

# wwPDB EM Validation Summary Report (i)

#### Feb 25, 2023 – 01:00 PM EST

PDB ID	:	7UI9
EMDB ID	:	EMD-26542
Title	:	Core Mediator-PICearly (Copy A)
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Deposited on	:	2022-03-28
Resolution	:	3.30 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 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	2.32.1
	: : : : :

## 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 3.30 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 $(\#Entries)$	$\mathop{\mathrm{EM}}\limits_{(\#\mathrm{Entries})}$
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	Q	uality of chain						
1	М	345	10%	90%						
2	Р	735	14%	86%						
3	Q	400	31%	69%						
4	S	309	• <b>•</b> 58%	41%						
5	a	566	13%	• 36%						
6	d	284	<b>•</b> 60%	• 40%						
7	f	295	10%	43%						
8	g	222	10%	• 24%						
9	h	223	61%	39%						

Continued on next page...



Mol	Chain	Length	Quality of chain								
10	i	149	55% • 44%								
11	j	157	93%	7%							
12	k	115	94%	6%							
13	n	1082	9% 57% 42%								
14	α	687	75%	25%							
15	r	307	82%	18%							
16		220	36%	10 %							
17	+	220	5/%								
10	U	140	21%								
18	u	140	5%	• 13%							
19	V	120	90%	• 9%							
20	W	127	81%	19%							
21	Z	25	96%	•							
22	А	1453	100%								
23	В	1224	96%	•							
24	С	318	85%	15%							
25	D	221	76%	24%							
26	Е	215	100%								
27	F	155	55% 45%								
28	G	171	99%	•							
29	Н	146	97%	•							
30	Ι	122	95%	5%							
31	J	70	100%								
32	K	120	97%	•							
33	L	70	7%         61%         39%								

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# 2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 63137 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
1	М	35	Total 263	C 169	N 41	O 49	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 2 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues		At	oms		AltConf	Trace	
2	Р	103	Total 861	C 554	N 142	0 162	${ m S} { m 3}$	0	0

• Molecule 3 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues		At	oms		AltConf	Trace	
3	Q	125	Total 1033	C 644	N 189	O 195	${ m S}{ m 5}$	0	0

• Molecule 4 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues		At	oms		AltConf	Trace	
4	S	181	Total 1436	C 893	N 256	0 279	S 8	0	0

• Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues		At		AltConf	Trace		
5	a	365	Total 3008	C 1932	N 478	O 588	S 10	0	0

• Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	d	171	Total 1388	C 875	N 233	O 276	${S \atop 4}$	0	0



• Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	f	169	Total 1407	C 905	N 234	O 262	${ m S}{ m 6}$	0	0

• Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	g	169	Total 1409	C 903	N 238	O 263	${ m S}{ m 5}$	0	0

• Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	h	136	Total 1126	C 709	N 199	0 215	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	i	83	Total 709	C 444	N 130	0 134	S 1	0	0

• Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	j	146	Total 1173	C 725	N 206	0 239	$\frac{S}{3}$	0	0

• Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	k	108	Total 876	C 546	N 149	0 177	${s \over 4}$	0	0

• Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues		At	AltConf	Trace			
13	n	625	Total 5139	C 3318	N 884	0 913	S 24	0	0

• Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 17.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	q	515	Total 4182	C 2674	N 707	O 788	S 13	0	0

• Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues		At	AltConf	Trace			
15	r	253	Total 1995	C 1271	N 331	O 383	S 10	0	0

• Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues		At	oms		AltConf	Trace	
16	s	81	Total 657	C 415	N 109	0 132	S 1	0	0

• Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues		Ate	AltConf	Trace			
17	t	210	Total 1609	C 1016	N 270	0 317	S 6	0	0

• Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	u	122	Total 978	C 611	N 163	0 199	${S \atop 5}$	0	0

• Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	v	109	Total 869	C 540	N 143	0 180	S 6	0	0

• Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	W	103	Total 871	C 575	N 135	0 155	${ m S}{ m 6}$	0	0

• Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB1.



Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
21	Z	25	Total 184	C 116	N 25	O 43	0	0

• Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues		A	AltConf	Trace			
	Δ	1452	Total	С	Ν	Ο	S	0	0
	A	1400	11425	7192	1995	2176	62	0	0

• Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues		Α	AltConf	Trace			
23	В	1172	Total 9336	C 5895	N 1637	0 1748	S 56	0	0

• Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	С	271	Total 2133	C 1340	N 355	0 424	S 14	0	0

• Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	D	169	Total 1353	C 838	N 237	0 275	${ m S} { m 3}$	0	0

• Molecule 26 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	Е	215	Total 1760	C 1116	N 310	O 322	S 12	0	0

• Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	F	86	Total 697	C 445	N 118	0 131	${ m S} { m 3}$	0	0

• Molecule 28 is a protein called DNA-directed RNA polymerase II subunit RPB7.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	G	171	Total 1340	C 861	N 222	O 249	S 8	0	0

• Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Н	141	Total 1126	C 706	N 189	O 226	${ m S}{ m 5}$	0	0

• Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues		A	toms	AltConf	Trace		
30	Ι	116	Total 943	C 580	N 171	0 181	S 11	0	0

• Molecule 31 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	J	70	Total 578	C 366	N 102	0 104	S 6	0	0

• Molecule 32 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	K	116	Total 929	C 596	N 158	0 173	${ m S} { m 2}$	0	0

• Molecule 33 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T.	43	Total	С	Ν	Ο	$\mathbf{S}$	0	0
00	Ц	10	344	211	69	60	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: Transcription initiation factor IIB









• Molecule 7: Mediator of RNA polymerase II transcription subunit 6



• Molecule 8: Mediator	of KINA polymerase	e II transcription subunit 7	
Chain g:	75%	• 24%	
MET ASN ASN ASP ASS GLU GLU SSI SSI ASN S11 S11 S11 S12 S14 S14 A40 S41	A22 GLN GLN THR ALA ASN ASN ASN ASN GLY GLY SER SER SER	E55 E56 E57 E57 E57 E57 A61 A61 A72 A74 C60 C80 C80 C80 C80 C80 C80 C80 C80 C80 C8	ASP LEU SER MET CLU THR CLU CLU
LEU TYR LYS LYS SER FIR EIO6 SIO9 N111 N111 K121 K121 L137	M143 Y144 E145 E145 E149 E149 P10 H15 H15 H15 H15	SER SER PRO PRO SER SER SER CLN CLN CLN	
• Molecule 9: Mediator	of RNA polymerase	e II transcription subunit 8	
Chain h:	61%	39%	
MET SER GLN SER GLN SER SER SER CLY CLY GLV GLV GLV CLY GLN GLN GLN	GLU ASP VAL SER SER PHE ASP CAS VAL CAS CAS CAS CAS CAS CAS CAS CAS CAS CAS	VAL THR THR ALA LEU LEU LEU LYS CASP CASP CASP CASP CASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LEU LEU VAL ARG
ASP SER SER PRO PRO PRO PRO PRO PRO PRO PRO ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	THR GLY GLV GLV CLU CLU CLS PRO TLE TLE TLE THR SER THR SER THR SER	SER SER ASN	
• Molecule 10: Mediator	of RNA polymera	se II transcription subunit 9	
Chain i:	55%	. 44%	
MET ASN LLEU GGLN ASN ASN VAL ASN CGLN CLEU CLEU LLEU TLEU THR	ASN PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	LLA EER LLA LLA LLA LLU LLU LLU LLU LLU LLU LLU	田和田田
		00 H 00 01 40 4 4 40 1 4 H 1 H 40 0 H 1 4 1 0	$\vdash \nabla                                   $
SER ASW GLY BG4 EG4 E107 SER SER SER SER SER F119 F119		. O F W W 4 O 4 4 4 O 1 4 H 1 H 4 O 0 F 1 4 H W	ΗΥΝΗΝ
• Molecule 11: Mediator	of RNA polymera	se II transcription subunit 10	Η Φ' Ω Η Ω
• Molecule 11: Mediator Chain j:	of RNA polymeras 76% 93%	se II transcription subunit 10	Η Φ' Ω Η Ω
<ul> <li>Molecule 11: Mediator</li> <li>Chain j:</li> </ul>	of RNA polymeras 76% 93% ≝ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩ ₩	se II transcription subunit 10 7%	R44 445 146 648 648 649 150 064 153 165 163 165 165 165 165 165 165 165 165 165 165
• Molecule 11: Mediator Chain j:	• of RNA polymera:         76%         93%         • • • • • • • • • • • • • • • • • • •	se II transcription subunit 10 7%	I104
• Molecule 11: Mediator Chain j: • 100 000 000 000 000 000 000 000 000 00	The second secon		H 104       H 16       H 16       H 16       H 15       H 15       H 16       H 16
<ul> <li>Molecule 11: Mediator</li> <li>Chain j:</li> <li>Molecule 21: Mediator</li> <li>Molecule 11: Mediator</li> <li>Molecule 21: Mediator</li> </ul>	Tool RNA polymera:         76%         93%         93%         1         1	se II transcription subunit 10 7% S B B B B B B B B B B B B B B B B B B B	1104       104         1105       1105         1106       145         1109       145         1112       146         1112       146         1112       146         1112       146         1112       146         1112       150         112       150         113       150         112       150         112       150         112       150         112       150         123       150         150       150         151       150         153       150         153       155         155       155         155       155         155       155         155       155         156       150         150       150         150       150         150       150         150       150         150       150         150       150         150       150         150       150         150       150         150





