

wwPDB EM Validation Summary Report (i)

Dec 19, 2023 – 08:07 pm GMT

PDB ID : 80EV

EMDB ID : EMD-16837

Title: Structure of the mammalian Pol II-SPT6-Elongin complex, lacking ELOA

latch (composite structure, structure 3)

Authors: Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.

Deposited on : 2023-03-13

Resolution : 2.86 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.dev70

MolProbity : 4.02b-467

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)

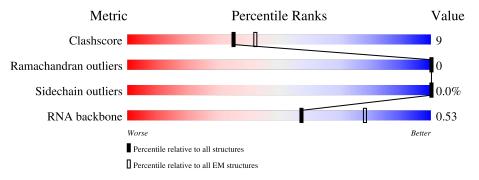
Validation Pipeline (wwPDB-VP) : 2.36

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 2.86 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	158937	4297
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	1970	61%	10%	28%
2	В	1251	76%		14% 10%
3	С	275	79%		15% 6%
4	D	184	40%	23% •	36%
5	Е	210	87%		12%
6	F	127	54%	7%	39%
7	G	172	78%		21%





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Mol	Chain	Length		Qualit	y of chain					
8	Н	150		86%						
9	I	125		80%			13% 7%			
10	J	67		87%			12% •			
11	K	117		87%			11% •			
12	L	58		59%	17%		24%			
13	N	48	40%	15	%	46%				
14	Р	46	22% •	•	72%					
15	Т	48	48%		31%		21%			
16	M	801	11% •		84%					
17	О	112	29%	66%		24%	10%			
18	Q	118	38%	%	22%	•	25%			
19	S	1729	31%	17%		52%				



2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 41781 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 II subunit RPB1.

Mo	l Chain	Residues		A		AltConf	Trace		
1	A	1409	Total 11159	C 7024	N 2000	O 2064	S 71	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		Atoms					Trace
2	D	1131	Total	С	N	О	S	0	0
	Б	1101	9047	5721	1592	1670	64	0	U

• Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues		Ato		AltConf	Trace		
3	С	258	Total 2072	C 1300	N 356	O 410	S 6	0	0

• Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	118	Total 967	C 608	N 167	O 188	S 4	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total 1721	C 1089	N 300	O 324	S 8	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues		Atoms					Trace
6	E	78	Total	С	N	О	S	0	0
	Г	10	626	401	106	114	5	0	0



• Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	C	171	Total	С	N	О	S	0	0
1	G	171	1347	872	218	249	8	U	U

• Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues		At	oms			AltConf	Trace
0	П	148	Total	С	N	О	S	0	0
0	п	140	1186	750	194	237	5	U	U

• Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues		Atoms					Trace
9	I	116	Total 932	C 577	N 165	O 179	S 11	0	0

• Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
10	Ţ	66	Total	С	N	О	S	0	0
10	1	66	524	339	88	91	6	0	U

• Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	K	115	Total 920	C 593	N 152	O 173	S 2	0	0

• Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
12	L	44	Total	С	N	О	S	0	0
			367	228	69	64	6		Ü

• Molecule 13 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues		\mathbf{A}_{1}	toms	AltConf	Trace		
13	N	26	Total 549	C 255	N 117	O 151	P 26	0	0

• Molecule 14 is a RNA chain called RNA.



Mol	Chain	Residues		\mathbf{At}	oms	AltConf	Trace		
14	Р	13	Total 280	C 125		O 88	P 13	0	0

• Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues		A	toms	AltConf	Trace		
15	Т	38	Total 769	C 365	N 130	O 236	P 38	0	0

• Molecule 16 is a protein called Elongin-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	М	128	Total	С	N	О	S	0	0
10	M	120	1074	680	195	192	7	U	U

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q14241
M	-1	ASN	-	expression tag	UNP Q14241
M	0	ALA	-	expression tag	UNP Q14241

• Molecule 17 is a protein called Elongin-C.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	О	101	Total 792		N 127	O 153	S 6	0	0

• Molecule 18 is a protein called Elongin-B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	Q	88	Total 696	C 437	N 121	O 135	S 3	0	0

• Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues		A	AltConf	Trace			
10	C	825	Total	С	N	О	S	0	0
19	b	029	6744	4289	1168	1253	34	0	U

There are 3 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP Q7KZ85
S	-1	ASN	-	expression tag	UNP Q7KZ85
S	0	ALA	-	expression tag	UNP Q7KZ85

• Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

M	[ol	Chain	Residues	Atoms		AltConf
2	0	A	1	Total 1	Mg 1	0

• Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

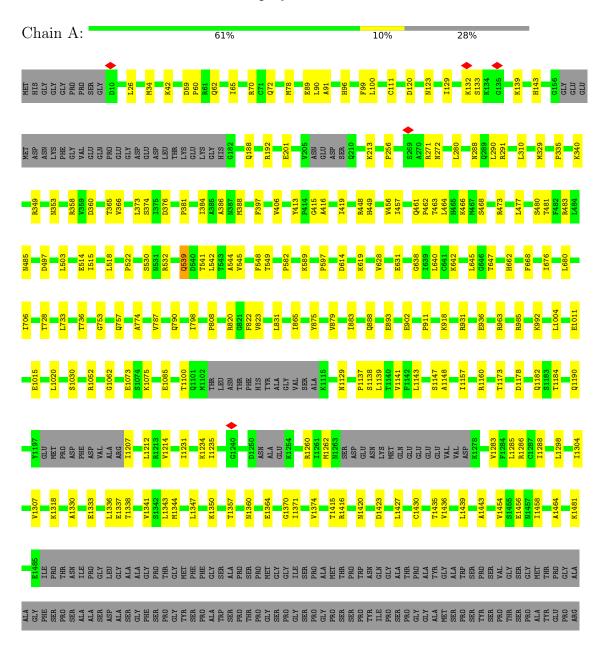
Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	В	1	Total Zn 1 1	0
21	С	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0



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.

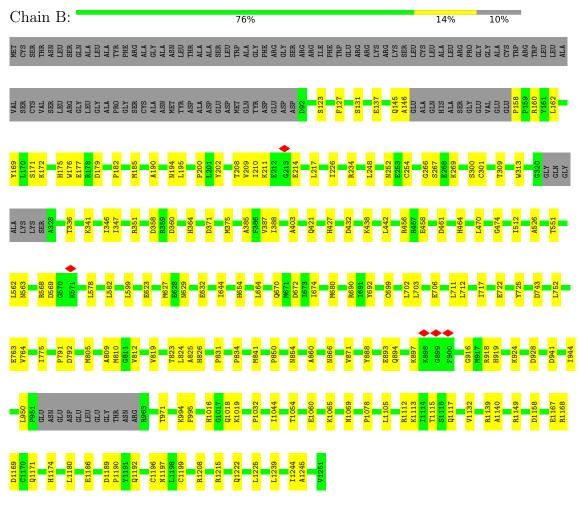
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





