wwPDB EM Validation Summary Report

Jun 26, 2024 – 09:37 PM JST

PDB ID	:	7YED
EMDB ID	:	EMD-33770
Title	:	In situ structure of polymerase complex of mammalian reovirus in the elongation state
Authors	:	Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.
Deposited on	:	2022-07-05
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

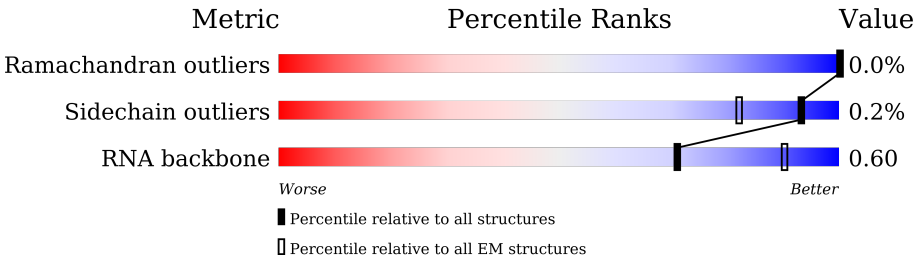
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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% 11%
1	B	1275	84% 16%
1	C	1275	85% 15%

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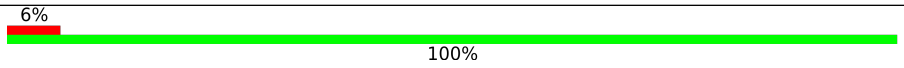
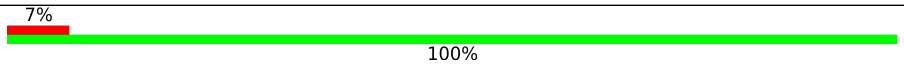
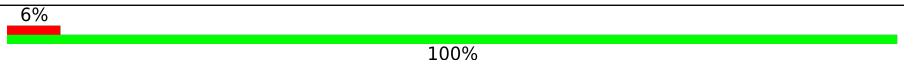
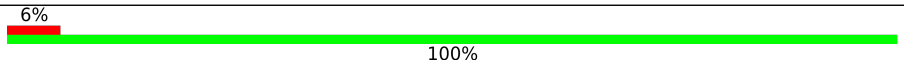
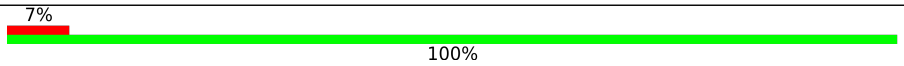
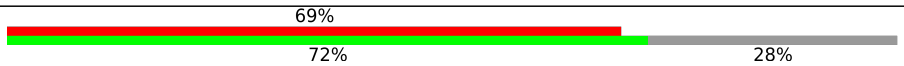
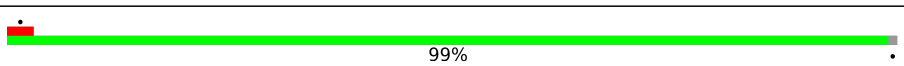
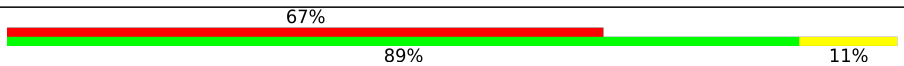
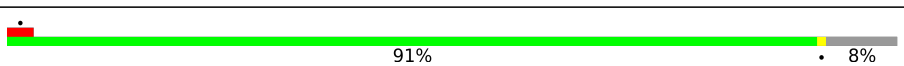
Mol	Chain	Length	Quality of chain
1	D	1275	
1	E	1275	
1	a	1275	
1	b	1275	
1	c	1275	
1	d	1275	
1	e	1275	
2	H	1289	
2	I	1289	
2	J	1289	
2	K	1289	
2	L	1289	
3	M	21	
4	N	36	
5	R	1267	
6	T	36	
7	U	736	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 158907 atoms, of which 291 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	139	Total	C	N	O	S	0	0
			1035	616	197	219	3		
1	2	139	Total	C	N	O	S	0	0
			1035	616	197	219	3		
1	3	138	Total	C	N	O	S	0	0
			1030	613	196	218	3		
1	4	131	Total	C	N	O	S	0	0
			969	577	183	206	3		
1	5	139	Total	C	N	O	S	0	0
			1035	616	197	219	3		
1	A	1129	Total	C	N	O	S	0	0
			8875	5659	1511	1652	53		
1	B	1075	Total	C	N	O	S	0	0
			8455	5397	1433	1574	51		
1	C	1086	Total	C	N	O	S	0	0
			8563	5469	1450	1592	52		
1	D	1051	Total	C	N	O	S	0	0
			8306	5309	1404	1544	49		
1	E	1058	Total	C	N	O	S	0	0
			8361	5342	1416	1554	49		
1	a	1080	Total	C	N	O	S	0	0
			8525	5448	1448	1578	51		
1	b	1078	Total	C	N	O	S	0	0
			8511	5439	1446	1575	51		
1	c	1080	Total	C	N	O	S	0	0
			8527	5448	1449	1579	51		
1	d	1087	Total	C	N	O	S	0	0
			8576	5476	1456	1593	51		
1	e	1087	Total	C	N	O	S	0	0
			8576	5476	1456	1593	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
			10143	6483	1699	1922	39		
2	I	1288	Total	C	N	O	S	0	0
			10143	6483	1699	1922	39		
2	J	1288	Total	C	N	O	S	0	0
			10143	6483	1699	1922	39		
2	K	1288	Total	C	N	O	S	0	0
			10143	6483	1699	1922	39		
2	L	1288	Total	C	N	O	S	0	0
			10143	6483	1699	1922	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	21	Total	C	N	O	P	0	0
			442	200	75	146	21		

- Molecule 4 is a RNA chain called RNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	26	Total	C	N	O	P	0	0
			540	247	91	178	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	1254	Total	C	N	O	S	0	0
			9919	6332	1699	1824	64		

- Molecule 6 is a RNA chain called RNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	36	Total	C	N	O	P	0	0
			753	342	126	250	35		

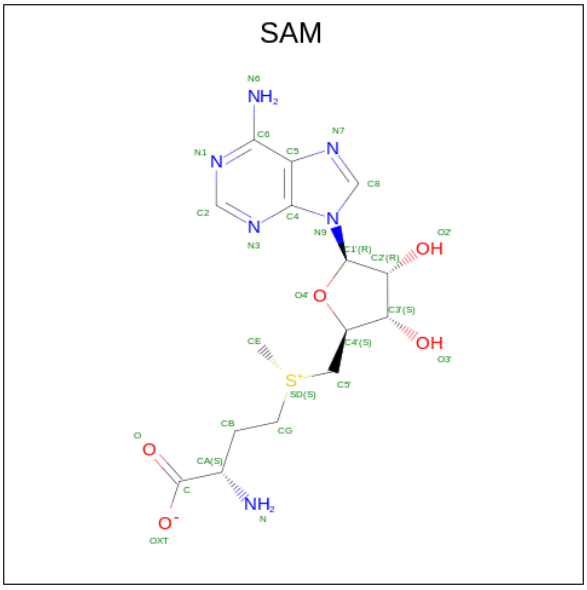
- Molecule 7 is a protein called Mu-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	679	Total	C	N	O	S	0	0
			5399	3460	917	991	31		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms	AltConf
9	H	1	Total C H N O S 49 15 22 6 5 1	0
9	H	1	Total C H N O S 49 15 22 6 5 1	0

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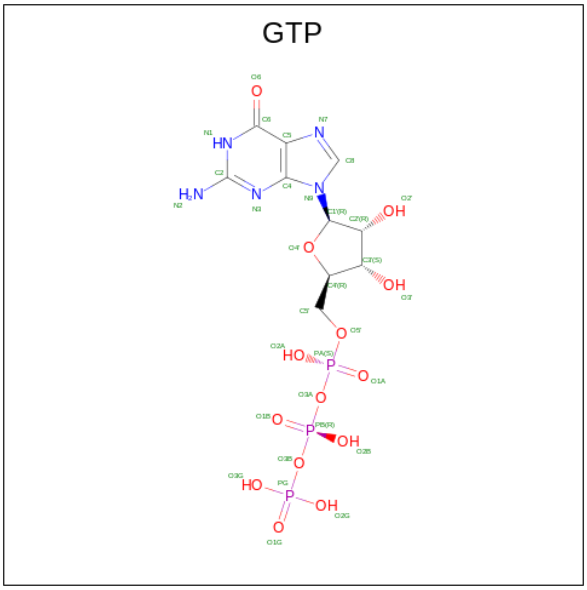
Mol	Chain	Residues	Atoms						AltConf
9	I	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	I	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	J	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	J	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	K	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	K	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
9	L	1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

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						AltConf
10	H	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
10	I	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
10	J	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

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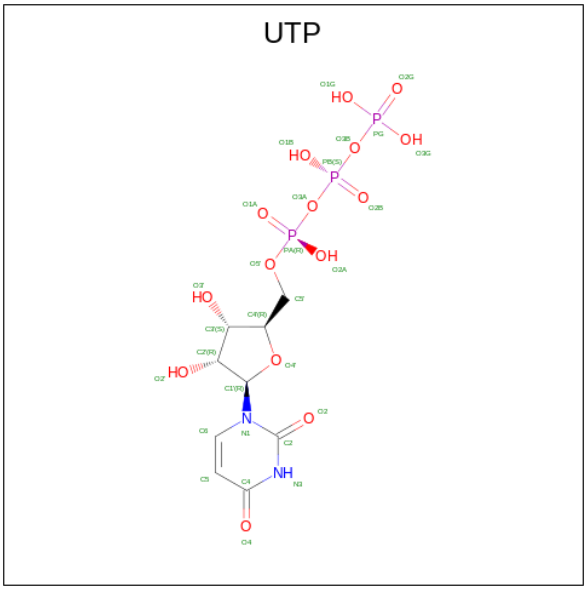
Mol	Chain	Residues	Atoms						AltConf
10	K	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
10	L	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 11 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



Mol	Chain	Residues	Atoms						AltConf
11	R	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

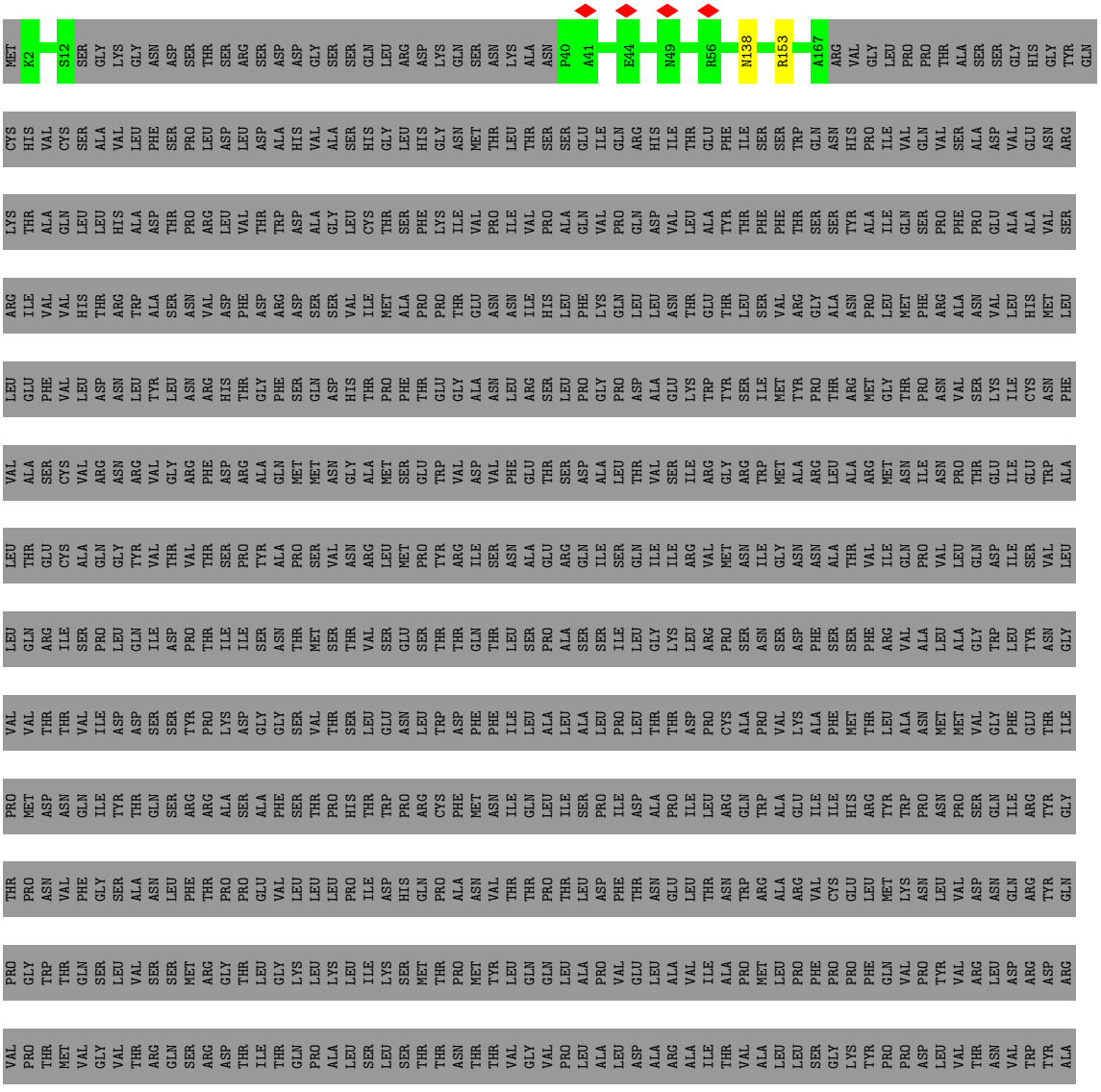
Mol	Chain	Residues	Atoms		AltConf
12	R	2	Total	Mg	0
			2	2	

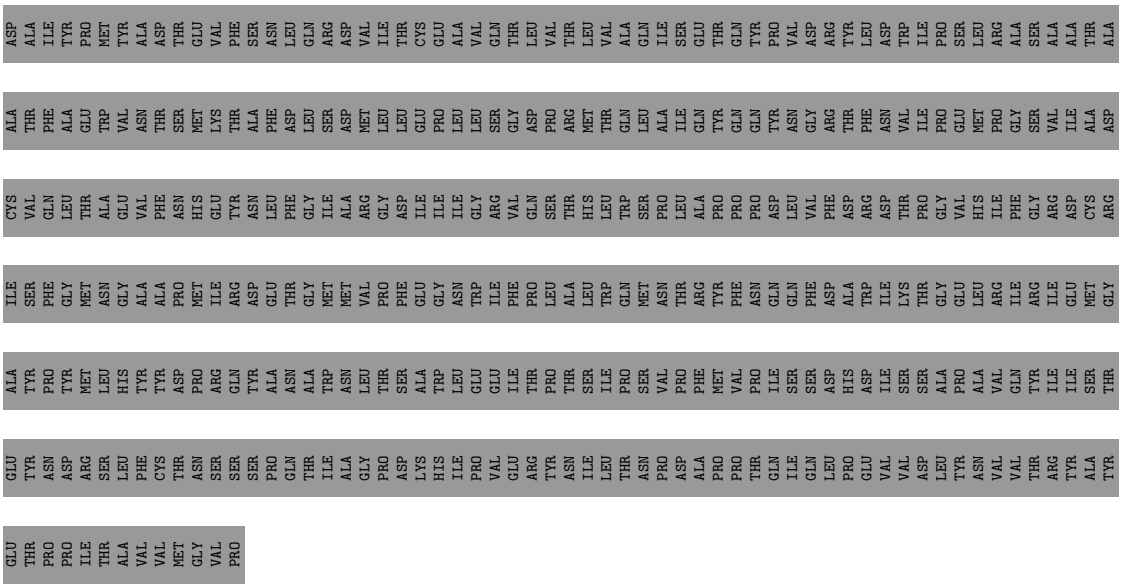
3 Residue-property plots (i)

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

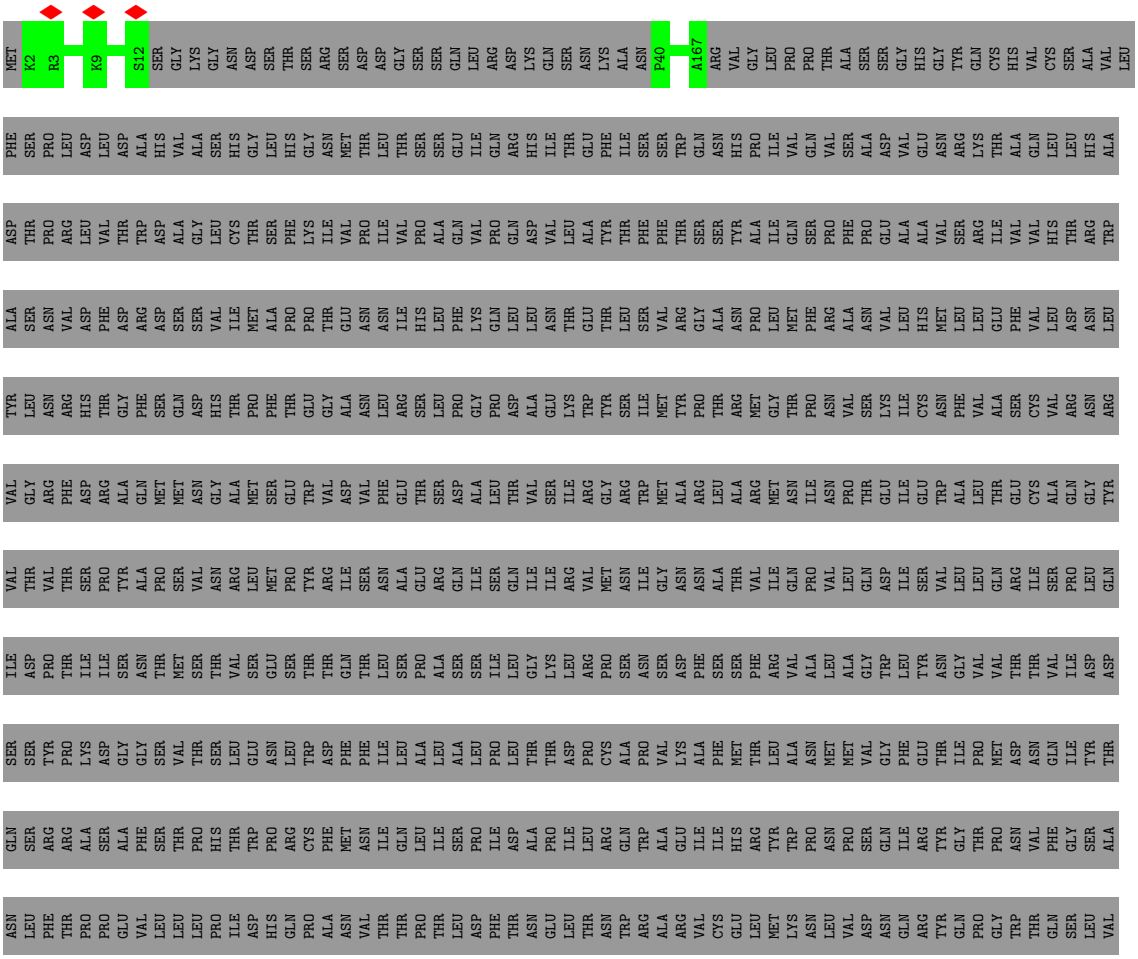
Chain 1:

