

# wwPDB EM Validation Summary Report (i)

#### Nov 26, 2022 – 02:55 PM EST

PDB ID	:	5SVA
EMDB ID	:	EMD-8305
Title	:	Mediator-RNA Polymerase II Pre-Initiation Complex
Authors	:	Robinson, P.J.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2016-08-05
Resolution	:	15.30  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)
:	2.31.3
	::

# 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 15.30 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)	${f EM} {f structures} \ (\#{f Entries})$
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	Quality of chain		
1	А	1733	70%	12% ·	18%
2	В	1224	83%		11% • 6%
3	С	318	74%	10%	16%
4	D	221	63% 10	6% •	19%
5	Е	215	88%		11%
6	F	155	50% 5%	46%	
7	G	171	<b>•</b> 90%		9% •
8	Н	146	76%	14	% • 9%
9	Ι	122	<b>•</b> 89%		8% •

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Mol	Chain	Length		Qualit	ty of chain		
10	J	70		74%		16	% • 7%
11	Κ	120	•	86%			10% •
12	L	70	46%		20%	3	4%
13	М	295	<b>–</b>		6%	47%	
14	N	223		68%		8%	25%
15	О	115		87%			• 10%
16	Р	687	<b>i</b>	66%		5%	29%
17	Q	307		74%		8%	18%
18	R	210	<b>•</b>	90%			10%
19	$\mathbf{S}$	121		84%			6% 10%
20	Т	284	29%	•	68%	6	
21	U	222		67%		•	30%
22	V	149	49%	)	7% •	43%	
23	W	140		80%		5	% 15%
24	Х	127	•	70%		•	28%
25	Υ	778		68%		•	28%
26	Ζ	843	<b></b>	6	6%	44%	
27	a	513	12%		88%		
28	b	72	33%	86%			• 12%
29	с	345	<b>–</b> 49%	)	6%	45%	
30	d	286	17%	•		59%	
31	е	122	19%	76%		7%	17%
32	f	735	19% •		80%		
33	g	400	40%	·		57%	
34	h	482	• 21% •		76%		

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Mol	Chain	Length	Quality of chain							
35	i	328	28%	8% •	63%					
36	j	240	10%	70%	• 25%					
37	k	25		68%	32%					
38	1	108	10%	57%	43%					
39	m	108	6%	57%	43%					
40	n	244	11%	82%	1	8%				



# 2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 66759 atoms, of which 626 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Λ	1499	Total	С	Ν	Ο	S	0	0
1	Л	1422	11174	7036	1954	2122	62	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	В	1156	Total	C 5791	N 1606	0	S 56	0	0
			9140	5761	1000	1097	00		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	266	Total 2095	C 1317	N 348	0 417	S 13	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total 1434	C 887	N 257	0 288	${S \over 2}$	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	214	Total 1752	C 1111	N 309	0 321	S 11	0	0

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

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
6	F	84	Total 679	C 434	N 115	0 127	${ m S} { m 3}$	0	0



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

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

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

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Н	133	Total 1068	C 673	N 180	0 211	$\frac{S}{4}$	0	0

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

Mol	Chain	Residues		A	toms			AltConf	Trace
9	Ι	119	Total 971	C 596	N 179	0 186	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total 532	C 339	N 93	0 94	S 6	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
11	K	115	Total 920	C 590	N 157	0 171	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	1

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

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
12	L	46	Total 363	С 224	N 72	O 63	$\frac{S}{4}$	0	0

• Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	М	156	Total 777	C 464	N 156	0 156	S 1	0	0

• Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 8.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
14	Ν	168	Total 891	C 542	N 172	O 177	0	0

• Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
15	О	103	Total 511	C 305	N 103	O 103	0	0

• Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues		Ator	AltConf	Trace		
16	Р	487	Total 2421	C 1447	N 487	O 487	0	0

• Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues		At	AltConf	Trace			
17	Q	253	Total 1979	C 1255	N 330	0 384	S 10	0	0

• Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	R	209	Total 1600	C 1011	N 269	0 315	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
19	$\mathbf{S}$	109	Total 544	C 326	N 109	O 109	0	0

• Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	Т	91	Total 756	C 475	N 125	0 154	${ m S} { m 2}$	0	0

• Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 7.



