

# wwPDB EM Validation Summary Report (i)

#### Sep 17, 2023 - 01:07 PM JST

PDB ID	:	7YCX
EMDB ID	:	EMD-33741
Title	:	The structure of INTAC-PEC complex
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Deposited on	:	2022-07-02
Resolution	:	4.18  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:

:	0.0.1.dev $50$
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35.1
	: : : : :

# 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 4.18 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	А	2190	8%	19%
2	В	1204	88%	12%
3	D	963	85%	• 14%
4	Е	1019	78%	22%
5	F	887	6%	37%
6	G	962	94%	• 5%
7	Н	995	93%	• 6%
8	Ι	658	96%	•

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Mol	Chain	Length	Quality of chain	
9	Κ	600	97% ···	
10	М	17	100%	•
11	Р	589	98%	
12	Q	309	95% 5%	
13	U	27	100%	•
14	1	1970	• 73% • 26%	
15	2	1174	94% 5%	
16	3	271	96% ·	
17	4	210	99%	
18	5	127	7%           63%         36%	
19	6	150	97%	
20	7	125	5% 94% 6%	
21	8	67	99%	
22	9	117	100%	•
23	a	58	78% • 21%	-
24	b	48	10% 75% 25%	
25	с	23	35% 65%	•
26	d	48	94% 6%	
27	е	528	12% 34% 65%	
28	f	580	83% 17%	
29	g	590	90% • 9%	
30	h	380	• 5%• 94%	
31	i	121	95%	
32	j	1087	<u>23%</u> 44% 56%	
33	k	172	98%	

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Mol	Chain	Length	Quality of chain		
			9%		
34	1	142	89%	•	10%



# 2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 113089 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 Integrator complex subunit 1.

Mol	Chain	Residues		Atoms					Trace
1	А	1779	Total 13054	C 8226	N 2322	0 2432	S 74	0	0

• Molecule 2 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues		Α	AltConf	Trace			
2	В	1061	Total 8328	C 5322	N 1412	O 1530	S 64	0	0

• Molecule 3 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues		А	AltConf	Trace			
2	Л	898	Total	С	Ν	Ο	$\mathbf{S}$	0	0
5	D	020	6205	3931	1085	1158	31	0	0

• Molecule 4 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues		At	AltConf	Trace			
4	Е	798	Total 5244	C 3284	N 988	O 958	S 14	0	0

• Molecule 5 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues		At	AltConf	Trace			
5	F	560	Total	С	Ν	Ο	$\mathbf{S}$	0	0
9	T,	500	4395	2809	750	813	23	0	0

• Molecule 6 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues		A	AltConf	Trace			
6	G	910	Total 6928	C 4382	N 1212	O 1293	S 41	0	0



• Molecule 7 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues		Α	AltConf	Trace			
7	Н	937	Total 7440	C 4761	N 1274	O 1361	S 44	0	0

• Molecule 8 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues		At	AltConf	Trace			
8	Ι	633	Total 4985	C 3210	N 815	O 926	S 34	0	0

• Molecule 9 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues		At	AltConf	Trace			
9	K	590	Total 4646	C 2964	N 806	0 841	S 35	0	0

• Molecule 10 is a protein called Unknown2.

Mol	Chain	Residues	1	Ator	ns	AltConf	Trace	
10	М	17	Total 85	C 51	N 17	O 17	0	0

• Molecule 11 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues		At	AltConf	Trace			
11	Р	581	Total 4527	C 2877	N 763	0 860	$\frac{\mathrm{S}}{27}$	0	0

• Molecule 12 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues		At	AltConf	Trace			
12	Q	293	Total 2366	C 1497	N 405	0 449	${ m S}$ 15	0	0

• Molecule 13 is a protein called Unknown.

Mol	Chain	Residues	1	Ator	$\mathbf{ns}$	AltConf	Trace	
13	U	27	Total 135	C 81	N 27	O 27	0	0



• Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB1,DNA-directed RNA polymerase II subunit RPB1, CTD1, CTD2, CTD3, CTD4.

