



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 6Z9Q / pdb_00006z9q
EMDB ID : EMD-11088
Title : Transcription termination intermediate complex 2
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2020-06-04
Resolution : 5.70 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:

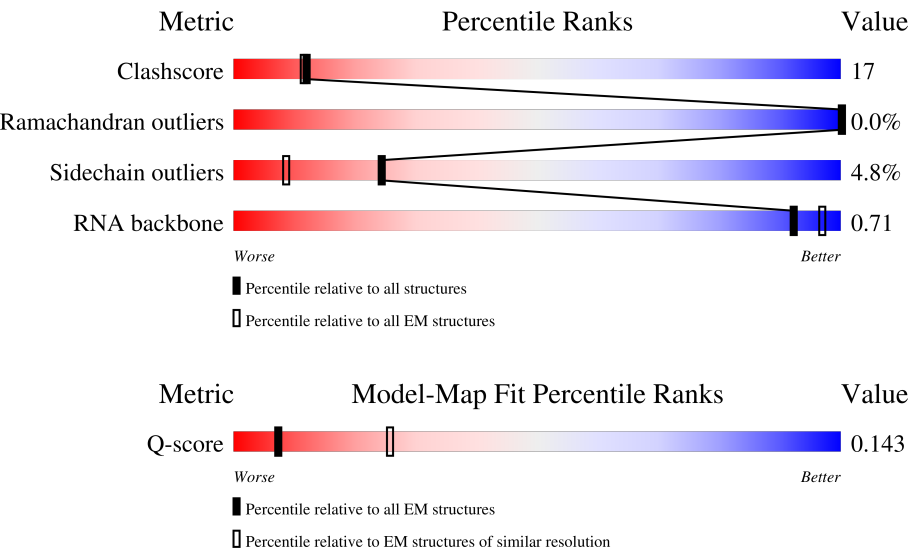
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	503 (5.20 - 6.20)

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

Mol	Chain	Length	Quality of chain
1	G	181	
2	a	419	
2	b	419	

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Mol	Chain	Length	Quality of chain
2	c	419	
2	d	419	
2	e	419	
2	f	419	
3	A	497	
4	U	329	
4	V	329	
5	W	91	
6	X	1342	
7	Y	1416	
8	K	50	
9	L	50	
10	R	99	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 52592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	112	Total	C	N	O	S	0	0
			906	573	167	160	6		

- Molecule 2 is a protein called Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	f	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
2	a	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
2	b	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
2	c	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
2	d	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
2	e	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		

- Molecule 3 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C3SSN7
A	0	ALA	-	expression tag	UNP C3SSN7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	235	Total	C	N	O	S	0	0
			1825	1135	325	359	6		
4	V	321	Total	C	N	O	S	0	0
			2504	1566	441	489	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	1358	Total	C	N	O	S	0	0
			10545	6620	1883	1992	50		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1408	LEU	-	expression tag	UNP C3SIA2
Y	1409	GLU	-	expression tag	UNP C3SIA2
Y	1410	VAL	-	expression tag	UNP C3SIA2
Y	1411	HIS	-	expression tag	UNP C3SIA2
Y	1412	HIS	-	expression tag	UNP C3SIA2
Y	1413	HIS	-	expression tag	UNP C3SIA2
Y	1414	HIS	-	expression tag	UNP C3SIA2
Y	1415	HIS	-	expression tag	UNP C3SIA2
Y	1416	HIS	-	expression tag	UNP C3SIA2

- Molecule 8 is a DNA chain called non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	36	Total	C	N	O	P	0	0
			748	353	145	214	36		

- Molecule 9 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	48	Total	C	N	O	P	0	0
			965	460	170	288	47		

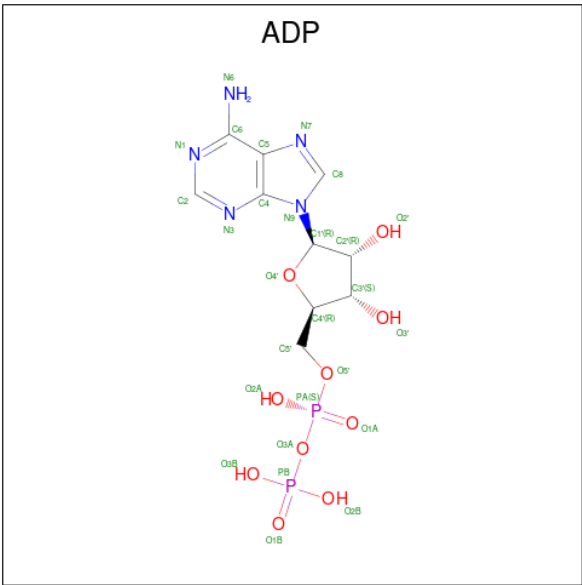
- Molecule 10 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	9	Total	C	N	O	P	0	0
			195	86	35	65	9		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	G	-	expression tag	GB 1227111474
R	2	G	-	expression tag	GB 1227111474
R	3	G	-	expression tag	GB 1227111474
R	72	U	-	insertion	GB 1227111474
R	77	U	-	expression tag	GB 1227111474
R	78	U	-	expression tag	GB 1227111474
R	79	A	-	expression tag	GB 1227111474
R	80	A	-	expression tag	GB 1227111474
R	81	A	-	expression tag	GB 1227111474
R	82	C	-	expression tag	GB 1227111474
R	83	C	-	expression tag	GB 1227111474
R	84	A	-	expression tag	GB 1227111474
R	85	C	-	expression tag	GB 1227111474
R	86	A	-	expression tag	GB 1227111474
R	87	C	-	expression tag	GB 1227111474
R	88	C	-	expression tag	GB 1227111474
R	89	U	-	expression tag	GB 1227111474
R	90	G	-	expression tag	GB 1227111474
R	91	G	-	expression tag	GB 1227111474
R	92	C	-	expression tag	GB 1227111474
R	93	G	-	expression tag	GB 1227111474
R	94	U	-	expression tag	GB 1227111474
R	95	G	-	expression tag	GB 1227111474
R	96	U	-	expression tag	GB 1227111474
R	97	G	-	expression tag	GB 1227111474
R	98	G	-	expression tag	GB 1227111474
R	99	C	-	expression tag	GB 1227111474

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

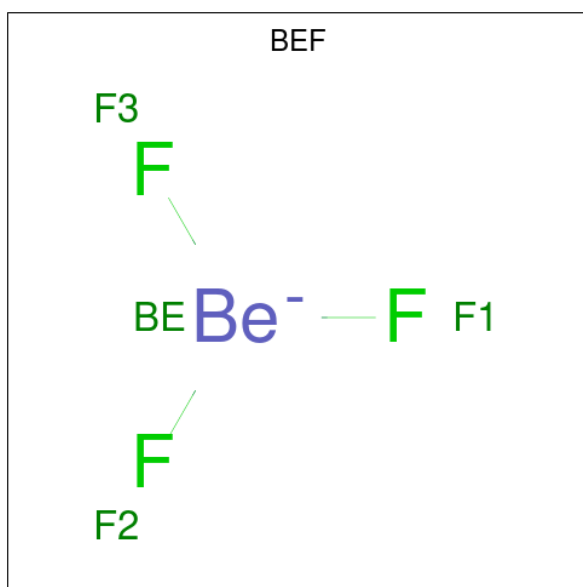


Mol	Chain	Residues	Atoms					AltConf
11	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	f	1	Total	Mg	0
			1	1	
12	b	1	Total	Mg	0
			1	1	
12	c	1	Total	Mg	0
			1	1	
12	d	1	Total	Mg	0
			1	1	
12	e	1	Total	Mg	0
			1	1	
12	Y	1	Total	Mg	0
			1	1	

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
13	f	1	Total	Be	F	0
			4	1	3	
13	b	1	Total	Be	F	0
			4	1	3	
13	c	1	Total	Be	F	0
			4	1	3	
13	d	1	Total	Be	F	0
			4	1	3	
13	e	1	Total	Be	F	0
			4	1	3	

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	Y	2	Total	Zn	0
			2	2	

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	f	3	Total	O	0
			3	3	
15	b	3	Total	O	0
			3	3	
15	c	3	Total	O	0
			3	3	

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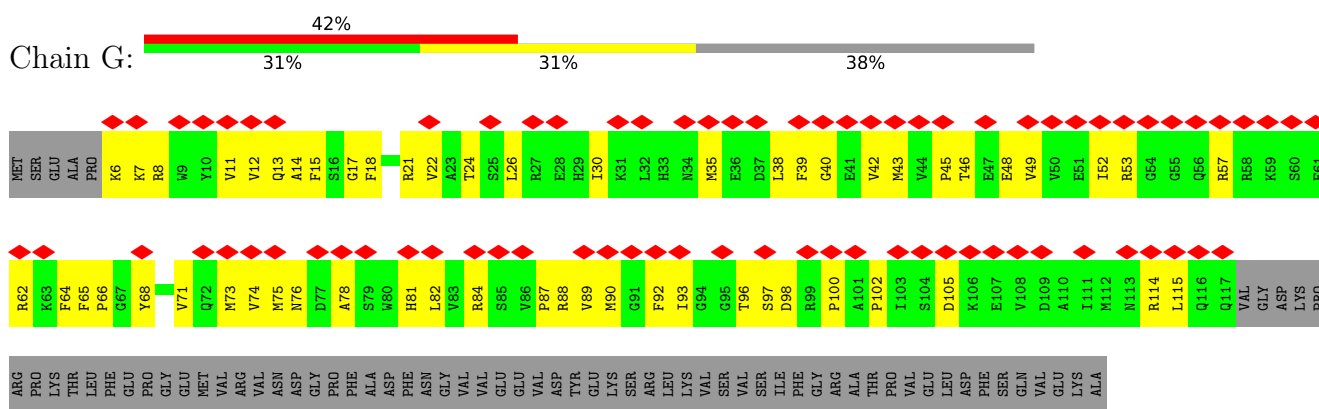
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Mol	Chain	Residues	Atoms		AltConf
15	d	3	Total	O	0
			3	3	
15	e	3	Total	O	0
			3	3	

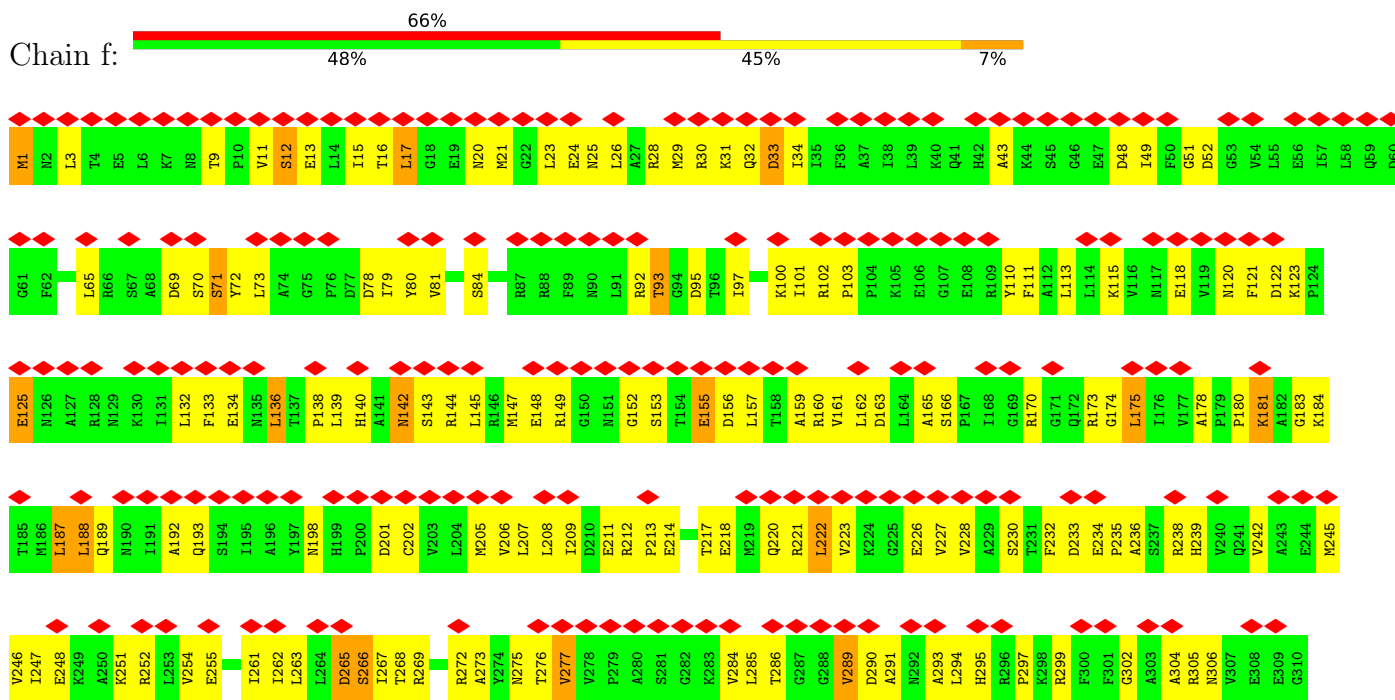
3 Residue-property plots

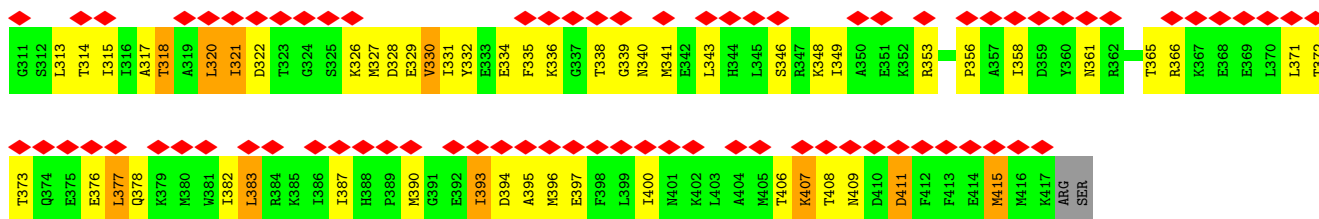
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Transcription termination/antitermination protein NusG

