



Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 01:30 AM JST

PDB ID : 7YFE
EMDB ID : EMD-33787
Title : In situ structure of polymerase complex of mammalian reovirus in virion
Authors : Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.
Deposited on : 2022-07-08
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
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

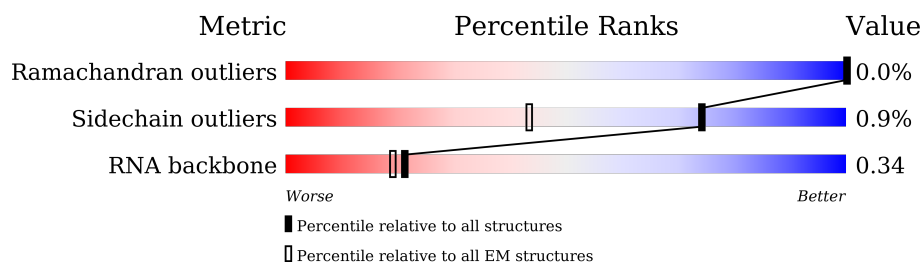
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.






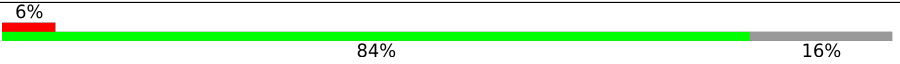
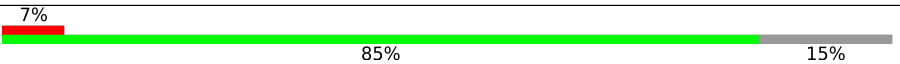

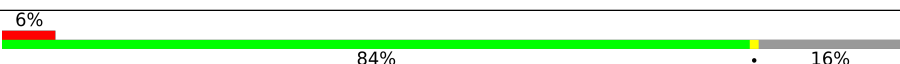
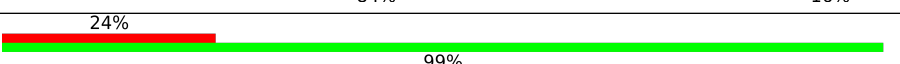
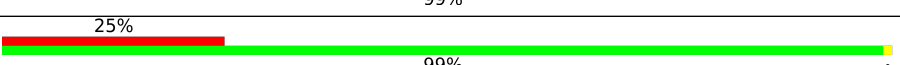
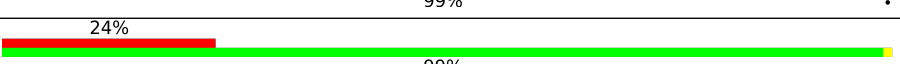
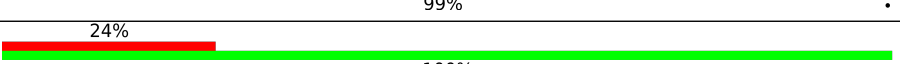
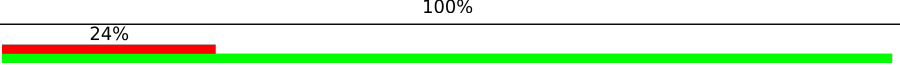
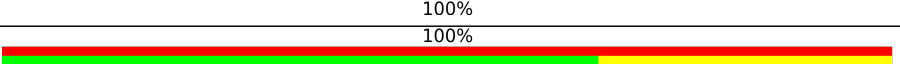


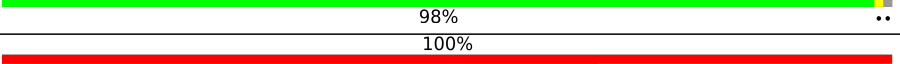

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	1275	10% . 89%
1	2	1275	10% . 89%
1	3	1275	11% 89%
1	4	1275	10% 90%
1	5	1275	10% . 89%
1	A	1275	86% 14%
1	B	1275	5% 83% . 16%
1	C	1275	7% 84% 15%

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Mol	Chain	Length	Quality of chain
1	D	1275	
1	E	1275	
1	a	1275	
1	b	1275	
1	c	1275	
1	d	1275	
1	e	1275	
2	H	1289	
2	I	1289	
2	J	1289	
2	K	1289	
2	L	1289	
3	M	3	
4	N	5	
5	R	1267	
6	T	9	
7	U	736	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 156282 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 RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	140	Total	C	N	O	S	0	0
			1041	619	198	221	3		
1	2	140	Total	C	N	O	S	0	0
			1041	619	198	221	3		
1	3	140	Total	C	N	O	S	0	0
			1040	618	198	221	3		
1	4	132	Total	C	N	O	S	0	0
			975	580	184	208	3		
1	5	143	Total	C	N	O	S	0	0
			1058	628	202	225	3		
1	A	1096	Total	C	N	O	S	0	0
			8628	5504	1462	1611	51		
1	B	1069	Total	C	N	O	S	0	0
			8412	5372	1425	1564	51		
1	C	1079	Total	C	N	O	S	0	0
			8510	5436	1440	1583	51		
1	D	1054	Total	C	N	O	S	0	0
			8327	5321	1408	1549	49		
1	E	1061	Total	C	N	O	S	0	0
			8385	5356	1420	1560	49		
1	a	1078	Total	C	N	O	S	0	0
			8504	5434	1445	1574	51		
1	b	1074	Total	C	N	O	S	0	0
			8470	5413	1437	1569	51		
1	c	1079	Total	C	N	O	S	0	0
			8514	5440	1446	1577	51		
1	d	1084	Total	C	N	O	S	0	0
			8547	5458	1451	1587	51		
1	e	1077	Total	C	N	O	S	0	0
			8497	5429	1444	1573	51		

- Molecule 2 is a protein called Lambda-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1288	Total	C	N	O	S	0	0
			10144	6483	1700	1922	39		
2	I	1288	Total	C	N	O	S	0	0
			10144	6483	1700	1922	39		
2	J	1288	Total	C	N	O	S	0	0
			10144	6483	1700	1922	39		
2	K	1288	Total	C	N	O	S	0	0
			10144	6483	1700	1922	39		
2	L	1288	Total	C	N	O	S	0	0
			10144	6483	1700	1922	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	3	Total	C	N	O	P	0	0
			63	28	10	22	3		

- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	5	Total	C	N	O	P	0	0
			105	47	17	36	5		

- Molecule 5 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	1255	Total	C	N	O	S	0	0
			9926	6336	1700	1826	64		

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*CP*GP*AP*UP*UP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

- Molecule 7 is a protein called Mu-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	666	Total	C	N	O	S	0	0
			5320	3414	905	971	30		

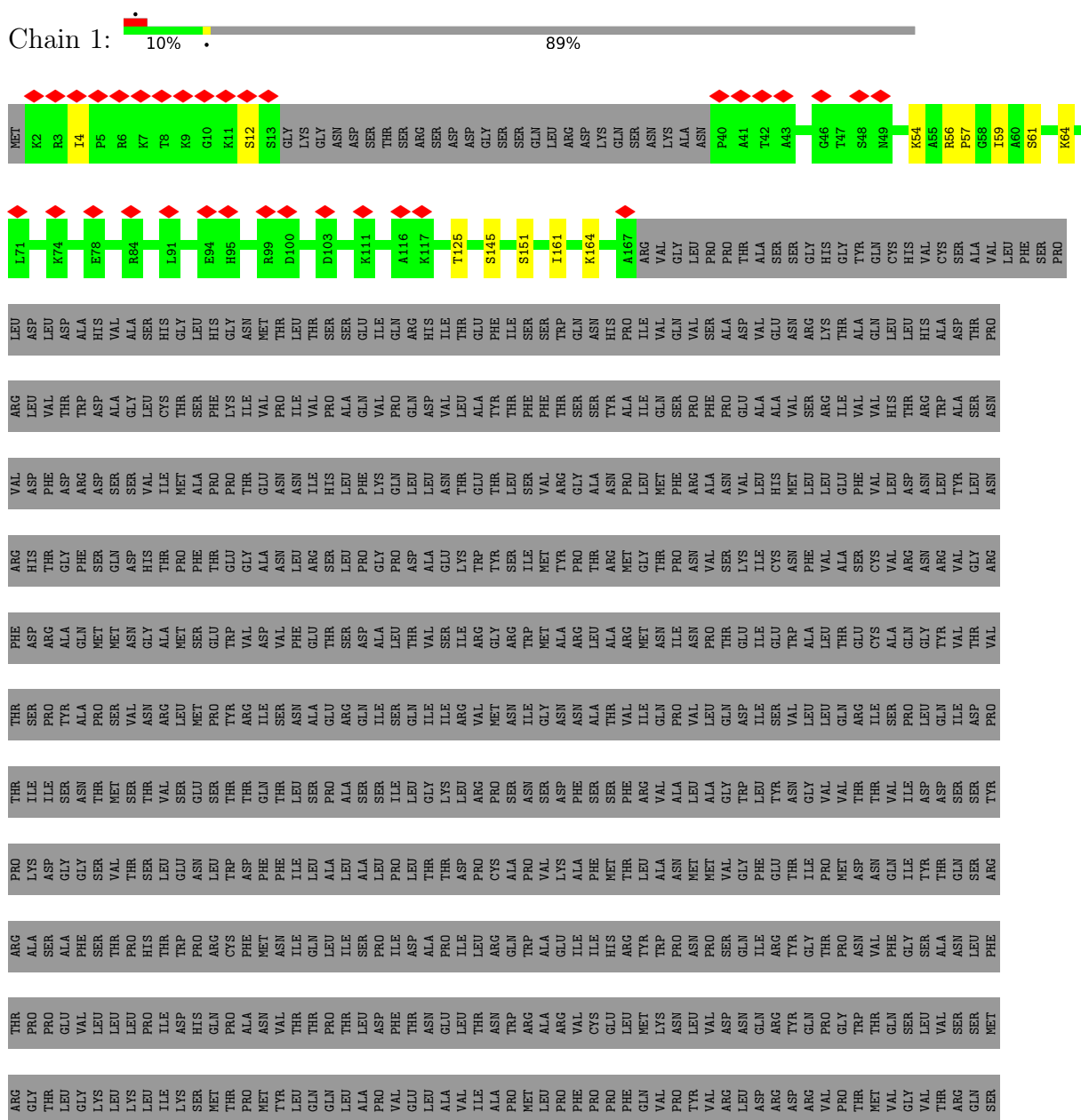
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total 1	Zn 1	0
8	C	1	Total 1	Zn 1	0
8	a	1	Total 1	Zn 1	0
8	b	1	Total 1	Zn 1	0
8	c	1	Total 1	Zn 1	0
8	d	1	Total 1	Zn 1	0
8	e	1	Total 1	Zn 1	0

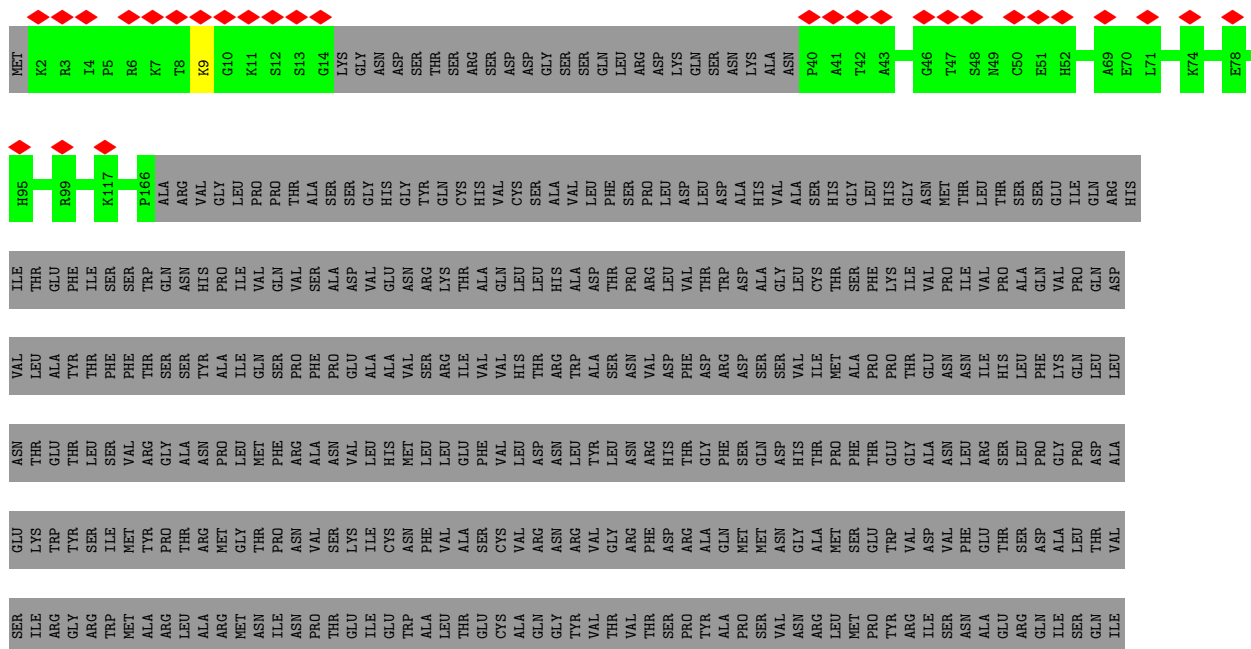
3 Residue-property plots

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

• Molecule 1: RNA helicase



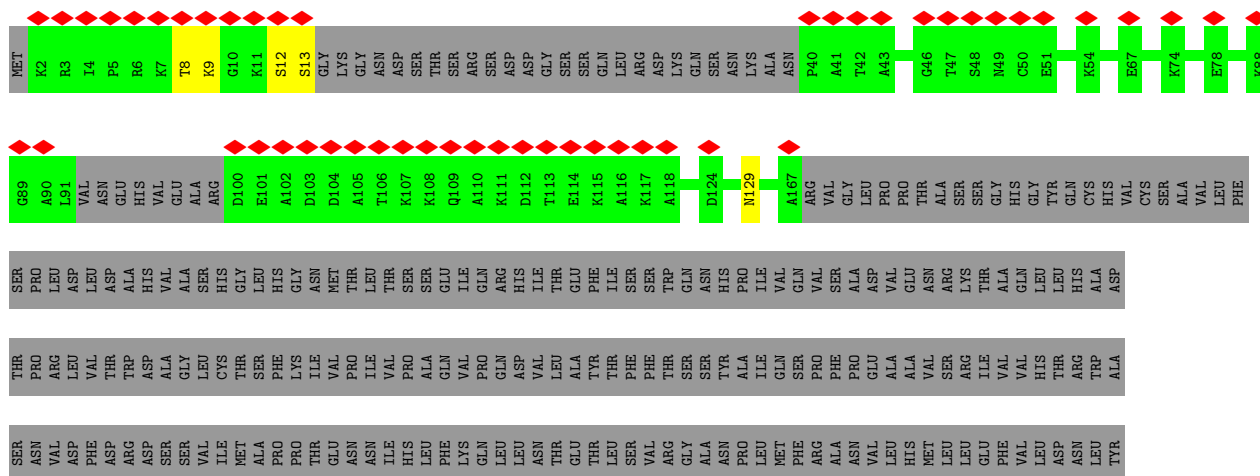




[illegible]