Mol	Chain	Residues		At	oms	AltConf	Trace		
21	U	156	Total 1310	C 847	N 220	O 238	${f S}{5}$	0	0

• Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	V	85	Total 720	C 451	N 133	0 135	S 1	0	0

• Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	W	119	Total 965	C 608	N 160	0 193	S 4	0	0

• Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	Х	92	Total 767	C 506	N 116	0 141	${f S}$ $4$	0	0

• Molecule 25 is a protein called DNA repair helicase RAD3.

Mol	Chain	Residues			AltConf	Trace				
25	Y	562	Total 5175	C 2901	Н 626	N 777	O 838	S 33	0	0

• Molecule 26 is a protein called DNA repair helicase RAD25.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	Z	469	Total 3769	C 2370	N 660	0 716	S 23	0	0

• Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
27	a	62	Total 518	C 334	N 83	O 101	0	0

• Molecule 28 is a protein called RNA polymerase II transcription factor B subunit 5.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
28	b	63	Total	C 216	N oo	0	S 2	0	0
20	U	05	499	316	88	93	2	0	

• Molecule 29 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
29	С	189	Total 1357	C 838	N 240	O 267	S 12	0	0

• Molecule 30 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace	
30	d	116	Total 956	C 599	N 159	0 195	${ m S} { m 3}$	0	0

• Molecule 31 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
31	е	101	Total 792	C 500	N 132	0 156	${S \atop 4}$	0	0

• Molecule 32 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	149	Total 1243	C 788	N 222	O 229	$\frac{S}{4}$	0	0

• Molecule 33 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	172	Total 1443	C 922	N 248	O 267	S 6	0	0

• Molecule 34 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace	
34	h	118	Total 960	C 625	N 158	0 172	${f S}{5}$	0	0

• Molecule 35 is a protein called Transcription initiation factor IIE subunit beta.



Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	120	Total 987	C 636	N 161	O 187	${ m S} { m 3}$	0	0

• Molecule 36 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace	
36	j	180	Total 1416	C 921	N 242	0 247	S 6	0	0

• Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	25	Total 184	C 116	N 25	O 43	0	0

• Molecule 38 is a DNA chain called 108bp HIS4 Promoter Non-template Strand (-92/+16).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	62	Total 1271	C 609	N 222	0 378	Р 62	0	0

• Molecule 39 is a DNA chain called 108bp HIS4 Promoter Template Strand (+16/-92).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	62	Total 1271	$\begin{array}{c} \mathrm{C} \\ 607 \end{array}$	N 236	O 366	Р 62	0	0

• Molecule 40 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms	AltConf	Trace
40	n	200	Total         C           200         200	0	200

• Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
41	А	2	Total Zn 2 2	0
41	В	1	Total Zn 1 1	0
41	С	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
41	Ι	2	Total Zn 2 2	0
41	J	1	Total Zn 1 1	0
41	L	1	Total Zn 1 1	0

• Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
42	А	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: DNA-directed RNA polymerase II subunit RPB1





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• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4





GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	SER ASP SER SER ASP GLY HIS ASP CLY CLYS LYS	ASP THR ASP GLY ASP GLU CALU CALU CLU GLY GLY	ASP PHE MET GLU VAL ASP GLU ASP ASP ASP	PRD VAL ASP ASR ASR GLU THR HIS LYS
THR 1182 8192 8231 8233 8233	AJA V248 P251 S252 S315 S18 S18 ASR ASR ASR ASR ASV V331	E342 E342 K349 F369 F370 F368 S58 S58 S58 S58 S58 S58 S58 S58 S58 S5	LTR LTR <b>G378</b> F331 F331 R392 R392 R420 A420	L452 V457 N471 E472 E477 L476 E477 V487
L493 P494 N532 D536 P544	F551 S574 F585 F585 F585 F515 F619 F619 F626	K627 P638 E654 A655 F669 F660	THK THR PHE SER ASP PHE LYS CLU CLU V670 V687	
• Molecule 17: ]	Mediator of RNA	polymerase II tr	anscription subu	mit 18
Chain Q:		74%	8%	18%
MET V2 E50 R55 R55 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C	M01 M01 D82 M86 F87 F87 F87 B86 D96 M101	108 1109 1109 ASN ASN THR VAL VAL VAL ASN ASN ASN	SER THR ASN GLU GLU ASP ASN ASN ASN SER LYS HIS	GLU ASP THR VAL ASN GLU SER ASR ASR ASP ASP
ASP TLE TLE ASP ASP ASP ASP ASP ALA SER PRO	PR0 SER 8158 8158 8158 8177 8177 8177 8177 8180 1217	1246 8260 8261 8261 1268 1268 1268 1275 1275 1275 1275 1275 1275 1275 1275	R299 V300 A301 A301 A301 A301 CLY LLEU LLEU LLEU	
• Molecule 18: 1	Mediator of RNA	polymerase II tr	anscription subu	unit 20
Chain R:		90%		10%
MET G2 M26 W35 W48 L49 P50	B52 L56 H64 K67 W116 L121	L135 1153 1153 1153 1158 1158 1187 1187 1189	D192 1193 1193 1200 1204 1210	
• Molecule 19: 1	Mediator of RNA	polymerase II tr	anscription subu	mit 22
Chain S:		84%	69	% 10%
M1 V19 D32 D32 V58 V58	ILE ILE PRO VAL THR GLU GLU CVS CVAL THR THR ARG F99	D100 E101 1102 1104 1121		
• Molecule 20: 1	Mediator of RNA	polymerase II tr	anscription subu	mit 4
Chain T:	29% •		68%	
MET SER VAL GLN GLN ASP ASP ALA ALA VAL ALA CLU SPHE SFR	MET GLY HIS GLY HIS AIG SER SER SER SER SER SER VAL VAL	ALA CLU THR ALA SER ASN ASN SER CLU ASP LT	K55 Y94 K99 K102 L115	N119 E120 E124 A127 LEU MET LEU GLU
GLN VAL GLU GLU FHE CYS ASN THR THR ILEU GLN GLN	ARG SER LYS LYS TLE ASN SER CLU CLU LEU LEU LEU LEU TYR	ALA LYS LEU SER LEU SER PHE THR LYS THR PRO PRO	PHE ASP LYS GLY GLY GLY PRO ASN ASN PRO THE	TRP PRO GLU GLU ASP ASP ASP ASP ASC GLY MET
LEU ALA MET ALA ALA SER LEU LEU CLU CLU LEU	ARC ARC PRO PRO GLU GLU GLU GLU GLU CLU VAL VAL	PRO THR VAL PRO PRO SER GLN GLU GLU CJ.N CJ.N	GLN MET ALA ALA LYS LYS CLV GLY THR PRO LYS THR TASP	SER PHE TILE PHE ASP ASP ALY ALA CTU VAL
GLY ASP GLU GLU ASP ASP LYS ASP LYS CYU GLU	GLU GLU ASN ASP ASP ALA ALA ASP ALA LEU ASP LEU ASP LEU LEU	ASP LEU ASP ASP ASP PHE PHE		