• Molecule 13: Mediator of RNA polymerase II transcription subunit 14





ASP ASP ASP ASP ASP ASP ASP ASS ASP ASP
ARIG GLU GLU GLU CLN ASN ASN ASN ASN ASS ASN ASS ASN ASS ASS
• Molecule 15: Mediator of RNA polymerase II transcription subunit 18
Chain r: 82% 18%
M1 NES SE4 SE4 SE5 SE5 SE5 SE5 SE5 SE5 SE5 SE5 SE5 SE5
PIC
• Molecule 16: Mediator of RNA polymerase II transcription subunit 19
36%           Chain s:         37%         63%
MET ARG ARG ASA ASA ASA ASA ASA ASA ASA ASA ASA AS
Re1 Kes Kes Kes Kes Kes Kes Krs Krs Krs Krs Krs Krs Krs Kr
ARG ARG ARS ARS ARS ARS ARS ARS ARS ARS CLEU CLEU ALA CLEU CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ALA ASS CLEA ASS ASS CLEA ASS ASS CLEA ASS ASS ASS ASS ASS ASS ASS ASS ASS A
SER SER SER SER SER ASN ASN ASN ASN ASN ASN ANG ARG ARG ARG ARG ARG ARG ARG ARG ARG AR
• Molecule 17: Mediator of RNA polymerase II transcription subunit 20
Chain t: 100%
There are no outlier residues recorded for this chain.
• Molecule 18: Mediator of RNA polymerase II transcription subunit 21
Chain u: 84% • 13%
MI 122 123 124 124 125 126 126 126 127 128 128 128 128 128 128 128 128



