wwPDB EM Validation Summary Report

Dec 17, 2022 – 02:28 pm GMT

PDB ID	:	6Z9T
EMDB ID	:	EMD-11091
Title	:	Transcription termination intermediate complex 5
Authors	:	Said, N.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2020-06-04
Resolution	:	4.10 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

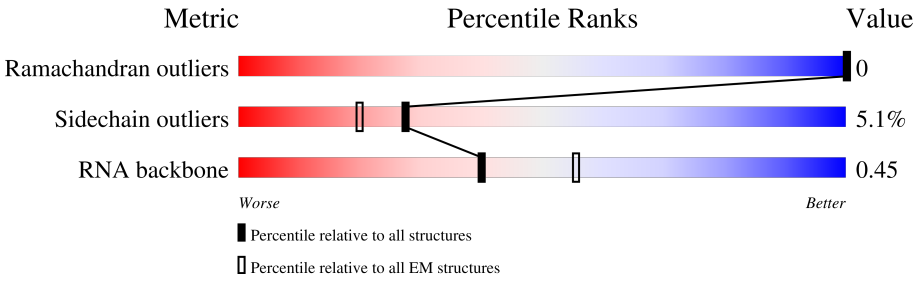
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.10 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	a	419	8% 89% 11%
1	b	419	5% 89% 11%
1	c	419	89% 10%
1	d	419	89% 11%
1	e	419	12% 89% 11%
1	f	419	14% 89% 11%
2	A	497	56% 99%
3	U	329	71% 29%

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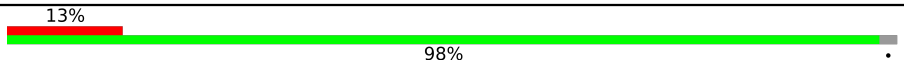
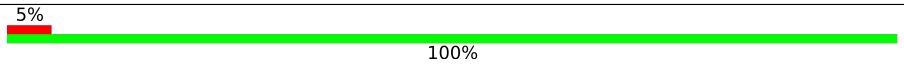
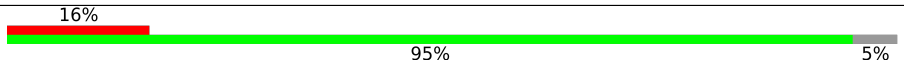
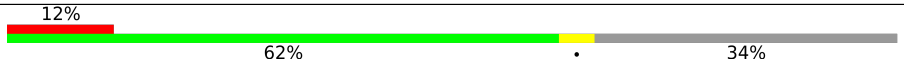
Mol	Chain	Length	Quality of chain
3	V	329	
4	W	91	
5	X	1342	
6	Y	1416	
7	L	50	
8	K	50	
9	R	99	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 51415 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 factor Rho.

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

- Molecule 2 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	495	Total 3850	C 2395	N 669	O 773	S 13	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	1343	Total	C	N	O	S	0	0
			10433	6550	1862	1971	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 7 is a DNA chain called template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	33	Total	C	N	O	P	0	0
			663	315	120	196	32		

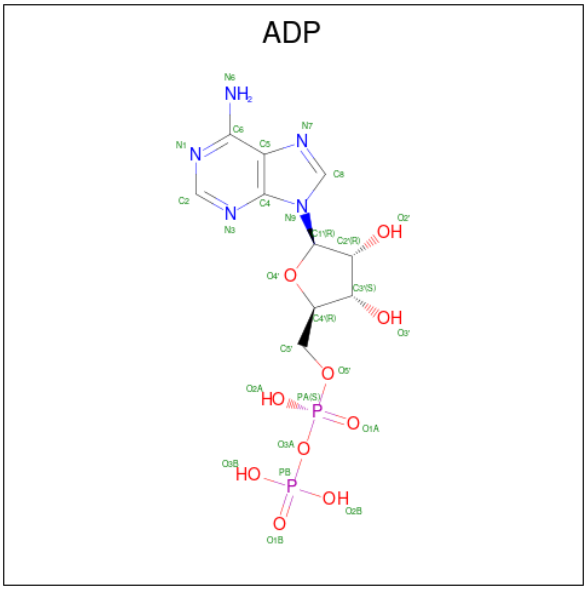
- Molecule 8 is a DNA chain called non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	21	Total	C	N	O	P	0	0
			437	205	86	125	21		

- Molecule 9 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	28	Total	C	N	O	P	0	0
			590	264	103	195	28		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	c	1	Total	Mg	0
			1	1	

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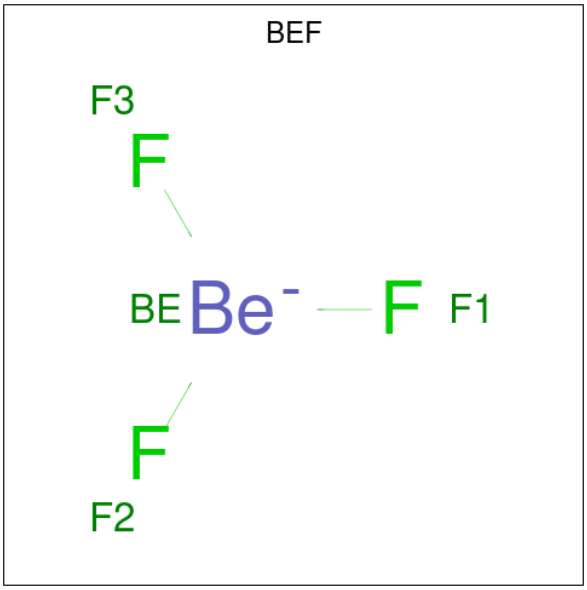
Mol	Chain	Residues	Atoms	AltConf
11	d	1	Total Mg 1 1	0
11	e	1	Total Mg 1 1	0
11	Y	1	Total Mg 1 1	0

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

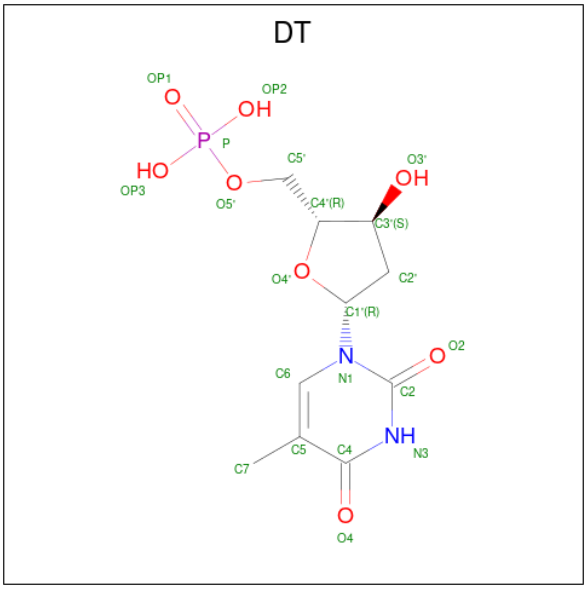


Mol	Chain	Residues	Atoms	AltConf
12	a	1	Total Be F 4 1 3	0
12	b	1	Total Be F 4 1 3	0
12	c	1	Total Be F 4 1 3	0
12	d	1	Total Be F 4 1 3	0
12	e	1	Total Be F 4 1 3	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

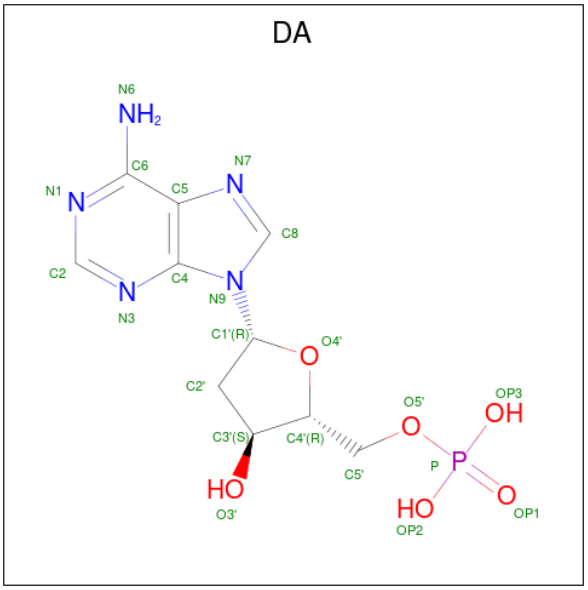
Mol	Chain	Residues	Atoms	AltConf
13	Y	2	Total Zn 2 2	0

- Molecule 14 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	Y	1	Total	C	N	O	P	0
			20	10	2	7	1	
14	L	1	Total	C	N	O	P	0
			20	10	2	7	1	

- Molecule 15 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: DA) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					AltConf
15	Y	1	Total	C	N	O	P	0
			21	10	5	5	1	

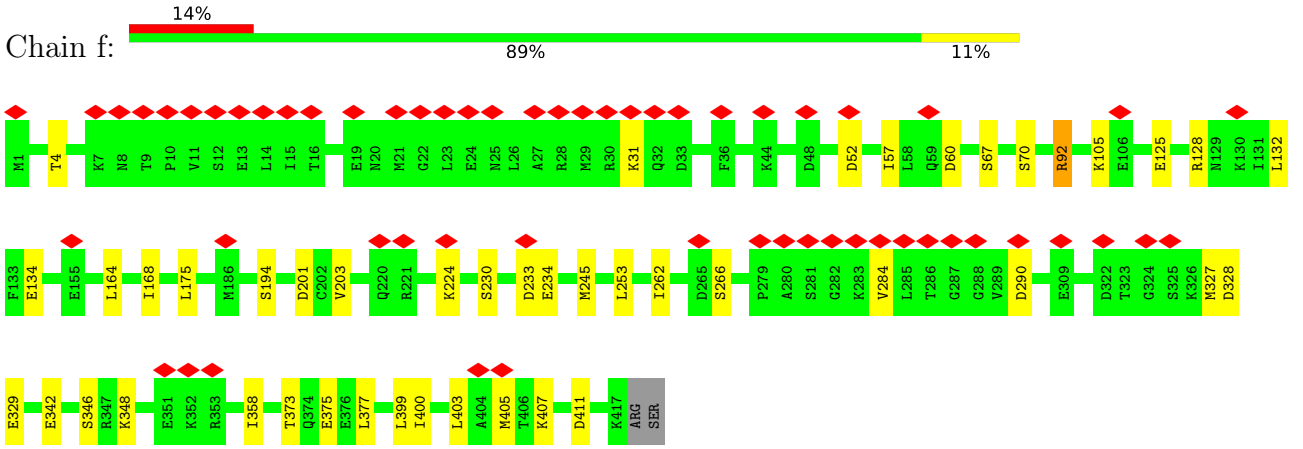
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	a	3	Total	O	0
			3	3	
16	b	3	Total	O	0
			3	3	
16	c	3	Total	O	0
			3	3	
16	d	3	Total	O	0
			3	3	
16	e	3	Total	O	0
			3	3	

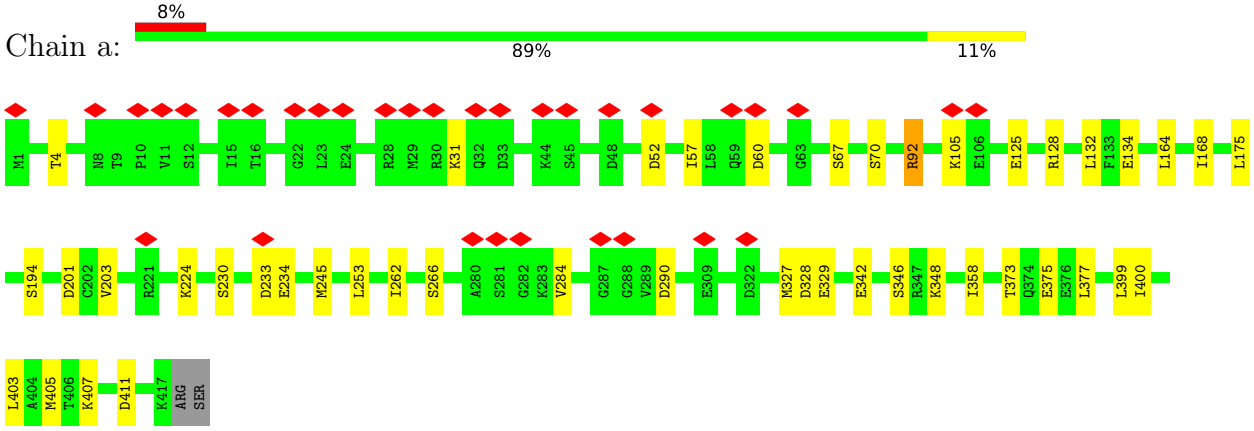
3 Residue-property plots (i)

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.

