



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 7DU2 / pdb\_00007du2  
EMDB ID : EMD-30865  
Title : RNA polymerase III EC complex in post-translocation state  
Authors : Li, L.; Yu, Z.; Zhao, D.; Ren, Y.; Hou, H.; Xu, Y.  
Deposited on : 2021-01-07  
Resolution : 3.35 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](mailto: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>.

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

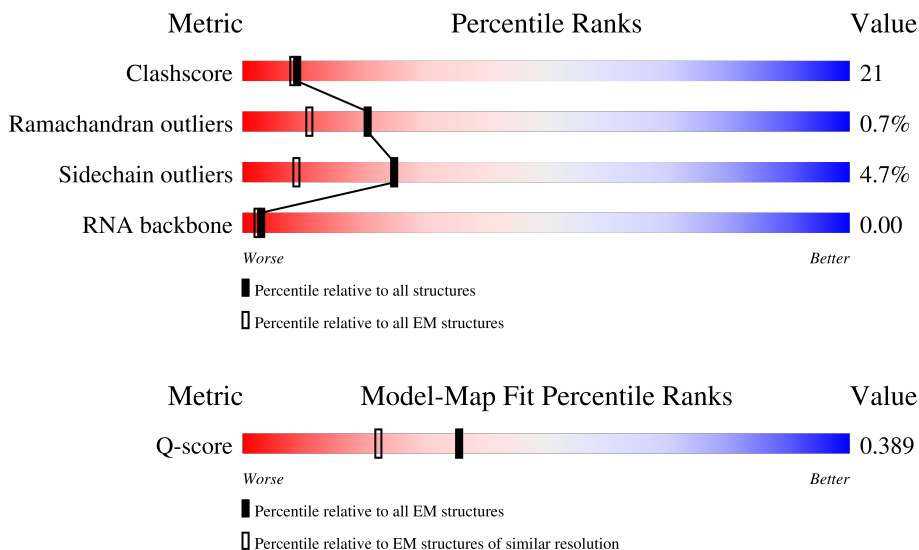
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.35 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.





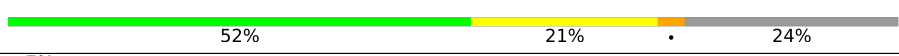





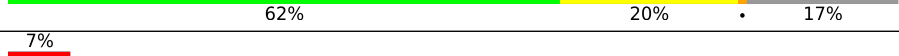
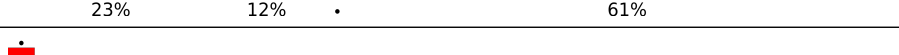
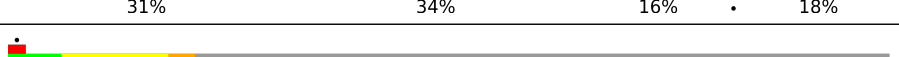
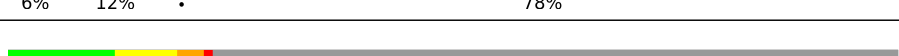

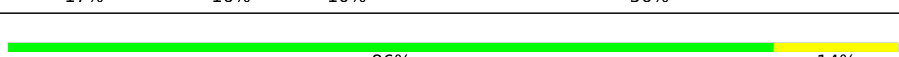
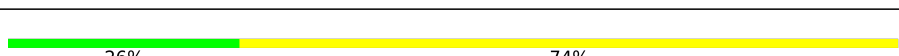
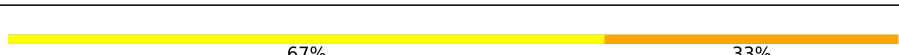

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 ( 2.85 - 3.85 )

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  $\geq 3$ , 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	A	1390	69% 22% 7%
2	B	1133	63% 26% 8%
3	C	346	63% 26% 5% 5%

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Mol	Chain	Length	Quality of chain
4	G	204	
5	K	133	
6	L	58	
7	P	316	
8	E	210	
9	F	127	
10	H	150	
11	J	67	
12	O	534	
13	Q	223	
14	D	148	
15	M	708	
16	N	398	
17	I	108	
18	X	14	
19	Y	19	
20	R	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	SF4	P	401	-	-	X	-

## 2 Entry composition i

There are 23 unique types of molecules in this entry. The entry contains 36616 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1293	10152	6430	1776	1875	71	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1044	8254	5238	1434	1514	68	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	330	2641	1667	469	494	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	166	1337	876	211	245	5	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	103	822	513	145	157	7	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	44	372	231	72	63	6	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	130	Total	C	N	O	S	0	0
			1008	636	166	196	10		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	194	Total	C	N	O	S	0	0
			1590	1014	276	292	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	122	Total	C	N	O	S	0	0
			1002	645	167	185	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	443	Total	C	N	O	S	0	0
			3546	2233	620	673	20		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	86	Total	C	N	O	S	0	0
			724	463	124	131	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	122	985	614	172	196	3	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	154	1272	809	226	232	5	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	92	697	445	117	131	4	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	47	340	210	65	60	5	0	0

- Molecule 18 is a DNA chain called DNA (5'-D(P\*GP\*TP\*CP\*TP\*GP\*AP\*TP\*CP\*TP\*C P\*GP\*GP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	X	14	288	137	52	85	14	0	0

- Molecule 19 is a DNA chain called DNA (5'-D(P\*TP\*TP\*CP\*CP\*GP\*AP\*GP\*AP\*TP\*C P\*AP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	Y	19	392	186	75	112	19	0	0

- Molecule 20 is a RNA chain called RNA (5'-R(P\*AP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	R	3	62	28	10	21	3	0	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

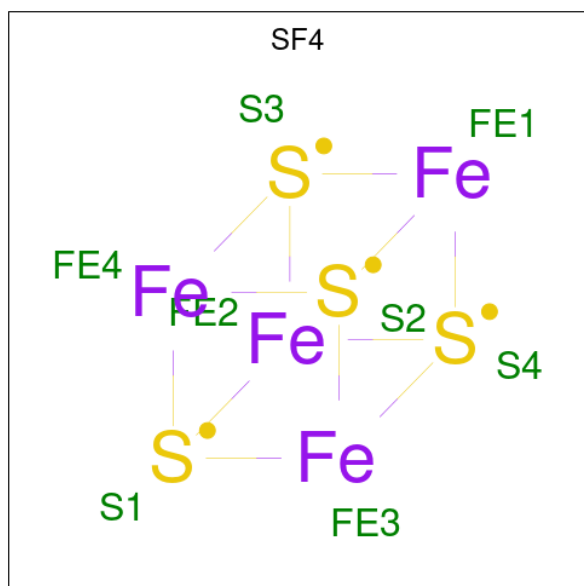
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	
22	J	1	Total	Zn	0
			1	1	
22	I	1	Total	Zn	0
			1	1	