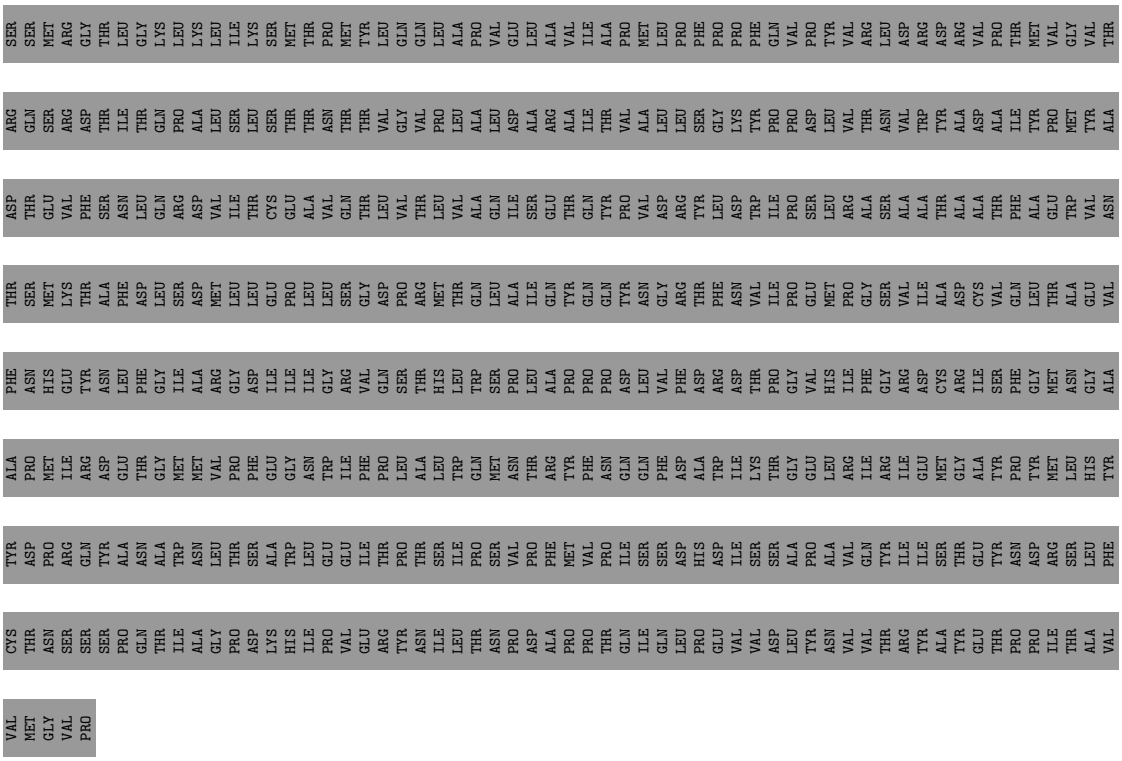




• Molecule 1: RNA helicase

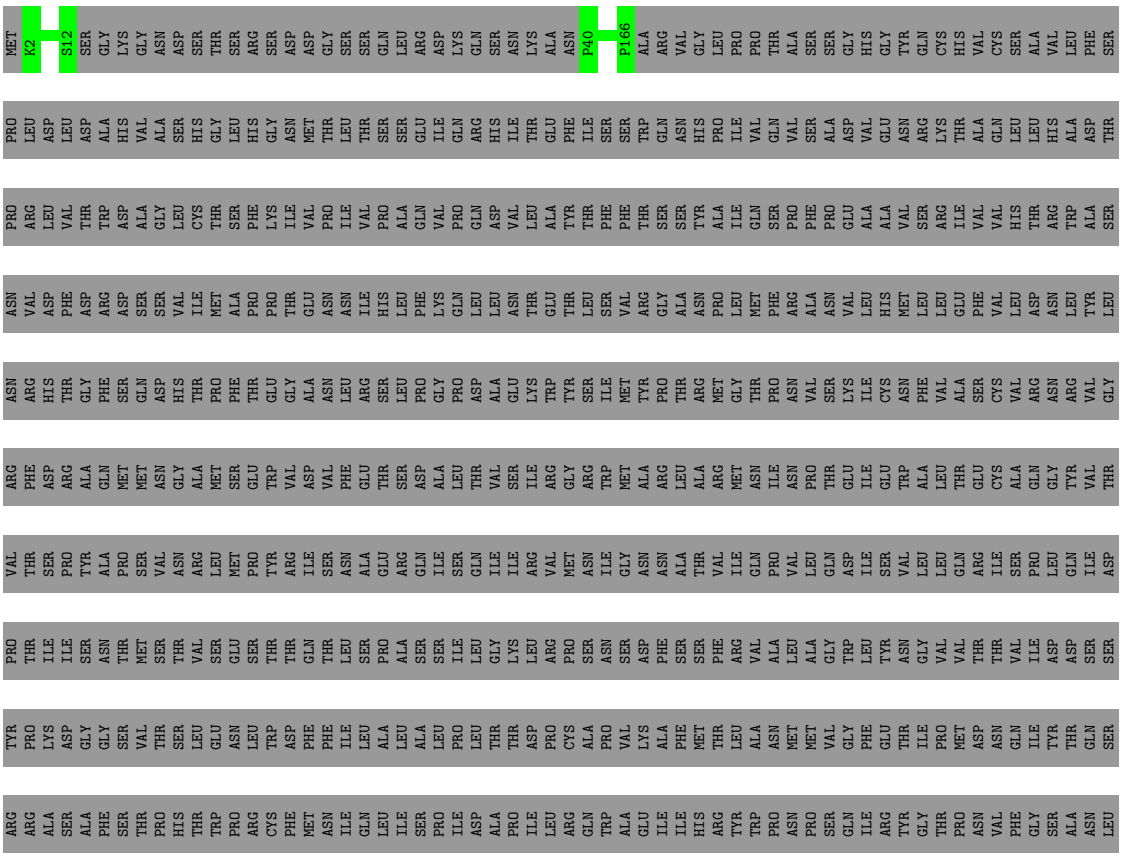
Chain 2: 11% 89%

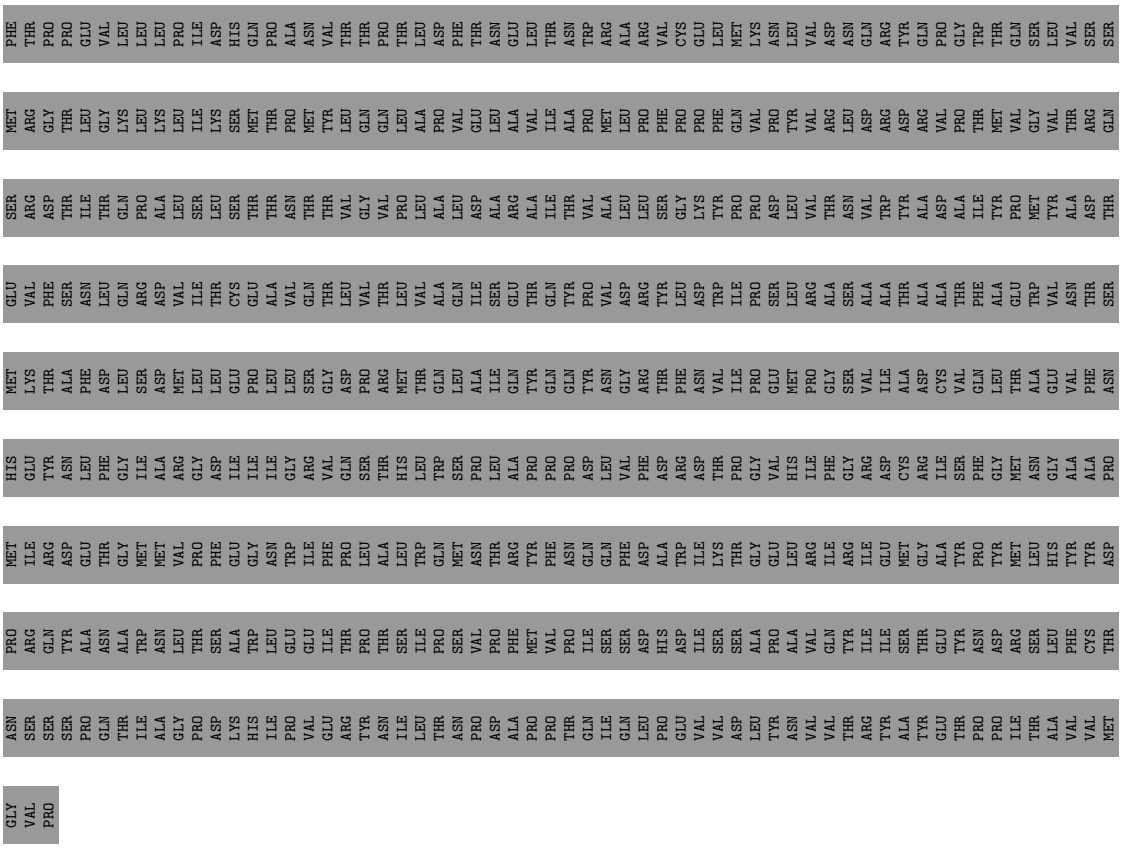




• Molecule 1: RNA helicase

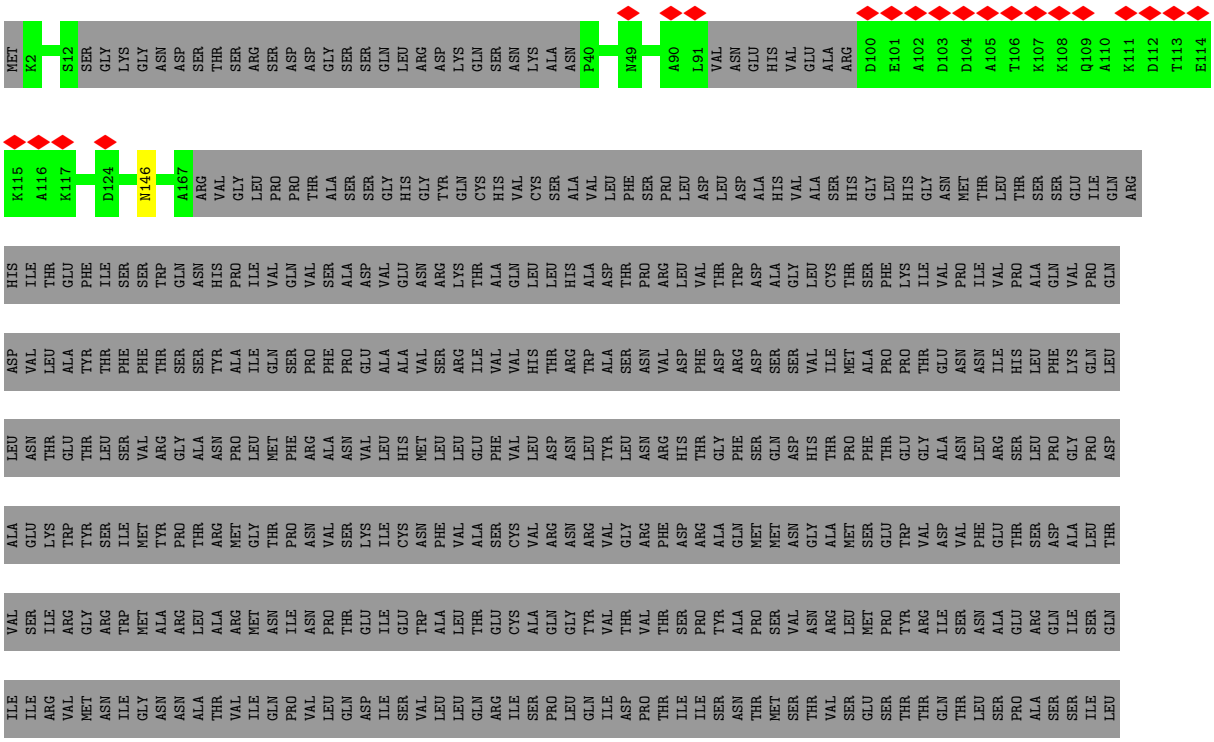
Chain 3: 11% 89%

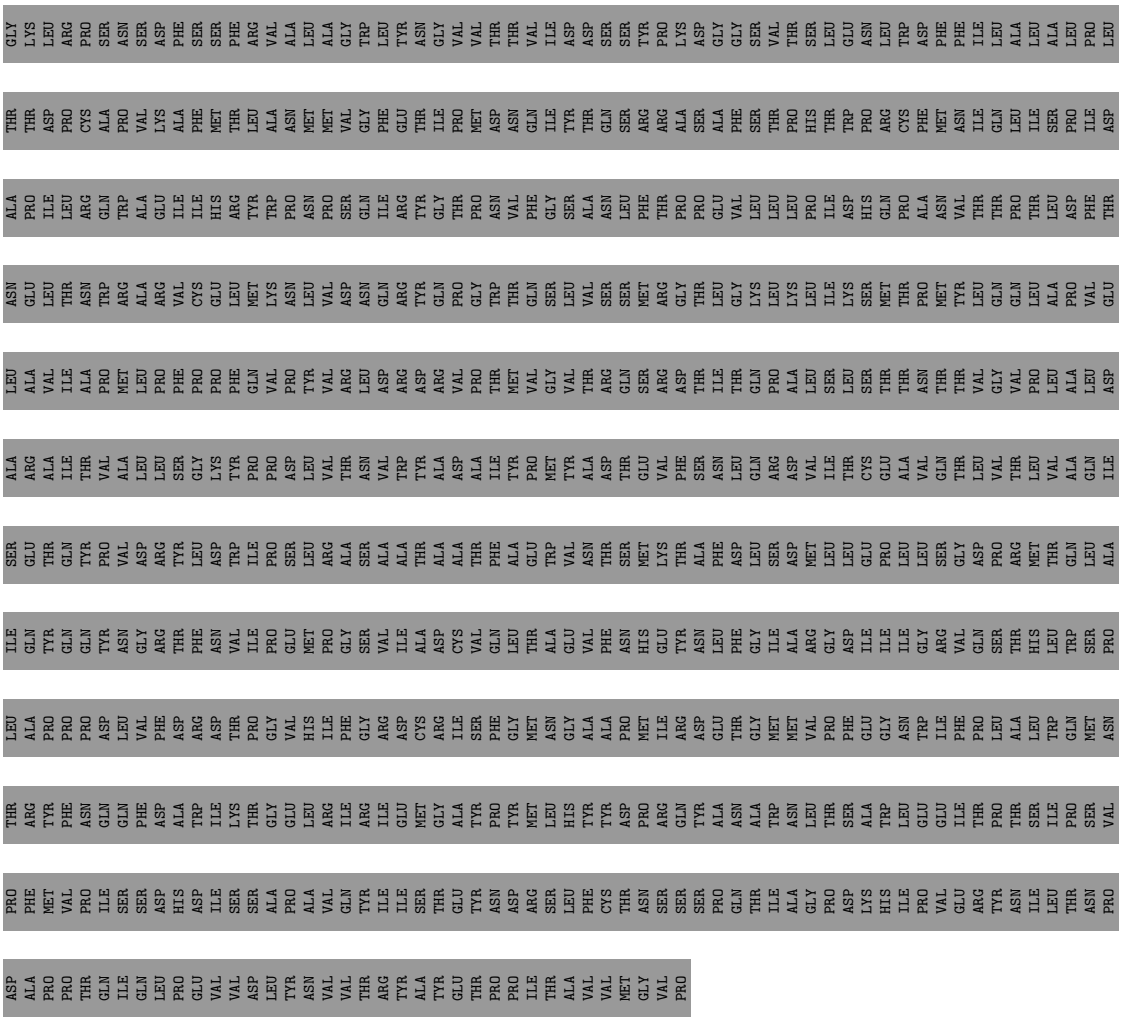




• Molecule 1: RNA helicase

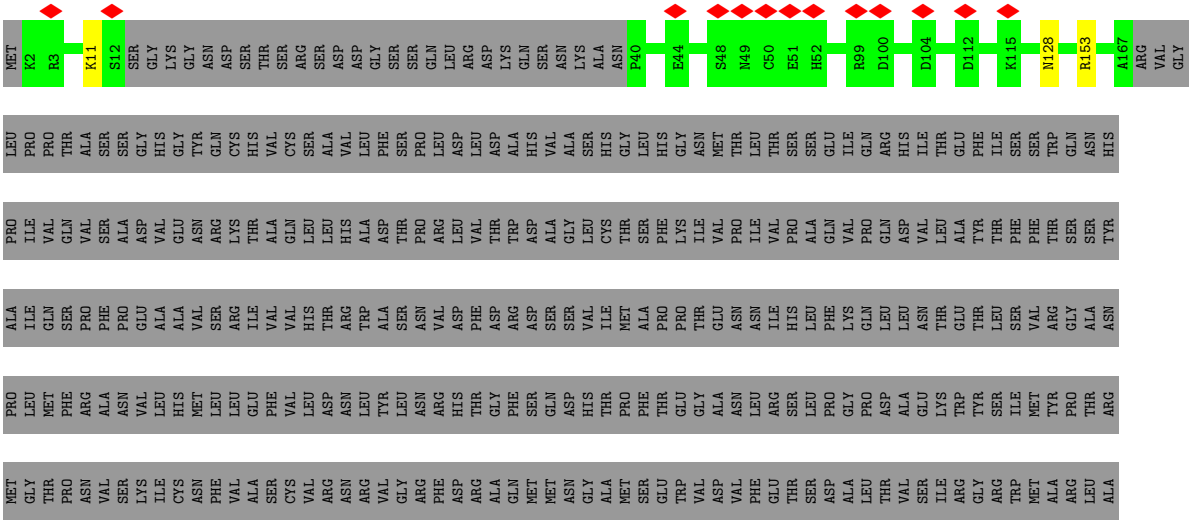
Chain 4:

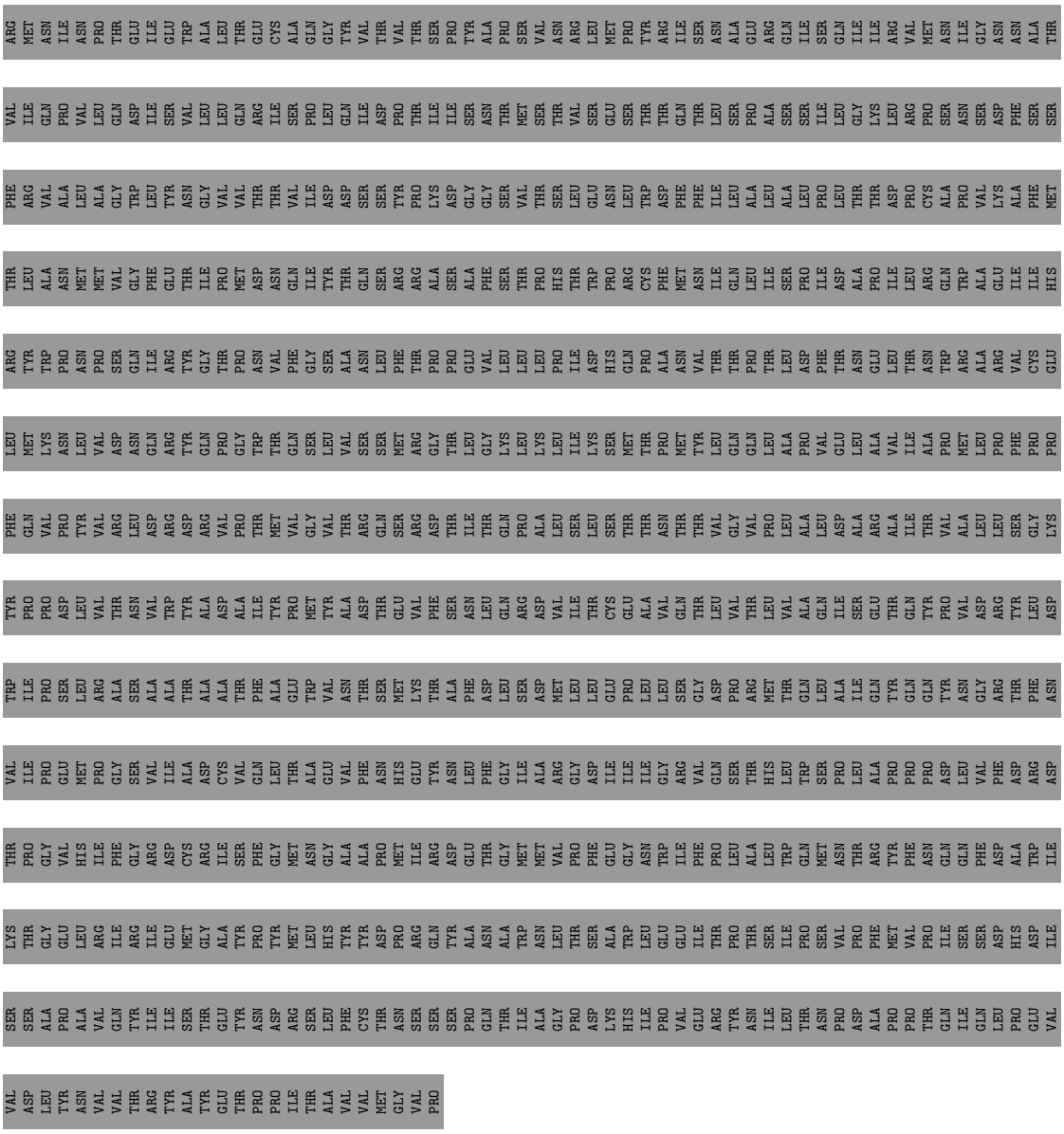




• Molecule 1: RNA helicase

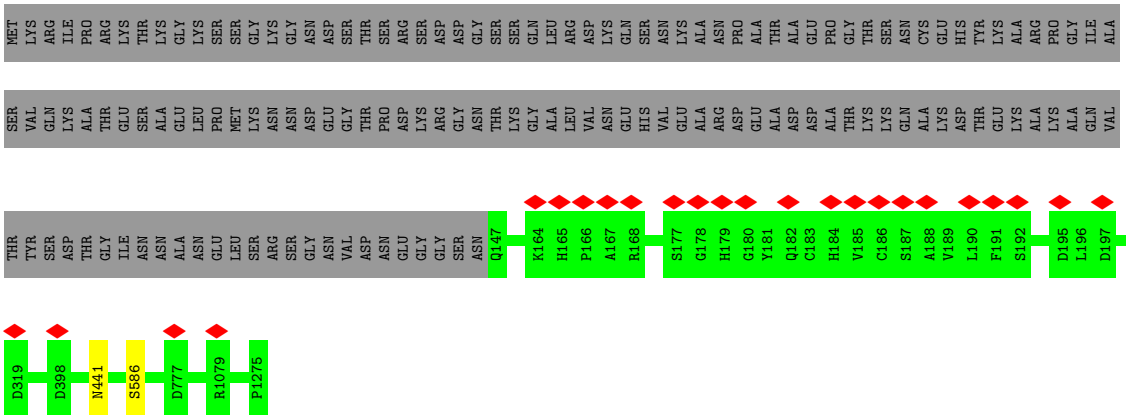
Chain 5:





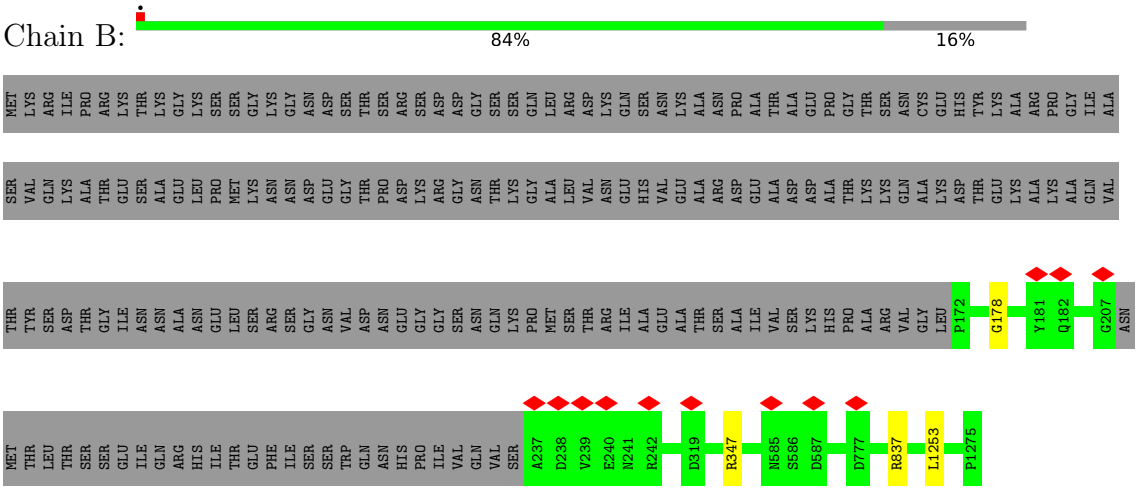
- Molecule 1: RNA helicase

Chain A:



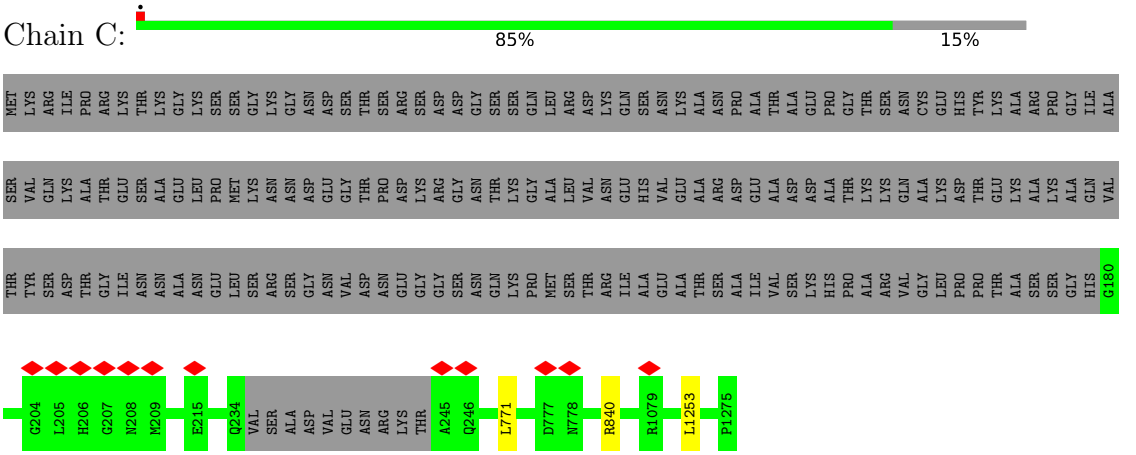
• Molecule 1: RNA helicase

Chain B:



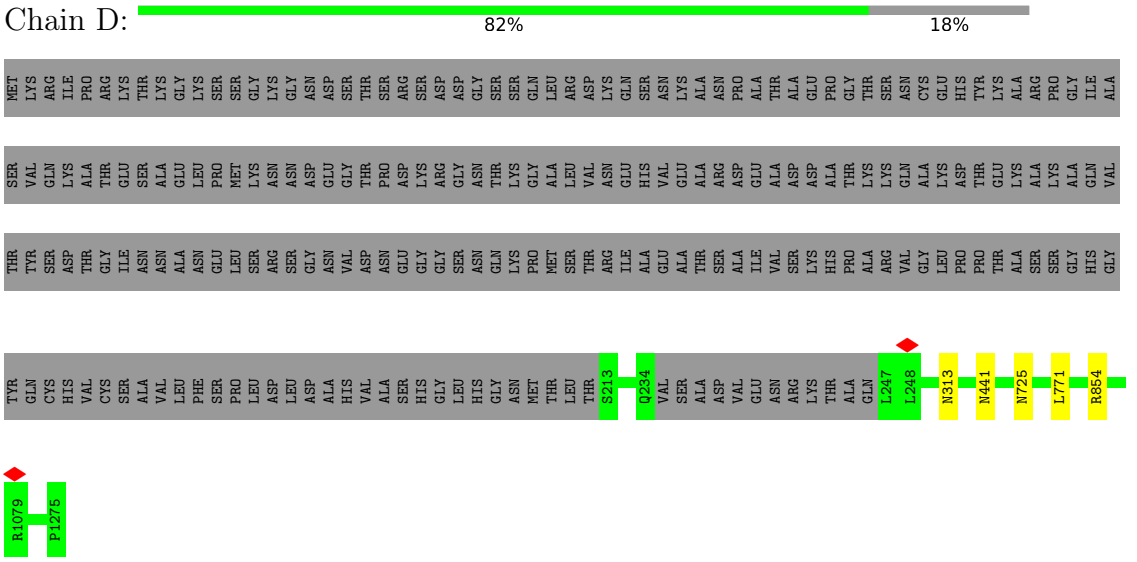
• Molecule 1: RNA helicase

Chain C:



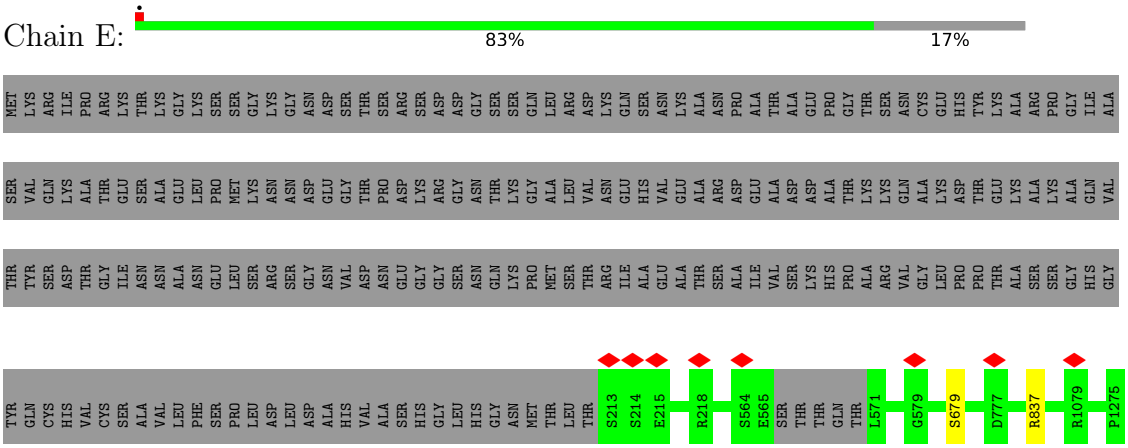
• Molecule 1: RNA helicase

Chain D:



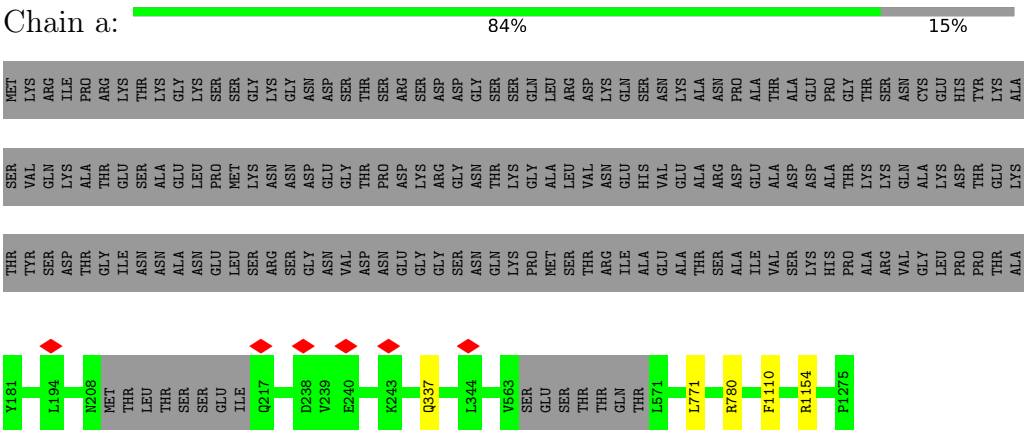
• Molecule 1: RNA helicase

Chain E:



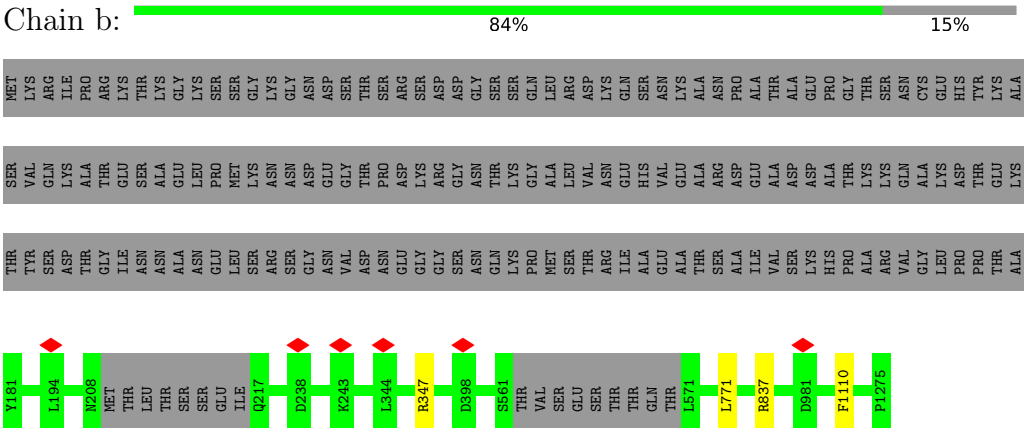
• Molecule 1: RNA helicase

Chain a:



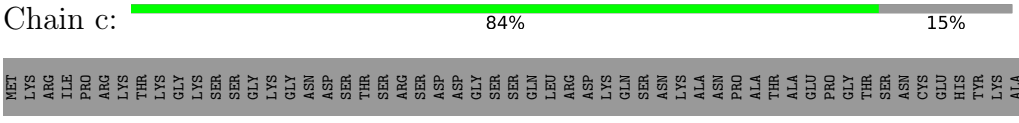
• Molecule 1: RNA helicase

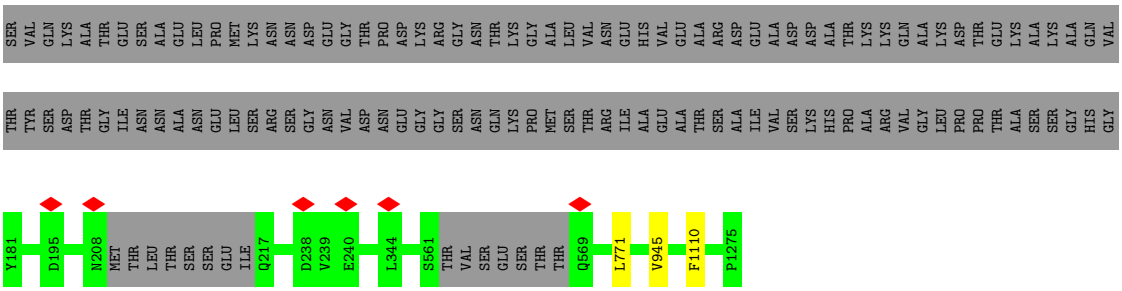
Chain b:



• Molecule 1: RNA helicase

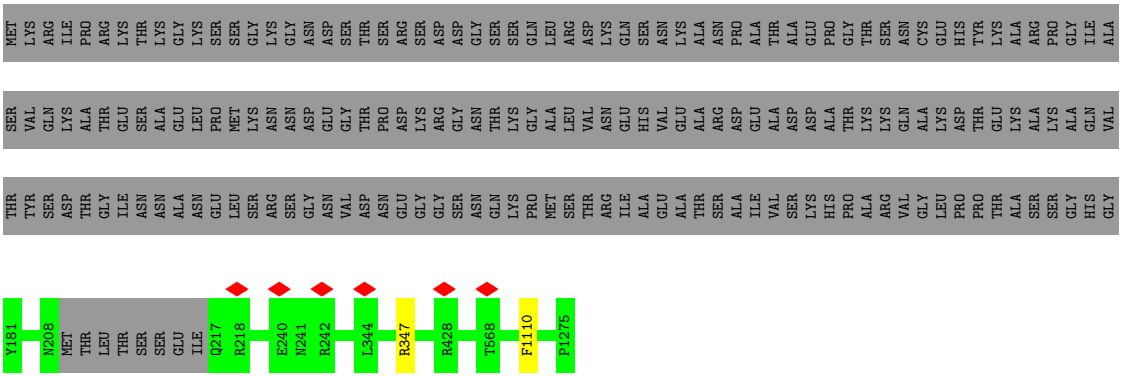
Chain c:





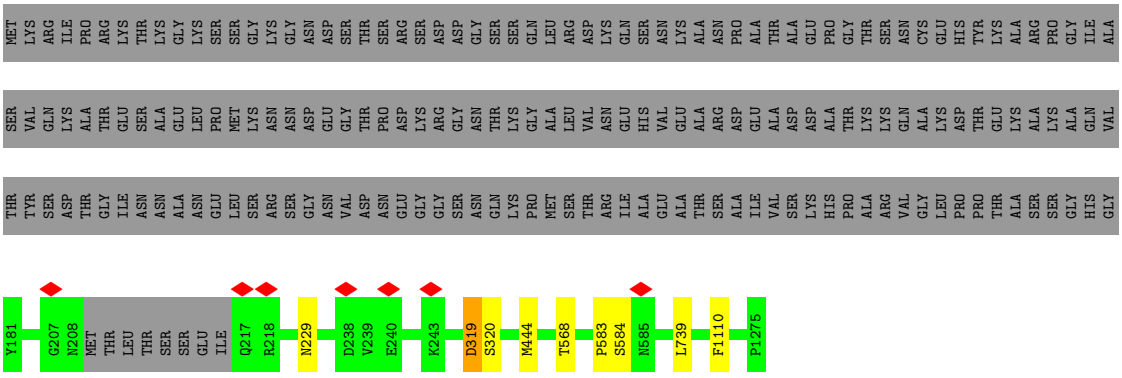
• Molecule 1: RNA helicase

Chain d:



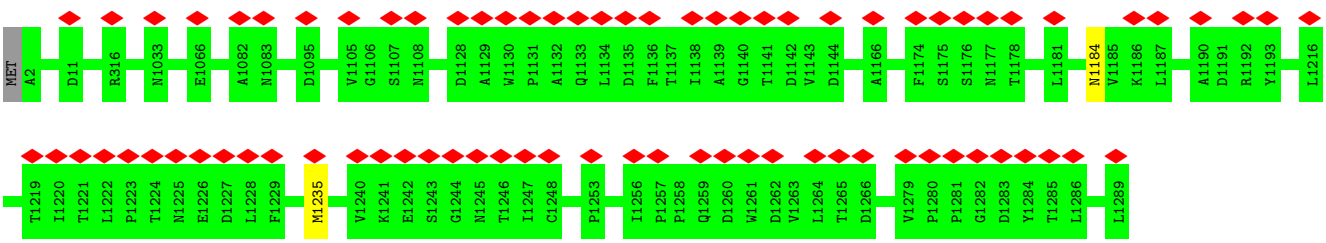
• Molecule 1: RNA helicase

Chain e:



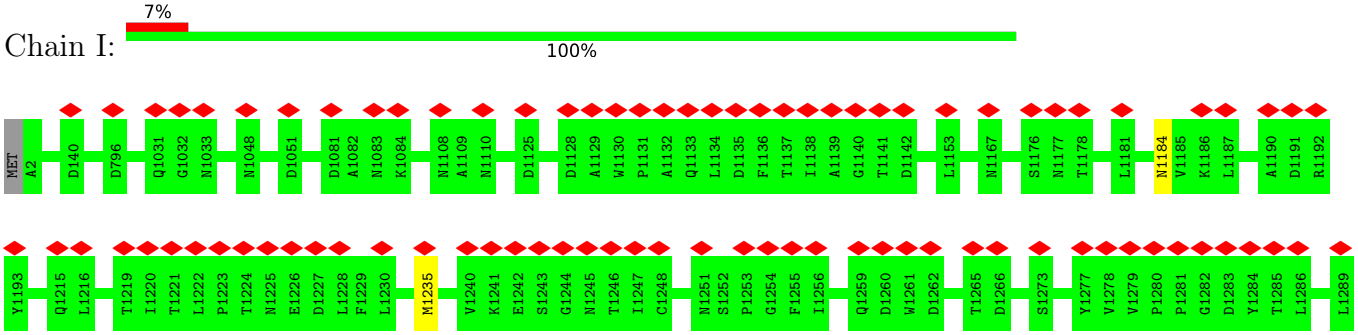
• Molecule 2: Lambda-2 protein

Chain H:



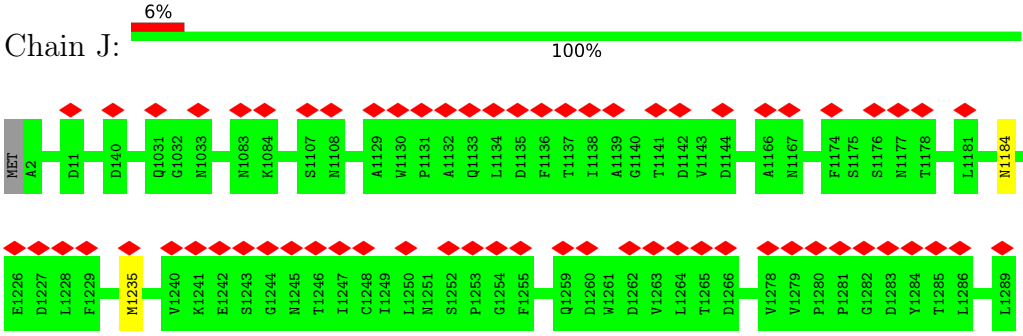
• Molecule 2: Lambda-2 protein

Chain I:



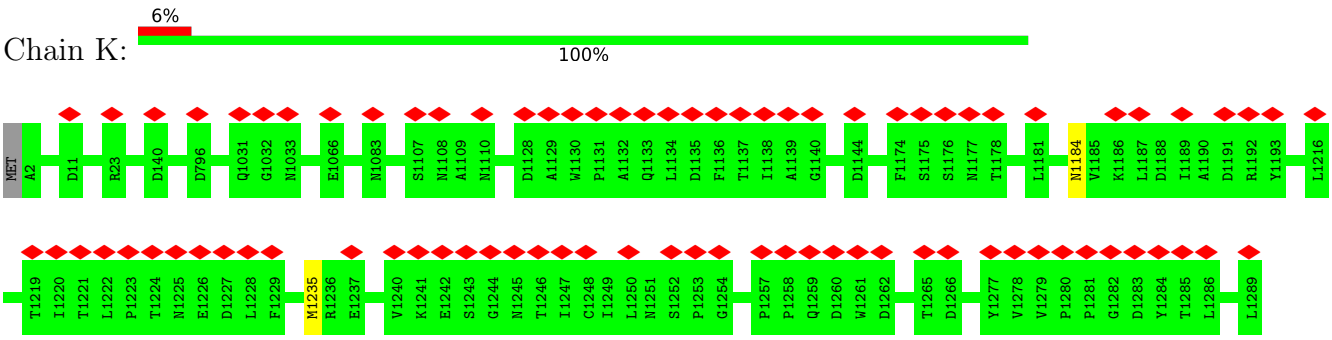
• Molecule 2: Lambda-2 protein

Chain J:



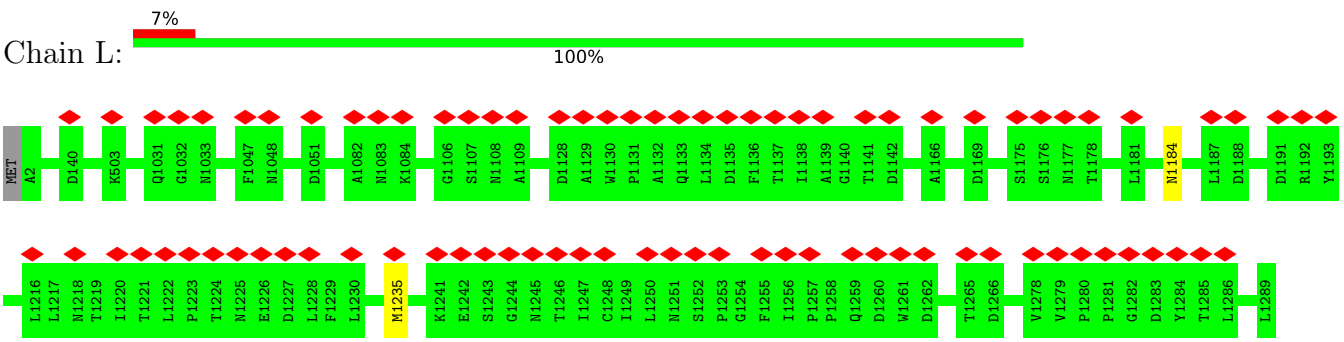
• Molecule 2: Lambda-2 protein

Chain K:



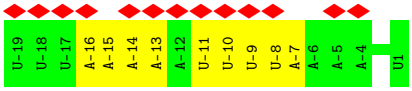
• Molecule 2: Lambda-2 protein

Chain L:



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

Chain M:

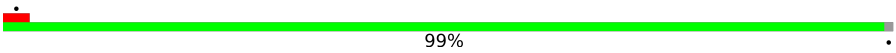


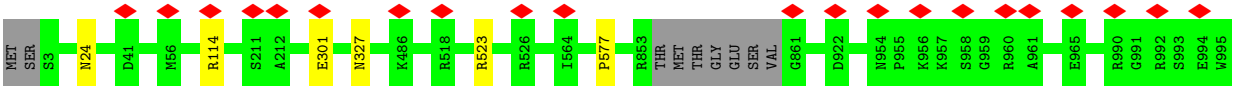
• Molecule 4: RNA (36-MER)

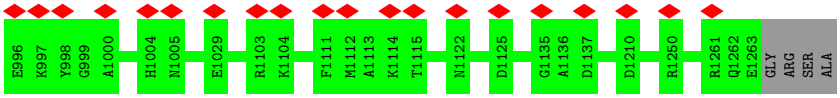
Chain N:

• Molecule 5: RNA-directed RNA polymerase

Chain R:

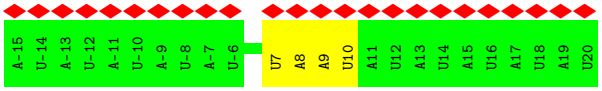






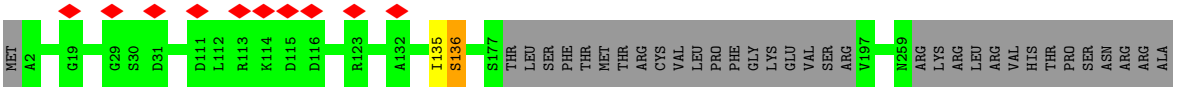
• Molecule 6: RNA (36-MER)

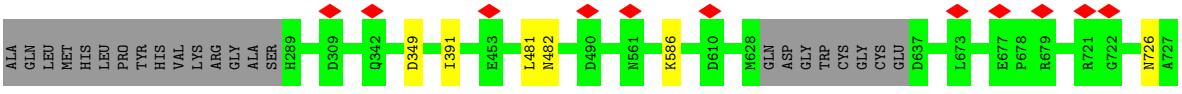
Chain T:

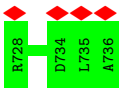


• Molecule 7: Mu-2 protein

Chain U:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100968	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	3.336	Depositor
Minimum map value	-1.852	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.205	Depositor
Recommended contour level	0.5	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, MG, UTP, 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	0.30	0/1046	0.45	0/1405
1	2	0.28	0/1046	0.47	0/1405
1	3	0.29	0/1041	0.46	0/1398
1	4	0.30	0/978	0.48	0/1311
1	5	0.32	0/1046	0.48	0/1405
1	A	0.34	0/9115	0.48	0/12486
1	B	0.33	0/8685	0.49	0/11897
1	C	0.34	0/8796	0.48	1/12049 (0.0%)
1	D	0.34	0/8532	0.48	1/11688 (0.0%)
1	E	0.34	0/8587	0.49	0/11761
1	a	0.33	0/8757	0.48	1/11995 (0.0%)
1	b	0.33	0/8743	0.47	1/11975 (0.0%)
1	c	0.33	0/8759	0.46	1/11997 (0.0%)
1	d	0.33	0/8809	0.47	0/12068
1	e	0.35	0/8809	0.49	3/12068 (0.0%)
2	H	0.30	0/10403	0.47	0/14203
2	I	0.30	0/10403	0.47	0/14203
2	J	0.30	0/10403	0.47	0/14203
2	K	0.30	0/10403	0.47	0/14203
2	L	0.30	0/10403	0.47	0/14203
3	M	0.25	0/494	0.80	0/765
4	N	0.19	0/603	0.72	0/933
5	R	0.32	0/10172	0.47	2/13813 (0.0%)
6	T	0.23	0/842	0.75	0/1306
7	U	0.32	0/5519	0.51	1/7494 (0.0%)
All	All	0.32	0/162394	0.48	11/222234 (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	B	0	1
1	E	0	1
1	a	0	2
1	b	0	1
1	c	0	2
1	d	0	1
1	e	0	2
7	U	0	3
All	All	0	13

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	349	ASP	CB-CG-OD1	7.08	124.67	118.30
1	D	771	LEU	CA-CB-CG	-6.58	100.17	115.30
1	C	771	LEU	CA-CB-CG	-6.00	101.50	115.30
5	R	301	GLU	N-CA-C	5.85	126.81	111.00
1	e	320	SER	N-CA-C	-5.50	96.16	111.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	178	GLY	Peptide
1	E	679	SER	Peptide
7	U	136	SER	Peptide
7	U	391	ILE	Peptide
7	U	586	LYS	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	135/1275 (11%)	122 (90%)	13 (10%)	0	100	100
1	2	135/1275 (11%)	123 (91%)	12 (9%)	0	100	100
1	3	134/1275 (10%)	122 (91%)	12 (9%)	0	100	100
1	4	125/1275 (10%)	111 (89%)	14 (11%)	0	100	100
1	5	135/1275 (11%)	124 (92%)	11 (8%)	0	100	100
1	A	1127/1275 (88%)	1042 (92%)	84 (8%)	1 (0%)	51	85
1	B	1071/1275 (84%)	997 (93%)	73 (7%)	1 (0%)	51	85
1	C	1082/1275 (85%)	997 (92%)	84 (8%)	1 (0%)	51	85
1	D	1047/1275 (82%)	975 (93%)	72 (7%)	0	100	100
1	E	1054/1275 (83%)	974 (92%)	80 (8%)	0	100	100
1	a	1074/1275 (84%)	1015 (94%)	59 (6%)	0	100	100
1	b	1072/1275 (84%)	1003 (94%)	69 (6%)	0	100	100
1	c	1074/1275 (84%)	1008 (94%)	66 (6%)	0	100	100
1	d	1083/1275 (85%)	1019 (94%)	64 (6%)	0	100	100
1	e	1083/1275 (85%)	1004 (93%)	77 (7%)	2 (0%)	47	82
2	H	1286/1289 (100%)	1154 (90%)	132 (10%)	0	100	100
2	I	1286/1289 (100%)	1156 (90%)	130 (10%)	0	100	100
2	J	1286/1289 (100%)	1155 (90%)	131 (10%)	0	100	100
2	K	1286/1289 (100%)	1156 (90%)	130 (10%)	0	100	100
2	L	1286/1289 (100%)	1154 (90%)	132 (10%)	0	100	100
5	R	1250/1267 (99%)	1161 (93%)	89 (7%)	0	100	100
7	U	671/736 (91%)	569 (85%)	98 (15%)	4 (1%)	25	64
All	All	19782/27573 (72%)	18141 (92%)	1632 (8%)	9 (0%)	100	100

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1253	LEU
7	U	481	LEU
1	A	586	SER
1	C	1253	LEU
7	U	136	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	111/1113 (10%)	109 (98%)	2 (2%)	59	85
1	2	111/1113 (10%)	111 (100%)	0	100	100
1	3	111/1113 (10%)	111 (100%)	0	100	100
1	4	104/1113 (9%)	103 (99%)	1 (1%)	76	91
1	5	111/1113 (10%)	108 (97%)	3 (3%)	44	77
1	A	995/1113 (89%)	994 (100%)	1 (0%)	93	98
1	B	946/1113 (85%)	944 (100%)	2 (0%)	93	98
1	C	960/1113 (86%)	959 (100%)	1 (0%)	93	98
1	D	932/1113 (84%)	928 (100%)	4 (0%)	91	97
1	E	937/1113 (84%)	936 (100%)	1 (0%)	93	98
1	a	954/1113 (86%)	952 (100%)	2 (0%)	93	98
1	b	952/1113 (86%)	950 (100%)	2 (0%)	93	98
1	c	954/1113 (86%)	954 (100%)	0	100	100
1	d	961/1113 (86%)	960 (100%)	1 (0%)	93	98
1	e	961/1113 (86%)	958 (100%)	3 (0%)	92	97
2	H	1117/1118 (100%)	1115 (100%)	2 (0%)	93	98
2	I	1117/1118 (100%)	1115 (100%)	2 (0%)	93	98
2	J	1117/1118 (100%)	1115 (100%)	2 (0%)	93	98
2	K	1117/1118 (100%)	1115 (100%)	2 (0%)	93	98
2	L	1117/1118 (100%)	1115 (100%)	2 (0%)	93	98
5	R	1074/1084 (99%)	1070 (100%)	4 (0%)	91	97
7	U	600/650 (92%)	599 (100%)	1 (0%)	93	98
All	All	17359/24019 (72%)	17321 (100%)	38 (0%)	93	98

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	523	ARG
1	e	229	ASN
7	U	726	ASN
1	b	347	ARG
1	e	444	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	726	ASN
1	e	217	GLN
1	a	313	ASN
1	b	929	GLN
1	e	731	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	20/21 (95%)	9 (45%)	1 (5%)
4	N	24/36 (66%)	0	0
6	T	35/36 (97%)	4 (11%)	1 (2%)
All	All	79/93 (84%)	13 (16%)	2 (2%)

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	-16	A
3	M	-15	A
3	M	-14	A
3	M	-13	A
3	M	-11	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	M	-8	U
6	T	9	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
9	SAM	H	1302	-	24,29,29	3.79	9 (37%)	23,42,42	3.37	9 (39%)
9	SAM	J	1302	-	24,29,29	1.01	2 (8%)	23,42,42	1.75	5 (21%)
11	UTP	R	1301	12	22,30,30	3.63	5 (22%)	27,47,47	2.34	7 (25%)
10	GTP	K	1303	-	26,34,34	3.49	9 (34%)	32,54,54	3.42	10 (31%)
10	GTP	H	1303	-	26,34,34	3.48	9 (34%)	32,54,54	3.42	10 (31%)
9	SAM	K	1301	-	24,29,29	3.79	9 (37%)	23,42,42	3.37	9 (39%)
10	GTP	I	1302	-	26,34,34	3.50	9 (34%)	32,54,54	3.42	10 (31%)
9	SAM	I	1301	-	24,29,29	1.06	3 (12%)	23,42,42	1.87	6 (26%)
10	GTP	J	1303	-	26,34,34	3.49	9 (34%)	32,54,54	3.42	10 (31%)
9	SAM	L	1302	-	24,29,29	1.05	3 (12%)	23,42,42	1.50	4 (17%)
9	SAM	L	1303	-	24,29,29	3.79	9 (37%)	23,42,42	3.38	9 (39%)
10	GTP	L	1301	-	26,34,34	3.49	9 (34%)	32,54,54	3.42	10 (31%)
9	SAM	H	1301	-	24,29,29	1.05	3 (12%)	23,42,42	1.49	5 (21%)
9	SAM	J	1301	-	24,29,29	3.79	9 (37%)	23,42,42	3.38	9 (39%)
9	SAM	I	1303	-	24,29,29	3.79	9 (37%)	23,42,42	3.37	9 (39%)
9	SAM	K	1302	-	24,29,29	0.99	1 (4%)	23,42,42	1.89	5 (21%)

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
9	SAM	H	1302	-	-	4/12/33/33	0/3/3/3
9	SAM	J	1302	-	-	4/12/33/33	0/3/3/3
11	UTP	R	1301	12	-	1/20/38/38	0/2/2/2
10	GTP	K	1303	-	-	2/18/38/38	0/3/3/3
10	GTP	H	1303	-	-	2/18/38/38	0/3/3/3
9	SAM	K	1301	-	-	4/12/33/33	0/3/3/3
10	GTP	I	1302	-	-	2/18/38/38	0/3/3/3
9	SAM	I	1301	-	-	5/12/33/33	0/3/3/3
10	GTP	J	1303	-	-	2/18/38/38	0/3/3/3
9	SAM	L	1302	-	-	3/12/33/33	0/3/3/3
9	SAM	L	1303	-	-	4/12/33/33	0/3/3/3
10	GTP	L	1301	-	-	2/18/38/38	0/3/3/3
9	SAM	H	1301	-	-	4/12/33/33	0/3/3/3
9	SAM	J	1301	-	-	4/12/33/33	0/3/3/3
9	SAM	I	1303	-	-	4/12/33/33	0/3/3/3
9	SAM	K	1302	-	-	4/12/33/33	0/3/3/3

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	1301	UTP	C6-N1	10.08	1.48	1.35
9	I	1303	SAM	C2-N3	10.04	1.48	1.32
9	L	1303	SAM	C2-N3	10.02	1.48	1.32
9	J	1301	SAM	C2-N3	10.01	1.48	1.32
9	H	1302	SAM	C2-N3	10.00	1.48	1.32

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	1303	GTP	O6-C6-N1	-9.07	109.94	120.65
9	L	1303	SAM	N3-C2-N1	-9.06	114.53	128.68
10	I	1302	GTP	O6-C6-N1	-9.05	109.96	120.65
9	J	1301	SAM	N3-C2-N1	-9.05	114.53	128.68
9	H	1302	SAM	N3-C2-N1	-9.04	114.55	128.68

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

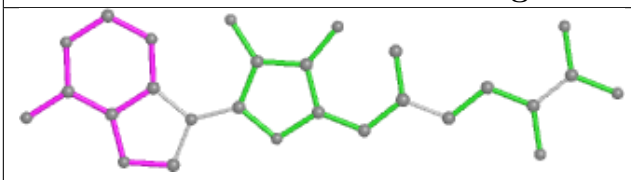
Mol	Chain	Res	Type	Atoms
9	H	1302	SAM	O-C-CA-N
9	I	1301	SAM	N-CA-CB-CG
9	I	1303	SAM	O-C-CA-N
9	J	1301	SAM	O-C-CA-N
9	J	1302	SAM	CA-CB-CG-SD

There are no ring outliers.