Mol	Chain	Residues		Α	AltConf	Trace			
14	1	1451	Total 11345	C 7135	N 2033	O 2109	S 68	0	0

• Molecule 15 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		А	AltConf	Trace			
15	2	1113	Total 8649	C 5489	N 1515	0 1581	S 64	0	0

• Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues		At	AltConf	Trace			
16	3	259	Total 2048	C 1289	N 354	O 399	S 6	0	0

• Molecule 17 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues		Ate	AltConf	Trace			
17	4	209	Total 1721	C 1089	N 300	0 324	S 8	0	0

• Molecule 18 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues		At	AltConf	Trace			
18	5	81	Total 649	C 413	N 111	O 120	${ m S}{ m 5}$	0	0

• Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	6	148	Total 1186	C 750	N 194	0 237	${f S}{5}$	0	0

• Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues		A	toms		AltConf	Trace	
20	7	117	Total 950	C 587	N 169	0 183	S 11	0	0

• Molecule 21 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
21	8	67	Total 533	$\begin{array}{c} \mathrm{C} \\ 345 \end{array}$	N 90	O 92	S 6	0	0

• Molecule 22 is a protein called RNA\_pol\_L\_2 domain-containing protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	9	117	Total 937	C 604	N 154	0 177	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 23 is a protein called RPB12.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
23	a	46	Total	C	N	0	S	0	0
			389	241	75	67	6		

• Molecule 24 is a DNA chain called non-template DNA.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
24	b	36	Total 752	C 351	N 153	0 212	Р 36	0	0

• Molecule 25 is a RNA chain called RNA.

Mol	Chain	Residues		At	$\mathbf{oms}$		AltConf	Trace	
25	С	23	Total 406	C 179	N 56	0 148	Р 23	0	0

• Molecule 26 is a DNA chain called template DNA.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
26	d	45	Total 909	C 431	N 157	0 276	Р 45	0	0

• Molecule 27 is a protein called Negative elongation factor A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	е	183	Total 1410	C 895	N 239	O 269	${ m S} 7$	0	0

• Molecule 28 is a protein called Negative elongation factor B.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
10	f	490	Total	С	Ν	Ο	0	0
20	1	400	1920	960	480	480	0	0

• Molecule 29 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues		At	AltConf	Trace			
29	g	534	Total 3764	C 2382	N 653	O 710	S 19	0	0

• Molecule 30 is a protein called Negative elongation factor E.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
30	h	22	Total 109	$\begin{array}{c} \mathrm{C} \\ 65 \end{array}$	N 22	O 22	0	0

• Molecule 31 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues		At	AltConf	Trace			
31	i	116	Total 911	C 570	N 159	0 173	S 9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	-3	GLY	-	expression tag	UNP P63272
i	-2	PRO	-	expression tag	UNP P63272
i	-1	GLY	-	expression tag	UNP P63272
i	0	SER	-	expression tag	UNP P63272

• Molecule 32 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues		At	AltConf	Trace			
32	j	482	Total 3854	C 2448	N 681	0 708	S 17	0	0

• Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues		At	AltConf	Trace			
33	k	171	Total 1299	C 849	N 205	O 238	${f S}{7}$	0	0

• Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB4.



Mol	Chain	Residues		At	AltConf	Trace			
34	1	128	Total 997	C 629	N 169	0 195	$\frac{S}{4}$	0	0

• Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
35	К	2	Total Zn 2 2	0
35	1	2	Total Zn 2 2	0
35	2	1	Total Zn 1 1	0
35	3	1	Total Zn 1 1	0
35	7	2	Total Zn 2 2	0
35	8	1	Total Zn 1 1	0
35	a	1	Total Zn 1 1	0

• Molecule 36 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	AltConf
36	Q	2	Total Mn 2 2	0

• Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
37	1	1	Total Mg 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: Integrator complex subunit 1











Chain G:

94%







There are no outlier residues recorded for this chain.



• Molecule 11: Serine/threenine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain P:										989	%					•
MET ALA ALA ALA ASP GLY ASP ASP	68	E23	E62	R221	L235	A242	K255	H304	D316	A589						

• Molecule 12: Serine/threenine-protein phosphatase 2A catalytic subunit alpha isoform

Chain Q:	95%	5%
MET D2 ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG		
• Molecule 13: Unknown		
Chain U:	100%	

There are no outlier residues recorded for this chain.

• Molecule 14: DNA-directed RNA polymerase II subunit RPB1, DNA-directed RNA polymerase II subunit RPB1, CTD1, CTD2, CTD3, CTD4









• Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC3











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#### LYS GLU ASN LEU VAL ASP GLY PHE

• Molecule 31: Transcription elongation factor SPT4









# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41201	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 $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	442.68002, 442.68002, 442.68002	wwPDB
Map dimensions	420, 420, 420	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: MN, 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).