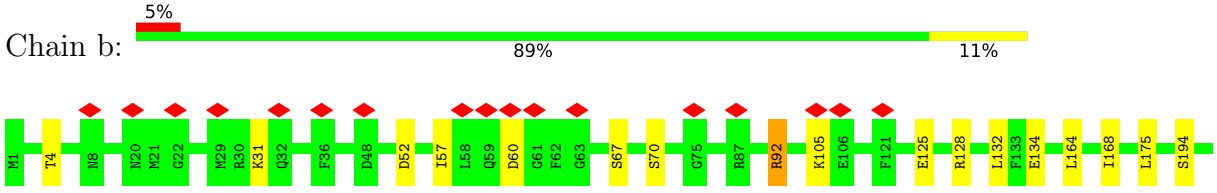
• Molecule 1: Transcription termination factor Rho

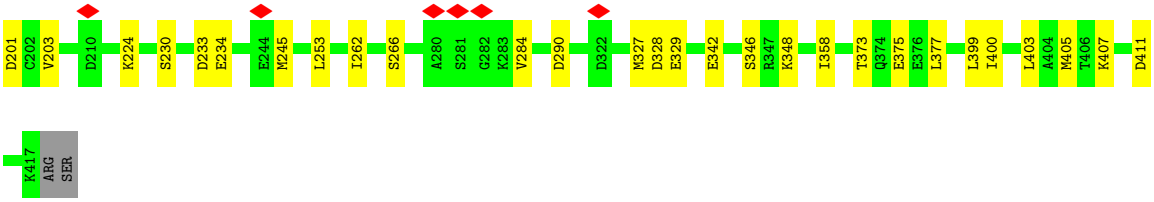


• Molecule 1: Transcription termination factor Rho

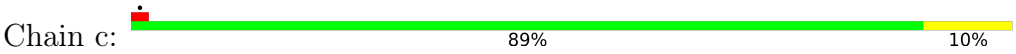


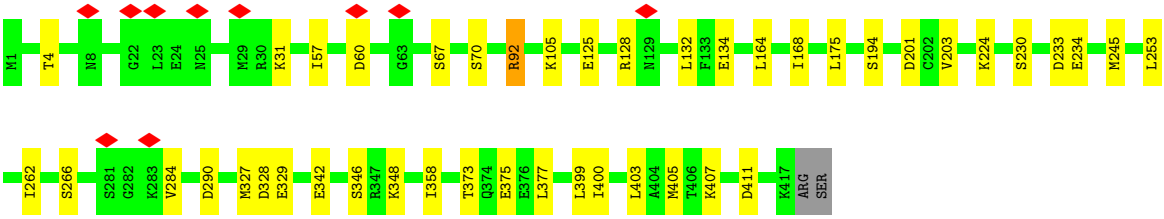
• Molecule 1: Transcription termination factor Rho



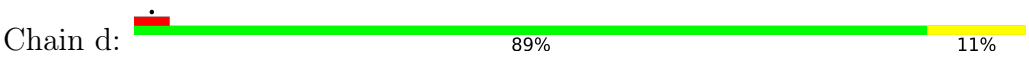


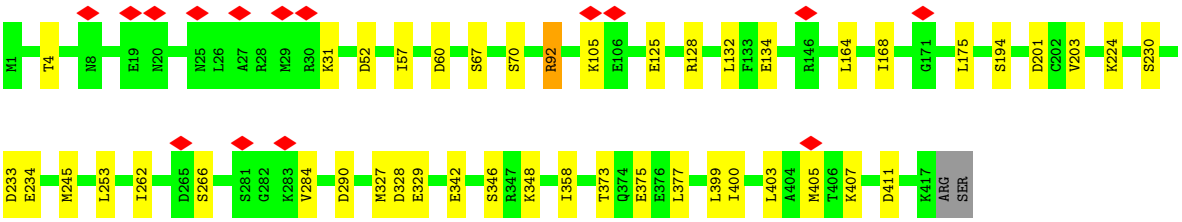
• Molecule 1: Transcription termination factor Rho



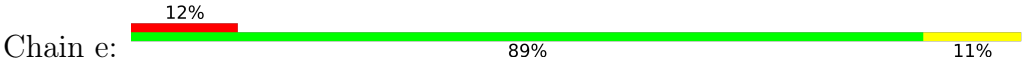


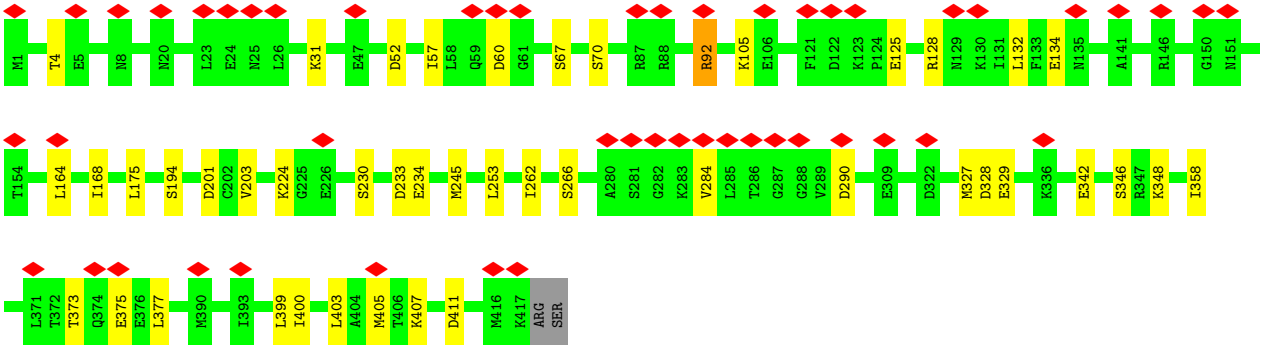
• Molecule 1: Transcription termination factor Rho



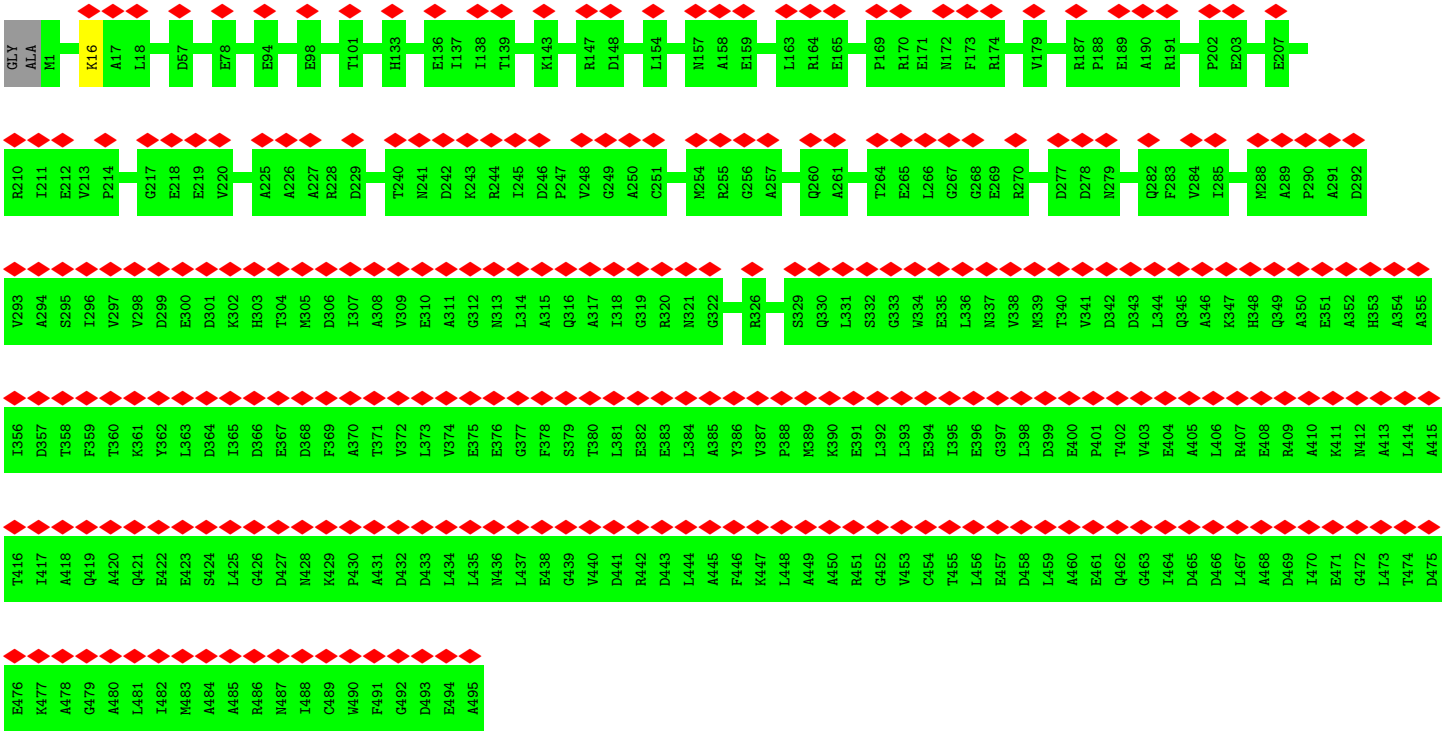


• Molecule 1: Transcription termination factor Rho



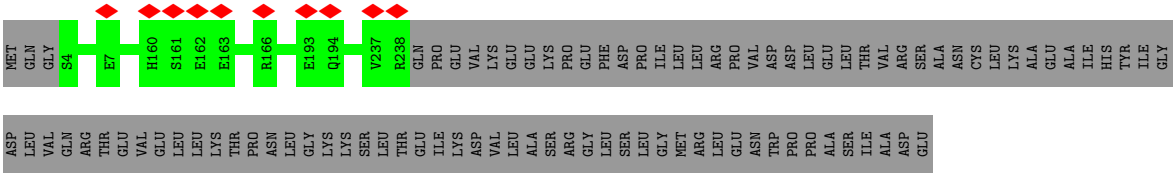


• Molecule 2: Transcription termination/antitermination protein NusA



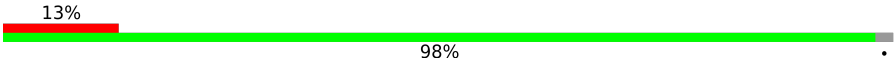
• Molecule 3: DNA-directed RNA polymerase subunit alpha