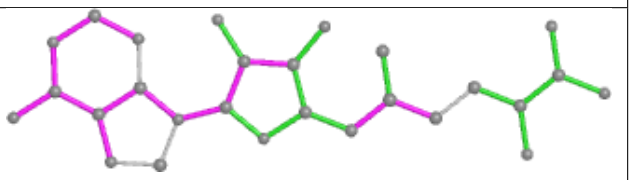
No monomer is involved in short contacts.

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.

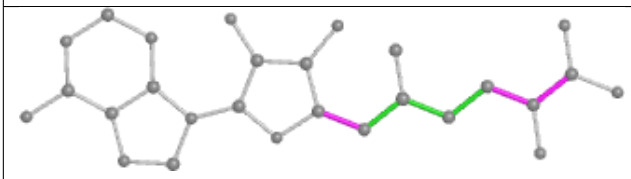
Ligand SAM H 1302



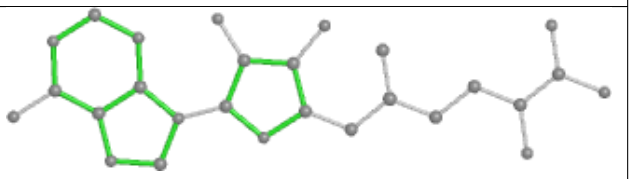
Bond lengths



Bond angles

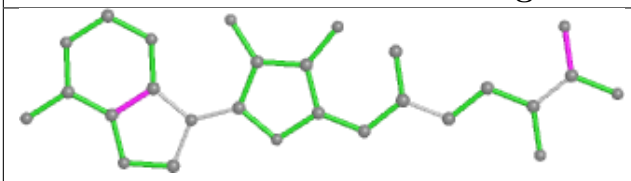


Torsions



Rings

Ligand SAM J 1302



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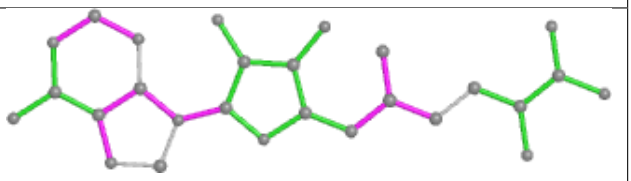
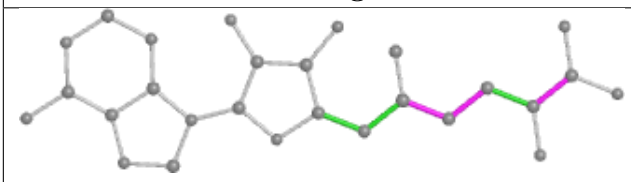
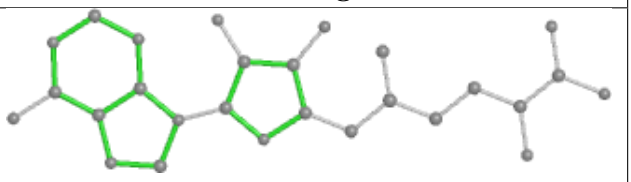


Bond angles

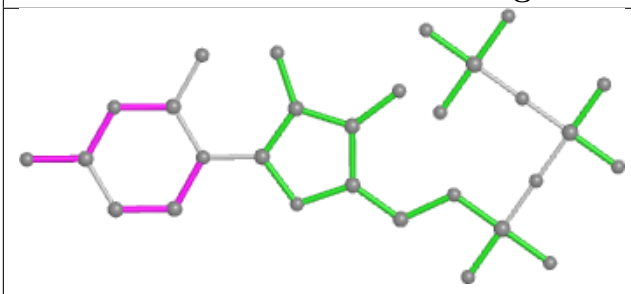


Torsions



Rings

Ligand UTP R 1301



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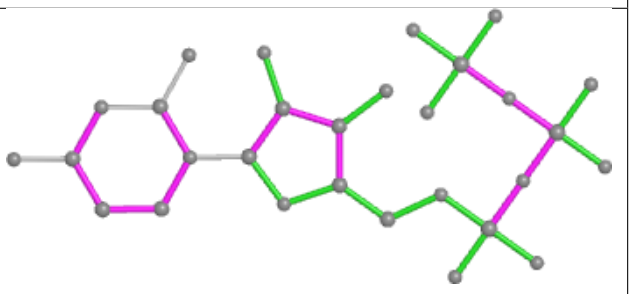
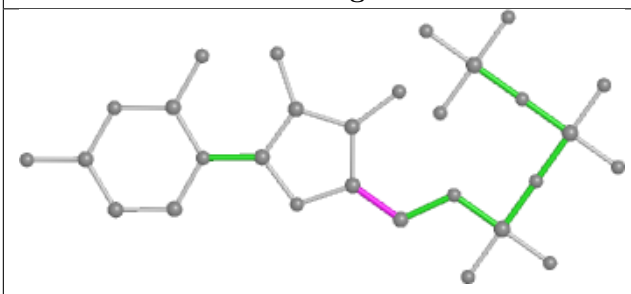


Bond angles



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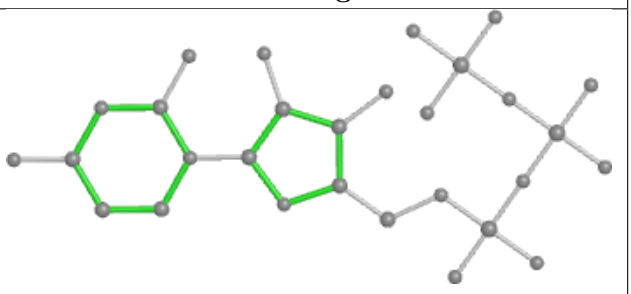
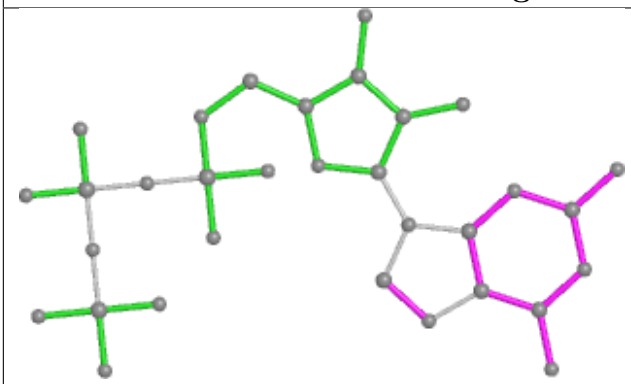
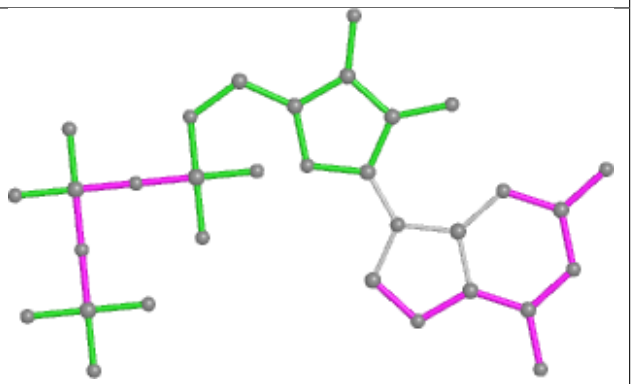


Rings

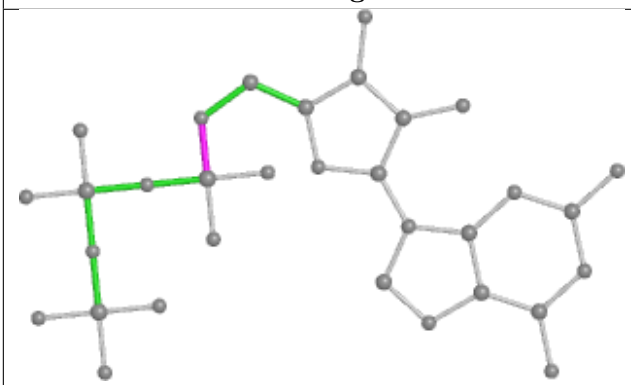
Ligand GTP K 1303



Bond lengths



Bond angles



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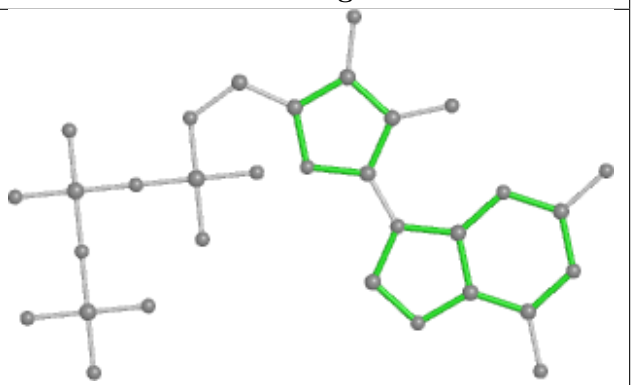
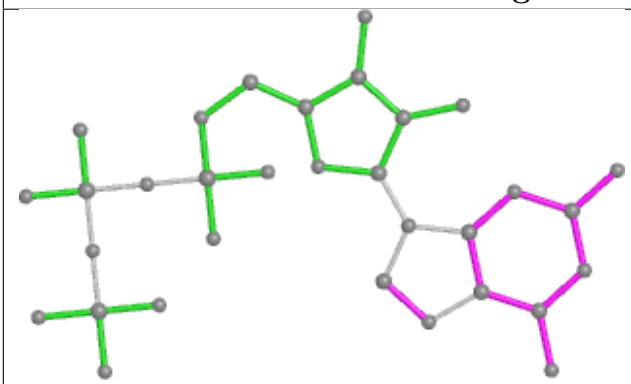


Rings

Ligand GTP H 1303



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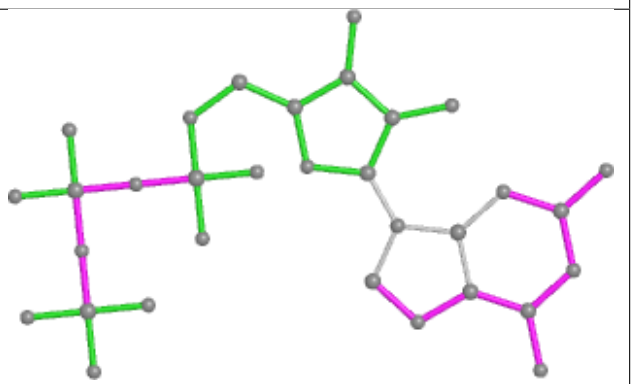

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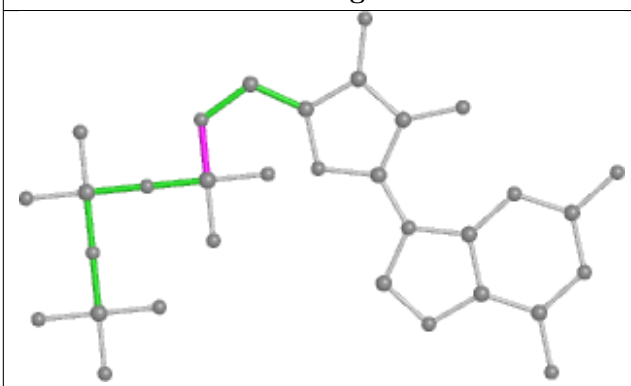

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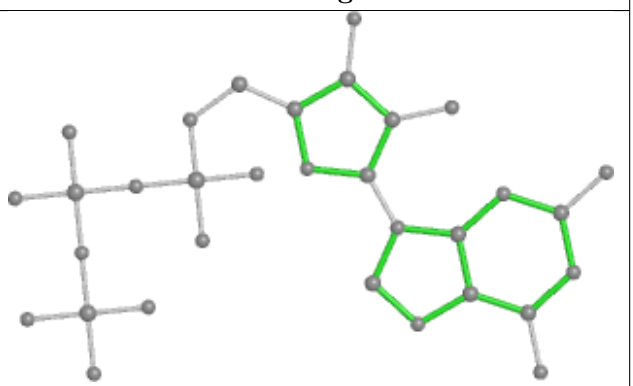
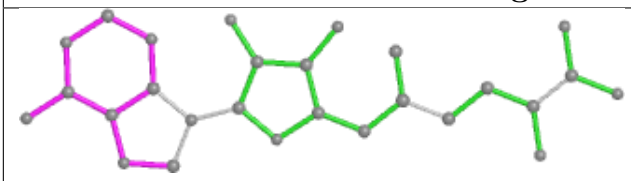


Rings

Ligand SAM K 1301



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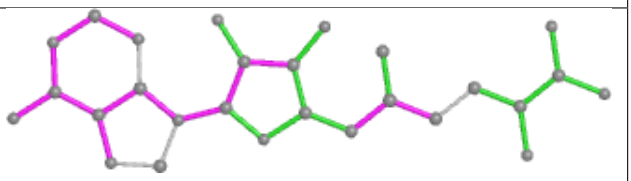

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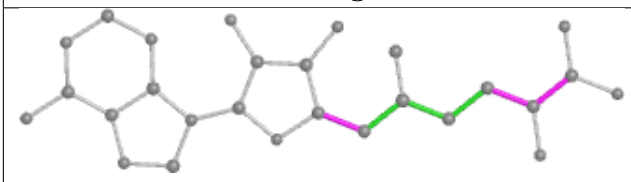

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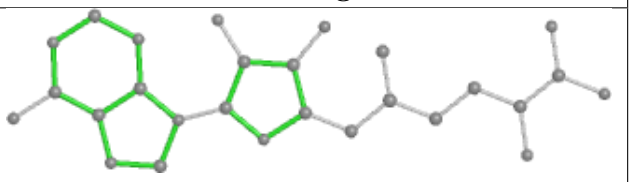
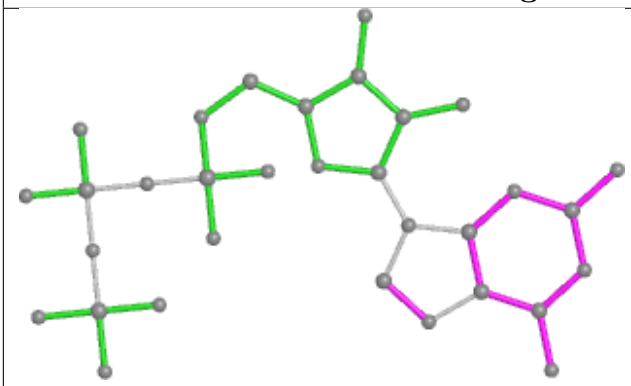


Rings

Ligand GTP I 1302



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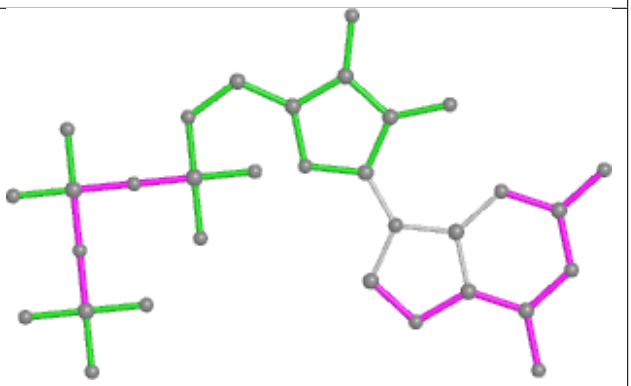

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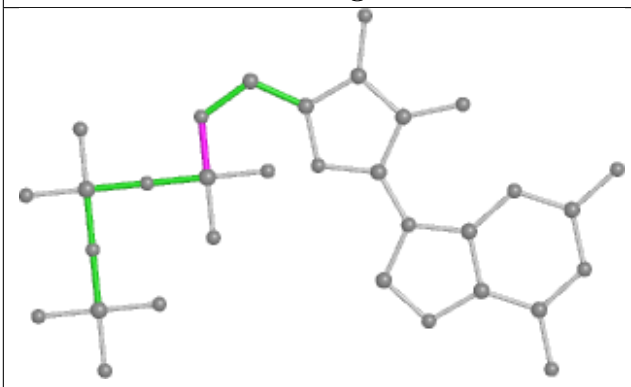

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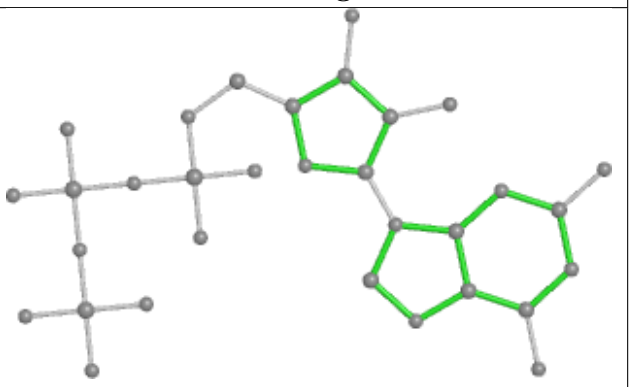