120 137 1140		
• Molecule 19:	Mediator of RNA polymerase II transcription subu	nit 22
Chain v:	90%	• 9%
M1 D36 D37 E38 G39 S40 F41	N45 VAL VAL THR GLU GLU GLU GLU GLU GLU GLU THR THR THR	
• Molecule 20:	Mediator of RNA polymerase II transcription subu	nit 31
Chain w:	81%	19%
MET SER SER THR ASN ASN ALA ALA ALA	PIAN PRA SER ASP ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	
• Molecule 21:	DNA-directed RNA polymerase II subunit RPB1	
Chain z:	96%	·
P1 821 825		
• Molecule 22:	DNA-directed RNA polymerase II subunit RPB1	
Chain A:	100%	
M1 V2 D156 A190 K330	M420 M421 M471 V1958 N1082 ♦ H1085 ♦ H1085 ♦ H1085 ♦ H11152 ♦ M1191 ♦ M1191 ♦ M1192 ↓ 111224 ♦ M1248 ♦ D1248 ♦ D1248 ♦	
• Molecule 23:	DNA-directed RNA polymerase II subunit RPB2	
Chain B:	96%	·
MET SER SER ALA ALA ALA ASN ASN SER CLU CLYS TYR	ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	R504 D505 D505 D668 ILE GLU GLV GLY CLY CLY CLY CLY CLY CLY VAL
GUU E678 ALA ALA ALA ASN ASN GUU GUU	ASP VAL ASP ASP ASP PRO ALA H733 H733 H733 H733 H733 H733 H733 F1220 F1224 F1224	
• Molecule 24:	DNA-directed RNA polymerase II subunit RPB3	
Chain C:	85%	15%





• Molecule 31: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:	100%
M1 P65 L66 D7 0	
• Molecule 32: DNA-d	irected RNA polymerase II subunit RPB11
Chain K:	97%
M A116 ASP ASP ALA PHE	

• Molecule 33: DNA-directed RNA polymerases I, II, and III subunit RPABC4

		7%										
	Chain L:				61%							39%
1		_						••	••	•	•	
	MET SER ARG GLU GLV PHE CLN	ILE PRO THR	ASP ASP ALA ALA ALA	ALA ALA GLY THR	SER GLN ALA ARG	THR ALA THR	K28	066	гь <i>(</i> Е68	A69	R70	



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1102984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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	Bo	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	М	0.26	0/267	0.47	0/362
2	Р	0.25	0/886	0.47	0/1198
3	Q	0.24	0/1049	0.48	0/1413
4	S	0.25	0/1462	0.48	0/1973
5	a	0.65	0/3067	0.86	4/4148~(0.1%)
6	d	0.27	0/1405	0.58	1/1889~(0.1%)
7	f	0.27	0/1440	0.50	0/1946
8	g	0.28	0/1434	0.50	1/1930~(0.1%)
9	h	0.26	0/1147	0.55	0/1552
10	i	0.26	0/720	0.63	1/965~(0.1%)
11	j	0.24	0/1188	0.45	0/1604
12	k	0.27	0/885	0.49	0/1183
13	n	0.24	0/5226	0.46	0/7051
14	q	0.26	0/4245	0.49	0/5702
15	r	0.26	0/2030	0.50	0/2747
16	s	0.24	0/669	0.43	0/906
17	t	0.26	0/1635	0.50	0/2215
18	u	0.28	0/984	0.58	0/1317
19	V	0.26	0/873	0.51	0/1177
20	W	0.26	0/897	0.42	0/1219
21	Z	0.25	0/194	0.40	0/270
22	А	0.28	0/11632	0.51	0/15735
23	В	0.27	0/9520	0.52	0/12839
24	С	0.27	0/2171	0.50	0/2941
25	D	0.24	0/1365	0.44	0/1831
26	Е	0.26	0/1796	0.49	0/2416
27	F	0.27	0/709	0.50	0/956
28	G	0.26	0/1368	0.49	0/1844
29	Н	0.28	0/1144	0.53	0/1548
30	Ι	0.25	0/961	0.55	0/1294
31	J	0.29	0/587	0.57	0/786
32	K	0.28	0/947	0.51	0/1279
33	L	0.25	0/346	0.61	0/457
All	All	0.29	0/64249	0.53	7/86693~(0.0%)



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	а	349	ARG	NE-CZ-NH1	7.21	123.91	120.30
5	a	67	TYR	CB-CG-CD2	-6.36	117.19	121.00
5	a	189	ARG	NE-CZ-NH1	6.24	123.42	120.30
10	i	73	LEU	CA-CB-CG	5.85	128.76	115.30
5	a	311	ARG	NE-CZ-NH1	5.45	123.03	120.30