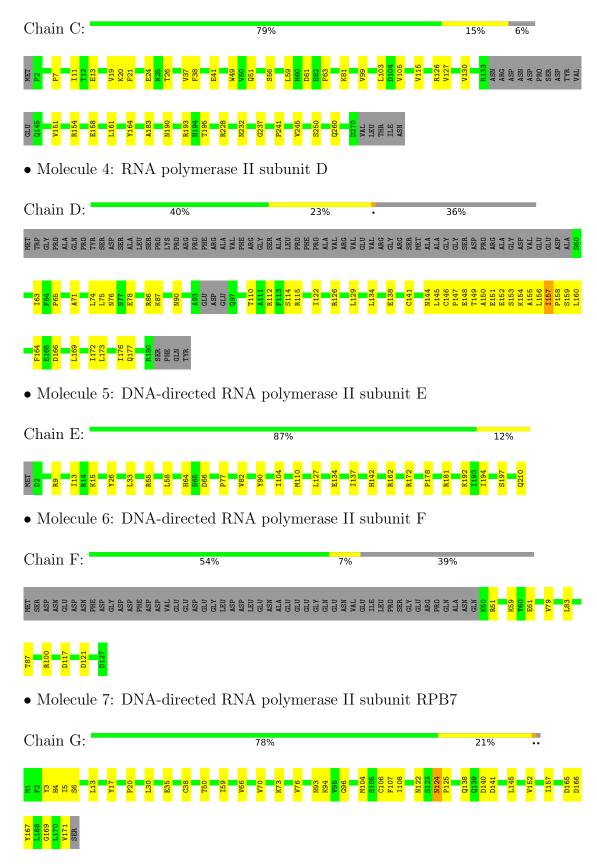


• Molecule 2: DNA-directed RNA polymerase subunit beta



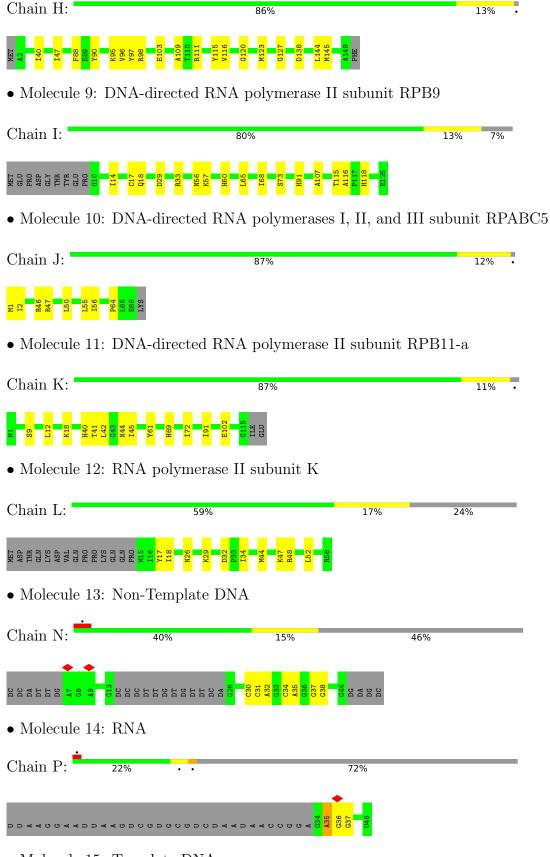
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3





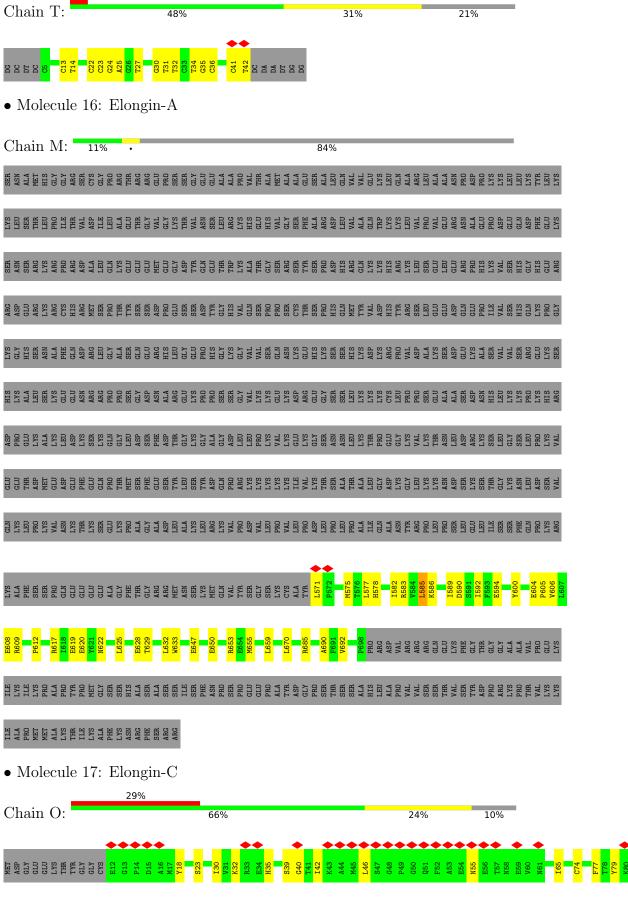
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