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

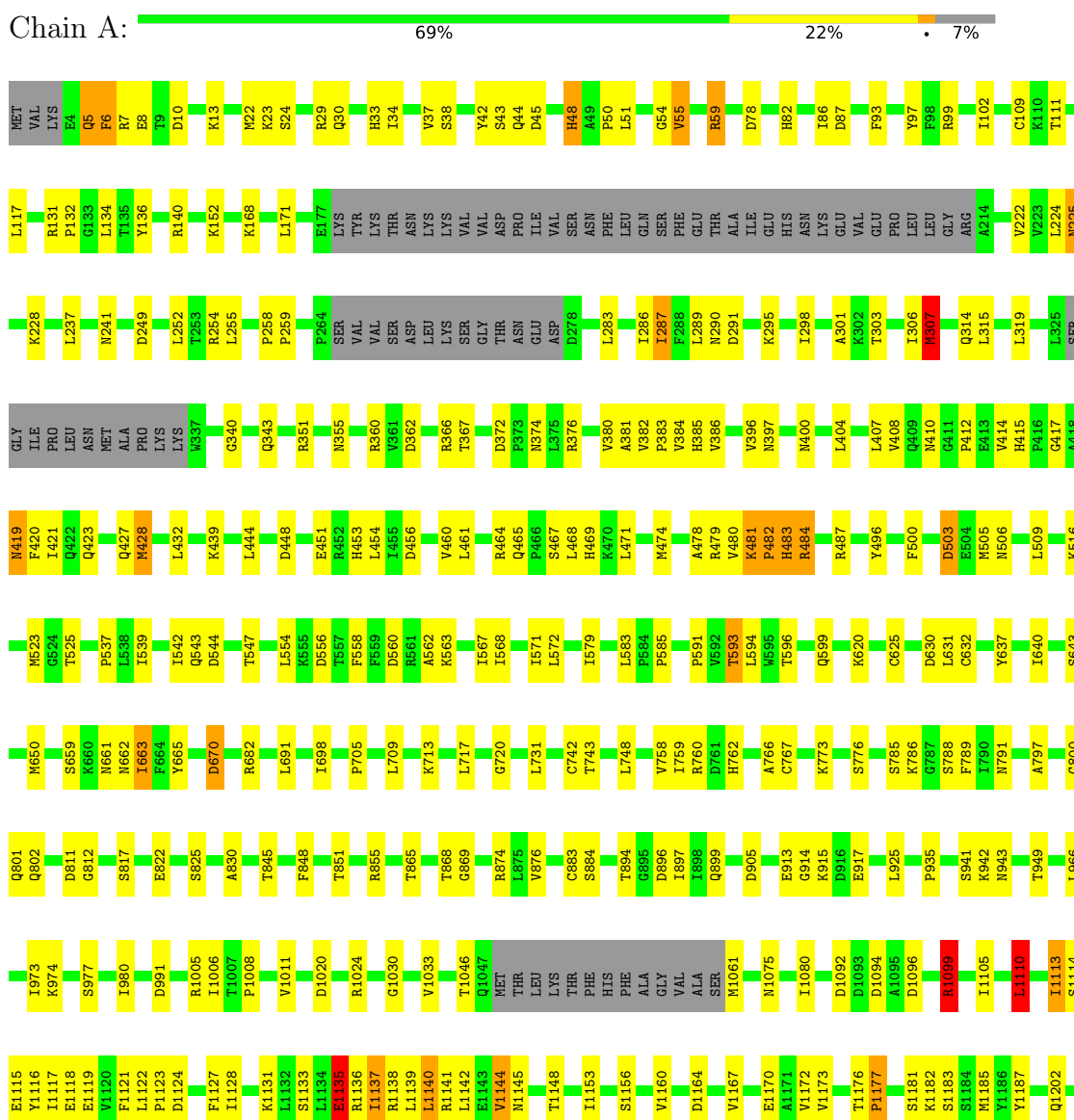


Mol	Chain	Residues	Atoms			AltConf
23	P	1	Total	Fe	S	0
			8	4	4	

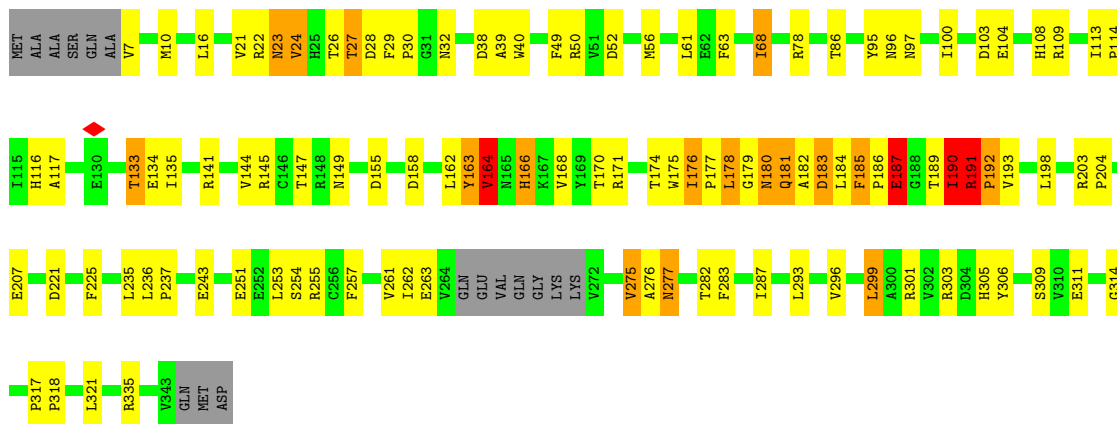
### 3 Residue-property plots [i](#)

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.

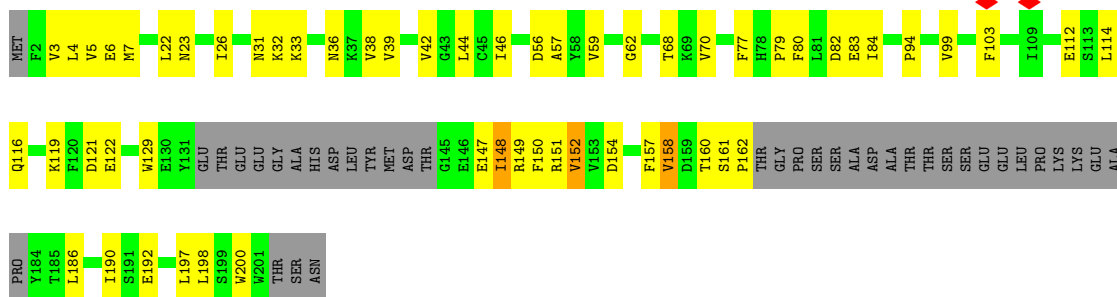
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



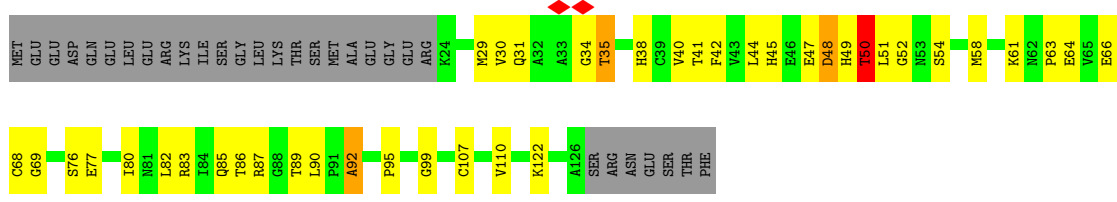




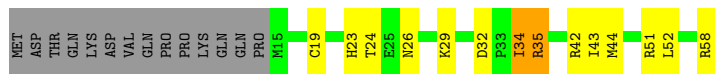
• Molecule 4: DNA-directed RNA polymerase III subunit RPC8



• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC2

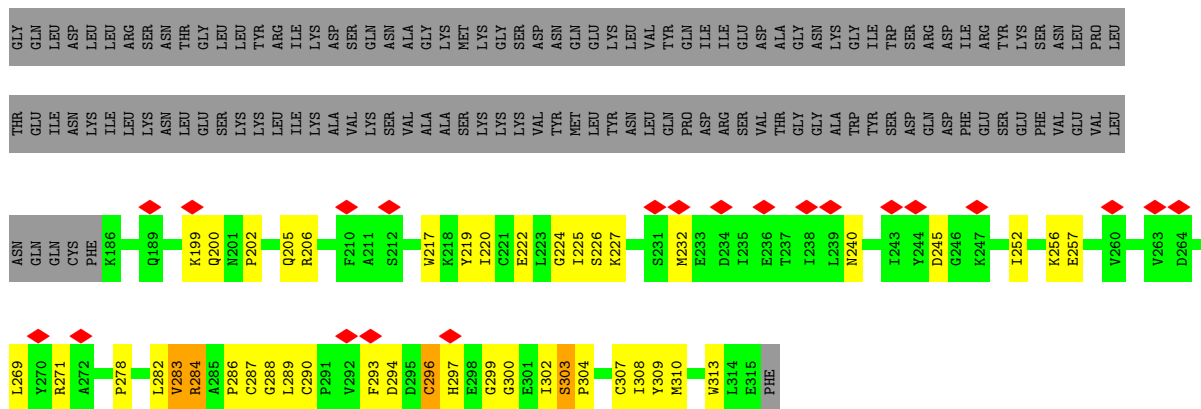


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC4

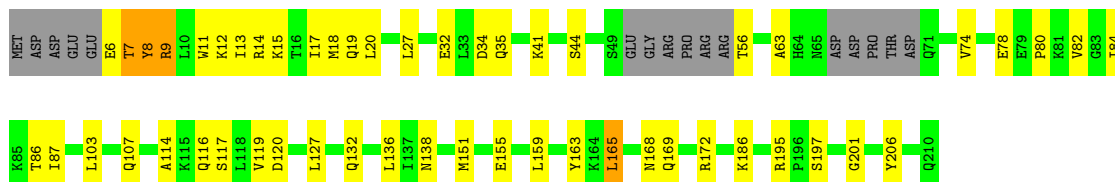


• Molecule 7: DNA-directed RNA polymerase III subunit RPC6

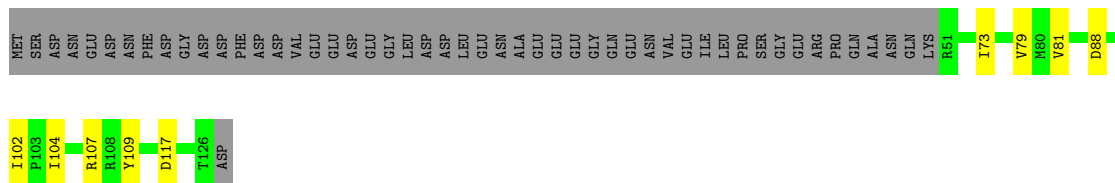




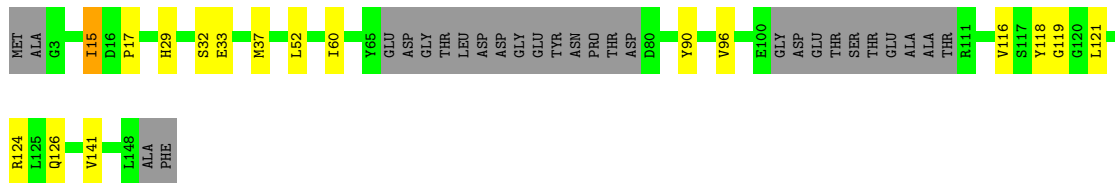
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



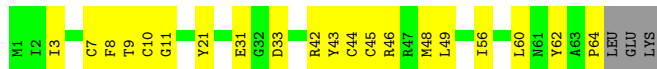
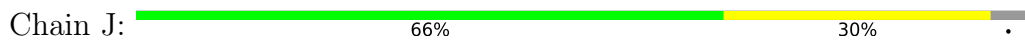
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

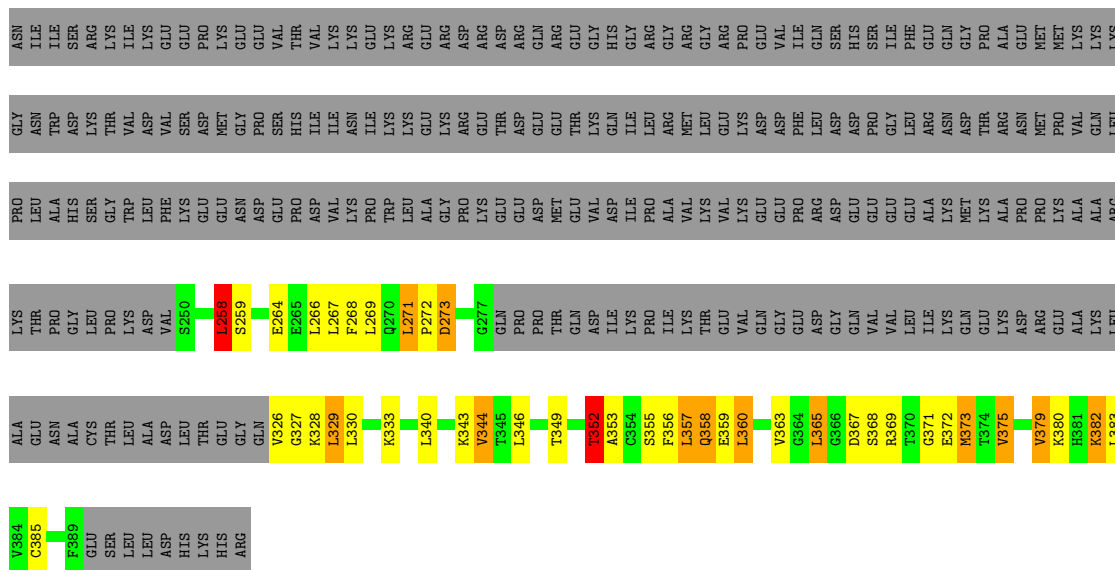


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

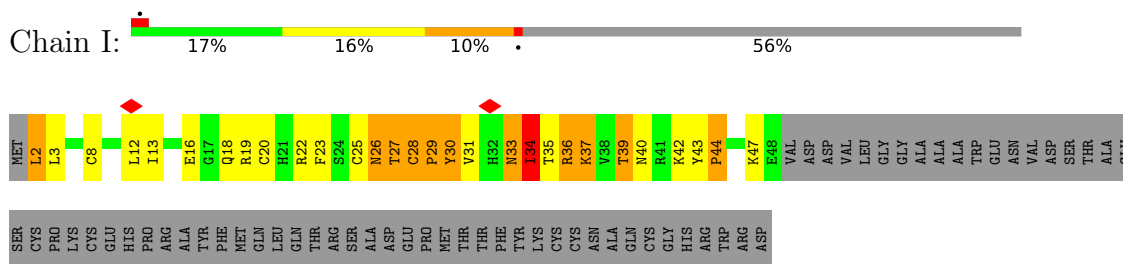




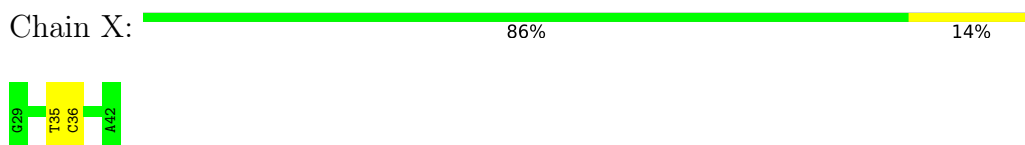




• Molecule 17: DNA-directed RNA polymerase III subunit RPC10



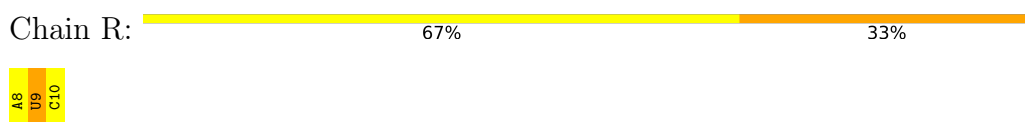
• Molecule 18: DNA (5'-D(P\*GP\*TP\*CP\*TP\*GP\*AP\*TP\*CP\*TP\*CP\*GP\*GP\*AP\*A)-3')



• Molecule 19: DNA (5'-D(P\*TP\*TP\*CP\*CP\*GP\*AP\*GP\*AP\*TP\*CP\*AP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*T)-3')



• Molecule 20: RNA (5'-R(P\*AP\*UP\*C)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	2.189	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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: ZN, MG, SF4