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

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	d Allowed Outliers		Percentiles	
1	М	33/345~(10%)	33 (100%)	0	0	100 100	
2	Р	99/735~(14%)	98~(99%)	1 (1%)	0	100 100	
3	Q	121/400~(30%)	121 (100%)	0	0	100 100	
4	S	179/309~(58%)	177 (99%)	2(1%)	0	100 100	
5	a	357/566~(63%)	343 (96%)	11 (3%)	3 (1%)	19 51	
6	d	165/284~(58%)	164 (99%)	1 (1%)	0	100 100	
7	f	163/295~(55%)	161 (99%)	2(1%)	0	100 100	
8	g	159/222~(72%)	159 (100%)	0	0	100 100	
9	h	132/223~(59%)	129 (98%)	3 (2%)	0	100 100	
10	i	79/149~(53%)	79 (100%)	0	0	100 100	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
11	j	142/157~(90%)	137~(96%)	5(4%)	0	100	100
12	k	104/115~(90%)	104 (100%)	0	0	100	100
13	n	611/1082~(56%)	607~(99%)	4 (1%)	0	100	100
14	q	505/687~(74%)	500 (99%)	5 (1%)	0	100	100
15	r	249/307~(81%)	244~(98%)	5 (2%)	0	100	100
16	S	77/220~(35%)	76~(99%)	1 (1%)	0	100	100
17	t	208/210~(99%)	206 (99%)	2(1%)	0	100	100
18	u	116/140~(83%)	115~(99%)	1 (1%)	0	100	100
19	v	105/120~(88%)	105 (100%)	0	0	100	100
20	W	99/127~(78%)	97~(98%)	2(2%)	0	100	100
21	Z	23/25~(92%)	21 (91%)	1 (4%)	1 (4%)	2	16
22	А	1451/1453 (100%)	1407 (97%)	43 (3%)	1 (0%)	51	81
23	В	1164/1224~(95%)	1132 (97%)	32 (3%)	0	100	100
24	С	269/318~(85%)	261~(97%)	8 (3%)	0	100	100
25	D	165/221~(75%)	163 (99%)	2 (1%)	0	100	100
26	Е	213/215~(99%)	210 (99%)	3 (1%)	0	100	100
27	F	84/155~(54%)	83~(99%)	1 (1%)	0	100	100
28	G	169/171~(99%)	166~(98%)	3 (2%)	0	100	100
29	Н	137/146~(94%)	133~(97%)	4 (3%)	0	100	100
30	Ι	114/122~(93%)	113 (99%)	1 (1%)	0	100	100
31	J	68/70~(97%)	65~(96%)	3 (4%)	0	100	100
32	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
33	L	41/70~(59%)	39~(95%)	2(5%)	0	100	100
All	All	7715/11003 (70%)	7560 (98%)	150 (2%)	5 (0%)	54	81

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All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	Z	21	SER
5	a	291	SER
5	a	306	ASN
5	a	289	CYS
22	А	958	VAL



