Full wwPDB EM Validation Report ⓘ

Jun 26, 2024 – 11:01 PM JST

PDB ID	:	7YEZ
EMDB ID	:	EMD-33779
Title	:	In situ structure of polymerase complex of mammalian reovirus in the reloaded state
Authors	:	Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.
Deposited on	:	2022-07-06
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:

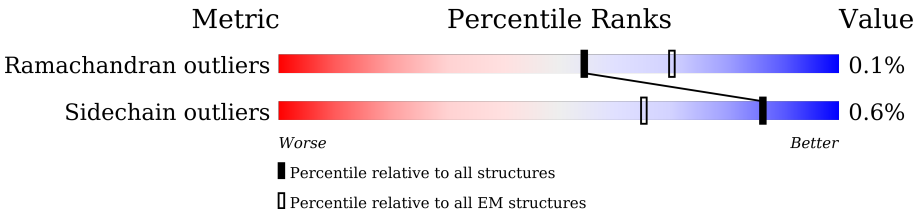
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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	154571	4023
Sidechain outliers	154315	3826

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	1	1275	11% 89%
1	2	1275	11% 89%
1	3	1275	11% 89%
1	4	1275	10% 90%
1	5	1275	11% 89%
1	A	1275	88% 12%
1	B	1275	83% 16%
1	C	1275	84% 15%
1	D	1275	81% 18%

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Mol	Chain	Length	Quality of chain
1	E	1275	82% 17%
1	a	1275	84% 15%
1	b	1275	85% 15%
1	c	1275	84% 15%
1	d	1275	84% 15%
1	e	1275	83% 16%
2	H	1289	29% 79% 21%
2	I	1289	31% 79% 21%
2	J	1289	29% 78% 21%
2	K	1289	28% 79% 21%
2	L	1289	28% 79% 21%
3	R	1267	19% 98%
4	U	736	17% 89% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 146162 atoms, of which 110 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	138	Total	C	N	O	S	0	0
			1026	610	195	218	3		
1	3	137	Total	C	N	O	S	0	0
			1023	608	195	217	3		
1	4	128	Total	C	N	O	S	0	0
			950	565	180	202	3		
1	5	139	Total	C	N	O	S	0	0
			1036	616	197	220	3		
1	A	1128	Total	C	N	O	S	0	0
			8868	5654	1510	1651	53		
1	B	1073	Total	C	N	O	S	0	0
			8442	5389	1431	1571	51		
1	C	1082	Total	C	N	O	S	0	0
			8535	5453	1444	1587	51		
1	D	1050	Total	C	N	O	S	0	0
			8300	5306	1403	1542	49		
1	E	1060	Total	C	N	O	S	0	0
			8376	5351	1419	1557	49		
1	a	1088	Total	C	N	O	S	0	0
			8580	5478	1457	1594	51		
1	b	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		
1	c	1080	Total	C	N	O	S	0	0
			8517	5444	1444	1578	51		
1	d	1085	Total	C	N	O	S	0	0
			8559	5467	1452	1589	51		
1	e	1075	Total	C	N	O	S	0	0
			8492	5422	1442	1578	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	I	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	J	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	K	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	L	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		

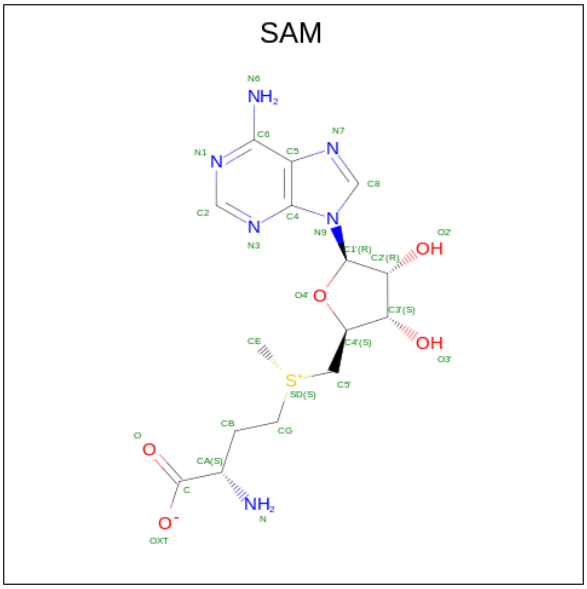
- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	1253	Total	C	N	O	S	0	0
			9913	6327	1697	1824	65		

- Molecule 4 is a protein called Mu-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	668	Total	C	N	O	S	0	0
			5322	3413	901	979	29		

- Molecule 5 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	H	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
5	I	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
5	J	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
5	K	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
5	L	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

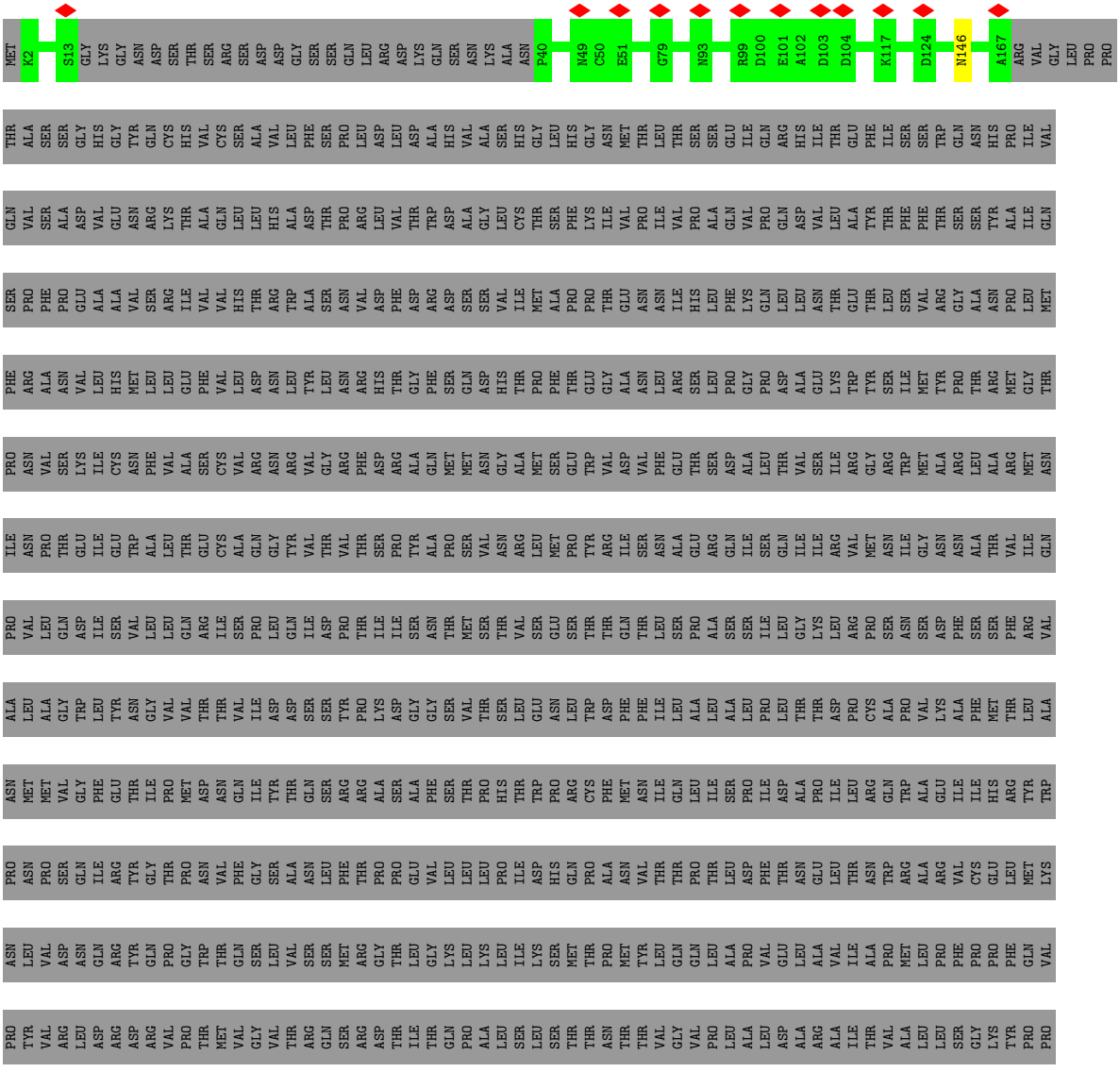
Mol	Chain	Residues	Atoms		AltConf
6	b	1	Total	Zn	0
			1	1	

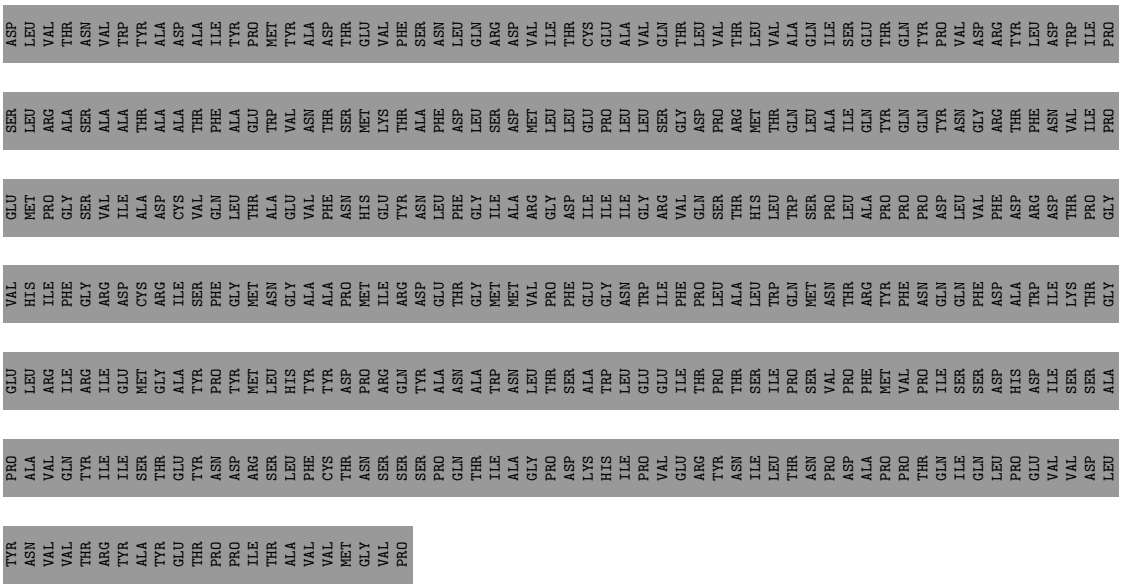
3 Residue-property plots (i)

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: RNA helicase

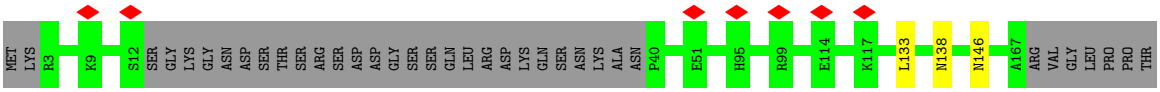
Chain 1:

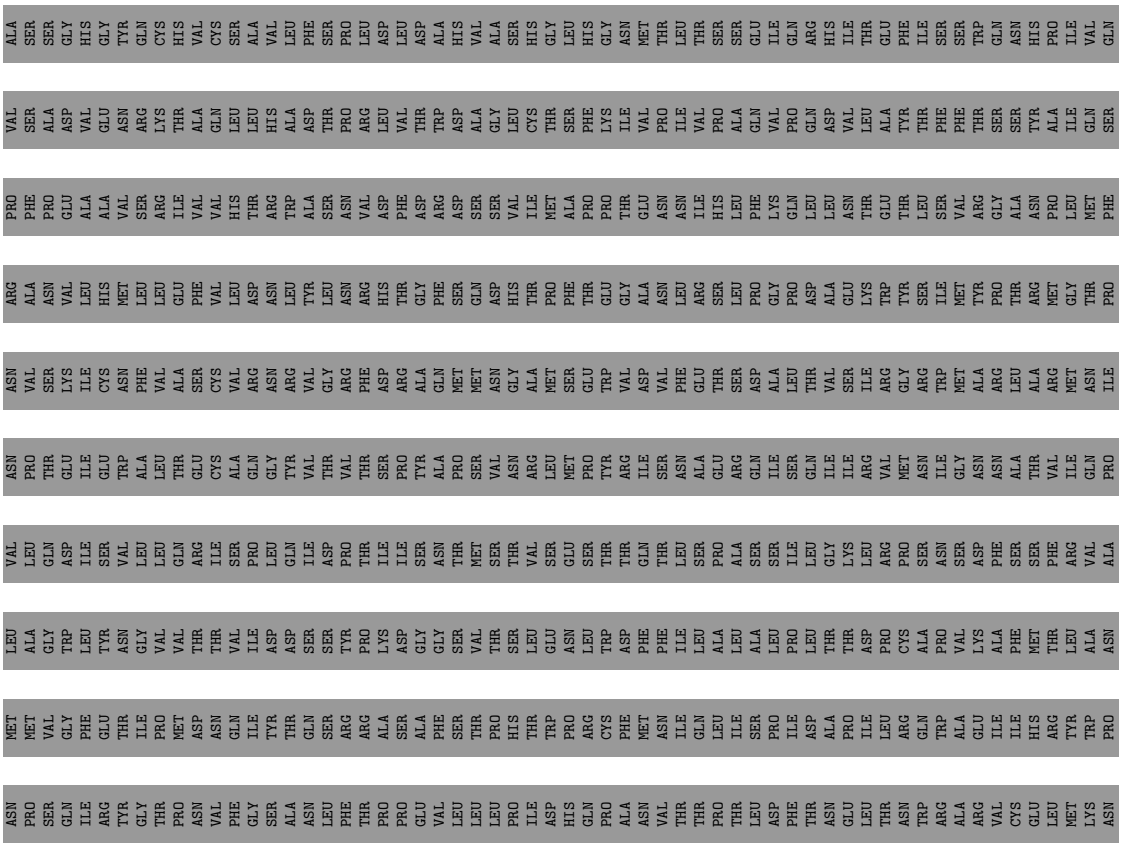


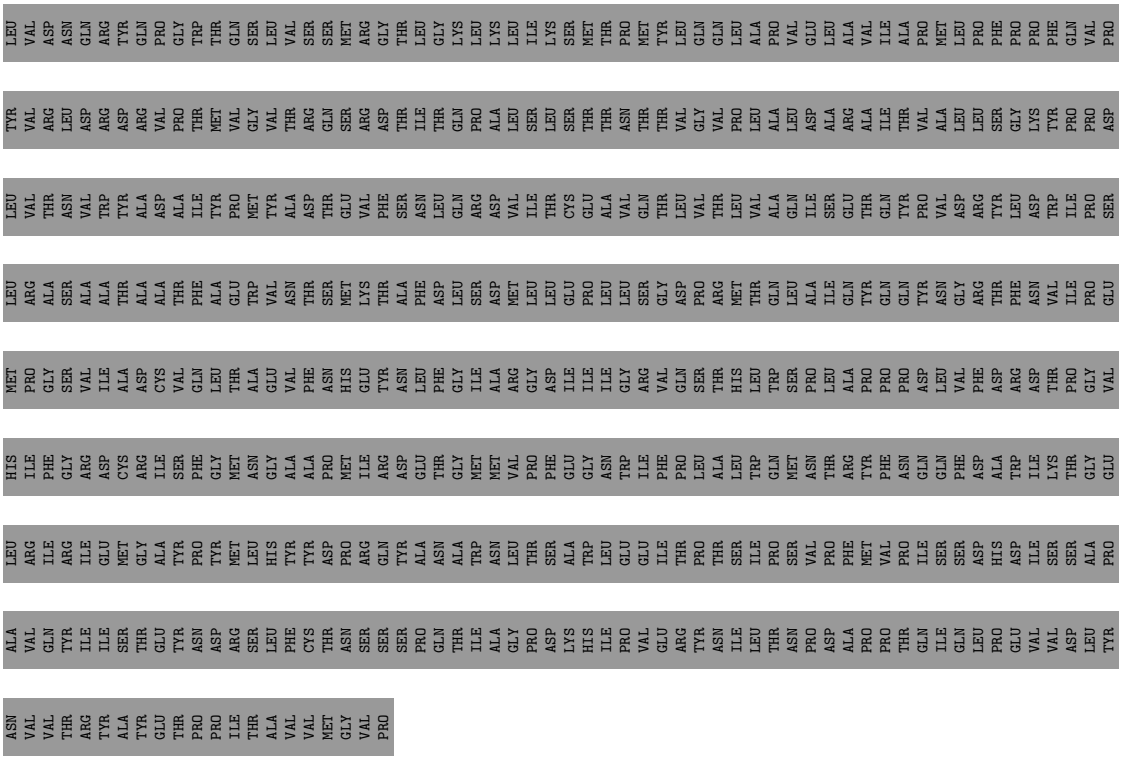


• Molecule 1: RNA helicase

Chain 2:

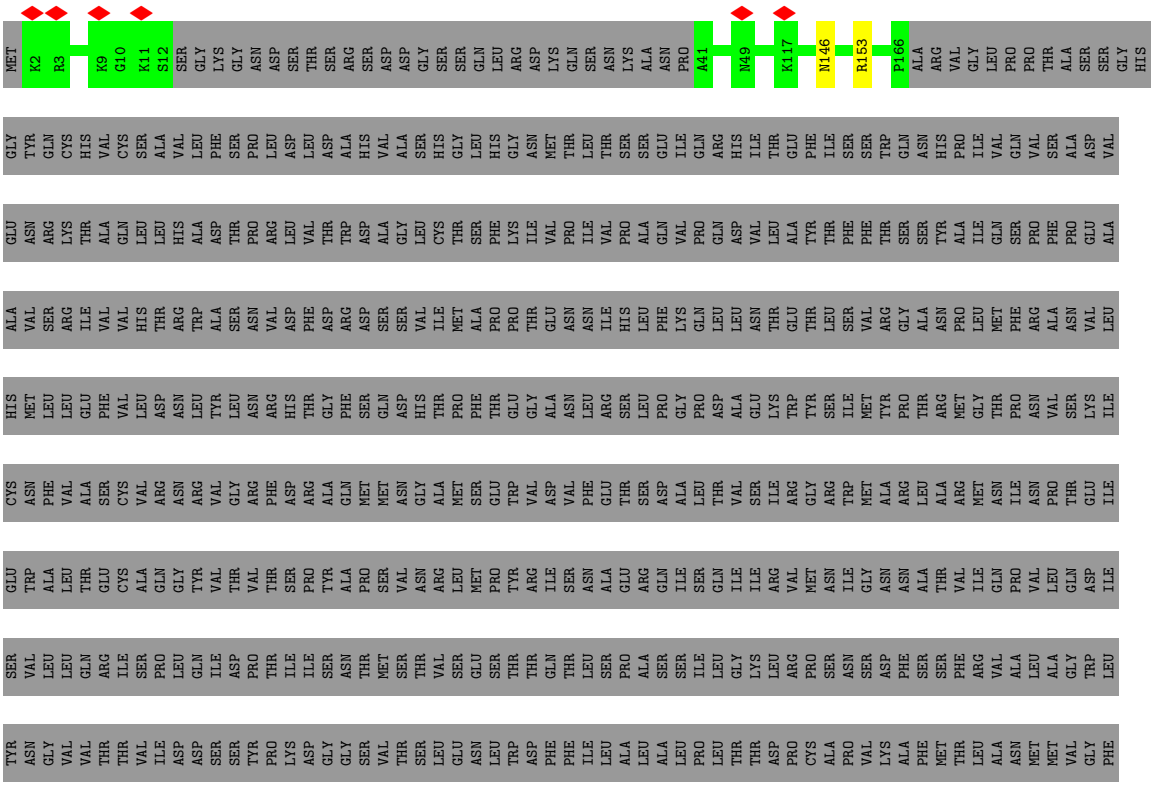


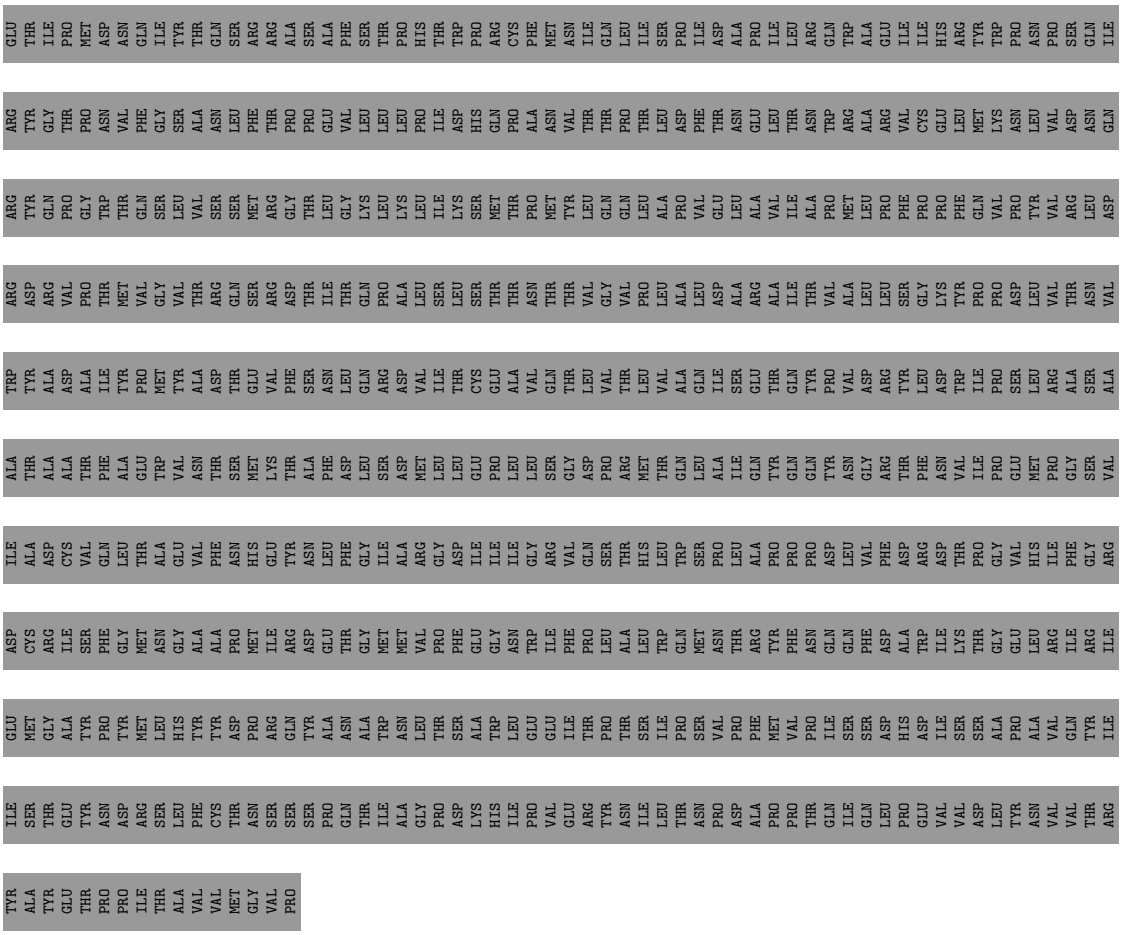




- Molecule 1: RNA helicase

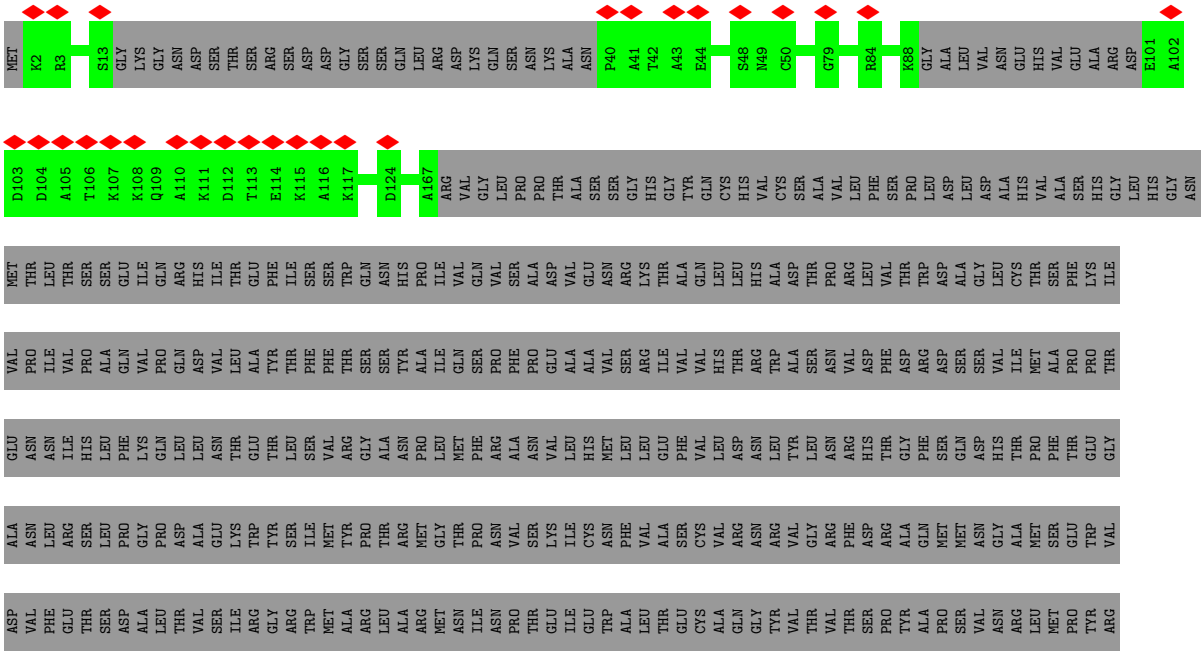
Chain 3:

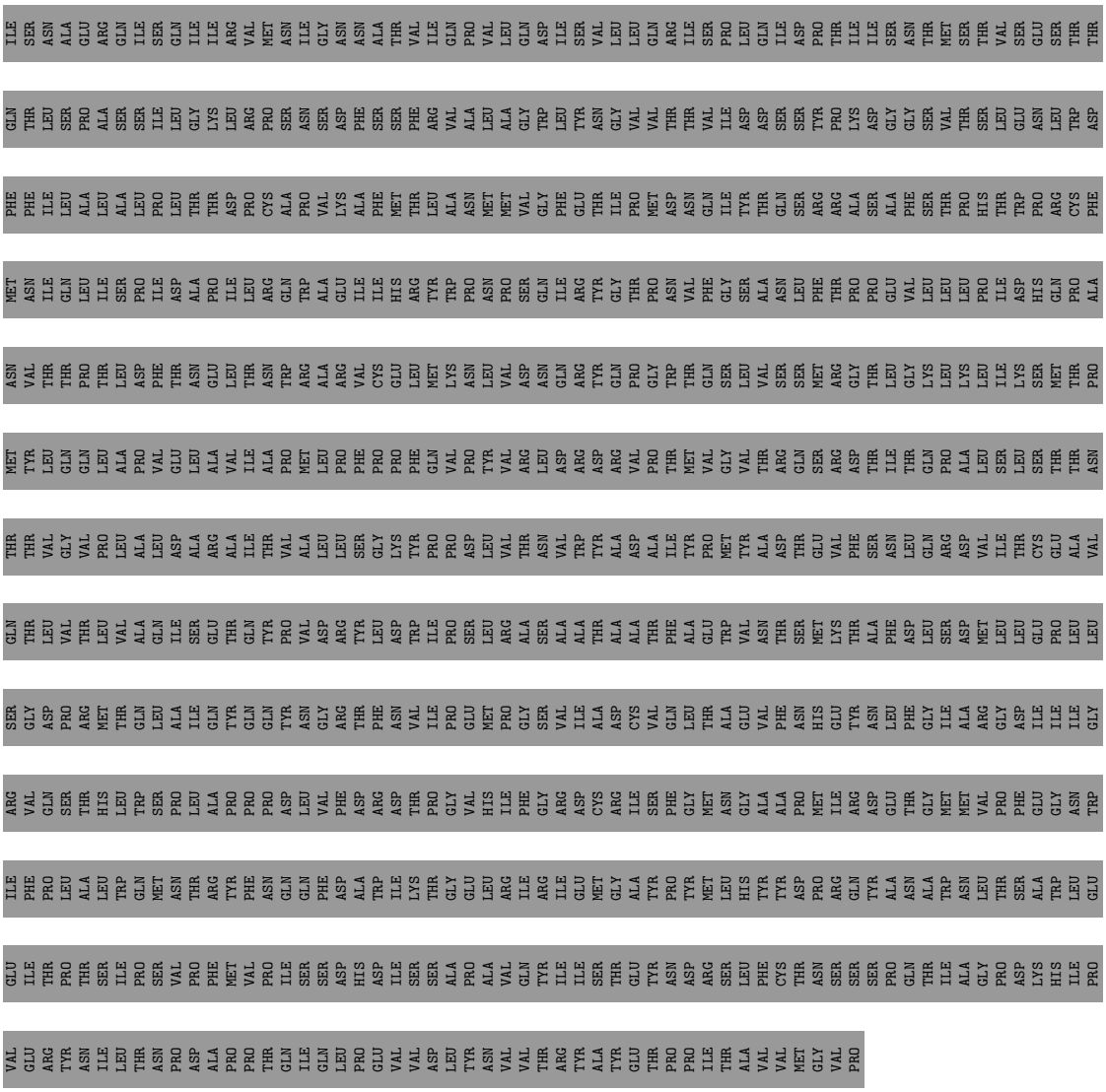




• Molecule 1: RNA helicase

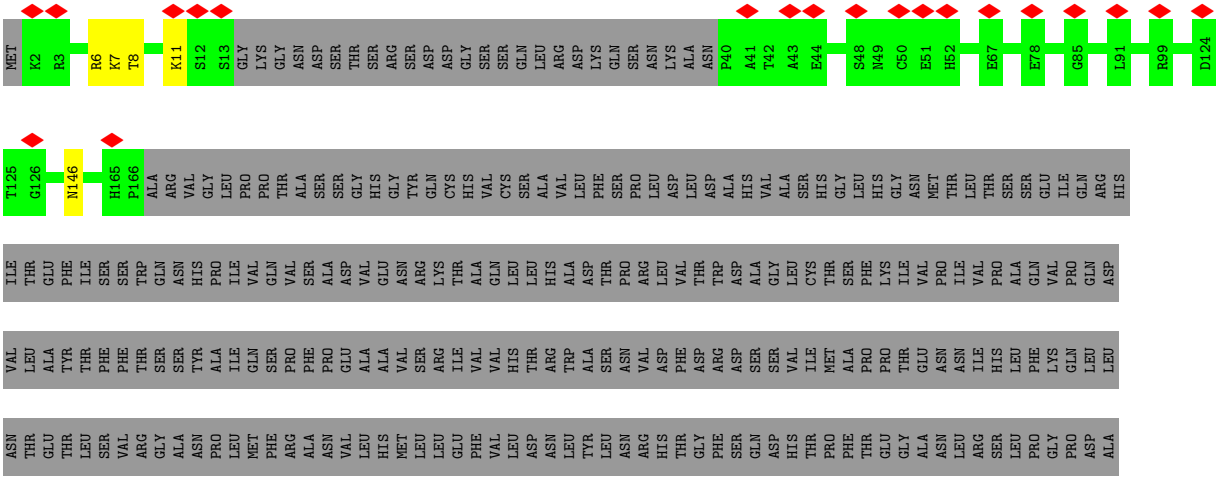
Chain 4:

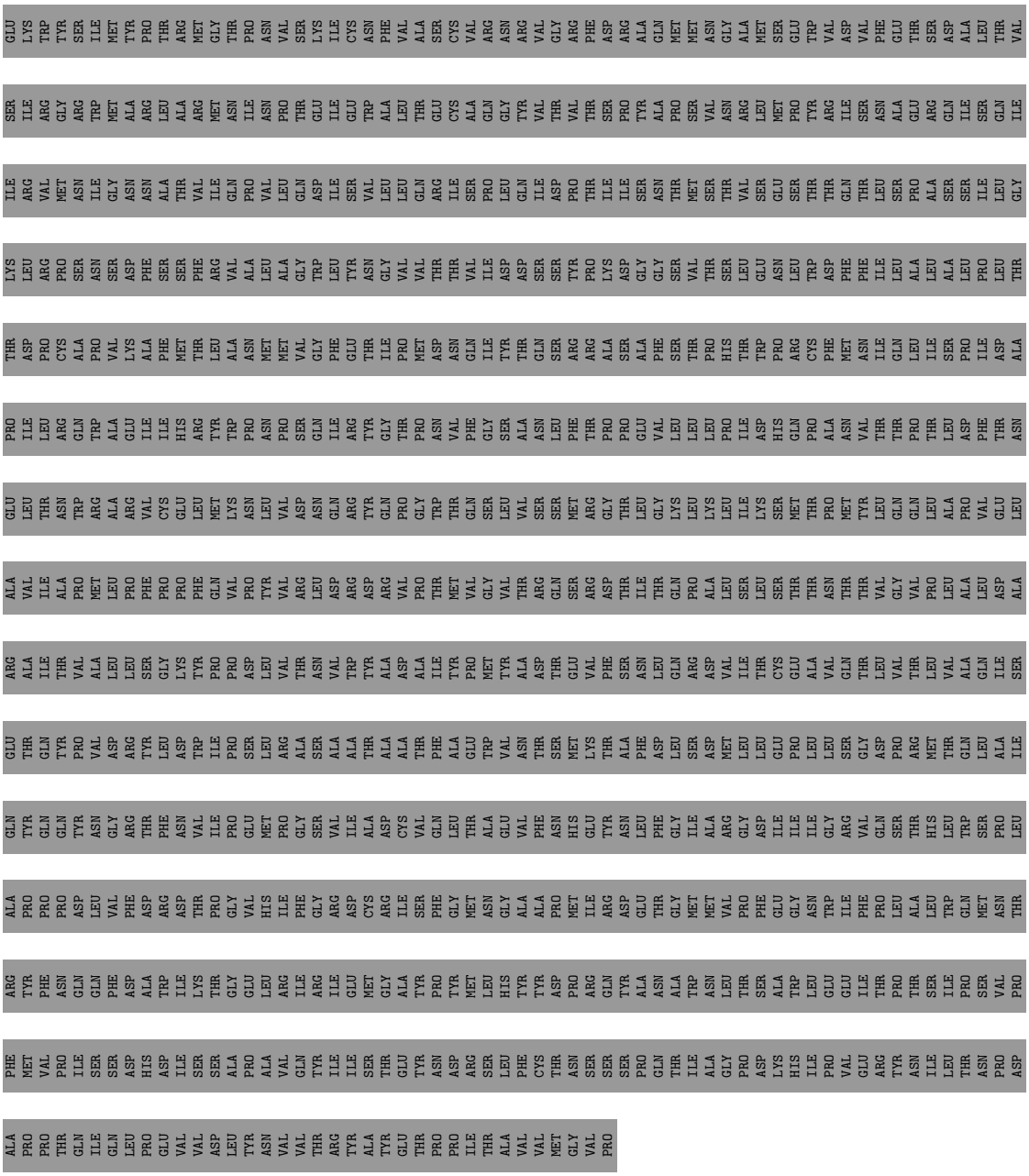




• Molecule 1: RNA helicase

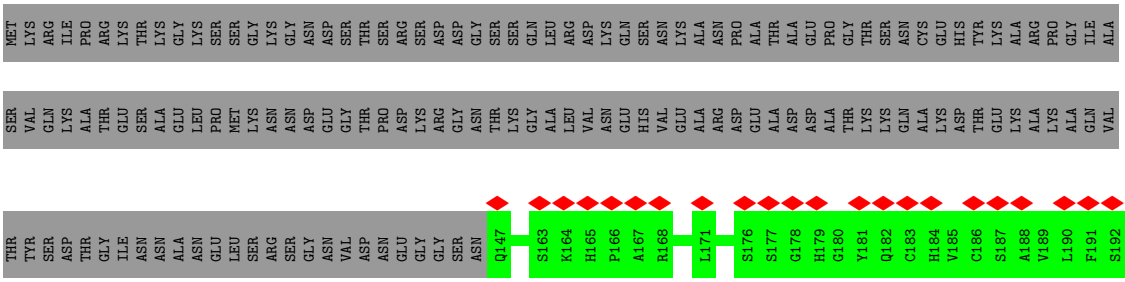
Chain 5:

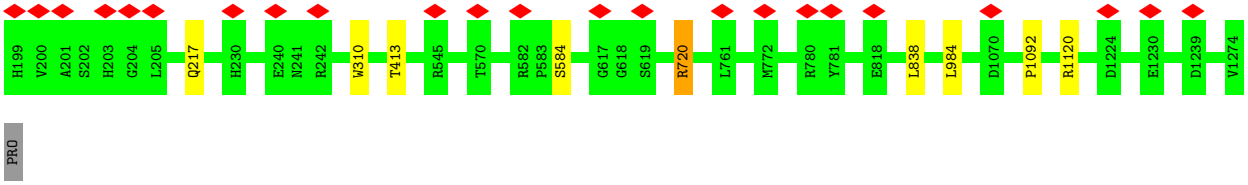




- Molecule 1: RNA helicase

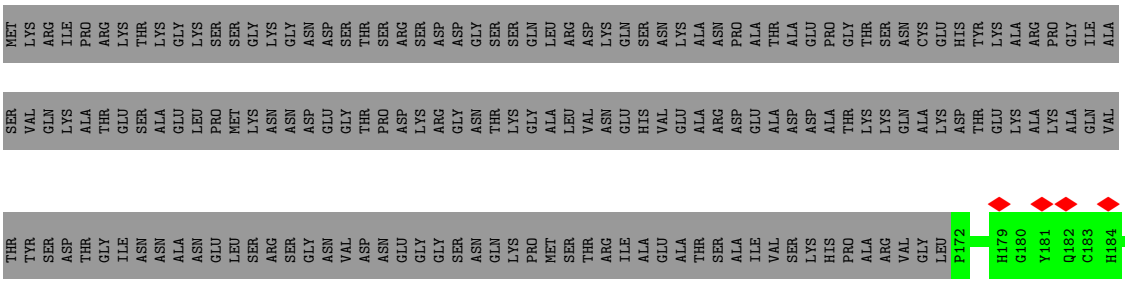
Chain A:





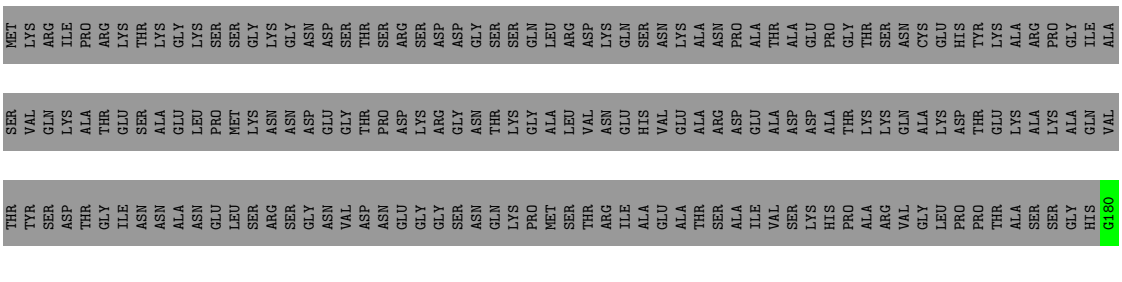
- Molecule 1: RNA helicase

Chain B:



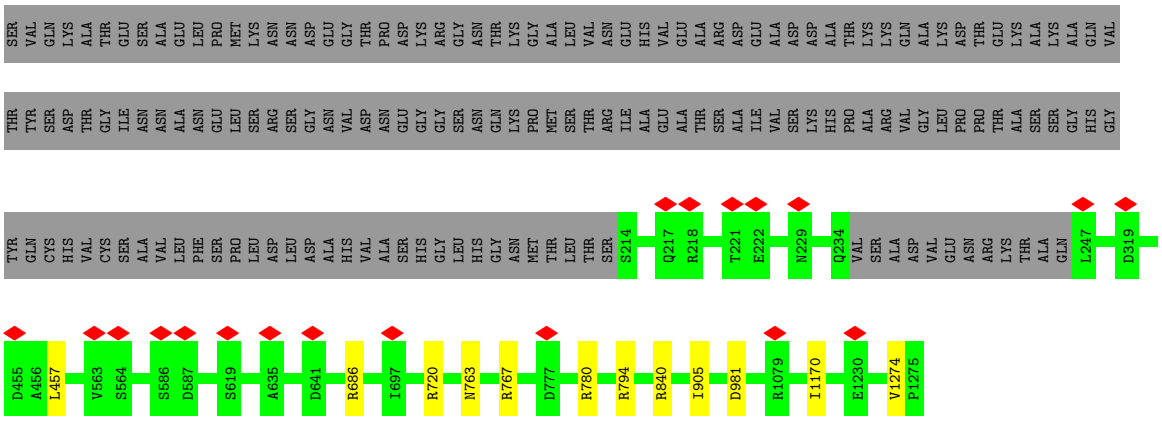
- Molecule 1: RNA helicase

Chain C:

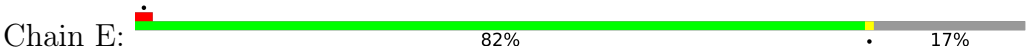


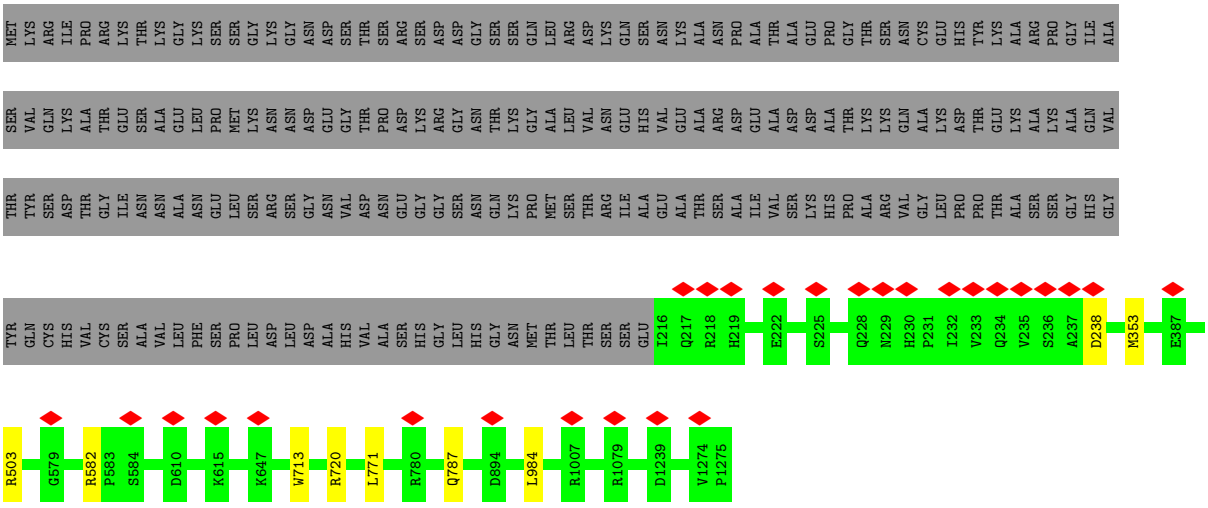
- Molecule 1: RNA helicase

Chain D:

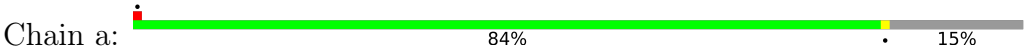


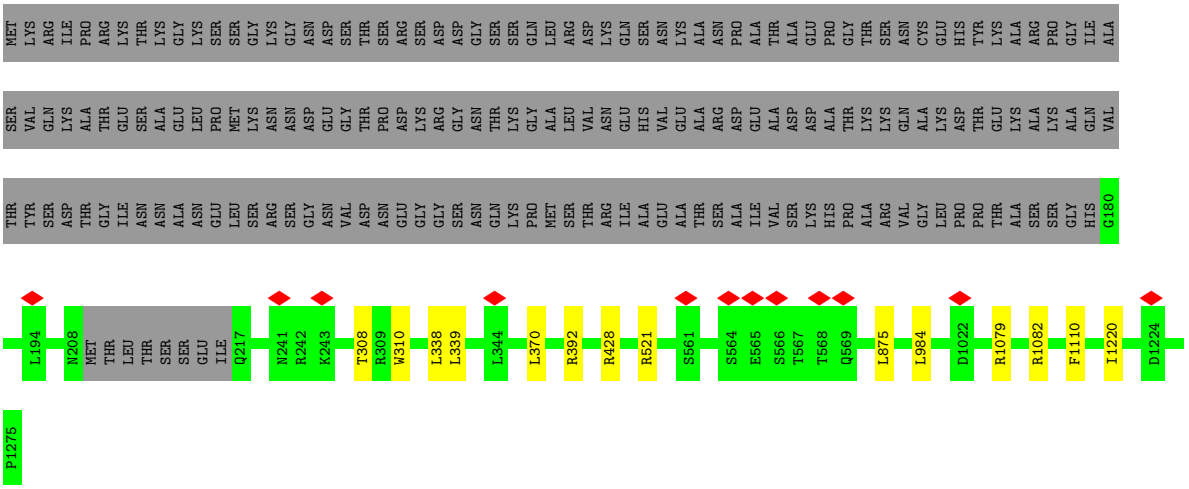
• Molecule 1: RNA helicase





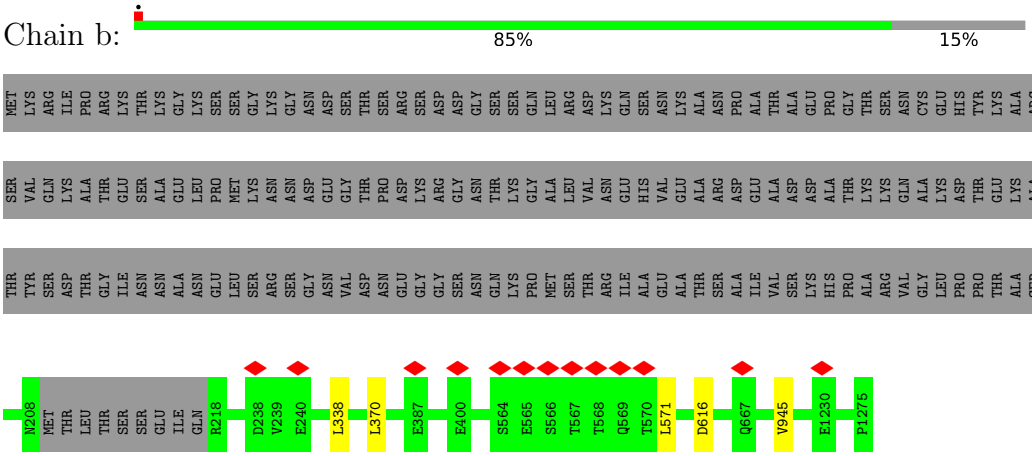
• Molecule 1: RNA helicase





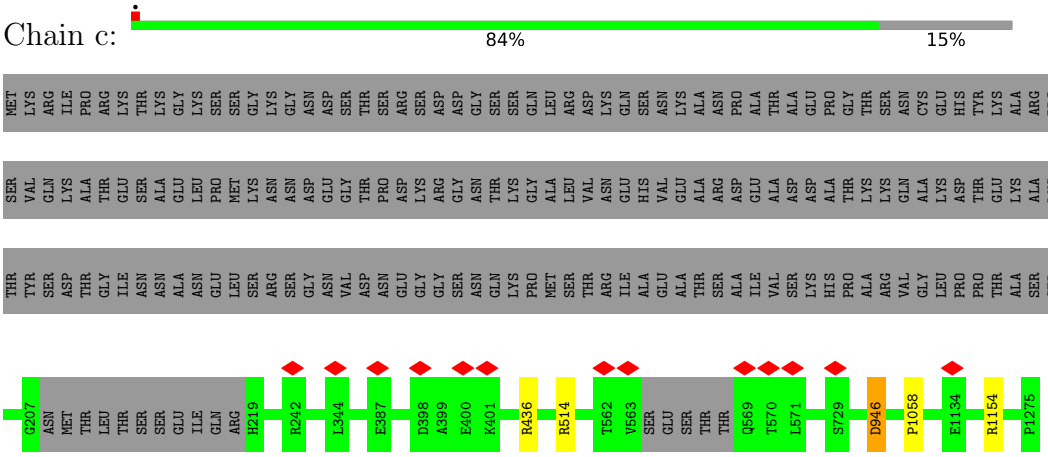
• Molecule 1: RNA helicase

Chain b:



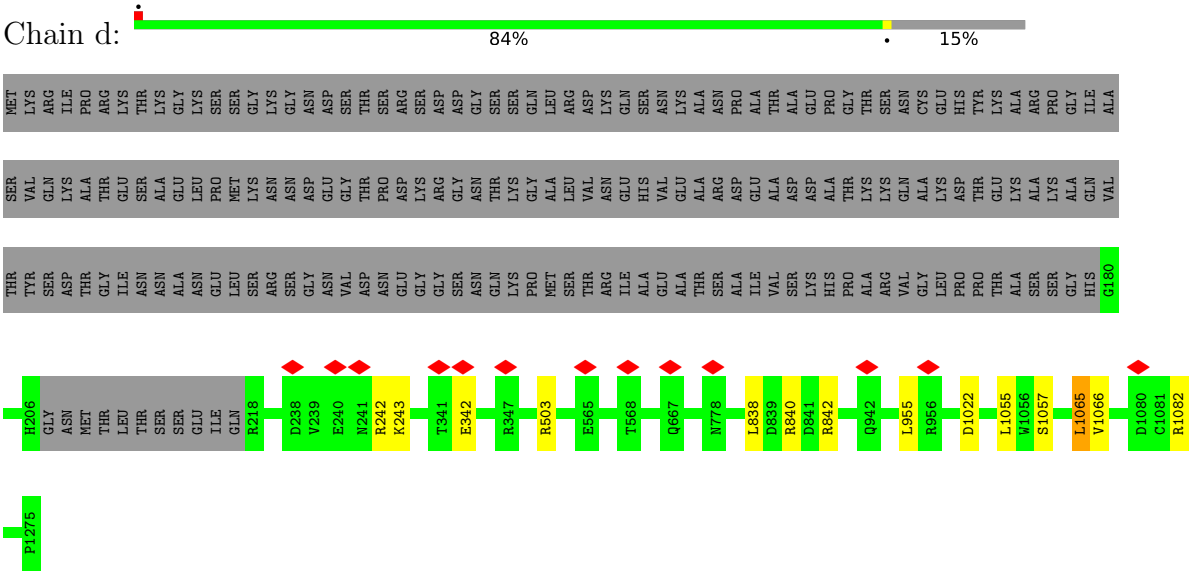
• Molecule 1: RNA helicase

Chain c:



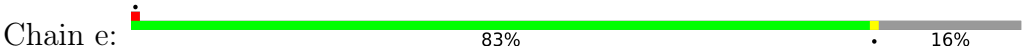
• Molecule 1: RNA helicase

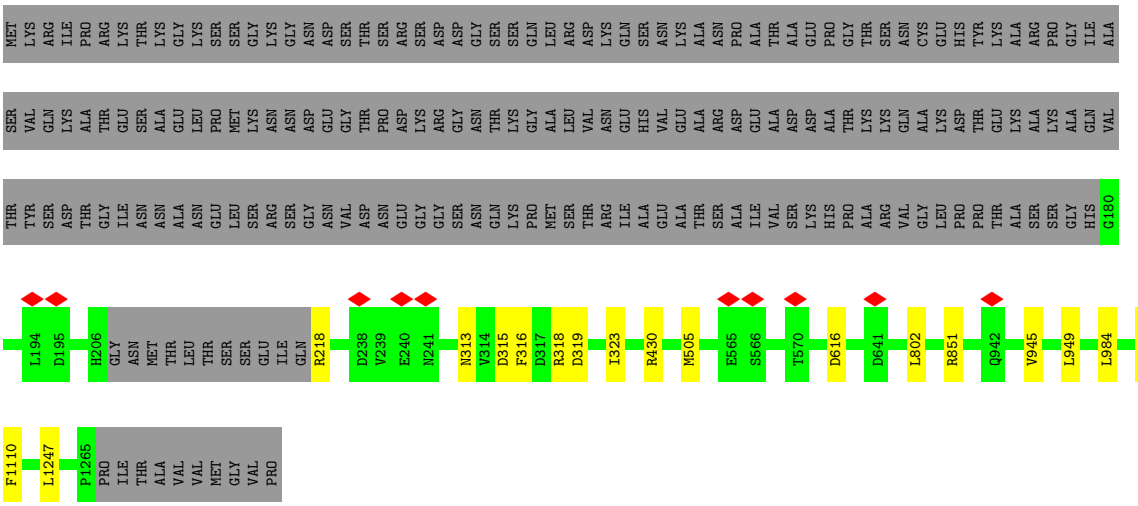
Chain d:



• Molecule 1: RNA helicase

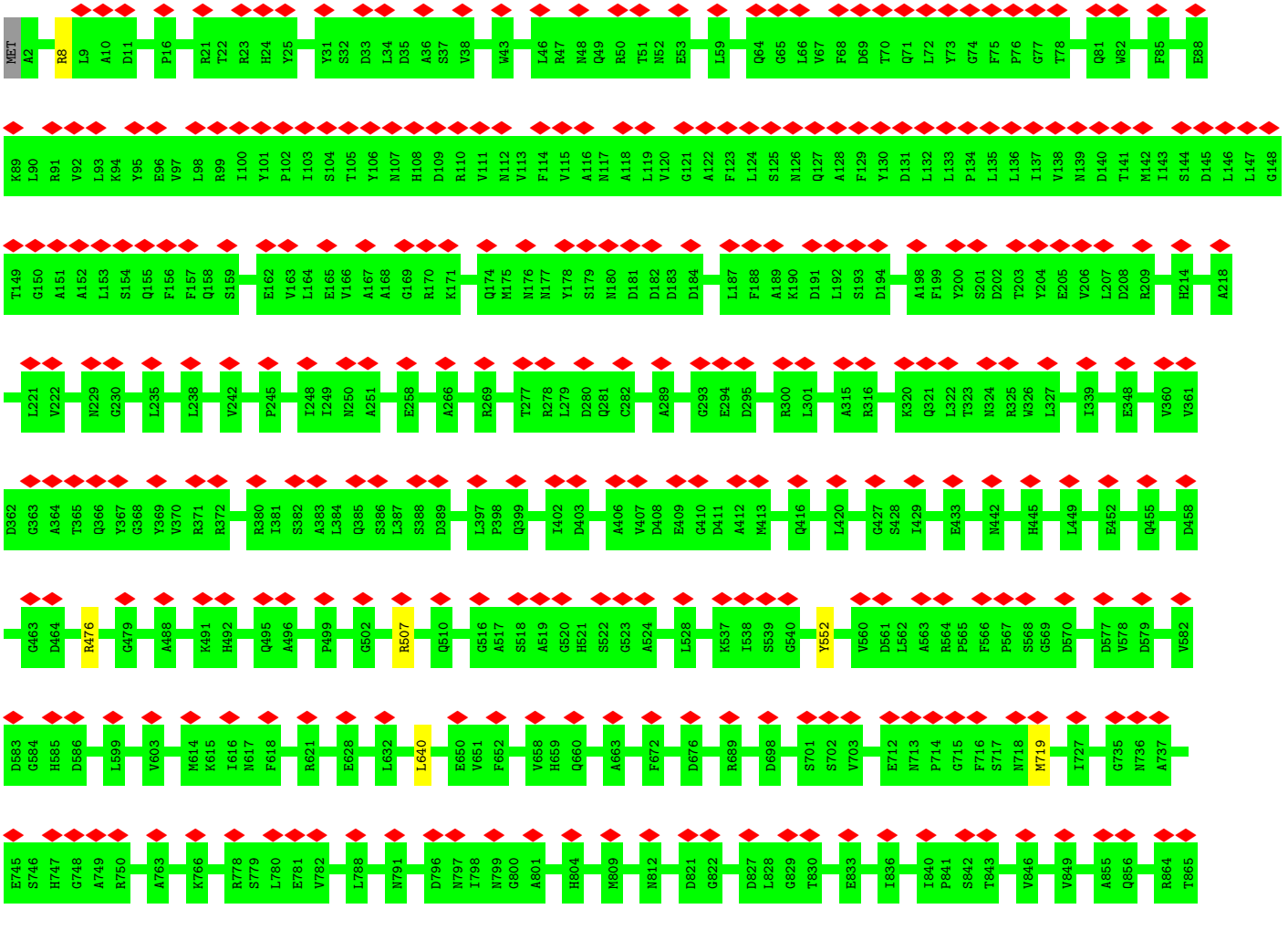
Chain e:

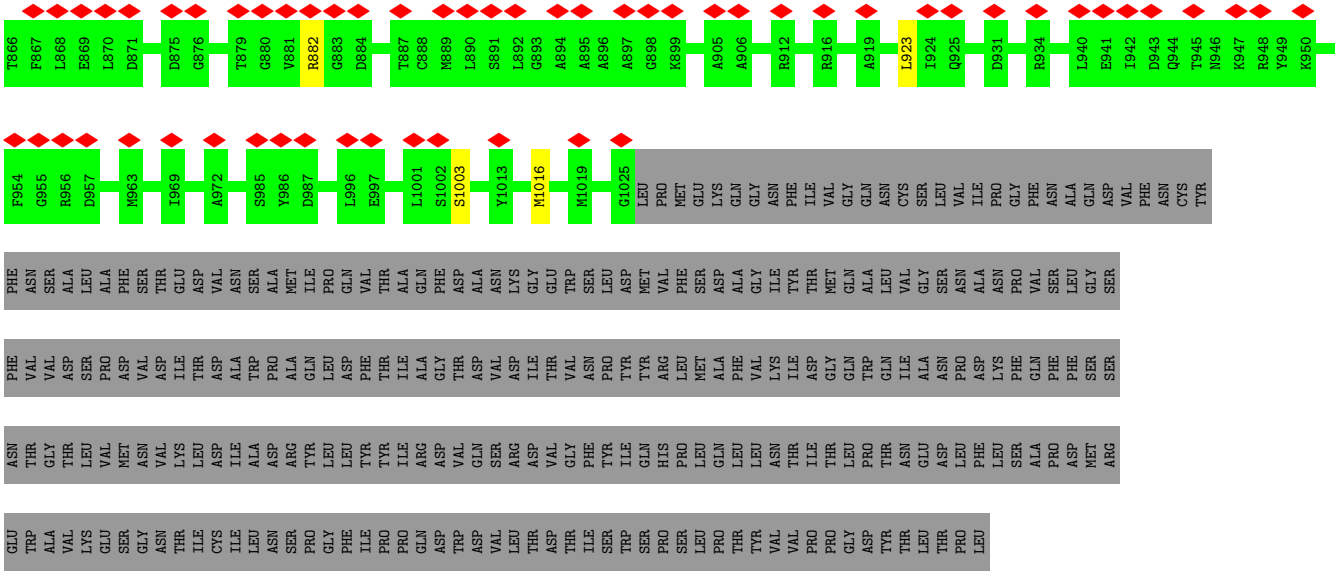




• Molecule 2: Lambda-2 protein

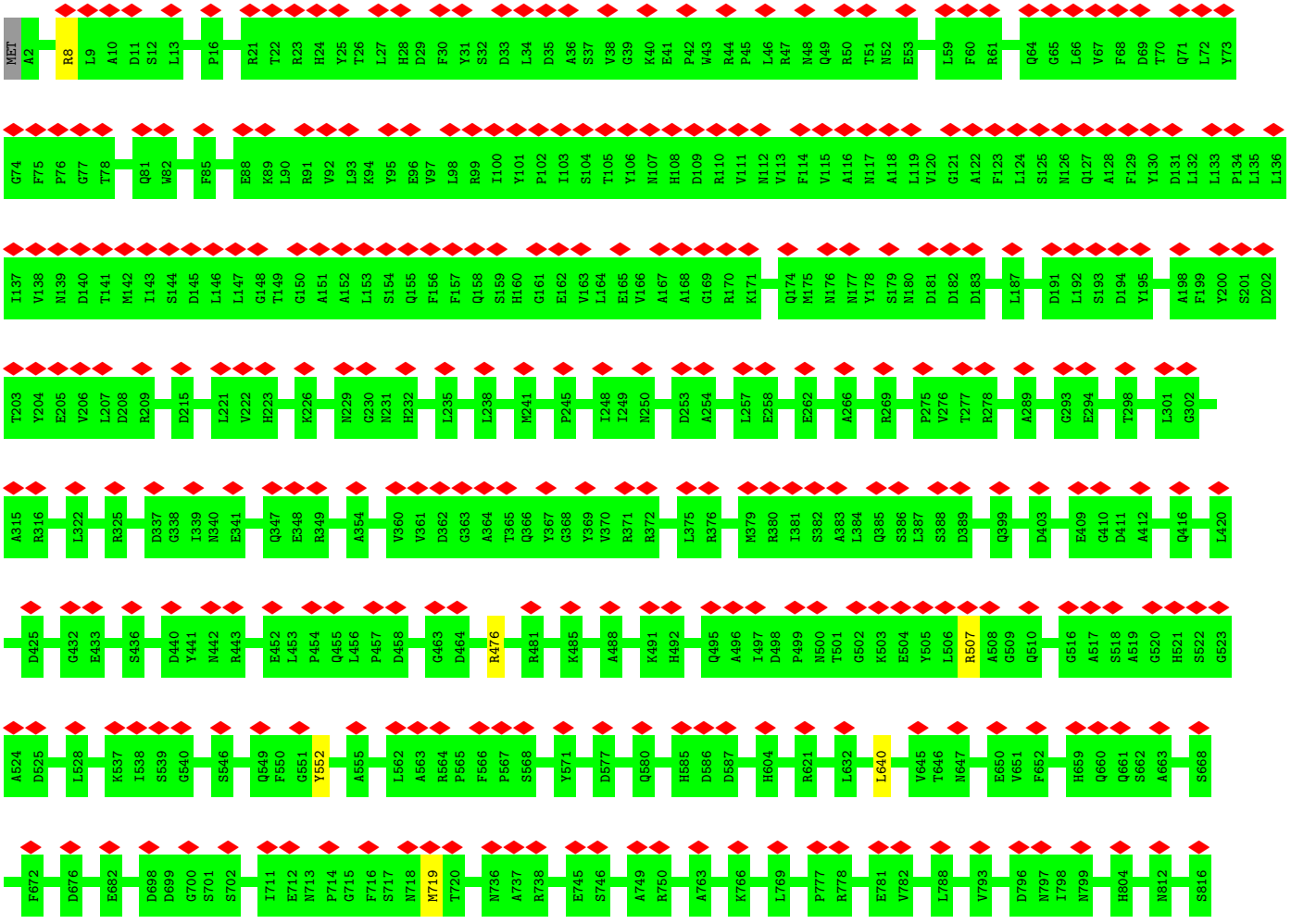
Chain H:

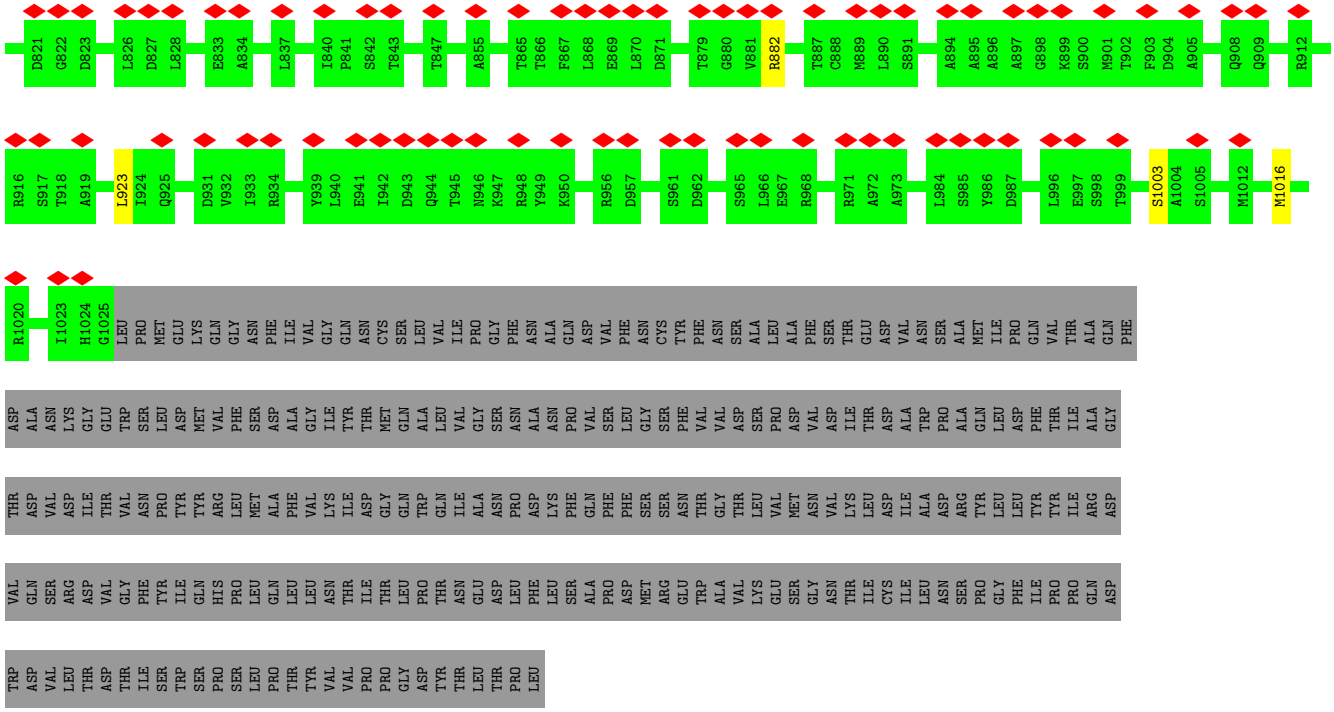




• Molecule 2: Lambda-2 protein

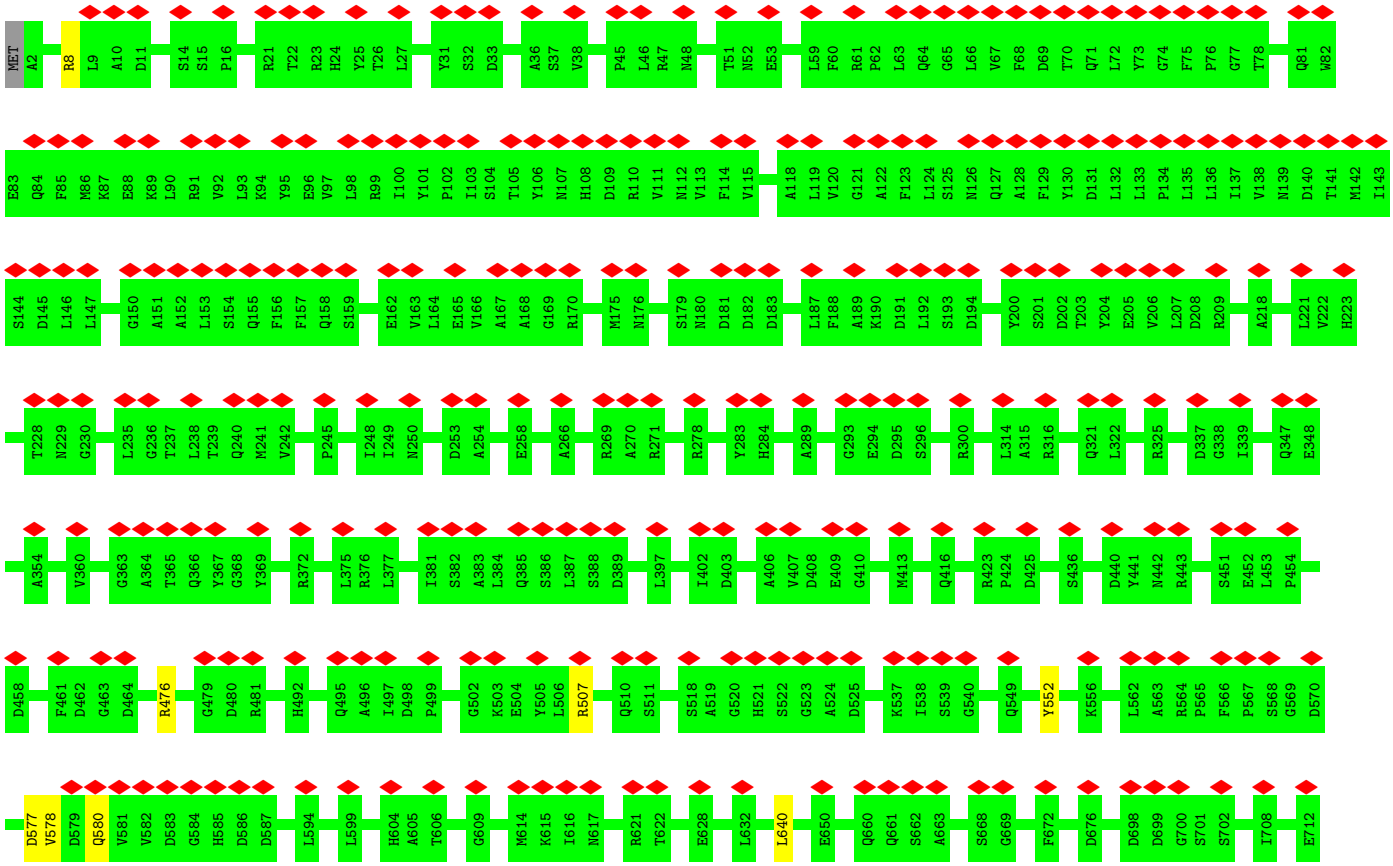
Chain I:

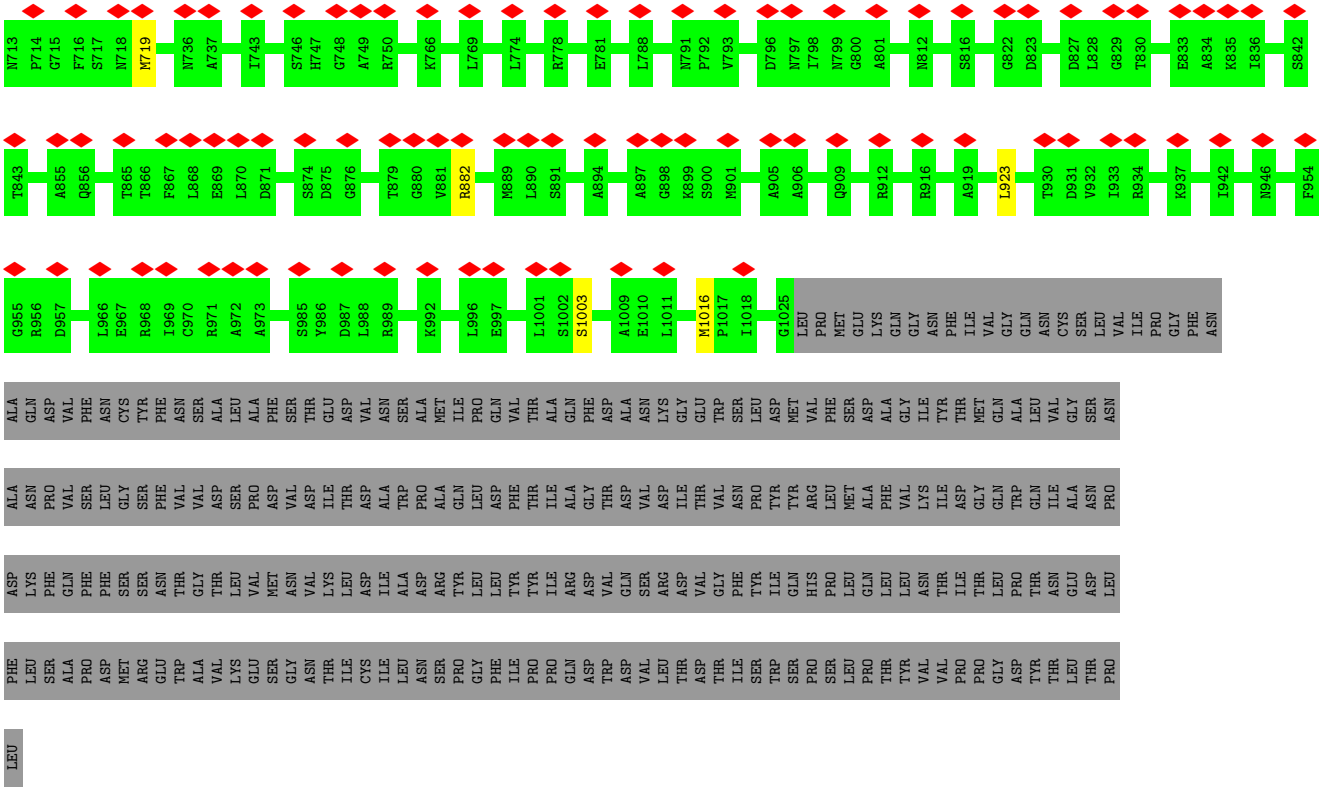




• Molecule 2: Lambda-2 protein

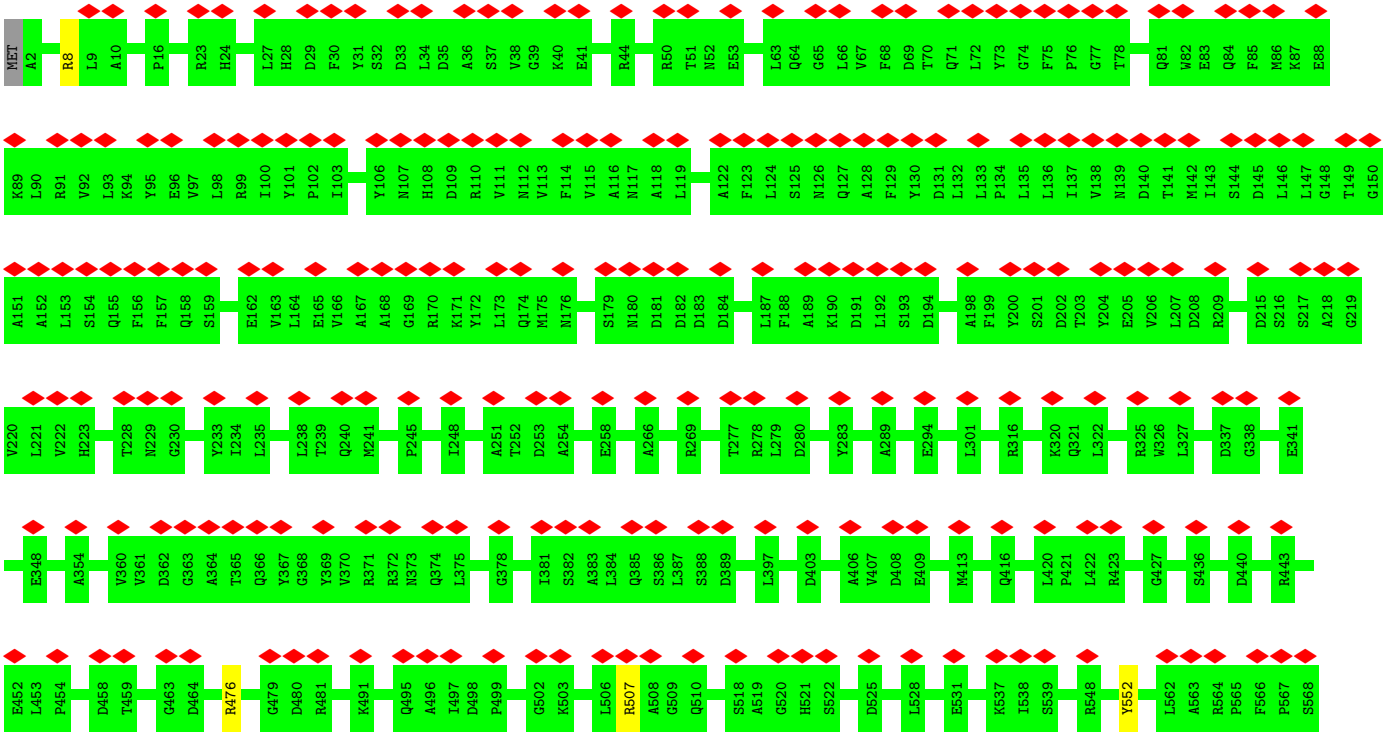
Chain J:

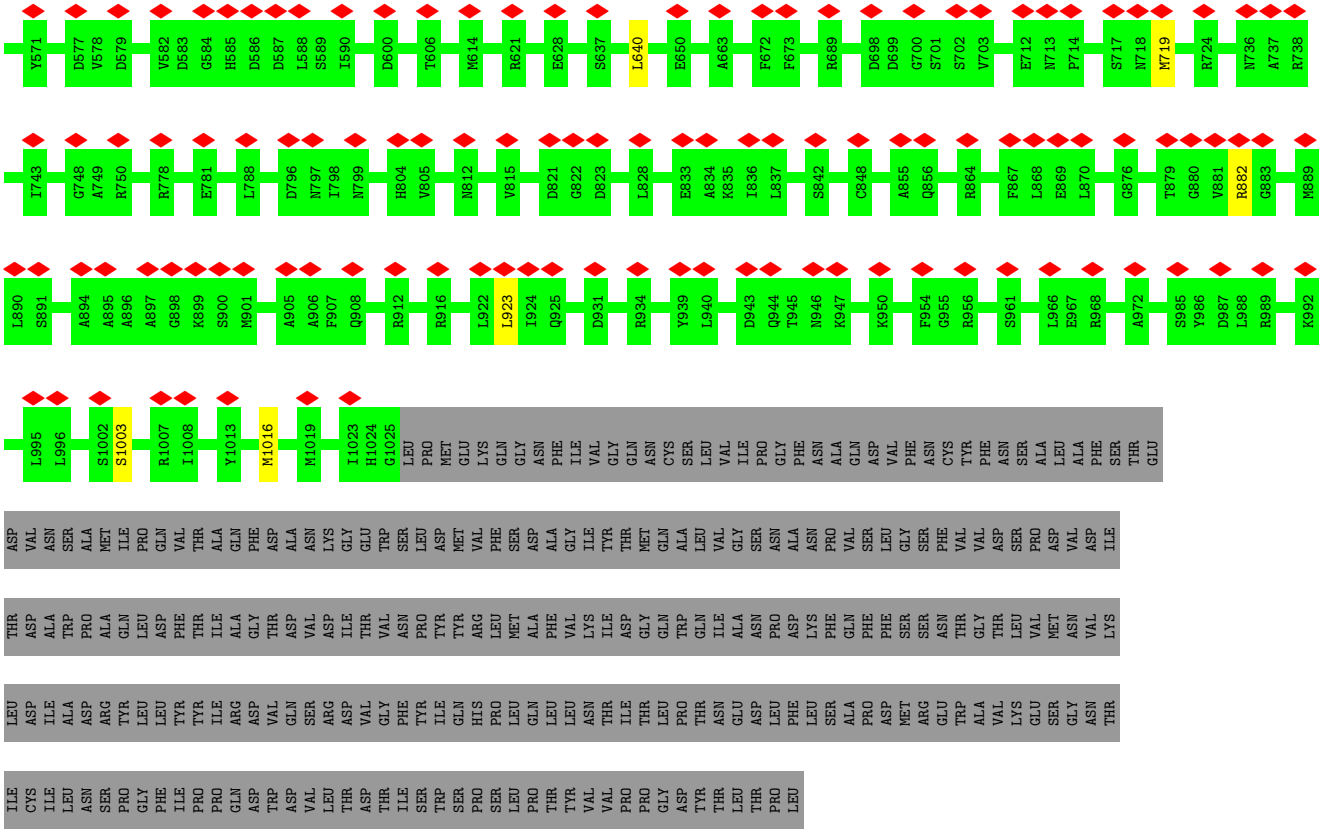




• Molecule 2: Lambda-2 protein

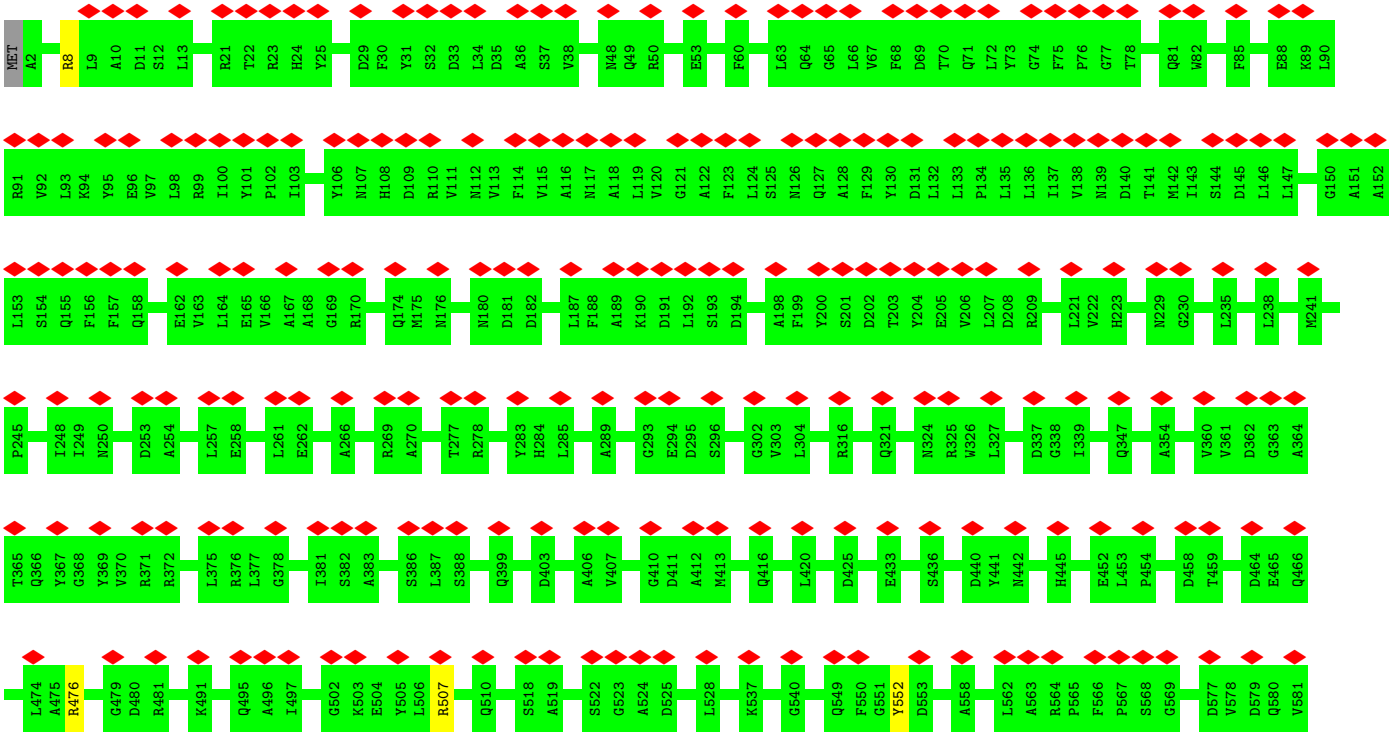
Chain K:

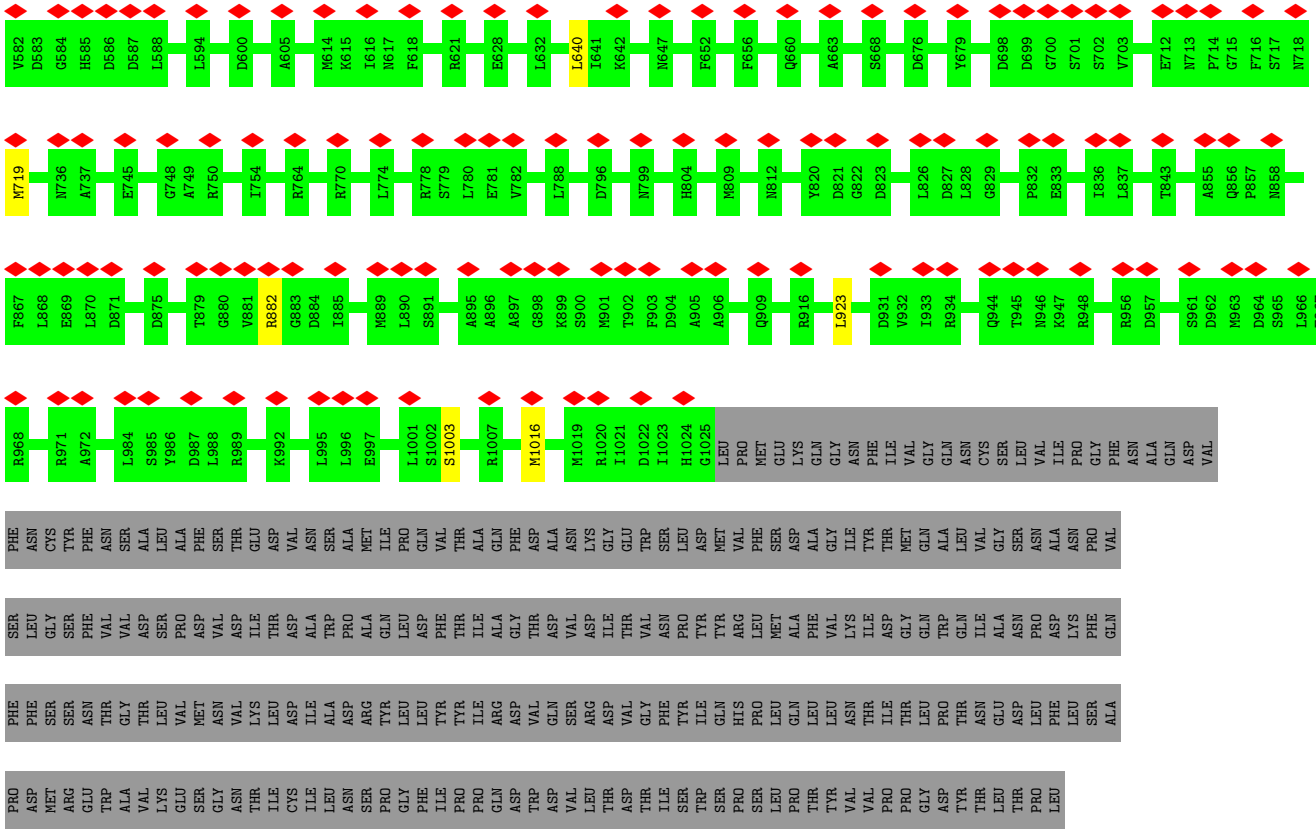




• Molecule 2: Lambda-2 protein

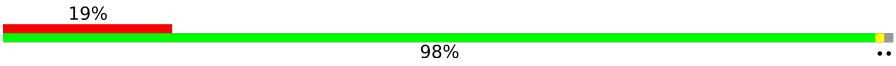
Chain L:

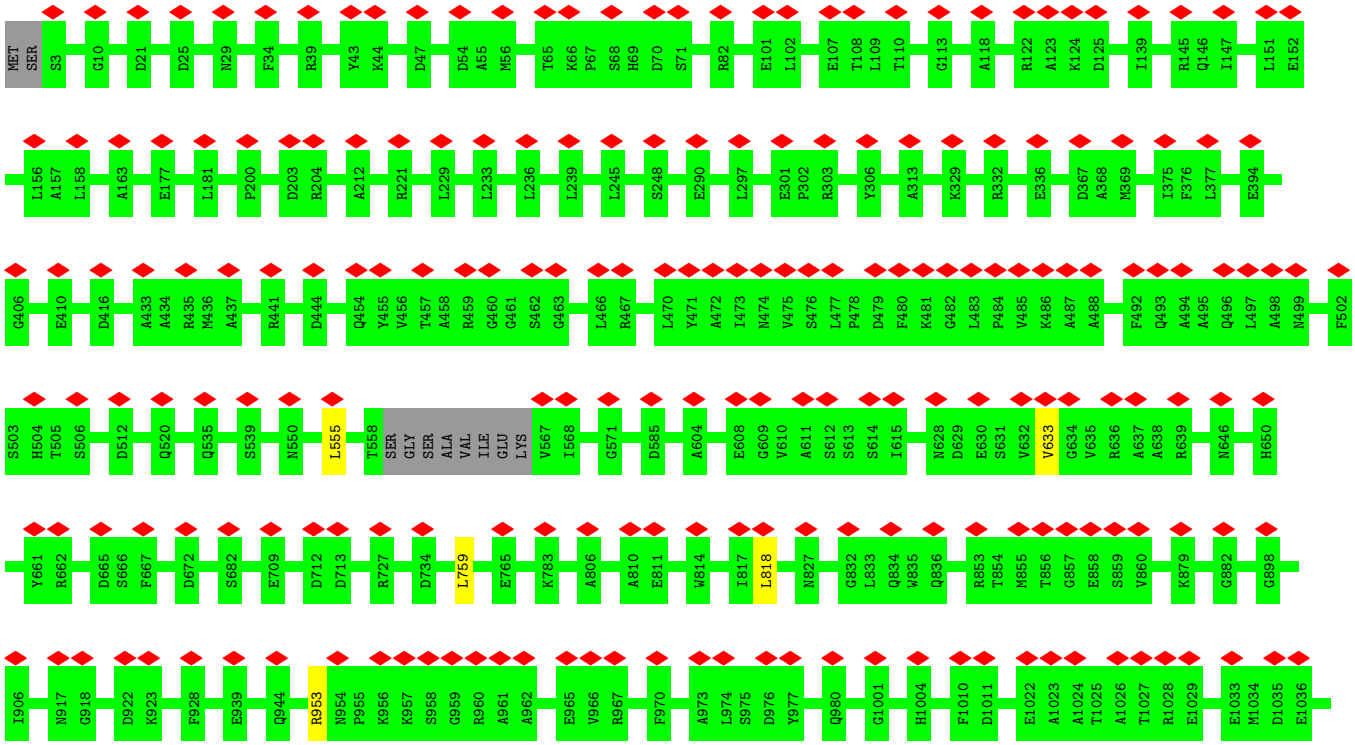


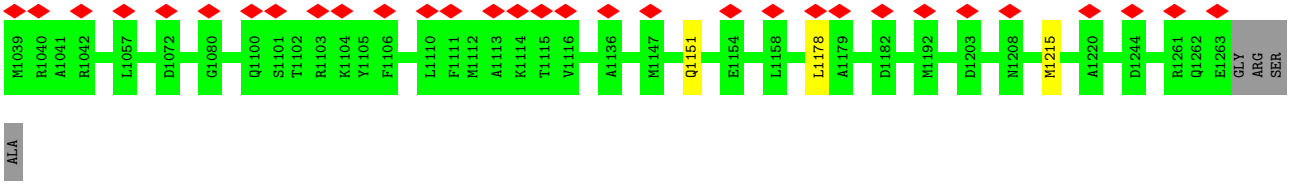


• Molecule 3: RNA-directed RNA polymerase

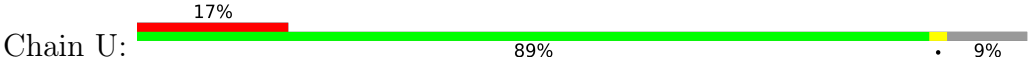
Chain R:







• Molecule 4: Mu-2 protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50491	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.244	Depositor
Minimum map value	-1.209	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, SAM

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	0.35	0/1052	0.58	0/1413
1	2	0.38	0/1037	0.60	1/1394 (0.1%)
1	3	0.36	0/1033	0.55	1/1387 (0.1%)
1	4	0.34	0/959	0.58	0/1285
1	5	0.37	0/1047	0.60	0/1406
1	A	0.42	0/9107	0.62	3/12474 (0.0%)
1	B	0.43	0/8671	0.63	3/11878 (0.0%)
1	C	0.42	1/8765 (0.0%)	0.62	1/12006 (0.0%)
1	D	0.43	0/8526	0.65	6/11680 (0.1%)
1	E	0.43	0/8603	0.63	2/11786 (0.0%)
1	a	0.41	0/8813	0.64	6/12073 (0.0%)
1	b	0.41	0/8804	0.62	4/12061 (0.0%)
1	c	0.41	0/8749	0.62	3/11985 (0.0%)
1	d	0.41	0/8792	0.63	3/12045 (0.0%)
1	e	0.42	0/8723	0.64	6/11948 (0.1%)
2	H	0.32	0/8275	0.59	2/11284 (0.0%)
2	I	0.32	0/8275	0.59	2/11284 (0.0%)
2	J	0.32	0/8275	0.59	2/11284 (0.0%)
2	K	0.32	0/8275	0.59	2/11284 (0.0%)
2	L	0.32	0/8275	0.59	2/11284 (0.0%)
3	R	0.40	0/10166	0.65	6/13806 (0.0%)
4	U	0.39	0/5439	0.68	4/7385 (0.1%)
All	All	0.39	1/149661 (0.0%)	0.62	59/204432 (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
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	a	0	2
1	b	0	1
1	c	0	1
1	d	0	4
1	e	0	2
4	U	0	1
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	PRO	C-N	-5.22	1.22	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	514	ARG	NE-CZ-NH2	12.79	126.69	120.30
1	D	1170	ILE	C-N-CA	9.91	146.47	121.70
1	B	1170	ILE	C-N-CA	7.87	141.38	121.70
1	c	514	ARG	NH1-CZ-NH2	-7.78	110.84	119.40
1	b	571	LEU	CA-CB-CG	7.70	133.02	115.30
3	R	555	LEU	CA-CB-CG	7.38	132.26	115.30
1	e	318	ARG	N-CA-C	-7.38	91.09	111.00
3	R	1215	MET	CA-CB-CG	7.37	125.83	113.30
1	E	984	LEU	CA-CB-CG	7.28	132.04	115.30
1	E	713	TRP	N-CA-C	-6.97	92.19	111.00
1	a	370	LEU	CA-CB-CG	6.96	131.31	115.30
1	a	338	LEU	CA-CB-CG	6.85	131.05	115.30
1	a	875	LEU	CA-CB-CG	6.54	130.33	115.30
3	R	818	LEU	CA-CB-CG	6.35	129.91	115.30
4	U	112	LEU	CA-CB-CG	6.35	129.90	115.30
1	D	686	ARG	CG-CD-NE	-6.29	98.59	111.80
1	e	949	LEU	CA-CB-CG	6.08	129.28	115.30
1	b	370	LEU	CA-CB-CG	6.07	129.27	115.30
1	C	543	LEU	CA-CB-CG	6.04	129.18	115.30
1	A	984	LEU	CA-CB-CG	6.01	129.12	115.30
1	c	946	ASP	CB-CG-OD1	5.95	123.66	118.30
1	b	338	LEU	CB-CG-CD1	-5.92	100.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	e	1247	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	838	LEU	CA-CB-CG	5.89	128.86	115.30
3	R	1178	LEU	CA-CB-CG	5.89	128.85	115.30
2	I	923	LEU	CA-CB-CG	5.67	128.35	115.30
2	H	923	LEU	CA-CB-CG	5.67	128.34	115.30
2	L	923	LEU	CA-CB-CG	5.65	128.30	115.30
2	K	923	LEU	CA-CB-CG	5.65	128.29	115.30
2	J	923	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	720	ARG	CA-CB-CG	5.59	125.71	113.40
1	a	984	LEU	CA-CB-CG	5.50	127.95	115.30
1	e	616	ASP	CB-CG-OD1	5.49	123.24	118.30
1	e	984	LEU	CA-CB-CG	5.45	127.82	115.30
3	R	759	LEU	CA-CB-CG	5.42	127.77	115.30
1	3	153	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	374	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	b	616	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	905	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	D	686	ARG	CB-CG-CD	5.29	125.36	111.60
1	d	1065	LEU	CA-CB-CG	5.29	127.46	115.30
4	U	729	LEU	CA-CB-CG	5.27	127.42	115.30
1	D	1274	VAL	C-N-CD	5.25	139.42	128.40
1	2	133	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	457	LEU	CA-CB-CG	5.22	127.31	115.30
1	d	955	LEU	CA-CB-CG	5.20	127.25	115.30
1	a	1082	ARG	NE-CZ-NH1	5.19	122.89	120.30
4	U	471	ASP	CB-CG-OD1	5.17	122.95	118.30
2	K	640	LEU	CA-CB-CG	5.09	127.00	115.30
2	I	640	LEU	CA-CB-CG	5.09	127.00	115.30
2	J	640	LEU	CA-CB-CG	5.08	126.99	115.30
4	U	650	LEU	CA-CB-CG	5.08	126.99	115.30
1	d	1022	ASP	CB-CG-OD1	5.08	122.87	118.30
2	L	640	LEU	CA-CB-CG	5.08	126.98	115.30
1	e	802	LEU	CA-CB-CG	5.07	126.96	115.30
2	H	640	LEU	CA-CB-CG	5.06	126.94	115.30
1	a	308	THR	C-N-CA	5.05	134.33	121.70
1	B	587	ASP	CB-CG-OD1	5.03	122.82	118.30
3	R	1151	GLN	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	PRO	Peptide
1	B	308	THR	Peptide
1	B	782	GLN	Peptide
1	C	317	ASP	Peptide
1	D	981	ASP	Peptide
1	E	238	ASP	Peptide
4	U	135	ILE	Peptide
1	a	1110	PHE	Peptide
1	a	1220	ILE	Peptide
1	b	945	VAL	Peptide
1	c	946	ASP	Peptide
1	d	1055	LEU	Peptide
1	d	1065	LEU	Peptide
1	d	342	GLU	Peptide
1	d	838	LEU	Peptide
1	e	1065	LEU	Peptide
1	e	1110	PHE	Peptide

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%)	120 (88%)	16 (12%)	0	100	100
1	2	134/1275 (10%)	119 (89%)	15 (11%)	0	100	100
1	3	133/1275 (10%)	124 (93%)	9 (7%)	0	100	100
1	4	122/1275 (10%)	108 (88%)	14 (12%)	0	100	100
1	5	135/1275 (11%)	124 (92%)	11 (8%)	0	100	100
1	A	1126/1275 (88%)	1030 (92%)	94 (8%)	2 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1069/1275 (84%)	978 (92%)	90 (8%)	1 (0%)	51	82
1	C	1076/1275 (84%)	985 (92%)	90 (8%)	1 (0%)	51	82
1	D	1046/1275 (82%)	961 (92%)	85 (8%)	0	100	100
1	E	1058/1275 (83%)	974 (92%)	83 (8%)	1 (0%)	51	82
1	a	1084/1275 (85%)	987 (91%)	95 (9%)	2 (0%)	47	78
1	b	1083/1275 (85%)	994 (92%)	89 (8%)	0	100	100
1	c	1074/1275 (84%)	989 (92%)	84 (8%)	1 (0%)	51	82
1	d	1081/1275 (85%)	995 (92%)	84 (8%)	2 (0%)	47	78
1	e	1071/1275 (84%)	970 (91%)	101 (9%)	0	100	100
2	H	1022/1289 (79%)	926 (91%)	95 (9%)	1 (0%)	51	82
2	I	1022/1289 (79%)	925 (90%)	96 (9%)	1 (0%)	51	82
2	J	1022/1289 (79%)	924 (90%)	97 (10%)	1 (0%)	51	82
2	K	1022/1289 (79%)	926 (91%)	95 (9%)	1 (0%)	51	82
2	L	1022/1289 (79%)	925 (90%)	96 (9%)	1 (0%)	51	82
3	R	1249/1267 (99%)	1129 (90%)	119 (10%)	1 (0%)	51	82
4	U	658/736 (89%)	587 (89%)	65 (10%)	6 (1%)	17	49
All	All	18445/27573 (67%)	16800 (91%)	1623 (9%)	22 (0%)	54	82

