1233	U1234	G1235	U1236	U1237	G1238	G1239	U1240	U1241	U1242	C1243	U1244	G1245	A1246	U1247	U1248	C1251	G1252	A1253	U1254	U1255	G1256	C1257	U1258	G1259	U1260	C1261	U1262	U1263	U1264	A1265	U1266	U1267	U1268	G1269	C1270	G1271	U1272	U1273	A1274	U1275	A1276	G1277	C1278	U1282	G1283	A1284	U1285	A1286	U1287						
G1288	C1289	U1290	C1291	G1292	U1293	U1294	U1295	C1296	U1297	C1298	U1299	G1300	A1301	U1302	U1303	A1304	C1305	C1306	U1307	A1308	U1312	U1313	C1314	C1315	U1316	G1317	U1318	U1319	C1320	A1321	U1322	G1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	G1331	C1332	U1333	G1334	C1335	U1336	U1339	U1340	G1341	U1342	G1343	U1344	C1345	G1346	A1347	C1348	A1349	C1350					
C1351	U1352	A1353	U1354	G1355	U1356	C1357	U1358	A1359	C1362	U1363	G1364	A1365	U1366	A1367	G1368	G1369	C1370	A1373	C1376	G1377	U1378	U1379	G1380	G1381	G1382	U1383	A1384	A1385	C1386	U1387	G1388	U1389	U1390	U1391	A1392	U1393	U1394	U1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	A1403	C1404	U1405	U1406	G1407	U1408	U1409	G1410	U1411	U1412	A1413						
C1414	U1415	C1416	C1417	G1418	U1419	A1420	G1421	G1422	G1423	U1424	G1425	U1426	C1427	C1428	A1431	G1432	U1433	A1434	G1435	G1436	U1437	U1438	U1439	U1440	G1441	U1442	U1443	G1444	G1445	U1446	C1447	U1448	C1451	U1452	A1453	C1454	U1457	U1458	G1459	U1460	C1461	C1462	C1463	G1464	G1465	U1469	A1470	G1471	C1472	G1473	U1474	C1475	U1476	A1477	G1478							
G1479	C1480	U1481	G1482	U1483	U1484	U1485	U1486	U1487	U1488	C1489	A1490	G1491	C1492	C1493	A1494	A1495	A1496	U1497	U1498	U1499	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	G1512	U1513	G1514	G1515	C1516	G1517	C1518	A1522	U1523	G1524	A1525	C1526	G1527	A1528	G1529	C1530	C1531	A1532	C1533	U1534	A1535	C1536	G1537	U1538	U1539	G1540	C1541					
A1544	U1545	G1546	C1547	U1548	U1549	C1550	A1551	A1552	U1553	U1554	U1555	C1556	C1557	C1558	U1559	G1560	C1561	U1562	U1563	C1564	C1565	A1566	G1567	G1568	A1569	U1570	A1571	U1572	G1573	C1574	G1575	U1576	C1577	U1578	A1579	G1580	C1582	U1583	U1584	A1585	C1586	A1587	U1588	U1589	U1590	C1592	A1593	U1594	C1595	A1596	U1597	A1598	U1599	C1600	G1601	U1602	A1603	C1604				
C1605	C1606	U1607	U1608	U1609	U1610	C1611	G1612	A1613	U1614	C1615	U1616	C1617	A1618	U1624	C1625	A1626	G1627	U1628	U1629	A1630	G1631	A1632	G1633	A1634	U1635	U1636	A1637	C1638	C1639	A1640	A1641	G1642	G1643	G1644	G1645	C1646	U1647	U1648	G1649	U1650	U1651	G1652	G1653	A1654	U1655	C1656	U1657	C1658	A1664	U1665	G1666	U1667	A1668	A1669	U1670	U1671	A1672					
G1673	G1674	U1675	U1676	U1677	U1678	U1679	U1680	G1681	G1684	C1685	U1686	C1687	U1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	G1696	G1697	A1698	G1699	U1700	A1701	G1702	G1703	C1704	A1705	C1706	G1707	C1708	U1709	G1710	A1711	U1712	U1713	U1714	G1715	U1716	U1717	G1718	U1719	U1720	G1721	U1722	G1723	G1724	U1725	C1726	U1727	U1728	U1729	C1730	G1731	C1732	G1733				
U1734	A1735	U1736	G1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765		U1768		U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795			
G1797	U1798	G1799	C1800	A1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833		U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856				
U1859	G1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	A1900	A1901	C1902	U1963	U1964	C1905	C1906	U1907	C1908	C1909		A1912	U1913	C1914	U1915	U1916	U1917	U1918	A1919	C1920	U1921	
U1982	U1983	G1984	C1985	C1986	A1987			C1990	C1993	U1993	U1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	U2007	U2008	C2009	U2010	U2011	C2012	C2013	A2014	U2015	U2016	U2017	C2018	A2019	A2020	C2021	U2022	C2023	C2024	C2025	U2026	C2027	U2028	C2029	C2030	A2031	C2032	A2033	U2034	C2035	C2036	A2037	C2040	U2041	A2042	C2043	C2044			
G1922	U1923	C1924	C1925	U1926	A1927	U1928	U1929	U1930	U1931	U1932	U19339																																																			

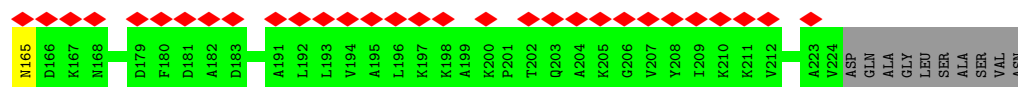
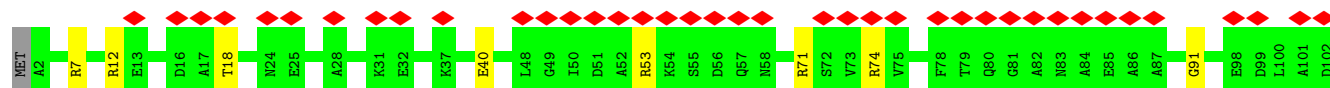
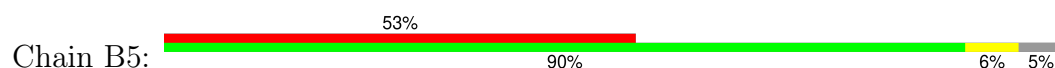




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13207	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	202.135	Depositor
Minimum map value	-122.001	Depositor
Average map value	-1.093	Depositor
Map value standard deviation	20.632	Depositor
Recommended contour level	27	Depositor
Map size (\AA)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.8, 2.8, 2.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 7MG, NH2, OMC, CM0, PSU, H2U, 6MZ, ACE, 5MU, FME