Mal	Chain	Bond	lengths	Bond angles				
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.26	0/13264	0.46	0/18049			
2	В	0.31	0/8474	0.48	0/11498			
3	D	0.31	0/6315	0.49	0/8583			
4	Е	0.26	0/5344	0.47	0/7312			
5	F	0.27	0/4508	0.49	0/6131			
6	G	0.32	0/7038	0.49	0/9532			
7	Н	0.27	0/7583	0.46	0/10280			
8	Ι	0.32	0/5110	0.49	0/6959			
9	K	0.30	0/4747	0.50	0/6412			
11	Р	0.27	0/4601	0.47	0/6246			
12	Q	0.29	0/2423	0.51	0/3285			
14	1	0.31	0/11492	0.52	0/15525			
15	2	0.32	0/8823	0.52	0/11947			
16	3	0.31	0/2091	0.50	0/2843			
17	4	0.26	0/1752	0.52	0/2366			
18	5	0.33	0/659	0.54	0/889			
19	6	0.30	0/1207	0.56	0/1628			
20	7	0.27	0/973	0.50	0/1316			
21	8	0.38	0/542	0.54	0/730			
22	9	0.28	0/956	0.48	0/1294			
23	a	0.31	0/395	0.63	0/524			
24	b	0.31	0/846	0.68	0/1304			
25	с	0.51	0/450	0.88	1/696~(0.1%)			
26	d	0.37	0/1014	0.73	0/1560			
27	е	0.24	0/1434	0.47	0/1948			
28	f	0.22	0/1913	0.40	0/2379			
29	g	0.25	0/3830	0.44	2/5236~(0.0%)			
30	h	0.27	0/108	0.74	$\overline{2/149}$ (1.3%)			
31	i	0.28	0/927	0.55	0/1250			
32	j	0.26	$0/3\overline{920}$	0.51	$0/5\overline{276}$			
33	k	0.26	0/1330	0.46	0/1813			
34	1	0.25	0/1011	0.46	0/1364			



Mal	[ol Chain Bond lengths		Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
All	All	0.29	0/115080	0.50	5/156324~(0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
25	с	38	G	C2'-C3'-O3'	5.75	122.90	113.70
29	g	60	PRO	N-CA-CB	5.70	110.14	103.30
30	h	5	PRO	N-CA-CB	5.62	110.05	103.30
30	h	6	PRO	N-CA-CB	5.59	110.01	103.30
29	g	76	PRO	N-CA-CB	5.02	109.33	103.30

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	Perce	ntiles
1	А	1755/2190~(80%)	1671~(95%)	82 (5%)	2 (0%)	51	85
2	В	1045/1204~(87%)	998~(96%)	47 (4%)	0	100	100
3	D	814/963~(84%)	754~(93%)	54 (7%)	6 (1%)	22	62
4	Ε	794/1019~(78%)	734~(92%)	57 (7%)	3~(0%)	34	71
5	F	554/887~(62%)	541 (98%)	13~(2%)	0	100	100
6	G	904/962~(94%)	830~(92%)	70 (8%)	4 (0%)	34	71
7	Н	933/995~(94%)	892 (96%)	41 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$\mathbf{ntiles}$
8	Ι	629/658~(96%)	592~(94%)	37~(6%)	0	100	100
9	Κ	586/600~(98%)	551 (94%)	33~(6%)	2 (0%)	41	75
11	Р	579/589~(98%)	559~(96%)	20 (4%)	0	100	100
12	Q	291/309~(94%)	267~(92%)	24 (8%)	0	100	100
14	1	1425/1970~(72%)	1335~(94%)	86~(6%)	4 (0%)	41	75
15	2	1099/1174~(94%)	995~(90%)	104 (10%)	0	100	100
16	3	255/271~(94%)	239 (94%)	16 (6%)	0	100	100
17	4	207/210~(99%)	201~(97%)	6 (3%)	0	100	100
18	5	79/127~(62%)	77~(98%)	2(2%)	0	100	100
19	6	146/150~(97%)	135~(92%)	11 (8%)	0	100	100
20	7	115/125~(92%)	111 (96%)	4 (4%)	0	100	100
21	8	65/67~(97%)	61 (94%)	4 (6%)	0	100	100
22	9	115/117~(98%)	108 (94%)	7~(6%)	0	100	100
23	a	44/58~(76%)	40 (91%)	4 (9%)	0	100	100
27	е	181/528~(34%)	177~(98%)	4(2%)	0	100	100
28	f	466/580~(80%)	451 (97%)	14 (3%)	1 (0%)	47	80
29	g	530/590~(90%)	501~(94%)	29~(6%)	0	100	100
30	h	20/380~(5%)	20 (100%)	0	0	100	100
31	i	114/121~(94%)	111~(97%)	3~(3%)	0	100	100
32	j	470/1087~(43%)	451~(96%)	19~(4%)	0	100	100
33	k	169/172~(98%)	162~(96%)	7~(4%)	0	100	100
34	1	126/142~(89%)	122~(97%)	4(3%)	0	100	100
All	All	$14510/18\overline{245}~(80\%)$	13686 (94%)	802 (6%)	22 (0%)	50	80

