wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 02:59 PM EDT

PDB ID	:	8SYL / pdb_00008syl
EMDB ID	:	EMD-40882
Title	:	Cryo-EM structure of the Escherichia coli 70S ribosome in complex with amikacin, mRNA, and A-, P-, and E-site tRNAs
Authors	:	Seely, S.M.; Gagnon, M.G.
Deposited on	:	2023-05-25
Resolution	:	2.90 Å(reported)
Based on initial model	:	8EKC

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 (i) 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 (i)) were used in the production of this report:

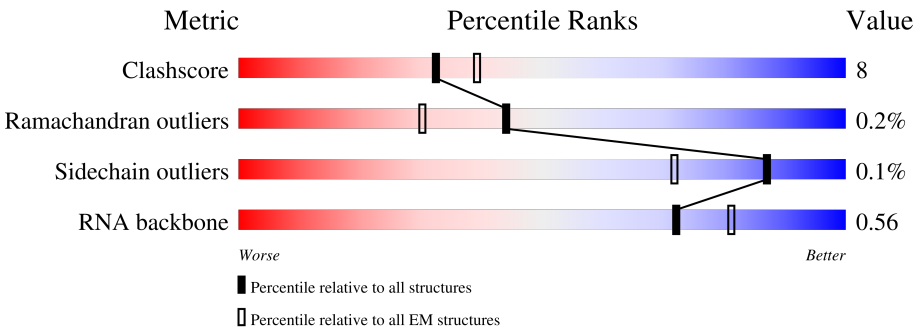
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

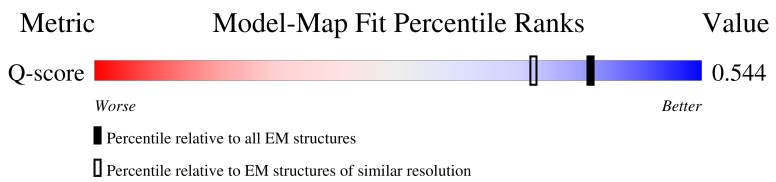
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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 <=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	54% 41% • •
2	b	241	29% 76% 17% 7%
3	c	233	61% 27% 12%

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Mol	Chain	Length	Quality of chain
4	d	206	60% 40%
5	e	167	74% 20% 7%
6	f	131	49% 28% 22%
7	g	156	83% 14%
8	h	130	75% 24%
9	i	130	66% 31%
10	j	103	81% 14% 6%
11	k	129	63% 27% 9%
12	l	124	70% 27%
13	m	118	78% 18%
14	n	101	76% 23%
15	o	89	69% 30%
16	p	82	76% 22%
17	q	84	69% 25% 6%
18	r	75	55% 17% 28%
19	s	92	61% 28% 11%
20	t	87	70% 28%
21	u	71	62% 15% 23%
22	w	76	45% 41% 12%
22	y	76	32% 43% 37% 14%
23	x	77	64% 30% 5%
24	v	24	33% 17% 50%
25	A	2904	59% 34% 5%
26	B	120	68% 27% 6%
27	C	273	77% 22%

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Mol	Chain	Length	Quality of chain
28	D	209	80% 20%
29	E	201	88% 12%
30	F	179	66% 32%
31	G	177	75% 24%
32	H	149	7% 23% 72%
33	L	142	79% 21%
34	M	123	79% 21%
35	N	144	78% 22%
36	O	136	74% 26%
37	P	127	72% 21% 7%
38	Q	117	74% 26%
39	R	115	83% 17%
40	S	118	83% 16%
41	T	103	89% 11%
42	U	110	79% 21%
43	V	100	77% 16% 7%
44	W	104	82% 16%
45	X	94	71% 29%
46	Y	85	84% 14%
47	Z	78	79% 19%
48	1	63	70% 27%
49	2	59	78% 20%
50	3	70	69% 17% 14%
51	4	57	70% 26%
52	5	55	76% 16% 7%

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Mol	Chain	Length	Quality of chain
53	6	46	83% 17%
54	7	65	85% 14%
55	8	38	82% 18%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 144591 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1528	32803	14637	6019	10619	1528	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1514	963	279	267	5	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	206	1613	1023	305	282	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1117	695	213	203	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	102	778	497	133	143	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	152	1054	656	204	190	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	129	969	611	169	183	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	126	937	586	183	166	2	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	j	97	673	428	130	115	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	117	860	531	168	158	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	modified residue	UNP A0A0H3PWX2

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	121	924	570	187	162	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	113	823	510	166	145	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	100	792	492	162	135	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	88	703	434	141	127	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	80	613	385	123	104	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	q	79	630	400	116	111	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	54	441	280	83	78	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	82	641	411	120	108	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	t	85	648	400	134	111	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	u	55	373	241	72	59	1	0	0

- Molecule 22 is a RNA chain called phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
22	w	74	1591	713	285	517	74	2	0	0
22	y	74	1585	707	285	518	74	1	0	0

- Molecule 23 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
23	x	76	1625	725	294	529	76	1	0	0

- Molecule 24 is a RNA chain called M-F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	v	12	255	115	46	82	12	0	0

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	A	2845	61097	27261	11245	19746	2845	0	0

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	B	120	2572	1145	470	837	120	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	C	271	2069	1282	417	363	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	D	209	1559	976	288	292	3	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	E	201	1538	966	282	285	5	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	F	177	1401	895	245	255	6	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	G	175	1299	818	237	242	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	H	41	303	194	54	54	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	N	144	1048	651	207	188	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	O	136	1075	686	205	177	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	modified residue	UNP E6BI61

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Q	116	876	541	175	160	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	R	114	913	573	178	161	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	U	110	850	529	163	155	3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	W	102	769	486	144	139	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	X	94	750	477	137	134	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Y	84	634	391	129	113	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	1	61	495	305	97	92	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	2	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	3	60	468	290	87	85	6	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	4	55	434	263	92	78	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	5	51	417	269	76	72	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	6	46	377	228	90	57	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	7	64	504	323	105	74	2	0	0

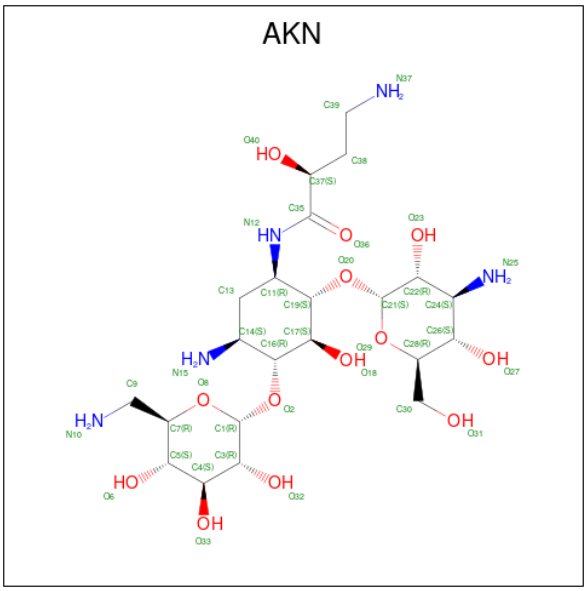
- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	8	38	302	185	65	48	4	0	0

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

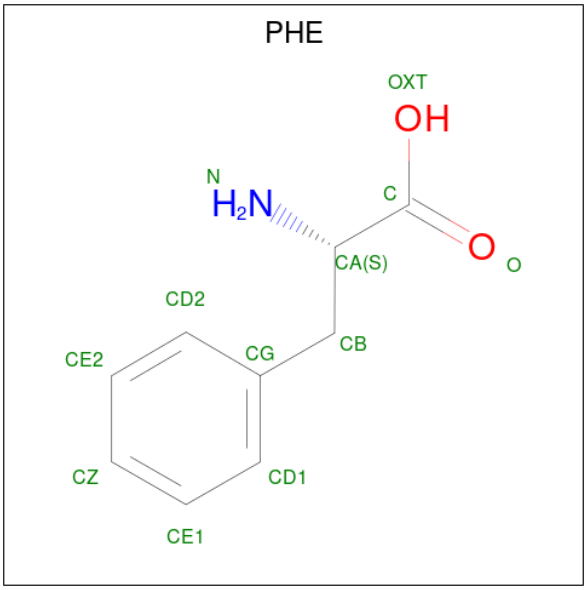
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	a	98	98	98	0
56	x	3	3	3	0
56	v	1	1	1	0
56	A	359	359	359	0
56	B	6	6	6	0
56	C	1	1	1	0
56	D	1	1	1	0
56	P	1	1	1	0
56	S	1	1	1	0
56	X	1	1	1	0
56	Y	1	1	1	0
56	4	1	1	1	0

- Molecule 57 is (2S)-N-[(1R,2S,3S,4R,5S)-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-5-azanyl-2-[(2S,3R,4S,5S ,6R)-4-azanyl-6-(hydroxymethyl)-3,5-bis(oxidanyl)oxan-2-yl]oxy-3-oxidanyl-cyclohexyl]-4-azanyl-2-oxidanyl-butanamide (CCD ID: AKN) (formula: $C_{22}H_{43}N_5O_{13}$).



Mol	Chain	Residues	Atoms				AltConf
57	a	1	Total 40	C 22	N 5	O 13	0
57	A	1	Total 40	C 22	N 5	O 13	0

- Molecule 58 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
58	w	1	Total 11	C 9	N 1	O 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	3	1	1	1	0
			Total	Zn	
59	8	1	1	1	0

- Molecule 60 is water.

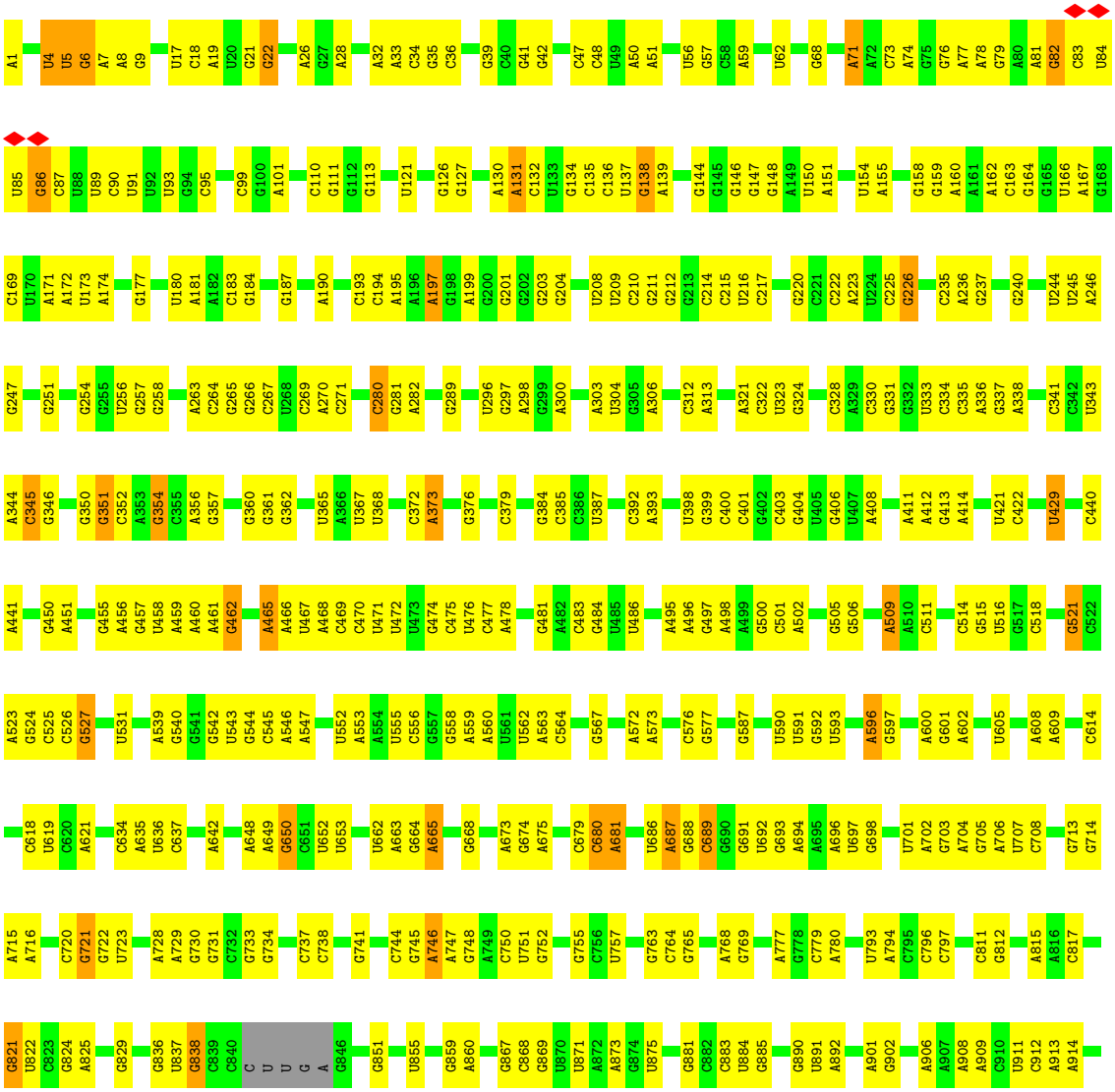
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	a	11	11	11	0
			Total	O	
60	n	1	1	1	0
			Total	O	
60	x	1	1	1	0
			Total	O	
60	A	60	60	60	0
			Total	O	
60	N	1	1	1	0

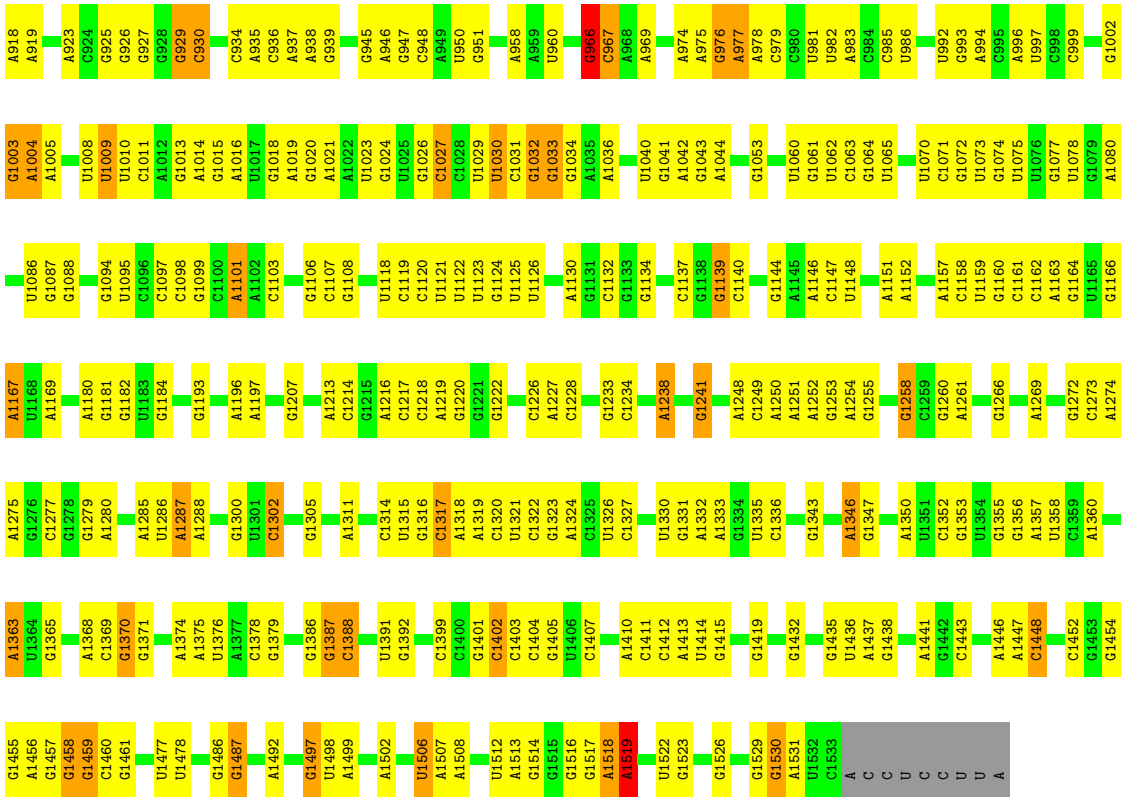
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA