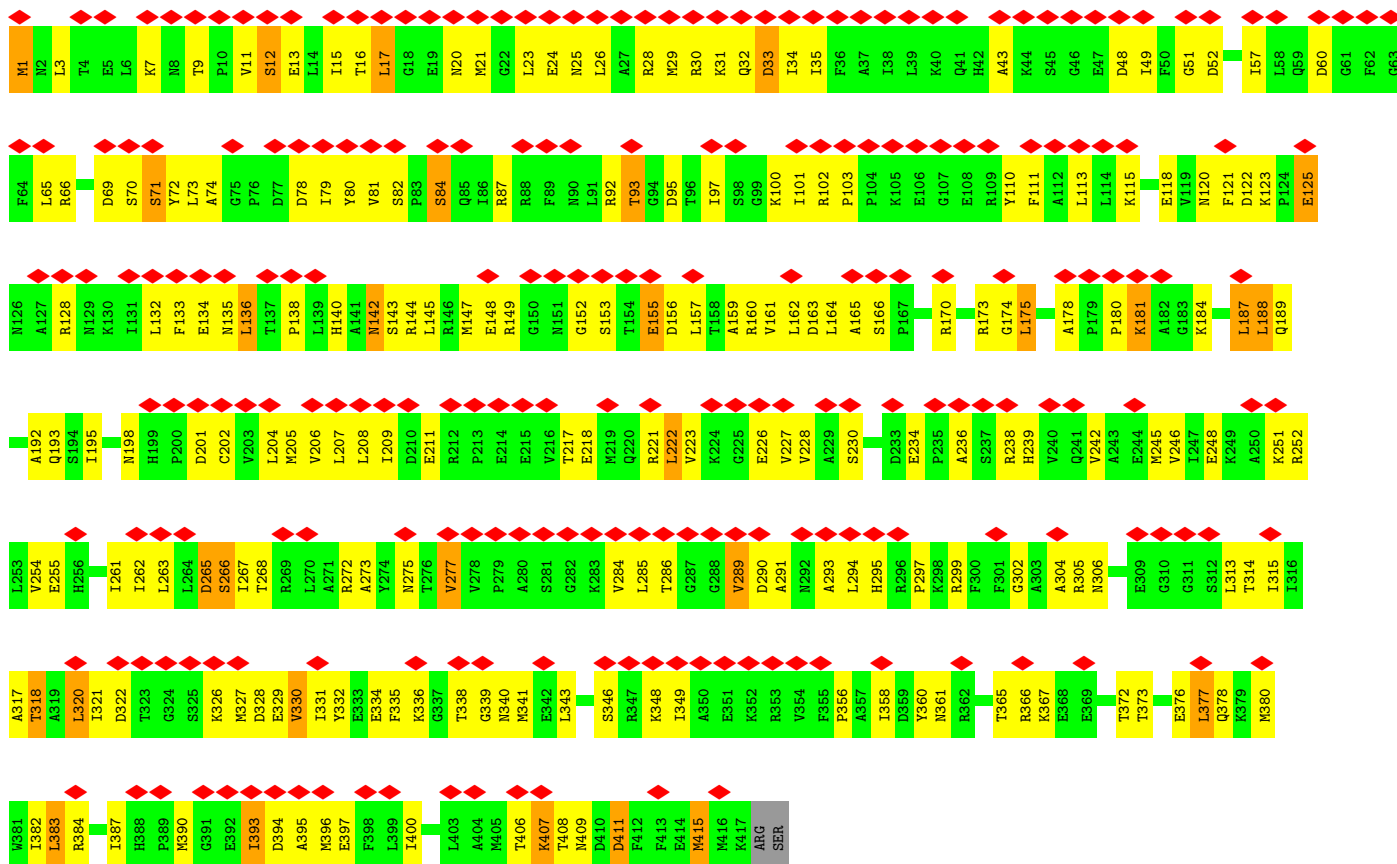


• Molecule 2: Transcription termination factor Rho

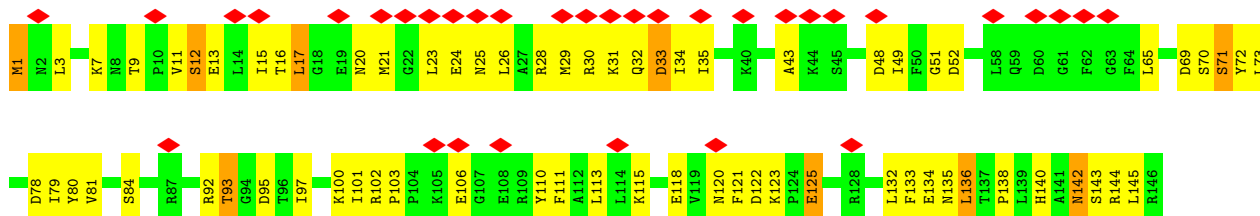


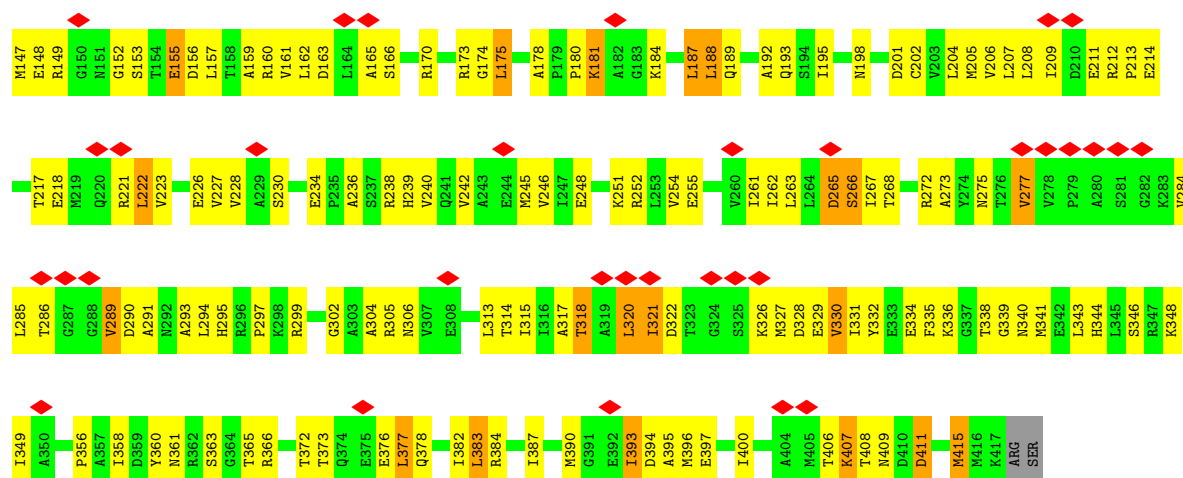


• Molecule 2: Transcription termination factor Rho

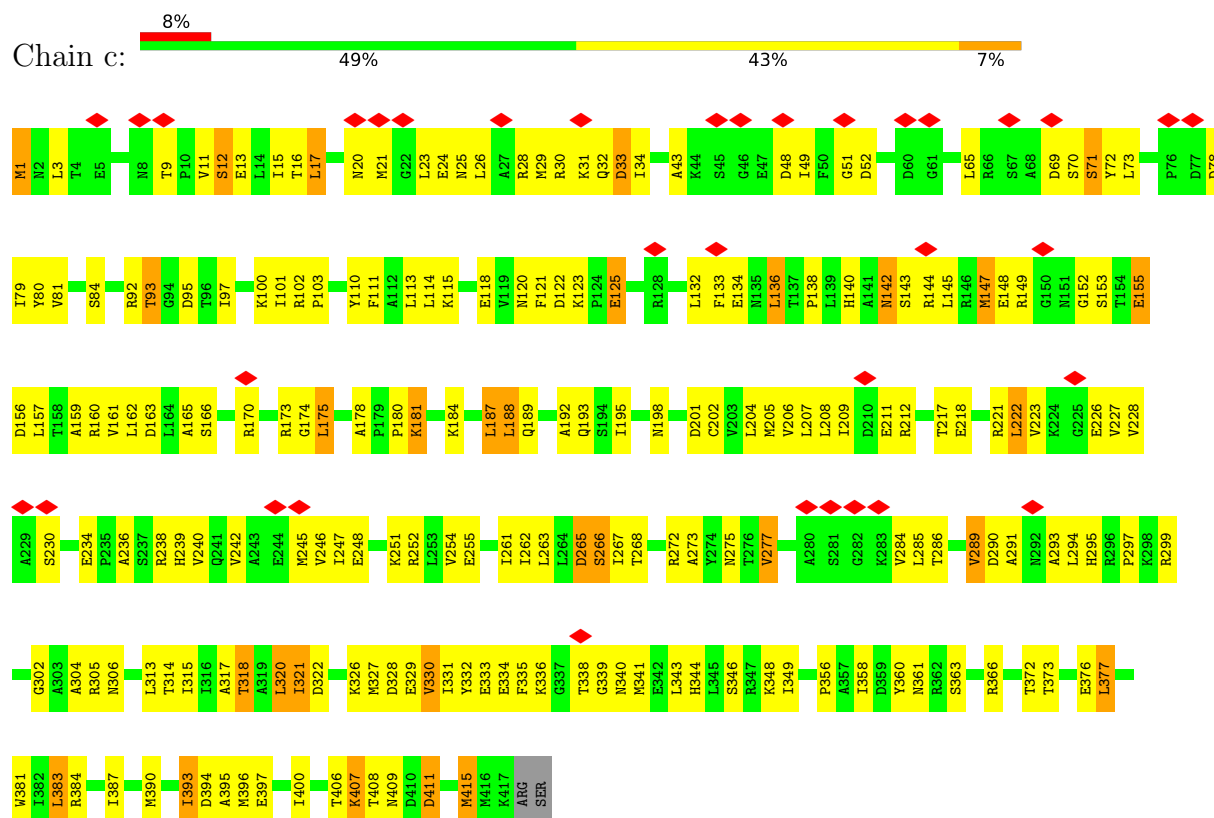


• Molecule 2: Transcription termination factor Rho

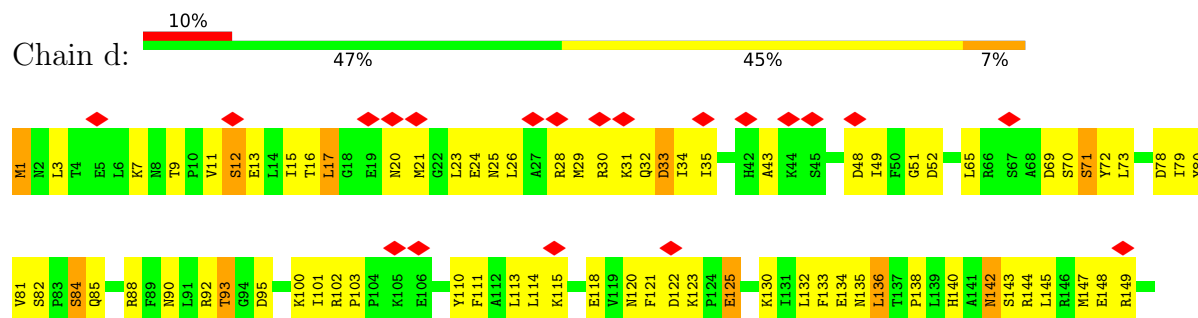


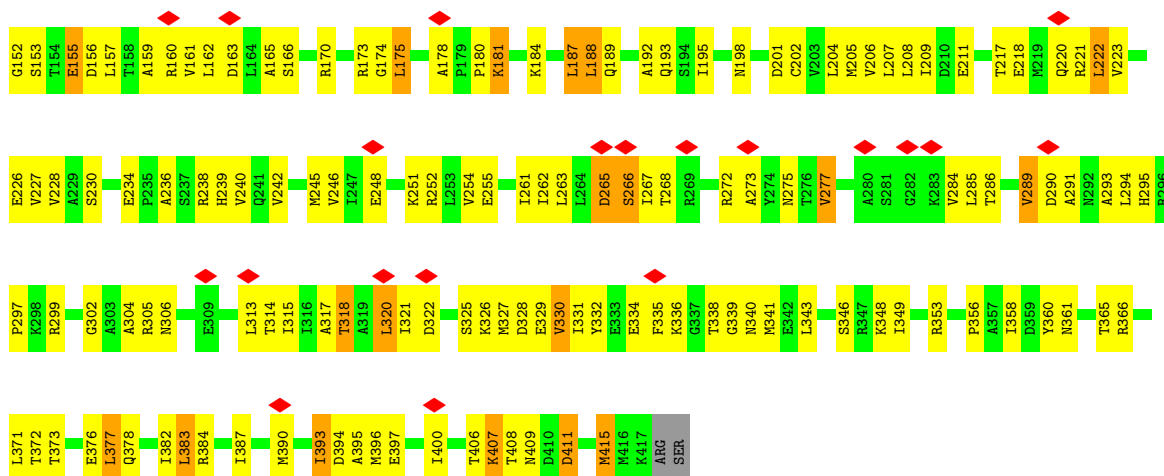


• Molecule 2: Transcription termination factor Rho