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	AB	0.70	0/1736	0.99	6/2340 (0.3%)
2	AC	0.73	0/1651	1.13	16/2225 (0.7%)
3	AD	0.75	0/1665	1.16	16/2227 (0.7%)
4	AE	0.69	0/1119	1.12	11/1506 (0.7%)
5	AF	0.72	0/835	1.09	6/1128 (0.5%)
6	AG	0.74	0/1188	1.23	15/1593 (0.9%)
7	AH	0.70	0/989	1.00	5/1326 (0.4%)
8	AI	0.79	0/1035	1.28	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	10/1079 (0.9%)
10	AK	0.74	0/894	1.23	11/1207 (0.9%)
11	AL	0.74	0/969	1.22	13/1300 (1.0%)
12	AM	0.76	0/884	1.30	14/1181 (1.2%)
13	AN	0.78	0/817	1.25	11/1088 (1.0%)
14	AO	0.72	0/722	1.19	8/964 (0.8%)
15	AP	0.77	0/648	1.19	8/870 (0.9%)
16	AQ	0.70	0/658	1.14	7/883 (0.8%)
17	AR	0.81	0/463	1.22	5/623 (0.8%)
18	AS	0.74	0/653	1.08	5/879 (0.6%)
19	AT	0.69	0/672	1.12	8/890 (0.9%)
20	AU	0.83	0/431	1.51	9/572 (1.6%)
21	AA	1.53	0/36759	2.21	1951/57346 (3.4%)
22	A1	1.55	0/1668	2.23	94/2595 (3.6%)
23	A2	1.46	1/343 (0.3%)	2.24	14/531 (2.6%)
24	A3	1.52	0/1722	2.20	88/2685 (3.3%)
25	BC	0.74	0/2121	1.26	28/2852 (1.0%)
26	BD	0.69	0/1586	1.17	11/2134 (0.5%)
27	BE	0.67	0/1571	1.18	13/2113 (0.6%)
28	BF	0.75	0/1444	1.24	15/1937 (0.8%)
29	BG	0.69	0/1343	1.17	10/1816 (0.6%)
30	BH	0.65	0/1122	1.07	4/1515 (0.3%)
31	BI	0.66	0/1046	1.00	2/1410 (0.1%)
32	BJ	0.71	0/1152	1.14	8/1551 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.70	0/947	1.28	11/1268 (0.9%)
34	BL	0.73	0/1054	1.32	13/1403 (0.9%)
35	BM	0.74	0/1093	1.15	10/1460 (0.7%)
36	BN	0.77	0/973	1.27	14/1301 (1.1%)
37	BO	0.73	0/902	1.28	12/1209 (1.0%)
38	BP	0.76	0/929	1.28	12/1242 (1.0%)
39	BQ	0.78	0/960	1.32	14/1278 (1.1%)
40	BR	0.73	0/829	1.16	8/1107 (0.7%)
41	BS	0.64	0/864	1.18	8/1156 (0.7%)
42	BT	0.64	0/744	1.21	7/994 (0.7%)
43	BU	0.69	0/787	1.17	7/1051 (0.7%)
44	BV	0.70	0/766	1.20	8/1025 (0.8%)
45	BW	0.73	0/604	1.28	9/799 (1.1%)
46	BX	0.76	0/635	1.31	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.71	0/453	1.22	5/605 (0.8%)
49	B0	0.74	0/450	1.31	8/599 (1.3%)
50	B1	0.74	0/417	1.16	3/556 (0.5%)
51	B2	0.81	0/380	1.48	8/498 (1.6%)
52	B3	0.72	0/513	1.18	4/676 (0.6%)
53	B4	0.67	0/303	1.29	4/397 (1.0%)
54	BA	1.41	1/69796 (0.0%)	2.21	4036/108888 (3.7%)
55	BB	1.41	0/2800	2.17	154/4367 (3.5%)
56	B5	0.64	0/1673	1.10	11/2255 (0.5%)
All	All	1.28	2/160085 (0.0%)	1.99	6823/239402 (2.9%)

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
3	AD	0	2
4	AE	0	1
21	AA	0	350
22	A1	0	14
23	A2	0	5
24	A3	0	16
25	BC	0	1
38	BP	0	1
54	BA	0	663
55	BB	0	31
All	All	0	1084

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	80	C	C4-N4	-5.22	1.29	1.33
54	BA	1314	C	C4-N4	-5.09	1.29	1.33

The worst 5 of 6823 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2740	A	O4'-C1'-N9	13.91	119.33	108.20
54	BA	1610	A	O4'-C1'-N9	13.75	119.20	108.20
54	BA	1584	U	O4'-C1'-N1	12.72	118.38	108.20
54	BA	280	U	O4'-C1'-N1	12.43	118.14	108.20
54	BA	1854	A	N1-C6-N6	-12.29	111.23	118.60

There are no chirality outliers.

5 of 1084 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	14	U	Sidechain
21	AA	6	G	Sidechain
3	AD	3	TYR	Sidechain
3	AD	36	ALA	Peptide
4	AE	148	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	1	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	1	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	4	0
22	A1	1627	0	832	1	0
23	A2	309	0	156	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B4	302	0	343	0	0
54	BA	62317	0	31339	3	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99657	11	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 0.

The worst 5 of 11 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)
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
21:AA:730:G:C5	21:AA:731:G:H1'	2.48	0.48
6:AG:148:LYS:HE3	10:AK:60:PHE:CZ	2.48	0.47
26:BD:125:TRP:CE3	26:BD:160:LYS:HE3	2.48	0.47
29:BG:1:SER:HA	54:BA:2749:A:OP1	2.18	0.43