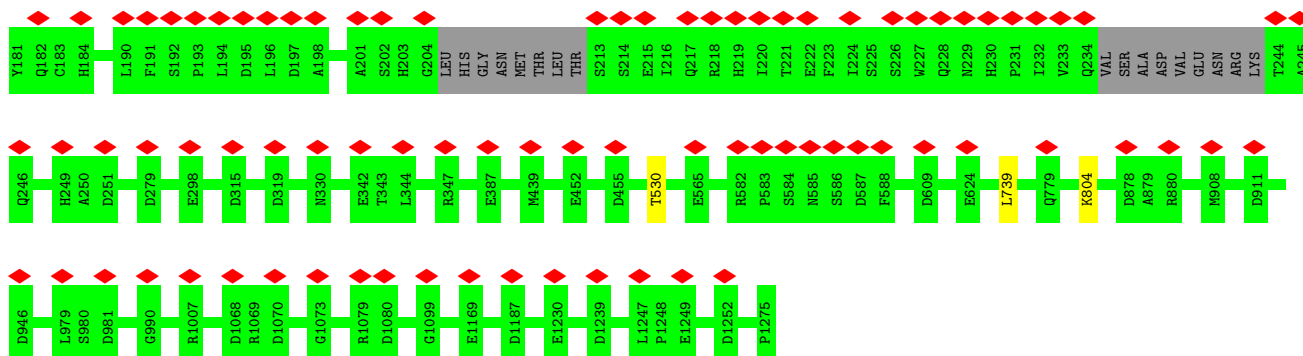
- Molecule 1: RNA helicase

Chain 4:  10% 90%

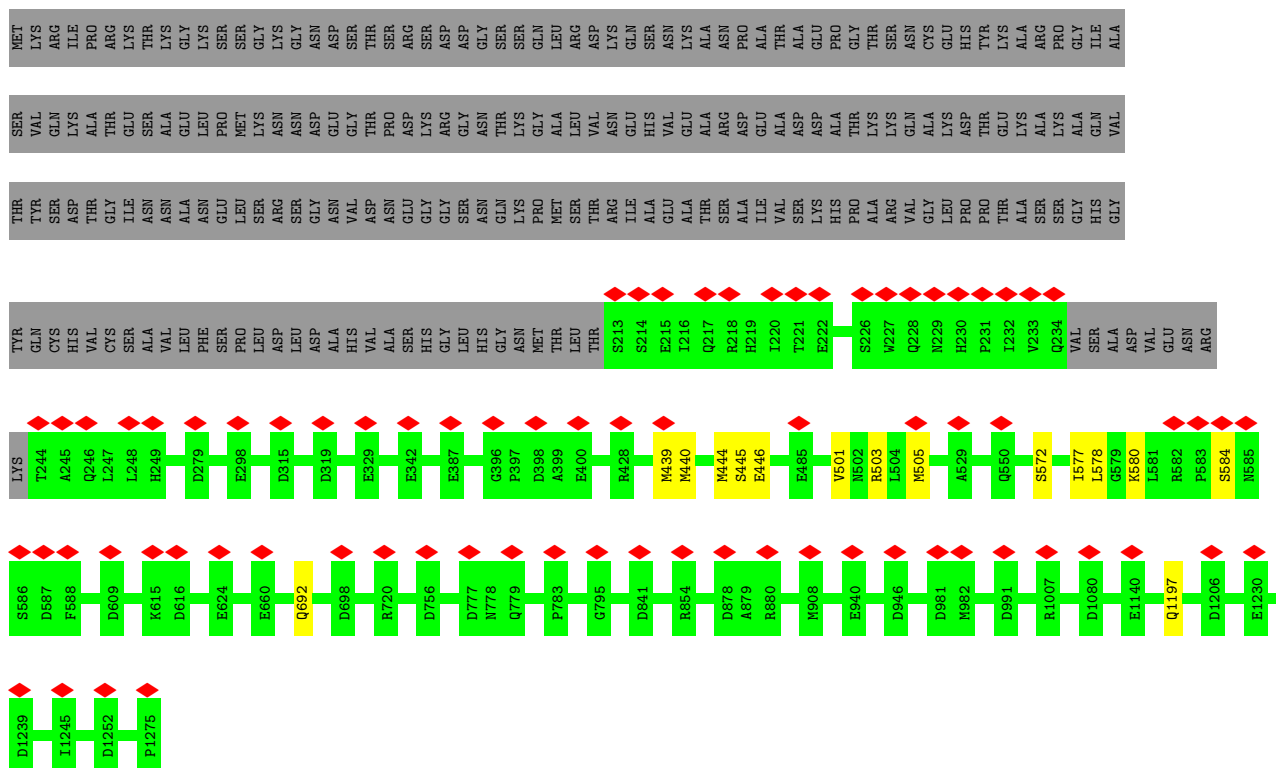
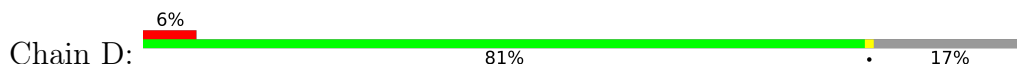




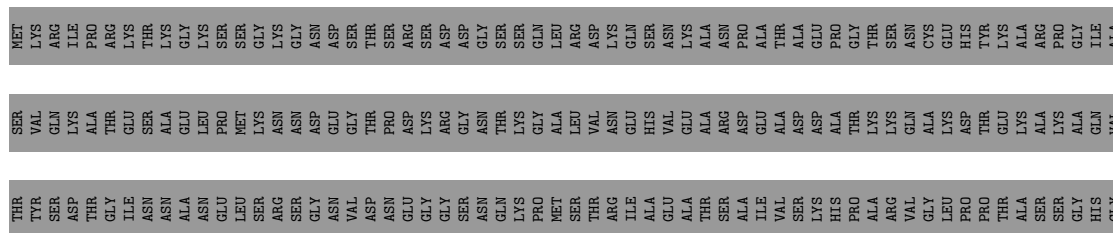
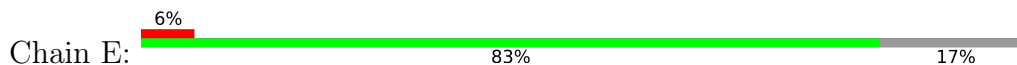


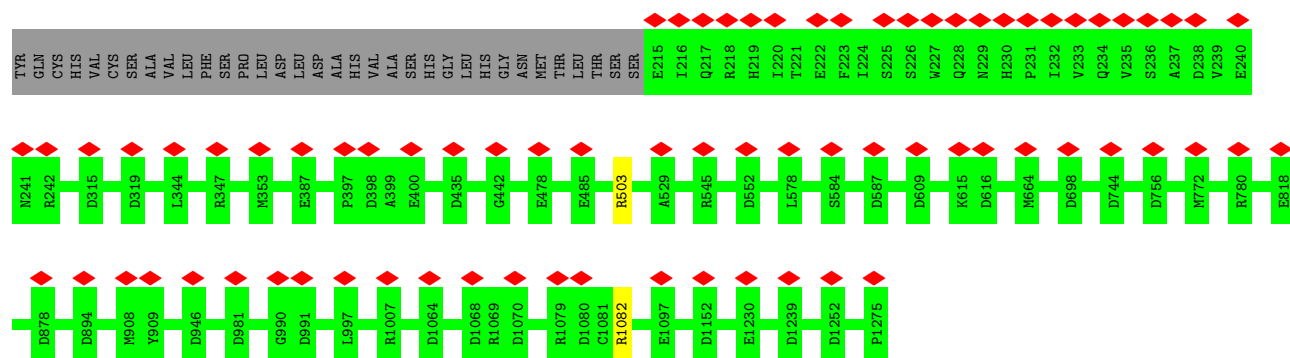


- Molecule 1: RNA helicase

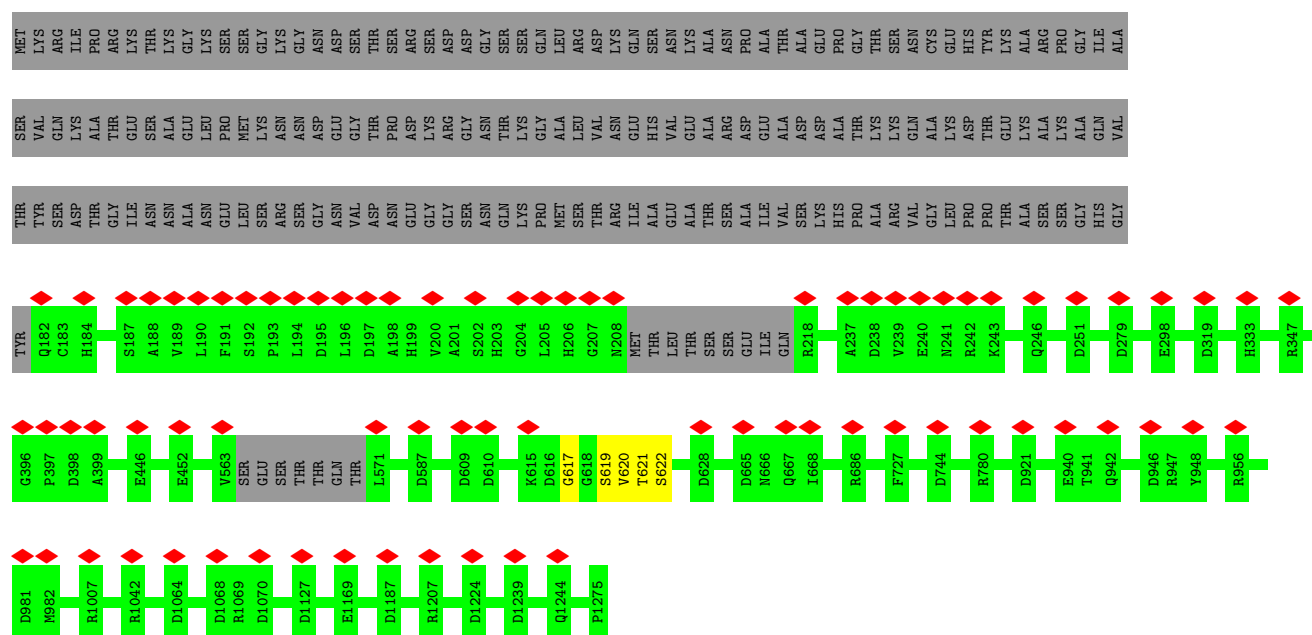
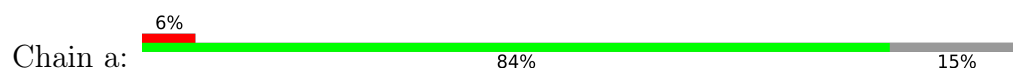


- Molecule 1: RNA helicase

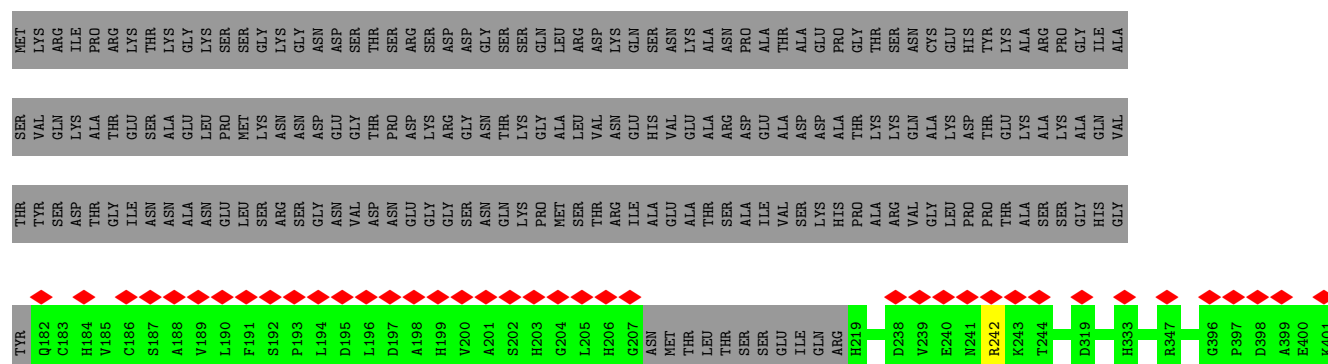
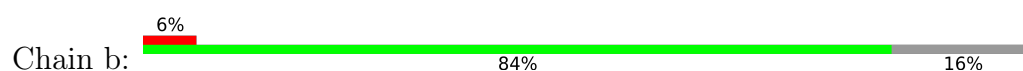