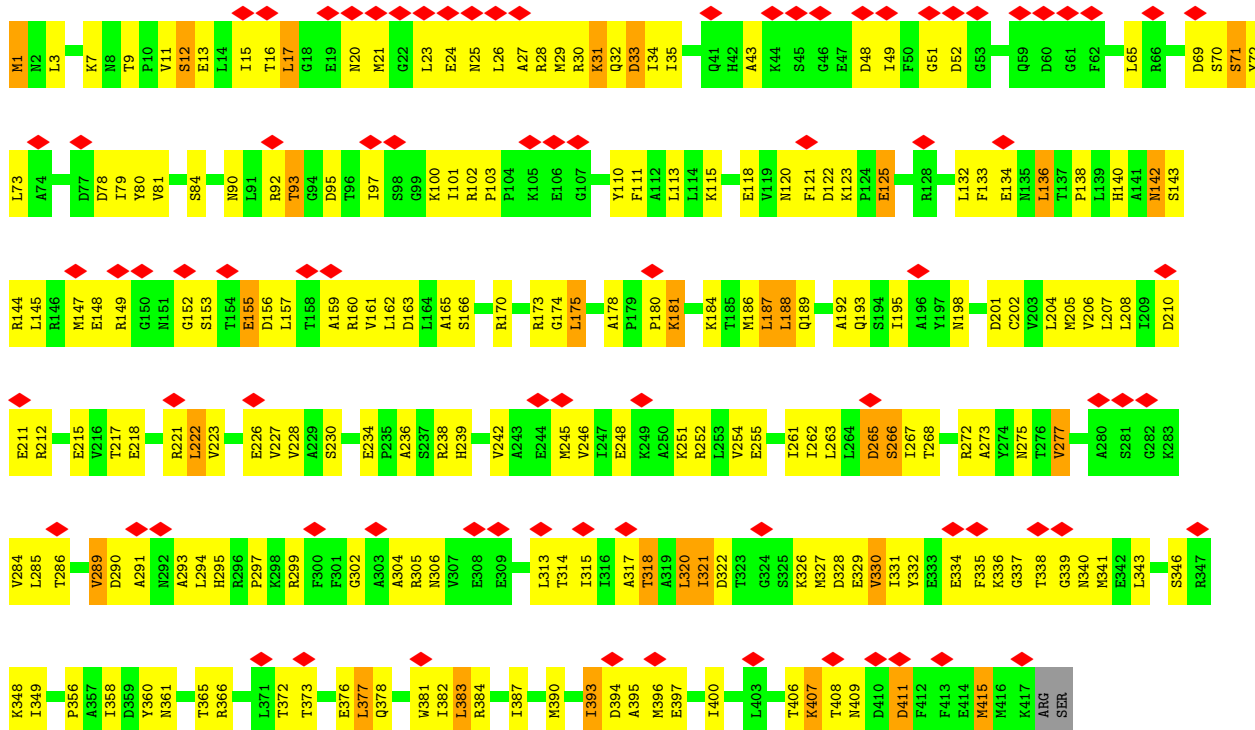


• Molecule 2: Transcription termination factor Rho

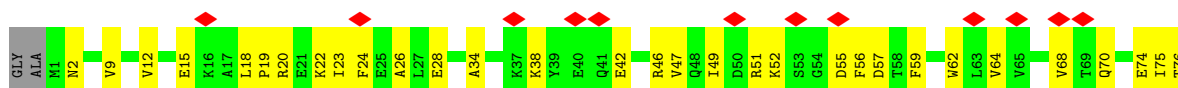


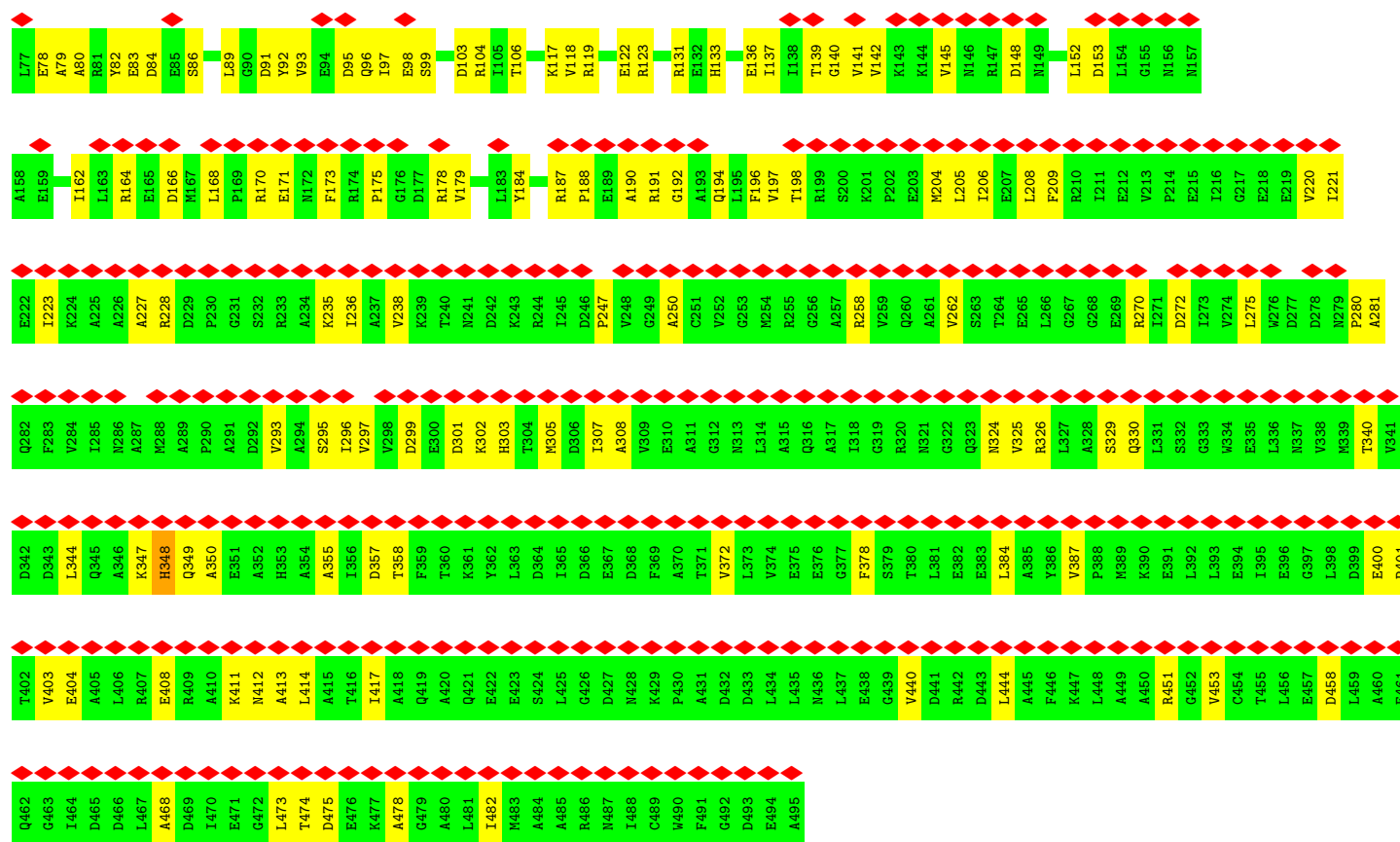


• Molecule 2: Transcription termination factor Rho

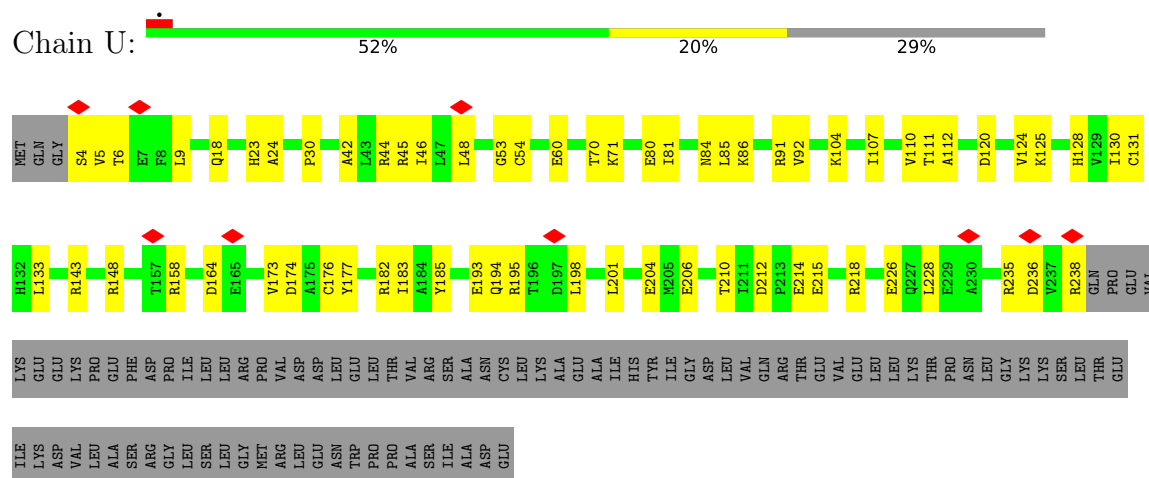


• Molecule 3: Transcription termination/antitermination protein NusA

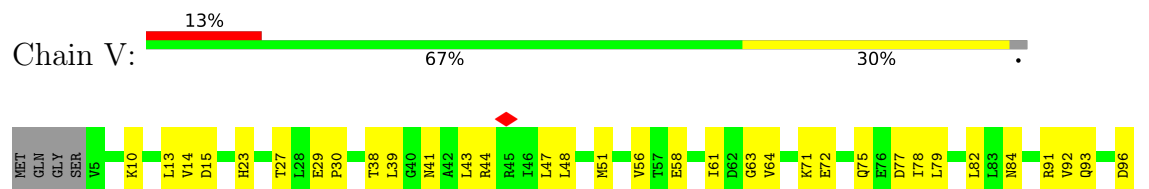


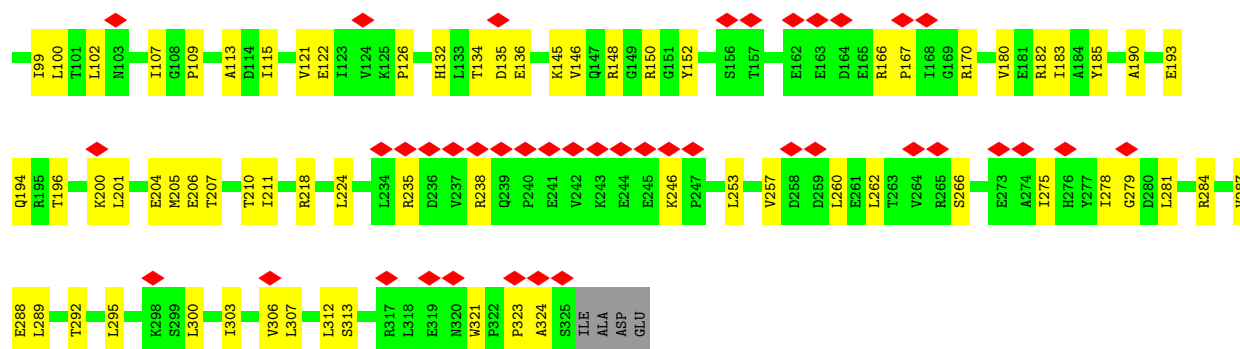