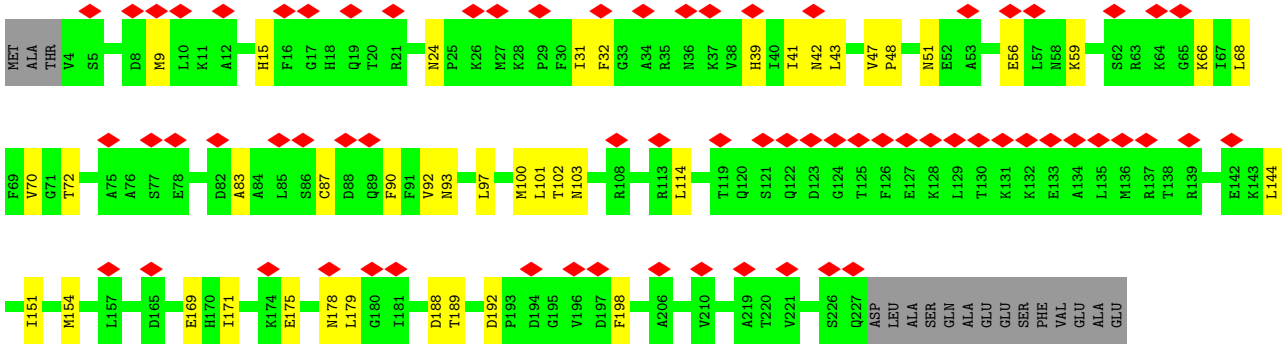
Chain a: 54% 41%





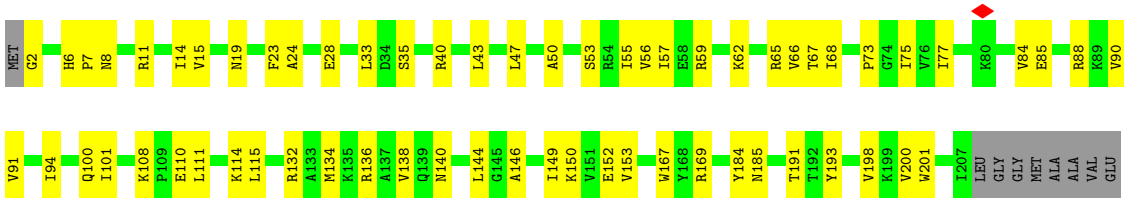
- Molecule 2: 30S ribosomal protein S2

Chain b:



- Molecule 3: 30S ribosomal protein S3

Chain c:



GLN PRO GLU LYS PRO ALA ALA GLN PRO LYS LYS GLN GLN ARG LYS GLY ARG LYS

- Molecule 4: 30S ribosomal protein S4

Chain d: 60% 40%

MET A2 R3 K8 L9 K10 L11 S12 R13 L19 F20 L21 K22 S23 R26 A27 I28 C32 K33 I34 E35 Q36 G39 R47 L48 S49 D50 Y51 G52 V53 Q54 L55 R56 E57 K58 Q59 K60 V61 R62 R63 E69 R70 Q71 N85 T86 G87 E88 N89 L93 L94 E95

L98 D99 N100 V101 R104 M105 T110 R111 A112 E113 A114 R115 V118 I123 M124 V125 I132 A133 S134 Y135 Q136 V137 N140 D141 V142 R146 K150 K151 Q152 V155 K156 L161 P168 T169 W170 L171 D174 M178 E179 G180 T181 F182 K185 P186 E187

R188 D194 I195 N196 E197 H198 L199 I200 V201 E202 L203 Y204 S205 K206

- Molecule 5: 30S ribosomal protein S5

Chain e: 74% 20% 7%

MET ALA HIS ILE GLU LYS GLN ALA GLY E10 T34 A35 L36 T37 V38 D41 R45 K52 A53 R54 A58 K62 L76 N77 N78 C79 T80 L81 Q82 G91 Q97 P98 G102 A107 V114 L115 V120 H121 N122 V123 L124 A125 I134 N135 R138

N148 S149 M152 L165 GLY LYS

- Molecule 6: 30S ribosomal protein S6

Chain f: 49% 28% 22%

MET R2 E5 I6 V10 V18 I22 T26 I29 A32 E33 G34 K35 I36 H37 R38 L39 W42 L47 A48 Y49 A57 H58 Y59 V60 L61 M62 N63 V64 E65 A66 P67 Q68 I71 D72 E73 L74 E75 F78 D82 A83 R86 S87 M88 V89

M102 V103 LYS ALA LYS ASP GLU ARG ARG GLU ARG ARG ASP ASP PHE ALA ASN GLU THR ALA ASP ASP ALA GLU ALA GLY ASP SER GLU GLU

- Molecule 7: 30S ribosomal protein S7

Chain g: 83% 14%

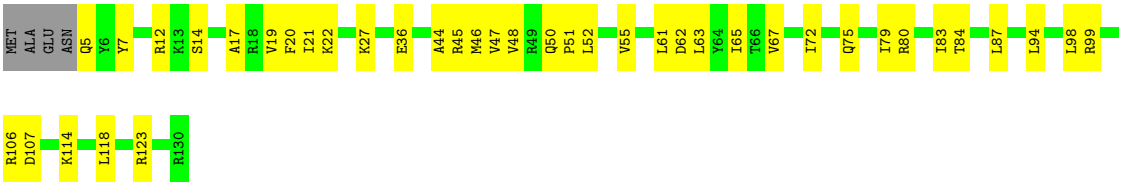
MET P2 G8 Q9 R10 F26 V27 N28 M31 G34 L47 F62 N68 V69 R70 P71 T72 V75 P93 R96 N97 A100 M101 D113 R119 L120 N130 M144 H153 TYR ARG TRP

- Molecule 8: 30S ribosomal protein S8

Chain h: 75% 24%

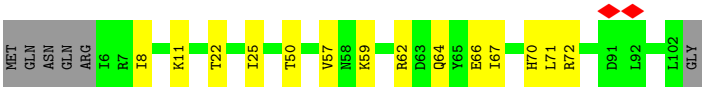
• Molecule 9: 30S ribosomal protein S9

Chain i:



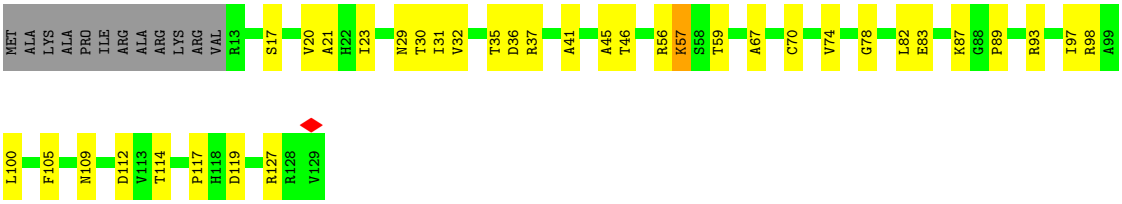
• Molecule 10: 30S ribosomal protein S10

Chain j:



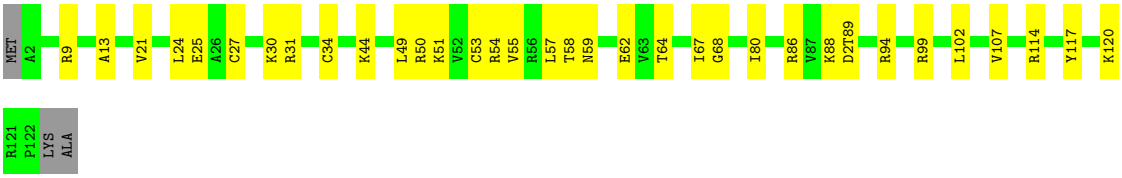
• Molecule 11: 30S ribosomal protein S11

Chain k:



• Molecule 12: 30S ribosomal protein S12

Chain l:

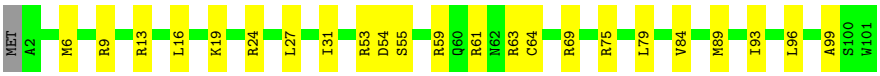


• Molecule 13: 30S ribosomal protein S13

Chain m:

• Molecule 14: 30S ribosomal protein S14

Chain n: 76% 23%

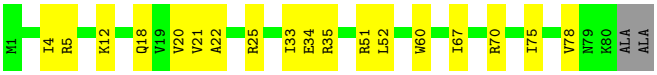


• Molecule 15: 30S ribosomal protein S15

Chain o: 69% 30%

• Molecule 16: 30S ribosomal protein S16

Chain p: 76% 22%

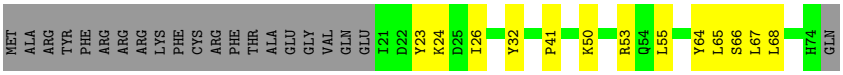


• Molecule 17: 30S ribosomal protein S17

Chain q: 69% 25% 6%

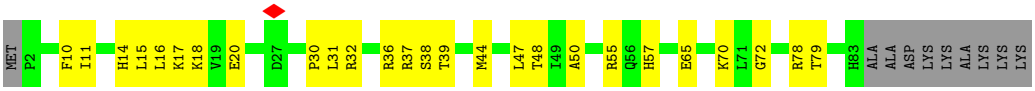
• Molecule 18: 30S ribosomal protein S18

Chain r: 55% 17% 28%



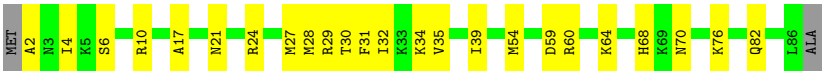
• Molecule 19: 30S ribosomal protein S19

Chain s: 61% 28% 11%



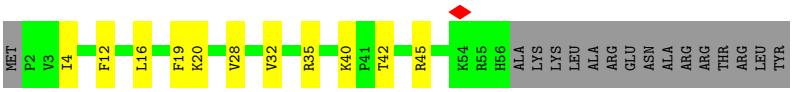
• Molecule 20: 30S ribosomal protein S20

Chain t: 70% 28%



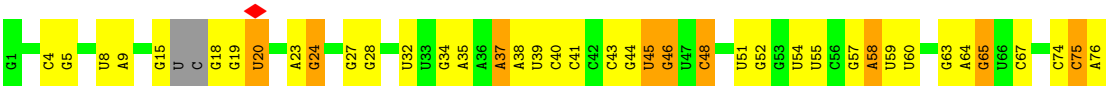
• Molecule 21: 30S ribosomal protein S21

Chain u:



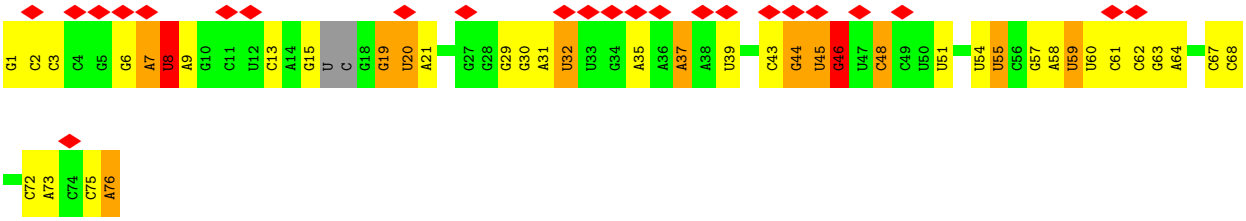
• Molecule 22: phenylalanine tRNA

Chain w:



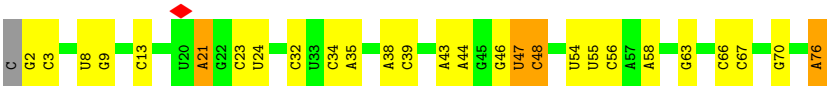
• Molecule 22: phenylalanine tRNA

Chain y:



• Molecule 23: P-site initiator tRNA

Chain x:

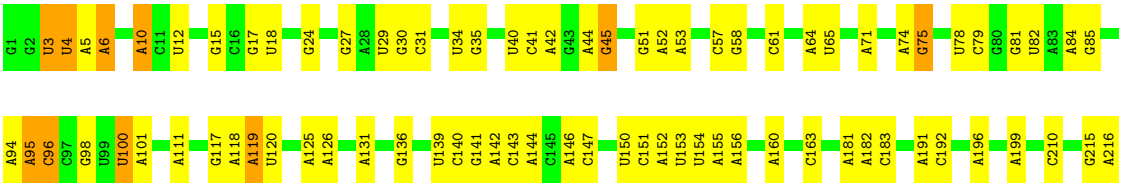


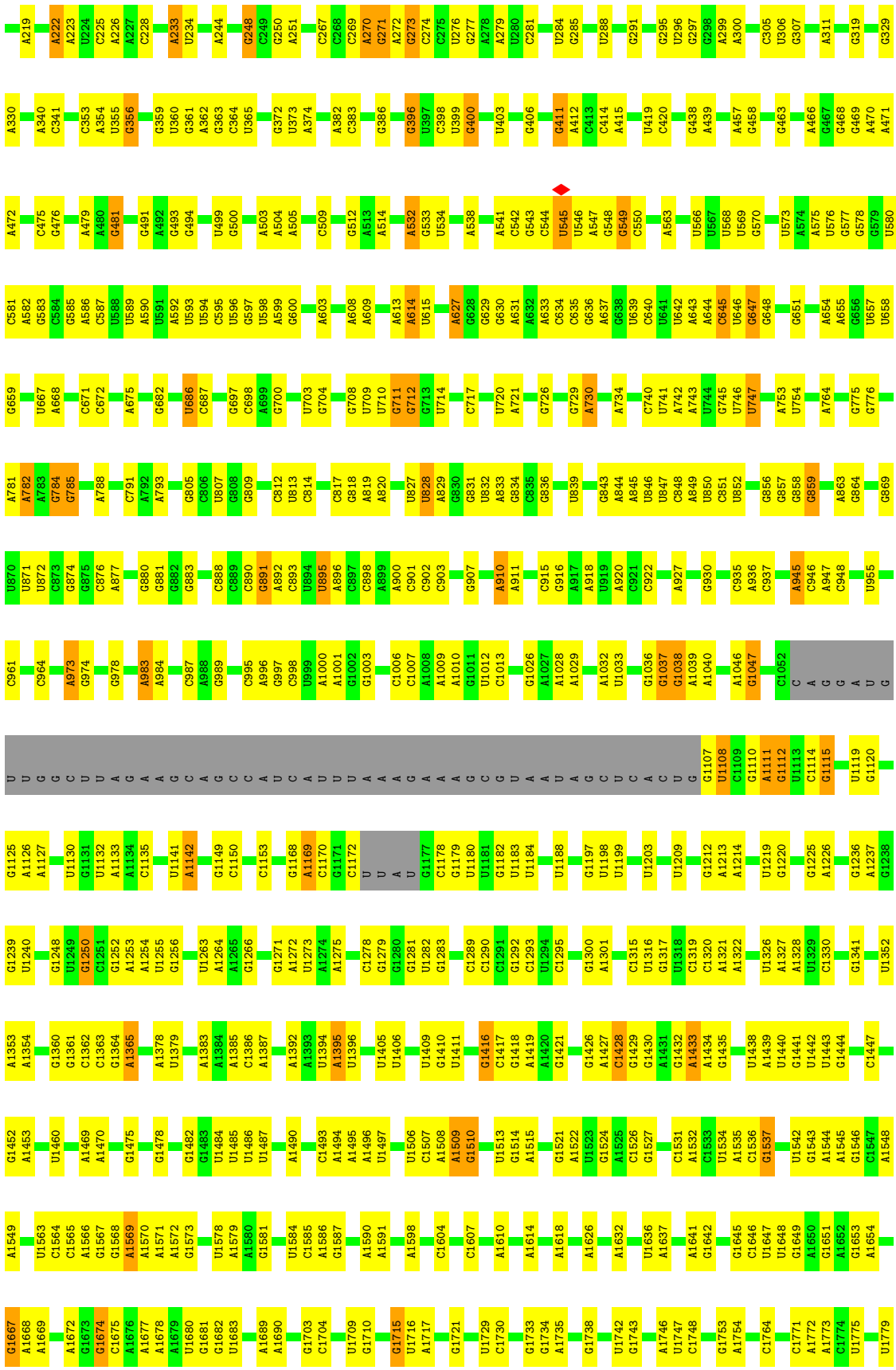
• Molecule 24: M-F-Stop mRNA

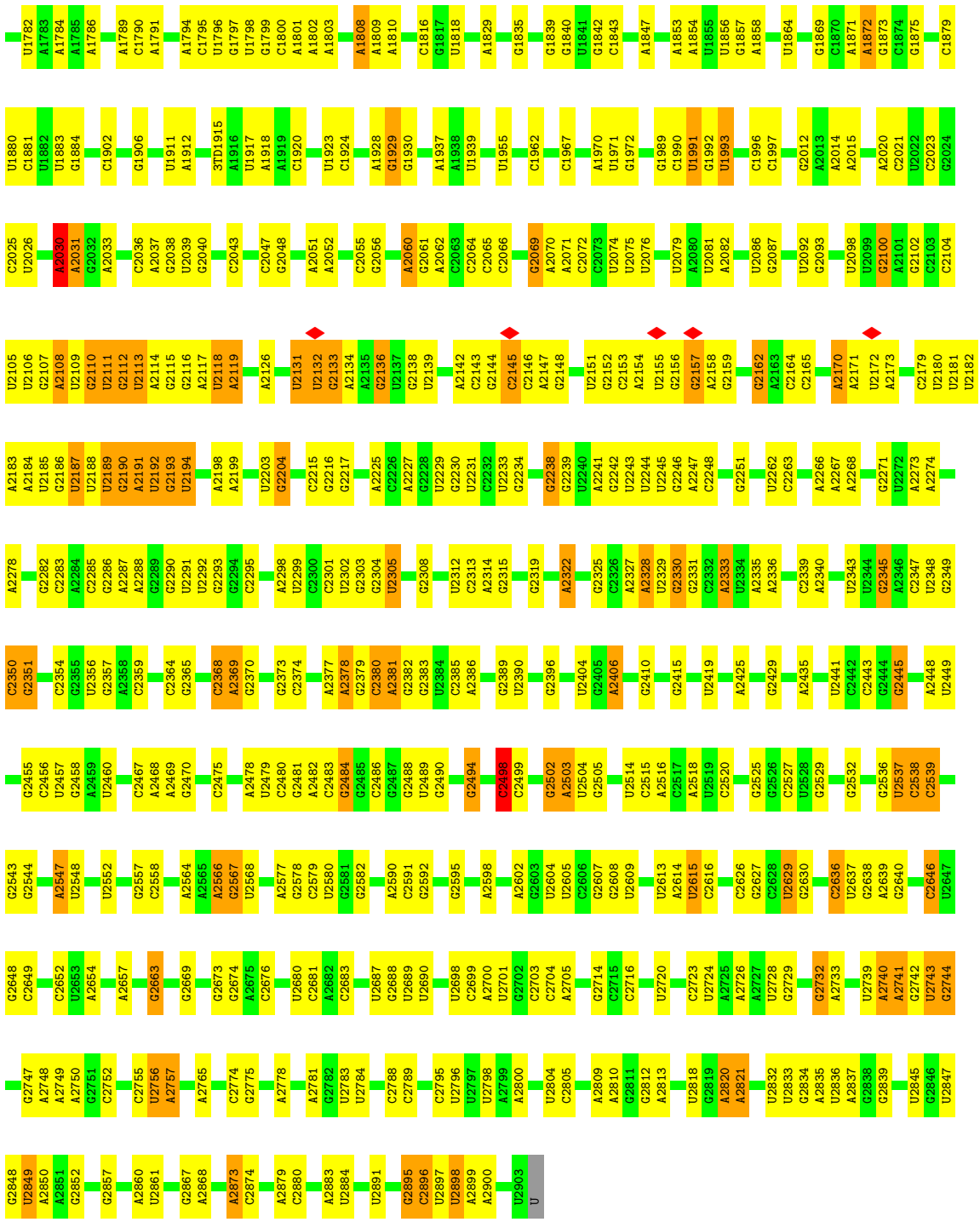
Chain v:

• Molecule 25: 23S Ribosomal RNA

Chain A:

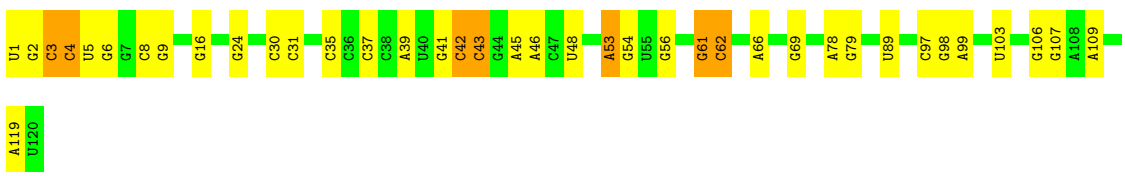



A219 A222 A223 U224 C225 A226 A227 C228 A233 U234 A244 G248 C249 G250 A251 C267 C268 C269 A270 G271 A272 G273 C274 C275 U276 G277 A278 A279 U280 C281 U284 G285 U288 G291 G295 U296 G297 G298 A299 A300 C305 U306 G307 A311 G319 G329
A330 A340 C341 C353 A354 U355 G356 G359 U360 G361 A362 G363 C364 U365 G372 U373 A374 A382 C383 G386 G396 U397 C398 U399 G400 U403 G406 G411 A412 C413 C414 A415 U419 C420 G438 A439 A457 G458 G463 A466 G467 G468 G469 A470 A471
A472 C475 G476 A479 A480 G481 G491 A492 G493 G494 U499 G500 A503 A504 A505 C509 G512 A513 A514 A532 G533 U534 A538 A541 C542 G543 C544 U545 U546 A547 G548 G549 C550 A563 U566 U567 U568 U569 G570 U573 A574 A575 U576 G577 G578 G579 U580
C581 A582 G583 C584 G585 A586 C587 U588 U589 A590 U591 A592 U593 U594 C595 U596 G597 U598 A599 G600 A603 A608 A609 A613 A614 U615 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 U641 U642 A643 A644 C645 U646 G647 G648 G651 A654 A655 G656 U657 U658
G659 U667 A668 C671 C672 A675 G682 U686 C687 G697 C698 A699 G700 U703 G704 G708 U709 U710 G711 G712 G713 U714 C717 U720 A721 G726 G729 A730 A734 C740 U741 A742 A743 U744 G745 U746 U747 A753 U754 A764 G775 G776
A781 A782 A783 G784 G785 A788 C791 A792 A793 G805 C806 U807 G808 G809 C812 U813 C814 C817 G818 A819 A820 U827 U828 A829 G830 G831 U832 A833 G834 C835 G836 U839 G843 A844 A845 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 A863 G864 G869
U870 U871 U872 C873 G874 G875 C876 A877 G880 G881 G882 G883 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 G907 A910 A911 C915 G916 A917 A918 U919 A920 C921 C922 A927 G930 C935 A936 C937 A945 C946 A947 C948 U955
C961 C964 A973 G974 G978 A983 A984 C987 A988 G989 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 G1026 A1027 A1028 A1029 A1032 U1033 G1036 G1037 G1038 A1039 A1040 A1046 G1047 C1052 C A G G A U G
U U G G C U U A G A A G C A G C C A U C A U U U A A A G A A A G C U C A C U G G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1119 G1120
G1125 A1126 A1127 U1130 G1131 U1132 A1133 A1134 C1135 U1141 A1142 G1149 C1150 C1153 G1168 A1169 C1170 G1171 C1172 U U A U G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 U1188 G1197 U1198 U1199 U1203 U1209 G1212 A1213 A1214 U1219 G1220 G1225 A1226 G1236 A1237 G1238
G1239 U1240 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 U1263 A1264 A1265 G1266 G1271 A1272 U1273 A1274 A1275 C1278 G1279 G1280 G1281 U1282 G1283 C1289 C1290 C1291 G1292 C1293 U1294 C1295 G1300 A1301 C1315 U1316 G1317 U1318 C1319 C1320 A1321 A1322 U1326 A1327 A1328 U1329 C1330 G1341 U1352
A1353 A1354 G1360 G1361 C1362 C1363 G1364 A1365 A1378 U1379 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394 A1395 U1396 U1405 U1406 U1409 G1410 U1411 G1416 C1417 G1418 A1419 A1420 G1421 G1426 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 U1438 A1439 U1440 G1441 U1442 U1443 G1444 C1447
G1452 A1453 U1460 A1469 A1470 G1475 G1478 G1482 G1483 U1484 U1485 U1486 U1487 A1490 C1493 A1494 A1495 A1496 U1497 U1506 C1507 A1508 A1509 G1510 U1513 G1514 A1515 G1521 A1522 U1523 G1524 A1525 C1526 G1527 C1531 A1532 C1533 U1534 A1535 C1536 G1537 U1542 G1543 A1544 A1545 G1546 C1547 A1548
A1549 U1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 A1572 G1573 U1578 A1579 A1580 G1581 U1584 C1585 A1586 G1587 A1590 A1591 A1598 C1604 C1607 A1610 A1614 A1618 A1626 A1632 U1636 A1637 A1641 G1642 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654
G1667 A1668 A1669 A1672 G1673 G1674 C1675 A1676 A1677 A1678 A1679 U1680 G1681 G1682 U1683 A1689 A1690 G1703 C1704 U1709 G1710 G1715 U1716 A1717 G1721 U1729 C1730 G1733 G1734 A1735 G1738 U1742 G1743 A1746 U1747 C1748 G1753 A1754 C1764 C1771 A1772 A1773 C1774 U1775 U1779



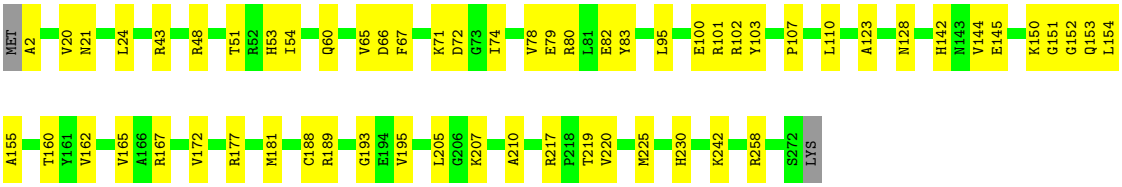
• Molecule 26: 5S Ribosomal RNA

Chain B:



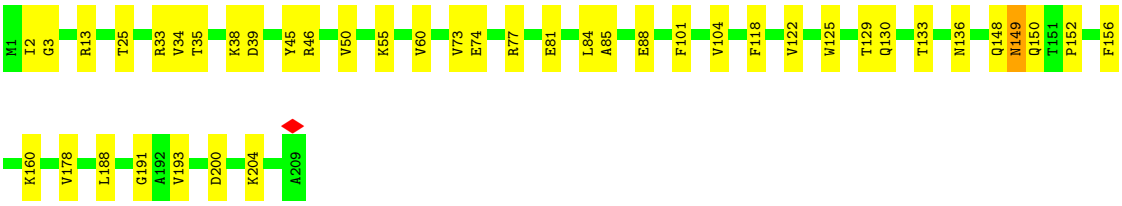
- Molecule 27: 50S ribosomal protein L2

Chain C:



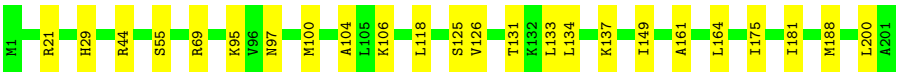
- Molecule 28: 50S ribosomal protein L3

Chain D:



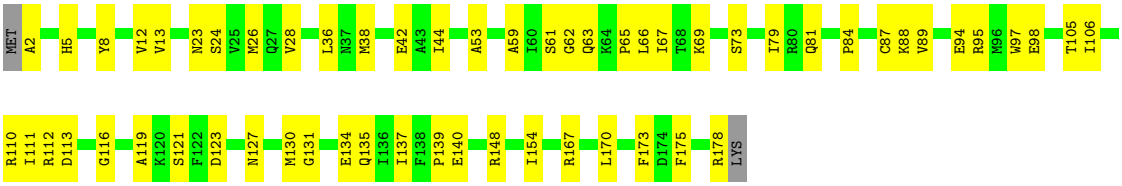
- Molecule 29: 50S ribosomal protein L4

Chain E:



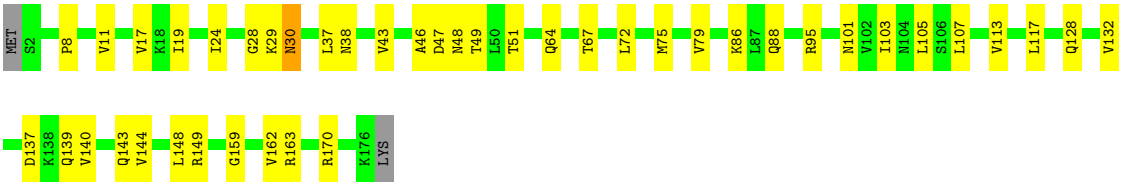
- Molecule 30: 50S ribosomal protein L5

Chain F:



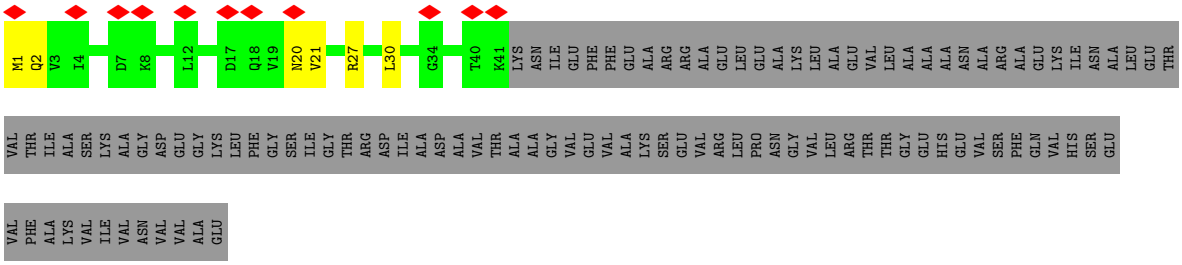
- Molecule 31: 50S ribosomal protein L6

Chain G:



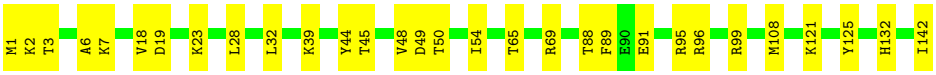
- Molecule 32: 50S ribosomal protein L9

Chain H: 7% 23% 72%



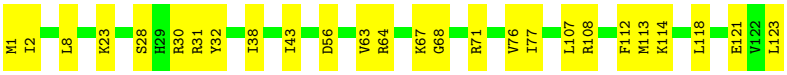
- Molecule 33: 50S ribosomal protein L13

Chain L: 79% 21%



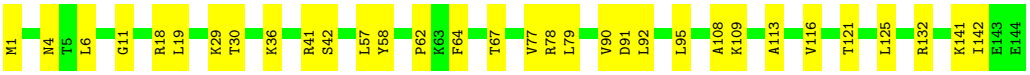
- Molecule 34: 50S ribosomal protein L14

