

wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 02:12 PM JST

PDB ID : 7D59

EMDB ID : EMD-30578

Title : cryo-EM structure of human RNA polymerase III in apo state

Authors: Wang, Q.; Wan, F.; Lan, P.; Wu, J.; Lei, M.

Deposited on : 2020-09-25

Resolution : 3.10 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 (i)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70

Mogul : 1.8.5 (274361), CSD as541be (2020)

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $MapQ \quad : \quad 1.9.13$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

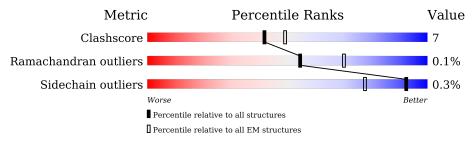
Validation Pipeline (wwPDB-VP) : 2.36

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 3.10 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1390	80%	19%
2	В	1133	81%	16%
3	С	346	85%	15%
4	D	148	61% 23%	15%
5	Е	210	84%	16%
6	F	127	50% 12% 38%	
7	G	204	69% 21%	10%
8	Н	150	81%	19% •

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Mol	Chain	Length		Qua	lity of cha	ain	
9	I	108	44	81%			19%
10	J	67	<u>-</u>	79%			21%
11	K	133	•	67%		14%	20%
12	L	58	<u>-</u>	64%		17%	19%
13	M	708	23%	8%		69%	
14	N	398	24%	10%		66%	
15	О	534	12%	71%		20%	8%
16	Р	316	30%	14%		56%	
17	Q	223	23%	1%	10%	46%	

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
19	SF4	Р	400	_	-	X	-



2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 39898 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		A	AltConf	Trace			
1	A	1386	Total 10881	C 6894	N 1897	O 2017	S 73	0	0

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

Mol	Chain	Residues		A	AltConf	Trace			
2	D	1095	Total	С	N	О	S	0	0
2	Б	1095	8668	5492	1513	1595	68	0	U

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

Mol	Chain	Residues		At	AltConf	Trace			
3	С	345	Total 2752	C 1732	N 490	O 518	S 12	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	126	Total 1013	C 634	N 176	O 200	S 3	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues		Ato	oms	AltConf	Trace		
5	Е	210	Total 1723	C 1088	N 301	O 325	S 9	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	F	79	Total	С	N	О	S	0	0
	-	10	636	407	108	116	5		



• Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	G	183	Total	С	N	О	S	0	0
'	G	100	1470	951	231	281	7	0	

• 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	1.40	Total	С	N	О	S	0	0
0	п	149	1197	759	195	238	5	U	U

• Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	I	108	Total 857	C 529	N 158	O 157	S 13	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	ī	67	Total	С	N	О	S	0	0
10	J	07	533	345	90	92	6	0	U

• Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms			AltConf	Trace		
11	К	107	Total 856	C 531	N 153	O 165	S 7	0	0

• Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

\mathbf{M}	ol	Chain	Residues		Ato	ms			AltConf	Trace
1:	2	L	47	Total 397	C 246	N 77	O 68	S 6	0	0

• Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
13	M	222	Total 1797	C 1134	N 307	O 346	S 10	0	0

• Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.



Mol	Chain	Residues	${f Atoms}$				AltConf	Trace	
1./	N	136	Total	С	N	О	S	0	0
14	11	130	1038	653	188	192	5		U

 \bullet Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	О	490	Total 3913	C 2468	N 678	O 742	S 25	0	0

• Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms				AltConf	Trace	
16	Р	139	Total 1103	C 700	N 178	O 214	S 11	0	0

• Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

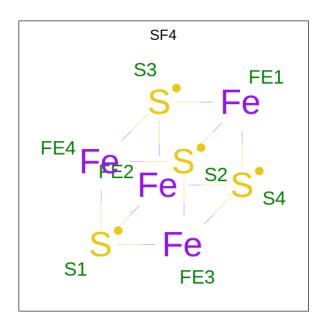
Mol	Chain	Residues	Atoms				AltConf	Trace	
17	0	191	Total	С	N	О	S	0	0
11	Q	Q 121	1049	667	166	210	6	0	

• Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

 \bullet Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe $_4$ S4).