• Molecule 4: DNA-directed RNA polymerase subunit alpha

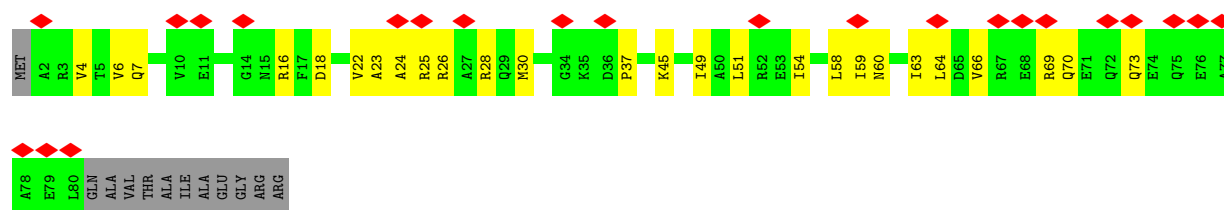


• Molecule 4: DNA-directed RNA polymerase subunit alpha

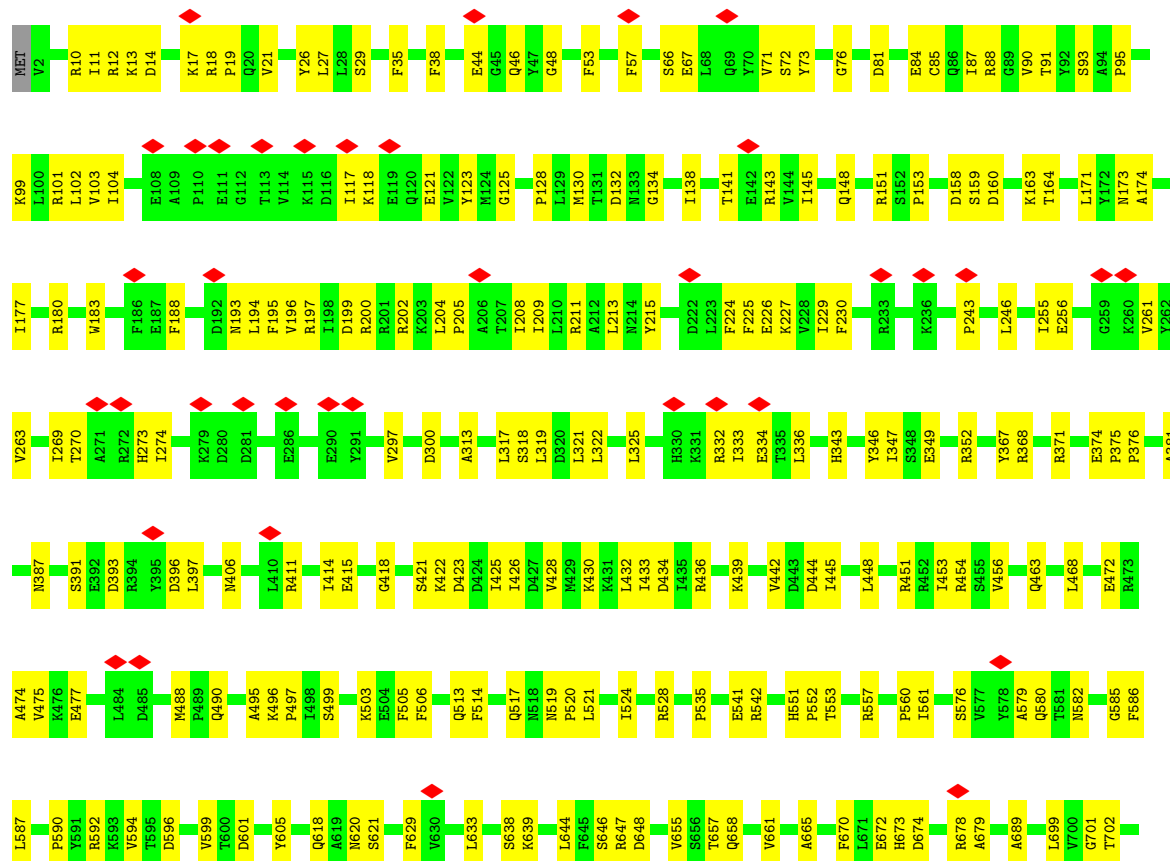


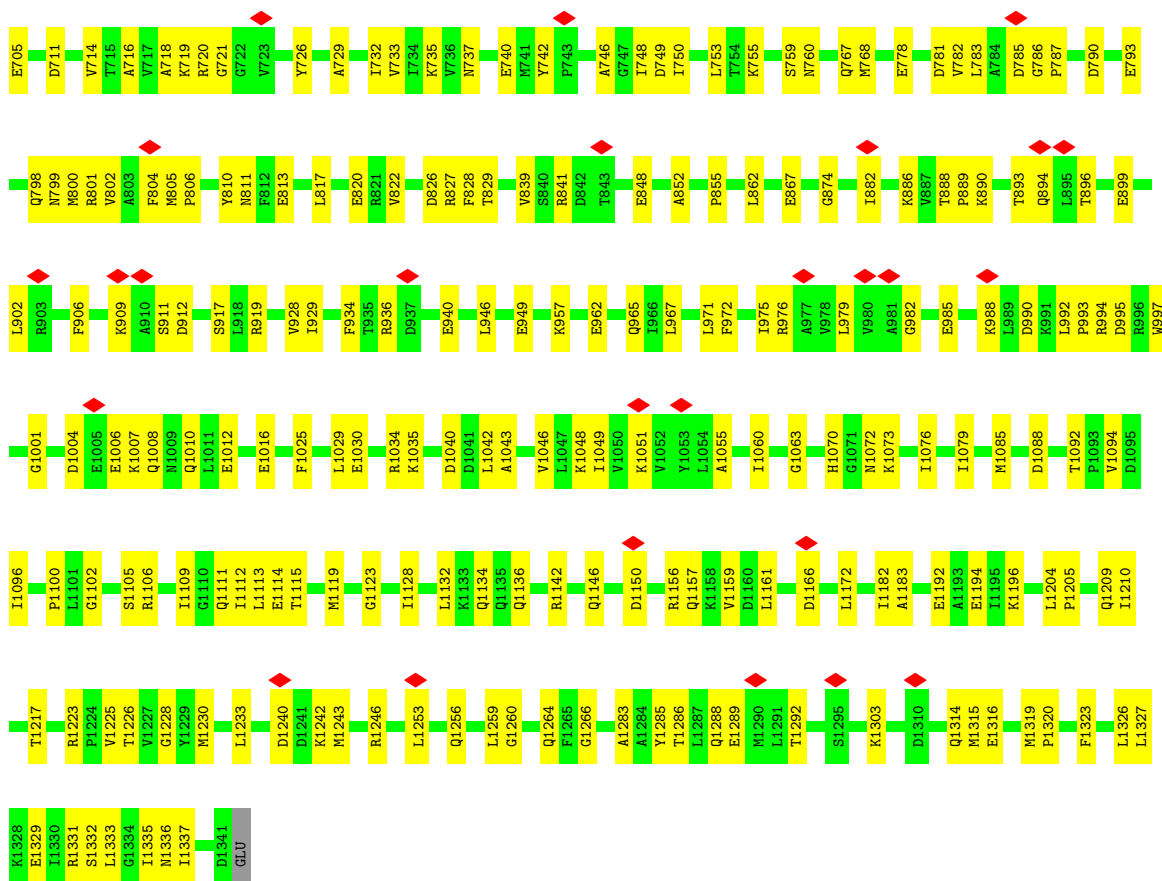


• Molecule 5: DNA-directed RNA polymerase subunit omega

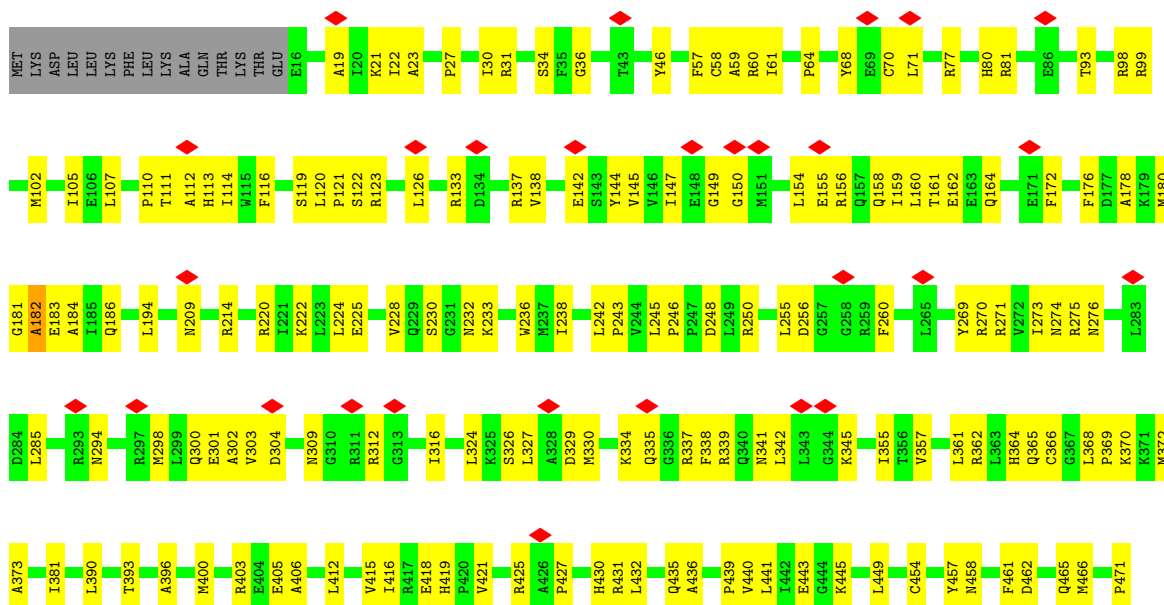


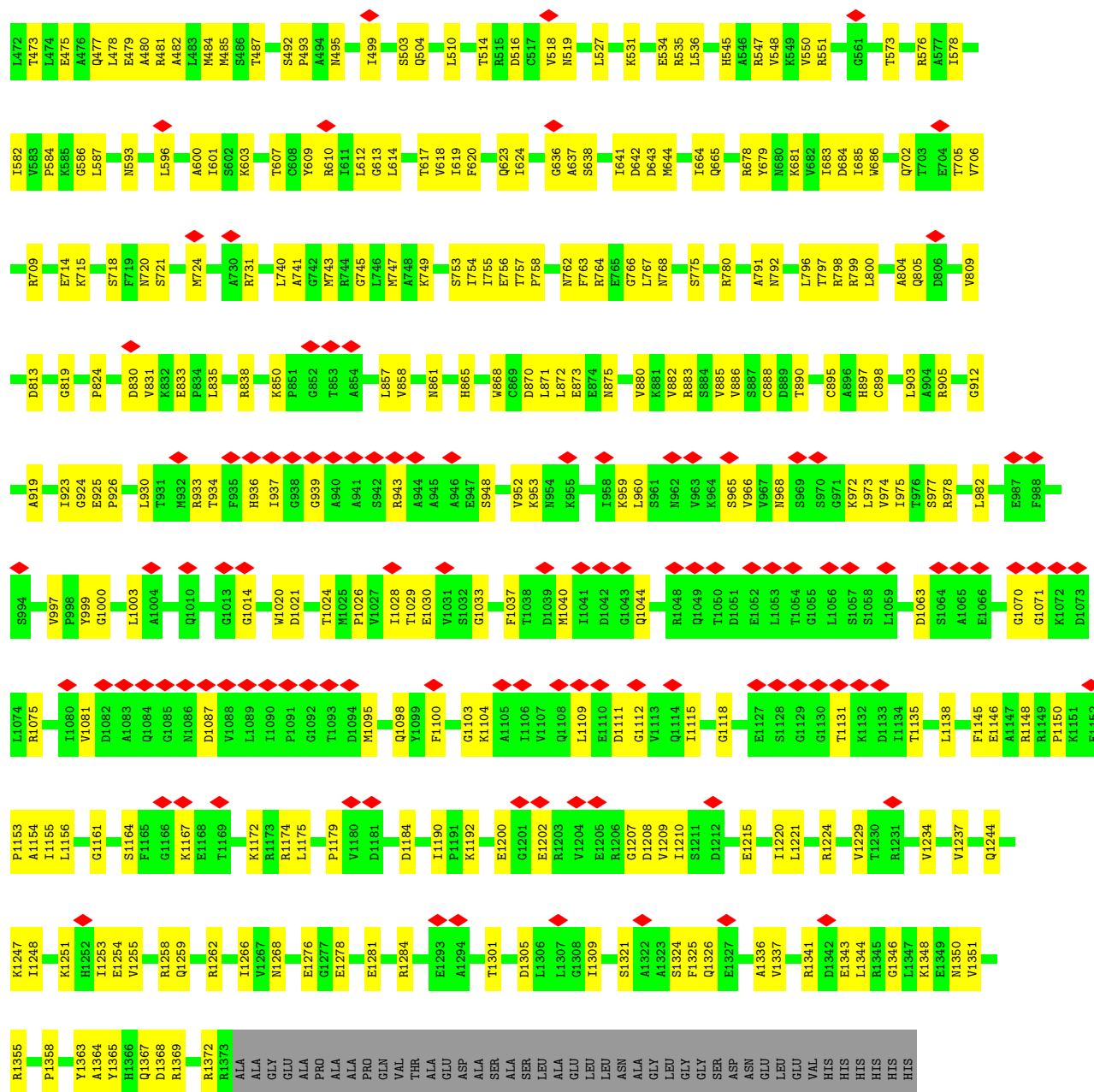
• Molecule 6: DNA-directed RNA polymerase subunit beta