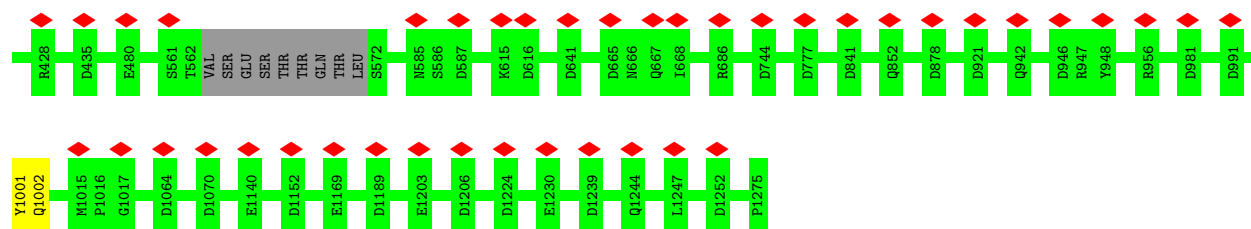


• Molecule 1: RNA helicase

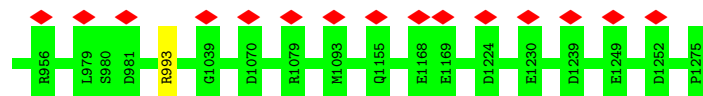
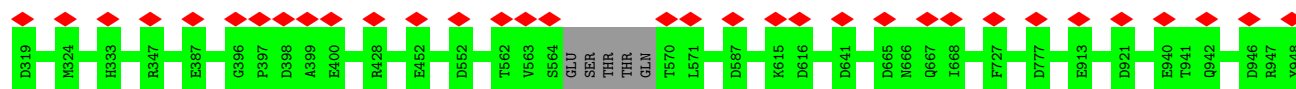
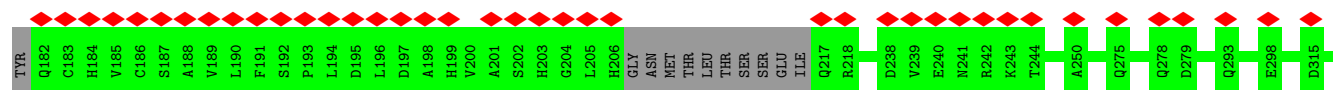
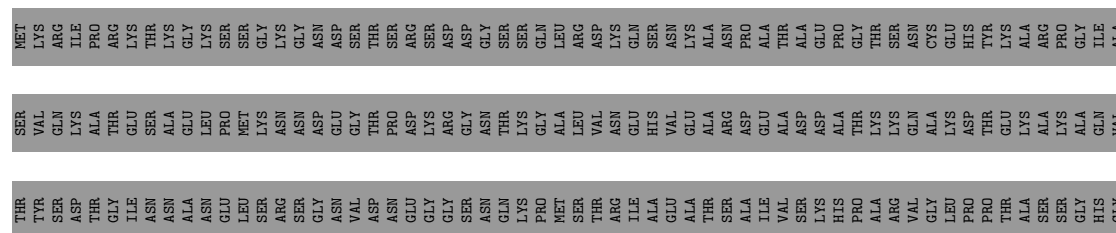
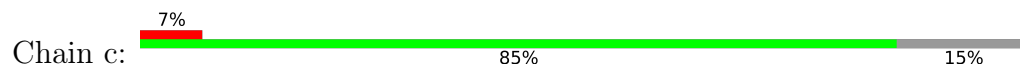


• Molecule 1: RNA helicase

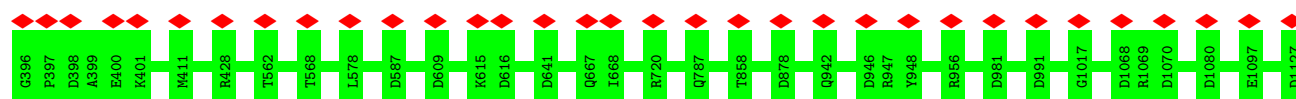
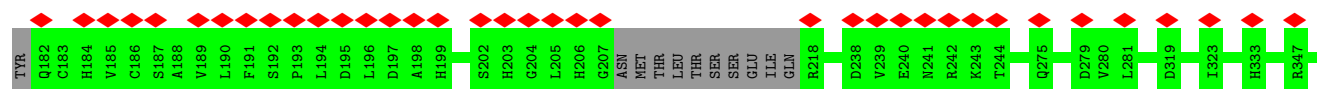
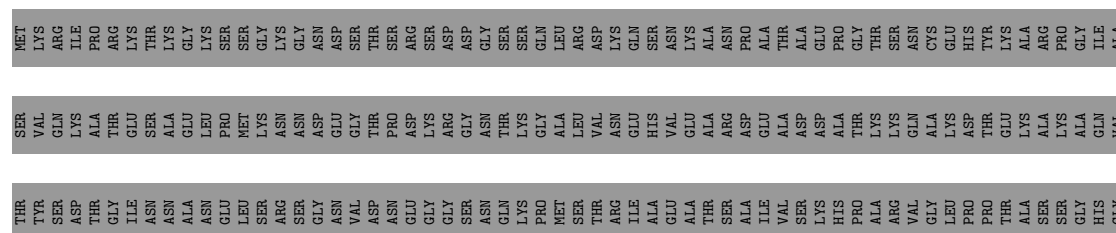
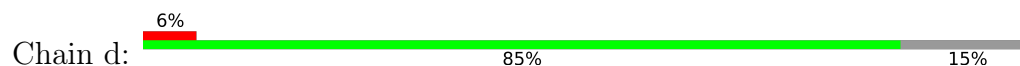




• Molecule 1: RNA helicase

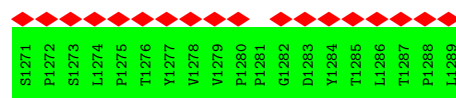
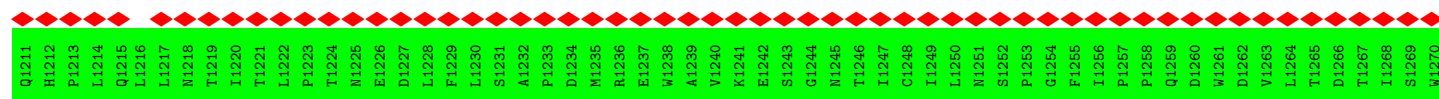
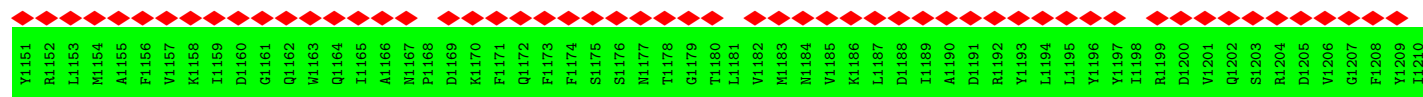
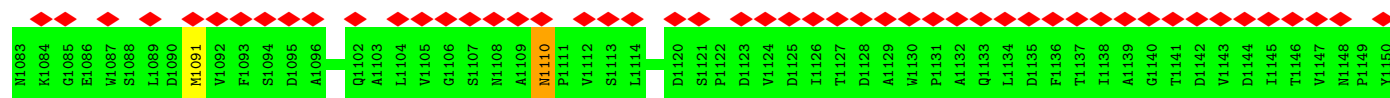
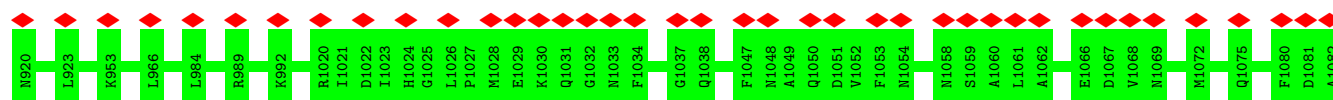
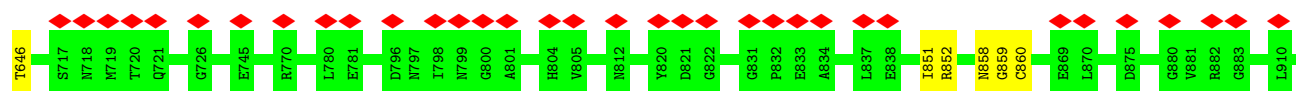
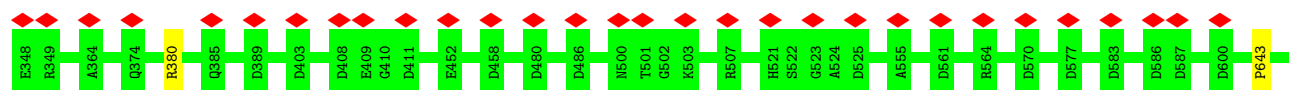
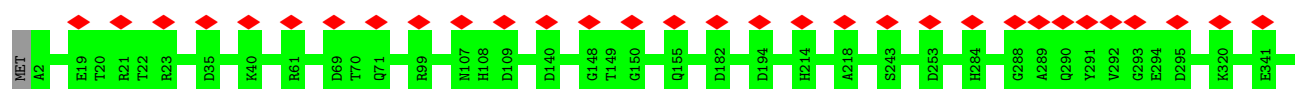


• Molecule 1: RNA helicase

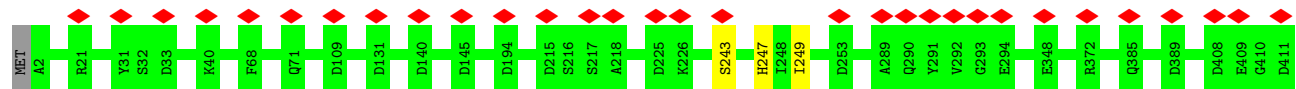


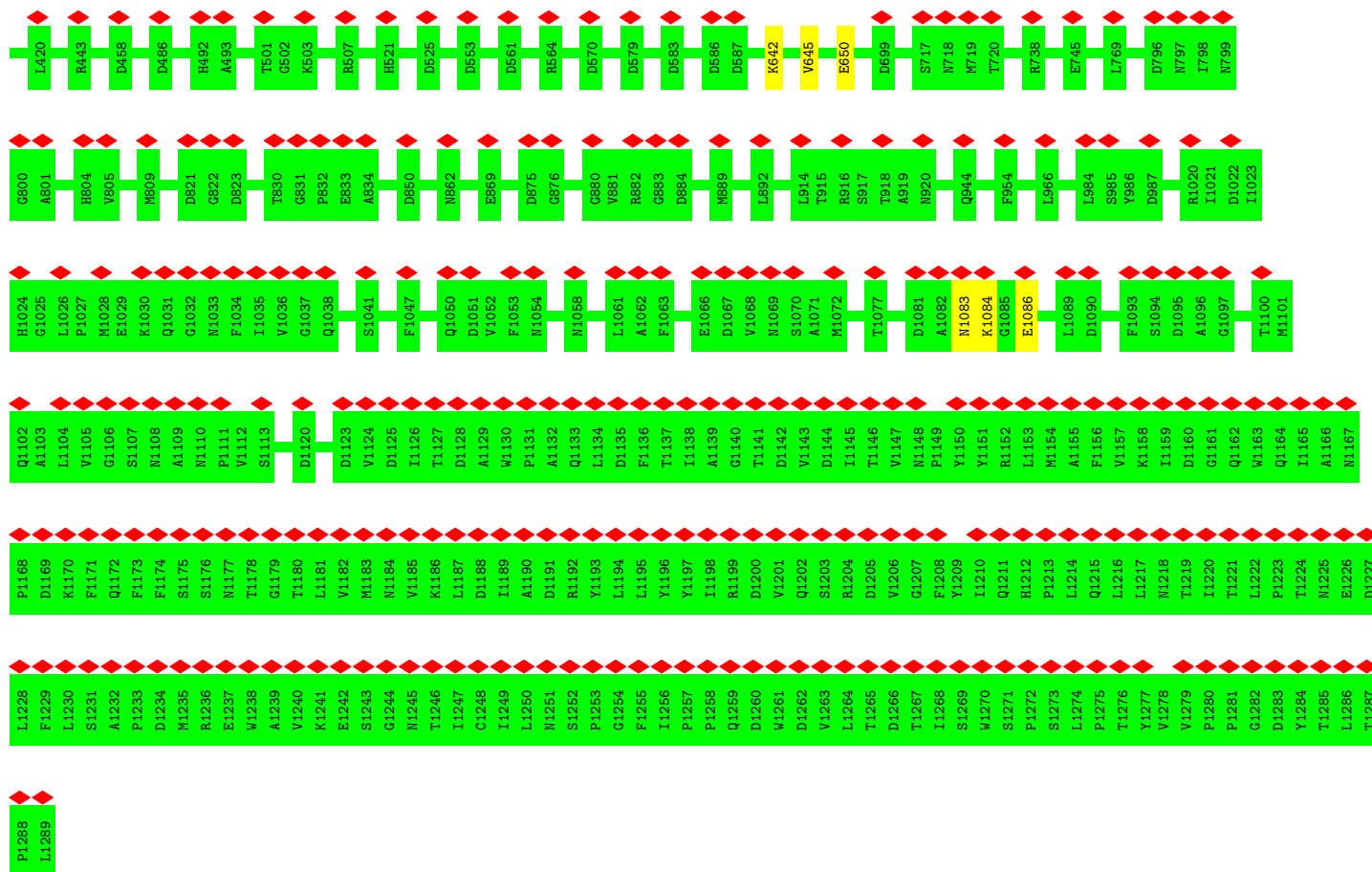


• Molecule 2: Lambda-2 protein



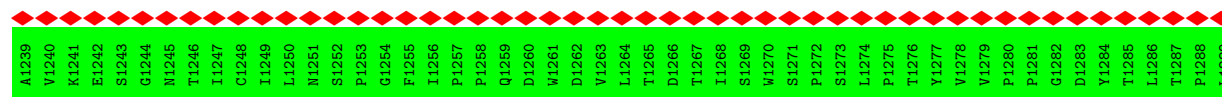
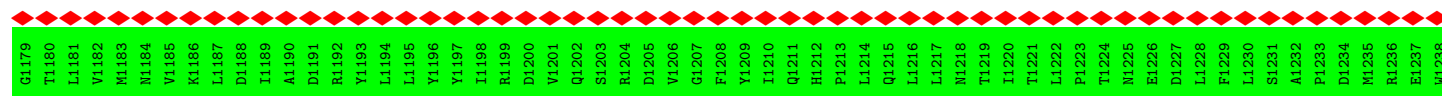
• Molecule 2: Lambda-2 protein