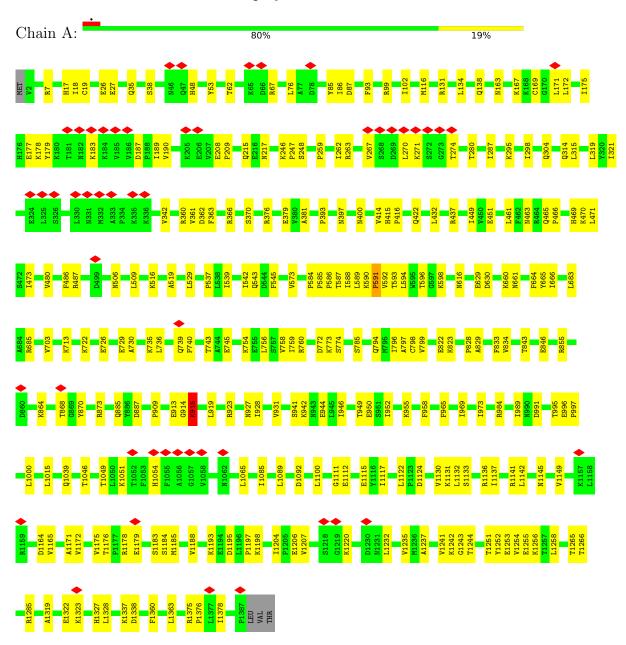
Mol	Chain	Residues	Atoms	AltConf
19	Р	1	Total Fe S 8 4 4	0



3 Residue-property plots (i)

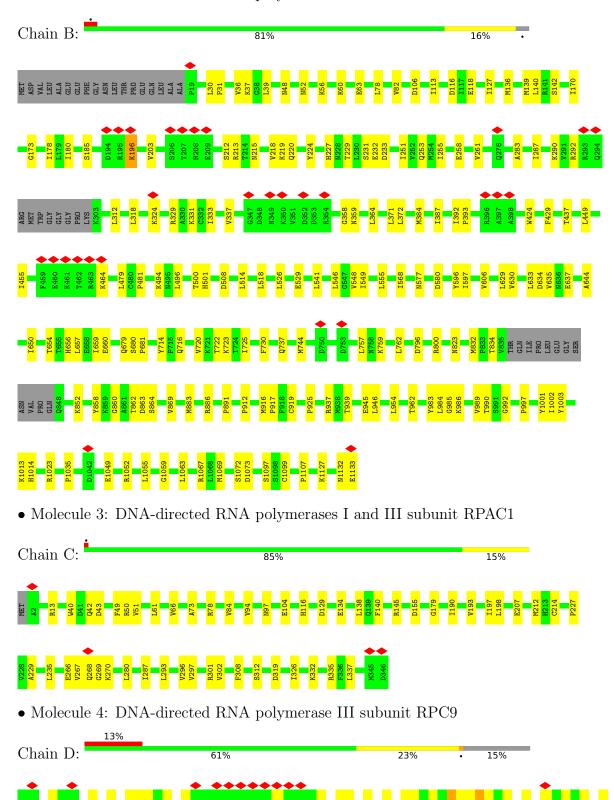
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 III subunit RPC1