#### 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	Percentile	
1	М	32/299~(11%)	32~(100%)	0	100	100
2	Р	95/641~(15%)	95~(100%)	0	100	100
3	Q	119/363~(33%)	118 (99%)	1 (1%)	81	89
4	S	158/274~(58%)	157 (99%)	1 (1%)	86	91
5	a	350/528~(66%)	347~(99%)	3 (1%)	78	87
6	d	158/258~(61%)	157 (99%)	1 (1%)	86	91
7	f	158/259~(61%)	157 (99%)	1 (1%)	86	91
8	g	160/208~(77%)	159 (99%)	1 (1%)	86	91
9	h	128/207~(62%)	127 (99%)	1 (1%)	81	89
10	i	82/144~(57%)	82 (100%)	0	100	100
11	j	134/145~(92%)	134 (100%)	0	100	100
12	k	101/108 (94%)	101 (100%)	0	100	100
13	n	591/1001~(59%)	588 (100%)	3 (0%)	88	93
14	q	482/642~(75%)	480 (100%)	2 (0%)	91	95
15	r	228/280~(81%)	228 (100%)	0	100	100
16	s	75/195~(38%)	75 (100%)	0	100	100
17	t	178/178~(100%)	178 (100%)	0	100	100
18	u	115/132~(87%)	110 (96%)	5 (4%)	29	59
19	V	101/112 (90%)	100 (99%)	1 (1%)	76	86
20	W	97/117~(83%)	97~(100%)	0	100	100
21	Z	25/25~(100%)	25 (100%)	0	100	100
22	А	1268/1268 (100%)	1265 (100%)	3 (0%)	93	97
23	В	1018/1061 (96%)	1015 (100%)	3 (0%)	92	96
24	С	239/274~(87%)	239 (100%)	0	100	100
25	D	150/200~(75%)	150 (100%)	0	100	100
26	Е	197/197~(100%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	F	76/137~(56%)	76~(100%)	0	100 100
28	G	152/152~(100%)	151~(99%)	1 (1%)	84 90
29	Н	124/128~(97%)	124 (100%)	0	100 100
30	Ι	110/116~(95%)	110 (100%)	0	100 100
31	J	65/65~(100%)	65~(100%)	0	100 100
32	Κ	99/102~(97%)	99~(100%)	0	100 100
33	L	38/57~(67%)	38 (100%)	0	100 100
All	All	7103/9873~(72%)	7076 (100%)	27 (0%)	91 95

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5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	u	1	MET
18	u	120	ARG
23	В	327	ARG
18	u	100	LYS
18	u	137	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such side chains are listed below:

Mol	Chain	Res	Type
22	А	471	ASN
22	А	1211	GLN
28	G	131	GLN
28	G	122	ASN
9	h	150	GLN

#### 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)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	q	1
18	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	С	319:LYS	Ν	5.82
1	u	80:LEU	С	81:PRO	Ν	3.18



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26542. 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: 180



Y Index: 180



Z Index: 180

#### 6.2.2 Raw map



X Index: 180

Y Index: 180

Z Index: 180

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: 166



Y Index: 178



Z Index: 193

#### 6.3.2 Raw map



X Index: 166

Y Index: 178

Z Index: 193

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



#### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.4.2 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.



## 6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

#### $6.5.1 \quad \mathrm{emd}\_26542\_\mathrm{msk}\_1.\mathrm{map}~(\mathrm{i})$





## 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  $1241~\rm{nm^3};$  this corresponds to an approximate mass of 1121 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 0.303  $\text{\AA}^{-1}$ 



## 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 0.303  $\mathrm{\AA^{-1}}$ 



## 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.30	-	-	
Author-provided FSC curve	3.30	3.79	3.34	
Unmasked-calculated*	3.91	4.70	4.00	

\*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 3.91 differs from the reported value 3.3 by more than 10 %



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26542 and PDB model 7UI9. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0125 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 (0.0125).



### 9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.8761	0.2940
А	0.9305	0.3960
В	0.9447	0.3960
С	0.9387	0.4190
D	0.9835	0.1810
E	0.9662	0.3800
F	0.9352	0.4230
G	0.9728	0.2730
Н	0.8944	0.4240
Ι	0.9194	0.3600
J	0.9089	0.3550
K	0.9258	0.4140
L	0.8399	0.3210
М	0.9731	0.4370
Р	0.8707	0.2170
Q	0.7460	0.1730
S	0.8023	0.2400
a	0.7465	0.1030
d	0.8756	0.1560
f	0.7747	0.1640
g	0.7730	0.1470
h	0.9836	0.2170
i	0.8916	0.1800
j	0.1585	0.0540
k	0.9480	0.2530
n	0.8220	0.1790
q	0.9320	0.2370
r	0.9399	0.4050
S	0.0234	0.0530
t	0.9432	0.4020
u	0.6935	0.1490
V	0.9222	0.2140
W	0.9334	0.1760
Z	0.9556	0.1970