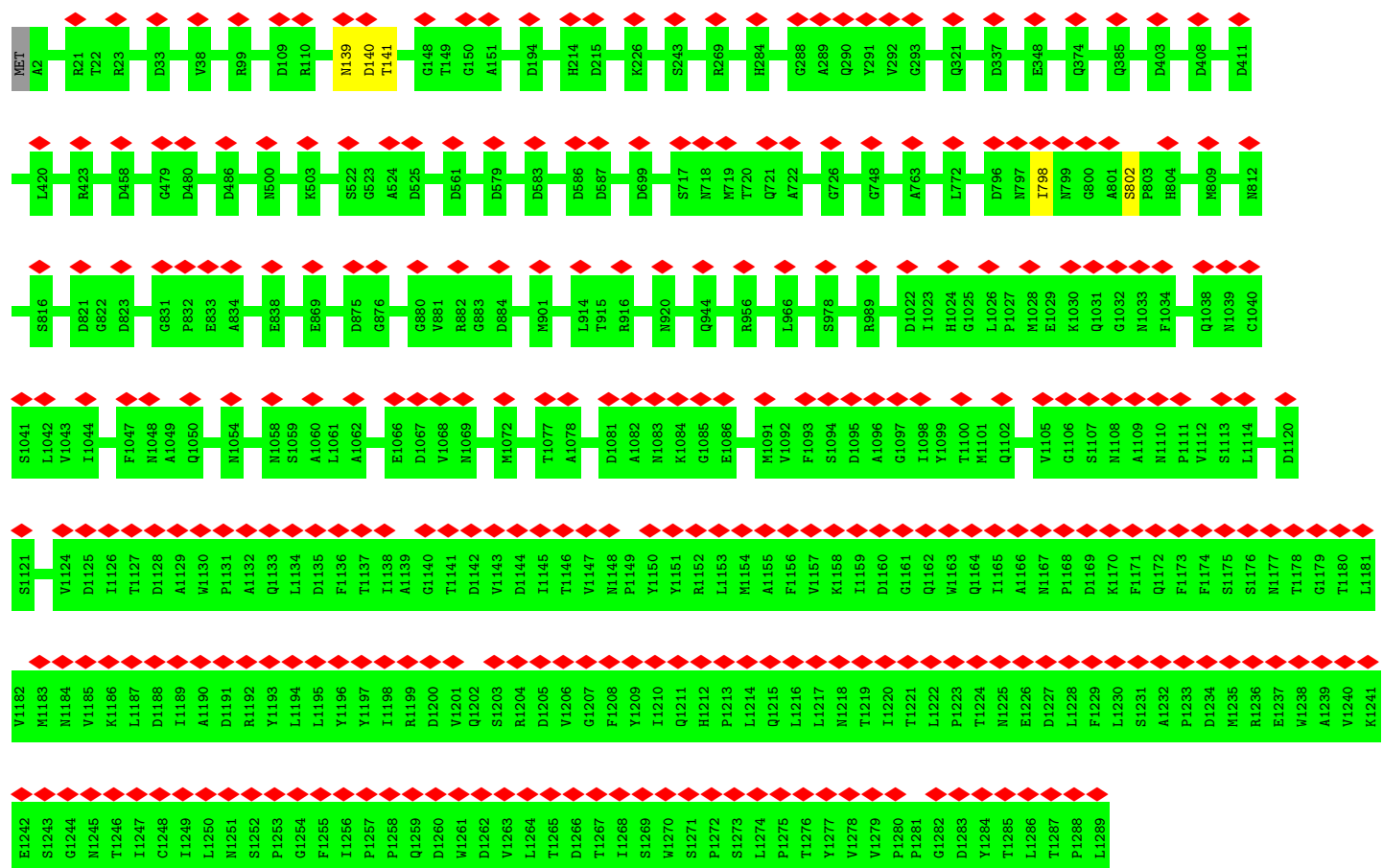


● Molecule 2: Lambda-2 protein





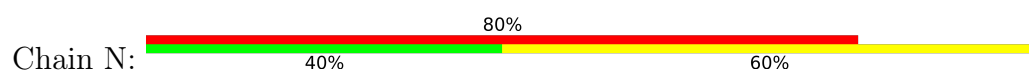
• Molecule 2: Lambda-2 protein

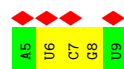


• Molecule 3: RNA (5'-R(P*GP*CP*U)-3')

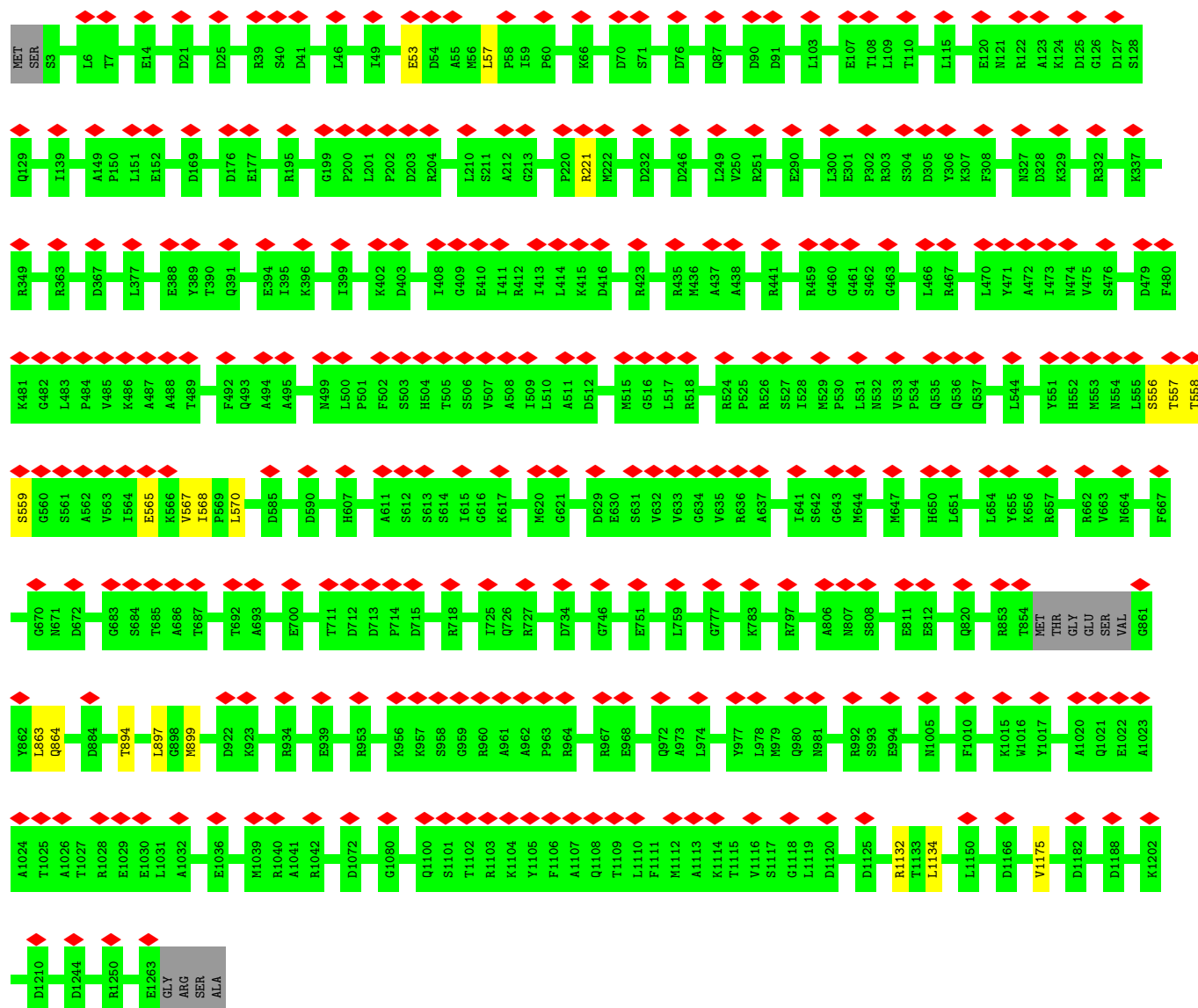


• Molecule 4: RNA (5'-R(P*AP*UP*CP*GP*U)-3')






• Molecule 5: RNA-directed RNA polymerase

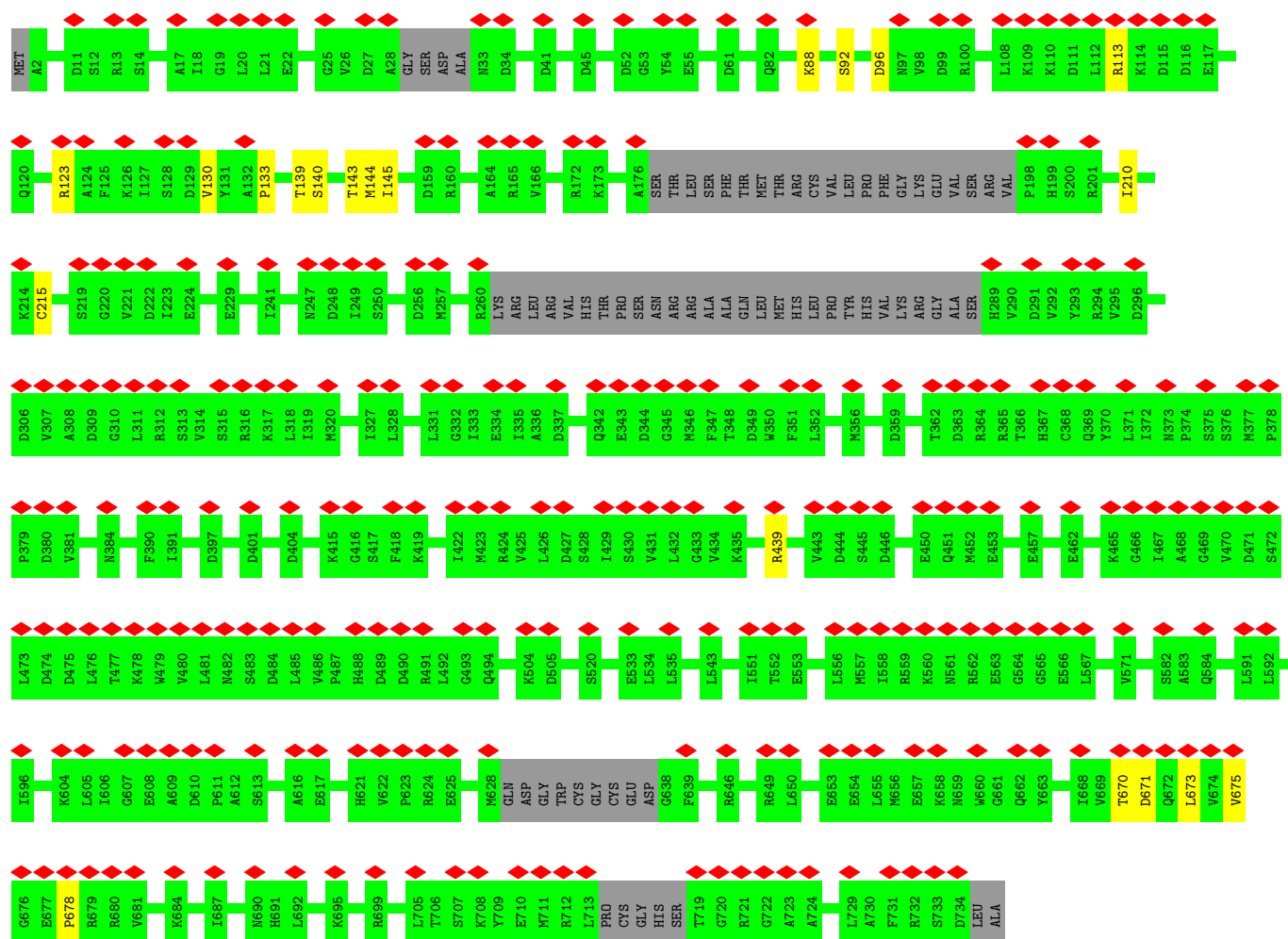


• Molecule 6: RNA (5'-R(P*AP*CP*GP*AP*UP*UP*AP*GP*C)-3')