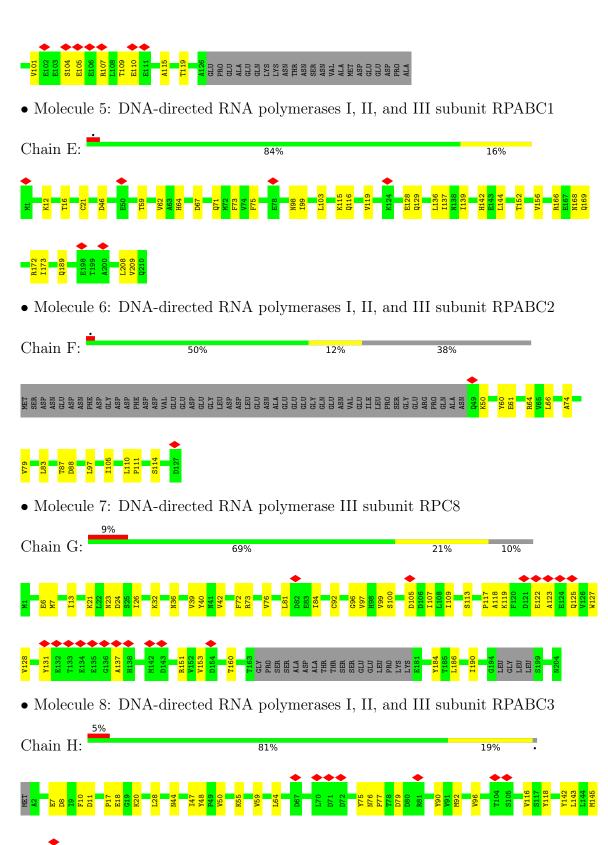




• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



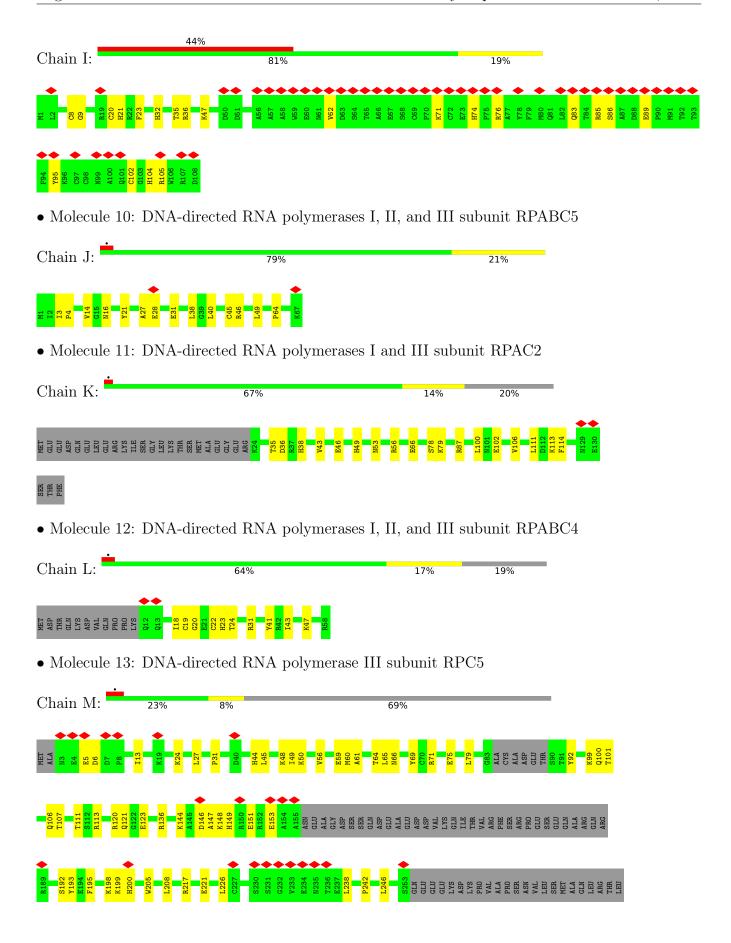




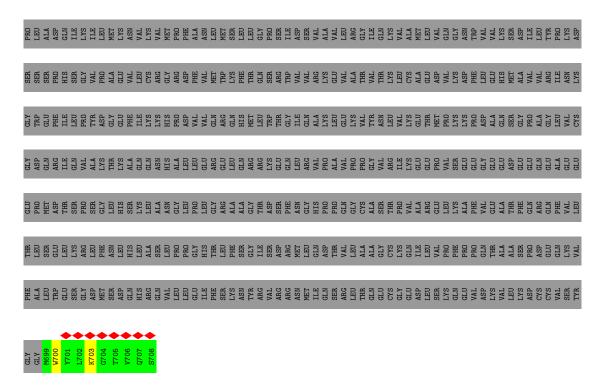


• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

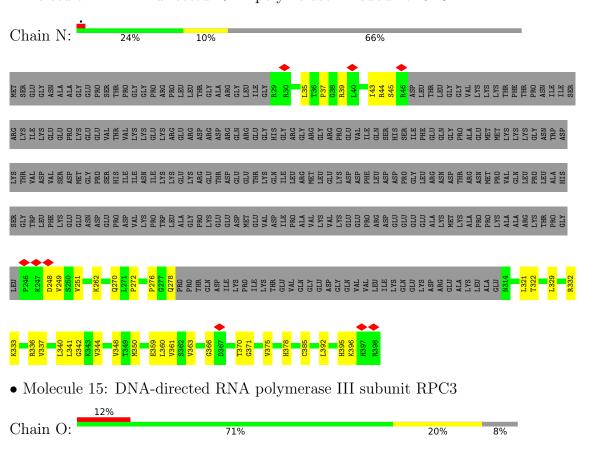




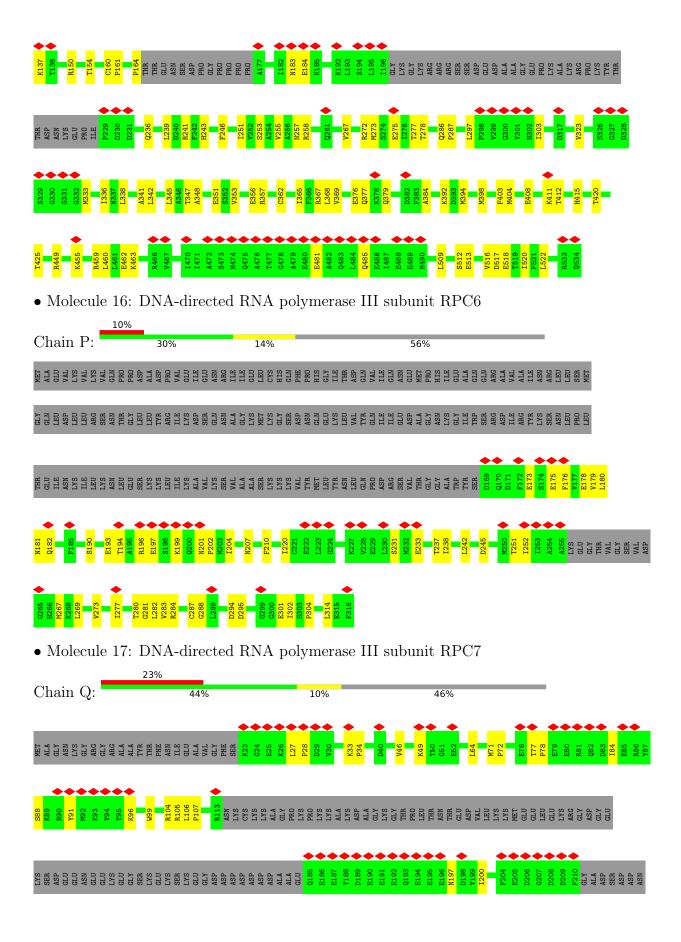




• Molecule 14: DNA-directed RNA polymerase III subunit RPC4













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	264514	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	366.24002, 366.24002, 366.24002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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, 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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.24	0/11078	0.41	0/14939
2	В	0.24	0/8833	0.41	0/11912
3	С	0.24	0/2806	0.42	0/3803
4	D	0.23	0/1026	0.41	0/1384
5	Е	0.24	0/1753	0.42	0/2368
6	F	0.23	0/646	0.39	0/873
7	G	0.25	0/1510	0.45	0/2054
8	Н	0.24	0/1219	0.43	0/1644
9	I	0.25	0/878	0.44	0/1186
10	J	0.23	0/542	0.39	0/730
11	K	0.23	0/871	0.39	0/1174
12	L	0.22	0/403	0.40	0/536
13	M	0.23	0/1837	0.42	0/2481