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	0.55	0/10329	0.81	8/13920 (0.1%)
2	B	0.64	1/8410 (0.0%)	0.90	11/11338 (0.1%)
3	C	0.65	0/2694	0.93	9/3653 (0.2%)
4	G	0.54	0/1374	0.97	4/1868 (0.2%)
5	K	0.66	0/837	0.89	1/1129 (0.1%)
6	L	0.56	0/377	0.77	0/500
7	P	0.53	0/1028	0.95	2/1391 (0.1%)
8	E	0.53	0/1616	0.78	2/2180 (0.1%)
9	F	0.56	0/620	0.74	1/839 (0.1%)
10	H	0.57	0/1019	0.81	0/1366
11	J	0.75	0/516	0.86	0/696
12	O	0.41	0/3604	0.75	3/4872 (0.1%)
13	Q	0.61	0/742	0.94	1/996 (0.1%)
14	D	0.86	0/997	1.42	6/1343 (0.4%)
15	M	0.91	1/1301 (0.1%)	1.44	16/1754 (0.9%)
16	N	0.87	0/703	1.46	4/946 (0.4%)
17	I	0.85	1/346 (0.3%)	1.45	5/469 (1.1%)
18	X	0.36	0/322	0.58	0/495
19	Y	0.32	0/440	0.55	0/677
20	R	0.41	0/68	0.89	0/103
All	All	0.60	3/37343 (0.0%)	0.91	73/50535 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	I	29	PRO	C-O	-6.42	1.18	1.24
2	B	692	GLN	CA-C	-5.51	1.45	1.52
15	M	45	LEU	N-CA	5.38	1.49	1.46

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	N-CA-C	-11.15	99.66	113.38
1	A	55	VAL	N-CA-C	-9.53	104.05	113.20
15	M	141	TYR	N-CA-C	-8.75	99.44	112.04
17	I	29	PRO	CB-CA-C	-8.12	105.05	111.87
15	M	66	ASN	N-CA-C	-7.82	99.70	109.64

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	A	10152	0	10382	334	0
2	B	8254	0	8364	325	0
3	C	2641	0	2615	156	0
4	G	1337	0	1306	108	0
5	K	822	0	810	64	0
6	L	372	0	382	20	0
7	P	1008	0	998	66	0
8	E	1590	0	1630	44	0
9	F	610	0	642	5	0
10	H	1002	0	999	12	0
11	J	507	0	524	25	0
12	O	3546	0	3585	146	0
13	Q	724	0	734	47	0
14	D	985	0	1006	125	0
15	M	1272	0	1264	157	0
16	N	697	0	742	70	0
17	I	340	0	306	64	0
18	X	288	0	159	1	0
19	Y	392	0	214	22	0
20	R	62	0	33	4	0
21	A	1	0	0	0	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1	0	0	0	0
23	P	8	0	0	4	0
All	All	36616	0	36695	1515	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 21.

The worst 5 of 1515 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)
15:M:31:PRO:HG2	15:M:136:ARG:CD	1.57	1.32
16:N:357:LEU:HD23	16:N:358:GLN:NE2	1.43	1.29
3:C:191:ARG:CB	3:C:192:PRO:HD3	1.61	1.27
12:O:356:GLU:OE1	13:Q:39:PRO:HD3	1.33	1.26
1:A:484:ARG:HH21	2:B:1017:LEU:CD2	1.49	1.26

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	A	1281/1390 (92%)	1154 (90%)	124 (10%)	3 (0%)	43	70
2	B	1030/1133 (91%)	925 (90%)	100 (10%)	5 (0%)	24	52
3	C	326/346 (94%)	293 (90%)	30 (9%)	3 (1%)	14	41
4	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100
5	K	101/133 (76%)	91 (90%)	8 (8%)	2 (2%)	6	24
6	L	42/58 (72%)	40 (95%)	1 (2%)	1 (2%)	4	21
7	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	16	44
8	E	188/210 (90%)	172 (92%)	15 (8%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	74/127 (58%)	68 (92%)	6 (8%)	0	100	100
10	H	116/150 (77%)	101 (87%)	15 (13%)	0	100	100
11	J	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
12	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	43	70
13	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	10	33
14	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	16	44
15	M	148/708 (21%)	110 (74%)	33 (22%)	5 (3%)	3	16
16	N	88/398 (22%)	80 (91%)	6 (7%)	2 (2%)	5	22
17	I	45/108 (42%)	33 (73%)	9 (20%)	3 (7%)	1	6
All	All	4426/6253 (71%)	3961 (90%)	436 (10%)	29 (1%)	20	46

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	523	VAL
2	B	802	PRO
3	C	190	ILE
3	C	191	ARG
6	L	35	ARG

### 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	1124/1212 (93%)	1094 (97%)	30 (3%)	39	60
2	B	912/988 (92%)	872 (96%)	40 (4%)	25	51
3	C	290/302 (96%)	268 (92%)	22 (8%)	12	38
4	G	149/181 (82%)	145 (97%)	4 (3%)	39	60
5	K	92/119 (77%)	90 (98%)	2 (2%)	45	63
6	L	41/55 (74%)	38 (93%)	3 (7%)	13	39
7	P	114/280 (41%)	112 (98%)	2 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	177/192 (92%)	175 (99%)	2 (1%)	65	73
9	F	66/111 (60%)	66 (100%)	0	100	100
10	H	110/131 (84%)	109 (99%)	1 (1%)	70	75
11	J	53/56 (95%)	53 (100%)	0	100	100
12	O	400/476 (84%)	393 (98%)	7 (2%)	51	66
13	Q	81/195 (42%)	74 (91%)	7 (9%)	10	33
14	D	114/136 (84%)	87 (76%)	27 (24%)	1	2
15	M	138/622 (22%)	120 (87%)	18 (13%)	4	16
16	N	81/347 (23%)	66 (82%)	15 (18%)	1	7
17	I	34/94 (36%)	26 (76%)	8 (24%)	1	2
All	All	3976/5497 (72%)	3788 (95%)	188 (5%)	25	50

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Q	79	GLU
14	D	99	LEU
13	Q	87	TYR
14	D	41	ASN
15	M	75	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
12	O	337	ASN
14	D	89	HIS
12	O	377	GLN
12	O	507	ASN
15	M	76	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	R	2/3 (66%)	2 (100%)	1 (50%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	R	9	U
20	R	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	R	9	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\# Z  > 2$
23	SF4	P	401	7	0,12,12	-	-	-		

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
23	SF4	P	401	7	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

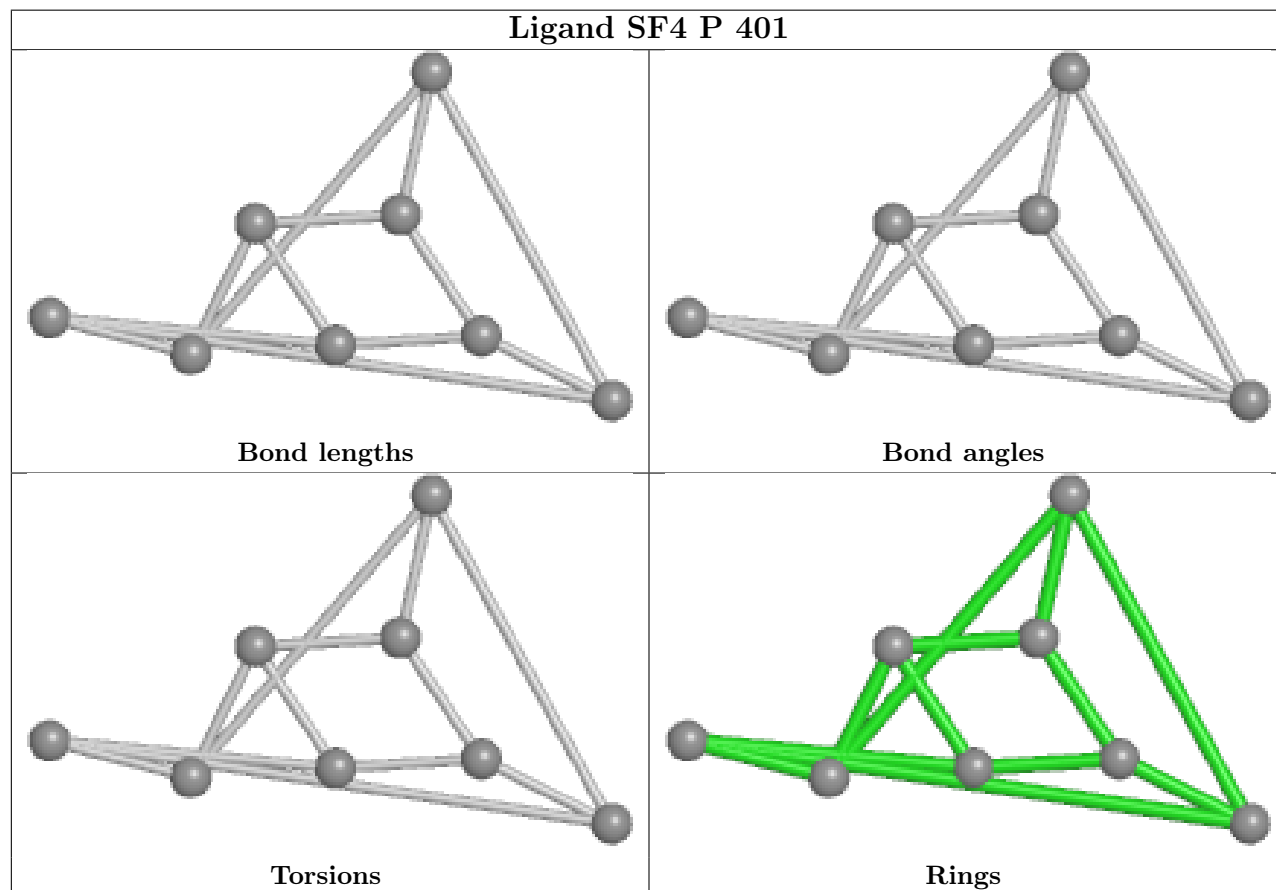
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	401	SF4	4	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.