Rings

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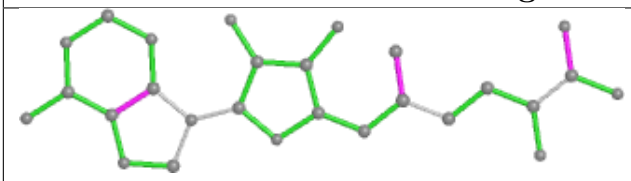

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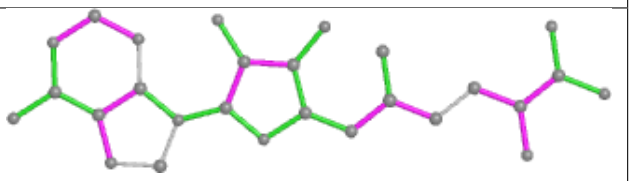

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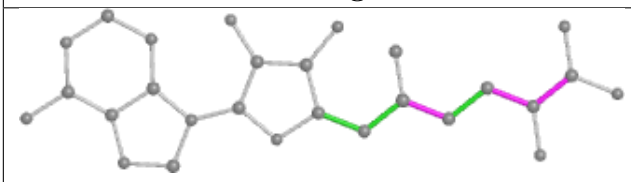

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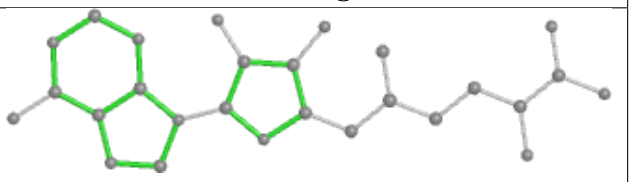
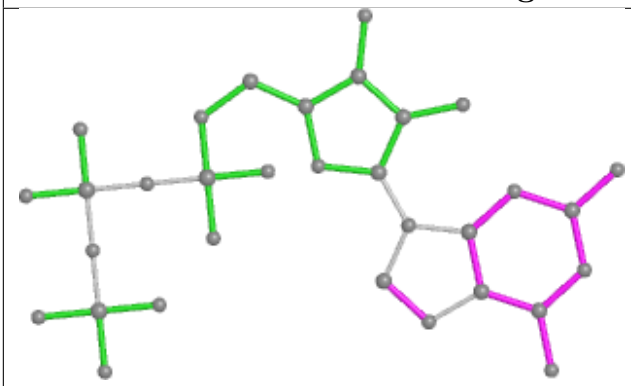


Rings

Ligand GTP J 1303



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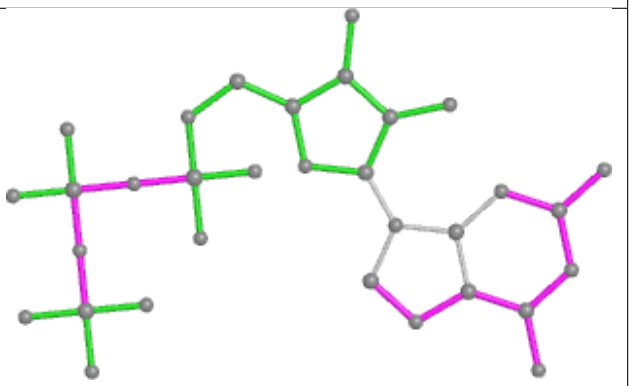
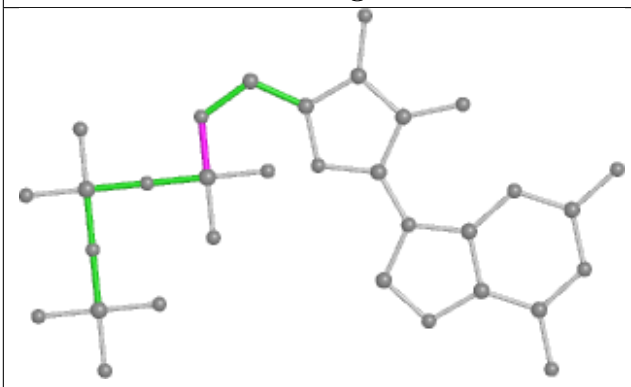


Bond angles



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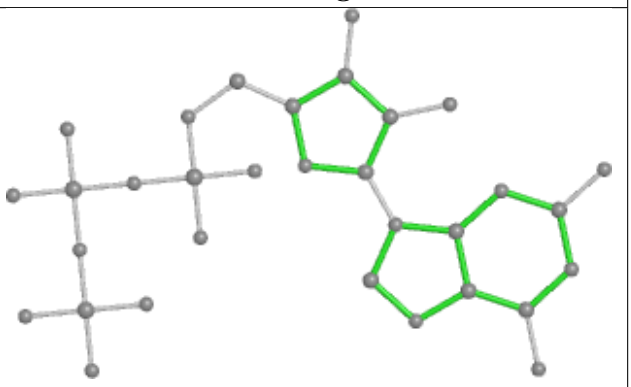
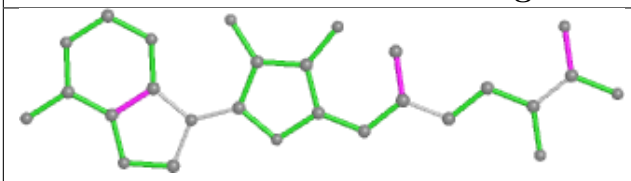
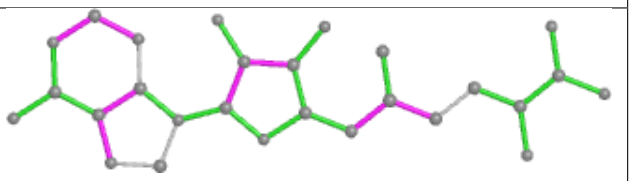
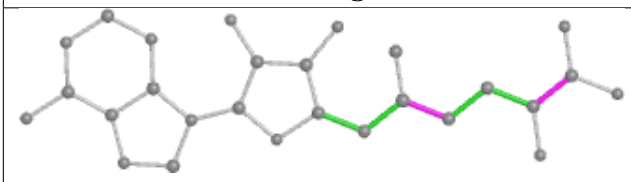
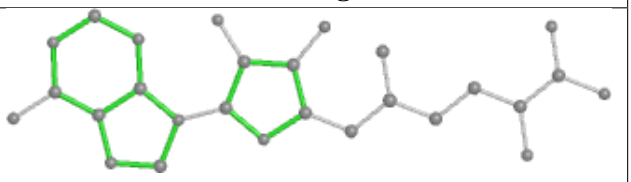


Rings

Ligand SAM L 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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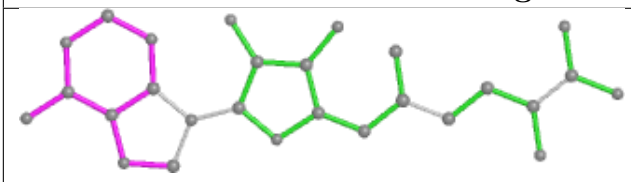
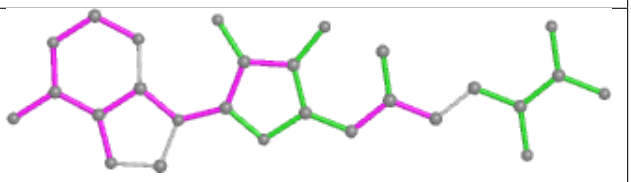
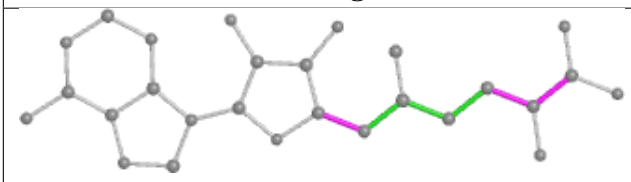
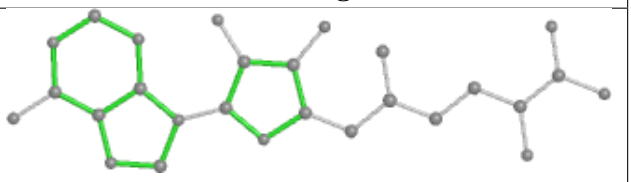
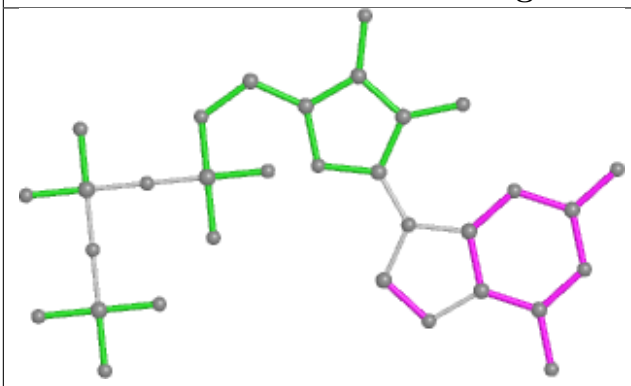
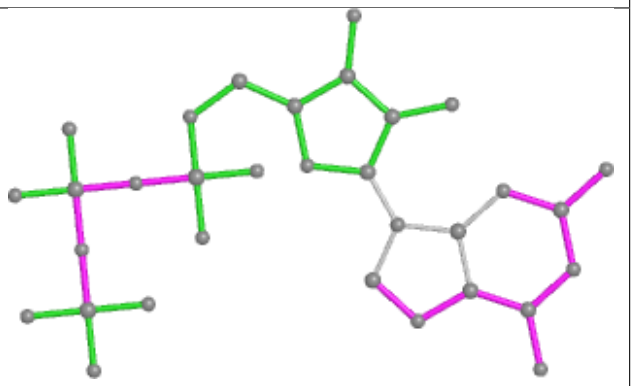
 Bond lengths	 Bond angles
 Torsions	 Rings

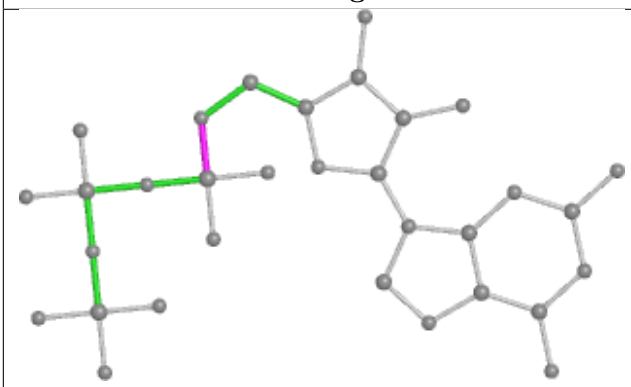
Ligand GTP L 1301



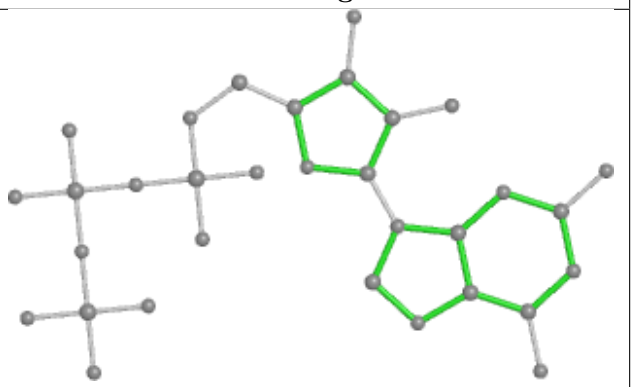
Bond lengths



Bond angles

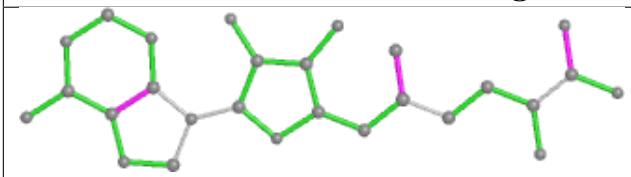


Torsions



Rings

Ligand SAM H 1301



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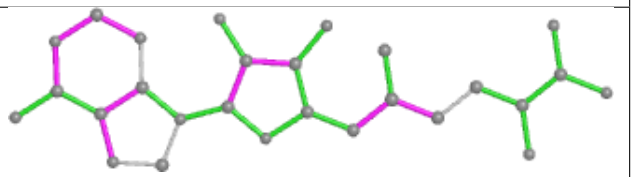
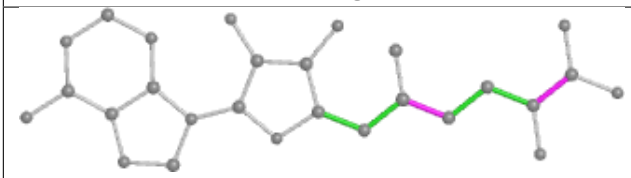


Bond angles



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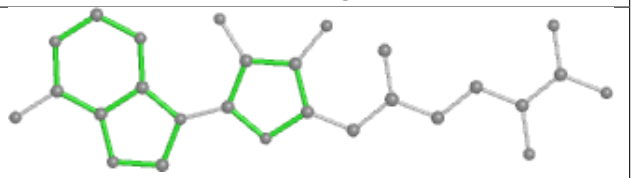
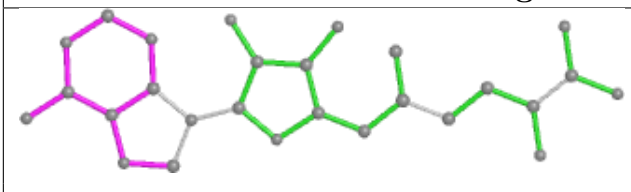


Rings

Ligand SAM J 1301



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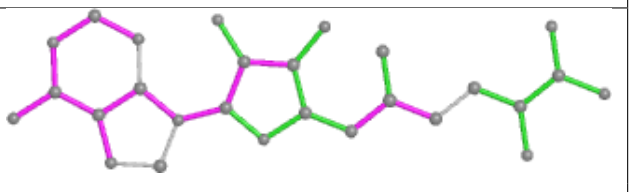
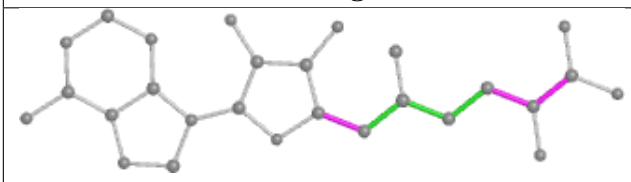
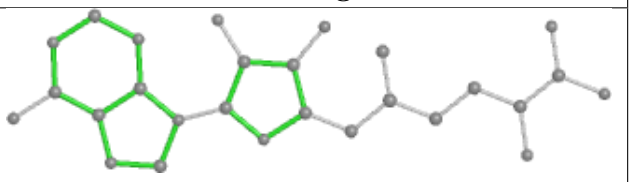


Bond angles

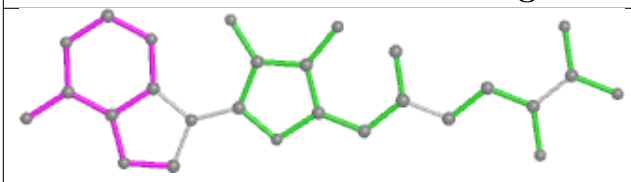


Torsions

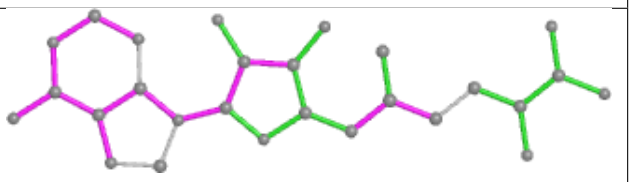


Rings

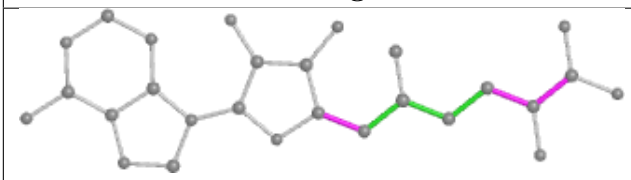
Ligand SAM I 1303



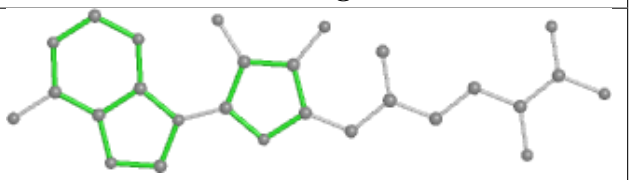
Bond lengths



Bond angles

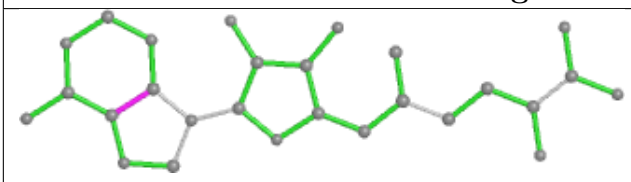


Torsions

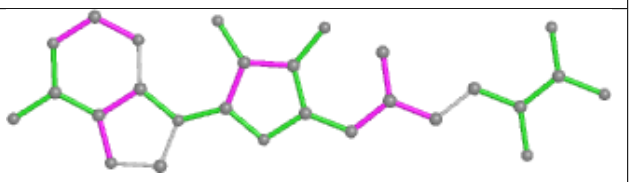


Rings

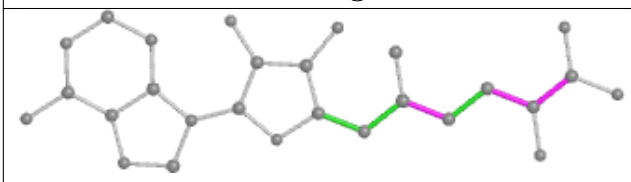
Ligand SAM K 1302



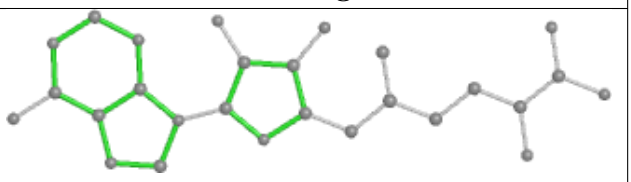
Bond lengths



Bond angles



Torsions



Rings

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.

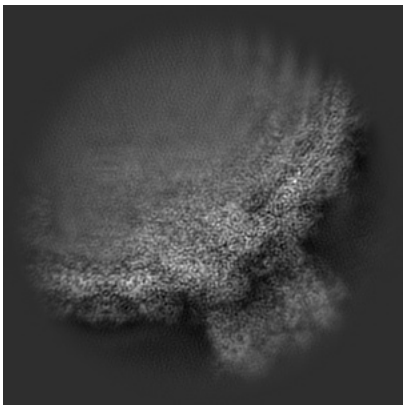
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33770. These allow visual inspection of the internal detail of the map and identification of artifacts.