• Molecule 15: Template DNA

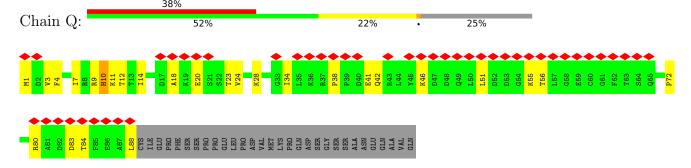




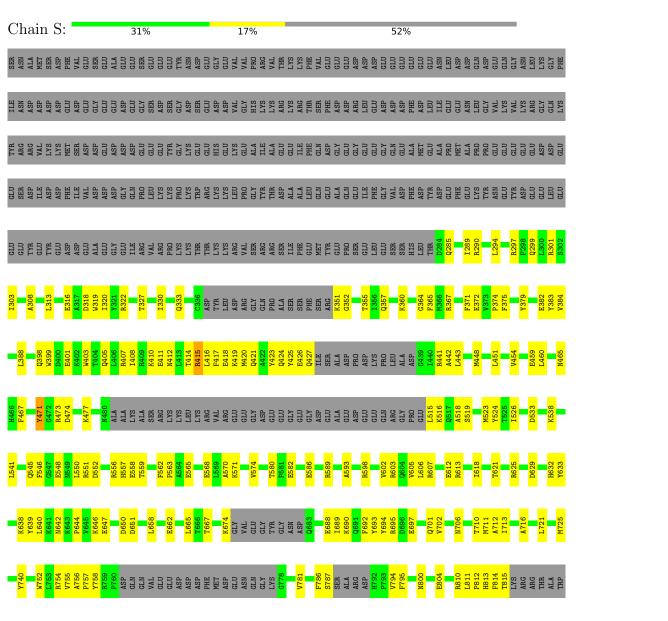




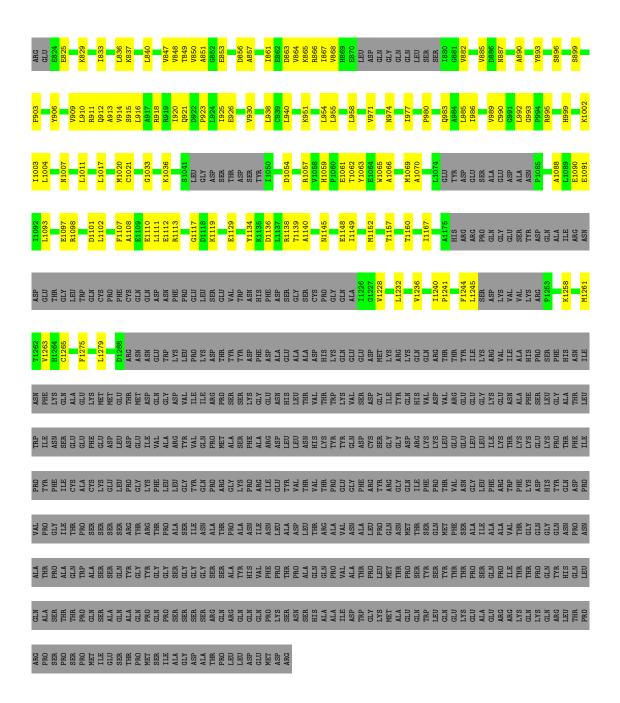
• Molecule 18: Elongin-B



• Molecule 19: Transcription elongation factor SPT6









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40.09	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.253	Depositor
Minimum map value	-16.528	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.086	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.28	0/11360	0.50	0/15328	
2	В	0.30	0/9227	0.49	$1/12454 \ (0.0\%)$	
3	С	0.31	0/2115	0.47	0/2873	
4	D	0.39	0/979	0.69	0/1312	
5	Е	0.28	0/1752	0.49	0/2366	
6	F	0.29	0/636	0.51	0/859	
7	G	0.33	0/1378	0.59	0/1870	
8	Н	0.29	0/1207	0.50	0/1628	
9	I	0.28	0/954	0.49	0/1293	
10	J	0.31	0/533	0.48	0/719	
11	K	0.31	0/939	0.48	0/1271	
12	L	0.30	0/372	0.58	0/493	
13	N	0.54	0/619	0.77	0/954	
14	Р	0.25	0/313	0.83	0/486	
15	Т	0.57	0/857	0.99	0/1319	
16	M	0.31	0/1098	0.58	1/1481 (0.1%)	
17	O	0.33	0/810	0.63	0/1097	
18	Q	0.30	0/707	0.73	1/952~(0.1%)	
19	S	0.30	0/6868	0.47	0/9250	
All	All	0.31	0/42724	0.53	3/58005~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	1
7	G	0	1
19	S	0	1

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\mathbf{Mol}	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
18	Q	10	HIS	C-N-CA	5.99	136.66	121.70
16	M	585	LEU	CB-CG-CD1	-5.39	101.83	111.00
2	В	824	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	GLN	Mainchain
4	D	157	ILE	Mainchain
7	G	124	ASN	Peptide
19	S	415	ARG	Sidechain

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	11159	0	11304	138	0
2	В	9047	0	9080	115	0
3	С	2072	0	2019	27	0
4	D	967	0	973	54	0
5	Ε	1721	0	1737	17	0
6	F	626	0	657	6	0
7	G	1347	0	1347	72	0
8	Н	1186	0	1147	11	0
9	I	932	0	856	12	0
10	J	524	0	540	5	0
11	K	920	0	942	8	0
12	L	367	0	367	10	0
13	N	549	0	289	4	0