• Molecule 7: DNA-directed RNA polymerase subunit beta'







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.282	Depositor
Minimum map value	-1.104	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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: ADP, BEF, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.16	0/925	0.42	0/1243
2	a	0.16	0/3329	0.41	0/4483
2	b	0.16	0/3329	0.41	0/4483
2	c	0.16	0/3329	0.41	0/4483
2	d	0.16	0/3329	0.41	0/4483
2	e	0.16	0/3329	0.41	0/4483
2	f	0.16	0/3329	0.41	0/4483
3	A	0.11	0/3897	0.34	0/5273
4	U	0.09	0/1847	0.27	0/2503
4	V	0.11	0/2538	0.31	0/3441
5	W	0.10	0/629	0.30	0/847
6	X	0.10	0/10736	0.29	0/14487
7	Y	0.11	0/10706	0.30	0/14456
8	K	0.15	0/839	0.30	0/1290
9	L	0.16	0/1078	0.46	2/1658 (0.1%)
10	R	0.10	0/217	0.20	0/337
All	All	0.13	0/53386	0.35	2/72433 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	23	DT	OP2-P-O3'	-8.45	82.64	108.00
9	L	23	DT	OP1-P-O3'	-8.30	83.11	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	906	0	909	61	0
2	a	3280	0	3359	162	0
2	b	3280	0	3357	156	0
2	c	3280	0	3357	151	0
2	d	3280	0	3357	168	0
2	e	3280	0	3358	181	0
2	f	3280	0	3358	172	0
3	A	3852	0	3835	105	0
4	U	1825	0	1853	43	0
4	V	2504	0	2558	72	0
5	W	627	0	634	22	0
6	X	10567	0	10585	294	0
7	Y	10545	0	10761	320	0
8	K	748	0	406	12	0
9	L	965	0	540	26	0
10	R	195	0	97	7	0
11	b	27	0	12	2	0
11	c	27	0	12	1	0
11	d	27	0	12	1	0
11	e	27	0	12	1	0
11	f	27	0	12	2	0
12	Y	1	0	0	0	0
12	b	1	0	0	0	0
12	c	1	0	0	0	0
12	d	1	0	0	0	0
12	e	1	0	0	0	0
12	f	1	0	0	0	0
13	b	4	0	0	0	0
13	c	4	0	0	0	0
13	d	4	0	0	1	0
13	e	4	0	0	0	0
13	f	4	0	0	1	0
14	Y	2	0	0	0	0
15	b	3	0	0	1	0
15	c	3	0	0	1	0
15	d	3	0	0	0	0
15	e	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	f	3	0	0	0	0
All	All	52592	0	52384	1812	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 1812 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:144:TYR:CE1	7:Y:180:MET:SD	2.08	1.47
7:Y:144:TYR:HE1	7:Y:180:MET:CE	1.42	1.32
7:Y:144:TYR:CE1	7:Y:180:MET:CE	2.19	1.25
7:Y:144:TYR:HE1	7:Y:180:MET:SD	1.50	1.24
7:Y:144:TYR:HE1	7:Y:180:MET:HE1	1.24	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	110/181 (61%)	91 (83%)	19 (17%)	0	100	100
2	a	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
2	b	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
2	c	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
2	d	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
2	e	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
2	f	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
3	A	493/497 (99%)	459 (93%)	33 (7%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	233/329 (71%)	223 (96%)	10 (4%)	0	100	100
4	V	319/329 (97%)	296 (93%)	23 (7%)	0	100	100
5	W	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
6	X	1338/1342 (100%)	1270 (95%)	68 (5%)	0	100	100
7	Y	1356/1416 (96%)	1307 (96%)	48 (4%)	1 (0%)	48	83
All	All	6416/6699 (96%)	6163 (96%)	251 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	348	HIS
7	Y	182	ALA

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	G	98/158 (62%)	98 (100%)	0	100	100
2	a	357/359 (99%)	313 (88%)	44 (12%)	4	17
2	b	357/359 (99%)	313 (88%)	44 (12%)	4	17
2	c	357/359 (99%)	313 (88%)	44 (12%)	4	17
2	d	357/359 (99%)	313 (88%)	44 (12%)	4	17
2	e	357/359 (99%)	313 (88%)	44 (12%)	4	17
2	f	357/359 (99%)	313 (88%)	44 (12%)	4	17
3	A	409/409 (100%)	409 (100%)	0	100	100
4	U	203/286 (71%)	203 (100%)	0	100	100
4	V	280/286 (98%)	280 (100%)	0	100	100
5	W	67/75 (89%)	67 (100%)	0	100	100
6	X	1155/1157 (100%)	1155 (100%)	0	100	100
7	Y	1134/1177 (96%)	1134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5488/5702 (96%)	5224 (95%)	264 (5%)	24 44

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	125	GLU
2	e	181	LYS
2	e	393	ILE
2	b	84	SER
2	b	33	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
6	X	760	ASN
7	Y	294	ASN
6	X	1010	GLN
6	X	1256	GLN
7	Y	488	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	R	8/99 (8%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
11	ADP	c	1000	12	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
11	ADP	f	1000	12	28,29,29	1.43	5 (17%)	43,45,45	1.83	9 (20%)
13	BEF	e	1002	-	0,3,3	-	-	-	-	-
11	ADP	e	1000	12	28,29,29	1.45	5 (17%)	43,45,45	1.87	8 (18%)
13	BEF	c	1002	-	0,3,3	-	-	-	-	-
11	ADP	b	1000	12	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
13	BEF	d	1002	-	0,3,3	-	-	-	-	-
13	BEF	f	1002	-	0,3,3	-	-	-	-	-
13	BEF	b	1002	-	0,3,3	-	-	-	-	-
11	ADP	d	1000	12	28,29,29	1.43	5 (17%)	43,45,45	1.82	8 (18%)

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
11	ADP	c	1000	12	-	2/16/32/32	0/3/3/3
11	ADP	f	1000	12	-	2/16/32/32	0/3/3/3
11	ADP	e	1000	12	-	2/16/32/32	0/3/3/3
11	ADP	b	1000	12	-	2/16/32/32	0/3/3/3
11	ADP	d	1000	12	-	1/16/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	e	1000	ADP	C5-C4	4.92	1.47	1.39
11	d	1000	ADP	C5-C4	4.76	1.47	1.39
11	f	1000	ADP	C5-C4	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1000	ADP	C5-C4	4.73	1.47	1.39
11	c	1000	ADP	C5-C4	4.71	1.47	1.39

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	1000	ADP	C5-C4-N3	-6.23	118.14	126.72
11	f	1000	ADP	C5-C4-N3	-5.83	118.69	126.72
11	b	1000	ADP	C5-C4-N3	-5.80	118.73	126.72
11	c	1000	ADP	C5-C4-N3	-5.78	118.76	126.72
11	d	1000	ADP	C5-C4-N3	-5.76	118.78	126.72

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	d	1000	ADP	C5'-O5'-PA-O1A
11	e	1000	ADP	O4'-C4'-C5'-O5'
11	c	1000	ADP	O4'-C4'-C5'-O5'
11	c	1000	ADP	C3'-C4'-C5'-O5'
11	e	1000	ADP	C3'-C4'-C5'-O5'

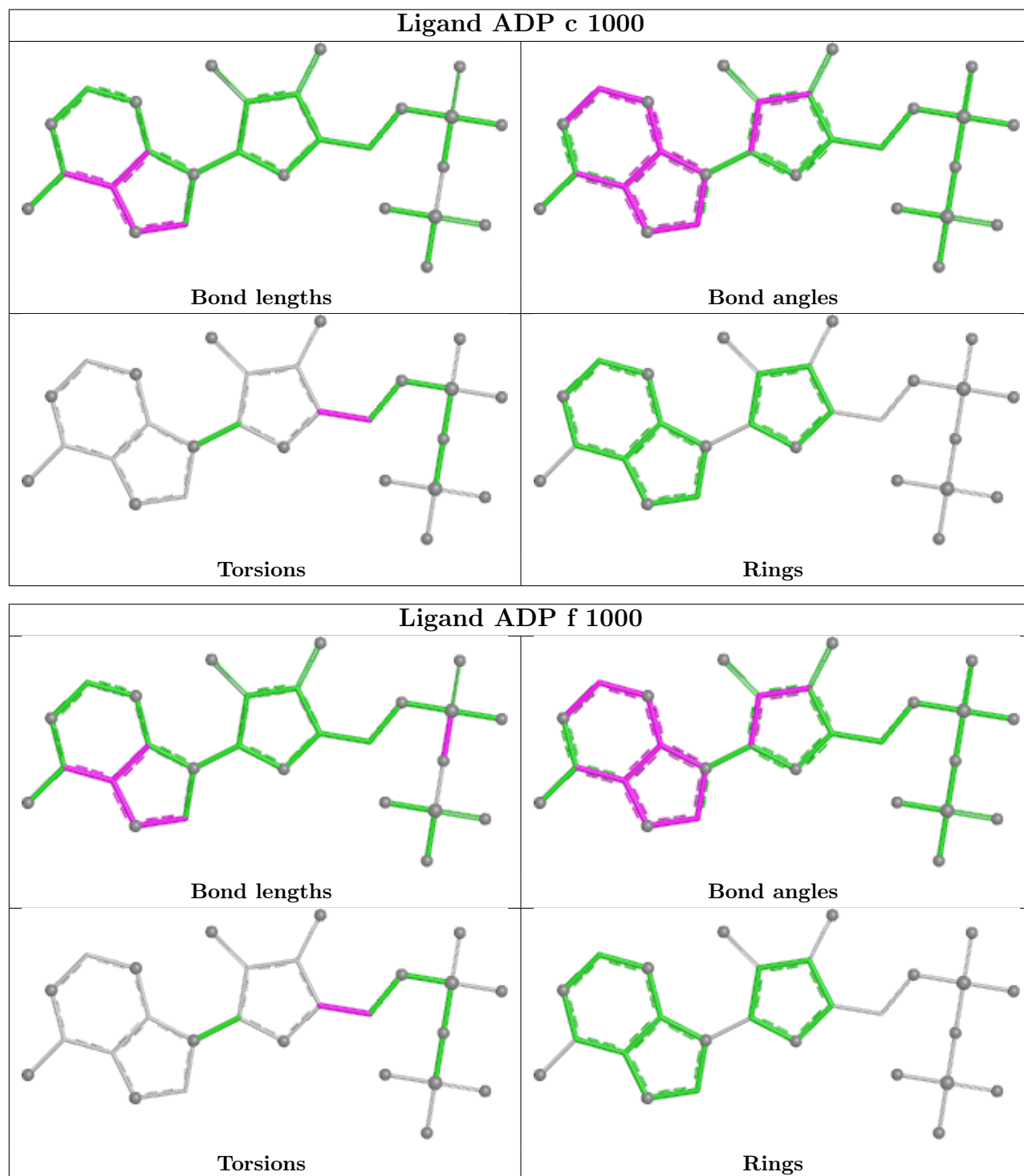
There are no ring outliers.