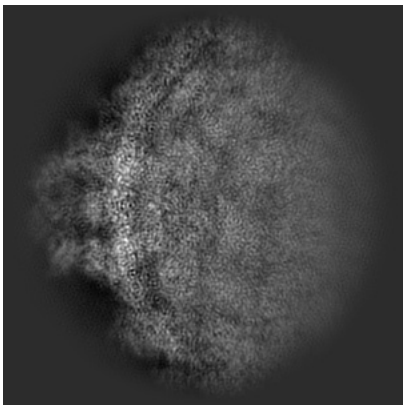
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

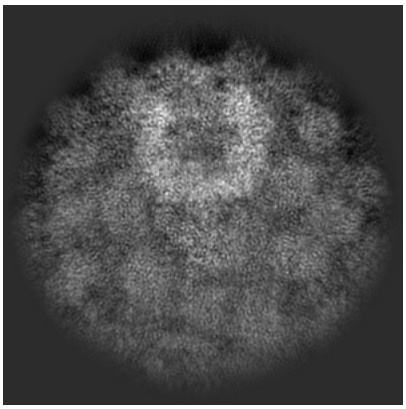
6.1.1 Primary map



X

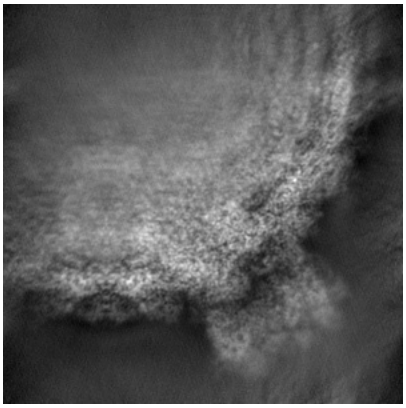


Y

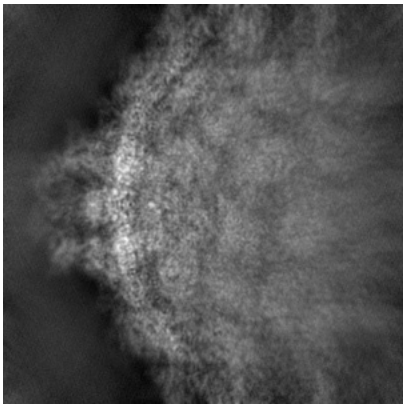


Z

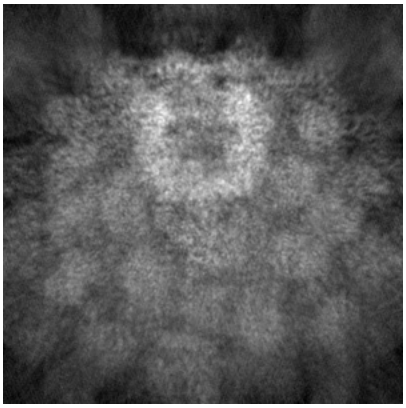
6.1.2 Raw map



X



Y

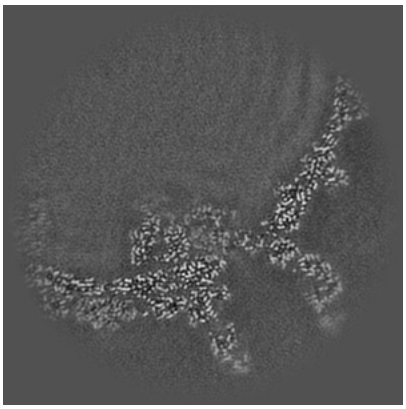


Z

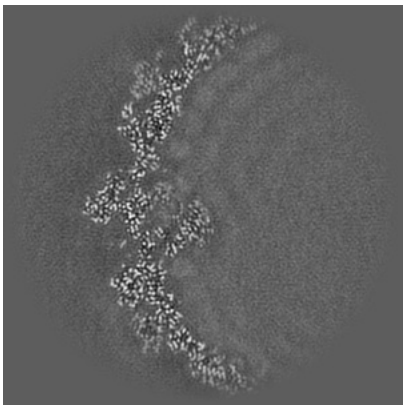
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

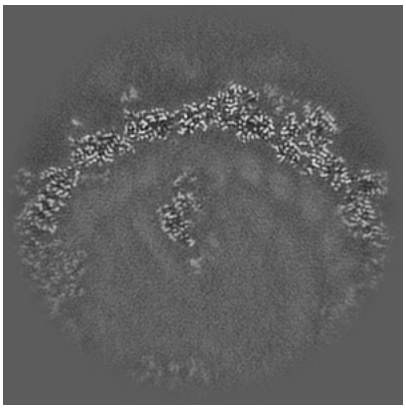
6.2.1 Primary map



X Index: 160

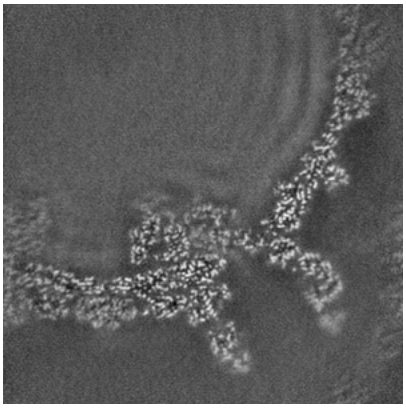


Y Index: 160

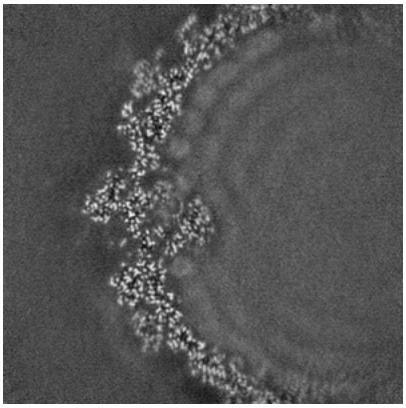


Z Index: 160

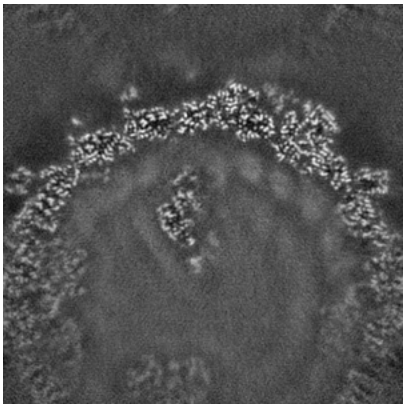
6.2.2 Raw map



X Index: 160



Y Index: 160

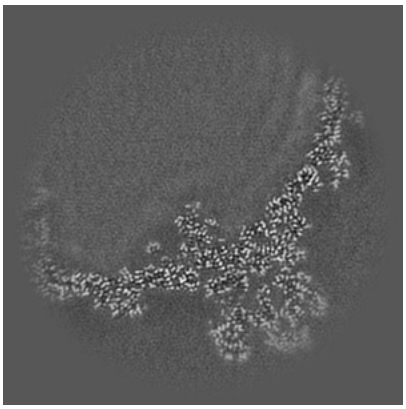


Z Index: 160

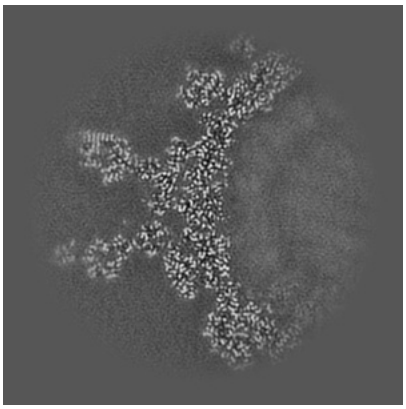
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

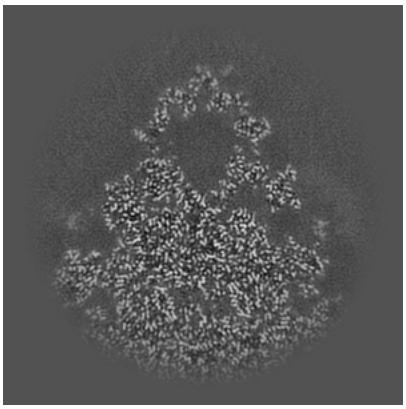
6.3.1 Primary map



X Index: 125

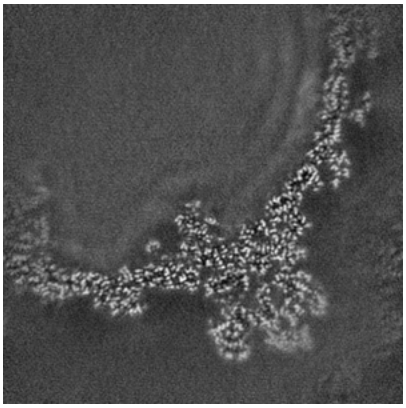


Y Index: 227

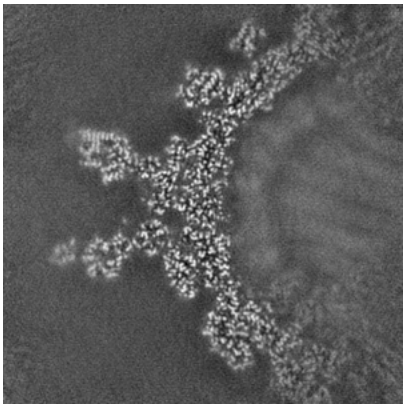


Z Index: 99

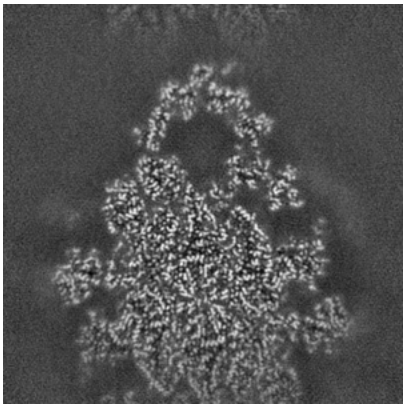
6.3.2 Raw map



X Index: 125



Y Index: 227

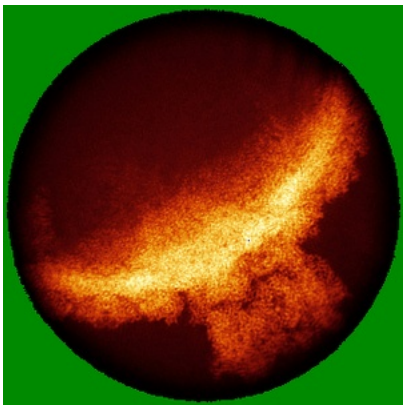


Z Index: 97

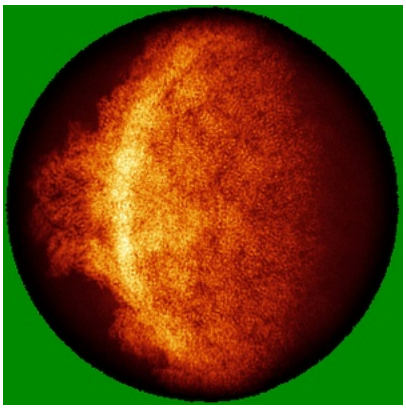
The images above show the largest variance slices of the map in three orthogonal directions.

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

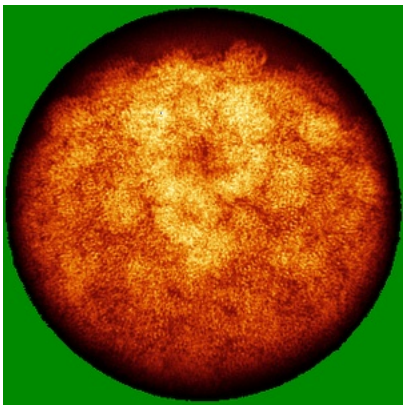
6.4.1 Primary map



X

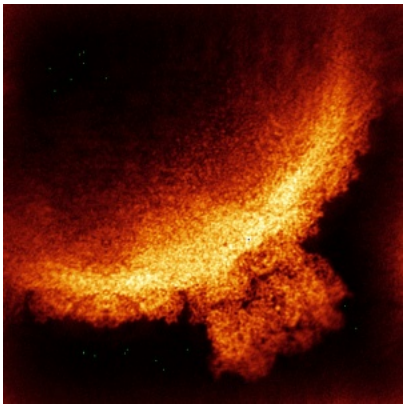


Y

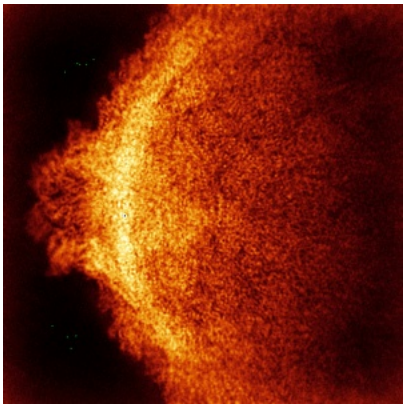


Z

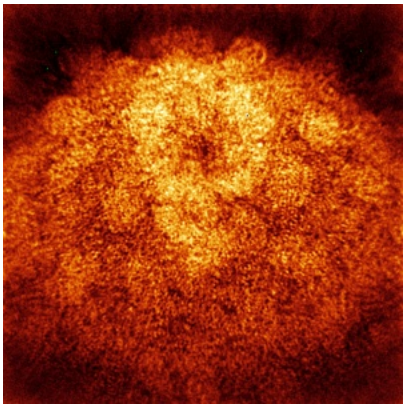
6.4.2 Raw map



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 0.5. 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

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.

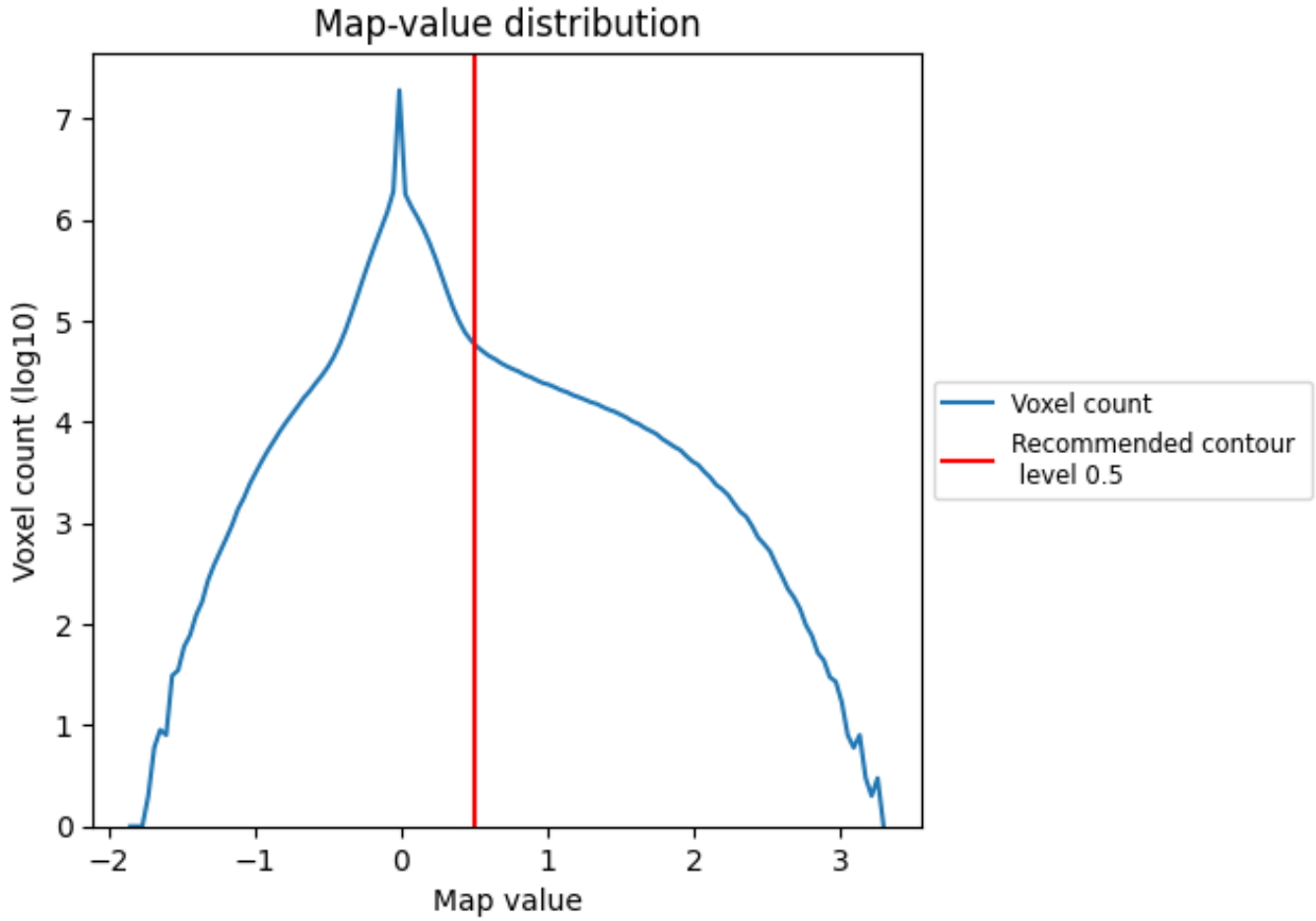
6.6 Mask visualisation (i)

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

7 Map analysis

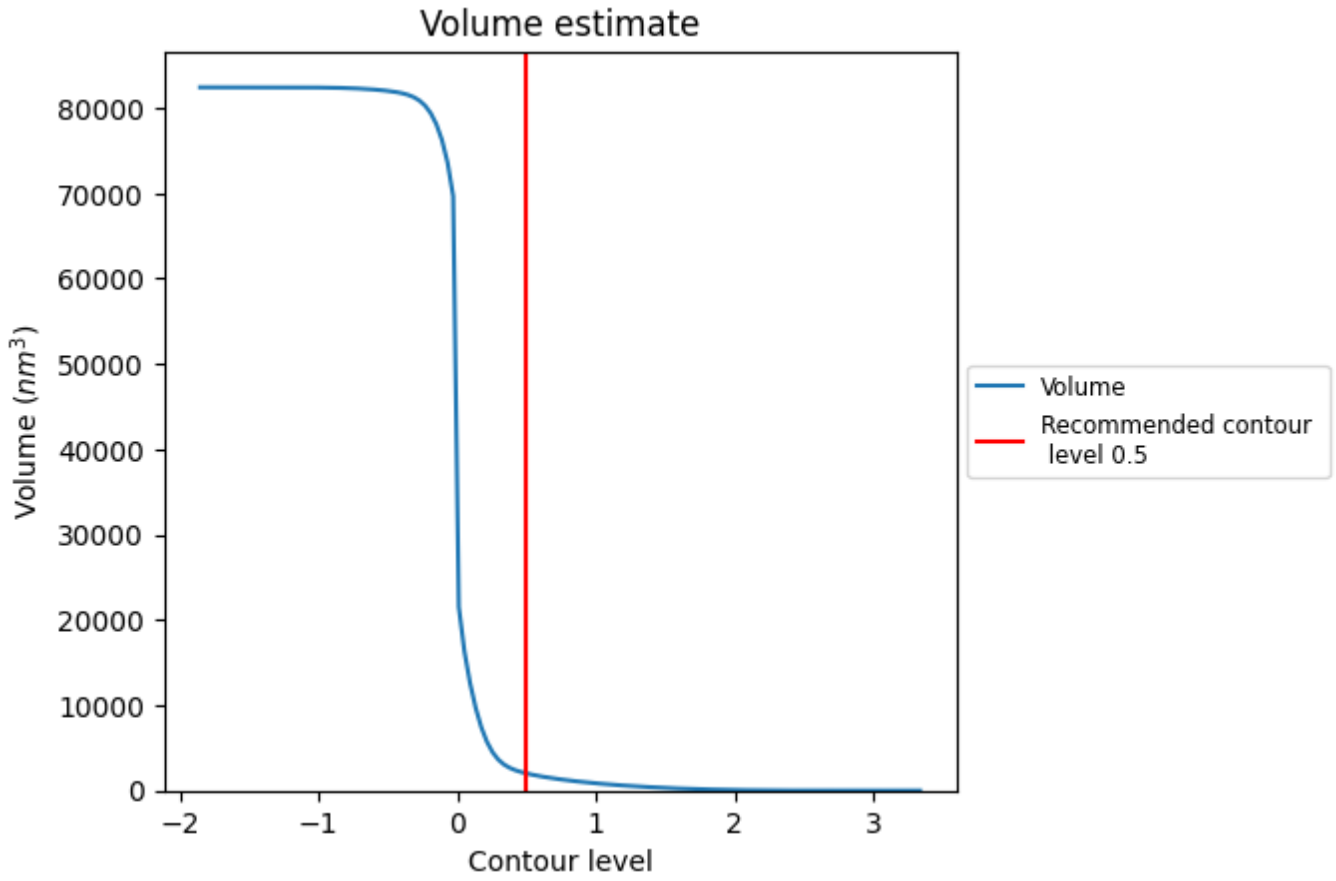
This section contains the results of statistical analysis of the map.