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	AB	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	25 64
2	AC	205/208 (99%)	190 (93%)	12 (6%)	3 (2%)	8 40
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	6 32
4	AE	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	4 25
5	AF	99/101 (98%)	90 (91%)	4 (4%)	5 (5%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AG	150/152 (99%)	130 (87%)	18 (12%)	2 (1%)	10	43
7	AH	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	55
8	AI	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	16	55
9	AJ	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	3	22
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	52
11	AL	121/124 (98%)	108 (89%)	11 (9%)	2 (2%)	7	37
12	AM	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	7	35
13	AN	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	6	32
14	AO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	3	20
15	AP	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	2	19
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	4	26
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	7	35
18	AS	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	10	43
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	36 (71%)	12 (24%)	3 (6%)	1	13
25	BC	270/273 (99%)	241 (89%)	22 (8%)	7 (3%)	4	26
26	BD	207/209 (99%)	172 (83%)	20 (10%)	15 (7%)	1	11
27	BE	199/201 (99%)	179 (90%)	17 (8%)	3 (2%)	8	40
28	BF	176/179 (98%)	142 (81%)	25 (14%)	9 (5%)	1	15
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	7	37
30	BH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3	21
31	BI	139/142 (98%)	128 (92%)	9 (6%)	2 (1%)	9	41
32	BJ	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	9	41
33	BK	121/123 (98%)	102 (84%)	15 (12%)	4 (3%)	3	21
34	BL	141/144 (98%)	111 (79%)	19 (14%)	11 (8%)	1	10
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5	29
36	BN	119/121 (98%)	108 (91%)	9 (8%)	2 (2%)	7	37
37	BO	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	4	25
39	BQ	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	4	26
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BS	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
42	BT	92/94 (98%)	77 (84%)	12 (13%)	3 (3%)	3	21
43	BU	101/104 (97%)	83 (82%)	12 (12%)	6 (6%)	1	13
44	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	12	47
45	BW	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	1	15
46	BX	75/79 (95%)	66 (88%)	8 (11%)	1 (1%)	10	43
47	BY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	8	38
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	15
49	B0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
50	B1	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	9
51	B2	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	5	28
52	B3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	1	14
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	25	64
All	All	5876/6008 (98%)	5234 (89%)	497 (8%)	145 (2%)	7	26

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	105	THR
9	AJ	74	VAL
12	AM	65	GLU
14	AO	45	HIS
16	AQ	39	ARG

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	AB	180/180 (100%)	180 (100%)	0	100	100
2	AC	170/171 (99%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	112 (99%)	1 (1%)	75	83
5	AF	87/87 (100%)	85 (98%)	2 (2%)	45	64
6	AG	123/123 (100%)	121 (98%)	2 (2%)	58	73
7	AH	104/105 (99%)	103 (99%)	1 (1%)	73	82
8	AI	105/105 (100%)	104 (99%)	1 (1%)	73	82
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	101 (98%)	2 (2%)	52	69
12	AM	91/92 (99%)	90 (99%)	1 (1%)	70	80
13	AN	83/84 (99%)	78 (94%)	5 (6%)	16	37
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	40	58
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	64 (98%)	1 (2%)	60	75
20	AU	44/44 (100%)	42 (96%)	2 (4%)	23	45
25	BC	216/217 (100%)	214 (99%)	2 (1%)	75	83
26	BD	164/164 (100%)	162 (99%)	2 (1%)	67	78
27	BE	165/165 (100%)	156 (94%)	9 (6%)	18	39
28	BF	149/150 (99%)	146 (98%)	3 (2%)	50	68
29	BG	137/138 (99%)	135 (98%)	2 (2%)	60	75
30	BH	114/114 (100%)	112 (98%)	2 (2%)	54	71
31	BI	109/110 (99%)	107 (98%)	2 (2%)	54	71
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	56	72
33	BK	103/103 (100%)	102 (99%)	1 (1%)	73	82
34	BL	102/103 (99%)	100 (98%)	2 (2%)	50	68
35	BM	109/109 (100%)	106 (97%)	3 (3%)	38	57
36	BN	100/100 (100%)	98 (98%)	2 (2%)	50	68
37	BO	86/87 (99%)	85 (99%)	1 (1%)	67	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	98 (99%)	1 (1%)	73	82
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	67	78
41	BS	93/93 (100%)	92 (99%)	1 (1%)	70	80
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	44	62
44	BV	78/78 (100%)	76 (97%)	2 (3%)	41	59
45	BW	59/59 (100%)	57 (97%)	2 (3%)	32	51
46	BX	67/68 (98%)	64 (96%)	3 (4%)	23	45
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	48	66
49	B0	47/48 (98%)	46 (98%)	1 (2%)	48	66
50	B1	45/45 (100%)	44 (98%)	1 (2%)	47	65
51	B2	38/38 (100%)	37 (97%)	1 (3%)	41	59
52	B3	51/52 (98%)	50 (98%)	1 (2%)	50	68
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	56	72
All	All	4842/4870 (99%)	4769 (98%)	73 (2%)	60	75

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BU	61	GLU
56	B5	40	GLU
44	BV	51	GLN
48	BZ	33	HIS
27	BE	7	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
10	AK	23	HIS
34	BL	35	HIS
44	BV	88	HIS
49	B0	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	251 (16%)	84 (5%)
22	A1	73/76 (96%)	10 (13%)	4 (5%)
23	A2	14/15 (93%)	8 (57%)	2 (14%)
24	A3	76/77 (98%)	13 (17%)	2 (2%)
54	BA	2902/2903 (99%)	462 (15%)	119 (4%)
55	BB	117/118 (99%)	18 (15%)	6 (5%)
All	All	4712/4722 (99%)	762 (16%)	217 (4%)

5 of 762 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A

5 of 217 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	615	U
54	BA	1383	A
54	BA	2571	U
54	BA	762	U
54	BA	1126	A

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

11 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	$\# Z > 2$
24	H2U	A3	21	24	18,21,22	1.29	2 (11%)	19,30,33	1.45	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	A3	56	24	18,21,22	0.85	0	21,30,33	1.34	2 (9%)
22	5MU	A1	54	22	19,22,23	0.72	0	27,32,35	1.32	3 (11%)
24	OMC	A3	33	24	19,22,23	0.69	0	25,31,34	1.06	2 (8%)
22	4SU	A1	7	22	18,21,22	1.47	2 (11%)	25,30,33	0.96	1 (4%)
24	4SU	A3	8	24	18,21,22	1.50	2 (11%)	25,30,33	0.90	1 (4%)
22	7MG	A1	46	22	23,26,27	4.10	3 (13%)	27,39,42	1.42	1 (3%)
24	5MU	A3	55	24	19,22,23	0.67	0	27,32,35	1.51	5 (18%)
22	6MZ	A1	37	22	17,25,26	1.09	1 (5%)	15,36,39	1.75	4 (26%)
22	PSU	A1	55	22	18,21,22	0.79	0	21,30,33	1.15	2 (9%)
22	CM0	A1	34	22,23	21,26,27	1.30	2 (9%)	26,37,40	1.53	2 (7%)

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
24	H2U	A3	21	24	-	1/7/38/39	0/2/2/2
24	PSU	A3	56	24	-	1/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	PSU	A1	55	22	-	2/7/25/26	0/2/2/2
22	CM0	A1	34	22,23	-	2/12/30/31	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-19.23	1.33	1.45
22	A1	7	4SU	C5-C4	-5.22	1.36	1.42
24	A3	8	4SU	C5-C4	-5.15	1.36	1.42
22	A1	34	CM0	O5-C5	-4.54	1.26	1.36
24	A3	21	H2U	C2-N3	-3.35	1.32	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.85	111.65	103.37
22	A1	34	CM0	C7-O5-C5	5.32	124.26	117.48
24	A3	56	PSU	C6-C5-C4	3.84	120.76	118.17
22	A1	37	6MZ	C9-N6-C6	3.65	126.23	122.85
22	A1	54	5MU	C5M-C5-C6	-3.62	117.95	122.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	55	PSU	C2'-C1'-C5-C4
24	A3	21	H2U	C4'-C5'-O5'-P
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C4

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0
22	A1	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
57	VAL	A1	101	58,22	4,6,7	0.77	0	6,7,9	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	FME	BA	3001	57	8,9,10	0.67	0	8,9,11	1.46	2 (25%)

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
57	VAL	A1	101	58,22	-	0/5/6/8	-
58	FME	BA	3001	57	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.48	118.39	124.77
58	BA	3001	FME	C-CA-N	2.38	114.08	109.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA
58	BA	3001	FME	O-C-CA-CB

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.