Chain M: 79% 21%



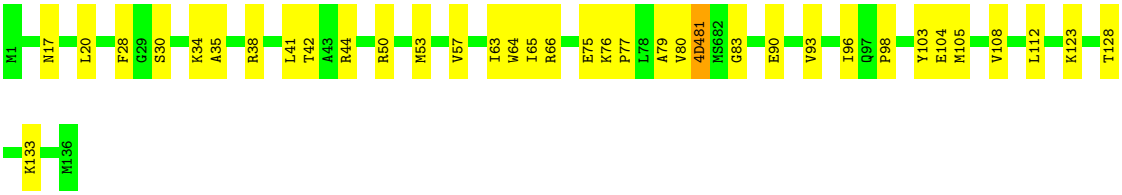
- Molecule 35: 50S ribosomal protein L15

Chain N: 78% 22%



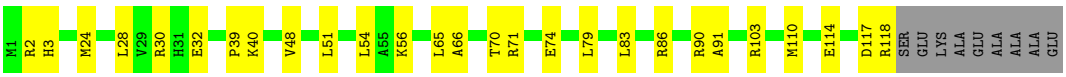
- Molecule 36: 50S ribosomal protein L16

Chain O: 74% 26%



- Molecule 37: 50S ribosomal protein L17

Chain P: 72% 21% 7%

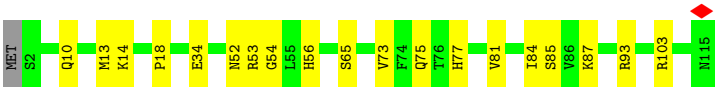


- Molecule 38: 50S ribosomal protein L18

Chain Q: 74% 26%

- Molecule 39: 50S ribosomal protein L19

Chain R: 83% 17%

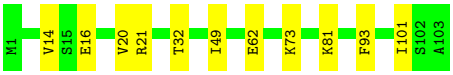


- Molecule 40: 50S ribosomal protein L20

Chain S: 83% 16%

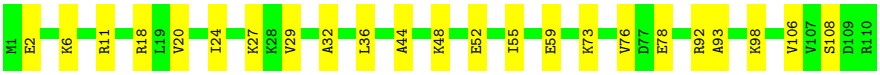
- Molecule 41: Ribosomal protein L21

Chain T: 89% 11%



- Molecule 42: 50S ribosomal protein L22

Chain U: 79% 21%



- Molecule 43: 50S ribosomal protein L23

Chain V: 77% 16% 7%

- Molecule 44: 50S ribosomal protein L24

Chain W: 82% 16%

- Molecule 45: 50S ribosomal protein L25

Chain X: 71% 29%

M1 A6 E7 V8 R9 K10 K14 R21 K25 A28 I29 I30 Y31 L38 A39 I40 E41 L42 V47 M50 Q51 Y57 I63 V64 V65 Q75 D76 V77 H80 P81 Y82 K83 P84 K85 L86 I89 A94

• Molecule 46: 50S ribosomal protein L27

Chain Y: 84% 14%

MET A2 K5 R11 R14 A18 V23 E29 V38 N50 D56 L59 V71 R77 I82 E85

• Molecule 47: 50S ribosomal protein L28

Chain Z: 79% 19%

MET S2 R3 V7 K10 N23 R28 N32 L33 H34 R37 F38 R50 M56 I59 D60 R74 G75 E76 K77 Y78

• Molecule 48: 50S ribosomal protein L29

Chain 1: 70% 27%

MET K2 L6 K9 S10 V11 L14 N15 L22 R29 Q39 L43 K44 Q45 V46 R47 R48 D49 R52 V53 K54 L57 N58 G62 ALA

• Molecule 49: 50S ribosomal protein L30

Chain 2: 78% 20%

MET A2 Q9 T10 R11 K19 L25 G26 L27 G28 L29 R38 F53 M54 V55 K56 V57 E58 E59

• Molecule 50: 50S ribosomal protein L31

Chain 3: 69% 17% 14%

M1 H6 E11 A14 M22 K23 I24 R25 S26 T27 L34 D35 S38 Q48 ARG ASP VAL ALA THR GLY G55 R56 R59 F64 N65 I66 PRO GLY SER LYS

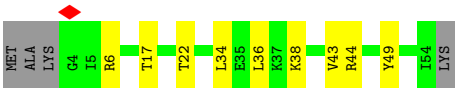
• Molecule 51: 50S ribosomal protein L32

Chain 4: 70% 26%

MET A2 V3 Q4 Q5 N6 K7 P8 S11 K12 M15 R16 D31 H38 L39 T44 A45 D46 R52 K53 V54 I55 A56 LYS

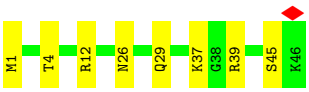
• Molecule 52: 50S ribosomal protein L33

Chain 5:



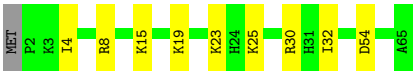
- Molecule 53: 50S ribosomal protein L34

Chain 6:



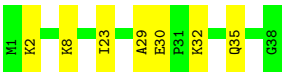
- Molecule 54: 50S ribosomal protein L35

Chain 7:



- Molecule 55: 50S ribosomal protein L36

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	234339	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 ($e^-/Å^2$)	40.5852	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.330	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, G7M, 3TD, 2MA, 6MZ, MS6, MG, 5MC, 4OC, 4SU, ZN, AKN, 7MG, OMU, 5MU, PSU, OMC, MEQ, 4D4, 1MG, OMG, 2MG, H2U, UR3, MA6, D2T, IAS

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	0.17	0/36450	0.26	0/56856
2	b	0.13	0/1542	0.32	0/2108
3	c	0.17	0/1640	0.34	0/2211
4	d	0.18	0/1665	0.40	0/2227
5	e	0.19	0/1130	0.35	0/1527
6	f	0.16	0/796	0.43	0/1086
7	g	0.15	0/1068	0.32	0/1452
8	h	0.17	0/979	0.33	0/1314
9	i	0.15	0/949	0.37	0/1276
10	j	0.14	0/682	0.31	0/933
11	k	0.34	0/867	0.50	0/1171
12	l	0.18	0/927	0.33	0/1249
13	m	0.12	0/831	0.28	0/1118
14	n	0.15	0/804	0.31	0/1072
15	o	0.18	0/711	0.32	0/952
16	p	0.15	0/623	0.33	0/842
17	q	0.17	0/639	0.39	0/859
18	r	0.15	0/447	0.26	0/601
19	s	0.14	0/658	0.33	0/889
20	t	0.19	0/654	0.36	0/871
21	u	0.12	0/380	0.37	0/518
22	w	0.24	0/1605	0.40	1/2494 (0.0%)
22	y	0.15	0/1606	0.24	0/2497
23	x	0.19	0/1725	0.24	0/2689
24	v	0.18	0/285	0.18	0/441
25	A	0.23	0/67852	0.28	0/105848
26	B	0.19	0/2876	0.28	0/4483
27	C	0.23	0/2108	0.32	0/2837
28	D	0.22	0/1569	0.32	0/2111
29	E	0.19	0/1557	0.28	0/2095
30	F	0.17	0/1425	0.32	0/1915

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	G	0.16	0/1319	0.37	1/1789 (0.1%)
32	H	0.10	0/306	0.29	0/413
33	L	0.21	0/1152	0.28	0/1551
34	M	0.21	0/955	0.29	0/1279
35	N	0.21	0/1057	0.32	0/1407
36	O	0.21	0/1073	0.29	0/1433
37	P	0.22	0/958	0.35	0/1281
38	Q	0.16	0/886	0.35	0/1192
39	R	0.20	0/925	0.27	0/1238
40	S	0.23	0/960	0.28	0/1278
41	T	0.21	0/829	0.31	0/1107
42	U	0.21	0/857	0.27	0/1149
43	V	0.17	0/744	0.27	0/994
44	W	0.18	0/777	0.33	0/1038
45	X	0.18	0/763	0.35	0/1022
46	Y	0.19	0/642	0.31	0/848
47	Z	0.20	0/635	0.24	0/848
48	1	0.17	0/496	0.31	0/660
49	2	0.21	0/453	0.26	0/605
50	3	0.10	0/475	0.22	0/633
51	4	0.21	0/440	0.28	0/588
52	5	0.16	0/424	0.27	0/565
53	6	0.22	0/380	0.29	0/498
54	7	0.20	0/513	0.31	0/676
55	8	0.22	0/303	0.31	0/397
All	All	0.20	0/155372	0.29	2/233031 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
36	O	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	w	75	C	OP1-P-O3'	13.05	147.14	108.00
31	G	30	ASN	N-CA-C	-6.15	106.75	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	O	81	4D4	Mainchain

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	a	32803	0	16528	474	0
2	b	1514	0	1322	27	0
3	c	1613	0	1686	43	0
4	d	1643	0	1707	73	0
5	e	1117	0	1132	23	0
6	f	778	0	731	26	0
7	g	1054	0	979	14	0
8	h	969	0	1014	22	0
9	i	937	0	921	35	0
10	j	673	0	628	12	0
11	k	860	0	854	28	0
12	l	924	0	955	23	0
13	m	823	0	838	15	0
14	n	792	0	817	21	0
15	o	703	0	719	19	0
16	p	613	0	608	21	0
17	q	630	0	657	17	0
18	r	441	0	467	13	0
19	s	641	0	648	20	0
20	t	648	0	677	20	0
21	u	373	0	339	11	0
22	w	1591	0	818	25	0
22	y	1585	0	804	26	0
23	x	1625	0	829	14	0
24	v	255	0	129	1	0
25	A	61097	0	30754	680	0
26	B	2572	0	1301	34	0
27	C	2069	0	2129	41	0
28	D	1559	0	1607	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	E	1538	0	1598	18	0
30	F	1401	0	1429	47	0
31	G	1299	0	1332	31	0
32	H	303	0	327	3	0
33	L	1129	0	1162	21	0
34	M	946	0	1023	18	0
35	N	1048	0	1123	27	0
36	O	1075	0	1146	25	0
37	P	945	0	989	19	0
38	Q	876	0	886	21	0
39	R	913	0	958	19	0
40	S	947	0	1019	18	0
41	T	816	0	839	9	0
42	U	850	0	911	15	0
43	V	738	0	807	10	0
44	W	769	0	812	14	0
45	X	750	0	773	20	0
46	Y	634	0	653	10	0
47	Z	625	0	652	12	0
48	1	495	0	526	15	0
49	2	449	0	488	11	0
50	3	468	0	460	11	0
51	4	434	0	445	12	0
52	5	417	0	451	7	0
53	6	377	0	418	8	0
54	7	504	0	572	8	0
55	8	302	0	340	7	0
56	4	1	0	0	0	0
56	A	359	0	0	0	0
56	B	6	0	0	0	0
56	C	1	0	0	0	0
56	D	1	0	0	0	0
56	P	1	0	0	0	0
56	S	1	0	0	0	0
56	X	1	0	0	0	0
56	Y	1	0	0	0	0
56	a	98	0	0	0	0
56	v	1	0	0	0	0
56	x	3	0	0	0	0
57	A	40	0	43	0	0
57	a	40	0	43	1	0
58	w	11	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	3	1	0	0	0	0
59	8	1	0	0	0	0
60	A	60	0	0	1	0
60	N	1	0	0	0	0
60	a	11	0	0	0	0
60	n	1	0	0	0	0
60	x	1	0	0	0	0
All	All	144591	0	94831	1966	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 8.

The worst 5 of 1966 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)
25:A:1047:G:HO2'	25:A:1110:G:H1	1.10	0.99
1:a:180:U:H3	1:a:195:A:H62	1.00	0.96
27:C:71:LYS:HD3	27:C:74:ILE:HD11	1.48	0.94
22:y:15:G:H22	22:y:48:C:H42	1.15	0.93
25:A:881:G:H1	25:A:895:U:H3	0.98	0.91

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%)	206 (93%)	16 (7%)	0	100	100
3	c	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	d	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	e	154/167 (92%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	100/131 (76%)	83 (83%)	14 (14%)	3 (3%)	3	14
7	g	150/156 (96%)	143 (95%)	7 (5%)	0	100	100
8	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	i	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
10	j	95/103 (92%)	90 (95%)	4 (4%)	1 (1%)	11	36
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
13	m	111/118 (94%)	107 (96%)	4 (4%)	0	100	100
14	n	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	o	86/89 (97%)	86 (100%)	0	0	100	100
16	p	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
17	q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	r	52/75 (69%)	51 (98%)	1 (2%)	0	100	100
19	s	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
20	t	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
21	u	53/71 (75%)	53 (100%)	0	0	100	100
27	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
28	D	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	54
29	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
30	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
31	G	173/177 (98%)	152 (88%)	21 (12%)	0	100	100
32	H	39/149 (26%)	36 (92%)	2 (5%)	1 (3%)	4	17
33	L	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
34	M	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
35	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
36	O	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
37	P	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
38	Q	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	14	41
39	R	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
40	S	115/118 (98%)	115 (100%)	0	0	100	100
41	T	101/103 (98%)	97 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	V	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
44	W	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
45	X	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
46	Y	82/85 (96%)	78 (95%)	3 (4%)	1 (1%)	10	34
47	Z	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
48	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
49	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	3	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
51	4	53/57 (93%)	53 (100%)	0	0	100	100
52	5	49/55 (89%)	49 (100%)	0	0	100	100
53	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	7	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	27
55	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5445/5886 (92%)	5219 (96%)	217 (4%)	9 (0%)	44	72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	37	HIS
6	f	68	GLN
38	Q	90	VAL
10	j	57	VAL
28	D	149	ASN

5.3.2 Protein sidechains (i)

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	115/199 (58%)	115 (100%)	0	100	100
3	c	167/190 (88%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	172/173 (99%)	172 (100%)	0	100	100
5	e	110/126 (87%)	110 (100%)	0	100	100
6	f	77/112 (69%)	77 (100%)	0	100	100
7	g	89/129 (69%)	89 (100%)	0	100	100
8	h	102/105 (97%)	102 (100%)	0	100	100
9	i	87/107 (81%)	87 (100%)	0	100	100
10	j	55/90 (61%)	55 (100%)	0	100	100
11	k	85/98 (87%)	82 (96%)	3 (4%)	32	66
12	l	97/103 (94%)	97 (100%)	0	100	100
13	m	78/96 (81%)	78 (100%)	0	100	100
14	n	78/84 (93%)	78 (100%)	0	100	100
15	o	74/77 (96%)	74 (100%)	0	100	100
16	p	58/65 (89%)	58 (100%)	0	100	100
17	q	70/78 (90%)	70 (100%)	0	100	100
18	r	46/65 (71%)	46 (100%)	0	100	100
19	s	68/79 (86%)	68 (100%)	0	100	100
20	t	61/66 (92%)	61 (100%)	0	100	100
21	u	28/61 (46%)	28 (100%)	0	100	100
27	C	213/218 (98%)	213 (100%)	0	100	100
28	D	161/163 (99%)	161 (100%)	0	100	100
29	E	161/165 (98%)	161 (100%)	0	100	100
30	F	146/150 (97%)	146 (100%)	0	100	100
31	G	133/138 (96%)	133 (100%)	0	100	100
32	H	32/114 (28%)	32 (100%)	0	100	100
33	L	116/116 (100%)	116 (100%)	0	100	100
34	M	104/104 (100%)	104 (100%)	0	100	100
35	N	102/103 (99%)	102 (100%)	0	100	100
36	O	107/107 (100%)	107 (100%)	0	100	100
37	P	98/103 (95%)	98 (100%)	0	100	100
38	Q	82/87 (94%)	82 (100%)	0	100	100
39	R	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	S	89/90 (99%)	89 (100%)	0	100	100
41	T	84/84 (100%)	84 (100%)	0	100	100
42	U	92/93 (99%)	92 (100%)	0	100	100
43	V	80/84 (95%)	80 (100%)	0	100	100
44	W	80/85 (94%)	80 (100%)	0	100	100
45	X	77/78 (99%)	77 (100%)	0	100	100
46	Y	62/63 (98%)	62 (100%)	0	100	100
47	Z	67/68 (98%)	67 (100%)	0	100	100
48	1	54/55 (98%)	54 (100%)	0	100	100
49	2	48/49 (98%)	48 (100%)	0	100	100
50	3	53/62 (86%)	53 (100%)	0	100	100
51	4	46/48 (96%)	46 (100%)	0	100	100
52	5	46/49 (94%)	46 (100%)	0	100	100
53	6	38/38 (100%)	38 (100%)	0	100	100
54	7	51/52 (98%)	51 (100%)	0	100	100
55	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4271/4803 (89%)	4268 (100%)	3 (0%)	87	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	k	56	ARG
11	k	57	LYS
11	k	59	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
33	L	131	ASN
41	T	89	HIS
34	M	89	ASN
38	Q	38	GLN
46	Y	57	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	207 (13%)	0
22	w	72/76 (94%)	12 (16%)	0
22	y	72/76 (94%)	17 (23%)	0
23	x	75/77 (97%)	8 (10%)	0
24	v	11/24 (45%)	3 (27%)	0
25	A	2842/2904 (97%)	399 (14%)	11 (0%)
26	B	119/120 (99%)	12 (10%)	3 (2%)
All	All	4717/4819 (97%)	658 (13%)	14 (0%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	2538	C
25	A	2756	U
26	B	61	G
26	B	3	C
26	B	42	C