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	n previous

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	Р	280	0	142	2	0
15	Τ	769	0	429	13	0
16	M	1074	0	1070	27	0
17	Ο	792	0	774	18	0
18	Q	696	0	694	15	0
19	S	6744	0	6723	266	0
20	A	1	0	0	0	0
21	A	2	0	0	0	0
21	В	1	0	0	0	0
21	С	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	Ĺ	1	0	0	0	0
All	All	41781	0	41090	712	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 9.

The worst 5 of 712 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
7:G:171:VAL:HG22	19:S:518:ALA:CB	1.43	1.48
7:G:171:VAL:CG2	19:S:518:ALA:HB1	1.58	1.32
7:G:171:VAL:CG2	19:S:518:ALA:CB	2.07	1.32
19:S:815:THR:O	19:S:829:LYS:HD2	1.11	1.24
7:G:122:ASN:HB2	19:S:405:GLN:NE2	1.57	1.18

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	Perce	ntiles
1	A	1395/1970 (71%)	1365 (98%)	30 (2%)	0	100	100
2	В	1123/1251 (90%)	1088 (97%)	35 (3%)	0	100	100
3	\mathbf{C}	254/275~(92%)	247 (97%)	7 (3%)	0	100	100
4	D	114/184 (62%)	106 (93%)	8 (7%)	0	100	100
5	\mathbf{E}	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	Н	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100
10	J	64/67~(96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	$42/58 \ (72\%)$	39 (93%)	3 (7%)	0	100	100
16	M	126/801 (16%)	119 (94%)	7 (6%)	0	100	100
17	О	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
18	Q	86/118 (73%)	73 (85%)	13 (15%)	0	100	100
19	S	799/1729 (46%)	770 (96%)	29 (4%)	0	100	100
All	All	4927/7466 (66%)	4757 (96%)	170 (4%)	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	Perce	ntiles
1	A	1239/1749 (71%)	1239 (100%)	0	100	100
2	В	991/1084 (91%)	991 (100%)	0	100	100
3	С	$235/252 \ (93\%)$	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	Е	191/192 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percei	ntiles
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	Н	129/131~(98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55~(73%)	40 (100%)	0	100	100
16	М	118/706 (17%)	118 (100%)	0	100	100
17	О	88/96 (92%)	88 (100%)	0	100	100
18	Q	75/103 (73%)	75 (100%)	0	100	100
19	S	731/1524 (48%)	730 (100%)	1 (0%)	93	98
All	All	4426/6590 (67%)	4425 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	471	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	887	ASN
19	S	1007	ASN
19	S	405	GLN
19	S	465	ASN
19	S	701	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/46~(26%)	3 (25%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	Р	35	A

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Mol	Chain	Res	Type
14	Р	36	G
14	Р	37	G

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.



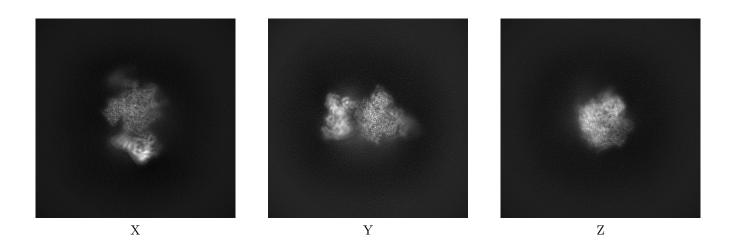
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16837. 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)

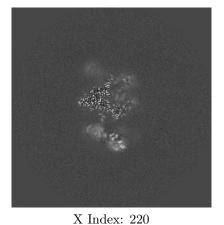
6.1.1 Primary map

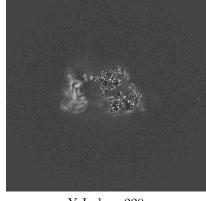


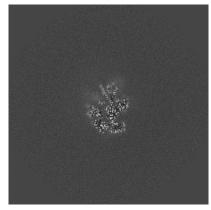
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map