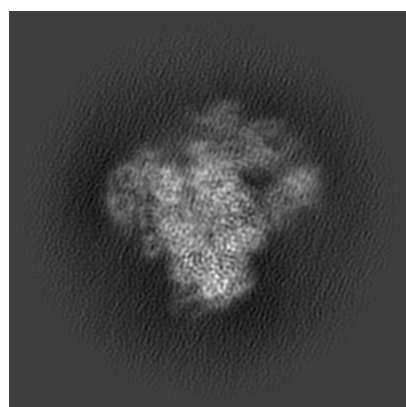
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30865. These allow visual inspection of the internal detail of the map and identification of artifacts.

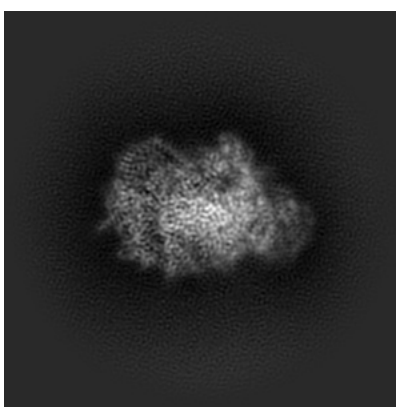
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

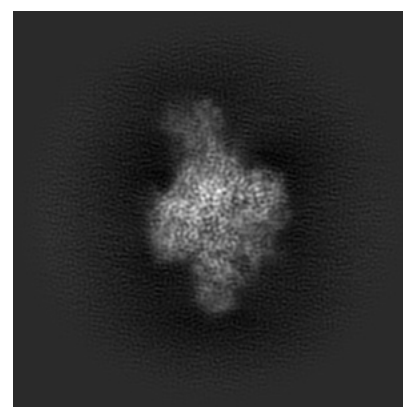
#### 6.1.1 Primary map



X



Y

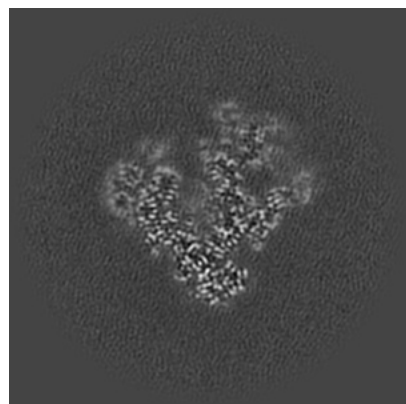


Z

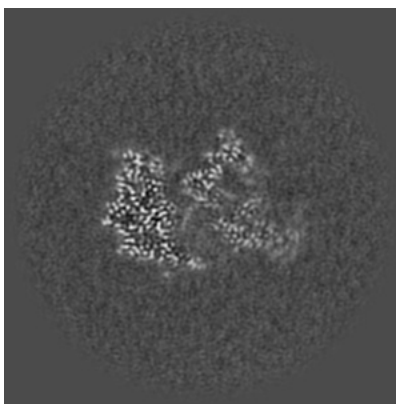
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

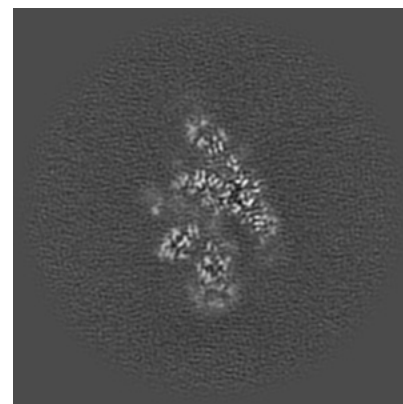
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

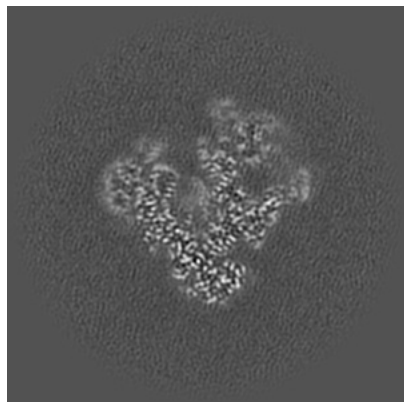


Z Index: 160

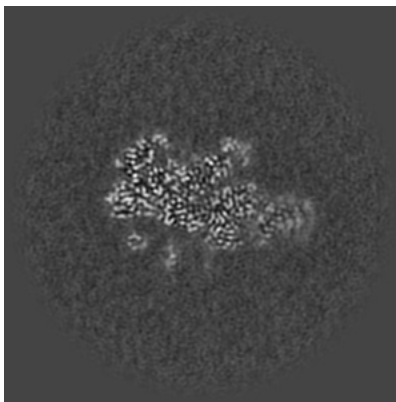
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

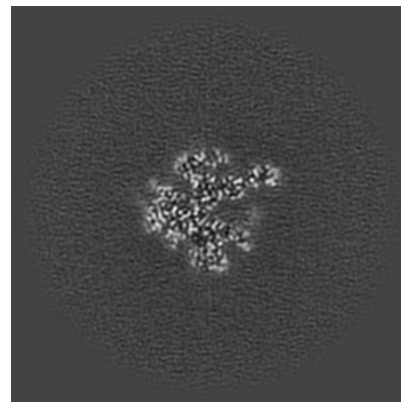
### 6.3.1 Primary map



X Index: 161



Y Index: 175

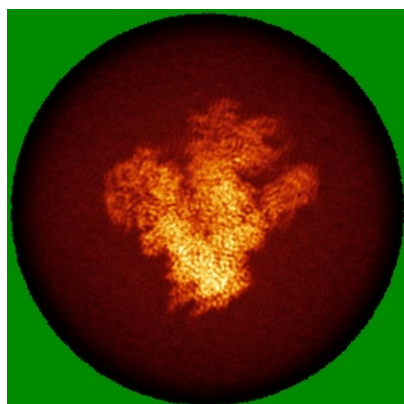


Z Index: 133

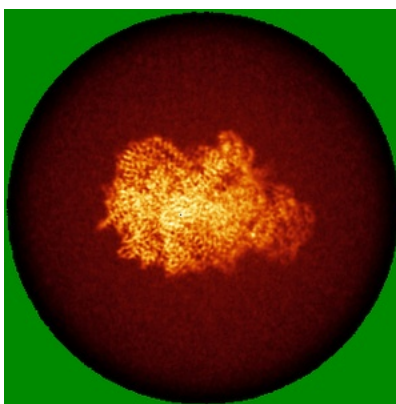
The images above show the largest variance slices of the map in three orthogonal directions.