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

58 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	$\#\|Z\| > 2$
25	PSU	A	746	25,56	18,21,22	1.40	3 (16%)	21,30,33	2.02	4 (19%)
36	MS6	O	82	36	5,7,8	0.56	0	2,7,9	1.24	0
22	MIA	w	37	22	28,31,32	2.33	6 (21%)	38,44,47	2.83	14 (36%)
1	5MC	a	1407	1	19,22,23	1.47	3 (15%)	26,32,35	1.13	3 (11%)
22	PSU	w	55	22	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
1	2MG	a	1516	1	23,26,27	1.23	4 (17%)	33,38,41	2.26	9 (27%)
25	G7M	A	2069	25	23,26,27	1.56	4 (17%)	34,39,42	1.68	5 (14%)
22	5MU	y	54	22	19,22,23	1.38	6 (31%)	27,32,35	2.07	6 (22%)
22	4SU	w	8	22	18,21,22	1.90	4 (22%)	25,30,33	2.10	4 (16%)
1	2MG	a	966	1	23,26,27	1.29	4 (17%)	33,38,41	2.21	7 (21%)
25	5MU	A	747	25	19,22,23	1.38	4 (21%)	27,32,35	2.20	6 (22%)
25	PSU	A	2604	25	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
25	PSU	A	2504	25	18,21,22	1.41	4 (22%)	21,30,33	2.04	3 (14%)
25	2MA	A	2503	25,56	22,25,26	1.46	5 (22%)	32,37,40	2.28	9 (28%)
25	3TD	A	1915	25	19,22,23	4.22	7 (36%)	23,32,35	1.83	4 (17%)
36	4D4	O	81	36	9,11,12	2.72	3 (33%)	7,13,15	0.81	0
25	PSU	A	2580	25	18,21,22	1.44	5 (27%)	21,30,33	2.17	4 (19%)
25	PSU	A	2605	25	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
25	OMU	A	2552	25	19,22,23	1.26	3 (15%)	25,31,34	1.82	5 (20%)
1	G7M	a	527	1	23,26,27	1.59	3 (13%)	34,39,42	1.78	5 (14%)
25	PSU	A	1911	25	18,21,22	1.40	3 (16%)	21,30,33	2.06	3 (14%)
23	5MU	x	54	23	19,22,23	1.36	5 (26%)	27,32,35	2.13	6 (22%)
23	PSU	x	55	23	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
23	4SU	x	8	23	18,21,22	1.86	4 (22%)	25,30,33	2.29	5 (20%)
22	PSU	y	55	22	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
22	7MG	w	46	22	23,26,27	1.31	3 (13%)	27,39,42	2.62	6 (22%)
1	2MG	a	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.20	7 (21%)
25	PSU	A	2457	25	18,21,22	1.42	4 (22%)	21,30,33	2.10	5 (23%)
1	MA6	a	1518	1	23,26,27	1.48	5 (21%)	33,38,41	2.39	13 (39%)
25	1MG	A	745	25	23,26,27	1.17	3 (13%)	33,39,42	1.77	5 (15%)
23	5MC	x	32	23	19,22,23	1.46	3 (15%)	26,32,35	1.23	3 (11%)
1	4OC	a	1402	1	20,23,24	0.75	0	25,32,35	0.95	1 (4%)
22	5MU	w	54	22	19,22,23	1.40	5 (26%)	27,32,35	1.94	5 (18%)
22	PSU	y	39	22	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
1	5MC	a	967	1	19,22,23	1.52	3 (15%)	26,32,35	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	UR3	a	1498	1	19,22,23	0.95	0	26,32,35	1.72	2 (7%)
22	7MG	y	46	22	23,26,27	1.31	3 (13%)	27,39,42	2.59	6 (22%)
25	6MZ	A	2030	25	22,25,26	1.45	5 (22%)	29,36,39	2.32	11 (37%)
25	OMG	A	2251	23,25	23,26,27	1.22	3 (13%)	32,38,41	1.97	6 (18%)
25	2MG	A	2445	25	23,26,27	1.27	3 (13%)	33,38,41	2.23	9 (27%)
22	PSU	w	32	22	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
22	4SU	y	8	22	18,21,22	1.83	4 (22%)	25,30,33	2.34	5 (20%)
25	5MU	A	1939	25	19,22,23	1.39	4 (21%)	27,32,35	2.15	6 (22%)
22	PSU	y	32	22	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
25	PSU	A	955	25	18,21,22	1.42	4 (22%)	21,30,33	2.08	3 (14%)
25	5MC	A	1962	25	19,22,23	1.41	3 (15%)	26,32,35	1.09	2 (7%)
12	D2T	l	89	12	8,9,10	1.98	1 (12%)	6,11,13	2.56	2 (33%)
25	6MZ	A	1618	25	22,25,26	1.44	5 (22%)	29,36,39	2.21	10 (34%)
25	2MG	A	1835	25	23,26,27	1.25	3 (13%)	33,38,41	2.27	9 (27%)
11	IAS	k	119	11	6,7,8	0.97	0	3,8,10	1.45	1 (33%)
1	MA6	a	1519	1	23,26,27	1.47	5 (21%)	33,38,41	2.43	13 (39%)
22	PSU	w	39	22	18,21,22	1.29	2 (11%)	21,30,33	2.26	3 (14%)
25	OMC	A	2498	25,56	19,22,23	0.82	0	25,31,34	0.95	1 (4%)
28	MEQ	D	150	28	8,9,10	0.51	0	5,10,12	0.34	0
22	MIA	y	37	22	21,24,32	1.56	4 (19%)	30,35,47	2.02	7 (23%)
1	PSU	a	516	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
25	PSU	A	1917	25	18,21,22	1.42	3 (16%)	21,30,33	2.01	3 (14%)
25	H2U	A	2449	25	18,21,22	1.11	3 (16%)	19,30,33	1.11	2 (10%)

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
25	PSU	A	746	25,56	-	2/7/25/26	0/2/2/2
36	MS6	O	82	36	-	4/4/6/8	-
22	MIA	w	37	22	-	2/15/33/34	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	w	55	22	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
25	G7M	A	2069	25	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	y	54	22	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
25	5MU	A	747	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	1/7/25/26	0/2/2/2
25	2MA	A	2503	25,56	-	0/7/25/26	0/3/3/3
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
36	4D4	O	81	36	-	2/11/12/14	-
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/9/27/28	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
23	5MU	x	54	23	-	0/7/25/26	0/2/2/2
23	PSU	x	55	23	-	0/7/25/26	0/2/2/2
23	4SU	x	8	23	-	0/7/25/26	0/2/2/2
22	PSU	y	55	22	-	3/7/25/26	0/2/2/2
22	7MG	w	46	22	-	2/7/37/38	0/3/3/3
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
23	5MC	x	32	23	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	1/9/29/30	0/2/2/2
22	5MU	w	54	22	-	0/7/25/26	0/2/2/2
22	PSU	y	39	22	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
22	7MG	y	46	22	-	6/7/37/38	0/3/3/3
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
25	OMG	A	2251	23,25	-	0/9/27/28	0/3/3/3
25	2MG	A	2445	25	-	0/9/27/28	0/3/3/3
22	PSU	w	32	22	-	0/7/25/26	0/2/2/2
22	4SU	y	8	22	-	2/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
22	PSU	y	32	22	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	1/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
11	IAS	k	119	11	-	3/7/7/8	-
1	MA6	a	1519	1	-	4/11/29/30	0/3/3/3
22	PSU	w	39	22	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25,56	-	1/9/27/28	0/2/2/2
28	MEQ	D	150	28	-	2/8/9/11	-
22	MIA	y	37	22	-	2/7/25/34	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.56	1.49	1.35
25	A	1915	3TD	C2-N1	9.74	1.49	1.37
22	w	37	MIA	C2-S10	-7.36	1.69	1.75
22	w	37	MIA	C13-C14	6.73	1.52	1.32
36	O	81	4D4	CZ-NE	6.33	1.45	1.33

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	w	37	MIA	C12-C13-C14	-9.20	110.50	127.01
22	w	46	7MG	N9-C4-N3	8.88	138.48	125.46
22	y	46	7MG	N9-C4-N3	8.75	138.28	125.46
25	A	2503	2MA	C5-C4-N3	-8.00	118.75	127.18
22	w	37	MIA	C5-C4-N3	-7.93	118.83	127.18

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1519	MA6	O4'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
22	w	37	MIA	C12-C13-C14-C16
22	y	55	PSU	C2'-C1'-C5-C4
36	O	82	MS6	CA-CB-CG-SD

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	w	37	MIA	2	0
1	a	966	2MG	2	0
25	A	2503	2MA	1	0
1	a	1518	MA6	3	0
1	a	1402	4OC	2	0
1	a	967	5MC	1	0
22	y	46	7MG	1	0
25	A	2030	6MZ	3	0
25	A	2445	2MG	1	0
22	y	8	4SU	2	0
22	y	32	PSU	2	0
1	a	1519	MA6	2	0
25	A	2498	OMC	2	0
28	D	150	MEQ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 479 ligands modelled in this entry, 476 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
58	PHE	w	101	22	10,11,12	1.70	1 (10%)	8,13,15	0.58	0
57	AKN	A	3360	-	41,42,42	1.96	11 (26%)	55,61,61	1.09	3 (5%)
57	AKN	a	3099	-	41,42,42	2.02	10 (24%)	55,61,61	1.22	6 (10%)

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
58	PHE	w	101	22	-	3/5/6/8	0/1/1/1
57	AKN	A	3360	-	-	6/23/83/83	0/3/3/3
57	AKN	a	3099	-	-	3/23/83/83	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	3360	AKN	C35-N12	5.87	1.46	1.34
57	a	3099	AKN	C35-N12	5.72	1.46	1.34
57	a	3099	AKN	C22-C24	-5.40	1.46	1.53
58	w	101	PHE	CB-CG	-5.21	1.39	1.51
57	A	3360	AKN	C22-C24	-5.06	1.47	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	a	3099	AKN	C13-C11-N12	-3.36	105.65	110.78
57	a	3099	AKN	C21-O20-C19	-3.00	110.86	117.98
57	A	3360	AKN	C21-O20-C19	-2.73	111.52	117.98
57	a	3099	AKN	C11-N12-C35	-2.69	118.57	123.25
57	a	3099	AKN	C19-C17-C16	2.59	114.35	109.11

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	3360	AKN	C14-C16-O2-C1
57	A	3360	AKN	C35-C37-C38-C39
57	A	3360	AKN	O40-C37-C38-C39
58	w	101	PHE	O-C-CA-CB
58	w	101	PHE	C-CA-CB-CG

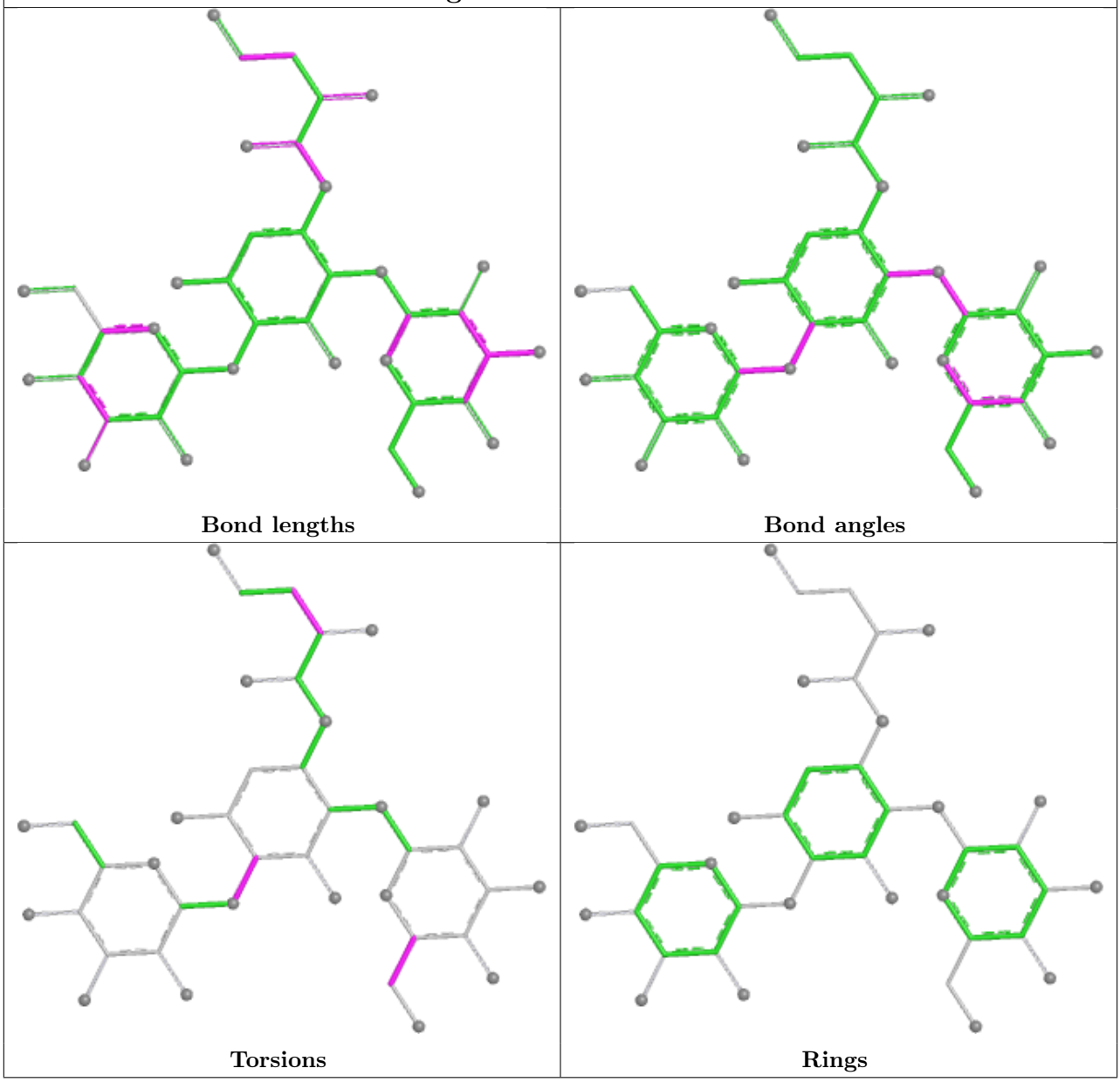
There are no ring outliers.