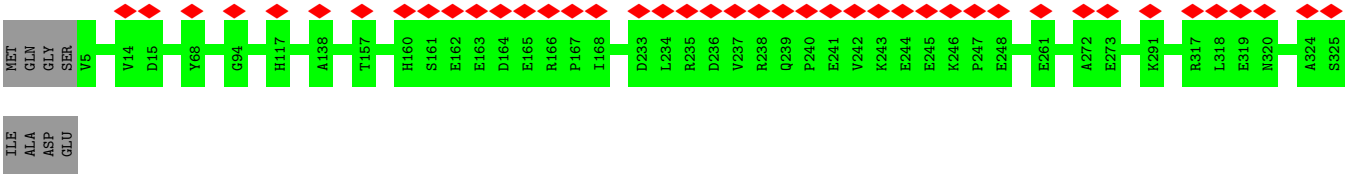
Chain U:



• Molecule 3: DNA-directed RNA polymerase subunit alpha

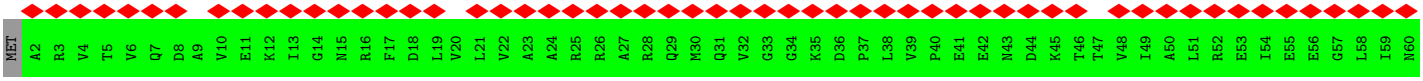
Chain V:

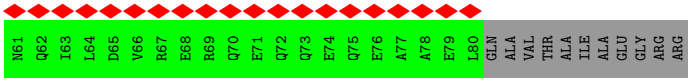




• Molecule 4: DNA-directed RNA polymerase subunit omega

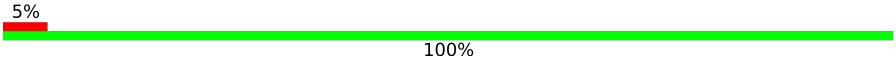
Chain W:

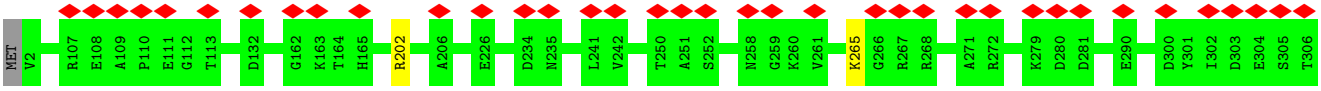


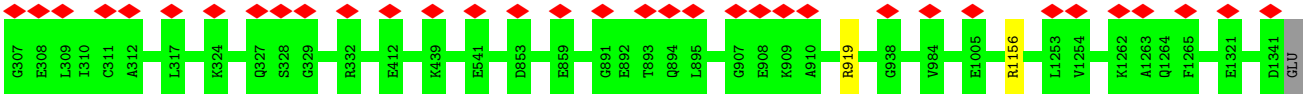


• Molecule 5: DNA-directed RNA polymerase subunit beta

Chain X:

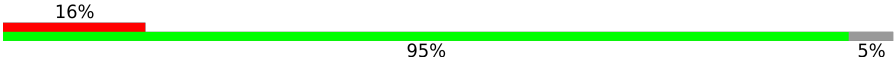


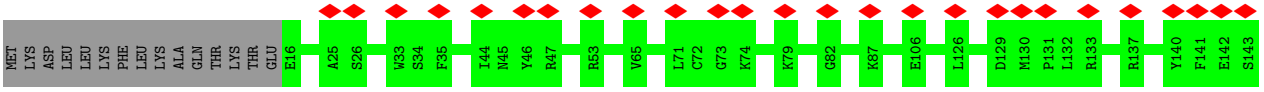


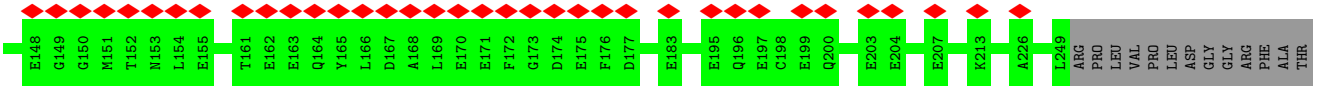


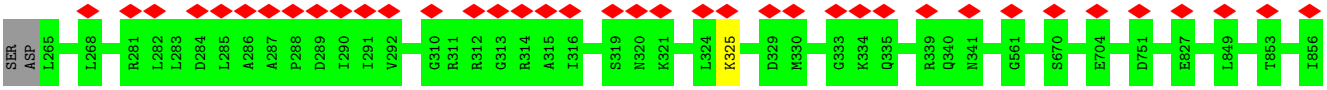
• Molecule 6: DNA-directed RNA polymerase subunit beta'

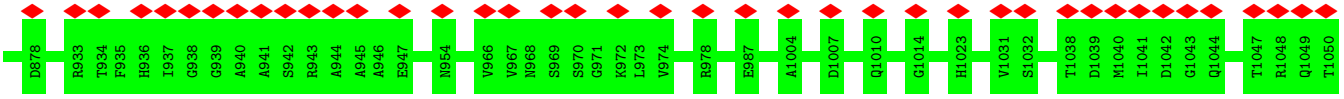
Chain Y:

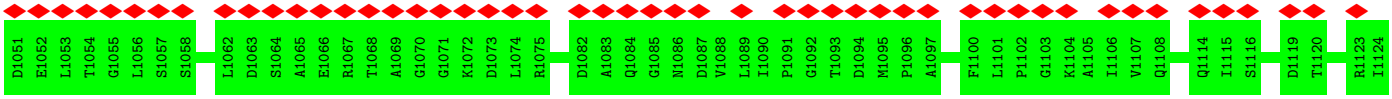


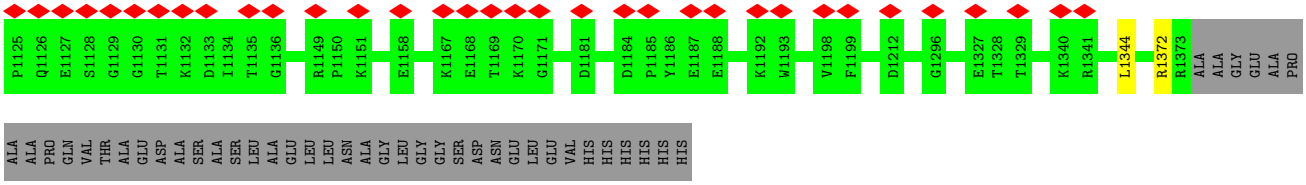






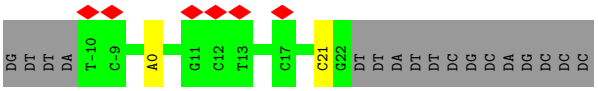






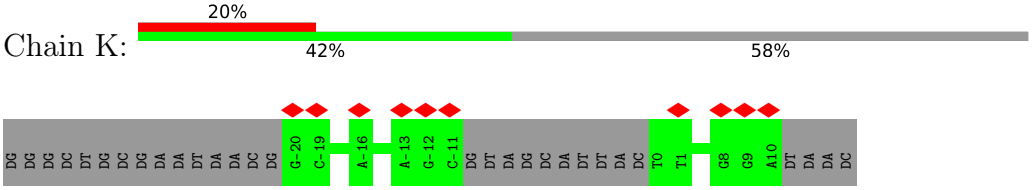
• Molecule 7: template strand

Chain L:



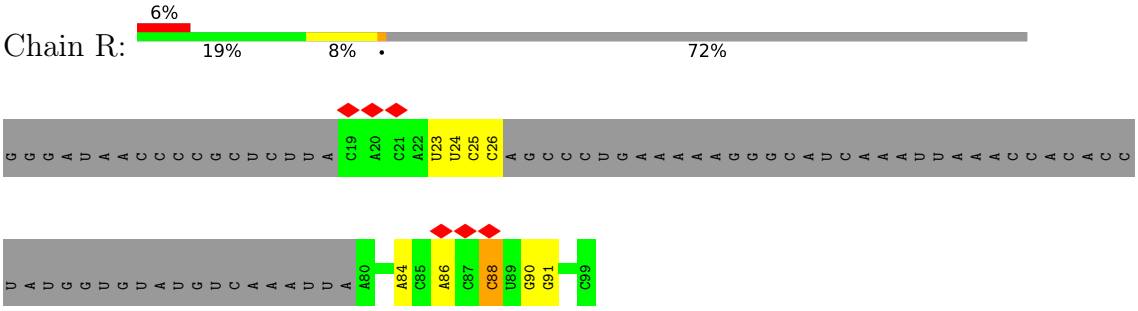
• Molecule 8: non template strand

Chain K:



• Molecule 9: rut RNA

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38054	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 ($e^-/Å^2$)	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	2.160	Depositor
Minimum map value	-1.113	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.063	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.27	0/3329	0.49	1/4483 (0.0%)
1	b	0.27	0/3329	0.49	1/4483 (0.0%)
1	c	0.27	0/3329	0.49	1/4483 (0.0%)
1	d	0.27	0/3329	0.49	1/4483 (0.0%)
1	e	0.27	0/3329	0.49	1/4483 (0.0%)
1	f	0.27	0/3329	0.49	1/4483 (0.0%)
2	A	0.24	0/3895	0.45	0/5270
3	U	0.23	0/1847	0.42	0/2503
3	V	0.23	0/2538	0.46	0/3441
4	W	0.22	0/629	0.39	0/847
5	X	0.25	0/10736	0.42	0/14487
6	Y	0.24	0/10590	0.43	1/14296 (0.0%)
7	L	0.68	1/741 (0.1%)	0.92	1/1139 (0.1%)
8	K	0.46	0/490	0.81	0/753
9	R	0.25	0/656	1.03	3/1016 (0.3%)
All	All	0.27	1/52096 (0.0%)	0.48	11/70650 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	21	DC	O3'-P	12.04	1.75	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	0	DA	O4'-C1'-N9	7.73	113.41	108.00
1	e	92	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	b	92	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	c	92	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	a	92	ARG	NE-CZ-NH2	6.88	123.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	b	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	c	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	d	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	e	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	f	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
2	A	493/497 (99%)	448 (91%)	45 (9%)	0	100	100
3	U	233/329 (71%)	224 (96%)	9 (4%)	0	100	100
3	V	319/329 (97%)	295 (92%)	24 (8%)	0	100	100
4	W	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	X	1338/1342 (100%)	1255 (94%)	83 (6%)	0	100	100
6	Y	1339/1416 (95%)	1257 (94%)	82 (6%)	0	100	100
All	All	6289/6518 (96%)	5965 (95%)	324 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	a	357/359 (99%)	312 (87%)	45 (13%)	4 22
1	b	357/359 (99%)	312 (87%)	45 (13%)	4 22
1	c	357/359 (99%)	313 (88%)	44 (12%)	4 22
1	d	357/359 (99%)	312 (87%)	45 (13%)	4 22
1	e	357/359 (99%)	312 (87%)	45 (13%)	4 22
1	f	357/359 (99%)	312 (87%)	45 (13%)	4 22
2	A	408/409 (100%)	407 (100%)	1 (0%)	93 96
3	U	203/286 (71%)	203 (100%)	0	100 100
3	V	280/286 (98%)	280 (100%)	0	100 100
4	W	67/75 (89%)	67 (100%)	0	100 100
5	X	1155/1157 (100%)	1151 (100%)	4 (0%)	92 95
6	Y	1122/1177 (95%)	1120 (100%)	2 (0%)	93 96
All	All	5377/5544 (97%)	5101 (95%)	276 (5%)	27 52