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

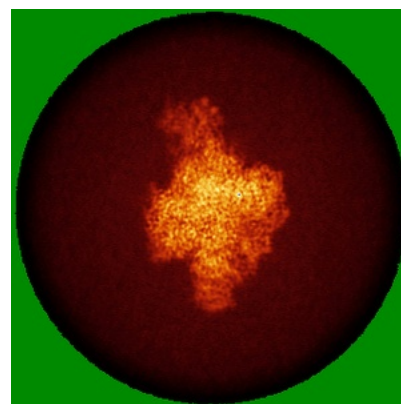
### 6.4.1 Primary map



X



Y

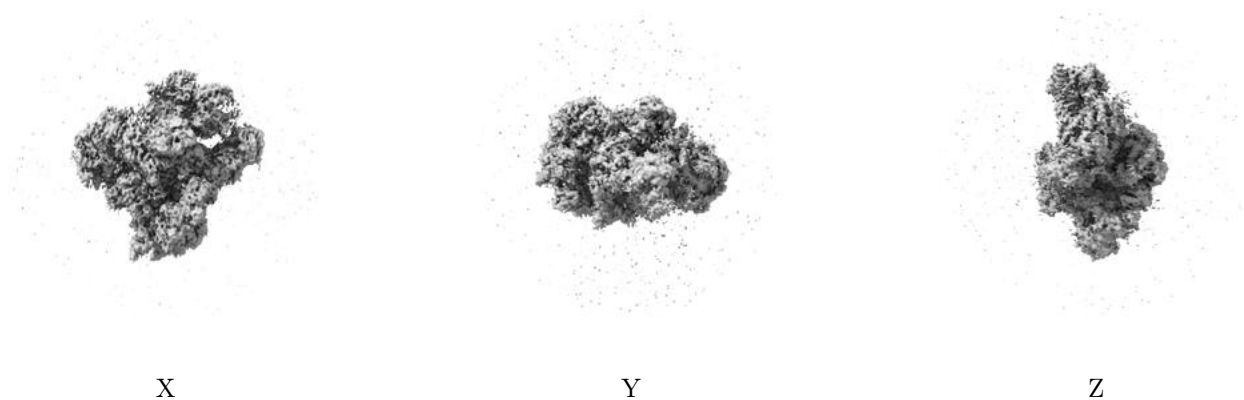


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

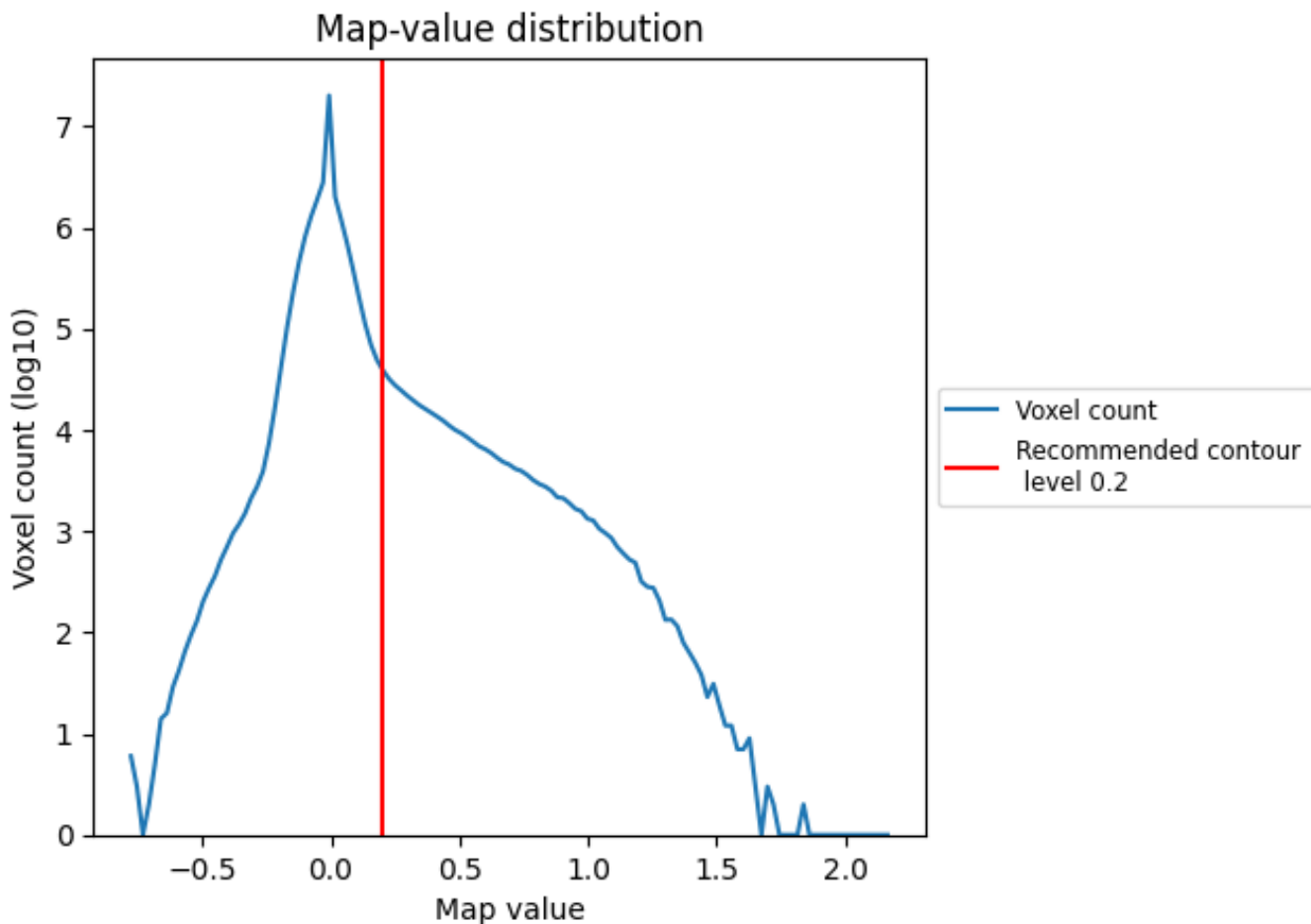
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