14	N	0.25	0/1051	0.46	0/1417
15	О	0.23	0/3972	0.41	0/5359
16	Р	0.24	0/1126	0.42	0/1522
17	Q	0.25	0/1076	0.40	0/1449
All	All	0.24	0/40627	0.41	0/54831

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
15	О	0	1
All	All	0	2

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	77	LYS	Peptide
15	О	68	HIS	Peptide

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	10881	0	11126	181	0
2	В	8668	0	8794	113	0
3	С	2752	0	2725	34	0
4	D	1013	0	1040	21	0
5	Е	1723	0	1745	22	0
6	F	636	0	667	13	0
7	G	1470	0	1409	28	0
8	Н	1197	0	1156	17	0
9	I	857	0	817	15	0
10	J	533	0	555	9	0
11	K	856	0	840	13	0
12	L	397	0	401	6	0
13	M	1797	0	1756	44	0
14	N	1038	0	1092	28	0
15	О	3913	0	3988	67	0
16	Р	1103	0	1066	38	0
17	Q	1049	0	985	17	0
18	A	2	0	0	0	0
18	В	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	Р	8	0	0	3	0
All	All	39898	0	40162	585	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 7.



The worst 5 of 585 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \AA) \end{array}$	Clash overlap (Å)
7:G:96:GLY:HA3	7:G:109:ILE:O	1.52	1.07
7:G:99:VAL:O	7:G:107:ILE:HB	1.75	0.85
8:H:92:MET:HB2	8:H:143:LEU:HB3	1.59	0.84