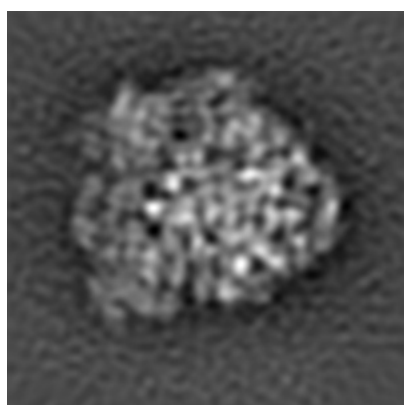
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1721. These allow visual inspection of the internal detail of the map and identification of artifacts.

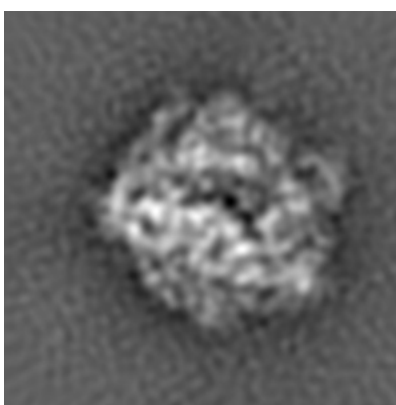
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

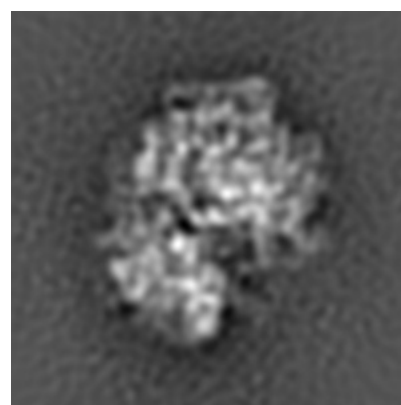
6.1.1 Primary map



X



Y

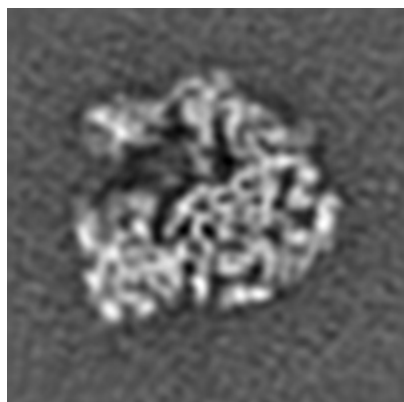


Z

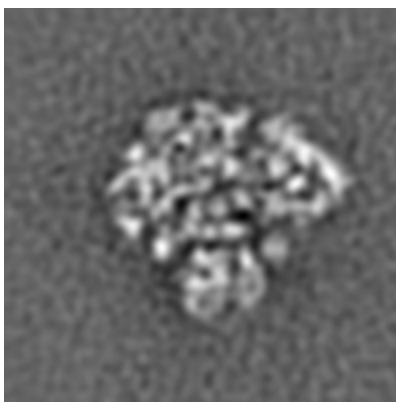
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

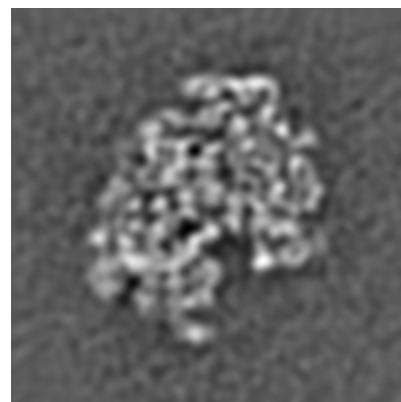
6.2.1 Primary map



X Index: 64



Y Index: 64

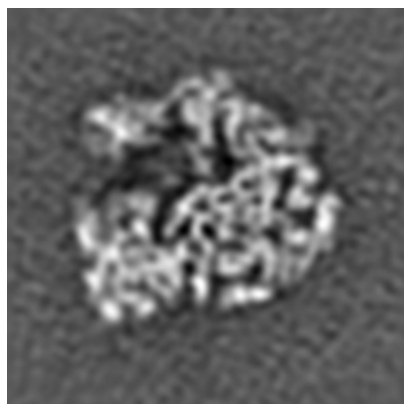


Z Index: 64

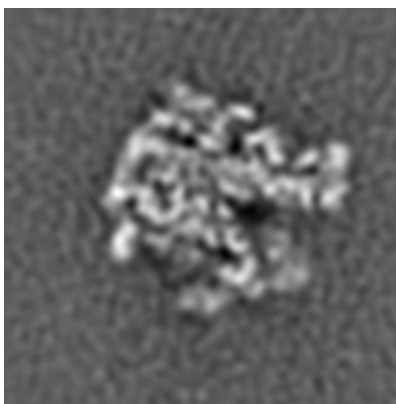
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

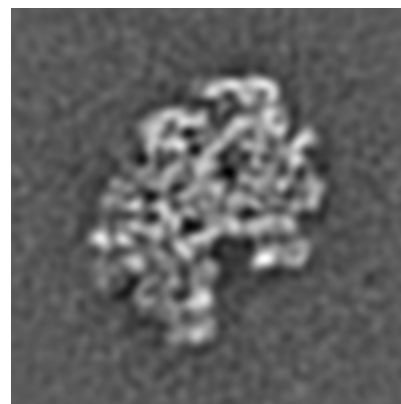
6.3.1 Primary map



X Index: 64



Y Index: 69

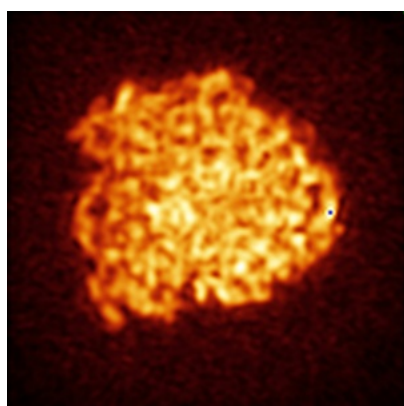


Z Index: 62

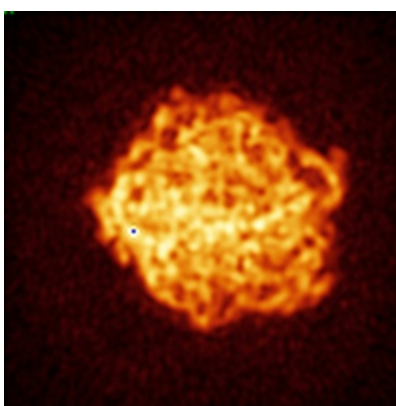
The images above show the largest variance slices of the map in three orthogonal directions.