Y Index: 220

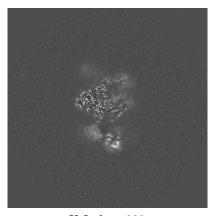


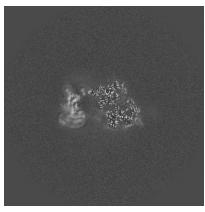
Z Index: 220

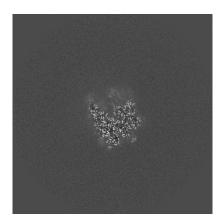
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map







X Index: 223

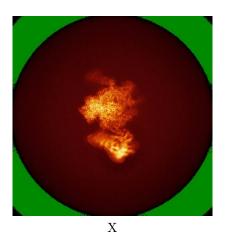
Y Index: 219

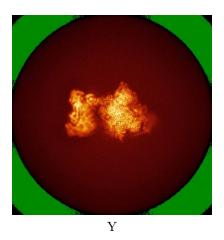
Z Index: 235

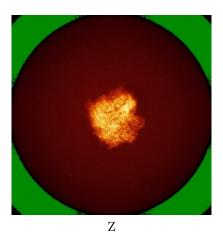
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map





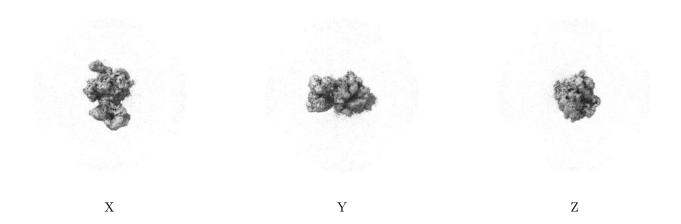


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 3.5. 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)

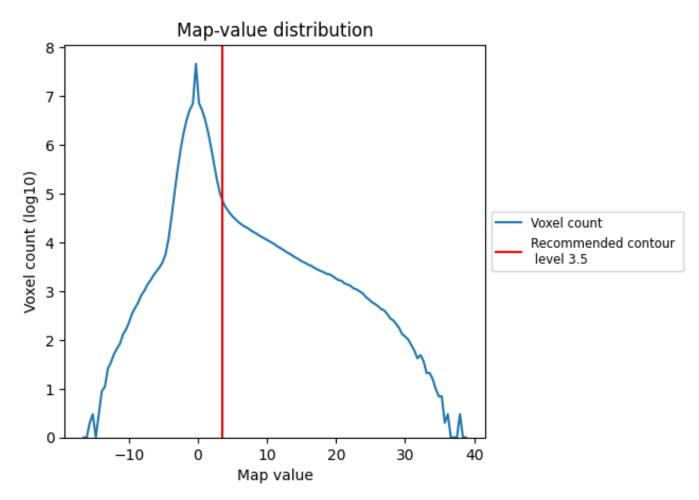
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

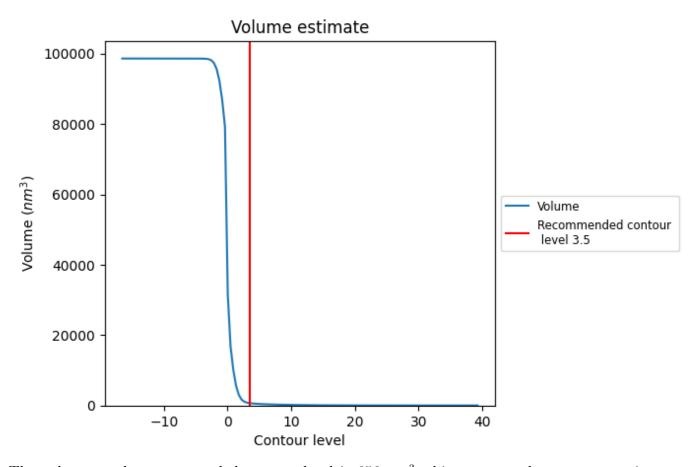
7.1 Map-value distribution (i)



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)