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	92	ARG
1	e	168	ILE
1	e	373	THR
1	b	92	ARG
1	b	60	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
5	X	1324	ASN
6	Y	232	ASN
6	Y	665	GLN
1	e	401	ASN
1	e	292	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	26/99 (26%)	9 (34%)	2 (7%)

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	24	U
9	R	25	C
9	R	26	C
9	R	84	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	90	G

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 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
12	BEF	a	1002	-	0,3,3	-	-	-		
12	BEF	e	1002	-	0,3,3	-	-	-		
10	ADP	c	1000	11	24,29,29	0.99	1 (4%)	29,45,45	1.58	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	DT	Y	1504	-	18,21,22	0.33	0	26,30,33	0.67	1 (3%)
10	ADP	d	1000	11,1	24,29,29	0.97	1 (4%)	29,45,45	1.49	4 (13%)
15	DA	Y	1505	-	18,23,24	0.67	0	17,33,36	0.71	0
12	BEF	c	1002	-	0,3,3	-	-	-		
12	BEF	d	1002	-	0,3,3	-	-	-		
12	BEF	b	1002	-	0,3,3	-	-	-		
10	ADP	a	1000	11,1	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
14	DT	L	101	-	18,21,22	0.31	0	26,30,33	0.84	0
10	ADP	e	1000	11,1	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
10	ADP	b	1000	11	24,29,29	0.96	1 (4%)	29,45,45	1.53	4 (13%)

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
10	ADP	c	1000	11	-	2/12/32/32	0/3/3/3
14	DT	Y	1504	-	-	1/7/21/22	0/2/2/2
10	ADP	d	1000	11,1	-	2/12/32/32	0/3/3/3
15	DA	Y	1505	-	-	1/3/21/22	0/3/3/3
10	ADP	a	1000	11,1	-	2/12/32/32	0/3/3/3
14	DT	L	101	-	-	5/7/21/22	0/2/2/2
10	ADP	e	1000	11,1	-	2/12/32/32	0/3/3/3
10	ADP	b	1000	11	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	1000	ADP	C5-C4	2.55	1.47	1.40
10	d	1000	ADP	C5-C4	2.52	1.47	1.40
10	a	1000	ADP	C5-C4	2.50	1.47	1.40
10	e	1000	ADP	C5-C4	2.50	1.47	1.40
10	b	1000	ADP	C5-C4	2.48	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1000	ADP	PA-O3A-PB	-4.03	118.99	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	c	1000	ADP	C3'-C2'-C1'	3.93	106.89	100.98
10	e	1000	ADP	PA-O3A-PB	-3.91	119.42	132.83
10	c	1000	ADP	PA-O3A-PB	-3.78	119.84	132.83
10	a	1000	ADP	C3'-C2'-C1'	3.66	106.49	100.98

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

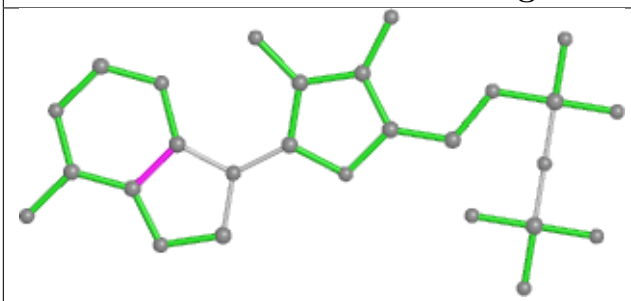
Mol	Chain	Res	Type	Atoms
10	b	1000	ADP	O4'-C4'-C5'-O5'
14	Y	1504	DT	O4'-C4'-C5'-O5'
14	L	101	DT	O4'-C1'-N1-C2
14	L	101	DT	O4'-C1'-N1-C6
10	c	1000	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

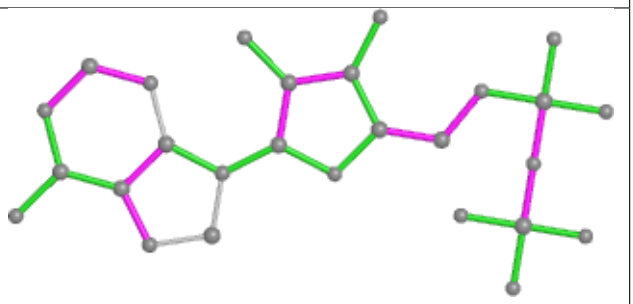
No monomer is involved in short contacts.

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.