• Molecule 7: Mu-2 protein

Chain U: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.522	Depositor
Minimum map value	-1.256	Depositor
Average map value	0.039	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.45	0/1052	0.61	1/1413 (0.1%)
1	2	0.42	0/1052	0.55	0/1413
1	3	0.28	0/1051	0.53	0/1411
1	4	0.30	0/984	0.51	0/1319
1	5	0.33	0/1069	0.60	1/1437 (0.1%)
1	A	0.26	0/8856	0.51	0/12127
1	B	0.26	0/8641	0.50	0/11837
1	C	0.26	0/8741	0.51	1/11973 (0.0%)
1	D	0.27	0/8553	0.52	0/11717
1	E	0.26	0/8612	0.52	0/11798
1	a	0.27	0/8735	0.51	1/11965 (0.0%)
1	b	0.25	0/8701	0.50	0/11919
1	c	0.25	0/8745	0.50	0/11979
1	d	0.26	0/8779	0.51	0/12027
1	e	0.29	0/8728	0.52	0/11955
2	H	0.26	0/10404	0.49	0/14205
2	I	0.25	0/10404	0.50	2/14205 (0.0%)
2	J	0.26	0/10404	0.49	0/14205
2	K	0.25	0/10404	0.49	0/14205
2	L	0.26	0/10404	0.50	0/14205
3	M	0.10	0/69	0.67	0/105
4	N	0.19	0/116	0.71	0/178
5	R	0.30	0/10179	0.53	1/13823 (0.0%)
6	T	0.24	0/214	0.79	0/331
7	U	0.29	0/5436	0.56	0/7375
All	All	0.27	0/160333	0.51	7/219127 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	57	PRO	N-CA-C	-6.28	95.77	112.10
1	C	739	LEU	CA-CB-CG	5.94	128.97	115.30
2	I	1110	ASN	N-CA-C	-5.76	95.44	111.00
1	a	617	GLY	N-CA-C	-5.76	98.70	113.10
5	R	1134	LEU	N-CA-C	-5.62	95.84	111.00
2	I	859	GLY	N-CA-C	5.57	127.03	113.10
1	5	10	GLY	N-CA-C	-5.25	99.97	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	136/1275 (11%)	134 (98%)	2 (2%)	0	100	100
1	2	136/1275 (11%)	133 (98%)	3 (2%)	0	100	100
1	3	136/1275 (11%)	134 (98%)	2 (2%)	0	100	100
1	4	126/1275 (10%)	121 (96%)	5 (4%)	0	100	100
1	5	139/1275 (11%)	137 (99%)	2 (1%)	0	100	100
1	A	1090/1275 (86%)	1043 (96%)	47 (4%)	0	100	100
1	B	1065/1275 (84%)	1021 (96%)	44 (4%)	0	100	100
1	C	1073/1275 (84%)	1027 (96%)	46 (4%)	0	100	100
1	D	1050/1275 (82%)	1016 (97%)	34 (3%)	0	100	100
1	E	1059/1275 (83%)	1013 (96%)	46 (4%)	0	100	100
1	a	1072/1275 (84%)	1021 (95%)	51 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	1068/1275 (84%)	1018 (95%)	50 (5%)	0	100	100
1	c	1073/1275 (84%)	1038 (97%)	35 (3%)	0	100	100
1	d	1080/1275 (85%)	1037 (96%)	43 (4%)	0	100	100
1	e	1071/1275 (84%)	1022 (95%)	49 (5%)	0	100	100
2	H	1286/1289 (100%)	1238 (96%)	48 (4%)	0	100	100
2	I	1286/1289 (100%)	1243 (97%)	42 (3%)	1 (0%)	48	78
2	J	1286/1289 (100%)	1245 (97%)	41 (3%)	0	100	100
2	K	1286/1289 (100%)	1238 (96%)	48 (4%)	0	100	100
2	L	1286/1289 (100%)	1243 (97%)	43 (3%)	0	100	100
5	R	1251/1267 (99%)	1198 (96%)	53 (4%)	0	100	100
7	U	654/736 (89%)	614 (94%)	38 (6%)	2 (0%)	37	66
All	All	19709/27573 (72%)	18934 (96%)	772 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	U	678	PRO
7	U	133	PRO
2	I	643	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	112/1113 (10%)	100 (89%)	12 (11%)	5	20
1	2	112/1113 (10%)	94 (84%)	18 (16%)	2	8
1	3	112/1113 (10%)	111 (99%)	1 (1%)	75	86
1	4	105/1113 (9%)	100 (95%)	5 (5%)	21	48
1	5	113/1113 (10%)	104 (92%)	9 (8%)	10	31
1	A	969/1113 (87%)	964 (100%)	5 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	942/1113 (85%)	935 (99%)	7 (1%)	81	88
1	C	954/1113 (86%)	952 (100%)	2 (0%)	92	96
1	D	934/1113 (84%)	919 (98%)	15 (2%)	58	75
1	E	940/1113 (84%)	938 (100%)	2 (0%)	92	96
1	a	952/1113 (86%)	948 (100%)	4 (0%)	89	93
1	b	948/1113 (85%)	945 (100%)	3 (0%)	91	95
1	c	954/1113 (86%)	953 (100%)	1 (0%)	92	97
1	d	958/1113 (86%)	958 (100%)	0	100	100
1	e	951/1113 (85%)	942 (99%)	9 (1%)	75	86
2	H	1117/1118 (100%)	1111 (100%)	6 (0%)	86	91
2	I	1117/1118 (100%)	1109 (99%)	8 (1%)	81	88
2	J	1117/1118 (100%)	1108 (99%)	9 (1%)	79	87
2	K	1117/1118 (100%)	1114 (100%)	3 (0%)	91	95
2	L	1117/1118 (100%)	1112 (100%)	5 (0%)	89	93
5	R	1075/1084 (99%)	1057 (98%)	18 (2%)	56	74
7	U	591/650 (91%)	573 (97%)	18 (3%)	36	61
All	All	17307/24019 (72%)	17147 (99%)	160 (1%)	74	86

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	ILE
1	1	12	SER
1	1	54	LYS
1	1	56	ARG
1	1	59	ILE
1	1	61	SER
1	1	64	LYS
1	1	125	THR
1	1	145	SER
1	1	151	SER
1	1	161	ILE
1	1	164	LYS
1	2	54	LYS
1	2	59	ILE
1	2	83	LYS

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Mol	Chain	Res	Type
1	2	84	ARG
1	2	88	LYS
1	2	91	LEU
1	2	92	VAL
1	2	114	GLU
1	2	121	THR
1	2	123	SER
1	2	125	THR
1	2	146	ASN
1	2	148	LYS
1	2	151	SER
1	2	161	ILE
1	2	162	VAL
1	2	163	SER
1	2	164	LYS
1	3	9	LYS
1	4	8	THR
1	4	9	LYS
1	4	12	SER
1	4	13	SER
1	4	129	ASN
1	5	8	THR
1	5	9	LYS
1	5	11	LYS
1	5	12	SER
1	5	42	THR
1	5	44	GLU
1	5	48	SER
1	5	50	CYS
1	5	51	GLU
1	A	851	ARG
1	A	855	ASP
1	A	859	GLN
1	A	911	ASP
1	A	914	VAL
1	B	664	MET
1	B	665	ASP
1	B	668	ILE
1	B	670	THR
1	B	671	GLN
1	B	780	ARG
1	B	825	MET

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Mol	Chain	Res	Type
1	C	530	THR
1	C	804	LYS
1	D	439	MET
1	D	440	MET
1	D	444	MET
1	D	445	SER
1	D	446	GLU
1	D	501	VAL
1	D	503	ARG
1	D	505	MET
1	D	572	SER
1	D	577	ILE
1	D	578	LEU
1	D	580	LYS
1	D	584	SER
1	D	692	GLN
1	D	1197	GLN
1	E	503	ARG
1	E	1082	ARG
2	H	98	LEU
2	H	103	ILE
2	H	104	SER
2	H	112	ASN
2	H	1050	GLN
2	H	1051	ASP
2	I	380	ARG
2	I	646	THR
2	I	851	ILE
2	I	852	ARG
2	I	858	ASN
2	I	860	CYS
2	I	1091	MET
2	I	1110	ASN
2	J	243	SER
2	J	247	HIS
2	J	249	ILE
2	J	642	LYS
2	J	645	VAL
2	J	650	GLU
2	J	1083	ASN
2	J	1084	LYS
2	J	1086	GLU

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Mol	Chain	Res	Type
2	K	380	ARG
2	K	1050	GLN
2	K	1051	ASP
2	L	139	ASN
2	L	140	ASP
2	L	141	THR
2	L	798	ILE
2	L	802	SER
5	R	53	GLU
5	R	57	LEU
5	R	221	ARG
5	R	556	SER
5	R	557	THR
5	R	558	THR
5	R	559	SER
5	R	565	GLU
5	R	567	VAL
5	R	568	ILE
5	R	570	LEU
5	R	863	LEU
5	R	864	GLN
5	R	894	THR
5	R	897	LEU
5	R	899	MET
5	R	1132	ARG
5	R	1175	VAL
7	U	88	LYS
7	U	92	SER
7	U	96	ASP
7	U	113	ARG
7	U	123	ARG
7	U	130	VAL
7	U	139	THR
7	U	140	SER
7	U	143	THR
7	U	144	MET
7	U	145	ILE
7	U	210	ILE
7	U	215	CYS
7	U	439	ARG
7	U	670	THR
7	U	671	ASP

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Mol	Chain	Res	Type
7	U	673	LEU
7	U	675	VAL
1	a	619	SER
1	a	620	VAL
1	a	621	THR
1	a	622	SER
1	b	242	ARG
1	b	1001	TYR
1	b	1002	GLN
1	c	993	ARG
1	e	312	SER
1	e	647	LYS
1	e	656	MET
1	e	661	THR
1	e	662	ILE
1	e	664	MET
1	e	668	ILE
1	e	676	SER
1	e	1032	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	146	ASN
1	2	86	ASN
1	3	119	GLN
1	4	63	GLN
1	4	129	ASN
1	4	146	ASN
1	5	63	GLN
1	5	76	ASN
1	A	340	ASN
1	A	1233	ASN
1	B	654	ASN
1	B	667	GLN
1	C	533	GLN
1	C	682	HIS
1	C	1123	ASN
1	D	692	GLN
1	D	1000	GLN
1	E	340	ASN
1	E	1088	ASN

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Mol	Chain	Res	Type
2	H	535	GLN
2	H	647	ASN
2	H	677	HIS
2	I	180	ASN
2	I	572	GLN
2	I	856	GLN
2	J	107	ASN
2	J	310	ASN
2	J	321	GLN
2	J	324	ASN
2	J	455	GLN
2	K	783	GLN
2	K	1164	GLN
2	L	139	ASN
2	L	347	GLN
2	L	352	GLN
2	L	526	GLN
5	R	439	GLN
5	R	732	GLN
5	R	864	GLN
5	R	1177	ASN
1	a	340	ASN
1	a	625	ASN
1	a	1213	ASN
1	b	1002	GLN
1	c	1003	GLN
1	d	246	GLN
1	d	524	ASN
1	e	234	GLN
1	e	307	HIS
1	e	313	ASN
1	e	654	ASN
1	e	812	GLN
1	e	1036	ASN
1	e	1205	ASN
1	e	1233	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	2/3 (66%)	1 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	N	4/5 (80%)	3 (75%)	1 (25%)
6	T	8/9 (88%)	3 (37%)	0
All	All	14/17 (82%)	7 (50%)	1 (7%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	2	C
4	N	6	U
4	N	7	C
4	N	8	G
6	T	5	U
6	T	6	U
6	T	7	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	N	7	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

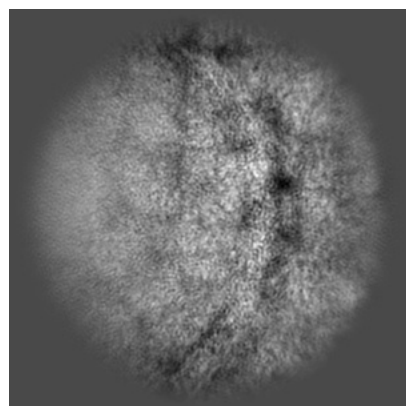
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33787. These allow visual inspection of the internal detail of the map and identification of artifacts.