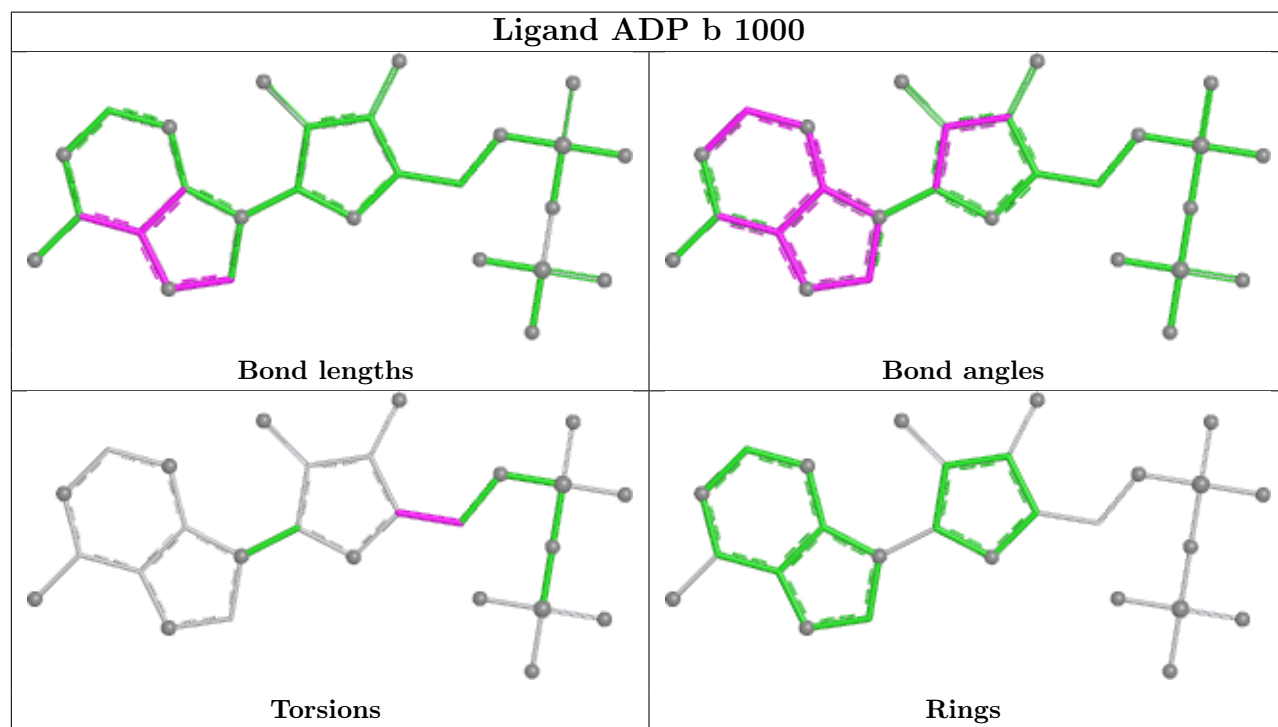
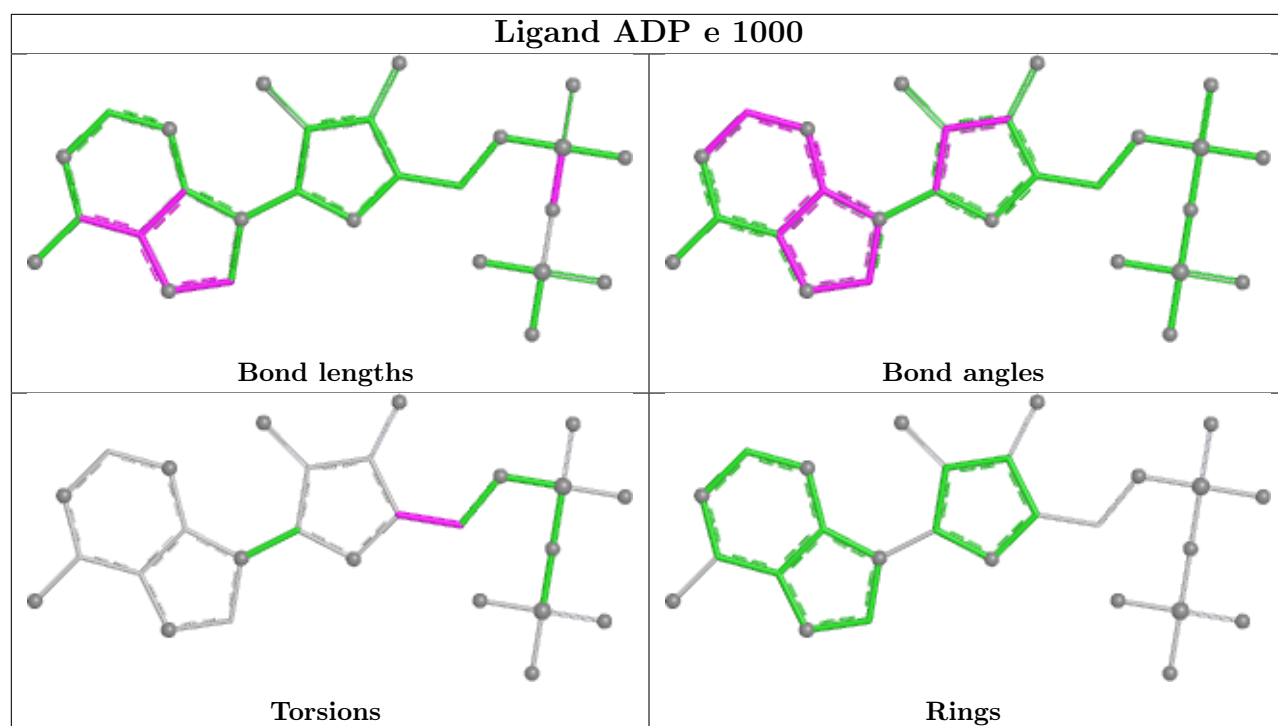
7 monomers are involved in 9 short contacts:

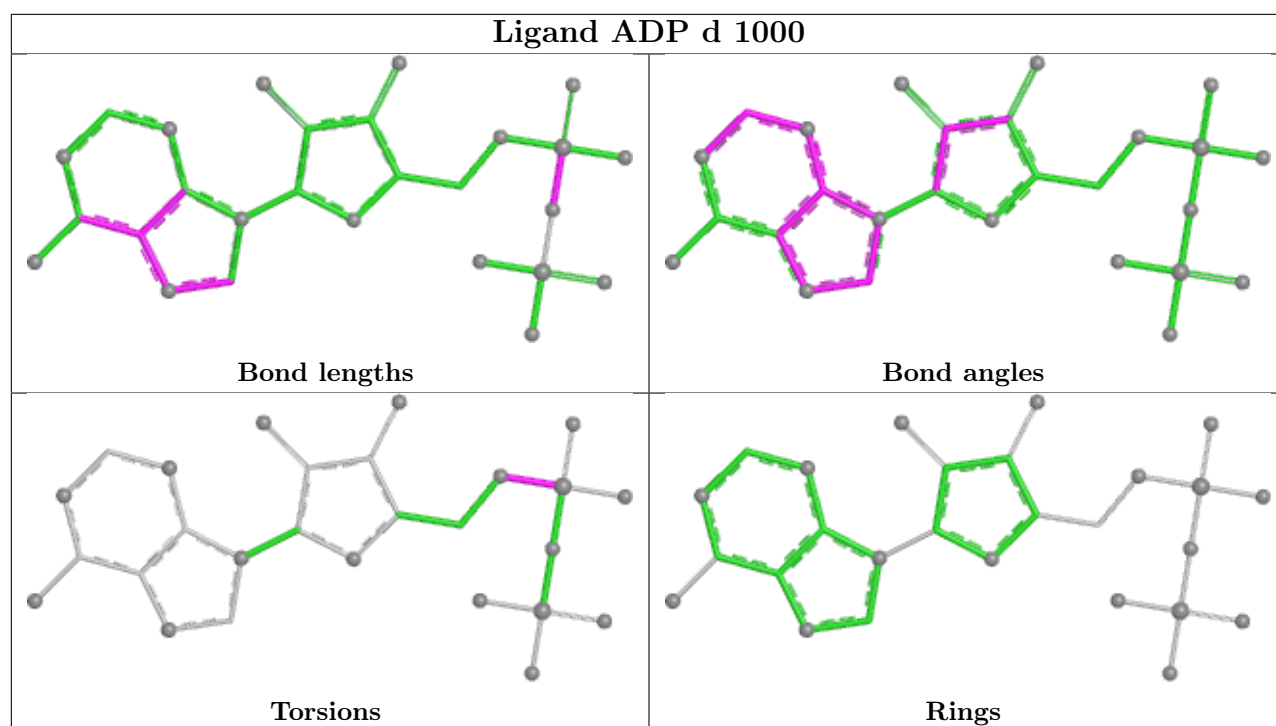
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	c	1000	ADP	1	0
11	f	1000	ADP	2	0
11	e	1000	ADP	1	0
11	b	1000	ADP	2	0
13	d	1002	BEF	1	0
13	f	1002	BEF	1	0
11	d	1000	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

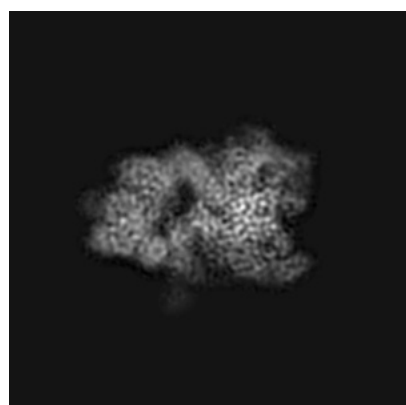
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11088. These allow visual inspection of the internal detail of the map and identification of artifacts.

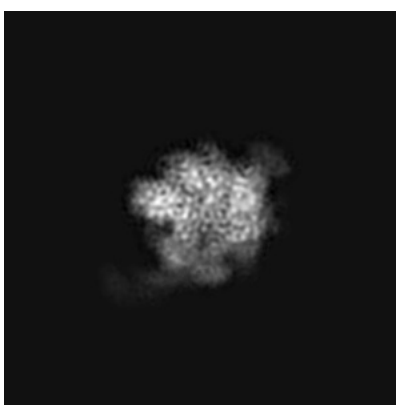
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

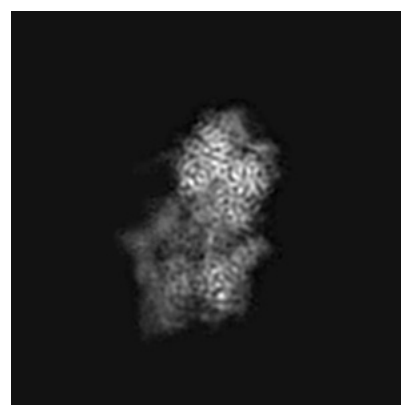
6.1.1 Primary map



X



Y

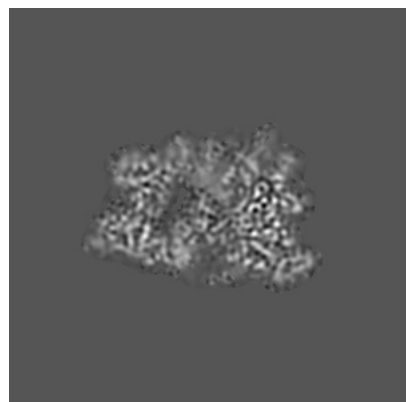


Z

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

6.2 Central slices [i](#)

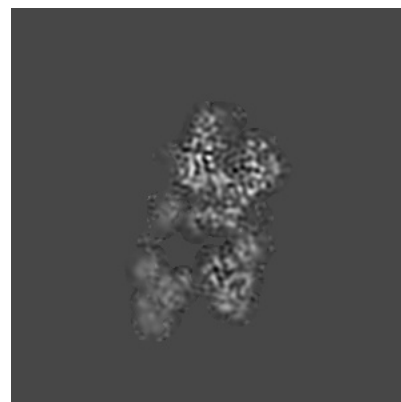
6.2.1 Primary map



X Index: 150



Y Index: 150

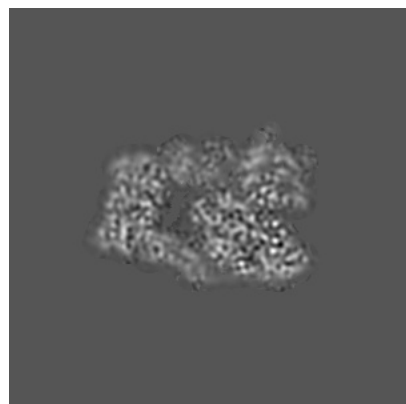


Z Index: 150

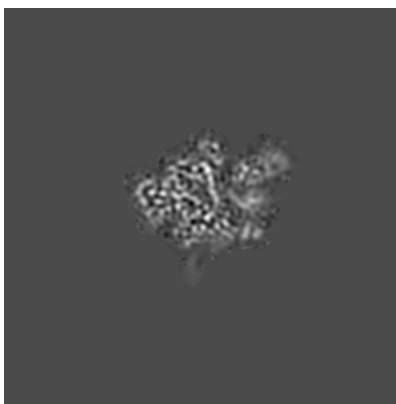
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 157



Y Index: 183

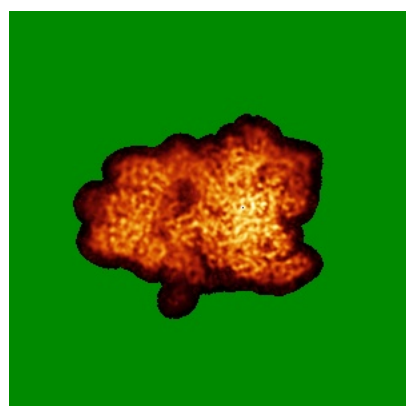


Z Index: 136

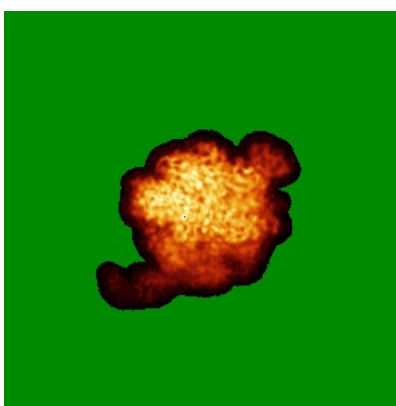
The images above show the largest variance slices of the map in three orthogonal directions.