1:A:913:GLU:HB2	1:A:919:LEU:HA	1.65	0.78
7:G:96:GLY:CA	7:G:109:ILE:O	2.34	0.75

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	1384/1390 (100%)	1316 (95%)	66 (5%)	2 (0%)	51	83
2	В	1089/1133 (96%)	1043 (96%)	46 (4%)	0	100	100
3	С	343/346 (99%)	314 (92%)	28 (8%)	1 (0%)	41	73
4	D	124/148 (84%)	117 (94%)	6 (5%)	1 (1%)	19	54
5	Е	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
6	F	77/127 (61%)	75 (97%)	2 (3%)	0	100	100
7	G	177/204 (87%)	167 (94%)	10 (6%)	0	100	100
8	Н	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
9	I	106/108 (98%)	100 (94%)	6 (6%)	0	100	100
10	J	65/67~(97%)	63 (97%)	2 (3%)	0	100	100
11	K	105/133~(79%)	104 (99%)	1 (1%)	0	100	100
12	L	45/58~(78%)	41 (91%)	4 (9%)	0	100	100
13	M	214/708 (30%)	210 (98%)	4 (2%)	0	100	100
14	N	130/398 (33%)	120 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
15	О	$484/534 \ (91\%)$	472 (98%)	12 (2%)	0	100	100
16	Р	135/316~(43%)	127 (94%)	8 (6%)	0	100	100
17	Q	115/223~(52%)	112 (97%)	3 (3%)	0	100	100
All	All	4948/6253 (79%)	4721 (95%)	223 (4%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	268	GLN
4	D	78	LEU
1	A	591	PRO
1	A	915	LYS