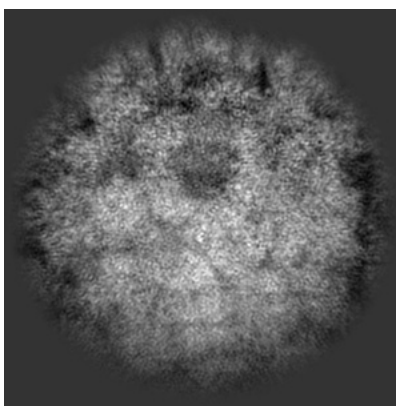
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

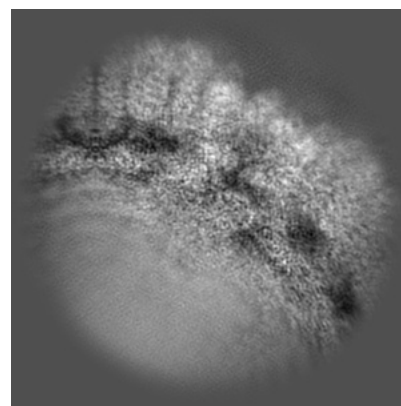
6.1.1 Primary map



X

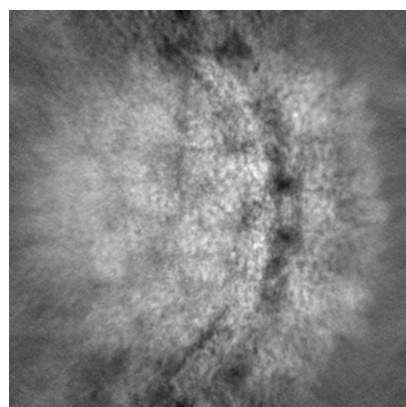


Y

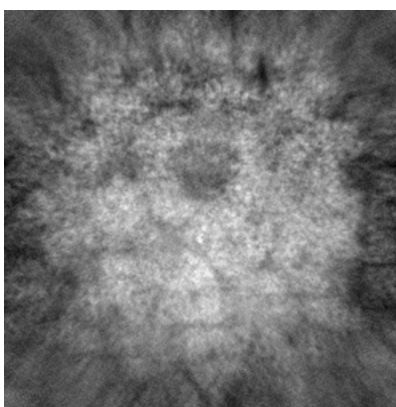


Z

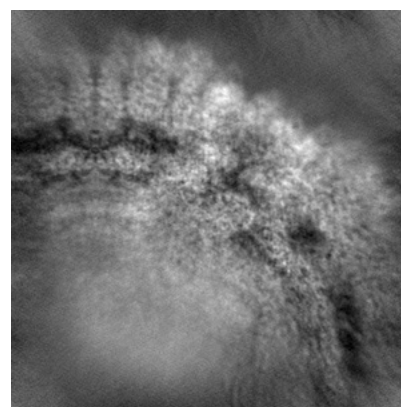
6.1.2 Raw map



X



Y

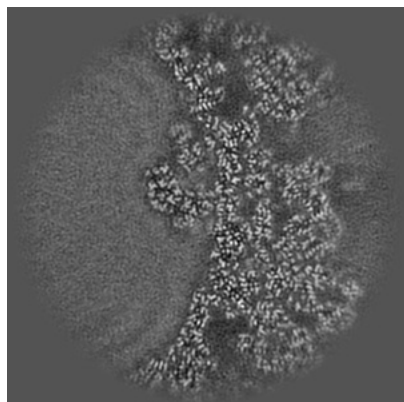


Z

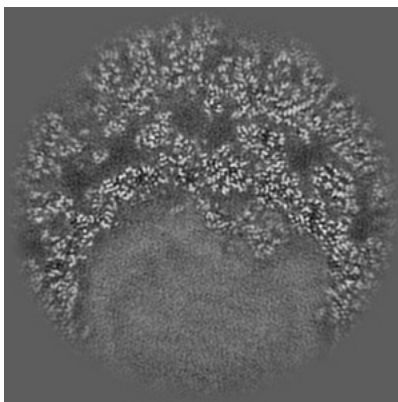
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

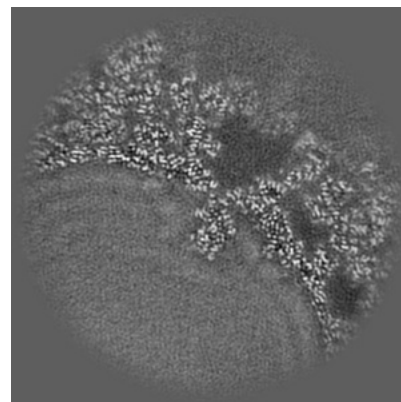
6.2.1 Primary map



X Index: 160

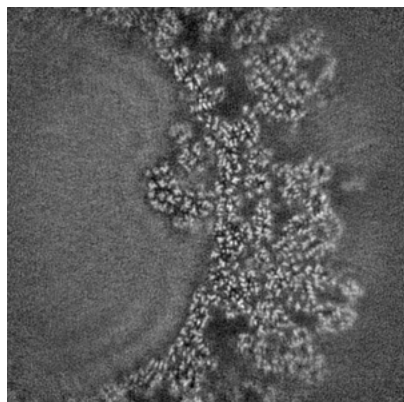


Y Index: 160

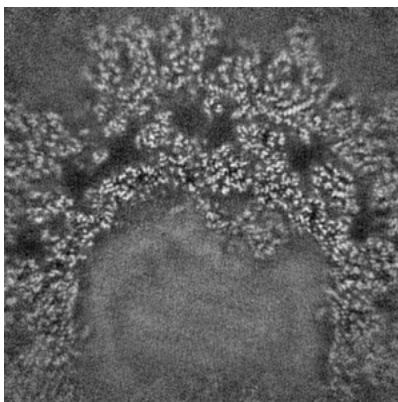


Z Index: 160

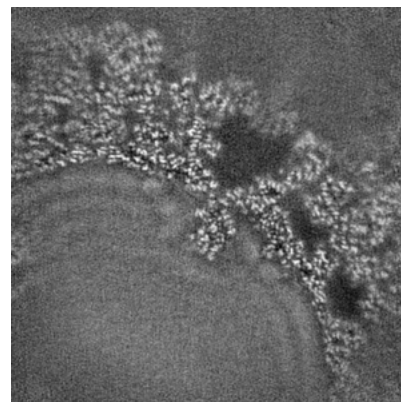
6.2.2 Raw map



X Index: 160



Y Index: 160

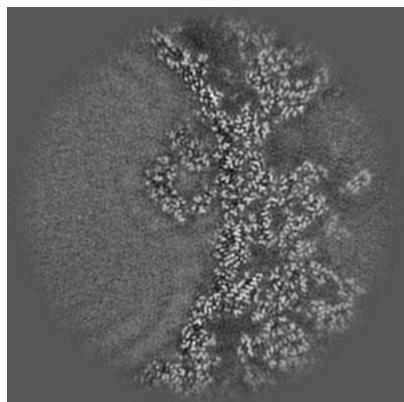


Z Index: 160

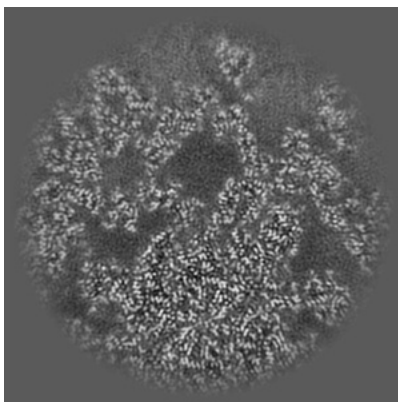
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

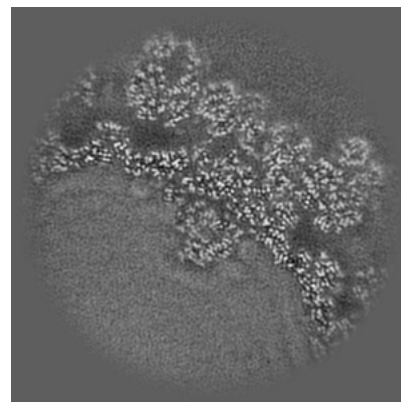
6.3.1 Primary map



X Index: 155

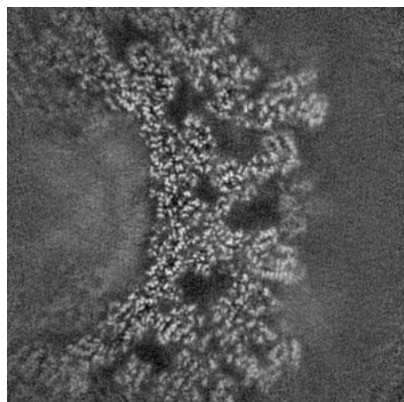


Y Index: 199

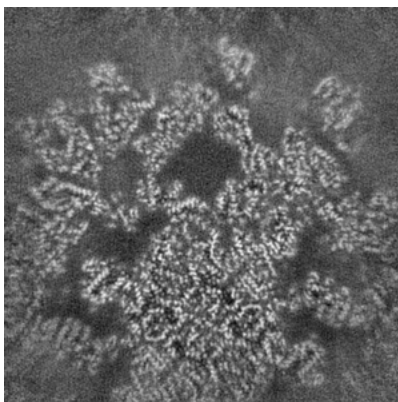


Z Index: 190

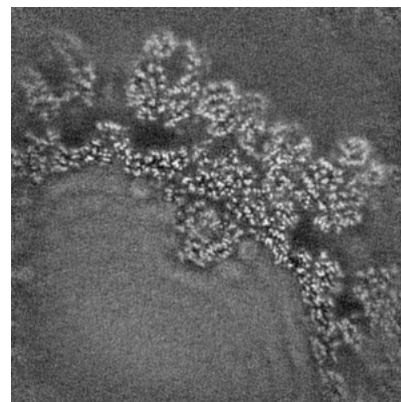
6.3.2 Raw map



X Index: 213



Y Index: 201

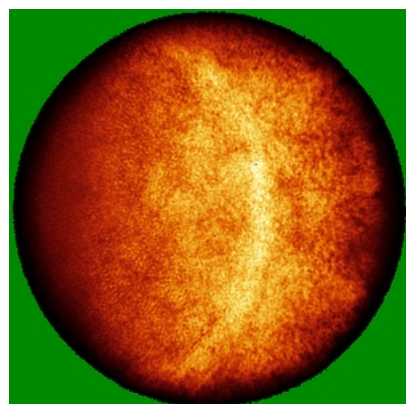


Z Index: 190

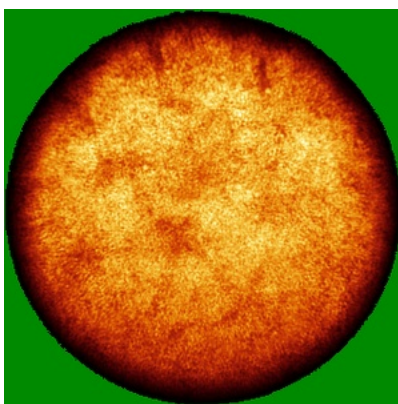
The images above show the largest variance slices of the map in three orthogonal directions.

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

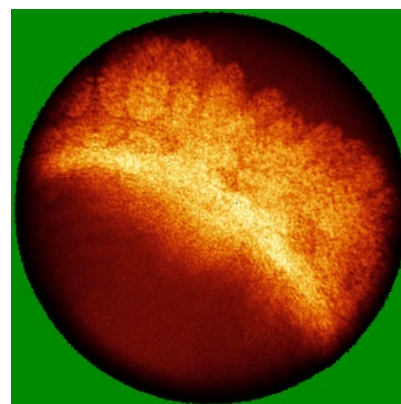
6.4.1 Primary map



X

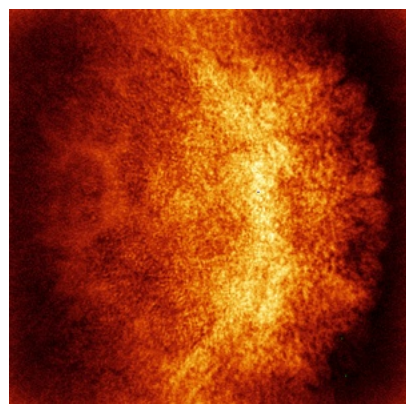


Y

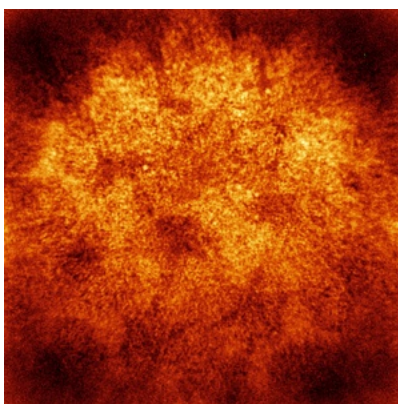


Z

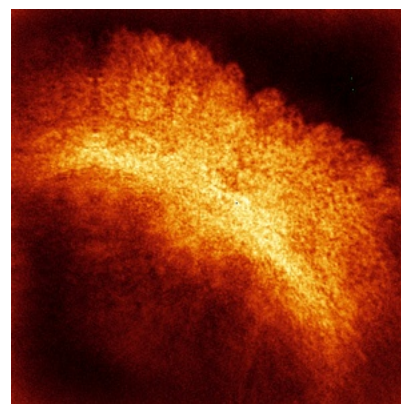
6.4.2 Raw map



X



Y

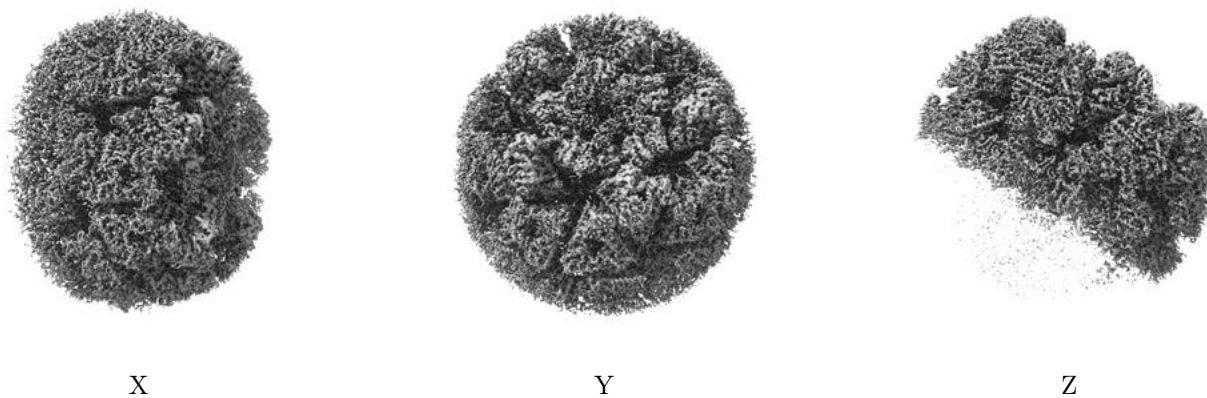


Z

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

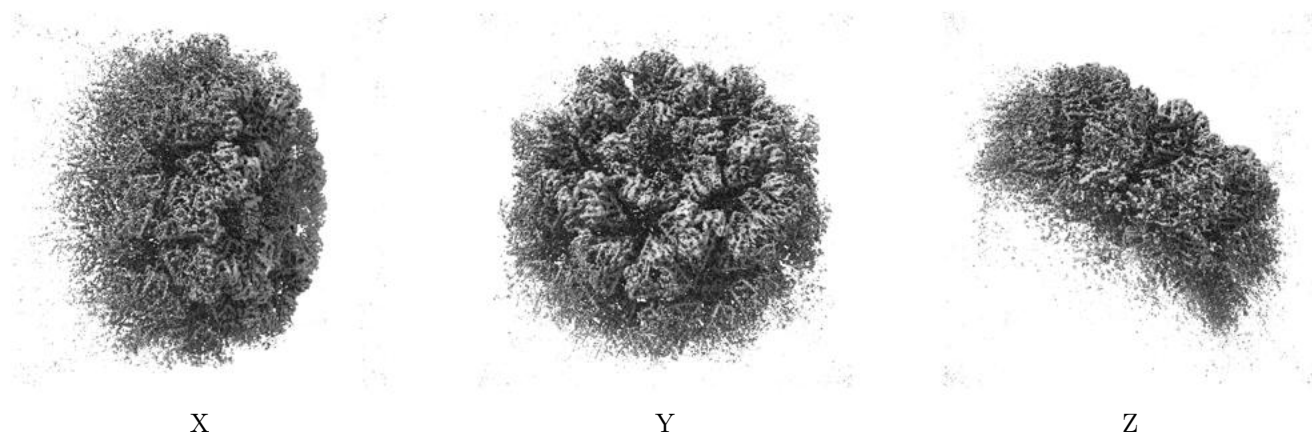
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