• Molecule 21: Mediator of RNA polymerase II transcription subunit 7















• Molecule 33: Transcription initiation factor IIF subunit beta







LYS SER ASP ASP <b>3126</b> 5126 5126 1135 1135 K127 K137 K140	D149 N154 N159 N159 N160 L163 L163 L163 L163 L165 N165 L165 L166 D167 D167	PR0 LYS LYS LYS C176 C176 C204 C204 C204 C204 C204 C205 C206 C206 C206 C206 C206 C206 C206 C206	D238 LYS THR PRO
R342 ASN ASN LEU LEU CYS CYS CYS CYS CYS CYS CYS CYS CYS LVX LVX LVX LVX	MET RTRP GLU ASN ASN CLEU FRO GLU FRO GLU ARG LTS LTS	LEU ASP CLEV CLEV CLEV CLEV CLEV CLEV CLEV ASER ASER ASER ASER ASE ASE ASE CLN CLES CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	LTS LYS ARG GLN
ARG LYS GLY LYS CLYS LYS THR ASN ASN HIS MET HIS CLFU LEU	LYS ASP TYR SER HIS ARG VAL		
• Molecule 36: TA	TA-box-binding protein	n	
Chain j:	70%	• 25%	
MET ALA ALA ALA GLU GLU CLYS GLU PHE CLYS GLU ALA ALA	LYS TLE TLE VAL VAL ASP ASP ASN ASN GLN GLU ASN	ARG ASP GLY GLY PRO PRO PRO PRO CLU ASP ALA ASP ALA ALA ALA ALA ALA CLU SER SER CLU SER CLU SER CLU SER CLU	ASF THR SER ALA THR
861 662 663 668 768 768 187 8107 ₹100 7109	R141 E129 K145 K151 D154 D154 V166 K107	F168 F169 F171 R171 R171 R220 C210 C223	
• Molecule 37: DN	A-directed RNA polyr	merase II subunit RPB1	
Chain k:	68%	32%	
P1 84 89 814 815 815 815 815 815 821 821 821	8 8		
• Molecule 38: 108	bp HIS4 Promoter No	on-template Strand (-92/+16)	
Chain l:	57%	43%	
DA DA DA DA DA DA DA DA DA	DD DD DD DD DD DD DD DD DD DD DD DD DD	Tts Tts Tts A67 A67 A67 A67 A69 D1 D1 D1 D1 D1 D1 D1 D1 D1 D1	DA DD DD DC DC DC
DT			
• Molecule 39: 108	bp HIS4 Promoter Ter	mplate Strand $(+16/-92)$	
Chain m:	57%	43%	I
DA DC DC DC DC DC DC DC DC DC DC DC DC DC	Ad DA DA DA DA DA DA DA DA DA DA DA DA DA	6120 6120 A129 0131 0131 0131 0130 0131 0131 0131 013	DT DT DT
• Molecule 40: Tra	nscription initiation fa	actor TFIID subunit 14	
Chain n:	82%	18%	
M1 T13 Q14 Q15 H16 117 P47 P47	F107 F107 L108 E110 S111 Y112 T137 GLU GLU GLU GLU GLU ASN	THR THR THR THR THR GLY GLY CLYS THR THR THR THR THR THR ARG THR ARG CLU CLY CLU CLY CLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	SER ALA SER THR VAL CYS GLY SER VAL
		WORLDWIDE PROTEIN DATA BANK	





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	15	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	503.8, 503.8, 503.8	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.29, 2.29, 2.29	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: MG, ZN

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.51	1/11374~(0.0%)	0.79	5/15384~(0.0%)	
2	В	0.48	0/9317	0.74	4/12567~(0.0%)	
3	С	0.49	0/2133	0.78	2/2891~(0.1%)	
4	D	0.51	0/1444	0.83	2/1935~(0.1%)	
5	Е	0.48	0/1788	0.72	0/2406	
6	F	0.58	0/691	0.79	0/933	
7	G	0.51	0/1368	0.81	0/1844	
8	Н	0.51	0/1086	0.80	0/1470	
9	Ι	0.47	0/989	0.78	0/1331	
10	J	0.54	0/541	0.88	1/727~(0.1%)	
11	Κ	0.48	0/938	0.71	0/1267	
12	L	0.54	0/365	0.79	0/485	
13	М	0.61	0/775	0.83	0/1077	
14	Ν	0.53	0/893	0.76	0/1237	
15	0	0.52	0/509	0.67	0/707	
16	Р	0.58	0/2417	0.79	2/3369~(0.1%)	
17	Q	0.56	0/2014	0.75	0/2728	
18	R	0.50	2/1626~(0.1%)	0.66	0/2205	
19	S	0.57	0/542	0.73	0/755	
20	Т	0.69	0/763	1.10	2/1025~(0.2%)	
21	U	0.43	0/1339	0.60	0/1808	
22	V	0.73	0/732	1.01	4/984~(0.4%)	
23	W	0.47	0/973	0.64	0/1308	
24	Х	0.39	0/789	0.53	0/1077	
25	Y	0.55	2/4616~(0.0%)	0.79	13/6196~(0.2%)	
26	Z	0.78	0/3837	0.98	8/5177~(0.2%)	
27	a	0.67	0/527	0.68	0/704	
28	b	0.60	0/504	0.69	1/679~(0.1%)	
29	с	0.29	0/1373	0.47	0/1863	
30	d	0.40	0/970	0.57	0/1310	
31	е	0.42	0/800	0.63	0/1080	
32	f	0.33	0/1267	0.82	9/1700~(0.5%)	



Mal	Chain	Bond lengths		Bond angles		
1VIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	g	0.66	0/1469	0.73	3/1972~(0.2%)	
34	h	0.96	0/978	1.11	1/1321~(0.1%)	
35	i	0.37	0/1003	0.61	0/1345	
36	j	0.41	0/1443	0.62	0/1942	
37	k	0.77	0/194	0.69	0/270	
38	1	0.43	0/1423	0.89	0/2195	
39	m	0.47	0/1427	0.89	0/2199	
All	All	0.54	5/67237~(0.0%)	0.78	57/91473~(0.1%)	