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	TRP
1	a	310	TRP
1	E	787	GLN
4	U	588	PHE
1	B	1214	SER
1	C	614	PRO
2	H	1003	SER
2	I	1003	SER
2	J	1003	SER
2	K	1003	SER
2	L	1003	SER
1	A	584	SER
4	U	136	SER
4	U	471	ASP
1	a	339	LEU

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Mol	Chain	Res	Type
4	U	133	PRO
3	R	633	VAL
4	U	134	LEU
4	U	456	PHE
1	d	1066	VAL
1	c	1058	PRO
1	d	1057	SER

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
1	1	112/1113 (10%)	111 (99%)	1 (1%)	78 90
1	2	110/1113 (10%)	108 (98%)	2 (2%)	59 79
1	3	110/1113 (10%)	109 (99%)	1 (1%)	78 90
1	4	103/1113 (9%)	103 (100%)	0	100 100
1	5	112/1113 (10%)	107 (96%)	5 (4%)	27 58
1	A	994/1113 (89%)	990 (100%)	4 (0%)	91 95
1	B	945/1113 (85%)	942 (100%)	3 (0%)	92 97
1	C	958/1113 (86%)	955 (100%)	3 (0%)	92 97
1	D	931/1113 (84%)	925 (99%)	6 (1%)	86 94
1	E	939/1113 (84%)	934 (100%)	5 (0%)	88 94
1	a	961/1113 (86%)	957 (100%)	4 (0%)	91 95
1	b	960/1113 (86%)	960 (100%)	0	100 100
1	c	953/1113 (86%)	951 (100%)	2 (0%)	93 98
1	d	959/1113 (86%)	953 (99%)	6 (1%)	86 94
1	e	951/1113 (85%)	941 (99%)	10 (1%)	73 86
2	H	884/1118 (79%)	877 (99%)	7 (1%)	81 91
2	I	884/1118 (79%)	877 (99%)	7 (1%)	81 91
2	J	884/1118 (79%)	874 (99%)	10 (1%)	73 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	K	884/1118 (79%)	877 (99%)	7 (1%)	81 91
2	L	884/1118 (79%)	877 (99%)	7 (1%)	81 91
3	R	1074/1084 (99%)	1073 (100%)	1 (0%)	93 98
4	U	592/650 (91%)	587 (99%)	5 (1%)	81 91
All	All	16184/24019 (67%)	16088 (99%)	96 (1%)	86 94

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	146	ASN
1	2	138	ASN
1	2	146	ASN
1	3	146	ASN
1	5	6	ARG
1	5	7	LYS
1	5	8	THR
1	5	11	LYS
1	5	146	ASN
1	A	217	GLN
1	A	413	THR
1	A	720	ARG
1	A	1120	ARG
1	B	353	MET
1	B	508	ARG
1	B	970	ASN
1	C	433	ARG
1	C	720	ARG
1	C	890	LYS
1	D	720	ARG
1	D	763	ASN
1	D	767	ARG
1	D	780	ARG
1	D	794	ARG
1	D	840	ARG
1	E	353	MET
1	E	503	ARG
1	E	582	ARG
1	E	720	ARG
1	E	771	LEU
2	H	8	ARG
2	H	476	ARG

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Mol	Chain	Res	Type
2	H	507	ARG
2	H	552	TYR
2	H	719	MET
2	H	882	ARG
2	H	1016	MET
2	I	8	ARG
2	I	476	ARG
2	I	507	ARG
2	I	552	TYR
2	I	719	MET
2	I	882	ARG
2	I	1016	MET
2	J	8	ARG
2	J	476	ARG
2	J	507	ARG
2	J	552	TYR
2	J	577	ASP
2	J	578	VAL
2	J	580	GLN
2	J	719	MET
2	J	882	ARG
2	J	1016	MET
2	K	8	ARG
2	K	476	ARG
2	K	507	ARG
2	K	552	TYR
2	K	719	MET
2	K	882	ARG
2	K	1016	MET
2	L	8	ARG
2	L	476	ARG
2	L	507	ARG
2	L	552	TYR
2	L	719	MET
2	L	882	ARG
2	L	1016	MET
3	R	953	ARG
4	U	113	ARG
4	U	212	THR
4	U	523	ARG
4	U	624	ARG
4	U	695	LYS

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Mol	Chain	Res	Type
1	a	392	ARG
1	a	428	ARG
1	a	521	ARG
1	a	1079	ARG
1	c	436	ARG
1	c	1154	ARG
1	d	242	ARG
1	d	243	LYS
1	d	503	ARG
1	d	840	ARG
1	d	842	ARG
1	d	1082	ARG
1	e	218	ARG
1	e	313	ASN
1	e	315	ASP
1	e	316	PHE
1	e	319	ASP
1	e	323	ILE
1	e	430	ARG
1	e	505	MET
1	e	851	ARG
1	e	945	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	63	GLN
1	1	76	ASN
1	1	86	ASN
1	5	63	GLN
1	A	219	HIS
1	A	228	GLN
1	A	375	HIS
1	A	382	HIS
1	A	527	ASN
1	A	569	GLN
1	A	731	ASN
1	A	1036	ASN
1	A	1116	GLN
1	A	1124	GLN
1	A	1125	GLN
1	B	293	GLN

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Mol	Chain	Res	Type
1	B	357	ASN
1	B	518	GLN
1	B	533	GLN
1	B	544	GLN
1	B	550	GLN
1	B	704	GLN
1	B	749	ASN
1	B	937	GLN
1	B	1000	GLN
1	B	1025	GLN
1	B	1116	GLN
1	C	182	GLN
1	C	278	GLN
1	C	357	ASN
1	C	524	ASN
1	C	527	ASN
1	C	544	GLN
1	C	749	ASN
1	C	832	GLN
1	C	1116	GLN
1	D	278	GLN
1	D	340	ASN
1	D	373	ASN
1	D	441	ASN
1	D	537	GLN
1	D	544	GLN
1	D	763	ASN
1	D	779	GLN
1	D	1000	GLN
1	D	1002	GLN
1	D	1036	ASN
1	D	1116	GLN
1	D	1123	ASN
1	D	1205	ASN
1	D	1246	GLN
1	E	228	GLN
1	E	246	GLN
1	E	518	GLN
1	E	654	ASN
1	E	704	GLN
1	E	774	ASN
1	E	782	GLN

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Mol	Chain	Res	Type
1	E	970	ASN
1	E	1002	GLN
1	E	1036	ASN
1	E	1051	GLN
1	E	1116	GLN
2	H	267	ASN
2	H	310	ASN
2	H	313	GLN
2	H	352	GLN
2	H	455	GLN
2	H	510	GLN
2	H	617	ASN
2	H	856	GLN
2	H	925	GLN
2	H	944	GLN
2	I	267	ASN
2	I	310	ASN
2	I	313	GLN
2	I	352	GLN
2	I	455	GLN
2	I	510	GLN
2	I	617	ASN
2	I	856	GLN
2	I	925	GLN
2	I	944	GLN
2	J	267	ASN
2	J	310	ASN
2	J	313	GLN
2	J	352	GLN
2	J	455	GLN
2	J	510	GLN
2	J	580	GLN
2	J	856	GLN
2	J	925	GLN
2	J	944	GLN
2	K	127	GLN
2	K	267	ASN
2	K	310	ASN
2	K	313	GLN
2	K	352	GLN
2	K	455	GLN
2	K	510	GLN

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Mol	Chain	Res	Type
2	K	617	ASN
2	K	856	GLN
2	K	925	GLN
2	K	944	GLN
2	L	267	ASN
2	L	274	GLN
2	L	310	ASN
2	L	313	GLN
2	L	352	GLN
2	L	455	GLN
2	L	510	GLN
2	L	617	ASN
2	L	856	GLN
2	L	925	GLN
2	L	944	GLN
3	R	79	ASN
3	R	283	HIS
3	R	499	ASN
3	R	535	GLN
3	R	550	ASN
3	R	836	GLN
3	R	1100	GLN
3	R	1208	ASN
4	U	82	GLN
4	U	451	GLN
1	a	293	GLN
1	a	518	GLN
1	a	527	ASN
1	a	731	ASN
1	a	832	GLN
1	a	970	ASN
1	a	1036	ASN
1	a	1124	GLN
1	a	1125	GLN
1	a	1149	HIS
1	a	1205	ASN
1	a	1233	ASN
1	b	340	ASN
1	b	415	ASN
1	b	527	ASN
1	b	667	GLN
1	b	1002	GLN

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Mol	Chain	Res	Type
1	b	1205	ASN
1	c	246	GLN
1	c	537	GLN
1	c	779	GLN
1	c	917	ASN
1	c	1003	GLN
1	c	1036	ASN
1	c	1205	ASN
1	c	1233	ASN
1	c	1244	GLN
1	d	184	HIS
1	d	246	GLN
1	d	369	ASN
1	d	550	GLN
1	d	787	GLN
1	d	1036	ASN
1	d	1255	ASN
1	e	234	GLN
1	e	278	GLN
1	e	527	ASN
1	e	1002	GLN
1	e	1124	GLN
1	e	1125	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	SAM	J	1301	-	24,29,29	1.01	2 (8%)	23,42,42	1.75	5 (21%)
5	SAM	K	1301	-	24,29,29	1.00	1 (4%)	23,42,42	1.89	5 (21%)
5	SAM	L	1301	-	24,29,29	1.20	4 (16%)	23,42,42	2.17	9 (39%)
5	SAM	H	1301	-	24,29,29	1.06	2 (8%)	23,42,42	1.48	5 (21%)
5	SAM	I	1301	-	24,29,29	1.07	3 (12%)	23,42,42	1.87	6 (26%)

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
5	SAM	J	1301	-	-	4/12/33/33	0/3/3/3
5	SAM	K	1301	-	-	4/12/33/33	0/3/3/3
5	SAM	L	1301	-	-	4/12/33/33	0/3/3/3
5	SAM	H	1301	-	-	4/12/33/33	0/3/3/3
5	SAM	I	1301	-	-	5/12/33/33	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1301	SAM	C5-C4	2.72	1.48	1.40
5	I	1301	SAM	OXT-C	-2.40	1.22	1.30
5	L	1301	SAM	OXT-C	-2.24	1.23	1.30
5	I	1301	SAM	C5-C4	2.11	1.46	1.40
5	H	1301	SAM	C5-C4	2.11	1.46	1.40
5	K	1301	SAM	C5-C4	2.09	1.46	1.40
5	J	1301	SAM	C5-C4	2.09	1.46	1.40
5	L	1301	SAM	C8-N7	2.05	1.38	1.34
5	I	1301	SAM	CE-SD	-2.03	1.66	1.78
5	L	1301	SAM	CE-SD	-2.01	1.66	1.78
5	J	1301	SAM	OXT-C	-2.01	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1301	SAM	OXT-C	-2.00	1.24	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	1301	SAM	CG-SD-C5'	5.81	118.23	103.40
5	J	1301	SAM	CG-SD-C5'	4.99	116.13	103.40
5	I	1301	SAM	CB-CA-N	4.17	121.10	110.17
5	L	1301	SAM	C4-C5-N7	-4.01	105.22	109.40
5	L	1301	SAM	C1'-N9-C4	-3.84	119.89	126.64
5	I	1301	SAM	CB-CA-C	3.84	119.44	110.30
5	L	1301	SAM	CG-SD-C5'	3.79	113.08	103.40
5	H	1301	SAM	N3-C2-N1	-3.79	122.75	128.68
5	K	1301	SAM	N3-C2-N1	-3.77	122.79	128.68
5	J	1301	SAM	N3-C2-N1	-3.67	122.95	128.68
5	I	1301	SAM	N3-C2-N1	-3.63	123.00	128.68
5	L	1301	SAM	C5-C6-N6	3.51	125.69	120.35
5	L	1301	SAM	C3'-C2'-C1'	3.47	106.21	100.98
5	K	1301	SAM	C4-C5-N7	-2.86	106.41	109.40
5	J	1301	SAM	C4-C5-N7	-2.76	106.52	109.40
5	L	1301	SAM	N3-C2-N1	-2.73	124.41	128.68
5	I	1301	SAM	C4-C5-N7	-2.66	106.63	109.40
5	H	1301	SAM	C3'-C2'-C1'	2.53	104.79	100.98
5	H	1301	SAM	C4-C5-N7	-2.49	106.81	109.40
5	H	1301	SAM	CG-SD-C5'	2.47	109.70	103.40
5	L	1301	SAM	OXT-C-CA	2.46	121.77	113.38
5	I	1301	SAM	C3'-C2'-C1'	2.46	104.68	100.98
5	L	1301	SAM	CB-CA-C	2.34	115.88	110.30
5	I	1301	SAM	CG-SD-C5'	2.31	109.31	103.40
5	K	1301	SAM	C3'-C2'-C1'	2.30	104.44	100.98
5	J	1301	SAM	CE-SD-C5'	2.22	118.02	100.54
5	L	1301	SAM	C2'-C3'-C4'	2.22	106.96	102.64
5	J	1301	SAM	C1'-N9-C4	-2.11	122.94	126.64
5	K	1301	SAM	CE-SD-C5'	2.03	116.46	100.54
5	H	1301	SAM	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1301	SAM	N-CA-CB-CG
5	J	1301	SAM	CA-CB-CG-SD

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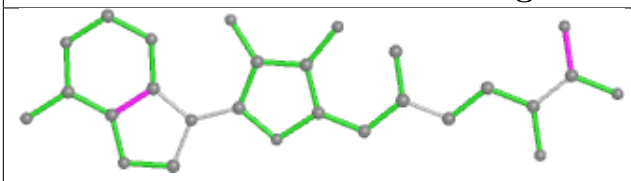
Mol	Chain	Res	Type	Atoms
5	K	1301	SAM	CB-CG-SD-C5'
5	L	1301	SAM	N-CA-CB-CG
5	L	1301	SAM	C-CA-CB-CG
5	H	1301	SAM	CB-CG-SD-CE
5	I	1301	SAM	CB-CG-SD-CE
5	L	1301	SAM	CB-CG-SD-CE
5	K	1301	SAM	N-CA-CB-CG
5	H	1301	SAM	OXT-C-CA-CB
5	K	1301	SAM	C-CA-CB-CG
5	H	1301	SAM	CB-CG-SD-C5'
5	I	1301	SAM	CB-CG-SD-C5'
5	J	1301	SAM	CB-CG-SD-C5'
5	L	1301	SAM	CB-CG-SD-C5'
5	J	1301	SAM	O-C-CA-CB
5	H	1301	SAM	O-C-CA-CB
5	J	1301	SAM	OXT-C-CA-CB
5	I	1301	SAM	O-C-CA-CB
5	I	1301	SAM	OXT-C-CA-CB
5	K	1301	SAM	OXT-C-CA-N

There are no ring outliers.

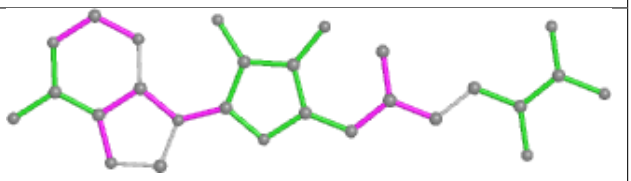
No monomer is involved in short contacts.

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.

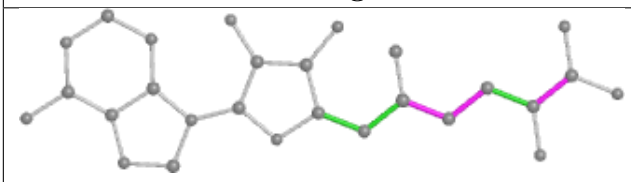
Ligand SAM J 1301



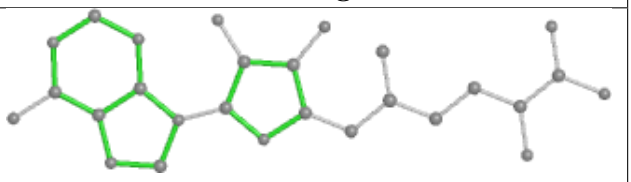
Bond lengths



Bond angles

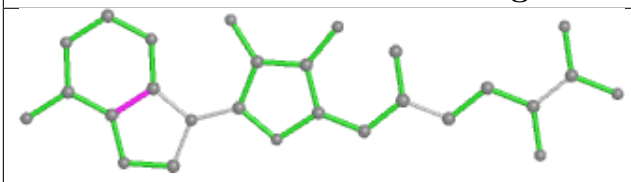


Torsions

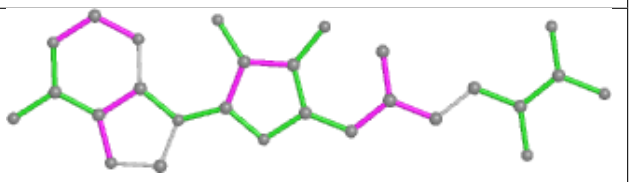


Rings

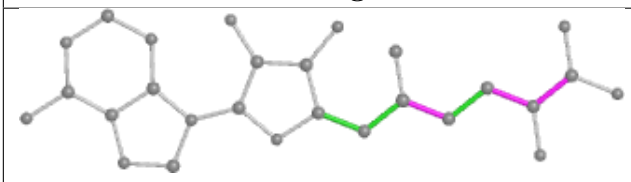
Ligand SAM K 1301



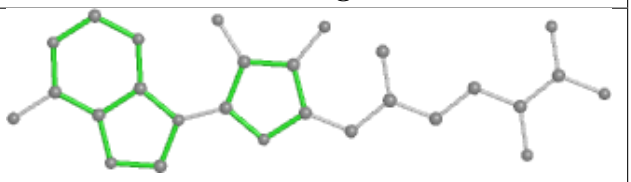
Bond lengths



Bond angles

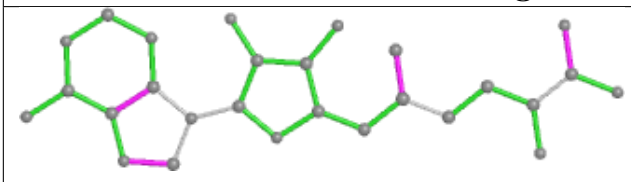


Torsions

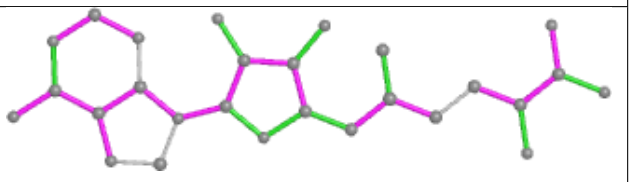


Rings

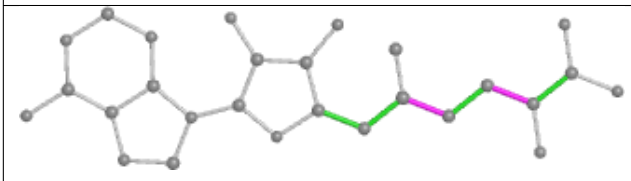
Ligand SAM L 1301



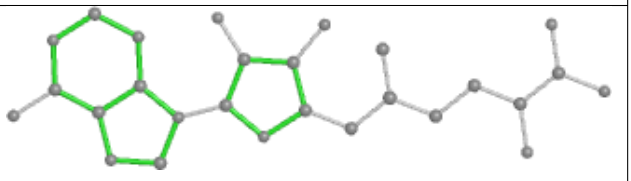
Bond lengths



Bond angles



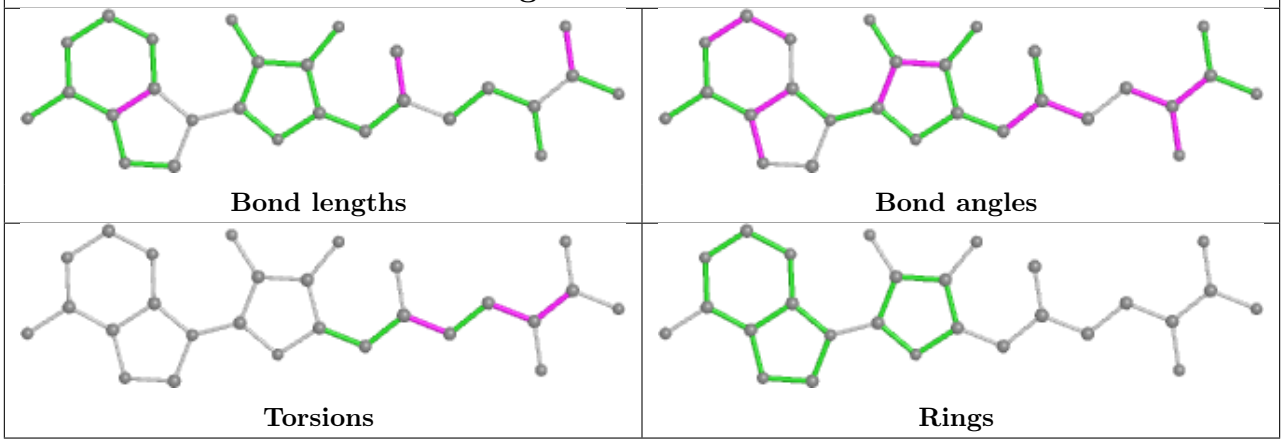
Torsions



Rings

Ligand SAM H 1301

Ligand SAM I 1301



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.