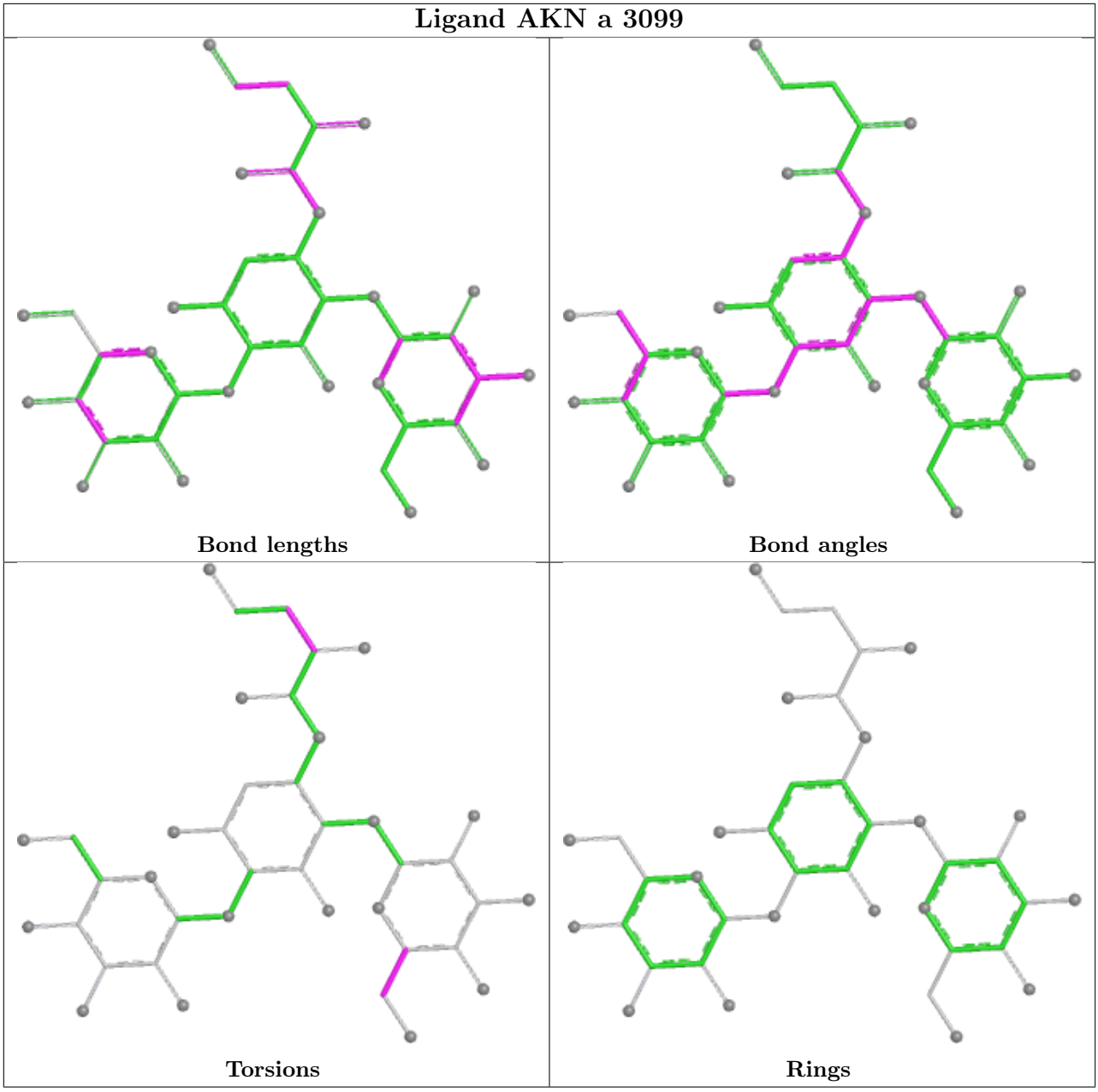
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	w	101	PHE	1	0
57	a	3099	AKN	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 then 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.

Ligand AKN A 3360





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.

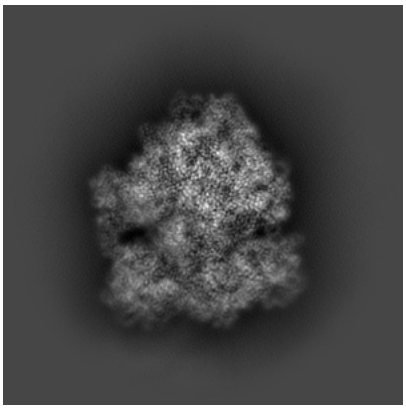
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40882. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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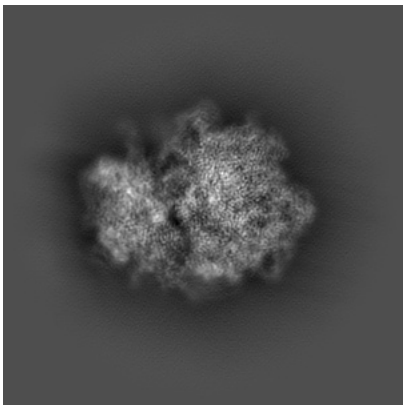

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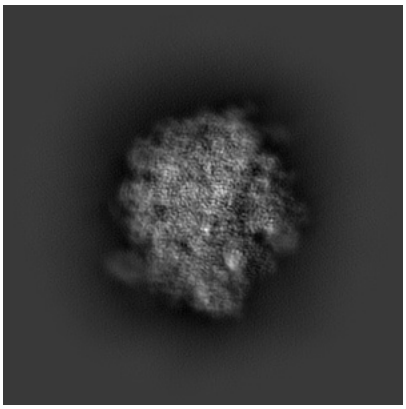
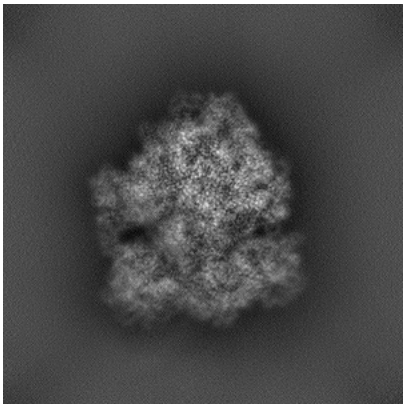


Z

6.1.2 Raw map



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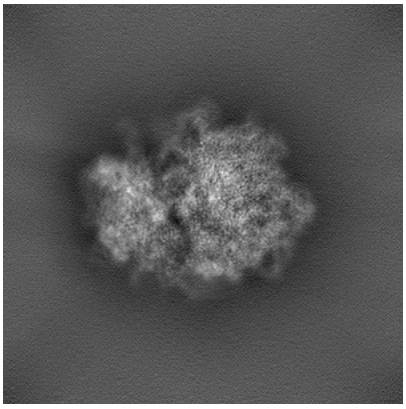

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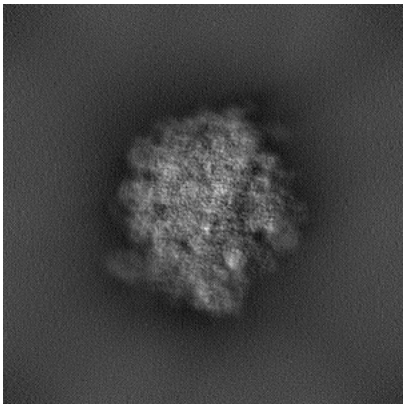
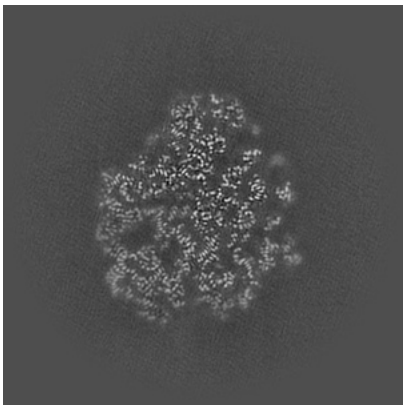


Z

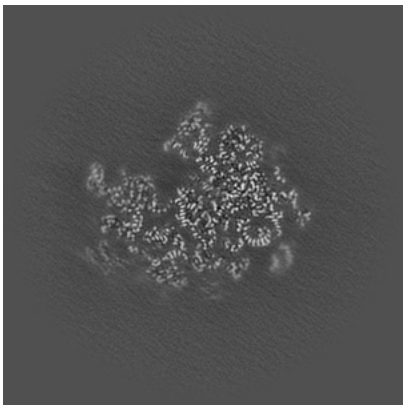
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

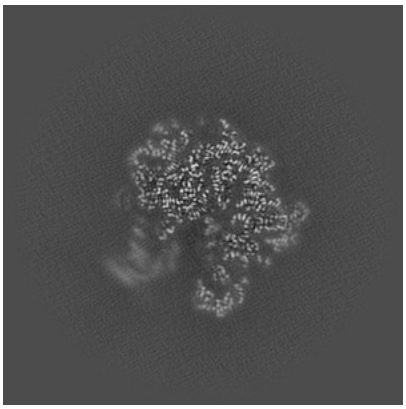
6.2.1 Primary map



X Index: 256

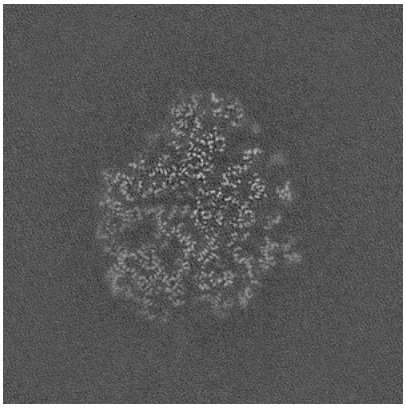


Y Index: 256

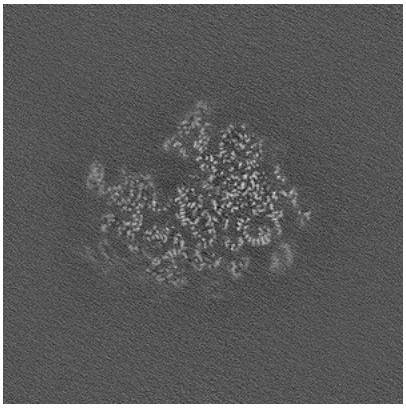


Z Index: 256

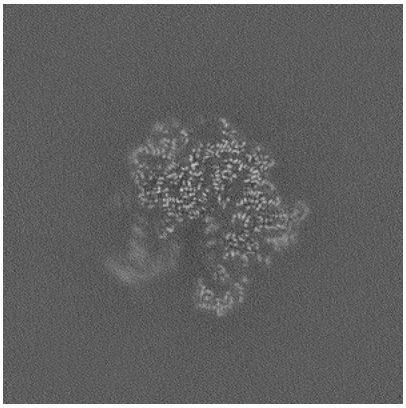
6.2.2 Raw map



X Index: 256



Y Index: 256

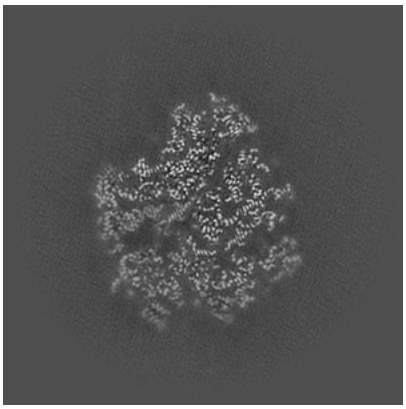


Z Index: 256

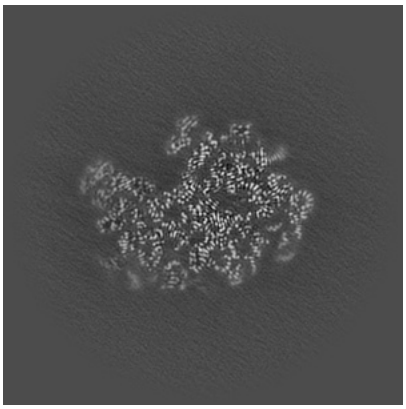
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

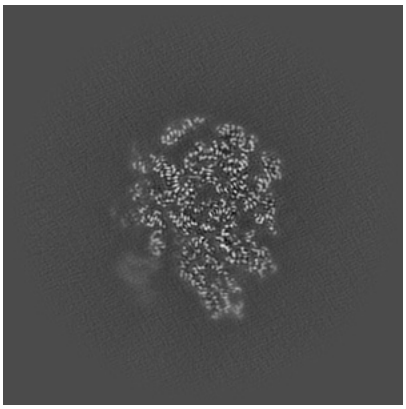
6.3.1 Primary map



X Index: 262

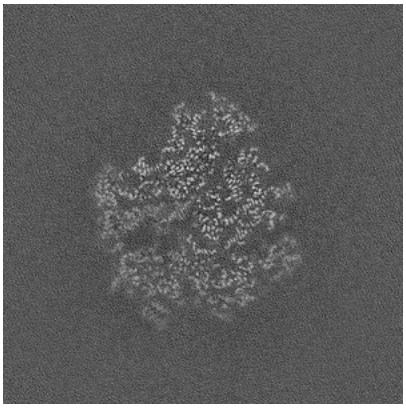


Y Index: 270

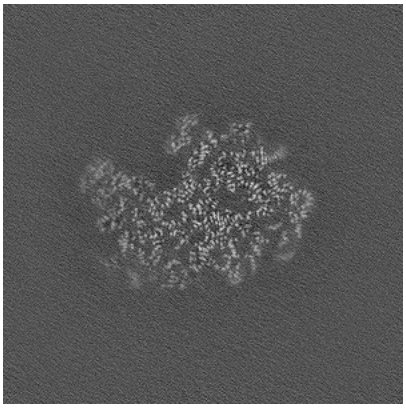


Z Index: 284

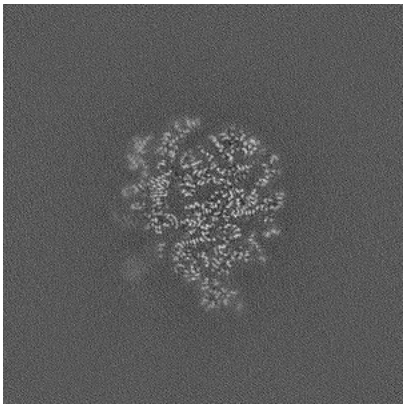
6.3.2 Raw map



X Index: 262



Y Index: 270

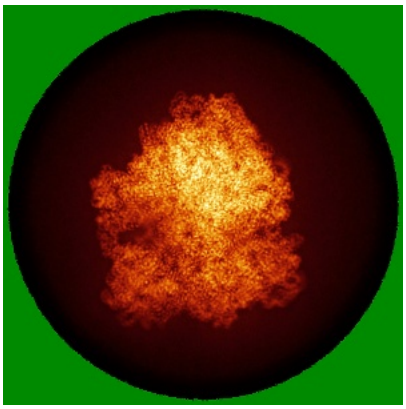


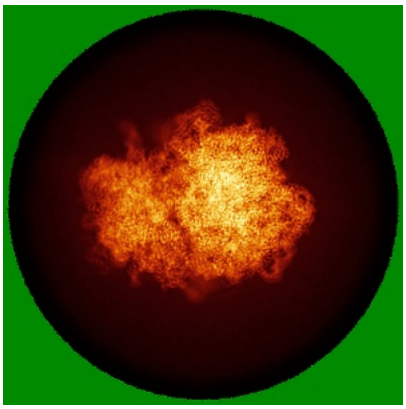
Z Index: 293

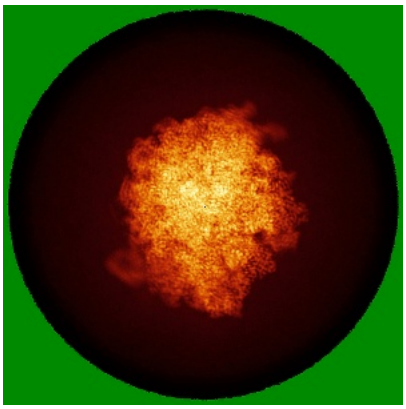
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