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
2	В	0	1
13	М	0	2
16	Р	0	3
17	Q	0	1
25	Y	0	1
26	Ζ	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	1394	THR	C-N	-6.29	1.21	1.33
25	Y	172	PRO	N-CD	5.61	1.55	1.47
25	Y	19	PRO	N-CD	5.51	1.55	1.47
18	R	35	TRP	CD2-CE2	5.06	1.47	1.41
18	R	116	TRP	CD2-CE2	5.04	1.47	1.41

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
25	Y	493	LEU	C-N-CD	-13.71	90.45	120.60
25	Y	533	THR	C-N-CD	-13.65	90.57	120.60
32	f	135	LEU	C-N-CD	-11.09	96.21	120.60
26	Ζ	505	ILE	CB-CA-C	-9.99	91.62	111.60
25	Y	433	PRO	CA-N-CD	-9.03	98.86	111.50

There are no chirality outliers.



Mol	Chain	Res	Type	Group
2	В	43	LEU	Mainchain
13	М	10	GLN	Peptide
13	М	138	GLY	Peptide
16	Р	471	ASN	Peptide
16	Р	532	ASN	Peptide

5 of 9 planarity outliers are listed below:

#### 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	P	erce	entiles
1	А	1414/1733~(82%)	1254 (89%)	112 (8%)	48 (3%)		3	26
2	В	1142/1224~(93%)	1022 (90%)	84 (7%)	36 (3%)		4	26
3	С	264/318~(83%)	242 (92%)	20 (8%)	2(1%)		19	60
4	D	174/221~(79%)	149 (86%)	17 (10%)	8 (5%)		2	21
5	Е	212/215~(99%)	195~(92%)	13~(6%)	4 (2%)		8	38
6	F	82/155~(53%)	75~(92%)	7 (8%)	0	1	L00	100
7	G	169/171~(99%)	157~(93%)	9~(5%)	3 (2%)		8	40
8	Н	129/146~(88%)	106 (82%)	14 (11%)	9~(7%)		1	14
9	Ι	117/122~(96%)	98 (84%)	16 (14%)	3(3%)		5	31
10	J	63/70~(90%)	51 (81%)	9 (14%)	3(5%)		2	21
11	K	113/120~(94%)	109 (96%)	4 (4%)	0	1	L00	100
12	L	44/70~(63%)	19~(43%)	14 (32%)	11 (25%)		0	1
13	М	152/295~(52%)	115 (76%)	20 (13%)	17 (11%)		0	7
14	N	164/223~(74%)	133 (81%)	16 (10%)	15 (9%)		1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
15	Ο	99/115~(86%)	92~(93%)	4 (4%)	3~(3%)	4	28
16	Р	479/687~(70%)	385~(80%)	61 (13%)	33~(7%)	1	15
17	$\mathbf{Q}$	249/307~(81%)	217 (87%)	25~(10%)	7 (3%)	5	30
18	R	207/210~(99%)	190~(92%)	12~(6%)	5 (2%)	6	33
19	S	105/121~(87%)	91~(87%)	7 (7%)	7 (7%)	1	15
20	Т	89/284~(31%)	69~(78%)	20 (22%)	0	100	100
21	U	150/222~(68%)	127 (85%)	22 (15%)	1 (1%)	22	63
22	V	83/149~(56%)	73~(88%)	5 (6%)	5 (6%)	1	17
23	W	115/140~(82%)	95~(83%)	18 (16%)	2 (2%)	9	42
24	Х	90/127~(71%)	86~(96%)	4 (4%)	0	100	100
25	Y	534/778~(69%)	503 (94%)	23 (4%)	8 (2%)	10	46
26	Ζ	461/843~(55%)	430 (93%)	26~(6%)	5 (1%)	14	52
27	a	60/513~(12%)	60 (100%)	0	0	100	100
28	b	61/72~(85%)	58~(95%)	3~(5%)	0	100	100
29	с	185/345~(54%)	164 (89%)	19 (10%)	2 (1%)	14	52
30	d	110/286~(38%)	103 (94%)	7 (6%)	0	100	100
31	е	97/122~(80%)	93~(96%)	4 (4%)	0	100	100
32	f	143/735~(20%)	130 (91%)	9 (6%)	4 (3%)	5	30
33	g	164/400~(41%)	148 (90%)	12 (7%)	4 (2%)	6	33
34	h	112/482~(23%)	100 (89%)	10 (9%)	2(2%)	8	40
35	i	114/328~(35%)	102 (90%)	9 (8%)	3 (3%)	5	31
36	j	178/240~(74%)	170 (96%)	5 (3%)	3 (2%)	9	42
37	k	23/25~(92%)	9~(39%)	6 (26%)	8 (35%)	0	0
All	All	8147/12614 (65%)	7220 (89%)	666 (8%)	261 (3%)	7	26