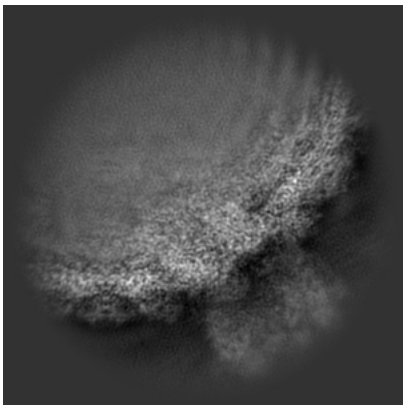
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33779. These allow visual inspection of the internal detail of the map and identification of artifacts.

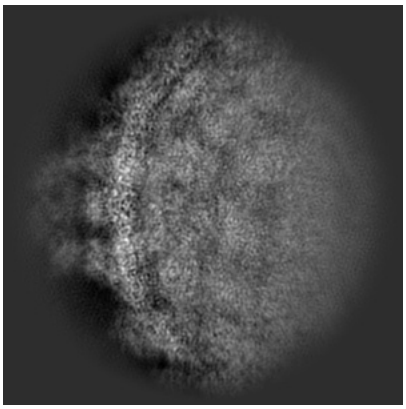
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

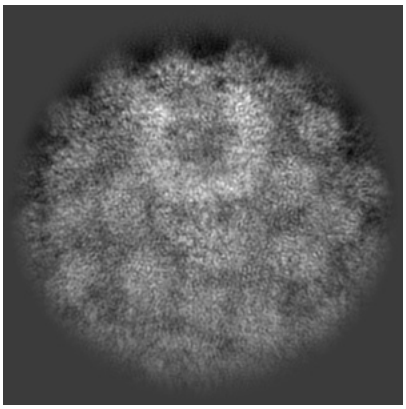
6.1.1 Primary map



X

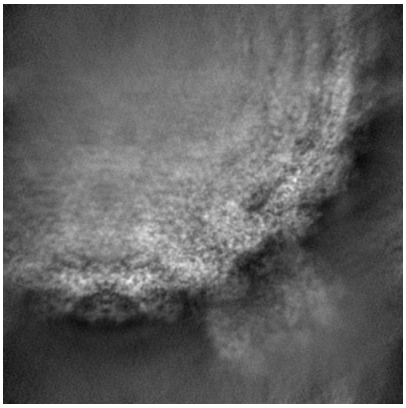


Y

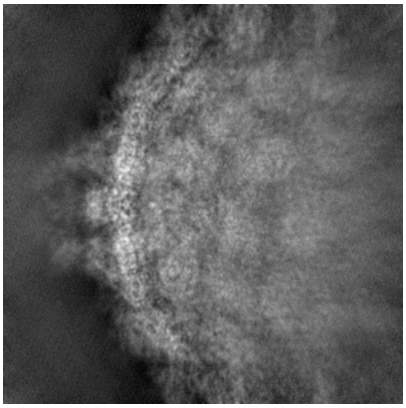


Z

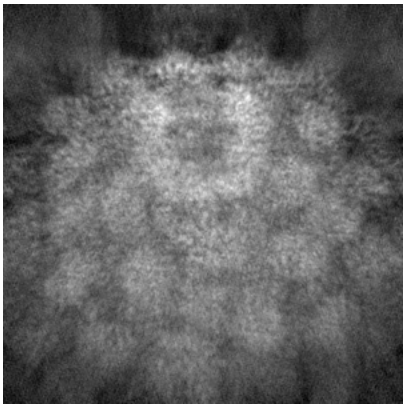
6.1.2 Raw map



X



Y

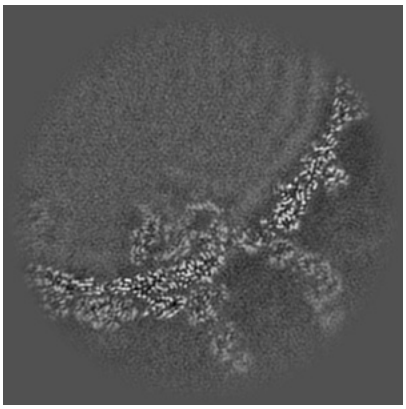


Z

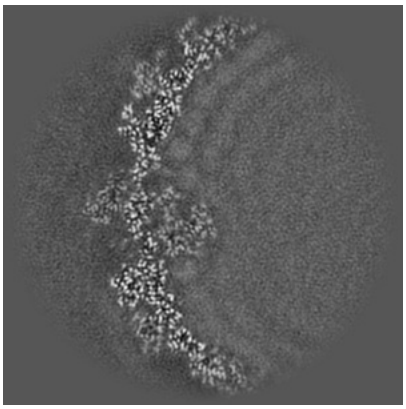
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

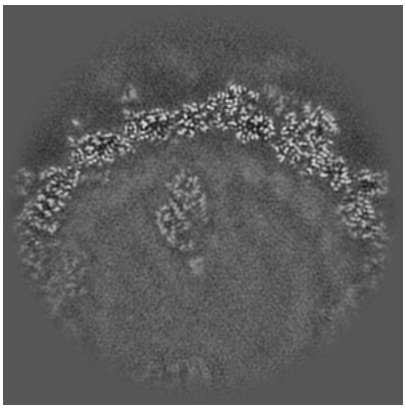
6.2.1 Primary map



X Index: 160

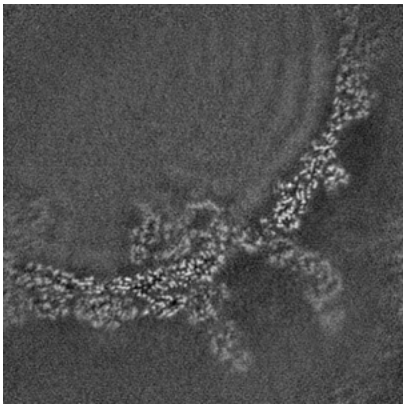


Y Index: 160

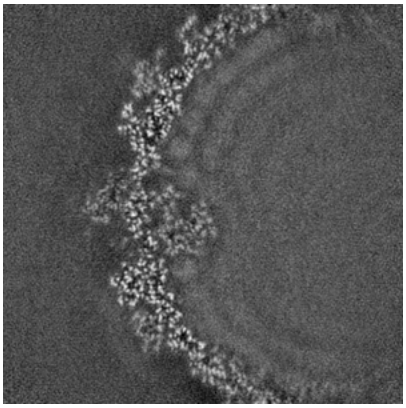


Z Index: 160

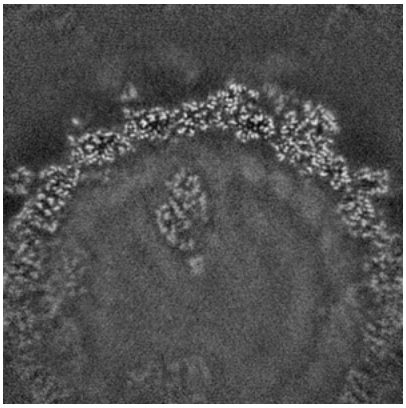
6.2.2 Raw map



X Index: 160



Y Index: 160

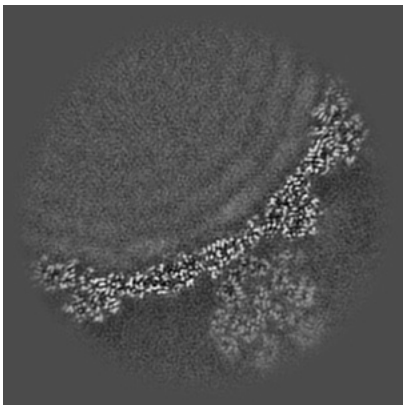


Z Index: 160

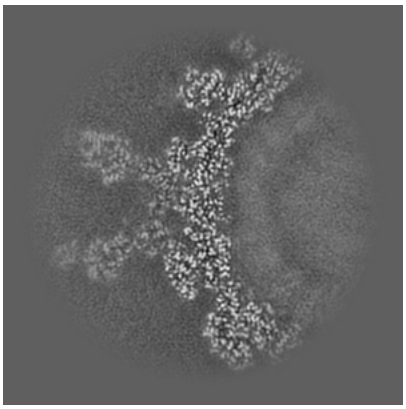
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

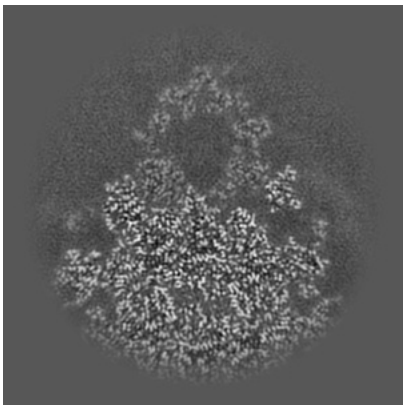
6.3.1 Primary map



X Index: 196

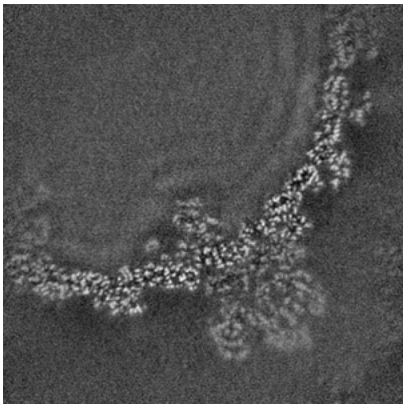


Y Index: 227

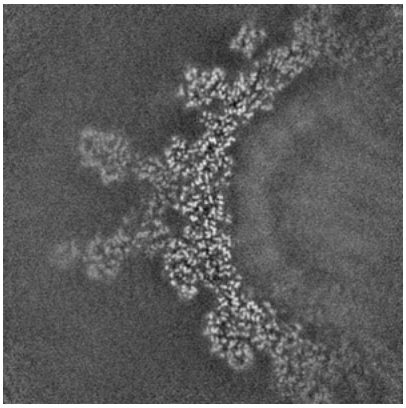


Z Index: 99

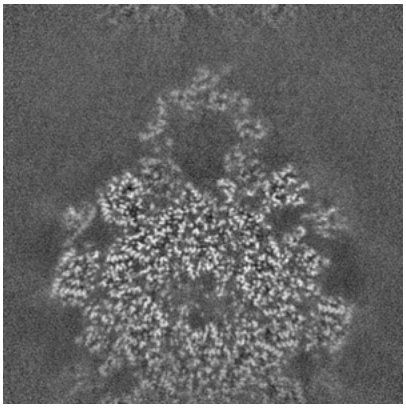
6.3.2 Raw map



X Index: 125



Y Index: 228

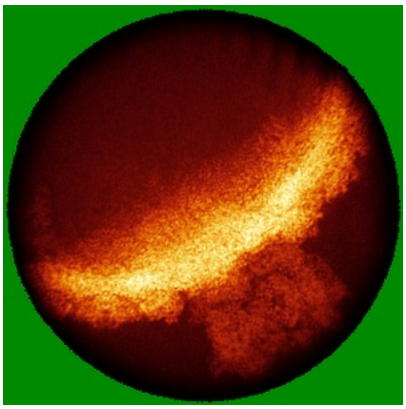


Z Index: 102

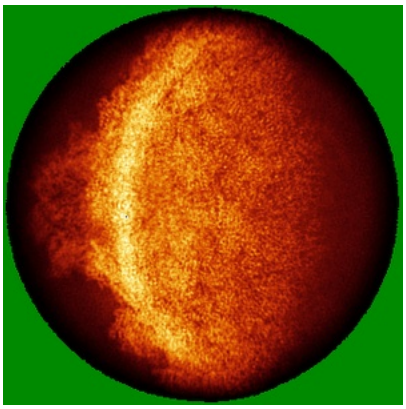
The images above show the largest variance slices of the map in three orthogonal directions.

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

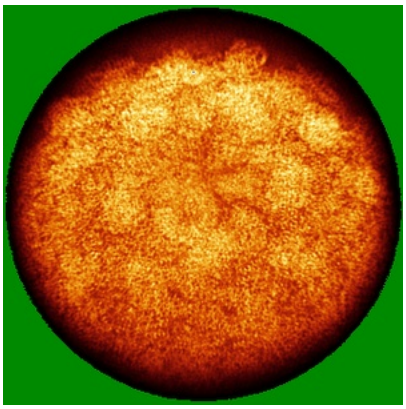
6.4.1 Primary map



X

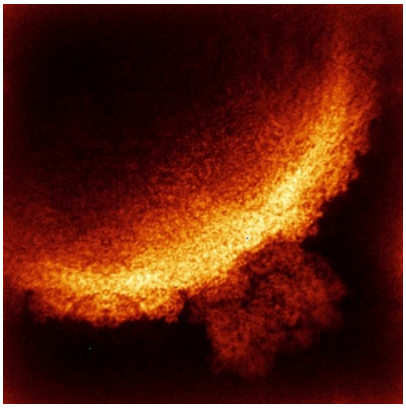


Y

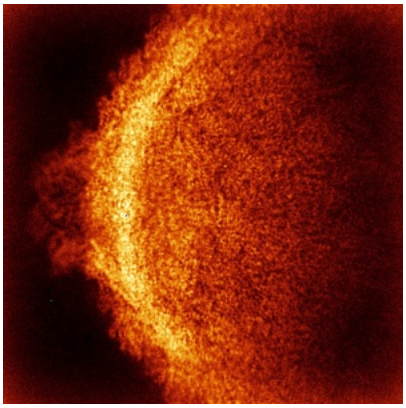


Z

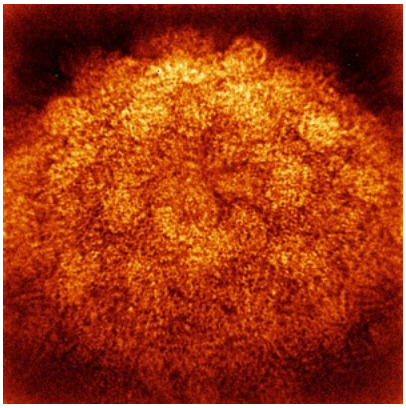
6.4.2 Raw map



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 0.4. 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.

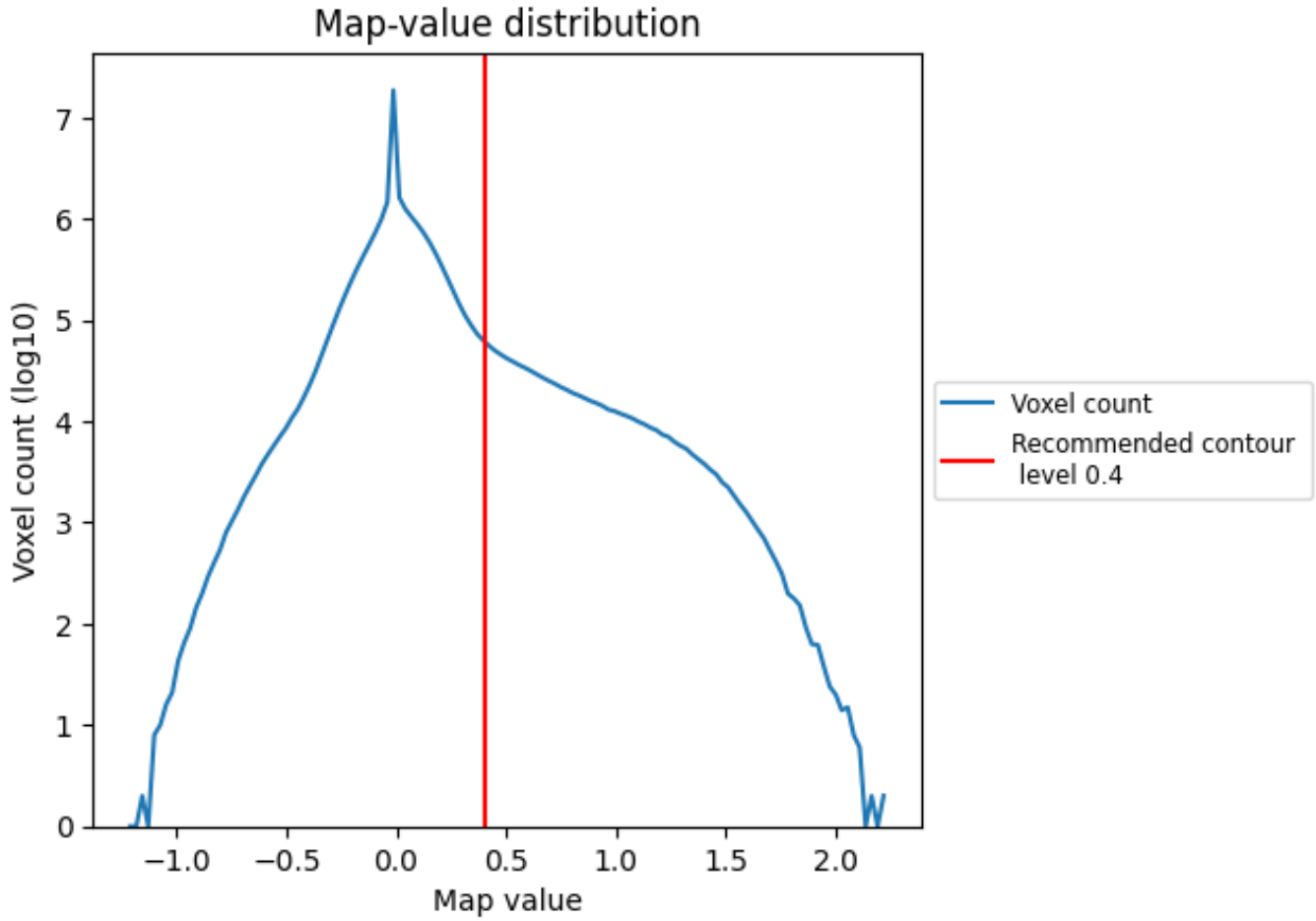
6.6 Mask visualisation (i)