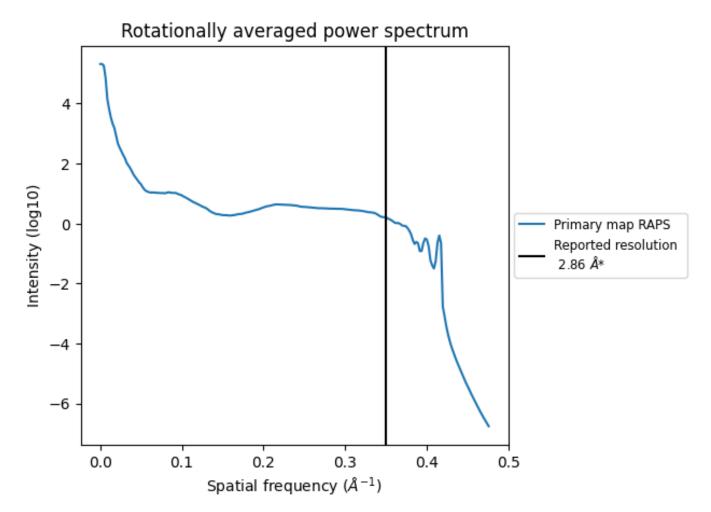


The volume at the recommended contour level is $656~\mathrm{nm^3}$; this corresponds to an approximate mass of $593~\mathrm{kDa}$.

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 0.350 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

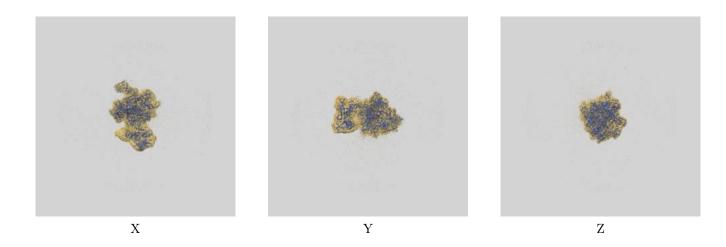
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16837 and PDB model 80EV. Per-residue inclusion information can be found in section 3 on page 8.

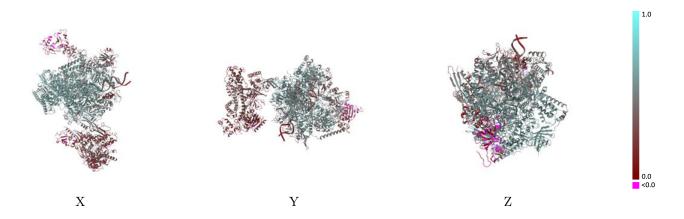
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

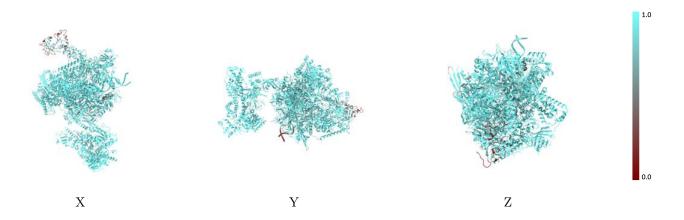


9.2 Q-score mapped to coordinate model (i)



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

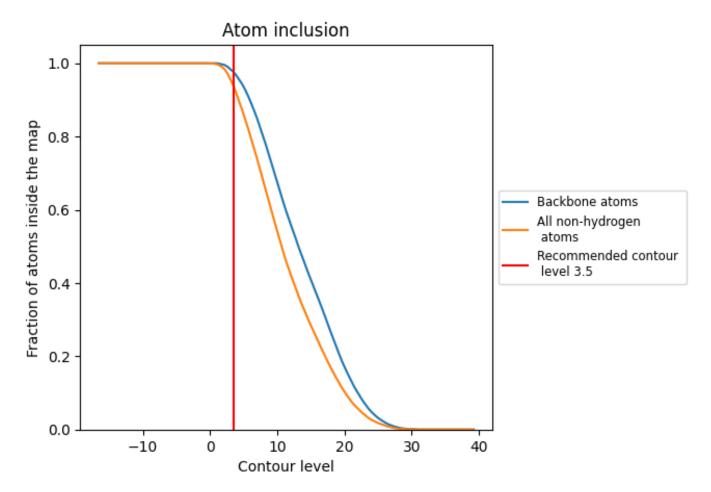
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.4680
A	0.9550	0.5510
В	0.9600	0.5650
С	0.9690	0.5950
D	0.9610	0.3040
Е	0.9520	0.5160
F	0.9620	0.5790
G	0.9500	0.4070
Н	0.9650	0.5760
I	0.9310	0.4670
J	0.9750	0.6040
K	0.9670	0.5950
L	0.9410	0.5120
M	0.8590	0.3090
N	0.8140	0.2840
O	0.5700	0.1210
Р	0.8820	0.4980
Q	0.4420	0.0670
S	0.9830	0.2530
T	0.8450	0.3850