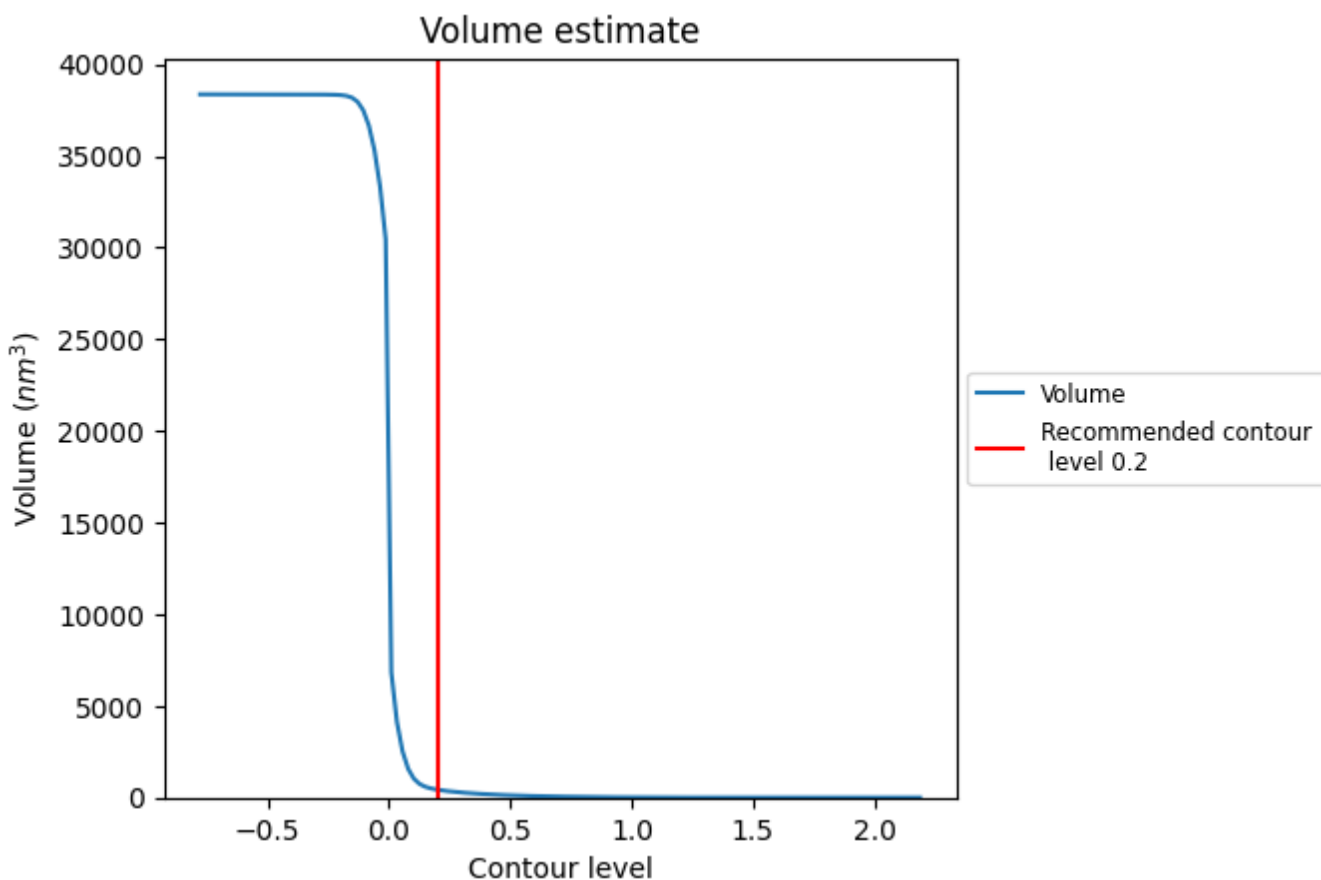
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

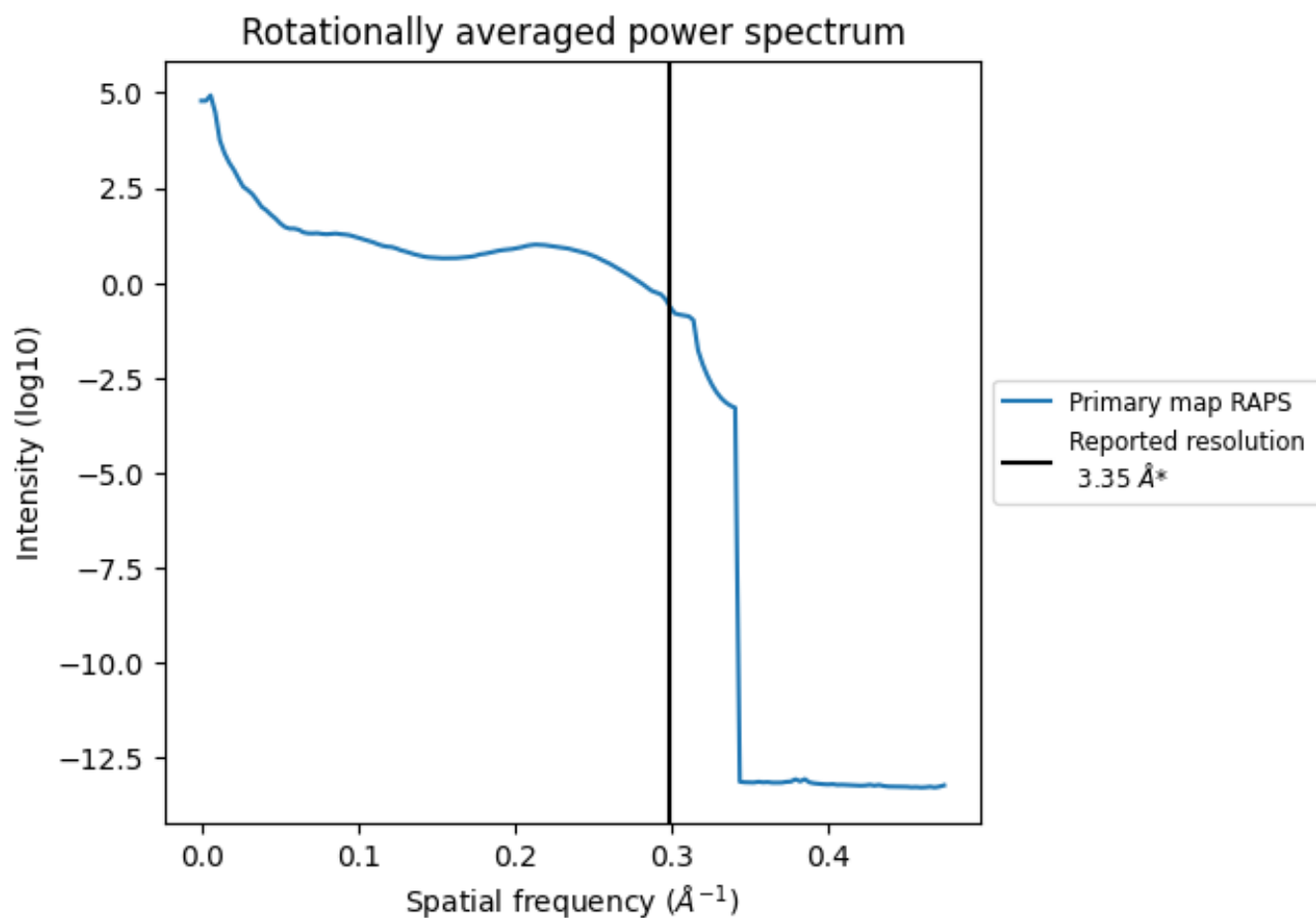
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm<sup>3</sup>; this corresponds to an approximate mass of 389 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 0.299 Å<sup>-1</sup>

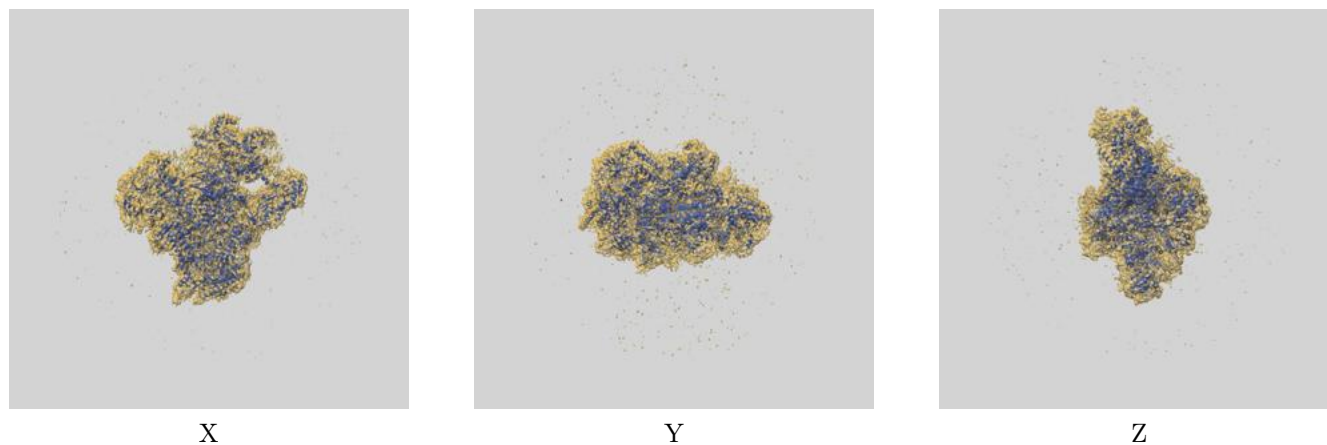
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