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

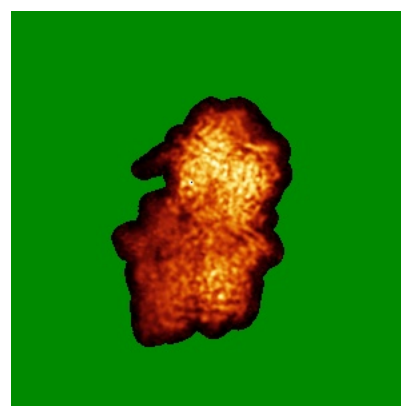
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

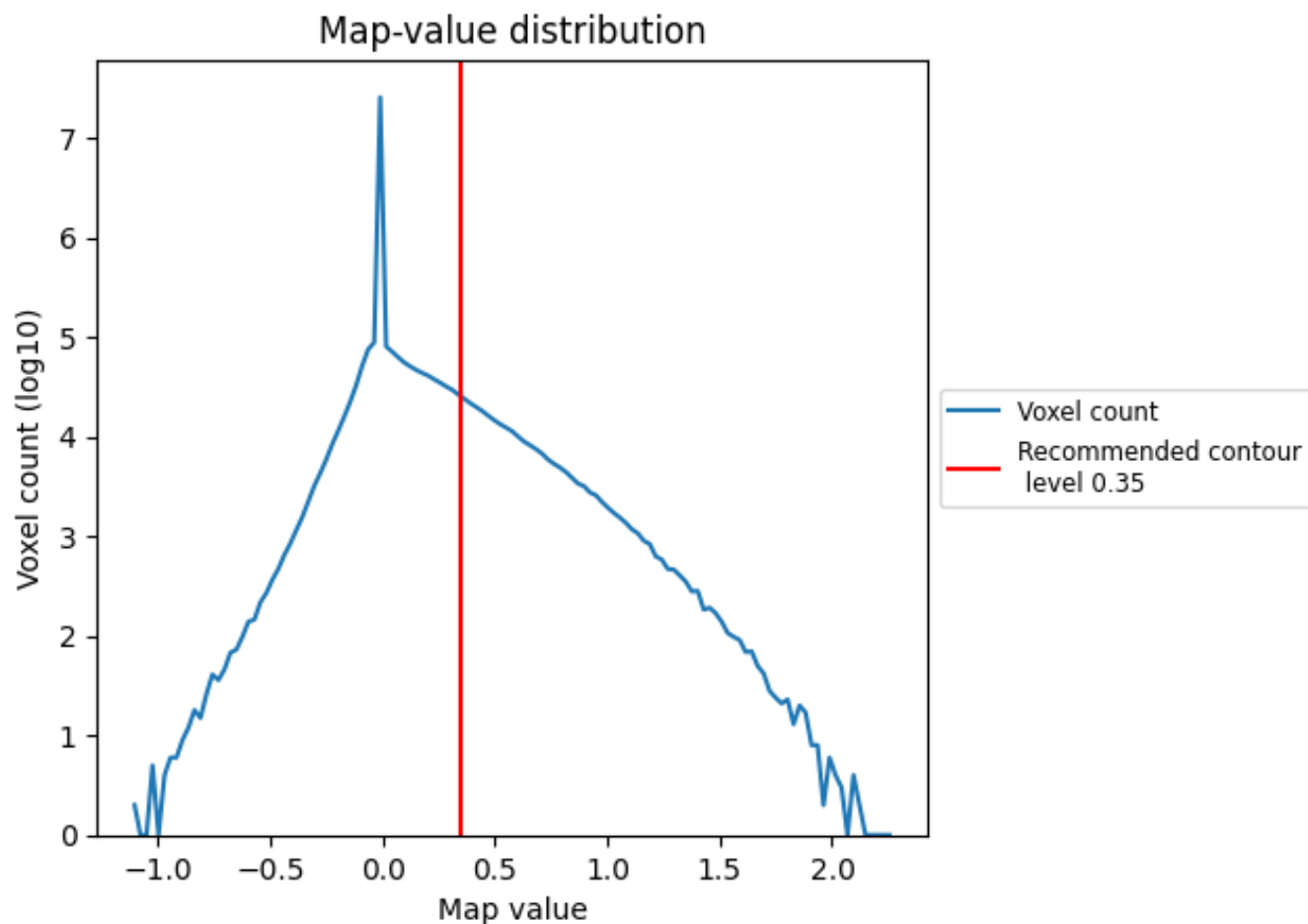
6.6 Mask visualisation

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

7 Map analysis [i](#)

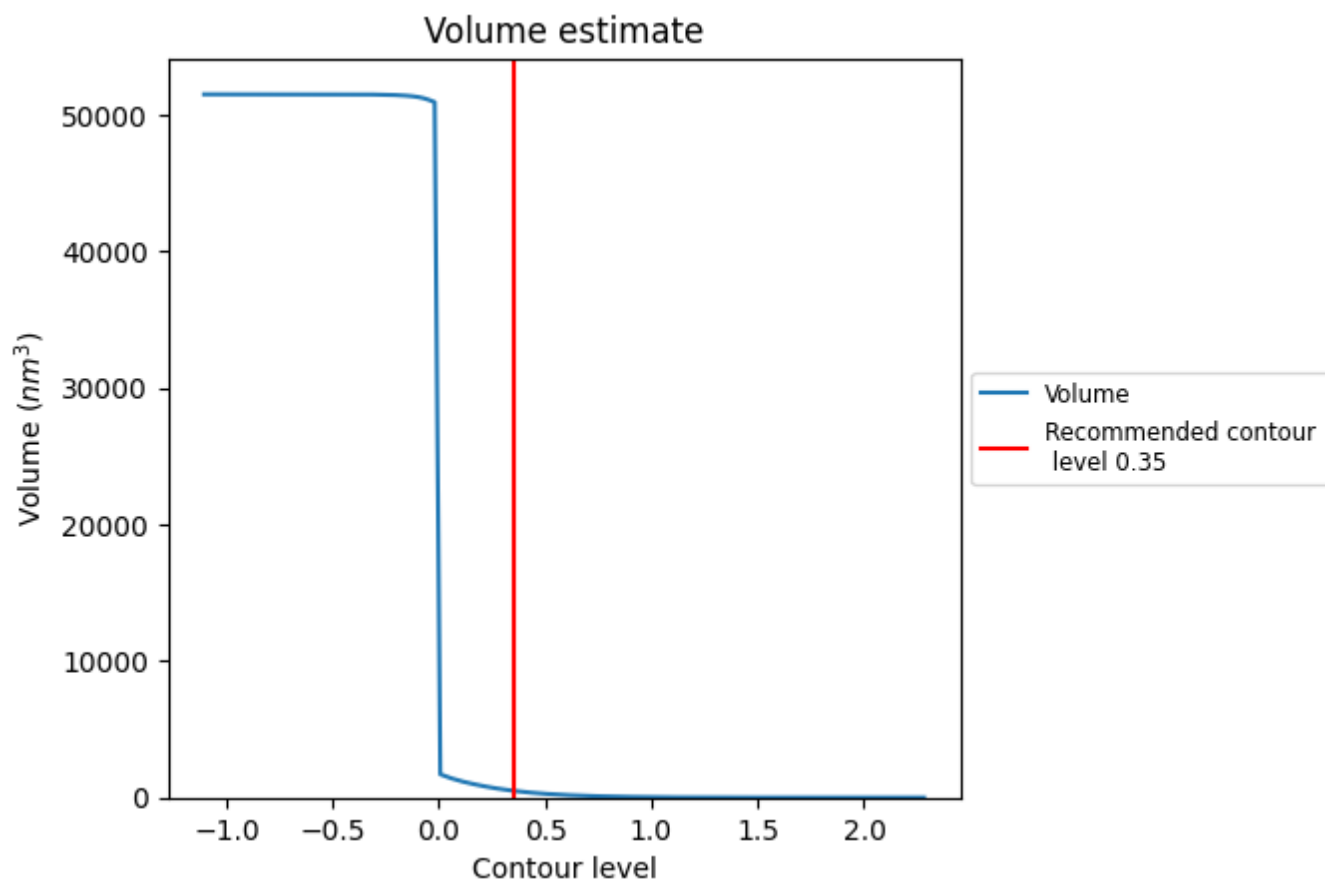
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

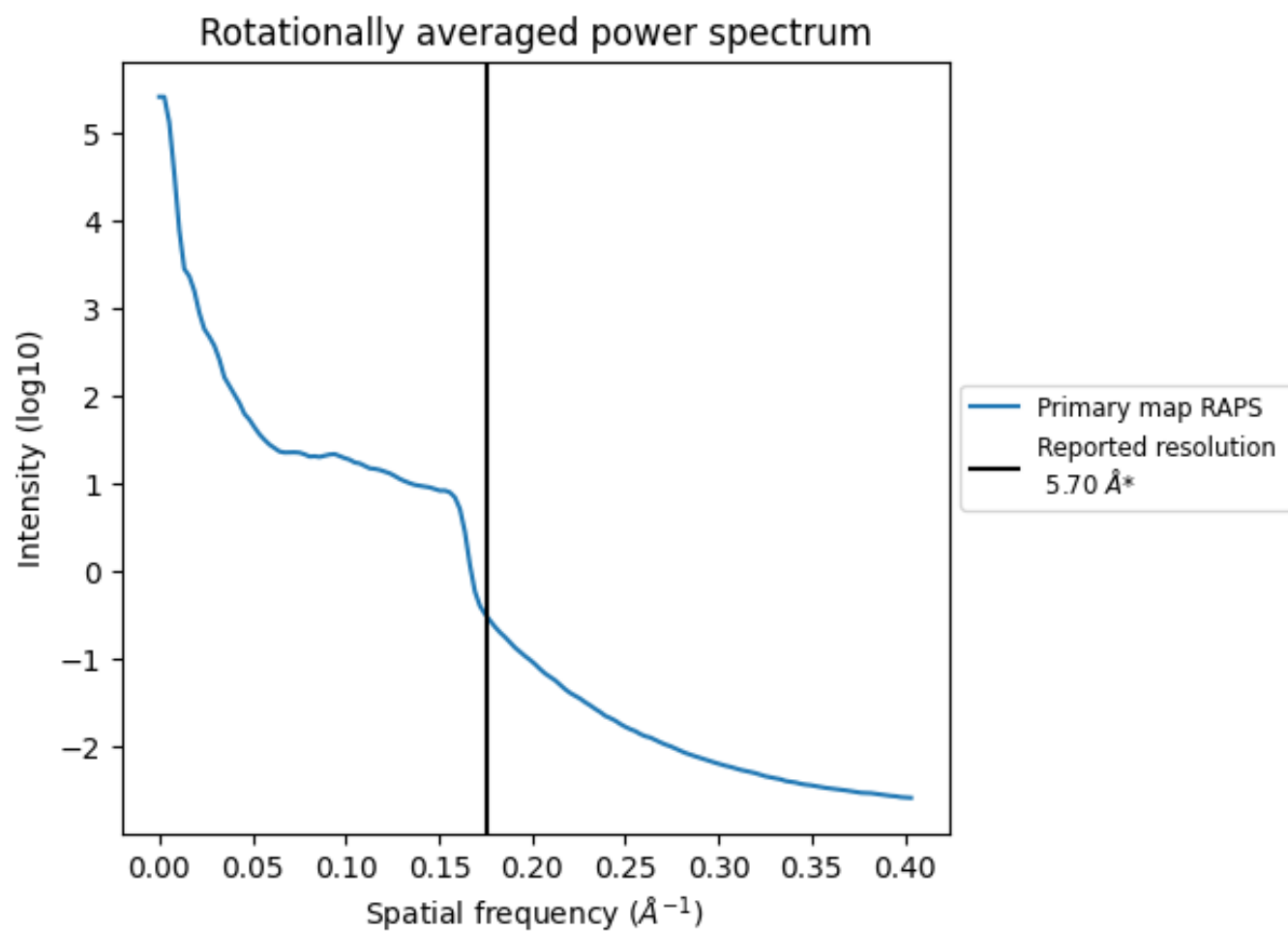
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