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

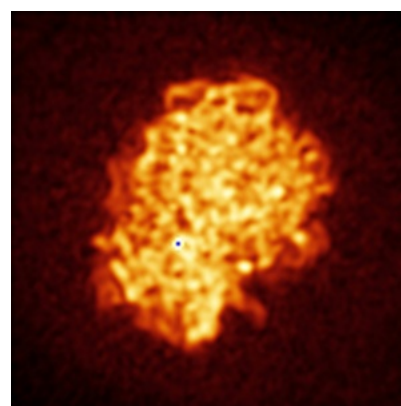
6.4.1 Primary map



X



Y

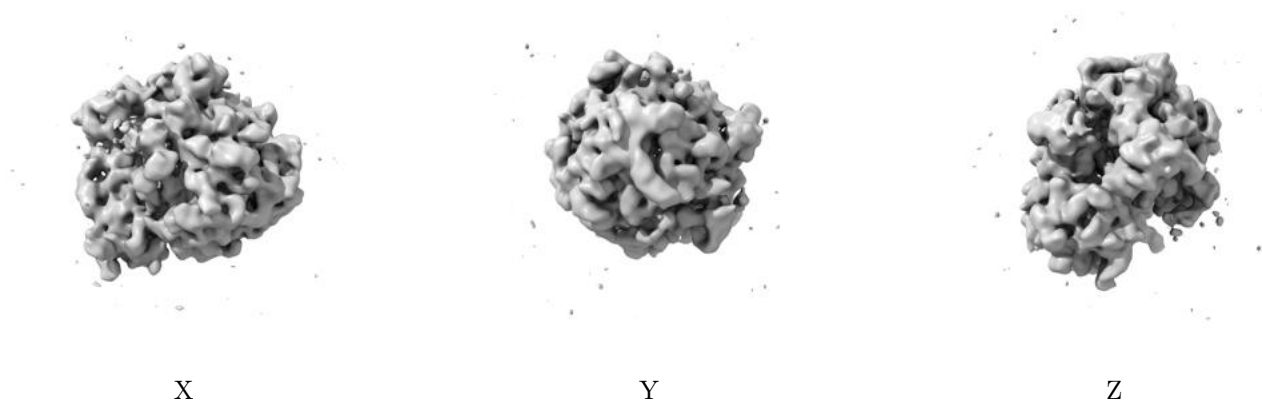


Z

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

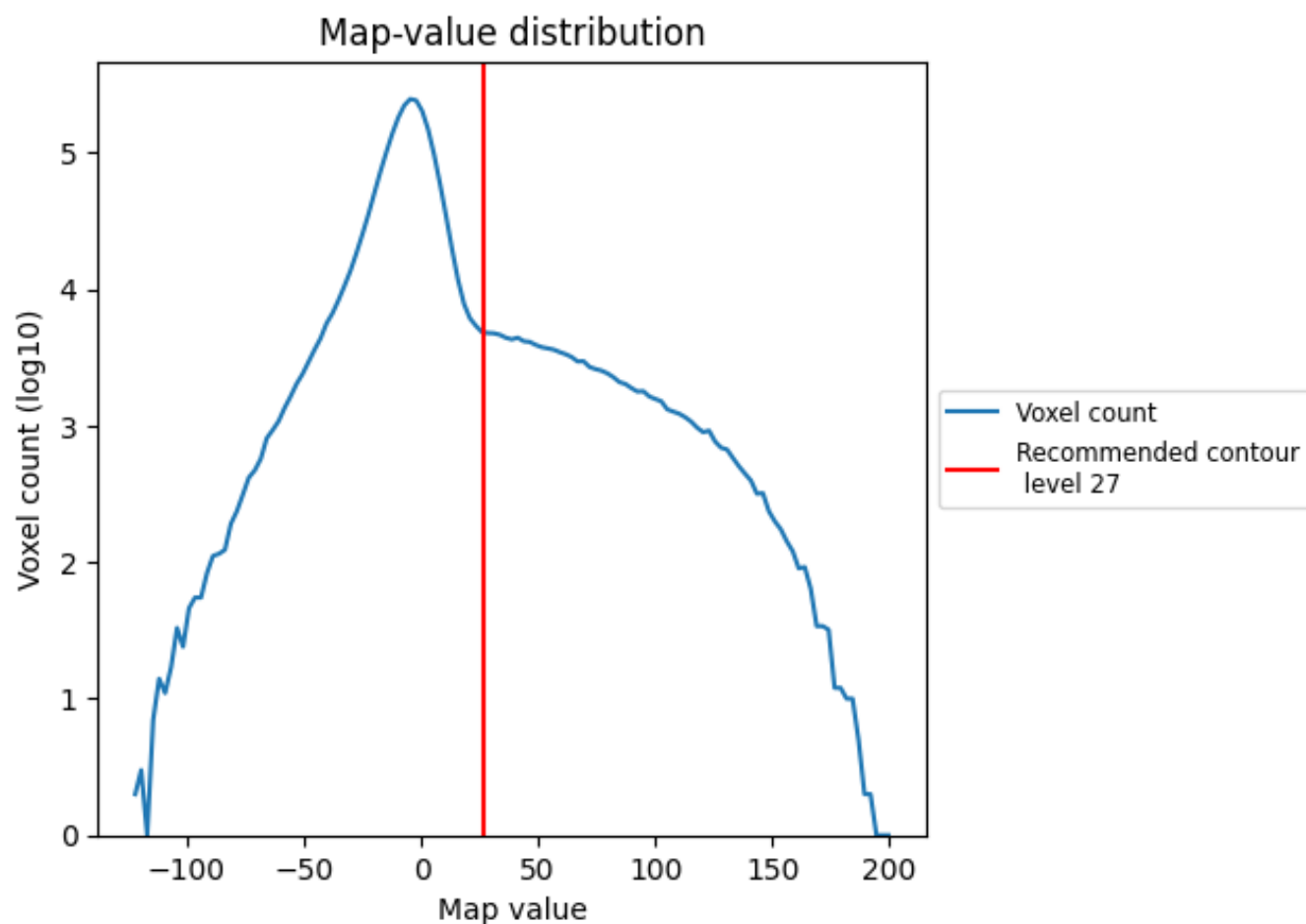
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