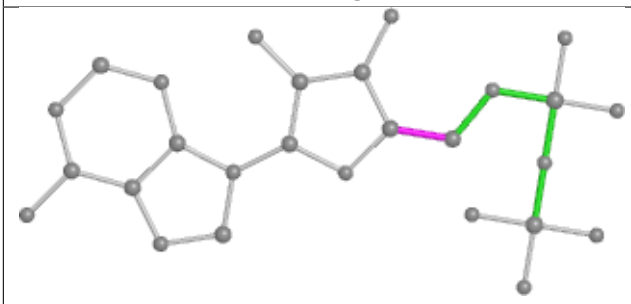
Ligand ADP c 1000



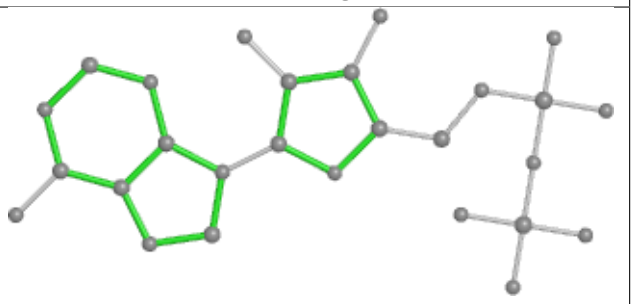
Bond lengths



Bond angles

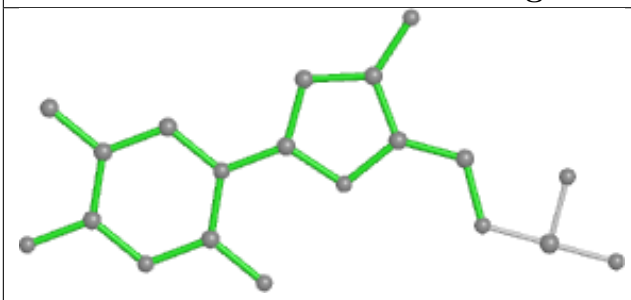


Torsions

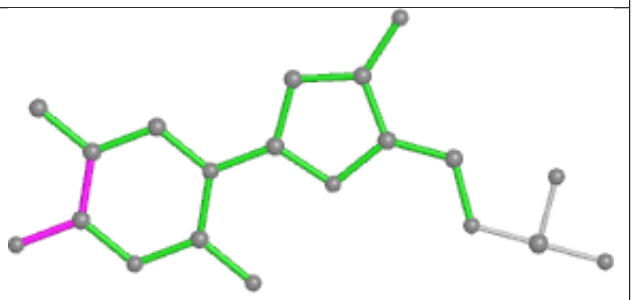


Rings

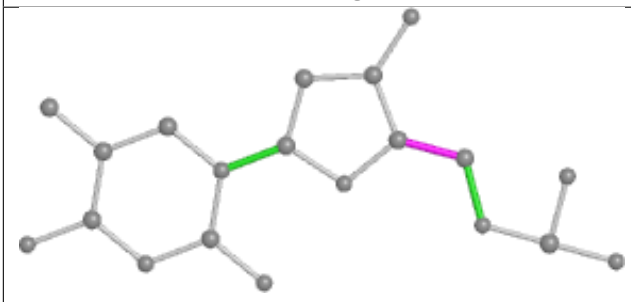
Ligand DT Y 1504



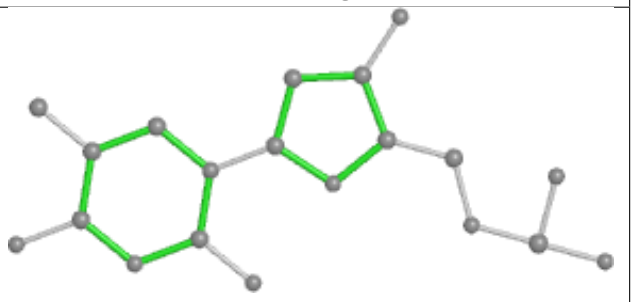
Bond lengths



Bond angles

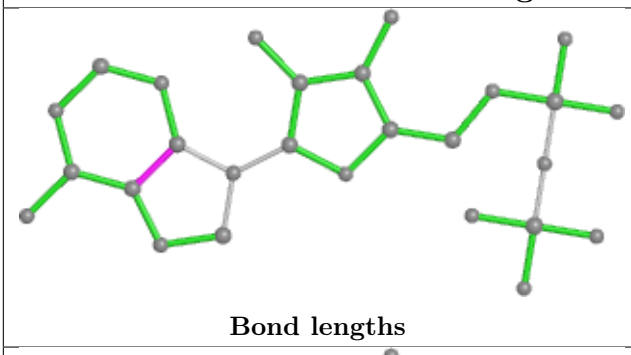


Torsions

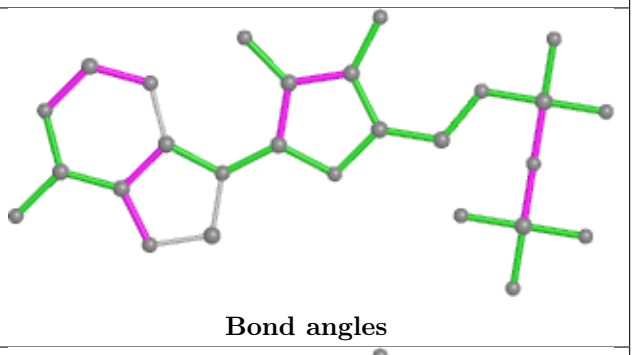


Rings

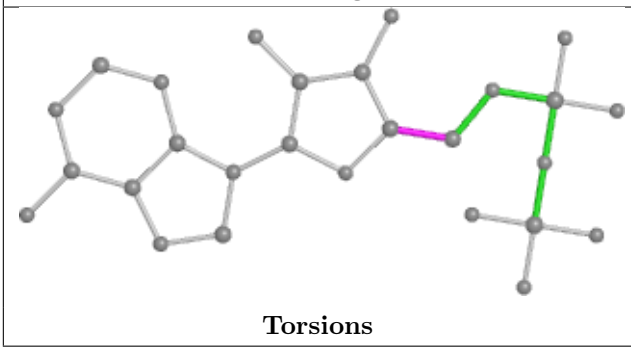
Ligand ADP d 1000



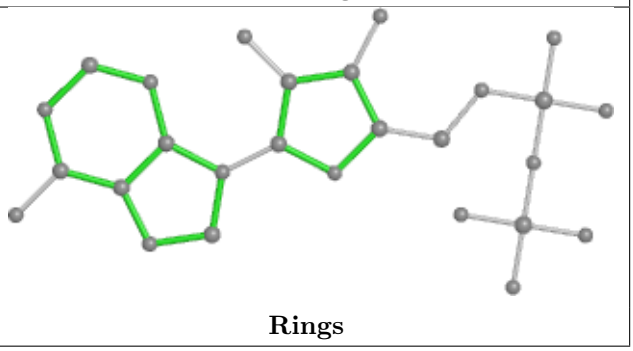
Bond lengths



Bond angles

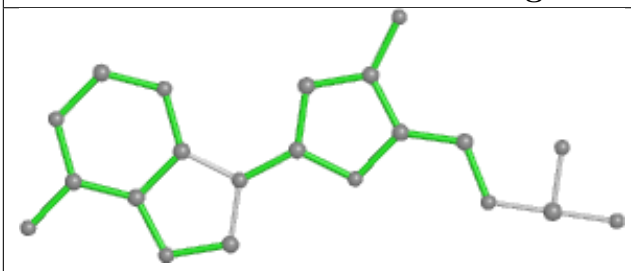


Torsions

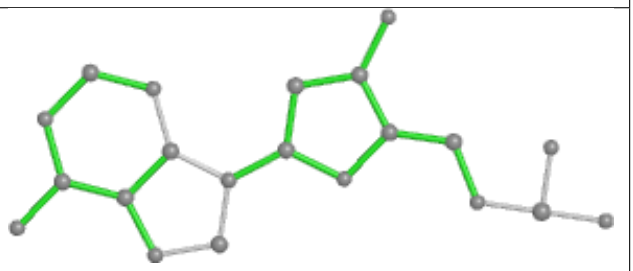


Rings

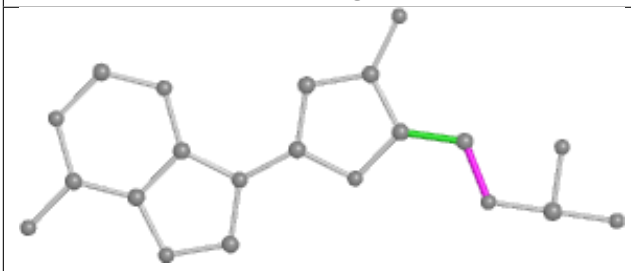
Ligand DA Y 1505



Bond lengths



Bond angles



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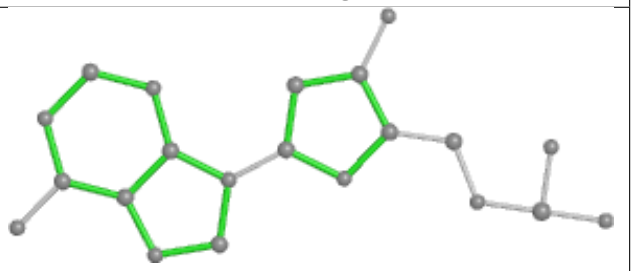
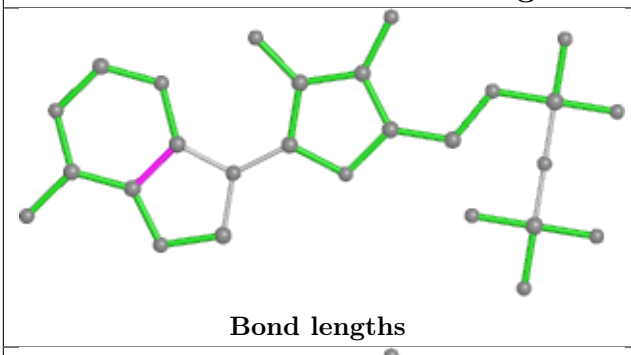
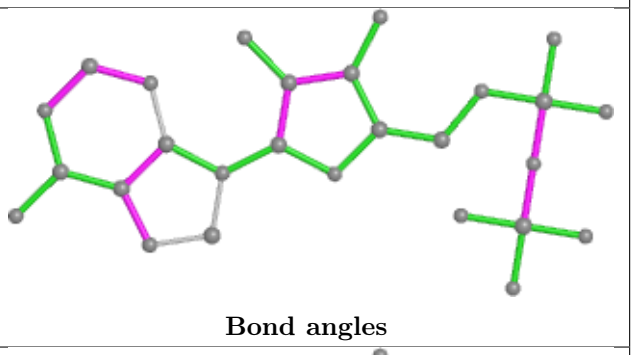