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	Percen	tiles
1	A	1208/1212 (100%)	1204 (100%)	4 (0%)	92	96
2	В	958/988 (97%)	956 (100%)	2 (0%)	93	97
3	С	301/302 (100%)	301 (100%)	0	100	100
4	D	117/136 (86%)	115 (98%)	2 (2%)	60	83
5	E	192/192 (100%)	192 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	164/181 (91%)	164 (100%)	0	100	100
8	Н	130/131 (99%)	130 (100%)	0	100	100
9	I	94/94 (100%)	94 (100%)	0	100	100
10	J	56/56~(100%)	56 (100%)	0	100	100
11	K	96/119 (81%)	96 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	200/622~(32%)	199 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
14	N	119/347~(34%)	118 (99%)	1 (1%)	81	92
15	О	439/476~(92%)	437 (100%)	2 (0%)	88	94
16	Р	125/280~(45%)	125 (100%)	0	100	100
17	Q	115/195~(59%)	114 (99%)	1 (1%)	78	91
All	All	4427/5497 (80%)	4414 (100%)	13 (0%)	92	96

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	80	LYS
13	M	144	LYS
17	Q	104	ARG
15	О	81	ARG
15	О	455	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	413	ASN
15	О	377	GLN
2	В	1082	GLN
15	О	302	ASN
17	Q	197	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 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	Pos	Link	B	Bond lengths		Bond angles		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
19	SF4	Р	400	16	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	SF4	Р	400	16	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Р	400	SF4	3	0

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.



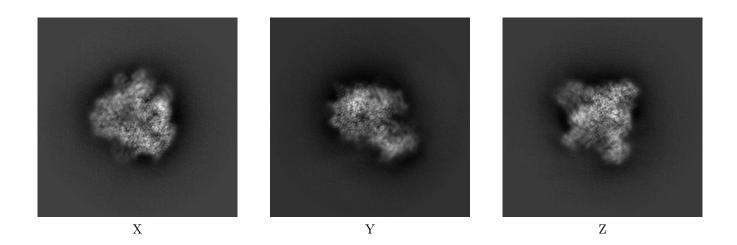
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30578. 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)

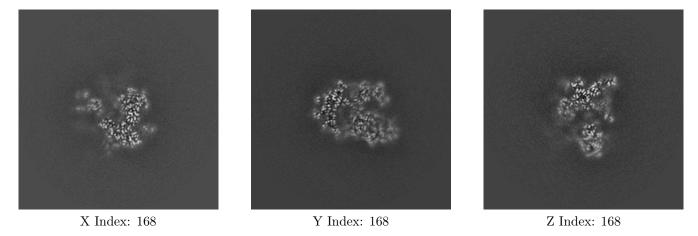
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map

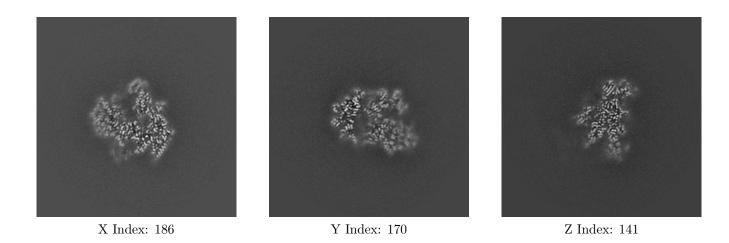




The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

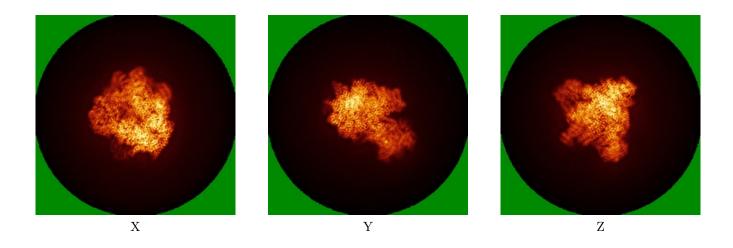
6.3.1 Primary map



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

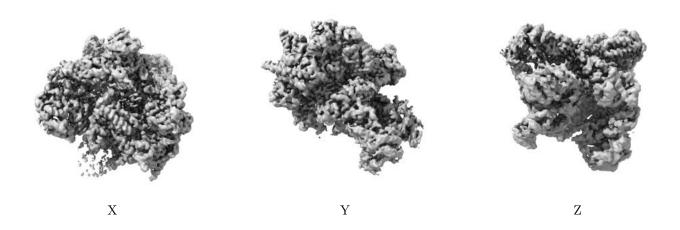


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 0.007. 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)