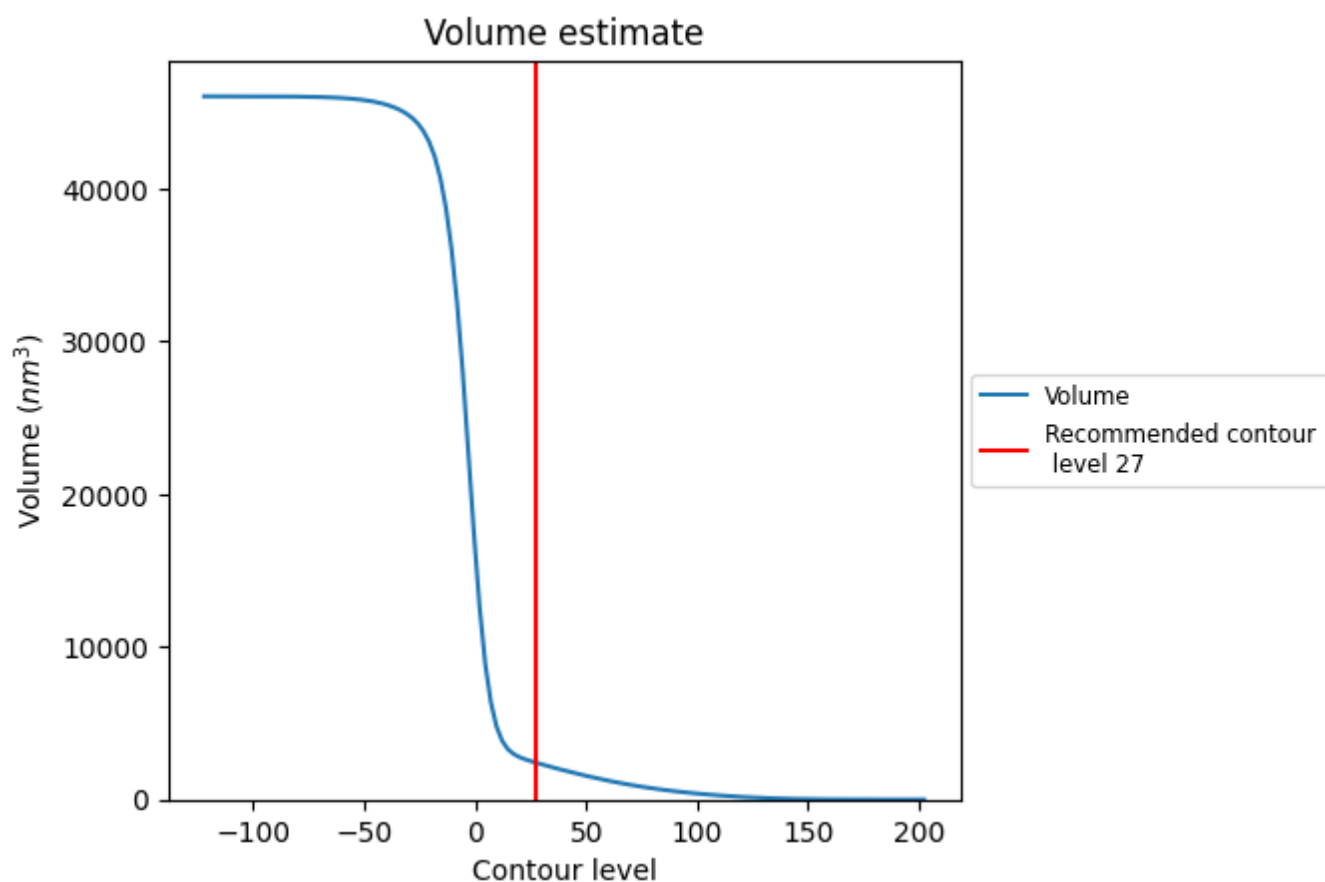
This section contains the results of statistical analysis of the map.

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.

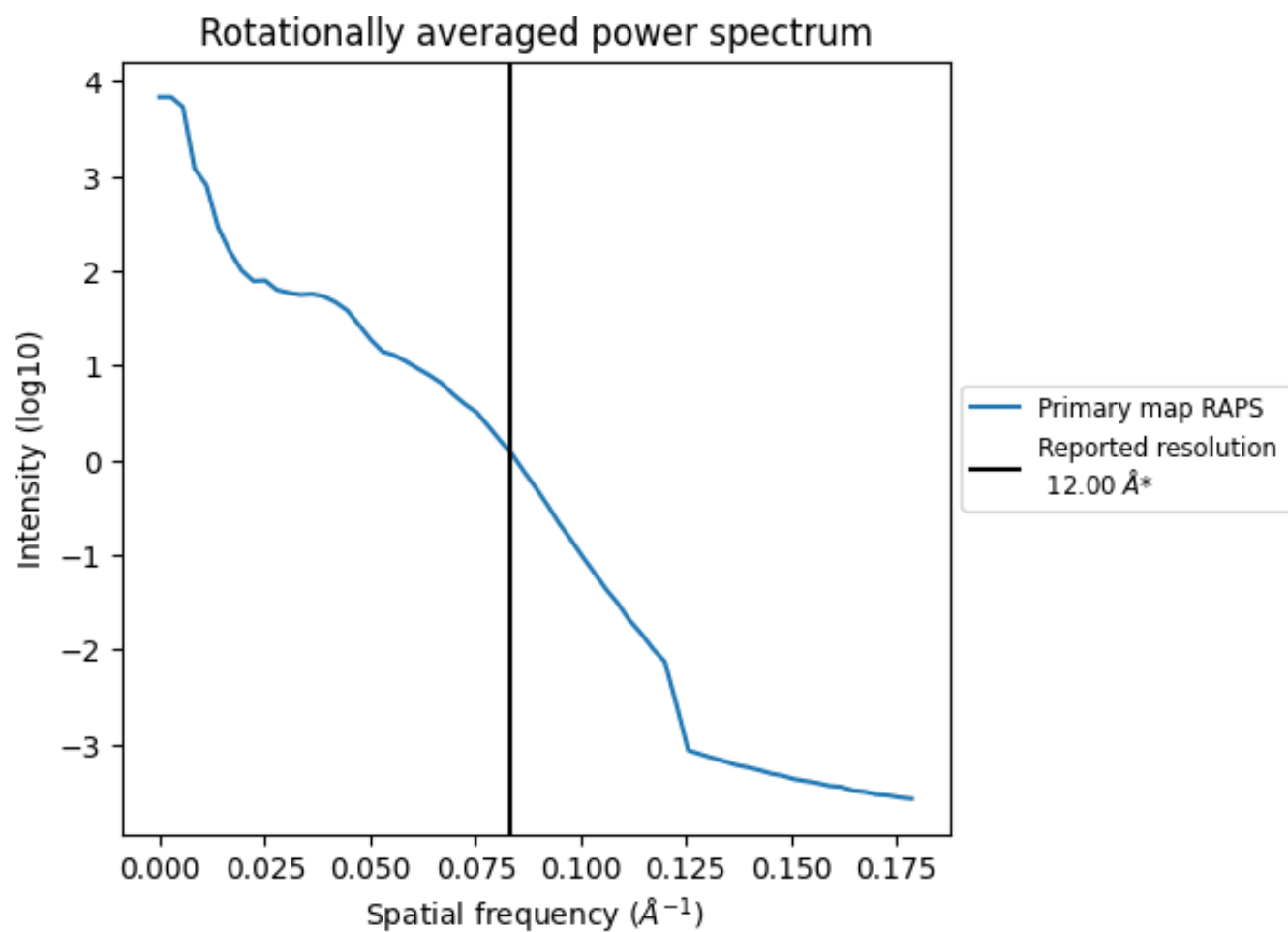
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2432 nm³; this corresponds to an approximate mass of 2196 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 0.083 Å⁻¹