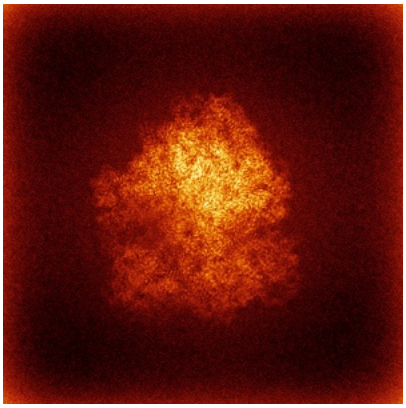
6.4.1 Primary map

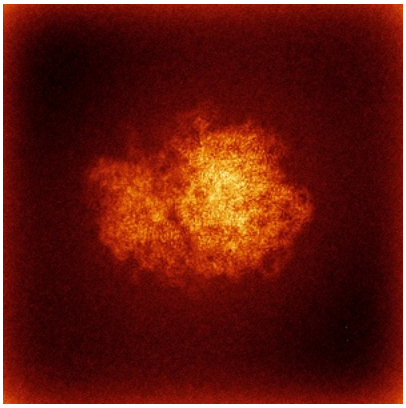

X

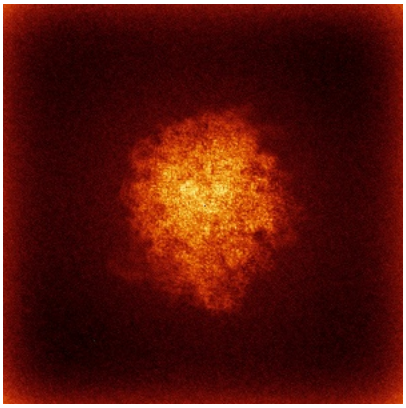

Y


Z

6.4.2 Raw map


X


Y

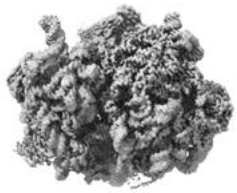

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

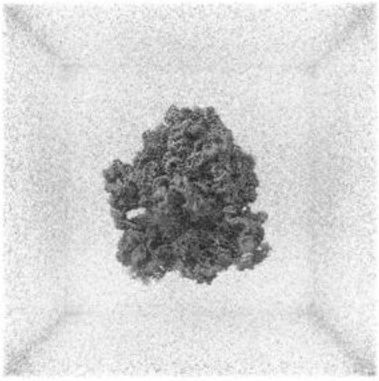


Y

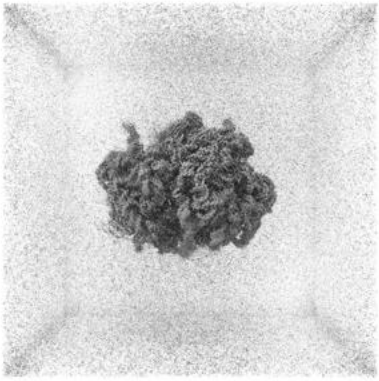
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

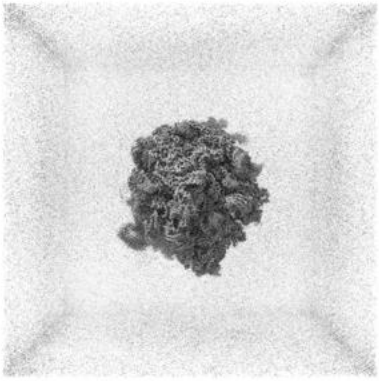
6.5.2 Raw map



X



Y



Z

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

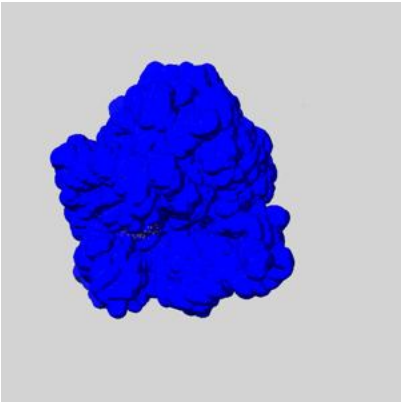
6.6 Mask visualisation (i)

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

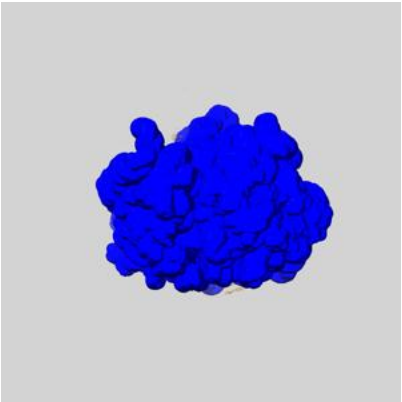
A mask typically either:

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

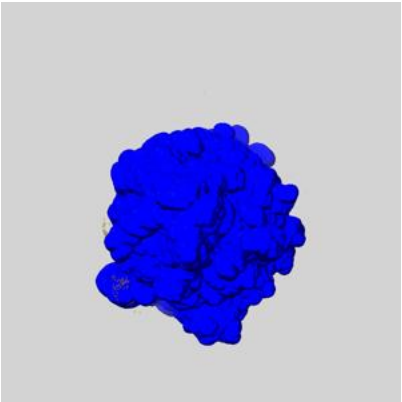
6.6.1 emd_40882_msk_1.map (i)



X



Y

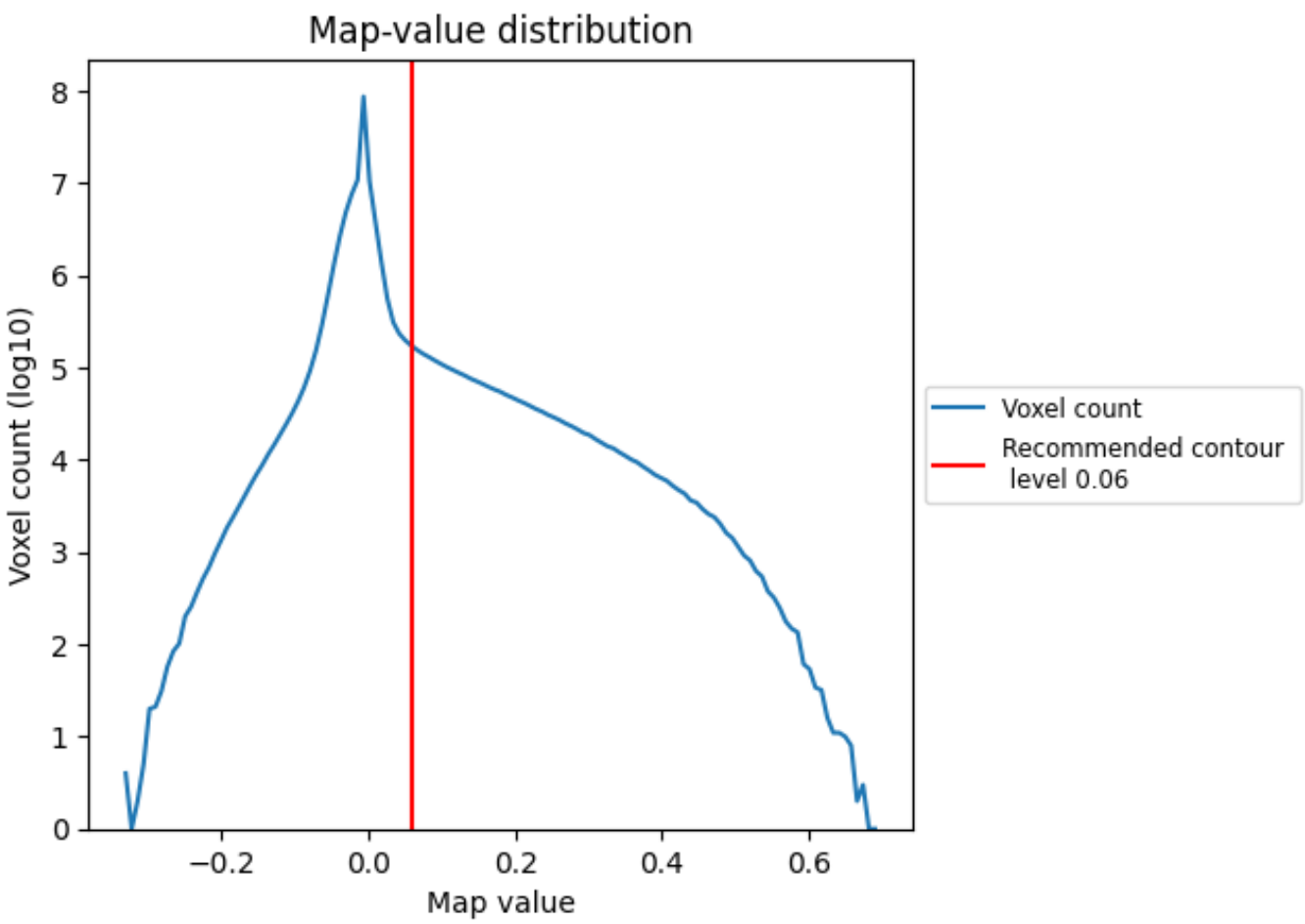


Z

7 Map analysis (i)

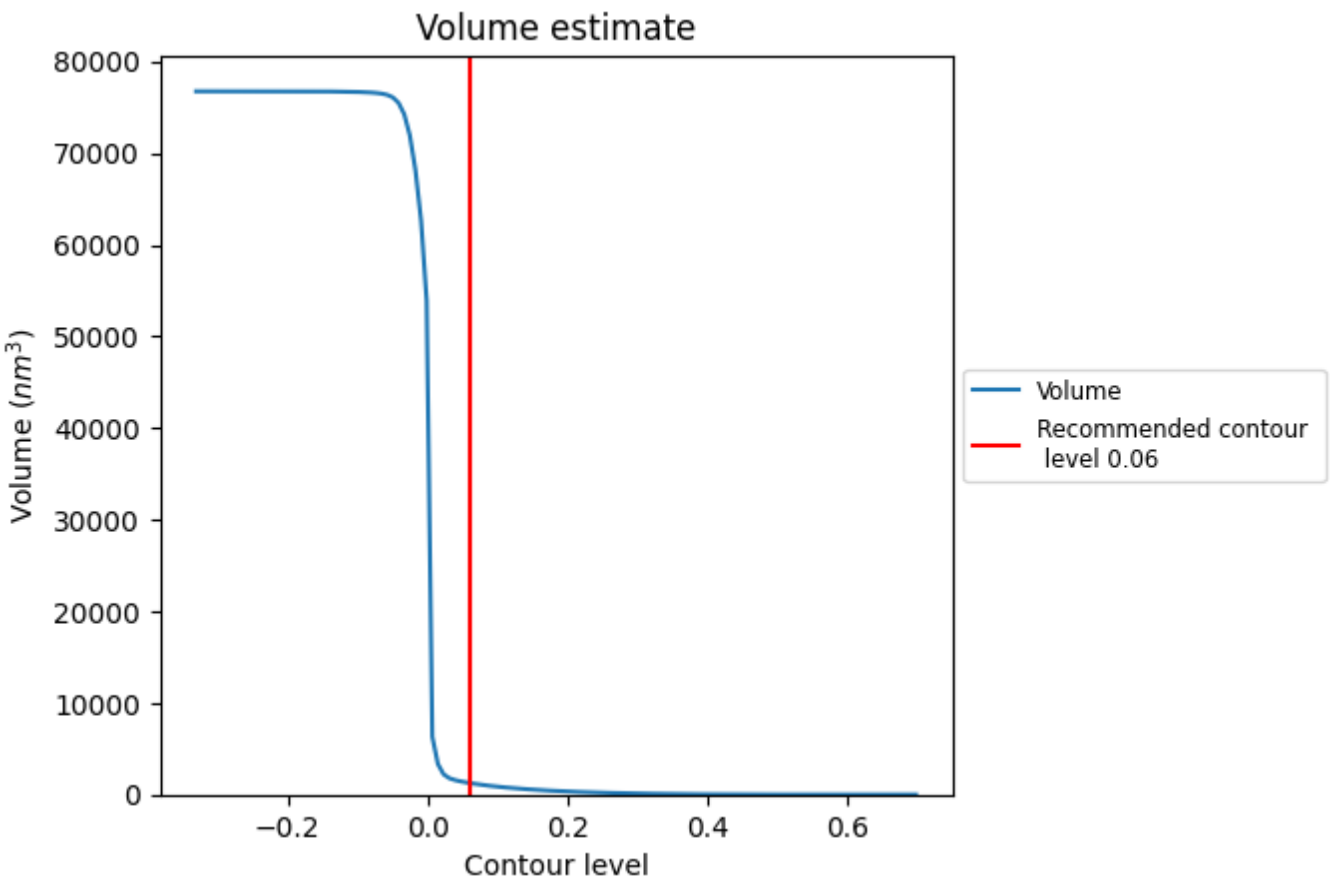
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

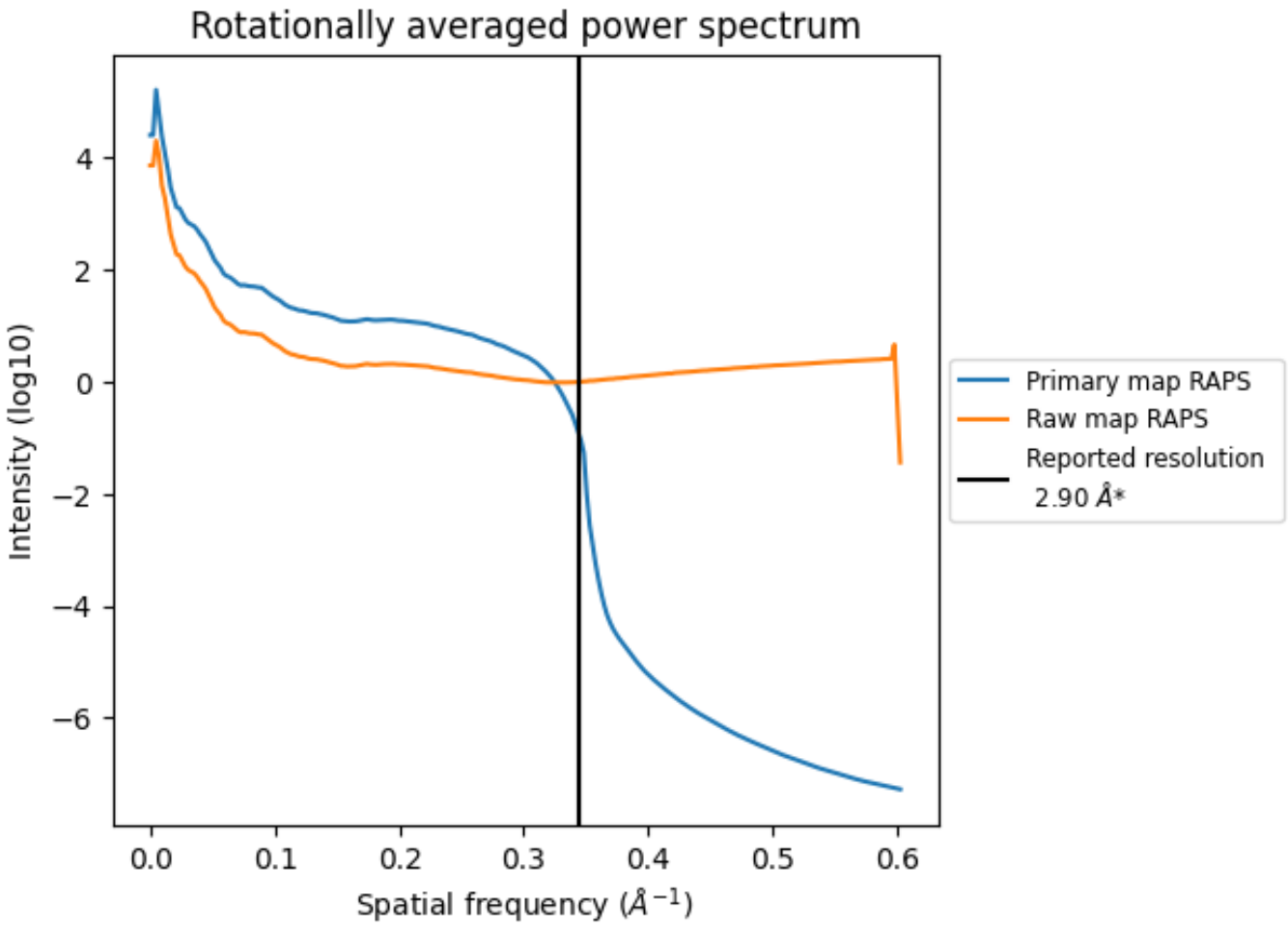
7.2 Volume estimate (i)



The volume at the recommended contour level is 1266 nm^3; this corresponds to an approximate mass of 1144 kDa.