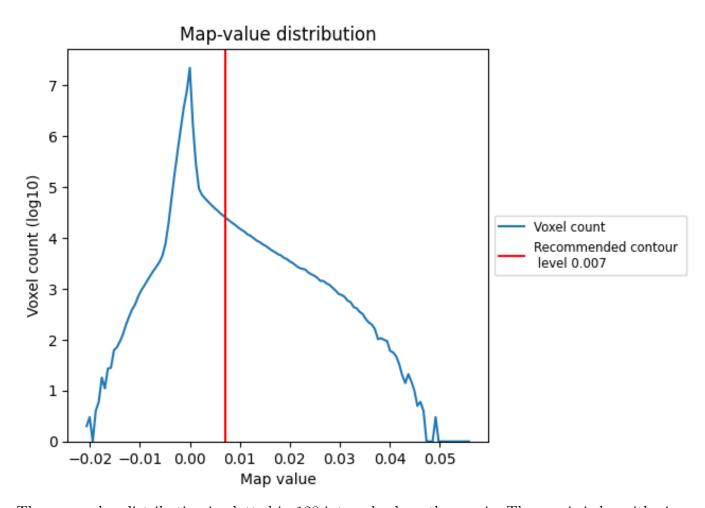
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

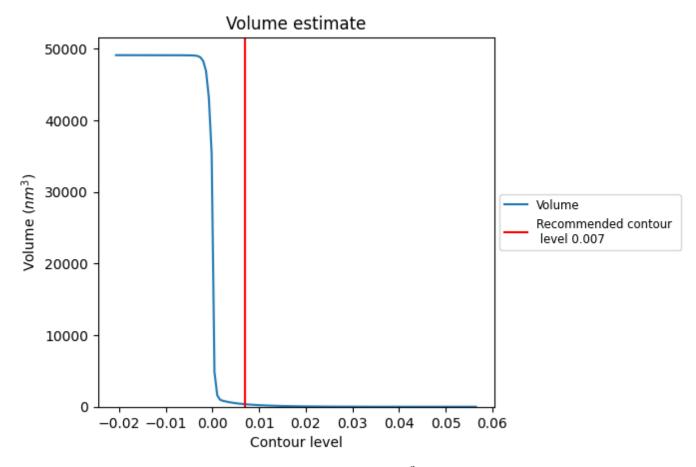
7.1 Map-value distribution (i)



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)

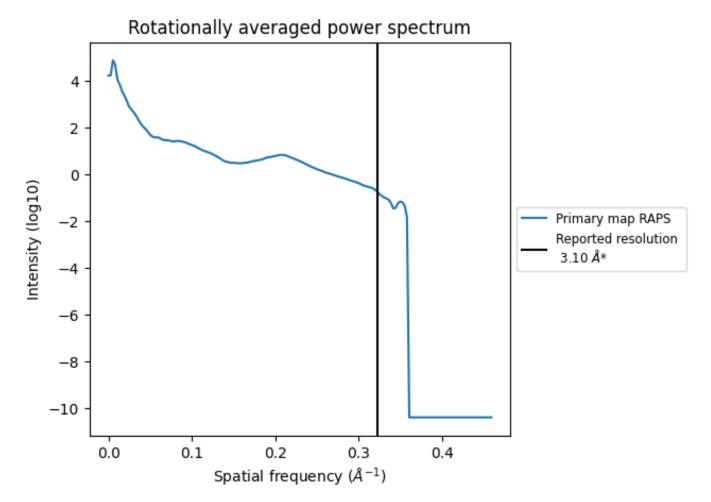


The volume at the recommended contour level is $357~\mathrm{nm}^3$; this corresponds to an approximate mass of $323~\mathrm{kDa}$.