Rings

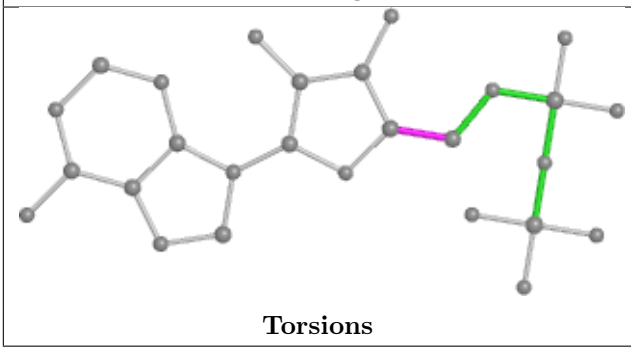
Ligand ADP a 1000



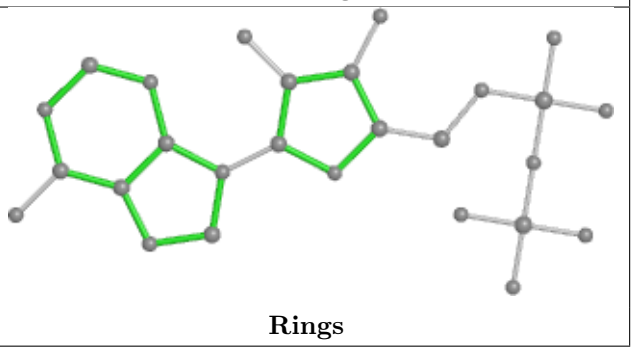
Bond lengths



Bond angles

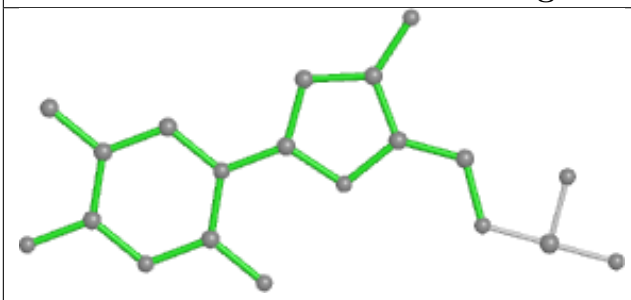


Torsions

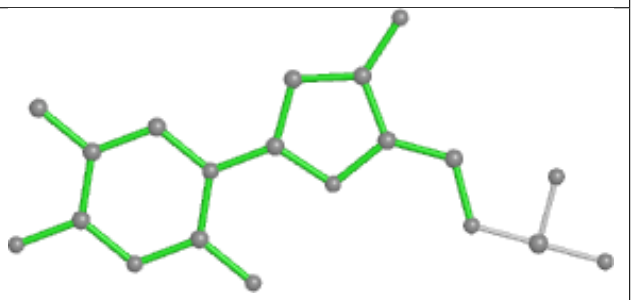


Rings

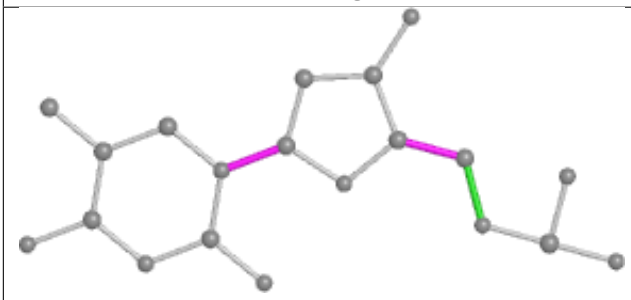
Ligand DT L 101



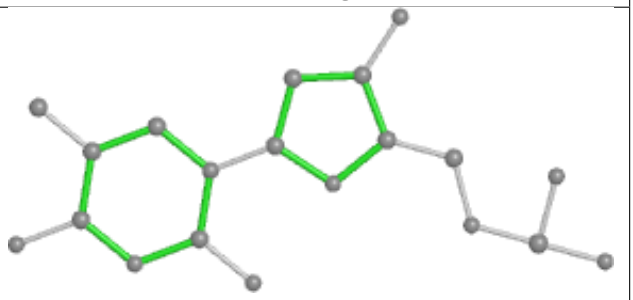
Bond lengths



Bond angles

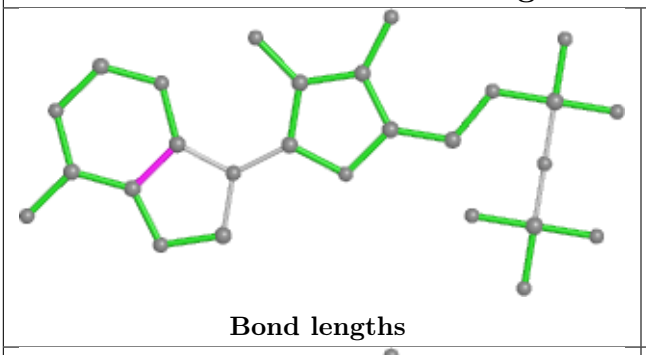


Torsions

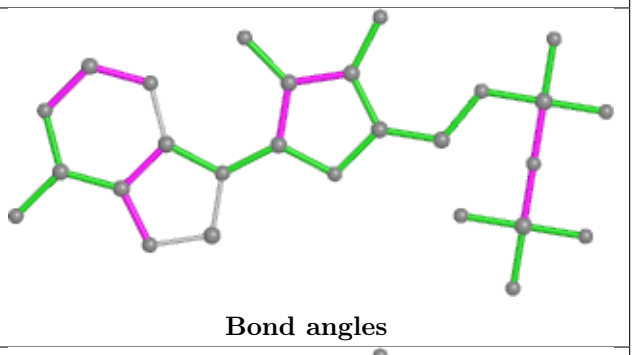


Rings

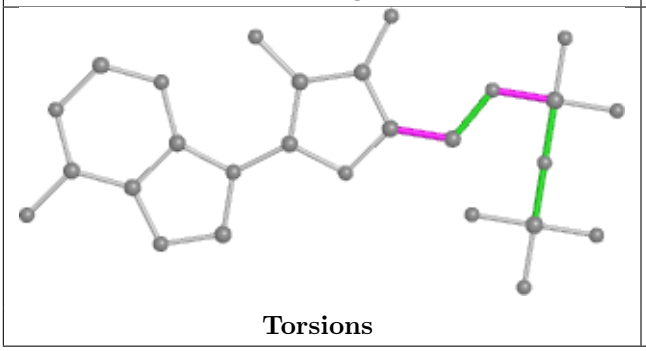
Ligand ADP e 1000



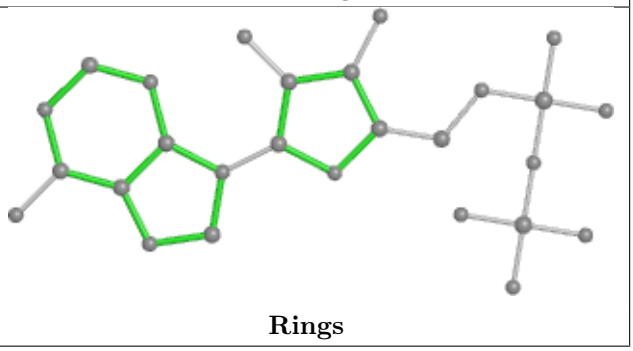
Bond lengths



Bond angles

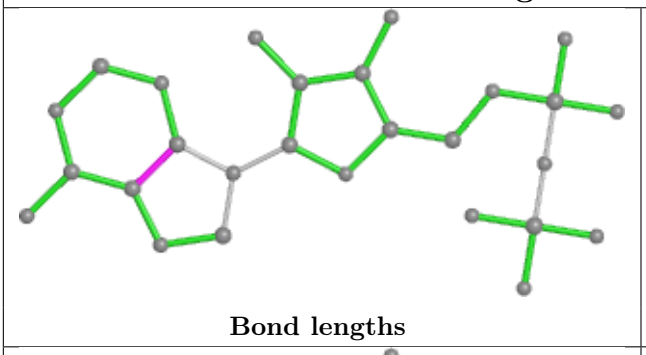


Torsions

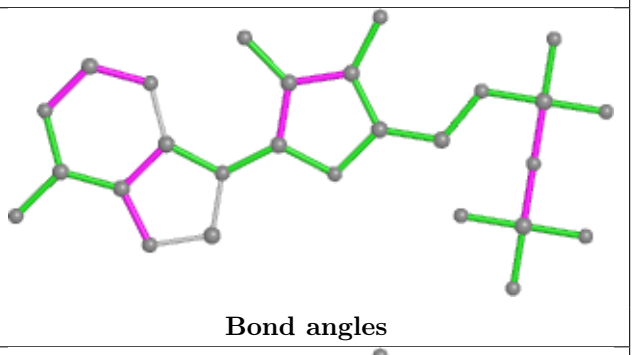


Rings

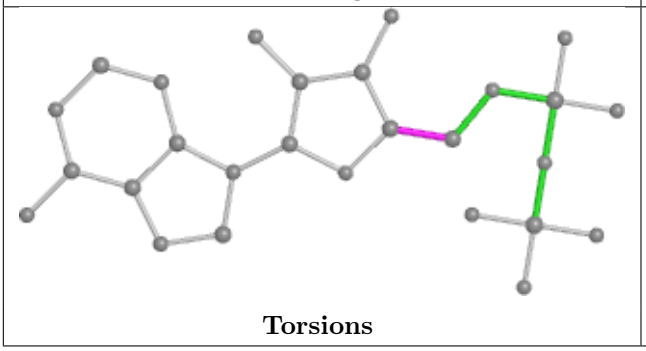
Ligand ADP b 1000



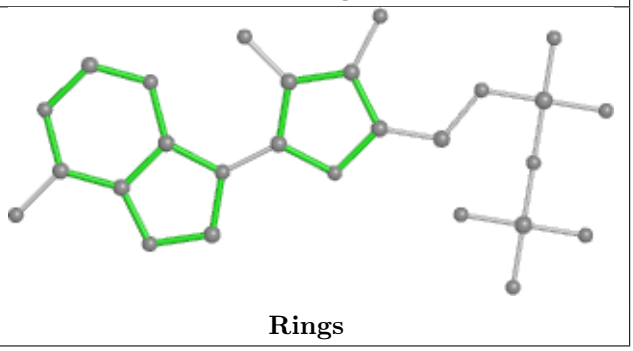
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	21:DC	O3'	22:DG	P	1.75

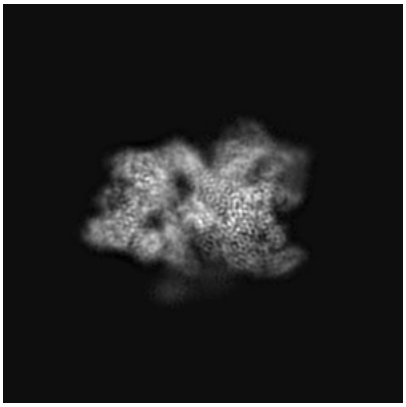
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11091. These allow visual inspection of the internal detail of the map and identification of artifacts.

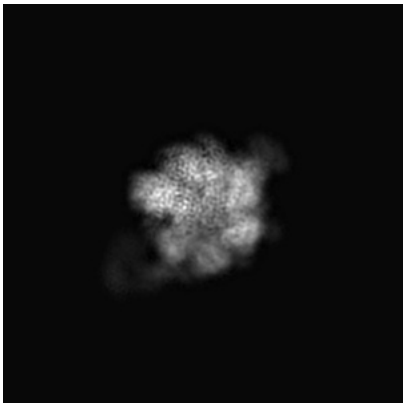
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

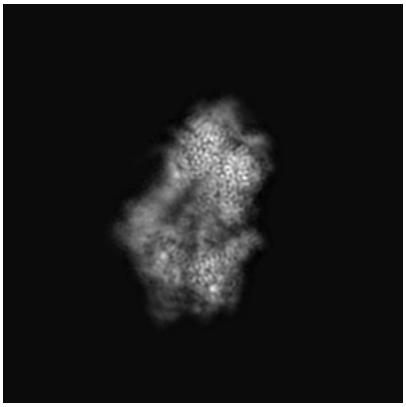
6.1.1 Primary map



X



Y

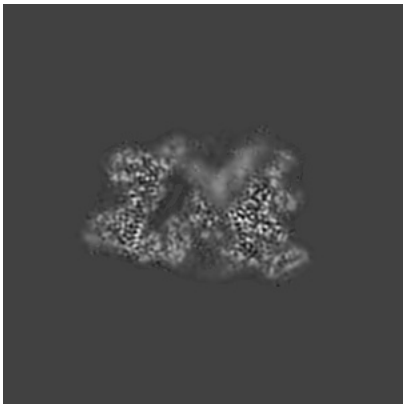


Z

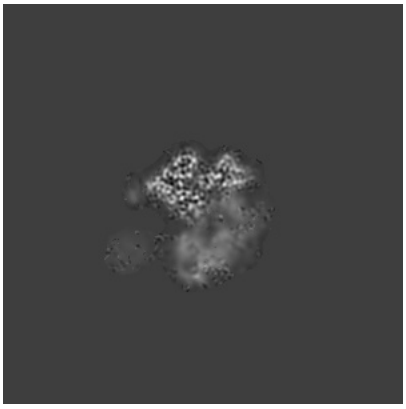
The images above show the map projected in three orthogonal directions.

6.2 Central slices

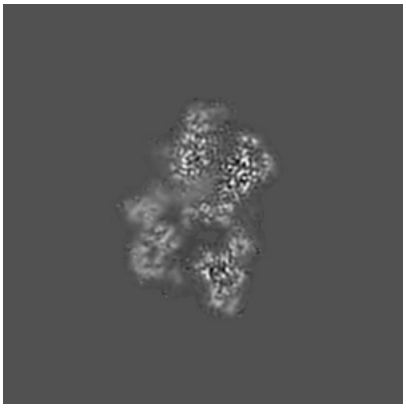
6.2.1 Primary map



X Index: 150



Y Index: 150

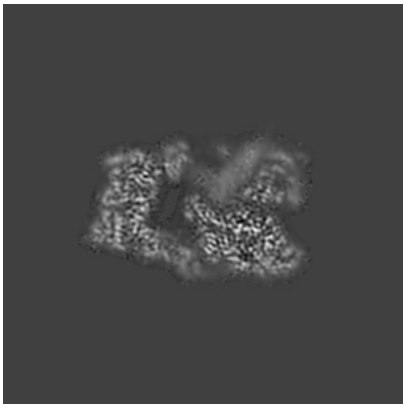


Z Index: 150

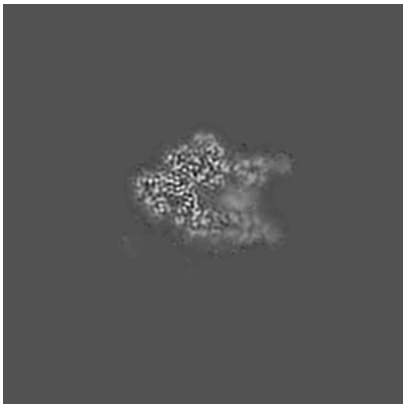
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

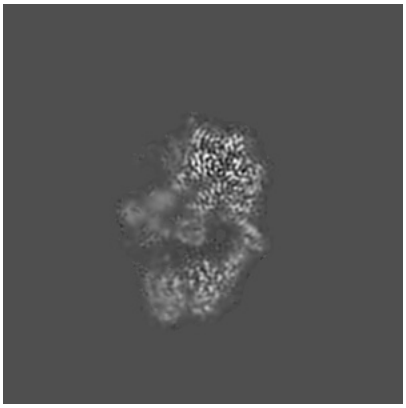
6.3.1 Primary map



X Index: 157



Y Index: 177

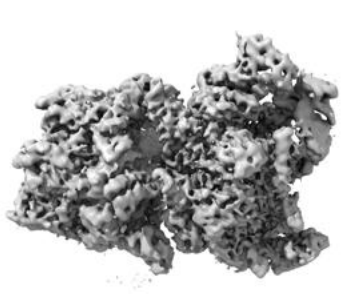


Z Index: 136

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

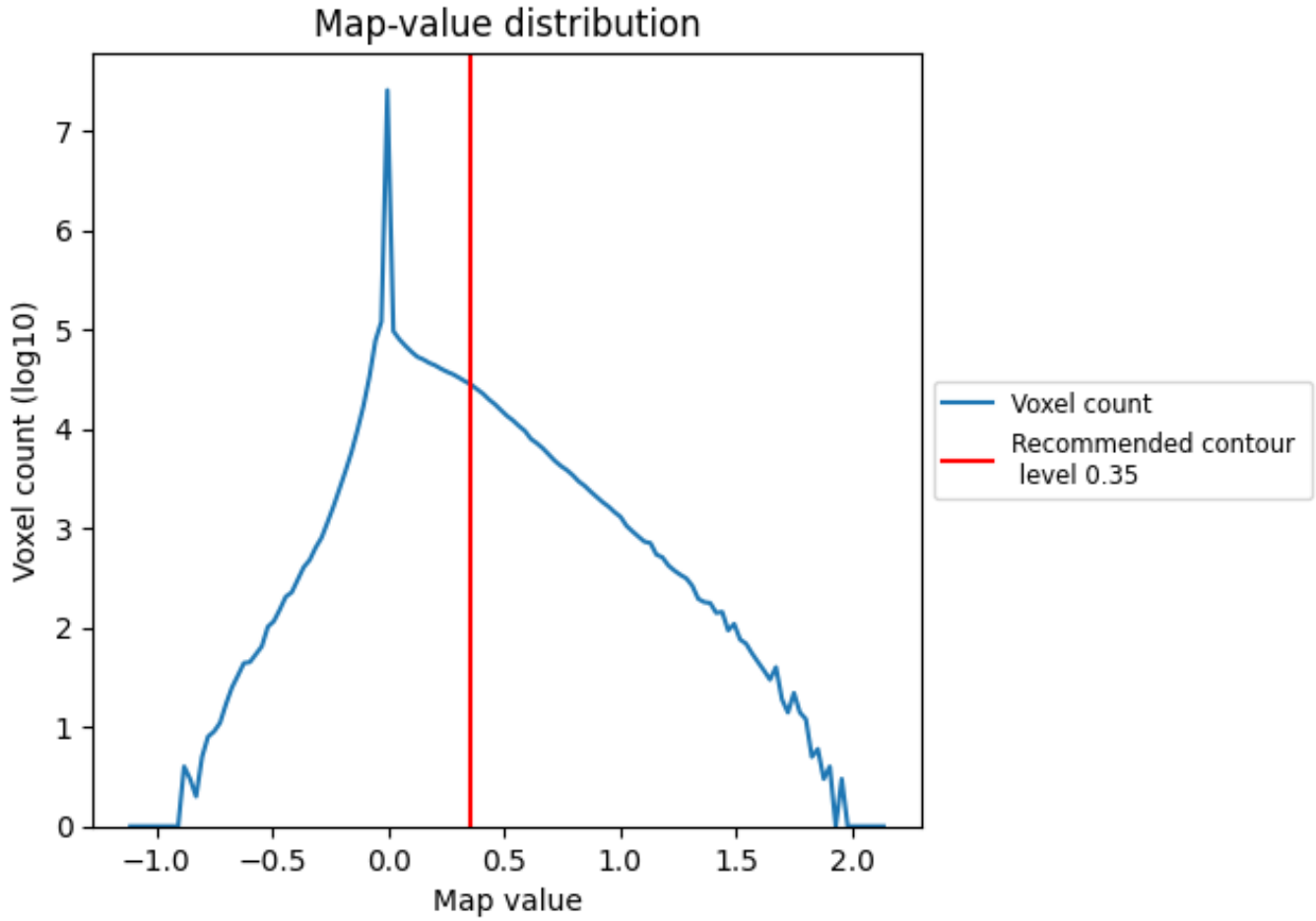
6.5 Mask visualisation (i)