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.

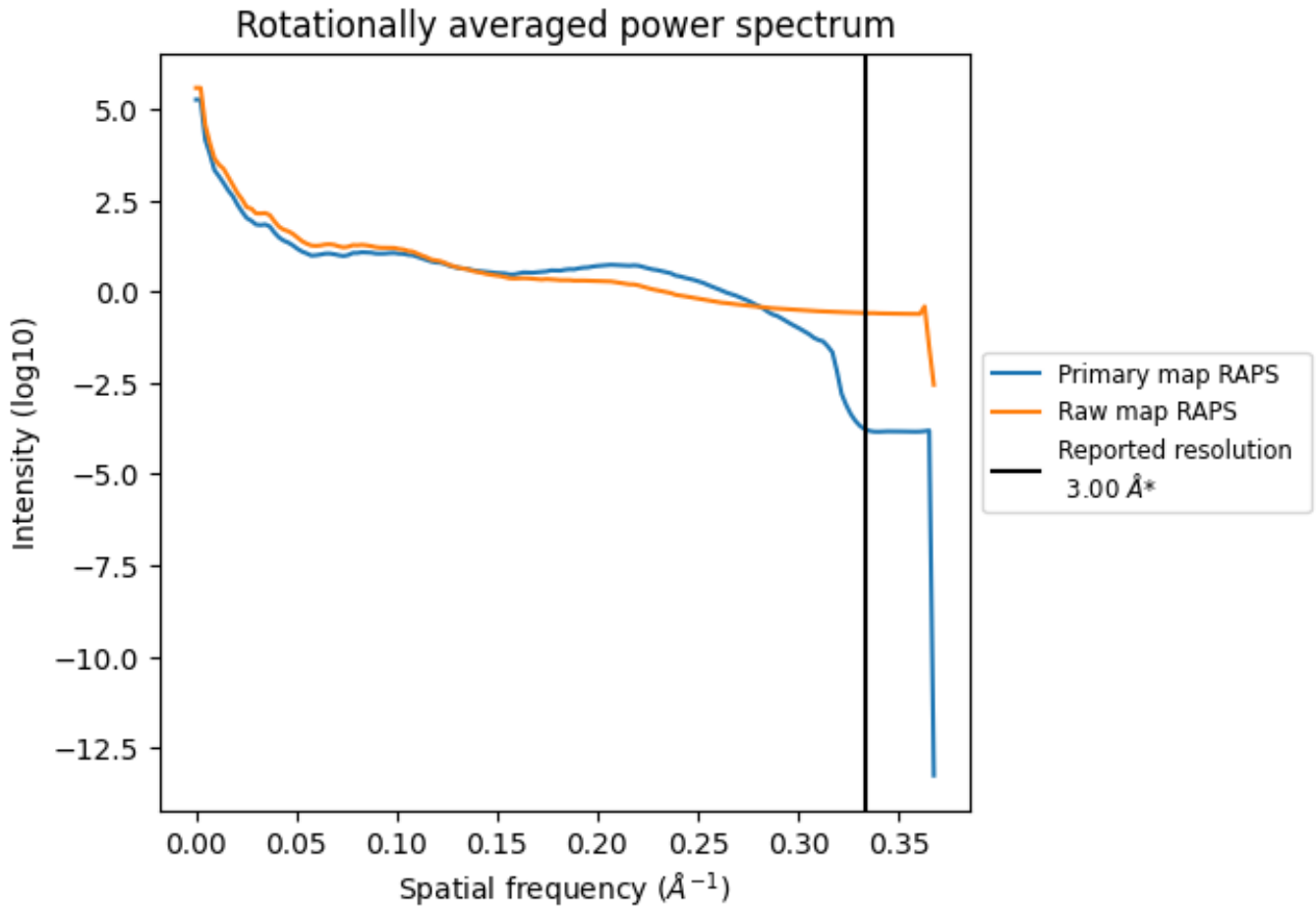
7.2 Volume estimate (i)



The volume at the recommended contour level is 2009 nm^3; this corresponds to an approximate mass of 1815 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)

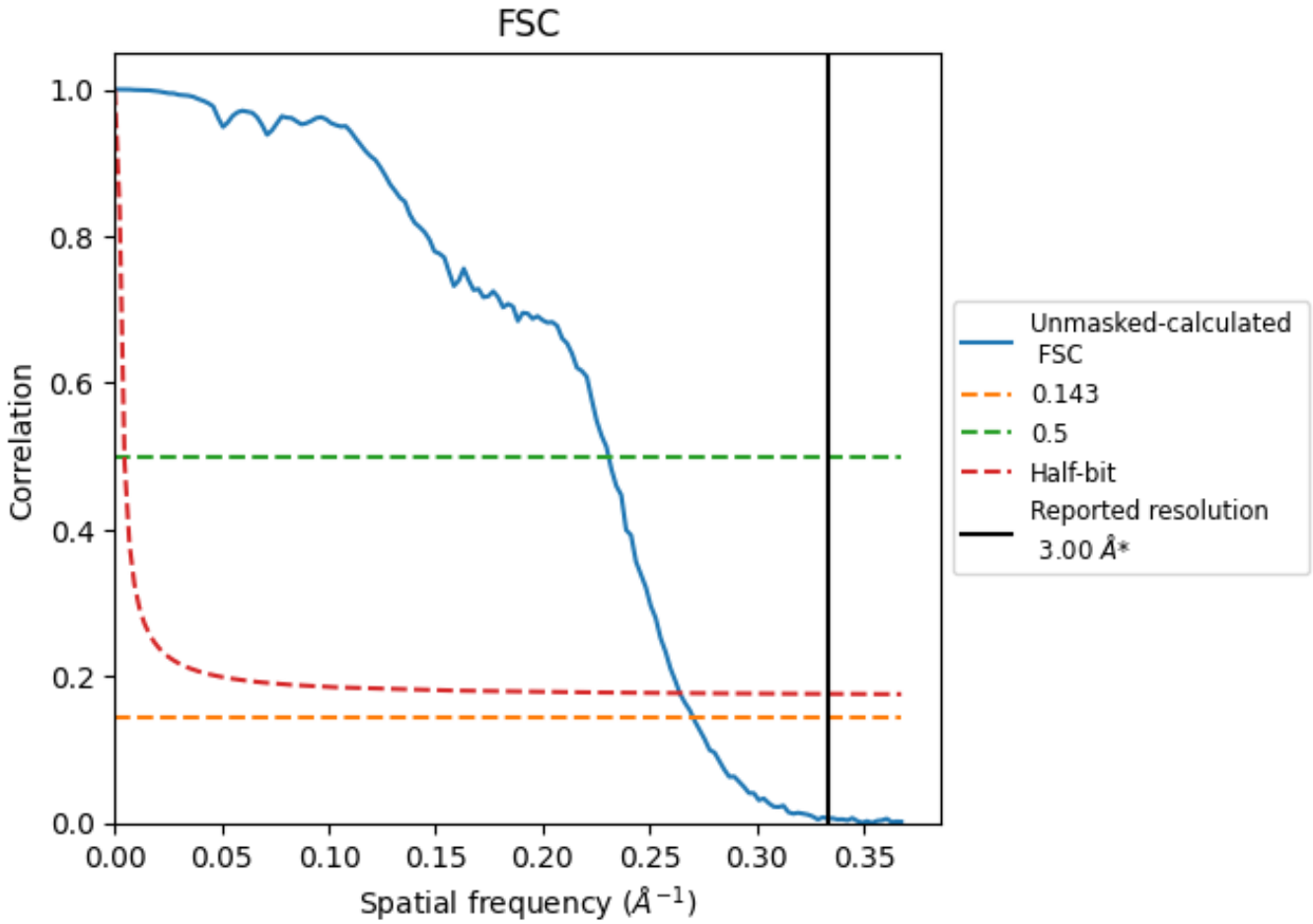


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

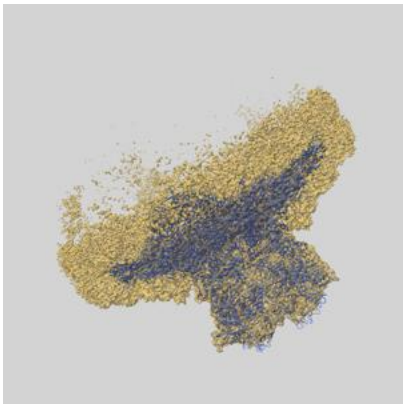
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.33	3.79

*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 3.70 differs from the reported value 3.0 by more than 10 %

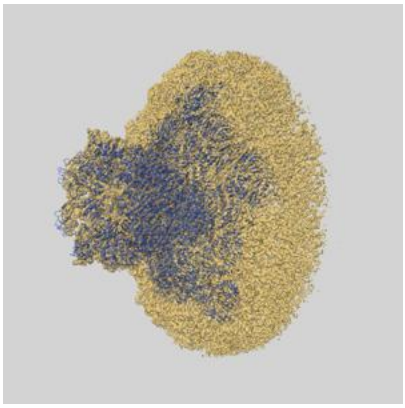
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33770 and PDB model 7YED. Per-residue inclusion information can be found in section 3 on page 9.

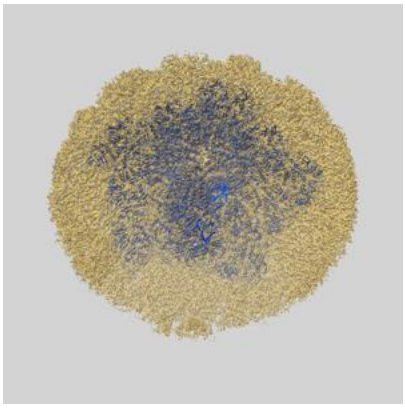
9.1 Map-model overlay



X



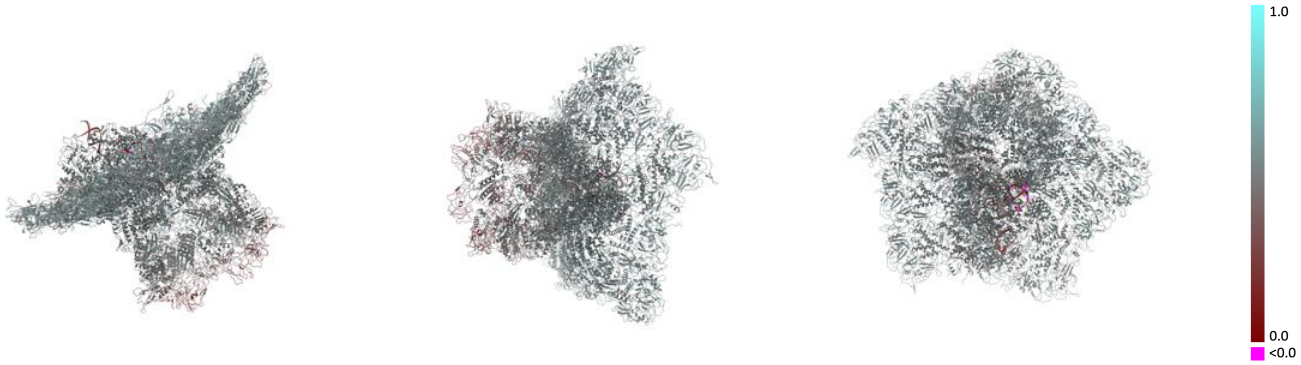
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

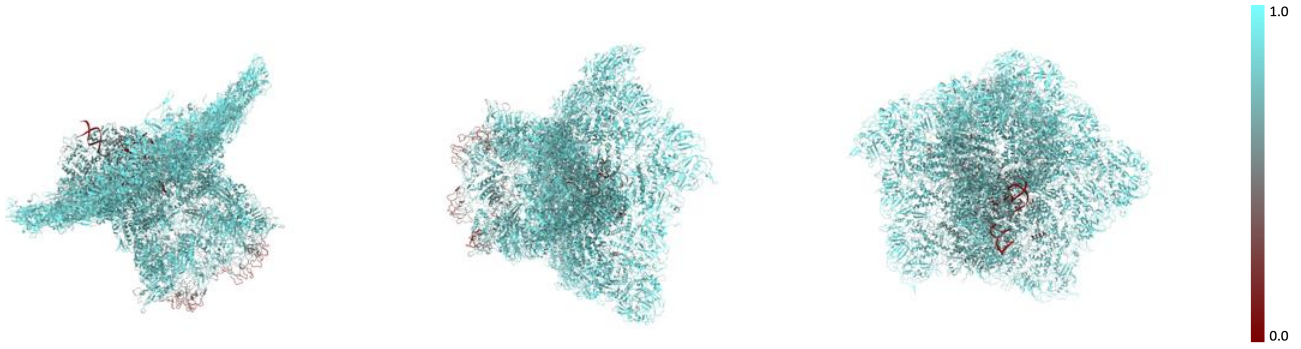
9.2 Q-score mapped to coordinate model (i)



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.

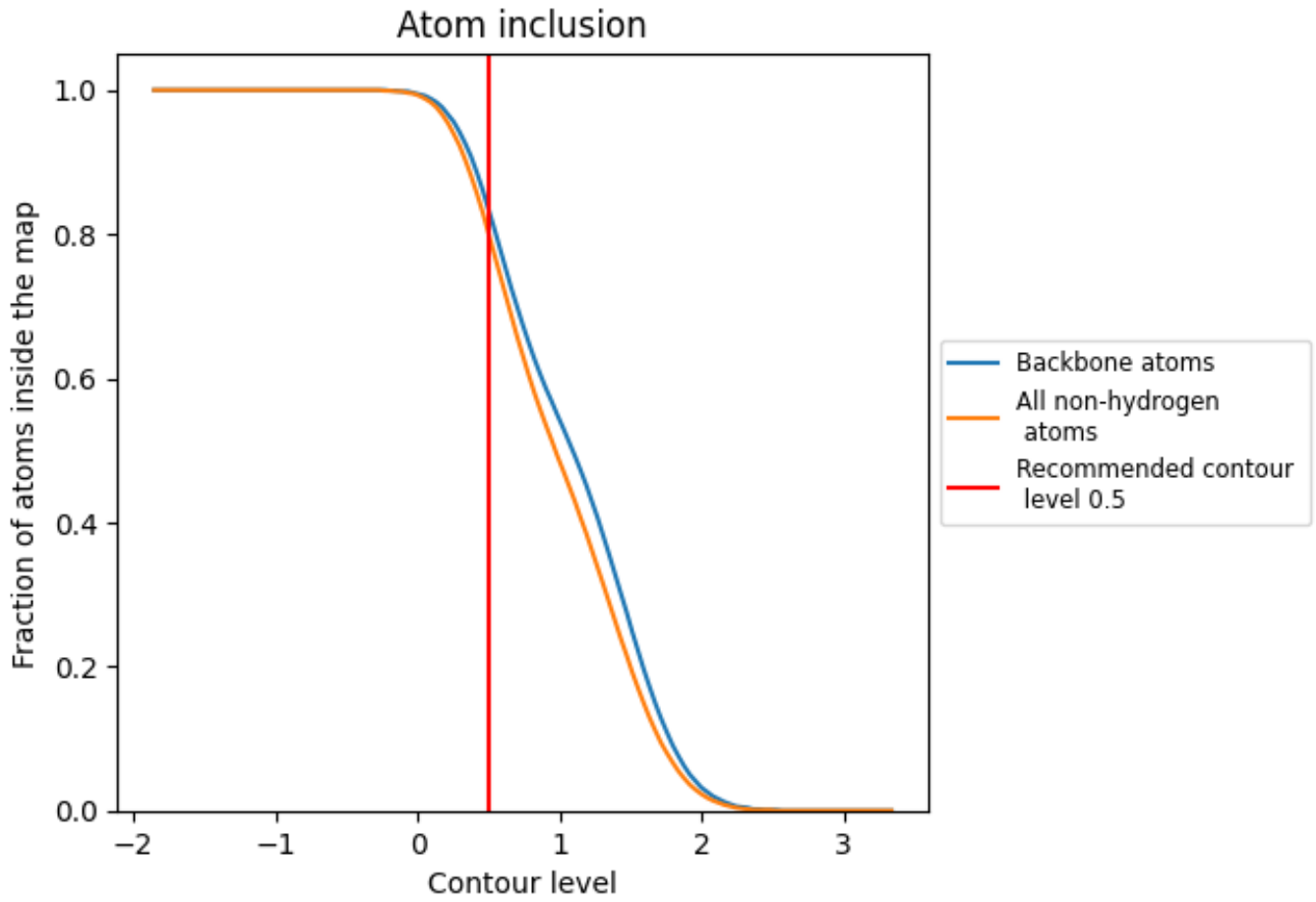
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% 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	0.8010	0.4980
1	0.7350	0.5050
2	0.7810	0.5090
3	0.7760	0.5090
4	0.6680	0.4840
5	0.6390	0.4930
A	0.8410	0.5210
B	0.8490	0.5250
C	0.8550	0.5250
D	0.8570	0.5260
E	0.8430	0.5220
H	0.7800	0.4650
I	0.7790	0.4640
J	0.7790	0.4650
K	0.7750	0.4640
L	0.7760	0.4630
M	0.3350	0.3100
N	0.0700	0.2090
R	0.7560	0.5000
T	0.2710	0.3060
U	0.7550	0.4910
a	0.8520	0.5240
b	0.8580	0.5230
c	0.8500	0.5250
d	0.8540	0.5230
e	0.8500	0.5220