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 0.323 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

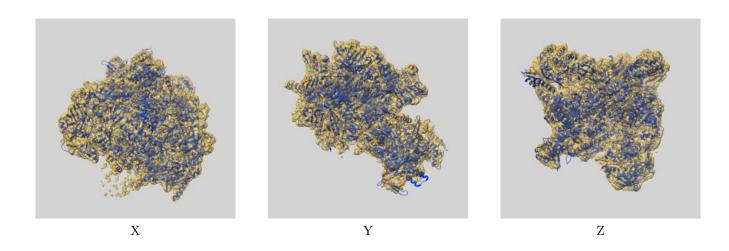
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30578 and PDB model 7D59. Per-residue inclusion information can be found in section 3 on page 8.

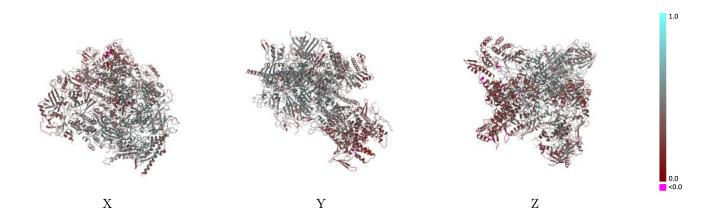
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

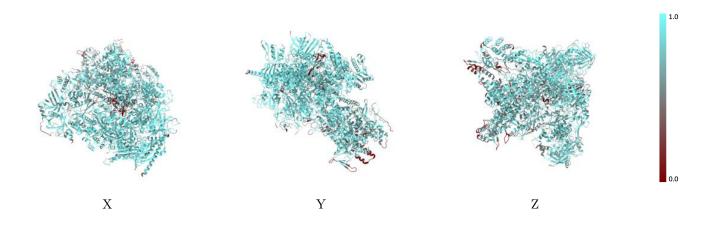


9.2 Q-score mapped to coordinate model (i)



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.

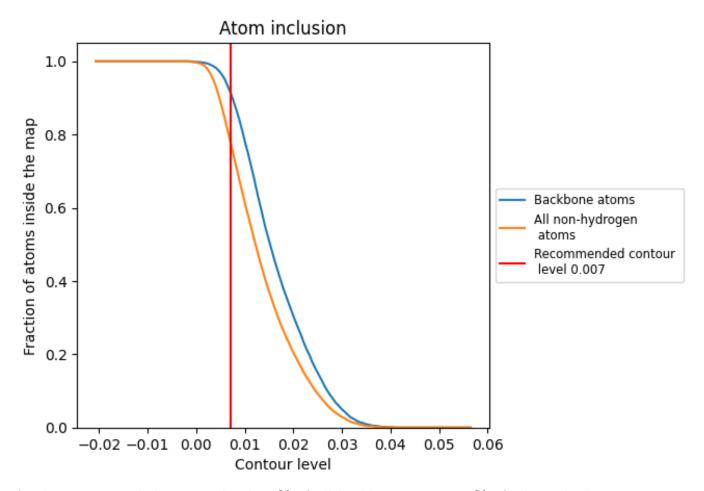
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).



9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.3910
A	0.8170	0.4260
В	0.8350	0.4390
С	0.8750	0.4430
D	0.6980	0.2680
Е	0.7980	0.3340
F	0.8820	0.4630
G	0.7460	0.3510
Н	0.8390	0.4270
I	0.4960	0.2940
J	0.8810	0.4840
K	0.8830	0.4390
L	0.8560	0.4320
M	0.7130	0.3070
N	0.7820	0.3700
О	0.6750	0.2960
Р	0.6120	0.2650
Q	0.4970	0.3050