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 $5~{\rm of}~261$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	74	MET
1	А	189	ARG
1	А	195	ASP
1	А	286	HIS
1	А	317	LYS



#### 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	Percentiles	
1	А	1240/1520~(82%)	1071~(86%)	169 (14%)	3	17
2	В	985/1061~(93%)	868~(88%)	117~(12%)	5	20
3	С	234/274~(85%)	206~(88%)	28 (12%)	5	20
4	D	160/200~(80%)	129 (81%)	31 (19%)	1	8
5	Е	196/197~(100%)	175 (89%)	21 (11%)	6	23
6	F	74/137~(54%)	67~(90%)	7 (10%)	8	27
7	G	152/152~(100%)	137~(90%)	15 (10%)	8	26
8	Н	117/128~(91%)	103 (88%)	14 (12%)	5	20
9	Ι	113/116~(97%)	106 (94%)	7~(6%)	18	43
10	J	60/65~(92%)	49 (82%)	11 (18%)	1	10
11	К	99/102~(97%)	87~(88%)	12 (12%)	5	20
12	L	40/57~(70%)	37~(92%)	3 (8%)	13	38
13	М	1/259~(0%)	1 (100%)	0	100	100
14	Ν	16/207~(8%)	14 (88%)	2 (12%)	4	19
17	Q	226/280~(81%)	206 (91%)	20 (9%)	10	31
18	R	177/178~(99%)	162 (92%)	15 (8%)	10	33
20	Т	87/258~(34%)	81 (93%)	6 (7%)	15	40
21	U	149/208~(72%)	142 (95%)	7(5%)	26	51
22	V	84/144~(58%)	80~(95%)	4 (5%)	25	51
23	W	113/132~(86%)	108 (96%)	5 (4%)	28	53
24	Х	87/117~(74%)	84 (97%)	3~(3%)	37	60
25	Y	512/707~(72%)	504 (98%)	8 (2%)	62	79
26	Ζ	412/737~(56%)	375 (91%)	37 (9%)	9	30
27	a	57/468~(12%)	57 (100%)	0	100	100
28	b	57/66~(86%)	57 (100%)	0	100	100
29	с	136/299~(46%)	118 (87%)	18 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
30	d	107/260~(41%)	104~(97%)	3~(3%)	43	65
31	е	91/108~(84%)	83~(91%)	8 (9%)	10	31
32	f	136/641~(21%)	135~(99%)	1 (1%)	84	90
33	g	162/363~(45%)	157~(97%)	5(3%)	40	62
34	h	108/429~(25%)	91~(84%)	17~(16%)	2	14
35	i	113/295~(38%)	86~(76%)	27 (24%)	0	4
36	j	152/205~(74%)	143~(94%)	9~(6%)	19	45
37	k	25/25~(100%)	25 (100%)	0	100	100
All	All	6478/10395~(62%)	5848 (90%)	630 (10%)	12	27

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 $5~{\rm of}~630$  residues with a non-rotameric side chain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
18	R	153	ILE
33	g	127	LYS
20	Т	120	GLU
18	R	121	LEU
26	Ζ	628	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
25	Y	138	ASN
36	j	88	HIS
26	Ζ	447	GLN
36	j	68	GLN
33	g	98	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 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-8305. 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.