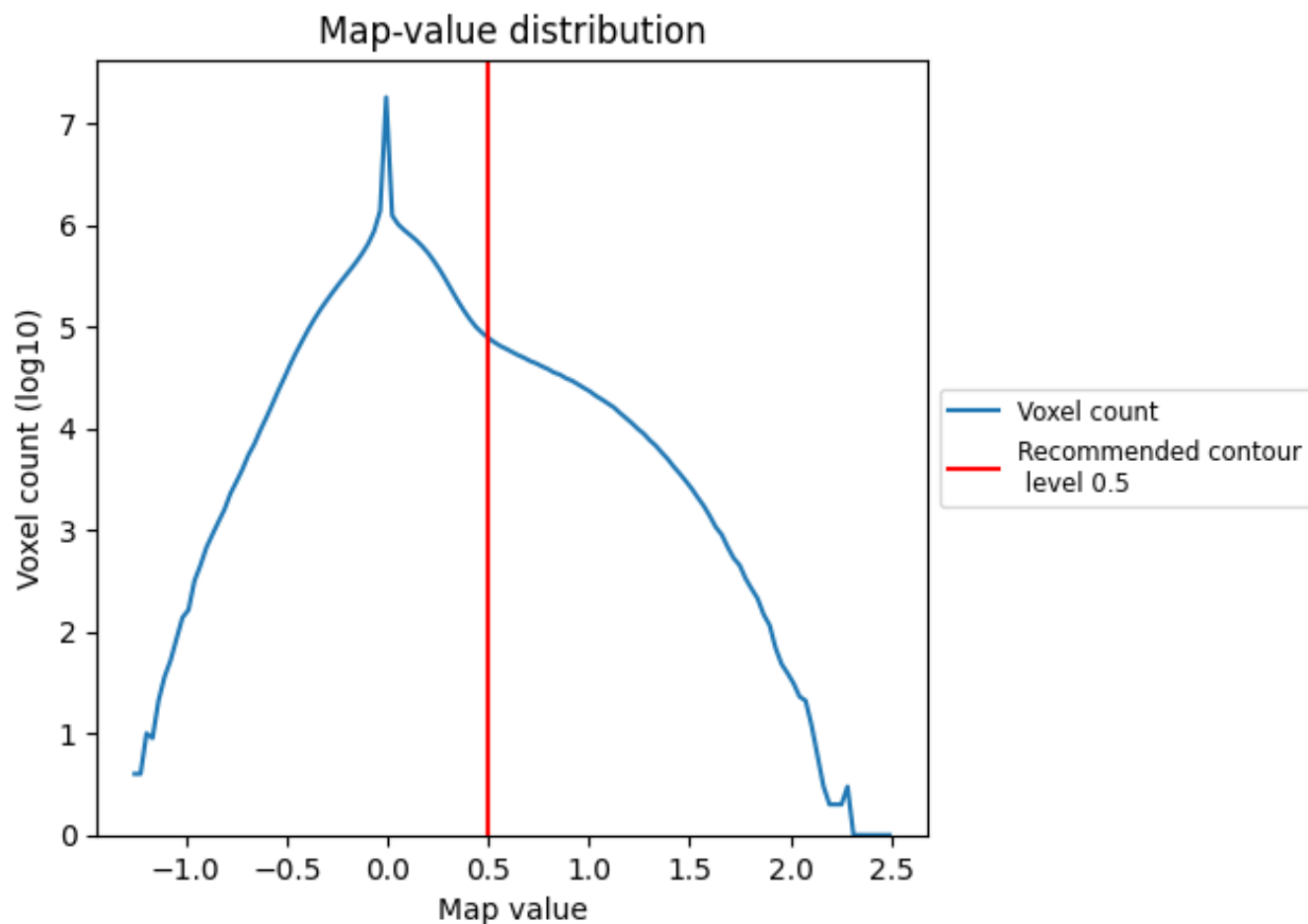
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

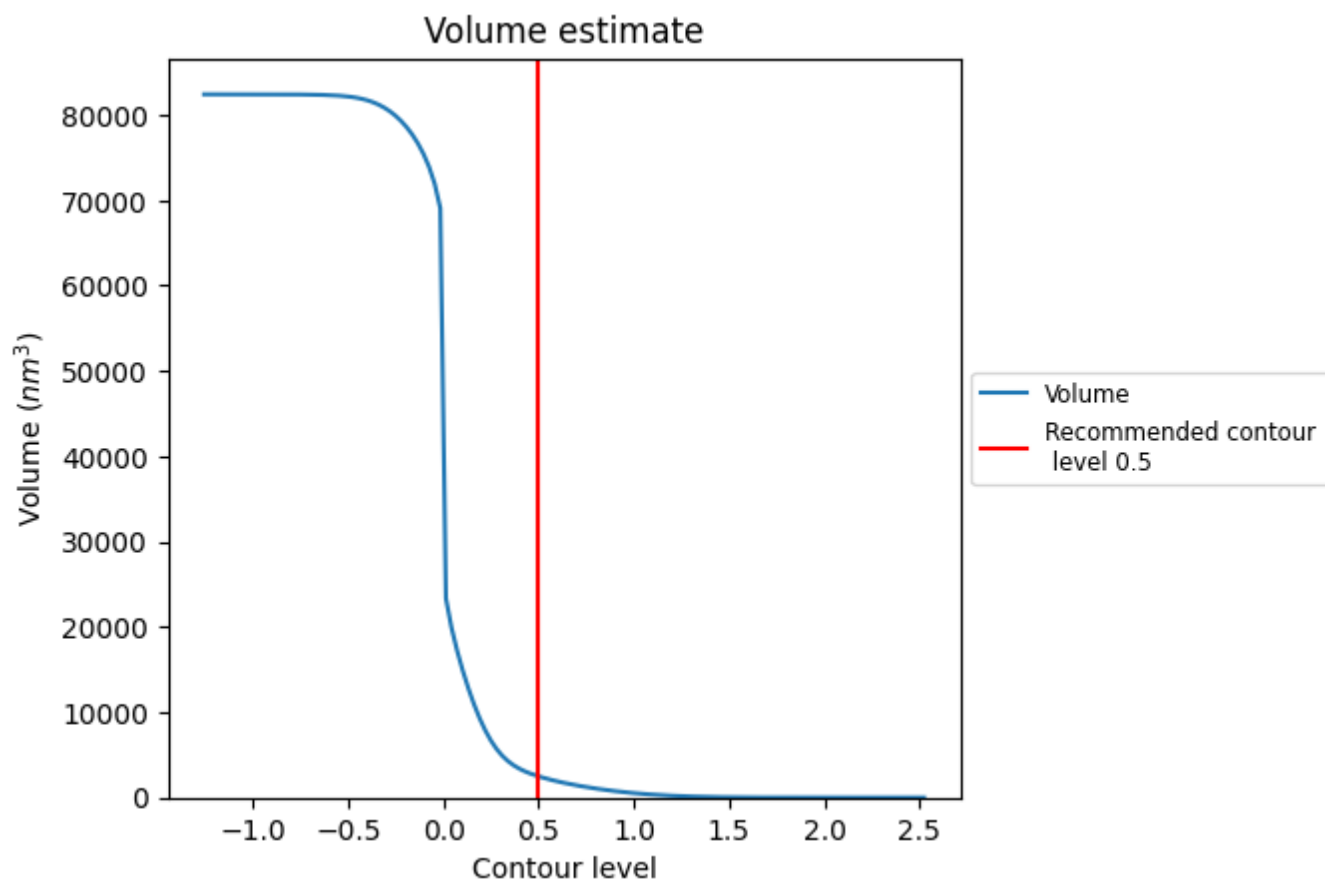
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

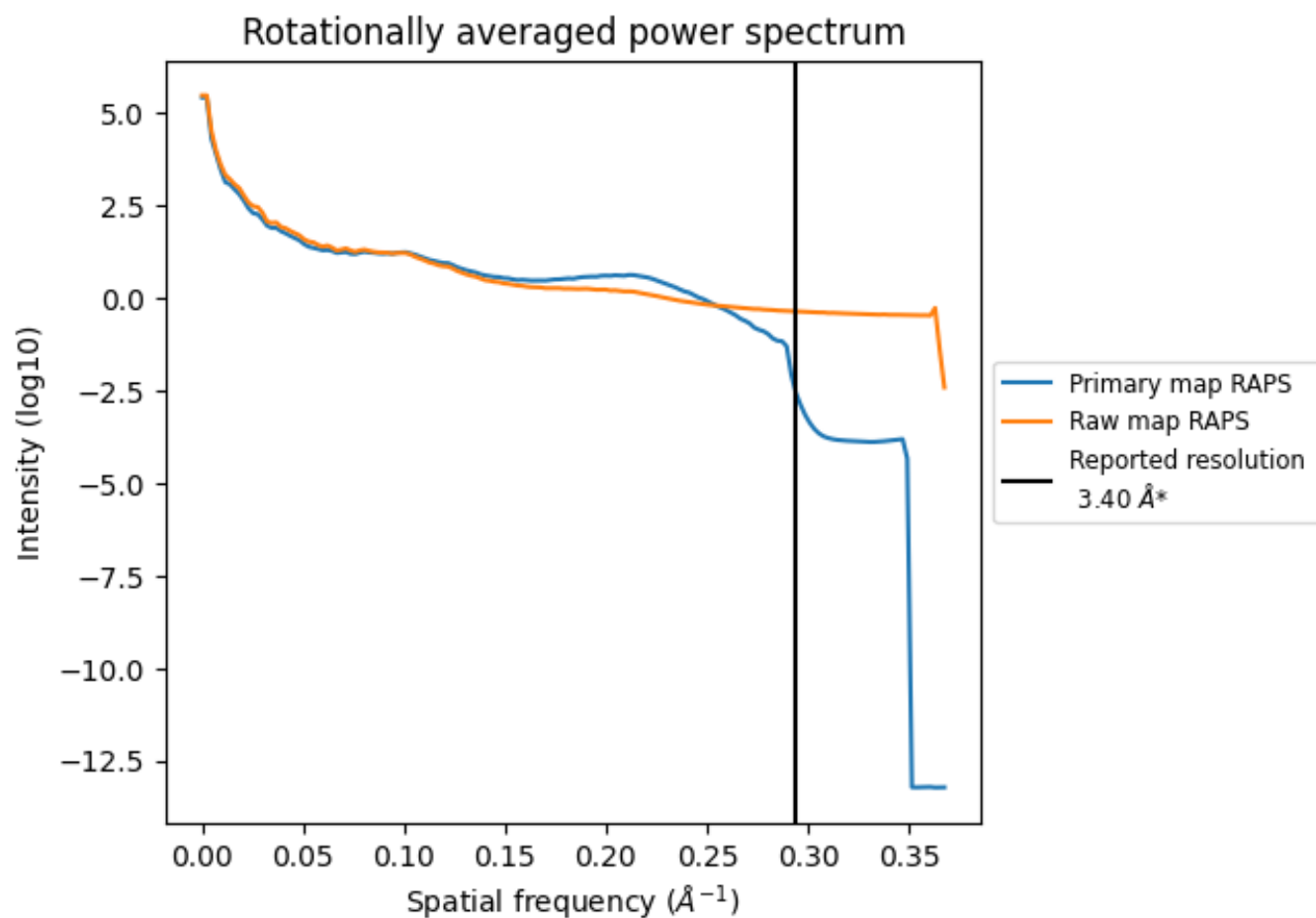
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2485 nm³; this corresponds to an approximate mass of 2245 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 ⓘ