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

7 Map analysis

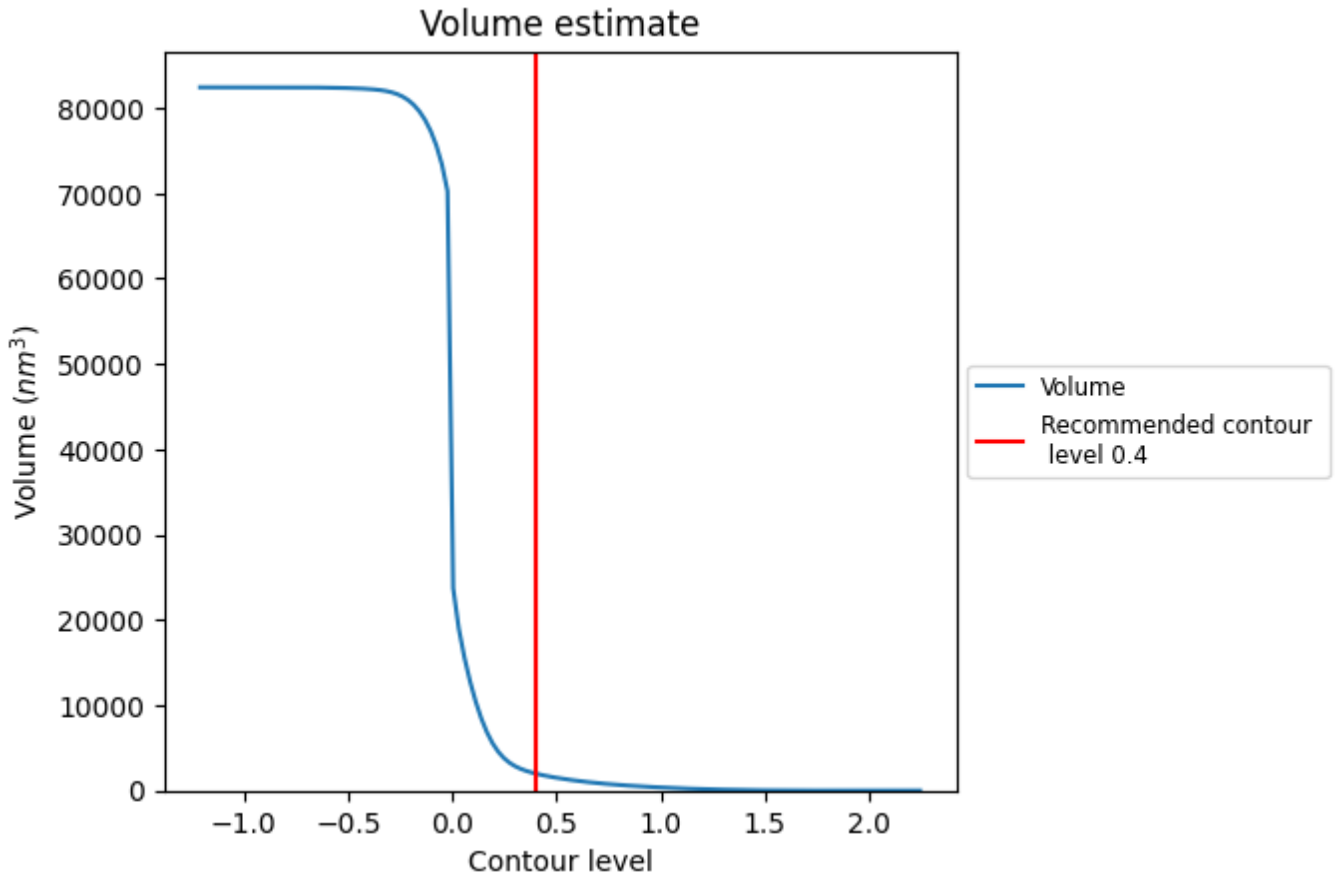
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

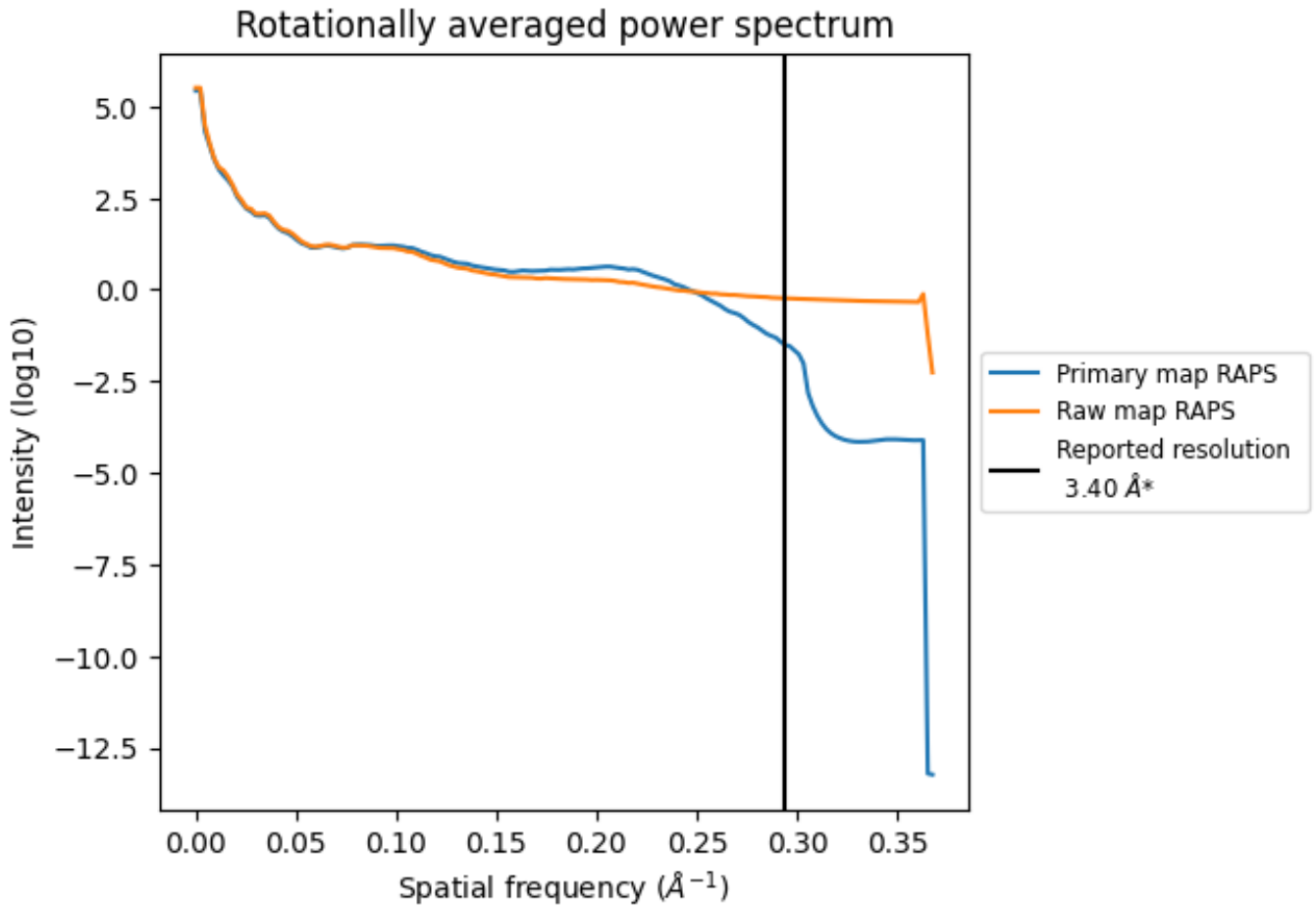
7.2 Volume estimate



The volume at the recommended contour level is 1994 nm^3; this corresponds to an approximate mass of 1801 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)

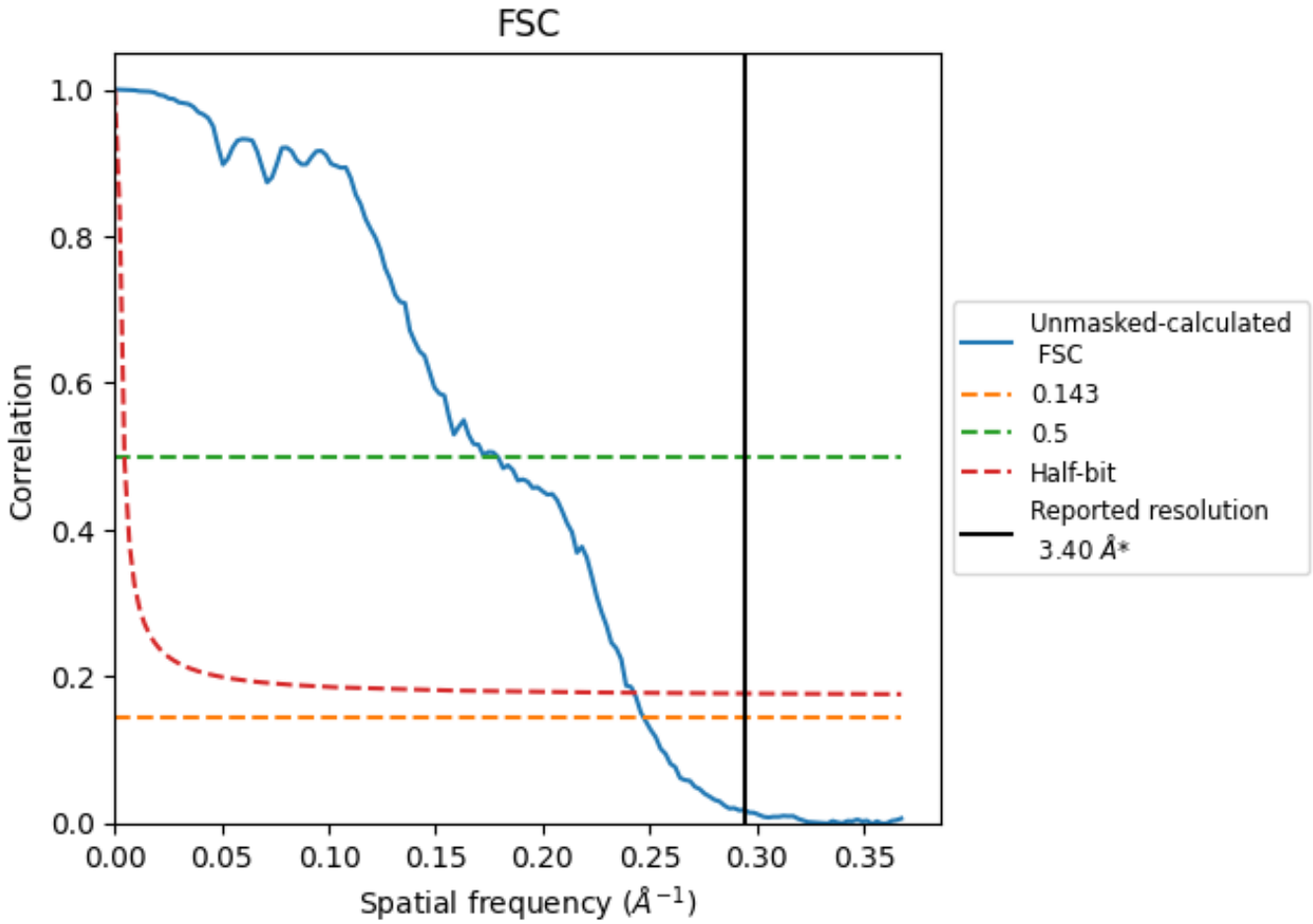


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

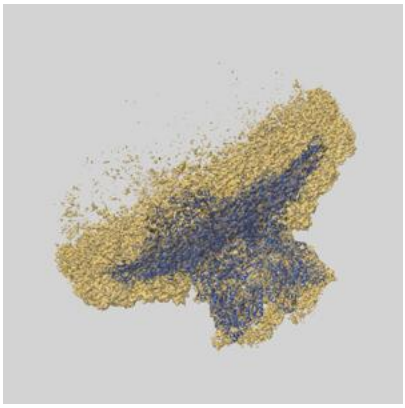
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	5.60	4.12

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

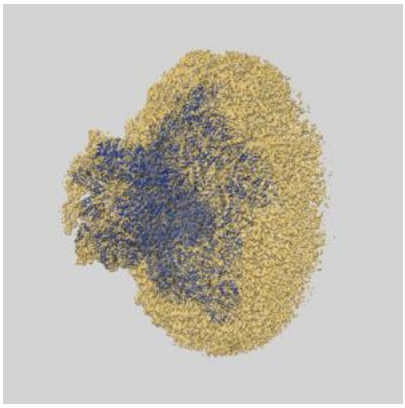
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33779 and PDB model 7YEZ. Per-residue inclusion information can be found in section 3 on page 7.

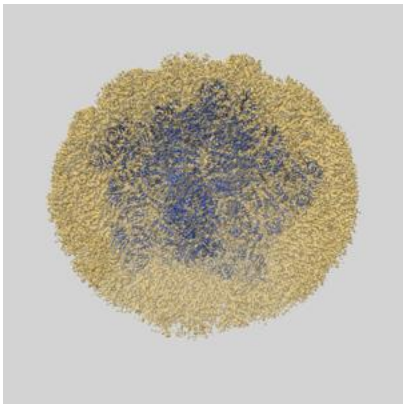
9.1 Map-model overlay



X



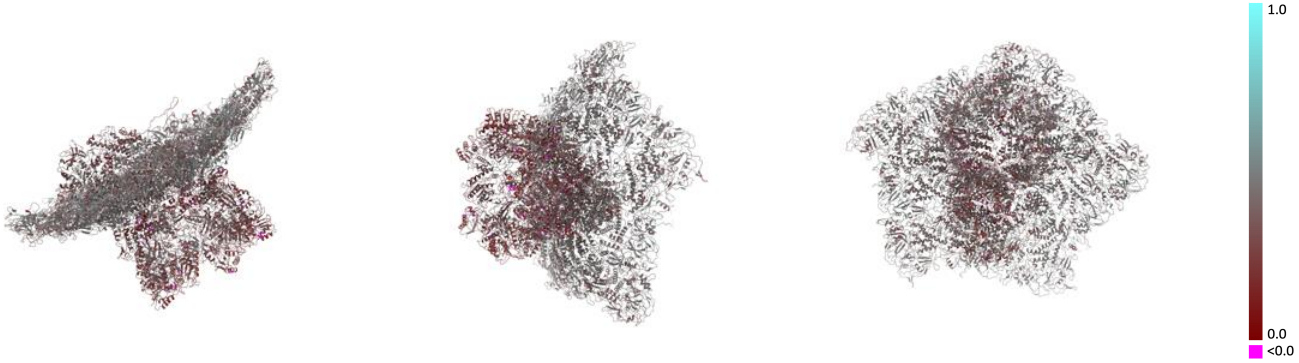
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

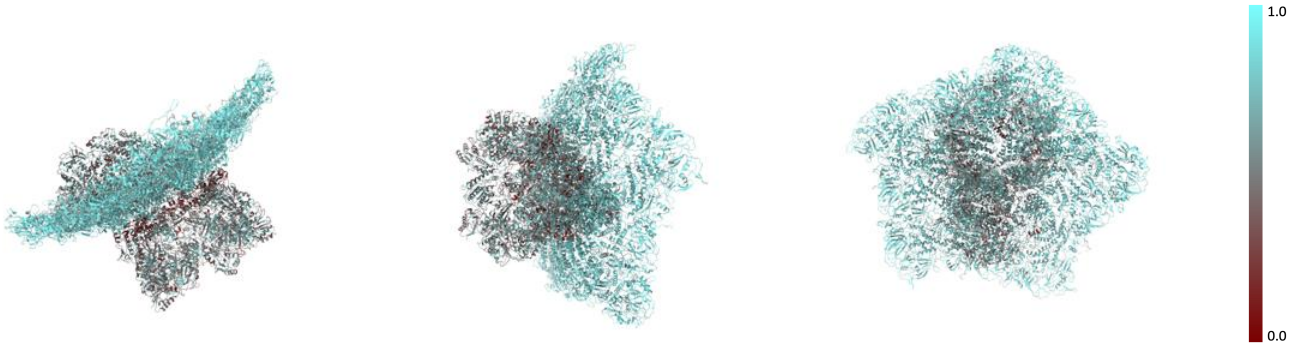
9.2 Q-score mapped to coordinate model



X Y Z

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.

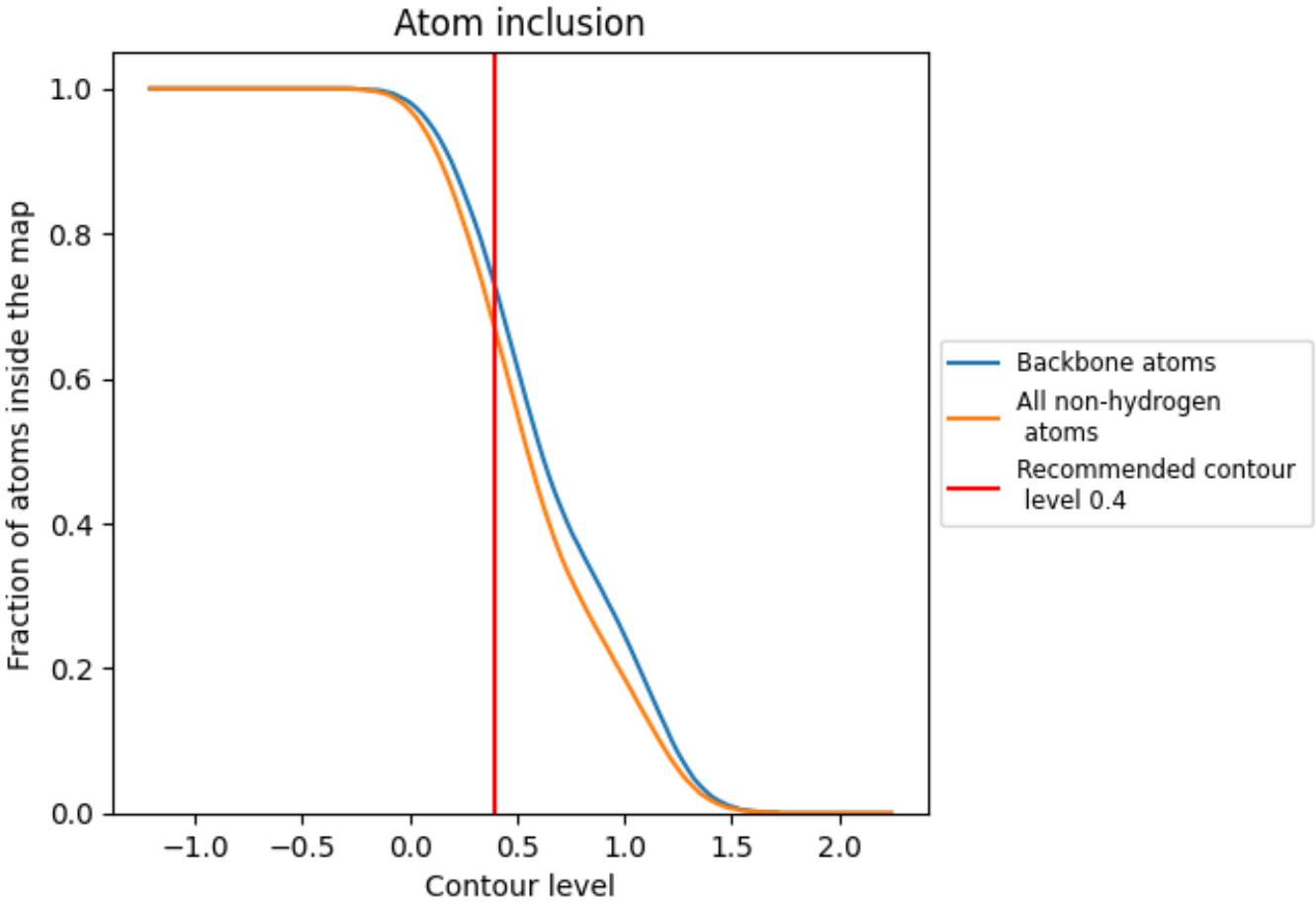
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.3840
1	0.6430	0.4010
2	0.7100	0.4080
3	0.6880	0.4160
4	0.5910	0.3840
5	0.5930	0.3750
A	0.7530	0.4170
B	0.7750	0.4250
C	0.7790	0.4230
D	0.7860	0.4280
E	0.7720	0.4250
H	0.4800	0.2980
I	0.4610	0.2860
J	0.4700	0.3070
K	0.4750	0.3130
L	0.4790	0.3100
R	0.5820	0.3460
U	0.5690	0.3640
a	0.7880	0.4250
b	0.7970	0.4330
c	0.7920	0.4320
d	0.7980	0.4310
e	0.7970	0.4270