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5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1816	PRO
3	D	63	PRO
3	D	106	SER
3	D	561	MET
4	Е	282	ILE



#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	1253/1907~(66%)	1248 (100%)	5~(0%)	91	94
2	В	946/1072~(88%)	943 (100%)	3~(0%)	92	95
3	D	617/845~(73%)	613 (99%)	4 (1%)	86	92
4	Ε	395/812~(49%)	392 (99%)	3 (1%)	81	89
5	F	490/796~(62%)	488 (100%)	2(0%)	91	94
6	G	744/840~(89%)	738 (99%)	6 (1%)	81	89
7	Н	822/896~(92%)	815 (99%)	7 (1%)	78	87
8	Ι	575/600~(96%)	574 (100%)	1 (0%)	93	96
9	K	505/520~(97%)	500 (99%)	5 (1%)	76	86
11	Р	508/512~(99%)	506 (100%)	2(0%)	91	94
12	Q	259/274~(94%)	259 (100%)	0	100	100
14	1	1239/1736~(71%)	1232 (99%)	7 (1%)	86	92
15	2	908/1027~(88%)	903 (99%)	5 (1%)	86	92
16	3	227/248~(92%)	227 (100%)	0	100	100
17	4	191/192~(100%)	189 (99%)	2(1%)	76	86
18	5	70/111~(63%)	69 (99%)	1 (1%)	67	80
19	6	129/131~(98%)	127 (98%)	2(2%)	62	78
20	7	105/112~(94%)	105 (100%)	0	100	100
21	8	56/56~(100%)	55 (98%)	1 (2%)	59	76
22	9	106/106~(100%)	106 (100%)	0	100	100
23	a	43/55~(78%)	42 (98%)	1 (2%)	50	69
27	е	158/451~(35%)	156 (99%)	2 (1%)	69	82
29	g	$\overline{339/513}~(66\%)$	336 (99%)	3 (1%)	78	87
31	i	$\overline{102/105~(97\%)}$	101 (99%)	1 (1%)	76	86
32	j	425/940 (45%)	423 (100%)	2 (0%)	88	93
33	k	$\overline{136/153}\ (89\%)$	134 (98%)	2 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
34	1	104/126~(82%)	103 (99%)	1 (1%)	76	86
All	All	11452/15136~(76%)	11384 (99%)	68 (1%)	86	92

 $5~{\rm of}~68$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
27	е	42	ARG
29	g	229	LYS
33	k	78	ARG
7	Н	493	LYS
7	Н	162	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such side chains are listed below:

Mol	Chain	Res	Type
15	2	1117	HIS
15	2	1129	ASN
34	l	47	GLN
5	F	462	GLN
5	F	225	GLN

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	с	22/23~(95%)	14~(63%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	с	25	A
25	с	26	U
25	с	27	А
25	с	28	А
25	с	29	С

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 13 ligands modelled in this entry, 13 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-33741. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

# 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



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



# 6.2 Central slices (i)

### 6.2.1 Primary map



X Index: 210





Z Index: 210

#### 6.2.2 Raw map



X Index: 210

Y Index: 210



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: 203



Y Index: 220



Z Index: 174

#### 6.3.2 Raw map



X Index: 207

Y Index: 220



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



6.4.2 Raw 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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

### 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 1216  $\rm nm^3;$  this corresponds to an approximate mass of 1099 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 0.239  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

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

### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.239  $\mathrm{\AA^{-1}}$ 



# 8.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	4.18	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	6.50	8.31	6.84	

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 4.18 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33741 and PDB model 7YCX. Per-residue inclusion information can be found in section 3 on page 11.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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 (0.015).



# 9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7930	0.3110
1	0.8490	0.3500
2	0.8960	0.4060
3	0.8970	0.4240
4	0.8170	0.2900
5	0.7870	0.3040
6	0.7760	0.2510
7	0.8220	0.2580
8	0.9190	0.4570
9	0.8390	0.3640
А	0.7480	0.2340
В	0.8730	0.3770
D	0.9070	0.4000
${ m E}$	0.7750	0.2950
F	0.7790	0.2680
G	0.9070	0.4090
Н	0.8120	0.2520
Ι	0.8410	0.3820
Κ	0.7610	0.3240
М	0.9650	0.2830
Р	0.8260	0.2400
Q	0.8950	0.3830
U	0.9410	0.4100
a	0.9140	0.4090
b	0.7000	0.1950
С	0.8100	0.2900
d	0.7810	0.2390
е	0.5240	0.1810
f	0.6490	0.2700
g	0.5480	0.2040
h	0.5780	0.2680
i	0.0210	0.1200
j	0.3860	0.1780
k	0.7400	0.2080
1	0.7450	0.1850