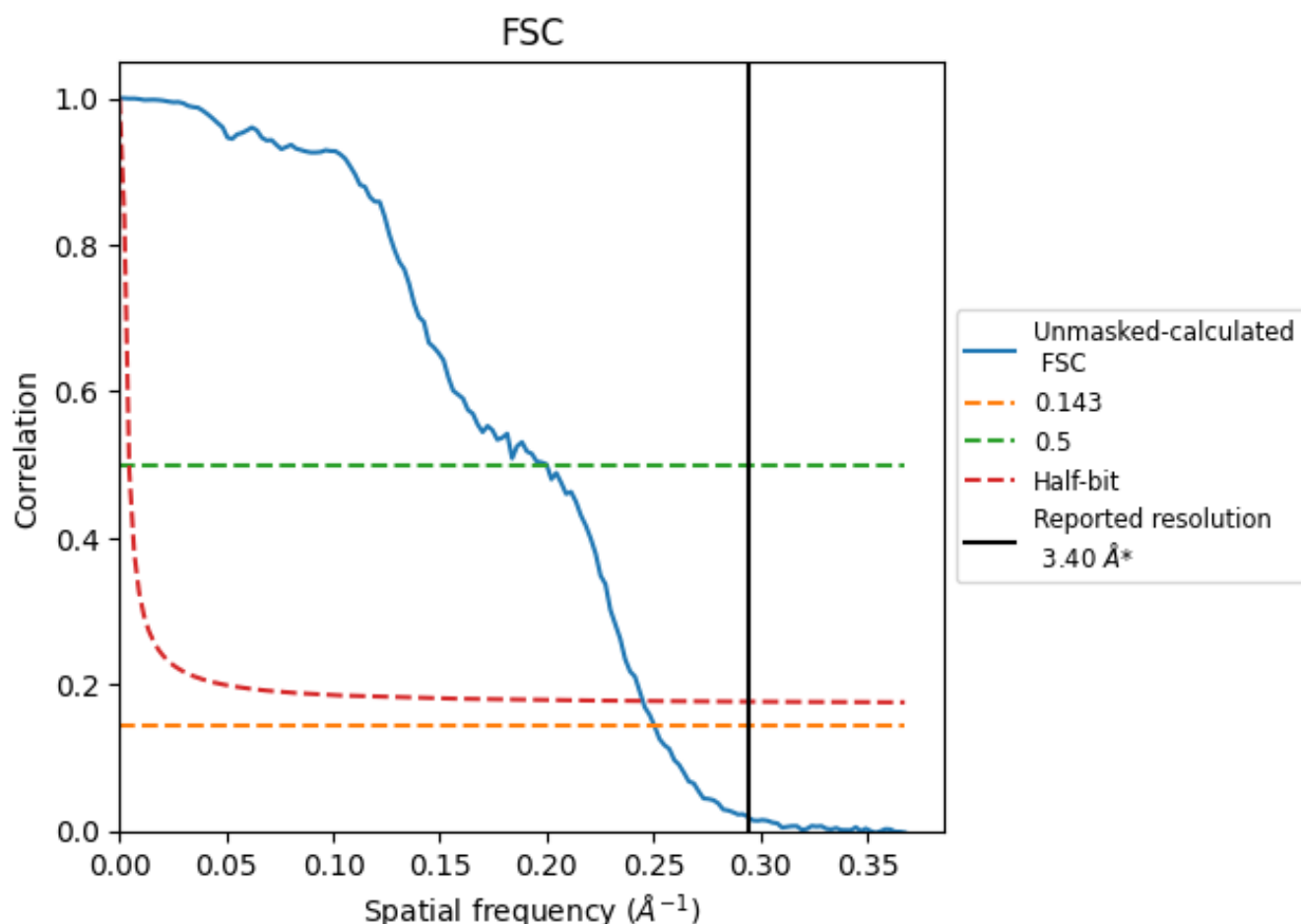


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

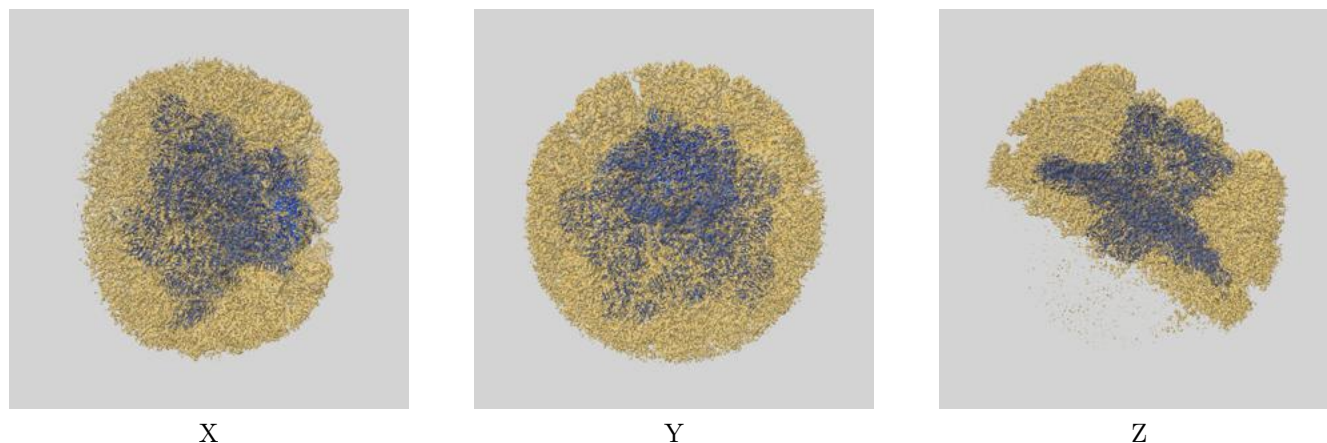
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	5.00	4.08

*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 3.99 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

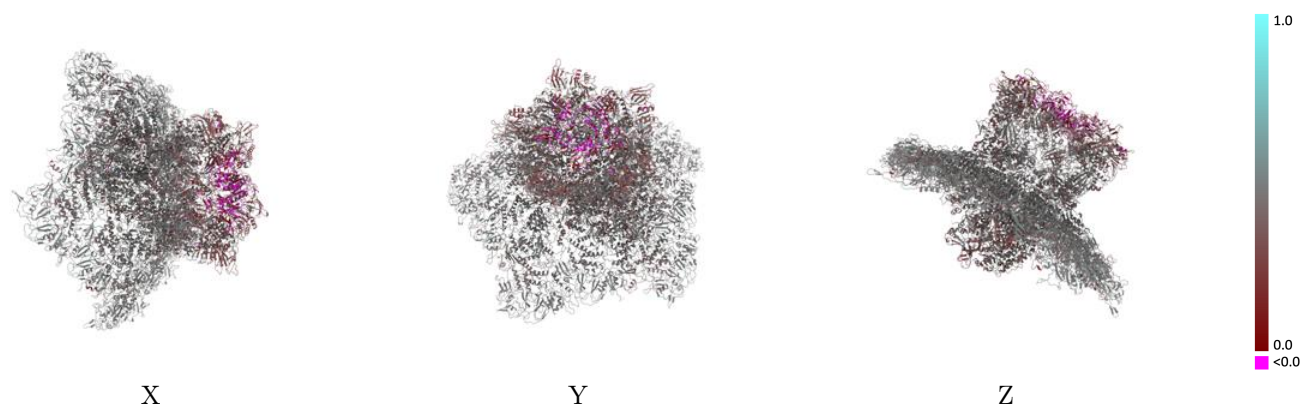
This section contains information regarding the fit between EMDB map EMD-33787 and PDB model 7YFE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



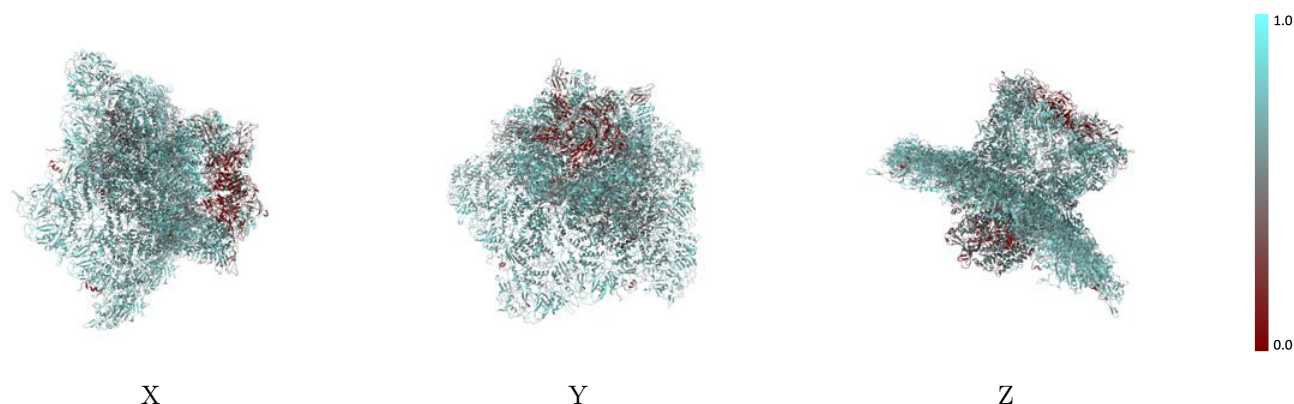
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



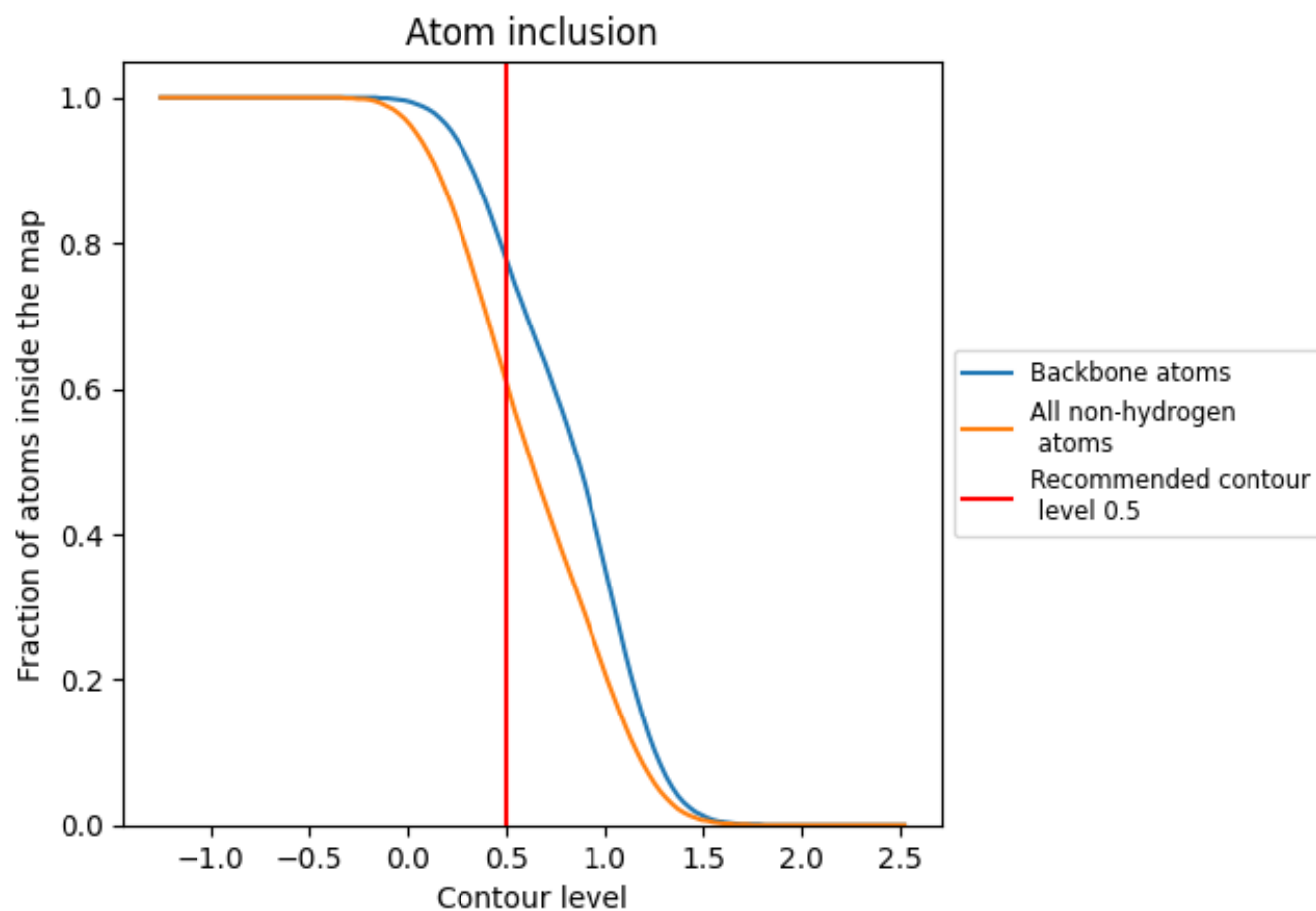
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.4220
1	 0.5350	 0.4410
2	 0.5270	 0.4310
3	 0.5320	 0.4280
4	 0.4540	 0.4180
5	 0.5060	 0.4270
A	 0.6800	 0.4630
B	 0.6730	 0.4610
C	 0.6700	 0.4560
D	 0.6690	 0.4580
E	 0.6700	 0.4590
H	 0.5620	 0.3630
I	 0.5620	 0.3600
J	 0.5630	 0.3630
K	 0.5630	 0.3590
L	 0.5690	 0.3620
M	 0.0640	 0.1960
N	 0.2290	 0.1290
R	 0.5310	 0.4190
T	 0.0880	 0.2270
U	 0.4350	 0.3950
a	 0.6580	 0.4640
b	 0.6570	 0.4620
c	 0.6470	 0.4570
d	 0.6510	 0.4570
e	 0.6640	 0.4640