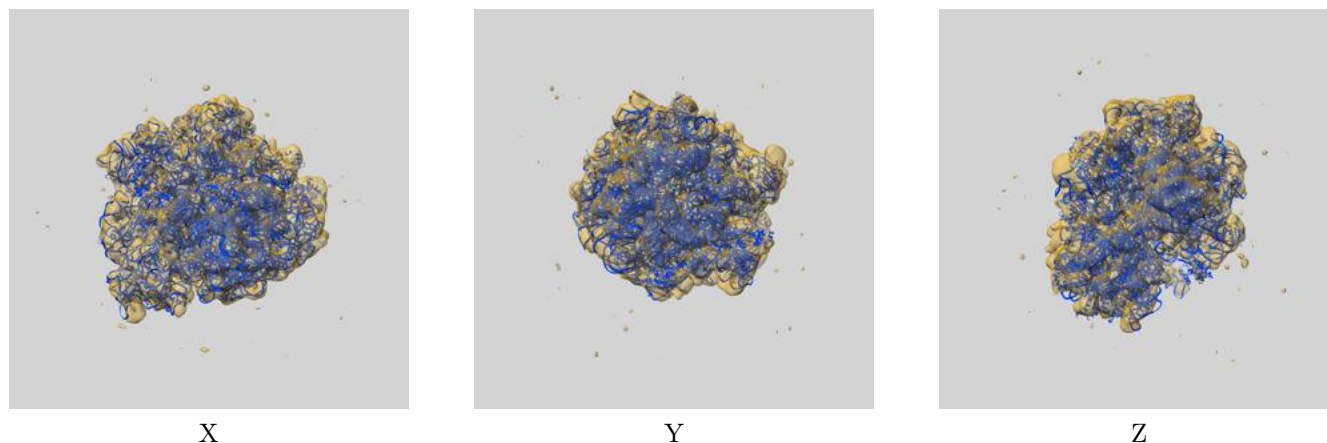
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

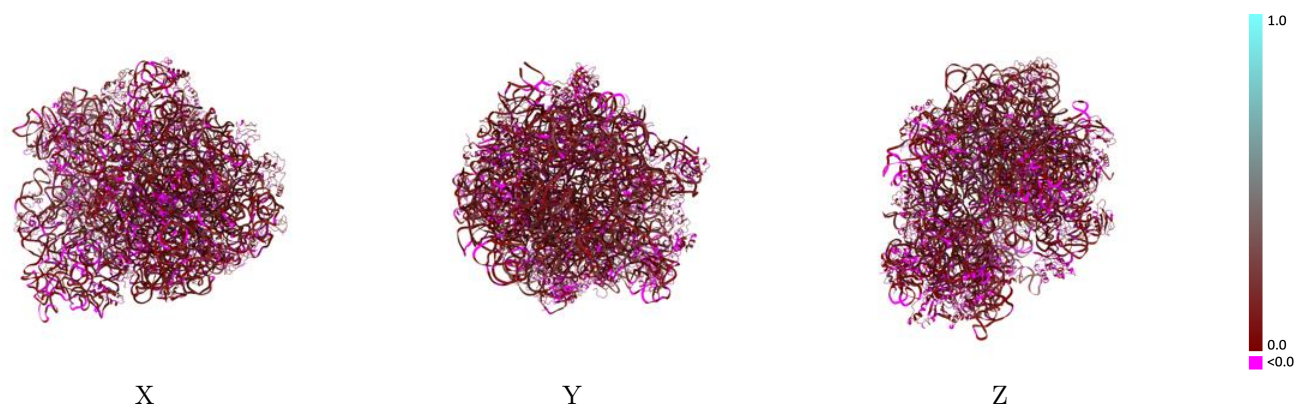
This section contains information regarding the fit between EMDB map EMD-1721 and PDB model 4V75. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



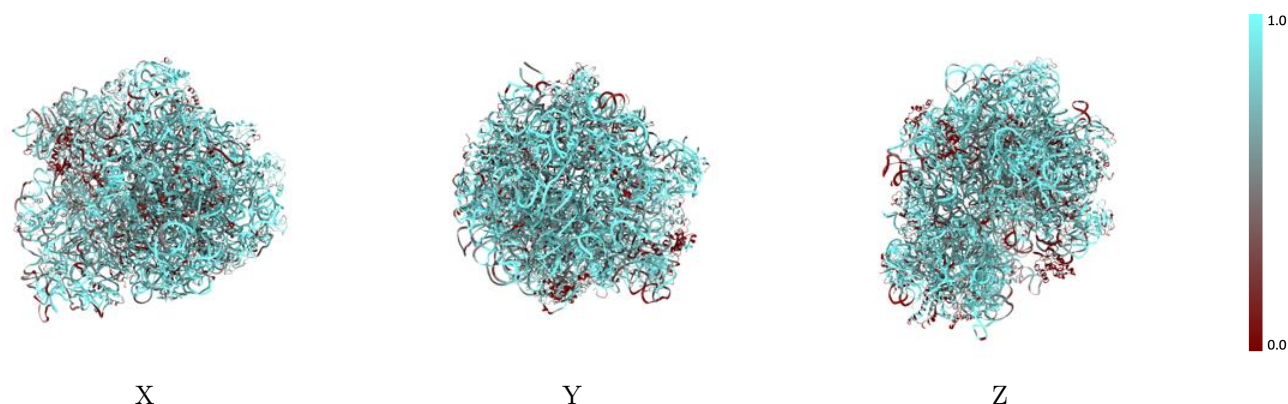
The images above show the 3D surface view of the map at the recommended contour level 27.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