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

7.3 Rotationally averaged power spectrum (i)

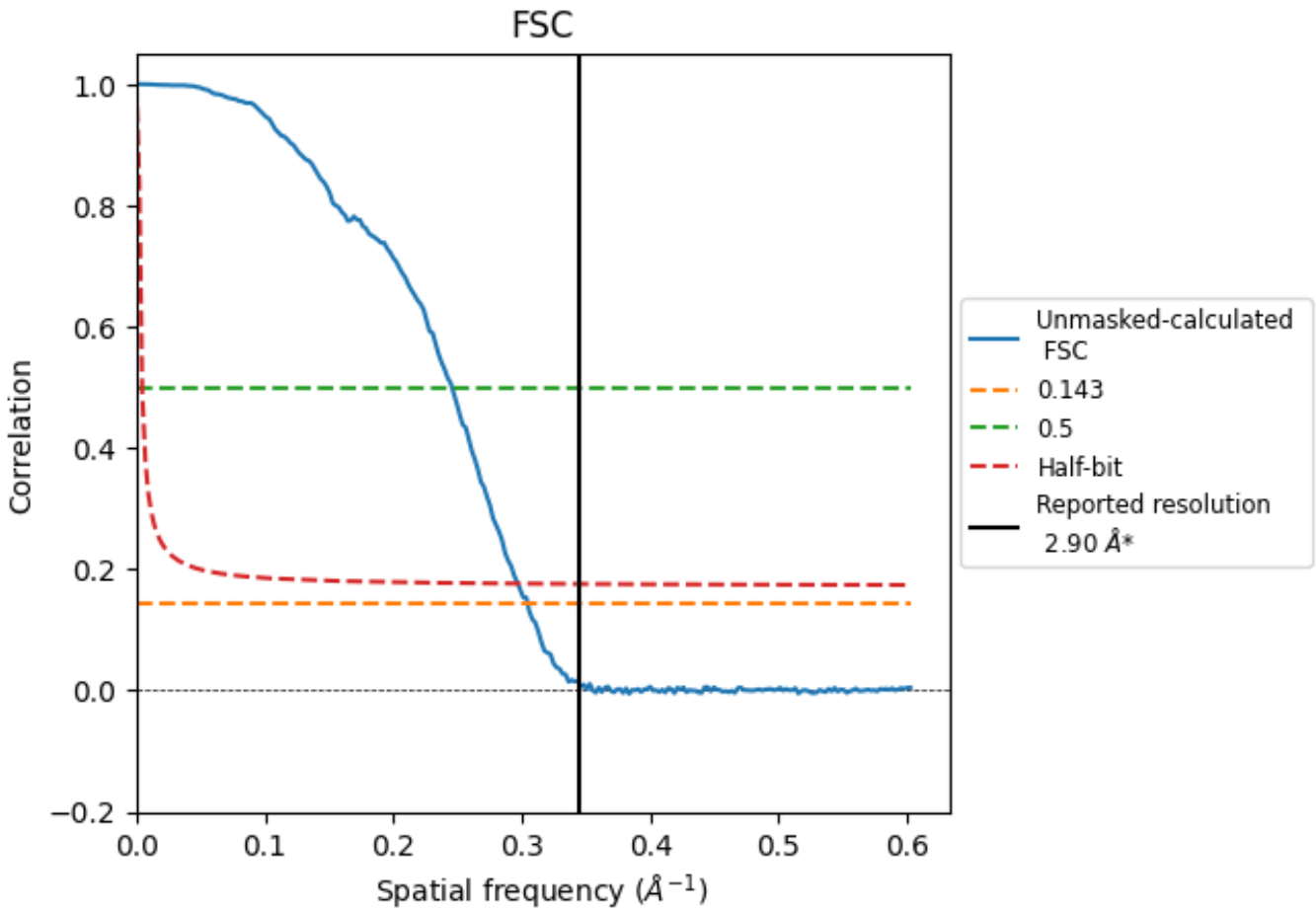


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

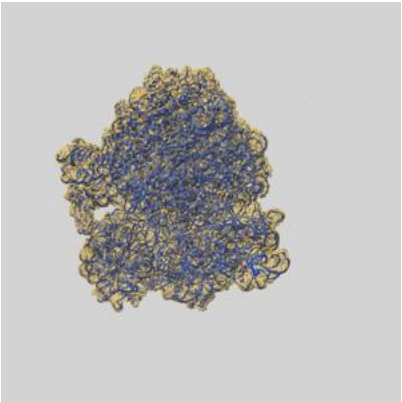
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.07	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.9 by more than 10 %

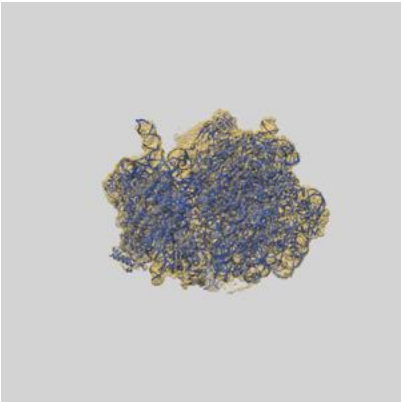
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40882 and PDB model 8SYL. Per-residue inclusion information can be found in section 3 on page 17.

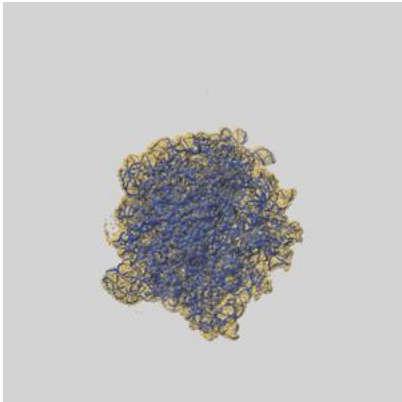
9.1 Map-model overlay (i)



X



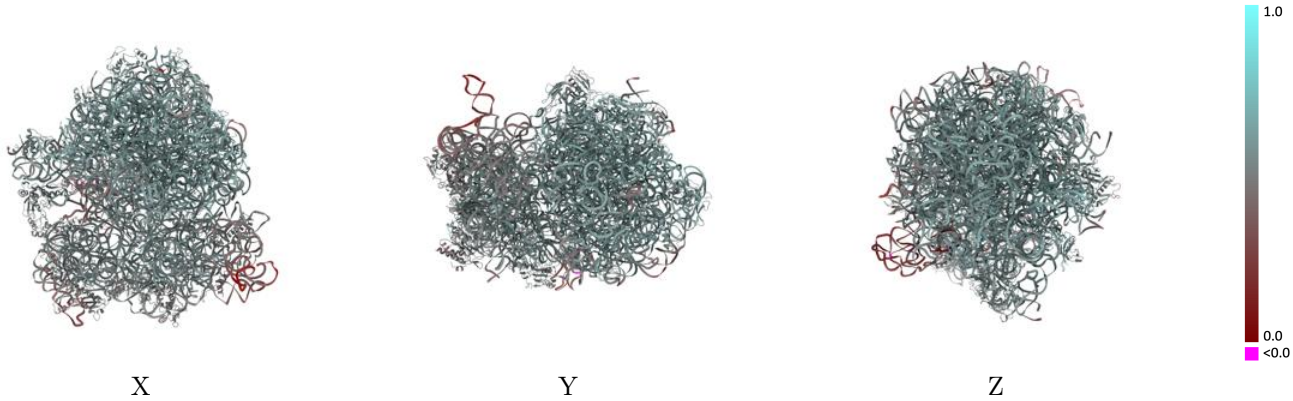
Y



Z

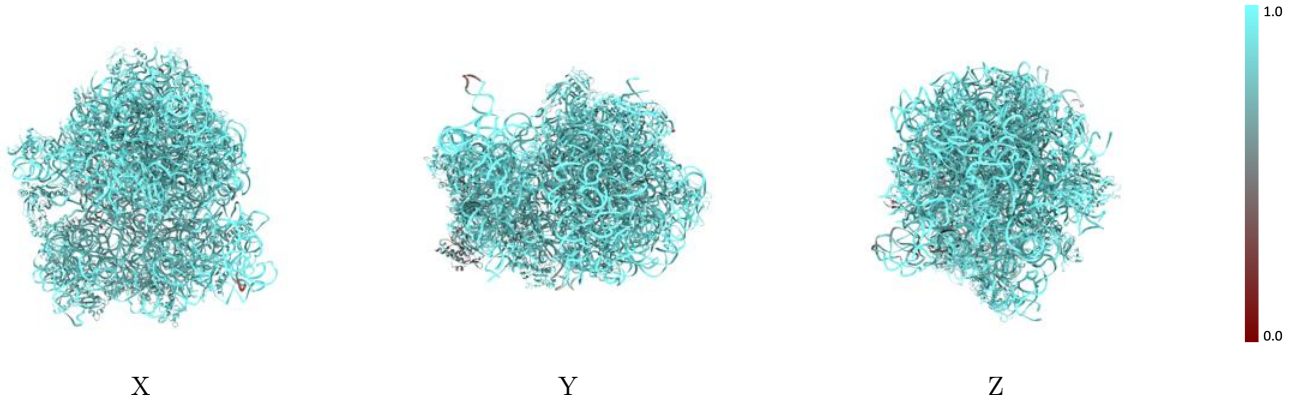
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



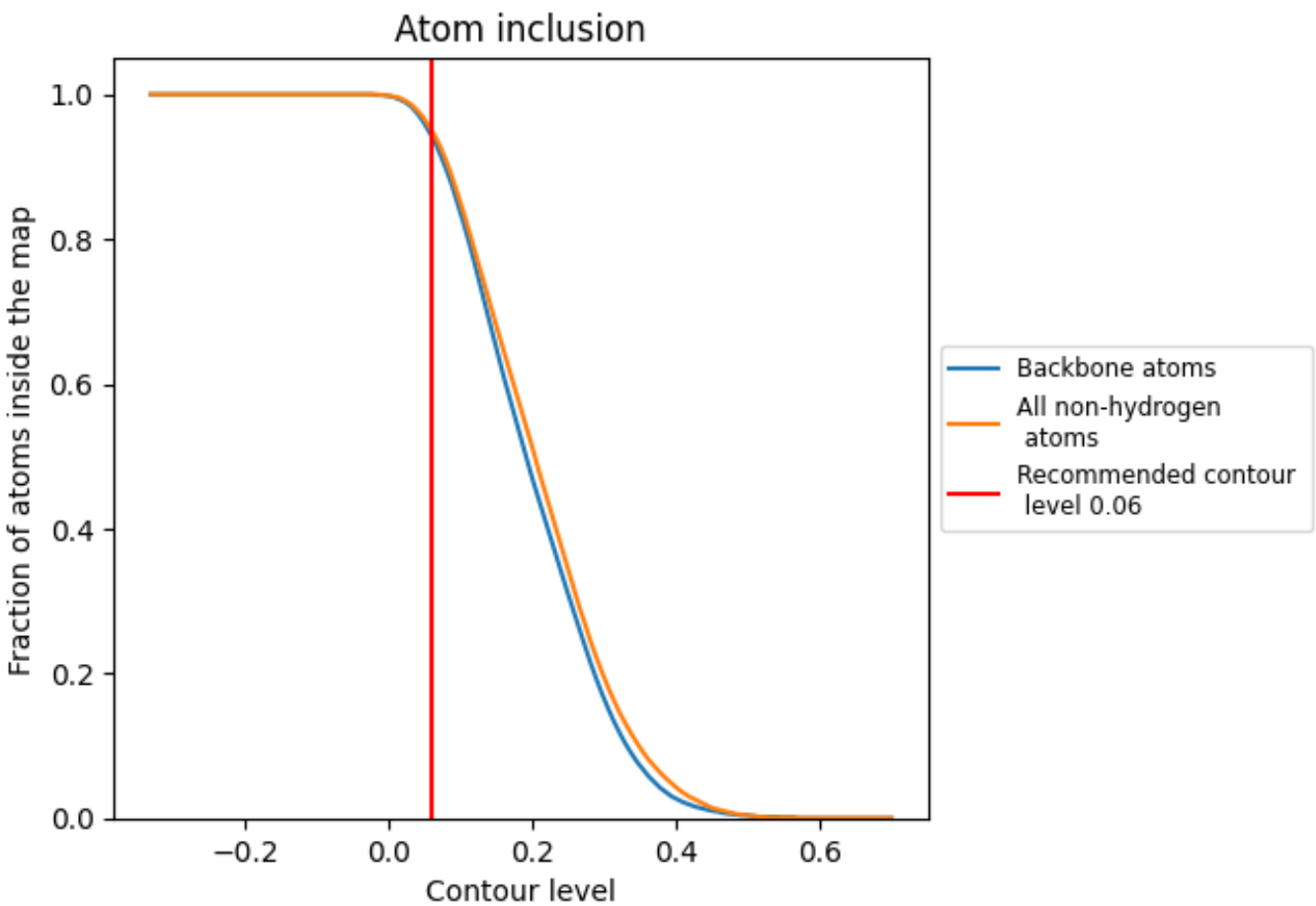
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.5440
1	0.9380	0.5210
2	0.9450	0.5780
3	0.8250	0.4950
4	0.9620	0.5920
5	0.8730	0.5670
6	0.9610	0.6030
7	0.9630	0.6060
8	0.9420	0.5770
A	0.9850	0.5650
B	0.9890	0.5450
C	0.9520	0.5930
D	0.9570	0.5890
E	0.9460	0.5760
F	0.8870	0.5130
G	0.9170	0.5230
H	0.5530	0.5060
L	0.9540	0.5890
M	0.9380	0.5900
N	0.9530	0.5790
O	0.9440	0.5880
P	0.9780	0.5990
Q	0.9540	0.5430
R	0.9230	0.5840
S	0.9780	0.5990
T	0.9520	0.5820
U	0.9510	0.5910
V	0.9150	0.5580
W	0.9430	0.5520
X	0.9240	0.5600
Y	0.9210	0.5870
Z	0.9580	0.5880
a	0.9780	0.5190
b	0.5300	0.4590
c	0.8340	0.5230

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Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8450	0.4770
e	0.9170	0.5530
f	0.8910	0.5000
g	0.9020	0.5020
h	0.9050	0.5360
i	0.9070	0.5050
j	0.8500	0.5110
k	0.8940	0.5350
l	0.9210	0.5660
m	0.9100	0.5190
n	0.8630	0.5180
o	0.9130	0.5340
p	0.9200	0.5050
q	0.8980	0.5270
r	0.9030	0.5300
s	0.8790	0.5050
t	0.8990	0.5000
u	0.7310	0.5210
v	0.9610	0.5640
w	0.8730	0.4950
x	0.9410	0.5370
y	0.5170	0.2430