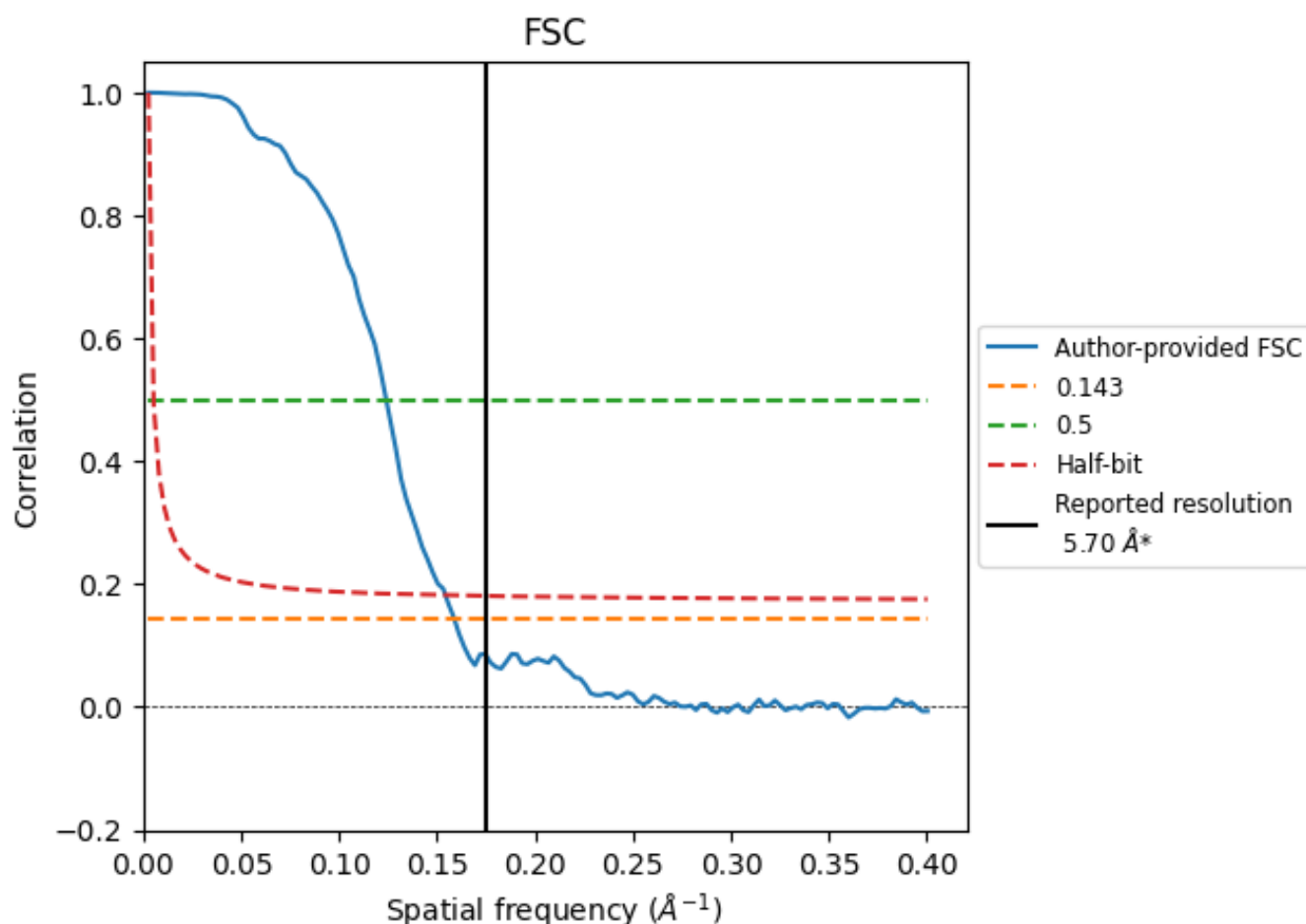


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8.2 Resolution estimates [i](#)

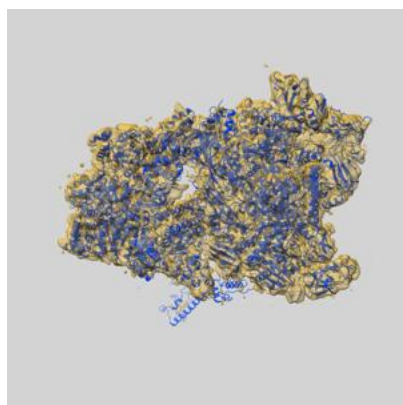
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	6.29	8.06	6.48
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 5.7 by more than 10 %

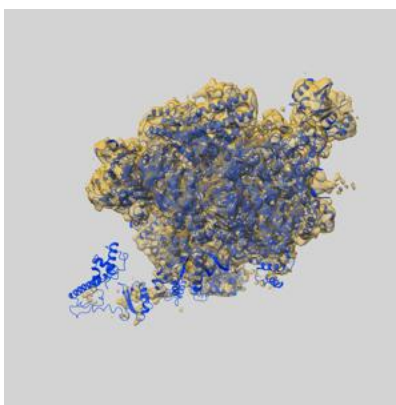
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11088 and PDB model 6Z9Q. Per-residue inclusion information can be found in section [3](#) on page [10](#).

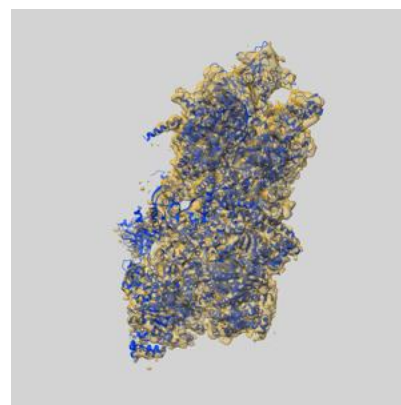
9.1 Map-model overlay [i](#)



X



Y



Z

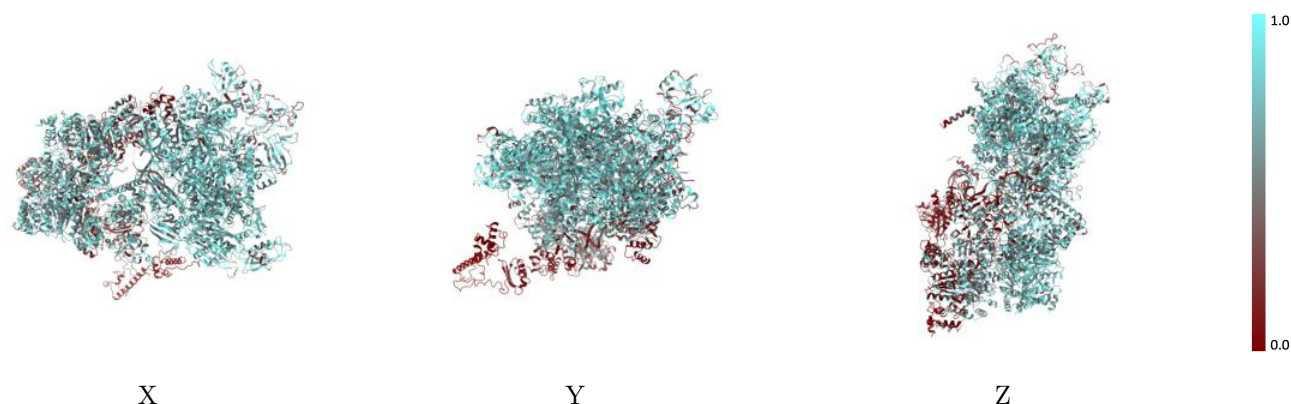
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



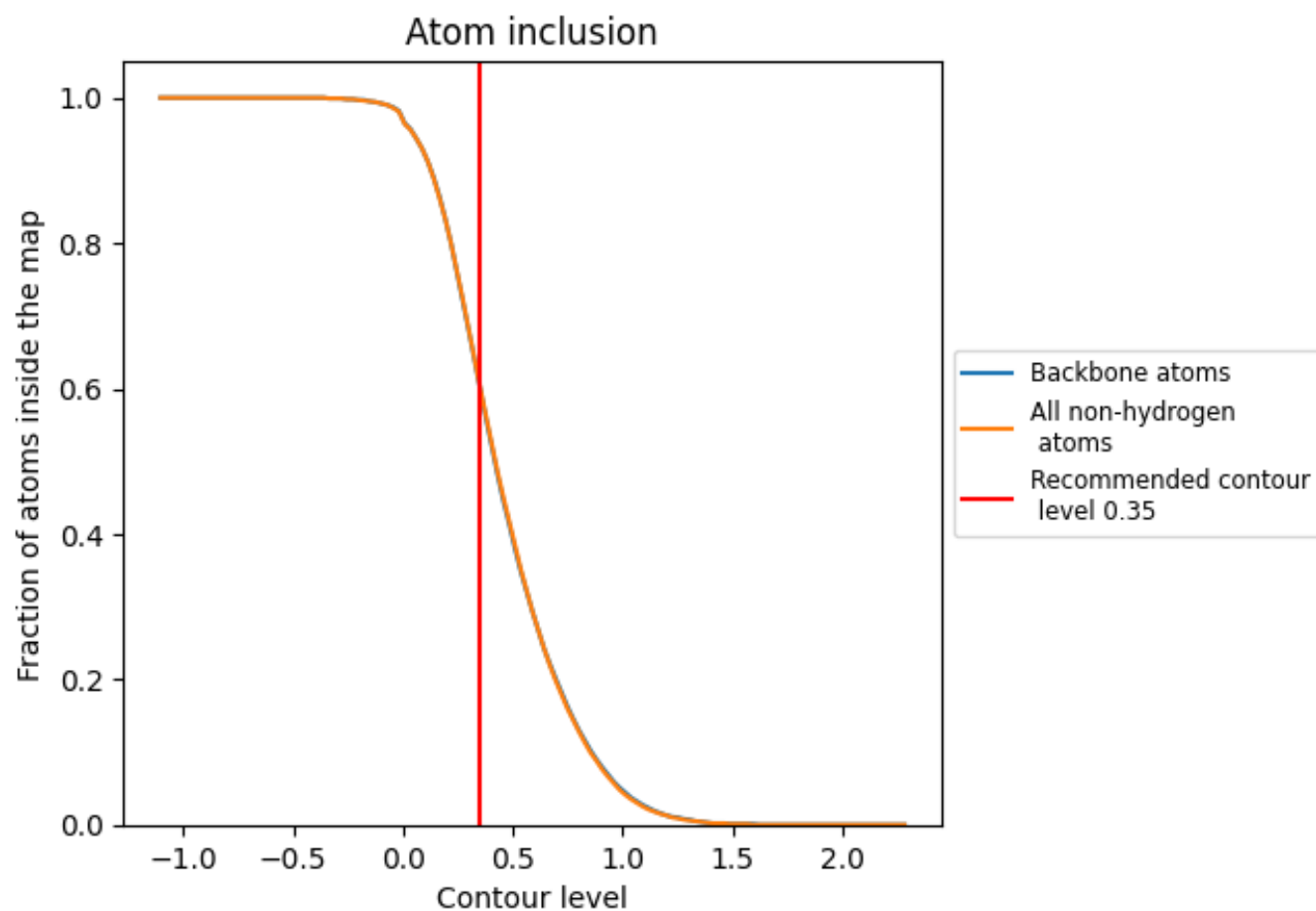
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6030	 0.1430
A	 0.2550	 0.0700
G	 0.2840	 0.1130
K	 0.5490	 0.0980
L	 0.6520	 0.1400
R	 0.8820	 0.2330
U	 0.7490	 0.1840
V	 0.6730	 0.1600
W	 0.5200	 0.1690
X	 0.7290	 0.1700
Y	 0.7040	 0.1660
a	 0.3740	 0.0950
b	 0.6580	 0.1380
c	 0.7080	 0.1590
d	 0.6820	 0.1430
e	 0.6200	 0.1380
f	 0.2940	 0.0860