#### Orthogonal projections (i) 6.1

#### 6.1.1**Primary** map



Х

![](_page_31_Picture_11.jpeg)

Ζ

6.1.2Raw map

![](_page_31_Picture_14.jpeg)

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

![](_page_31_Picture_16.jpeg)

#### 6.2 Central slices (i)

#### 6.2.1 Primary map

![](_page_32_Picture_5.jpeg)

X Index: 110

![](_page_32_Picture_7.jpeg)

Y Index: 110

![](_page_32_Picture_9.jpeg)

Z Index: 110

#### 6.2.2 Raw map

![](_page_32_Picture_12.jpeg)

X Index: 110

Y Index: 110

Z Index: 110

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

![](_page_32_Picture_17.jpeg)

#### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map

![](_page_33_Picture_5.jpeg)

X Index: 90

![](_page_33_Picture_7.jpeg)

Y Index: 86

![](_page_33_Picture_9.jpeg)

Z Index: 103

#### 6.3.2 Raw map

![](_page_33_Picture_12.jpeg)

X Index: 90

Y Index: 86

Z Index: 103

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

![](_page_33_Picture_17.jpeg)

#### 6.4 Orthogonal surface views (i)

6.4.1 Primary map

![](_page_34_Picture_5.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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

![](_page_34_Picture_8.jpeg)

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.

![](_page_34_Picture_10.jpeg)

#### Mask visualisation (i) 6.5

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

#### $emd_{8305}msk_{1.map}$ (i) 6.5.1

![](_page_35_Picture_9.jpeg)

![](_page_35_Picture_11.jpeg)

# 7 Map analysis (i)

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

### 7.1 Map-value distribution (i)

![](_page_36_Figure_6.jpeg)

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.

![](_page_36_Picture_8.jpeg)

#### 7.2 Volume estimate (i)

![](_page_37_Figure_4.jpeg)

The volume at the recommended contour level is 3796  $\rm nm^3;$  this corresponds to an approximate mass of 3429 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.

![](_page_37_Picture_7.jpeg)

### 7.3 Rotationally averaged power spectrum (i)

![](_page_38_Figure_4.jpeg)

\*Reported resolution corresponds to spatial frequency of 0.065  ${\rm \AA^{-1}}$ 

![](_page_38_Picture_6.jpeg)

# 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)

![](_page_39_Figure_6.jpeg)

\*Reported resolution corresponds to spatial frequency of 0.065  $\mathrm{\AA^{-1}}$ 

![](_page_39_Picture_8.jpeg)

# 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	15.30	-	-	
Author-provided FSC curve	15.27	17.24	15.97	
Unmasked-calculated*	15.70	17.27	16.05	

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

![](_page_40_Picture_6.jpeg)

# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8305 and PDB model 5SVA. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay (i)

![](_page_41_Picture_6.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

![](_page_41_Picture_8.jpeg)

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

![](_page_42_Figure_4.jpeg)

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)

![](_page_42_Figure_7.jpeg)

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 (0.025).

![](_page_42_Picture_9.jpeg)

#### 9.4 Atom inclusion (i)

![](_page_43_Figure_4.jpeg)

At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

![](_page_43_Picture_6.jpeg)

1.0

0.0 <0.0

#### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9567	0.0490
А	0.9933	0.0610
В	0.9962	0.0400
С	0.9898	0.0500
D	0.9780	0.0630
E	0.9930	0.0720
F	0.9970	0.0640
G	0.9758	0.0570
Н	0.9510	0.0380
Ι	0.9440	0.0490
J	1.0000	0.0810
K	0.9746	0.0720
L	1.0000	0.0570
М	0.9665	0.0290
N	0.9989	0.0450
0	1.0000	0.0700
Р	0.9851	0.0610
Q	0.9923	0.0460
R	0.9810	0.0630
S	1.0000	0.0330
Т	0.9798	0.0460
U	0.9961	0.0700
V	0.9772	0.1040
W	0.9958	0.0940
X	0.9854	0.0070
Y	0.9923	0.0450
Z	0.9340	0.0360
a	0.6090	-0.0120
b	0.6037	0.0000
С	0.9679	0.0260
d	0.5480	0.0070
e	0.7375	0.0220
f	0.9133	0.0170
g	0.9823	0.0240
h	0.9606	0.0620

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![](_page_44_Picture_7.jpeg)

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Chain	Atom inclusion	Q-score
i	1.0000	0.0750
j	0.8256	0.0390
k	1.0000	-0.0140
1	0.7679	0.0630
m	0.8253	0.0540
n	0.8600	0.0390

![](_page_45_Picture_5.jpeg)