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

7 Map analysis

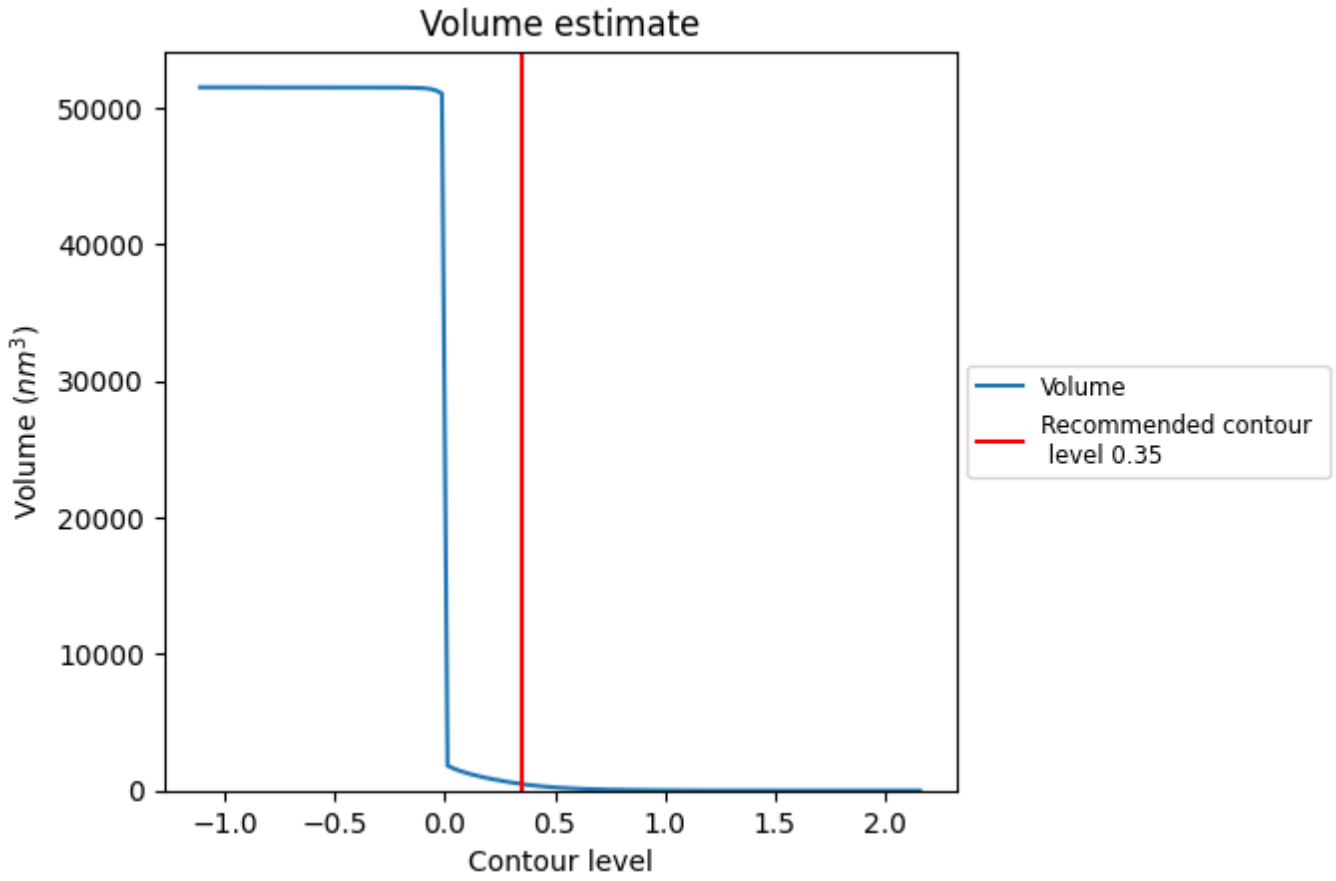
This section contains the results of statistical analysis of the map.

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.

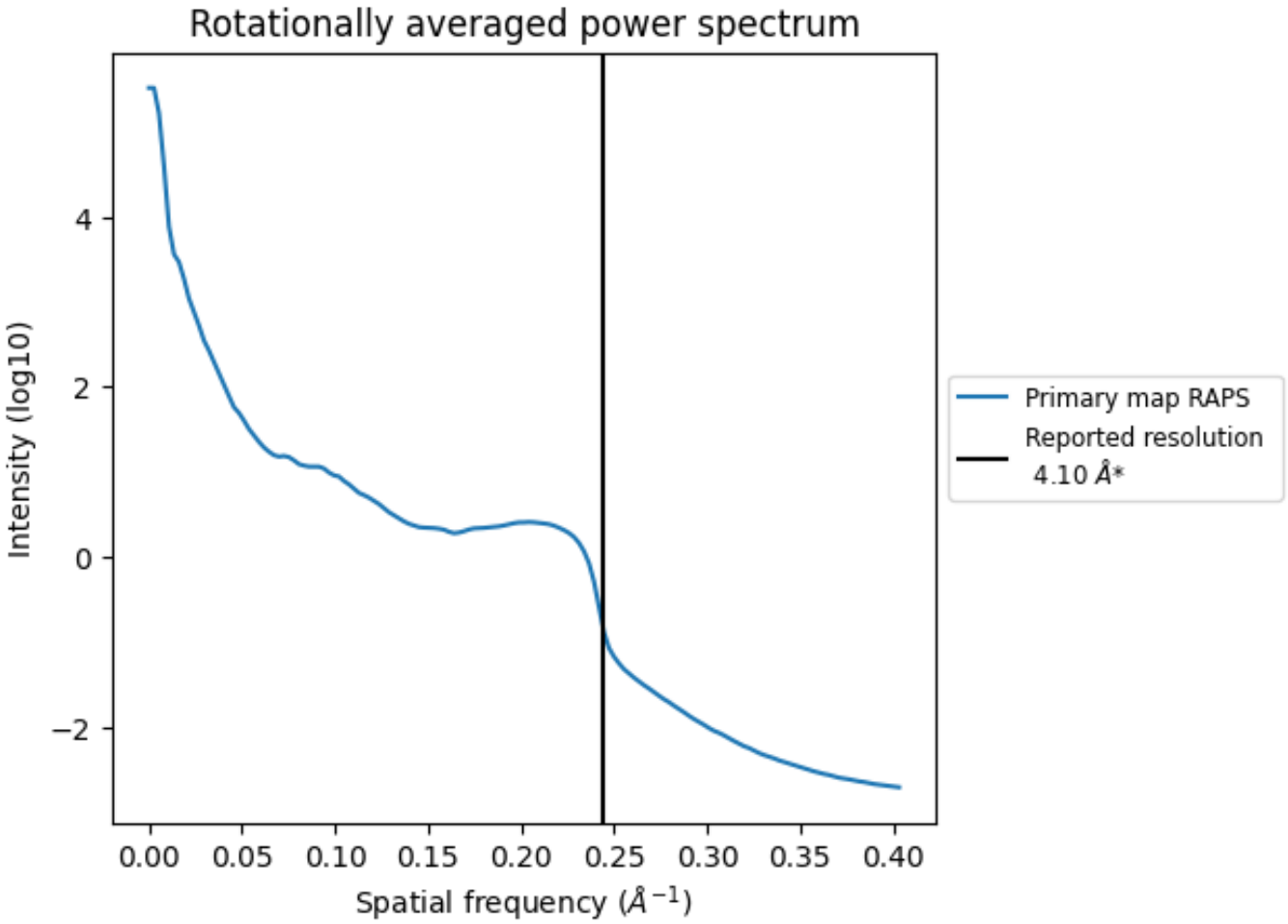
7.2 Volume estimate (i)



The volume at the recommended contour level is 477 nm^3; this corresponds to an approximate mass of 431 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)