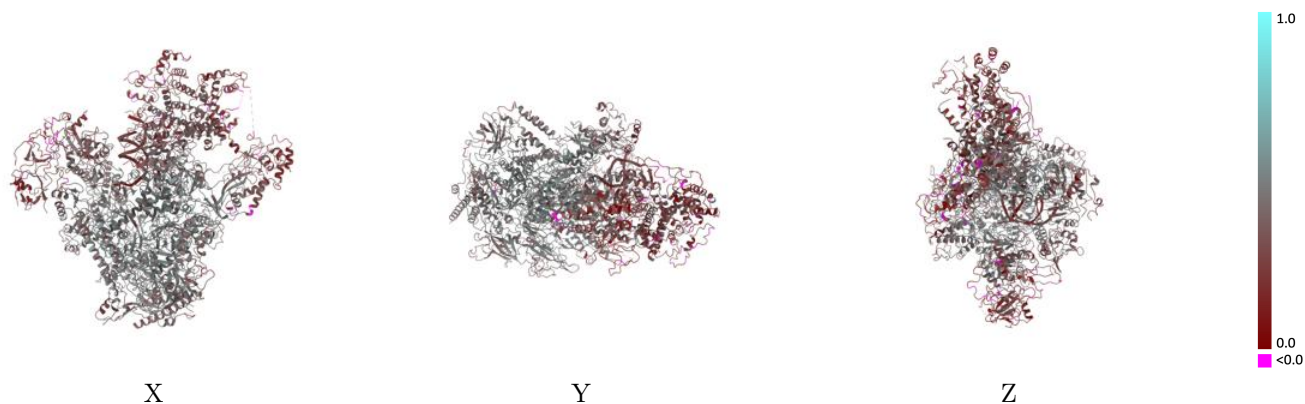
This section contains information regarding the fit between EMDB map EMD-30865 and PDB model 7DU2. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



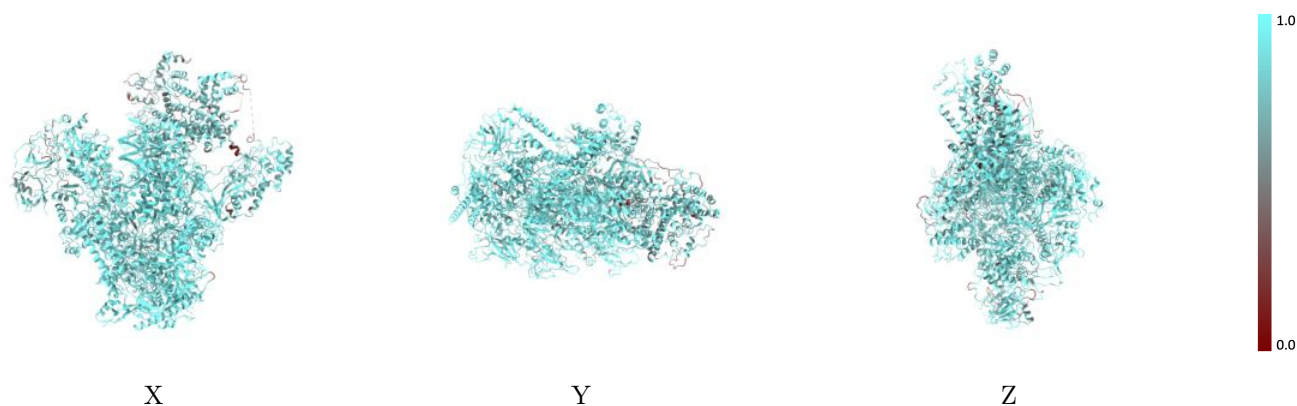
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



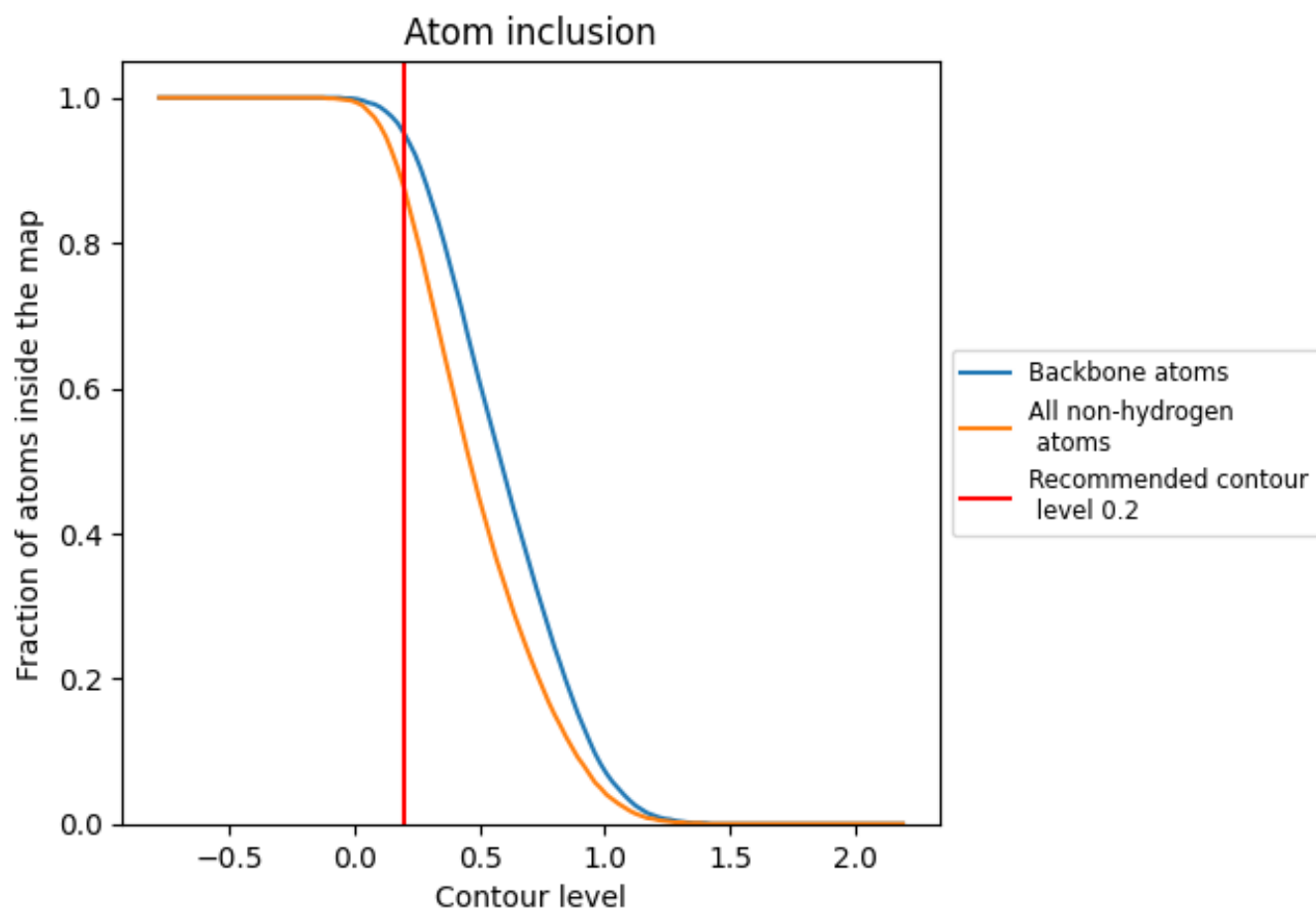
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.3890
A	 0.9100	 0.4470
B	 0.9070	 0.4500
C	 0.9110	 0.4230
D	 0.8070	 0.2150
E	 0.9090	 0.3820
F	 0.9480	 0.4800
G	 0.8820	 0.3320
H	 0.9120	 0.4300
I	 0.8230	 0.2920
J	 0.9330	 0.4620
K	 0.9170	 0.4210
L	 0.9470	 0.4200
M	 0.7560	 0.1990
N	 0.7980	 0.2740
O	 0.7730	 0.2850
P	 0.6900	 0.2070
Q	 0.6460	 0.2540
R	 0.6130	 0.2660
X	 0.9200	 0.2460
Y	 0.9340	 0.3170