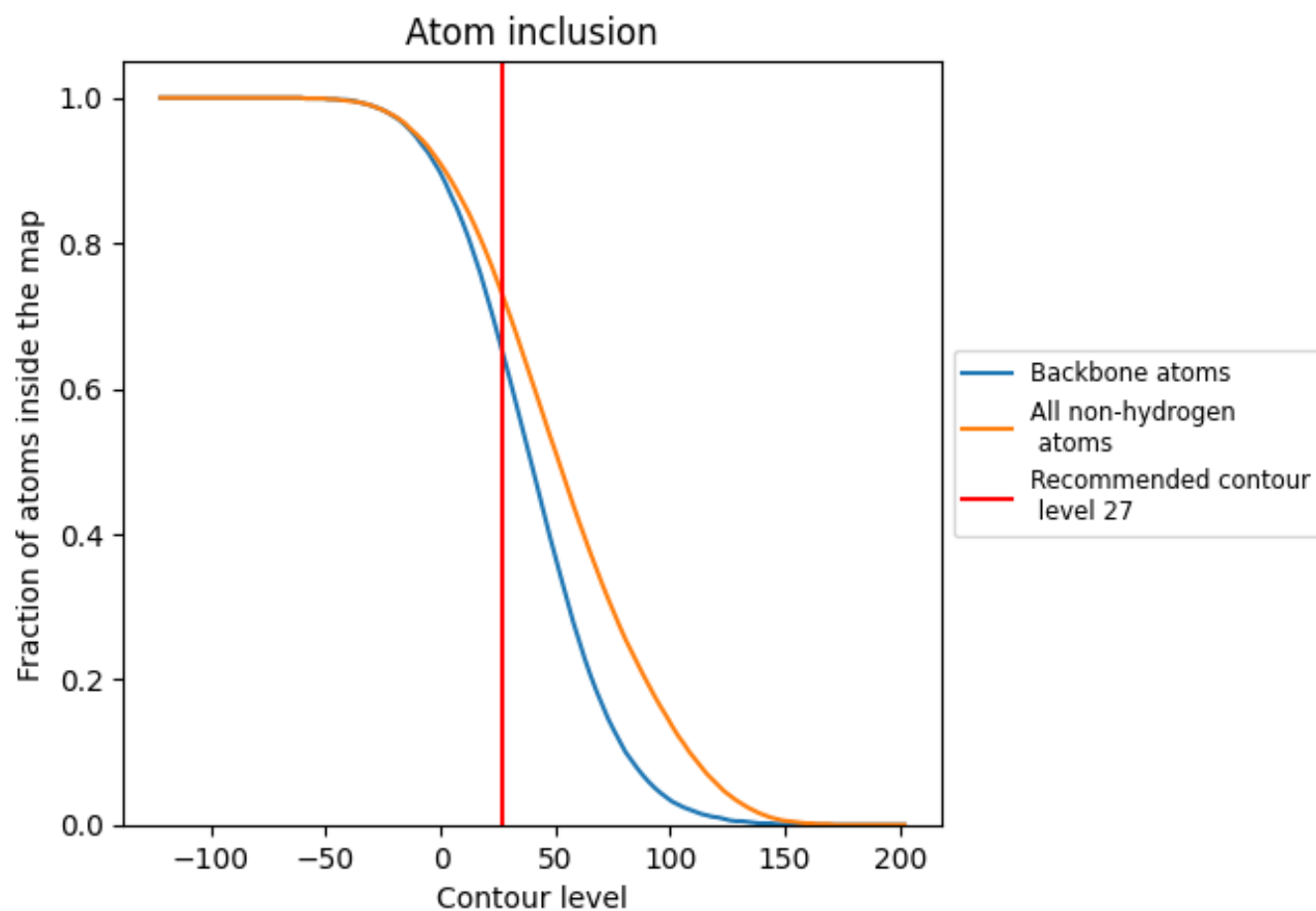
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (27).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 73% 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 (27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.0720
A1	 0.6500	 0.0960
A2	 0.5920	 0.0590
A3	 0.5400	 0.0610
AA	 0.8090	 0.0810
AB	 0.6030	 0.0610
AC	 0.6120	 0.0470
AD	 0.6200	 0.0320
AE	 0.6310	 0.0690
AF	 0.7180	 0.0780
AG	 0.6480	 0.0570
AH	 0.6450	 0.0510
AI	 0.6830	 0.0270
AJ	 0.5100	 0.0090
AK	 0.7170	 0.0570
AL	 0.6500	 0.0410
AM	 0.7100	 0.0720
AN	 0.5930	 0.0150
AO	 0.6670	 0.0410
AP	 0.5400	 0.0440
AQ	 0.6410	 0.0680
AR	 0.4510	 0.0160
AS	 0.6150	 0.0200
AT	 0.6700	 0.0090
AU	 0.4250	 -0.0020
B0	 0.6190	 0.0430
B1	 0.5790	 0.0530
B2	 0.4250	 0.0420
B3	 0.3810	 0.0100
B4	 0.5410	 -0.0020
B5	 0.4320	 0.0320
BA	 0.8020	 0.0900
BB	 0.7530	 0.0550
BC	 0.4990	 0.0430
BD	 0.5140	 0.0360



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Chain	Atom inclusion	Q-score
BE	 0.6760	 0.0610
BF	 0.7380	 0.0580
BG	 0.7370	 0.0770
BH	 0.3010	 0.0310
BI	 0.0490	 0.0220
BJ	 0.5080	 0.0280
BK	 0.4790	 0.0490
BL	 0.4660	 -0.0000
BM	 0.5120	 0.0410
BN	 0.5860	 0.0350
BO	 0.8200	 0.0410
BP	 0.5440	 0.0400
BQ	 0.4980	 0.0270
BR	 0.6460	 0.0530
BS	 0.5710	 0.0500
BT	 0.7040	 0.0490
BU	 0.6440	 0.0440
BV	 0.6520	 0.0560
BW	 0.5740	 0.0240
BX	 0.6420	 0.0430
BY	 0.5150	 0.0330
BZ	 0.6770	 0.0460