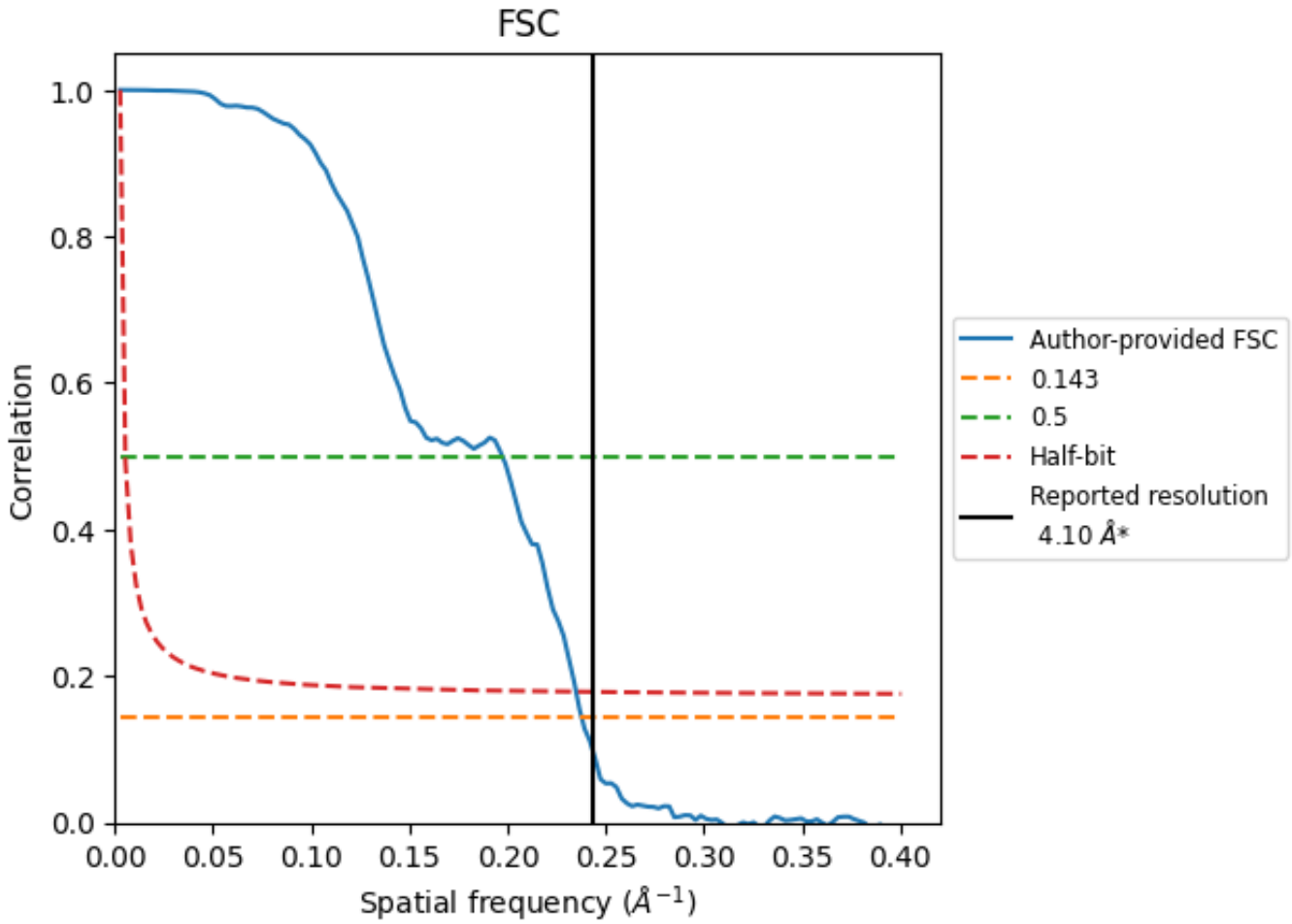


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

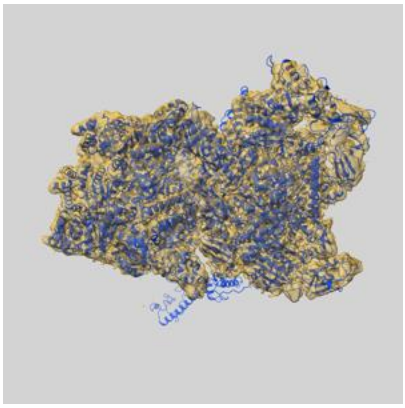
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.21	5.07	4.26
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

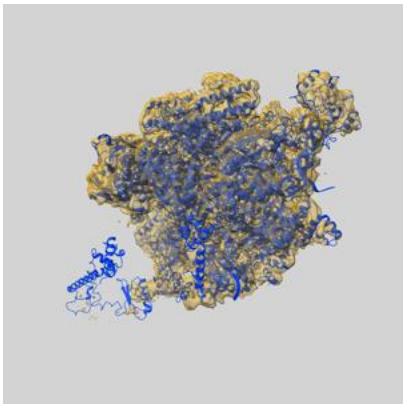
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11091 and PDB model 6Z9T. Per-residue inclusion information can be found in section 3 on page 10.

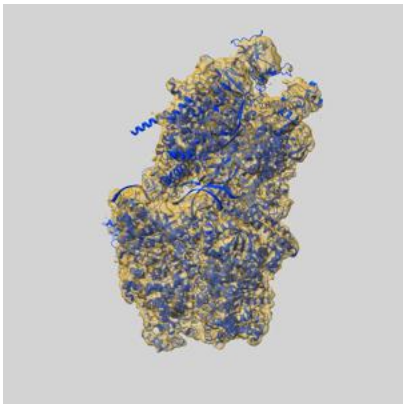
9.1 Map-model overlay



X



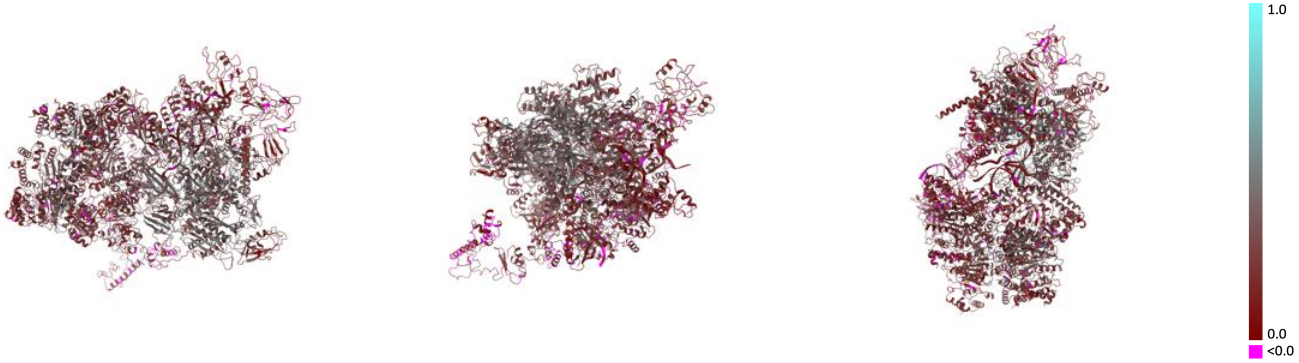
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

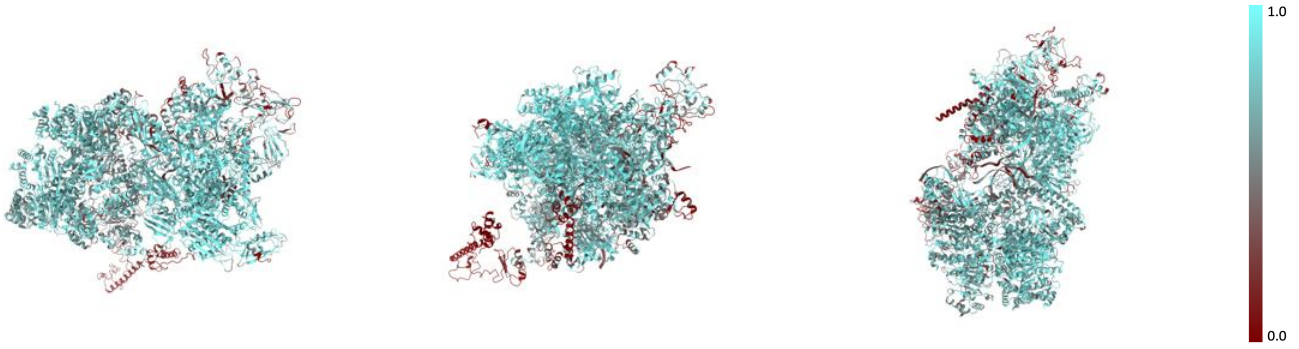
9.2 Q-score mapped to coordinate model



X Y Z

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

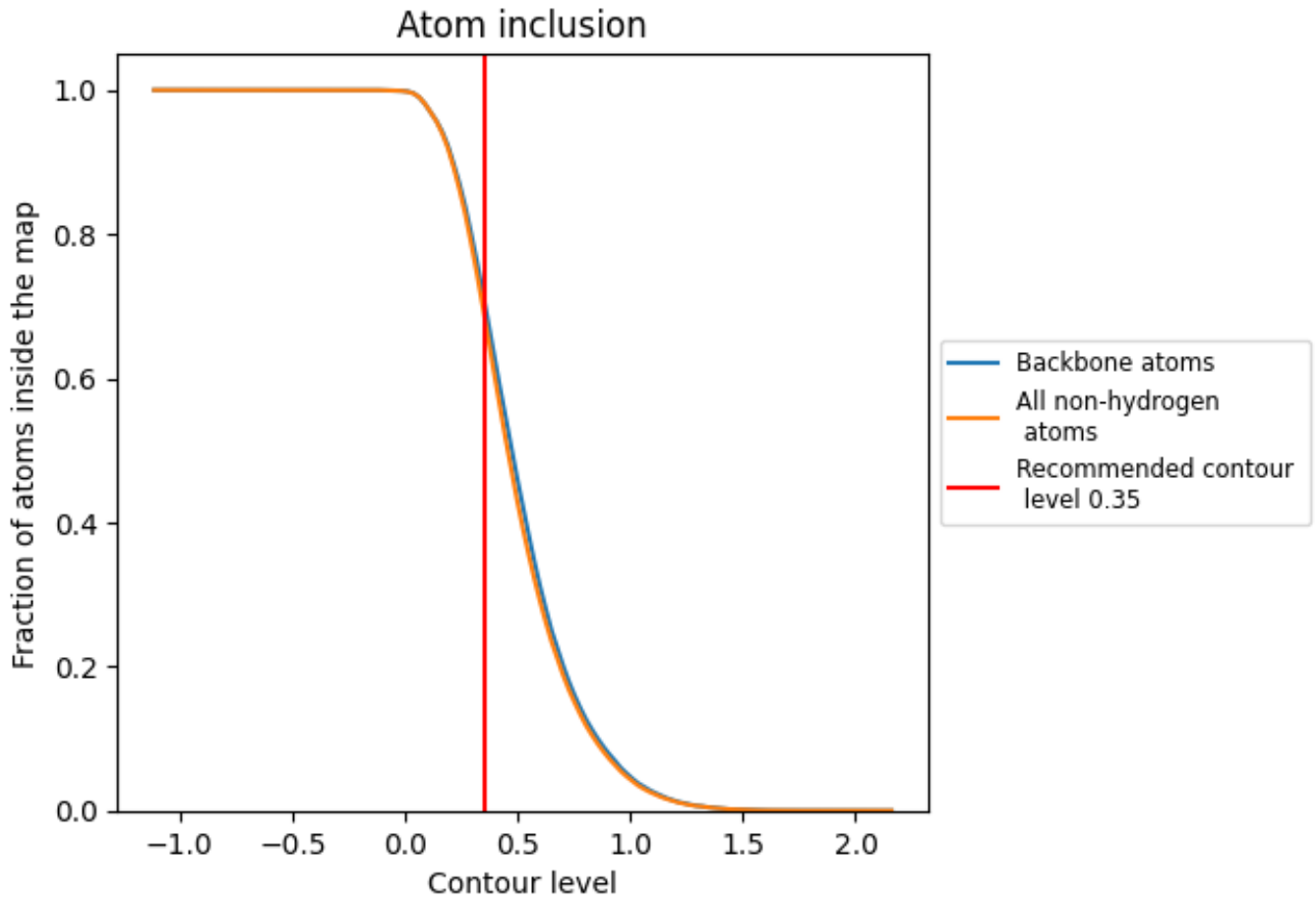
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 69% 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	0.6918	0.2580
A	0.3532	0.1520
K	0.4805	0.0860
L	0.6091	0.1150
R	0.7203	0.1680
U	0.8263	0.3720
V	0.7113	0.2800
W	0.0753	0.2110
X	0.7925	0.3320
Y	0.6950	0.2620
a	0.7332	0.2320
b	0.7622	0.2670
c	0.7877	0.2830
d	0.7609	0.2600
e	0.6691	0.2000
f	0.6680	0.1820