

wwPDB EM Validation Summary Report (i)

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PDB ID	:	80EU
EMDB ID	:	EMD-16835
Title	:	Structure of the mammalian Pol II-SPT6 complex (composite structure, Struc-
		ture 4)
Authors	:	Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.
Deposited on	:	2023-03-13
Resolution	:	3.04 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.dev70
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36
	: : : : :

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 3.04 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ 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 $\leq=5\%$ 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	Qualit	ty of chain	
1	А	1970	6 1%	10%	28%
2	В	1251	• 74%	16% 10%	
3	С	275	75%		19% 6%
4	D	184	47%	17%	36%
5	Е	210	83%		16%
6	F	127	- 57%	5%	39%
7	G	172	74%		24% •••



Mol	Chain	Length		Quality of c	hain					
8	Н	150		89%		10% •				
9	Ι	125	<u></u>	80%						
10	J	67	•	87%		12% •				
11	Κ	117		86%						
12	L	58	• 67	%	9%	24%				
13	Ν	48	15%	15%	46%					
14	Р	46	7%		72%					
15	Т	48	17%		23%	21%				
16	S	1729	37%	10%	53%					

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2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 39178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues		A	AltConf	Trace			
1	Λ	1400	Total	С	Ν	Ο	\mathbf{S}	0	0
	Л	1409	11159	7024	2000	2064	71	U	0

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

Mol	Chain	Residues		Α	AltConf	Trace			
2	В	1131	Total 9047	C 5721	N 1592	O 1670	S 64	0	0

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	118	Total 967	C 608	N 167	0 188	${S \atop 4}$	0	0

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

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

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

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
6	F	78	Total 626	C 401	N 106	0 114	${S \atop 5}$	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 1347	C 872	N 218	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	Atoms			AltConf	Trace		
8	Н	148	Total 1186	C 750	N 194	0 237	${S \atop 5}$	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	Ι	116	Total 932	C 577	N 165	0 179	S 11	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	66	Total 524	C 330	N 88	O 01	S 6	0	0
			024	000	00	51	0		

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
11	K	115	Total 920	C 593	N 152	0 173	${S \over 2}$	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace		
12	L	44	Total 367	C 228	N 69	O 64	S 6	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
13	Ν	26	Total 549	C 255	N 117	0 151	Р 26	0	0

• Molecule 14 is a RNA chain called RNA.



Mol	Chain	Residues		Atoms					Trace
14	Р	13	Total 280	C 125	N 54	O 88	Р 13	0	0

• Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Т	38	Total 769	C 365	N 130	O 236	Р 38	0	0

• Molecule 16 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms				AltConf	Trace	
16	S	819	Total 6703	C 4260	N 1164	0 1246	S 33	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

• Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
17	А	1	Total Mg 1 1	0

• Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
18	А	2	Total Zn 2 2	0
18	В	1	Total Zn 1 1	0
18	С	1	Total Zn 1 1	0
18	Ι	2	Total Zn 2 2	0
18	J	1	Total Zn 1 1	0



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Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total Zn 1 1	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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











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



1134 113 1137 115 1145 114 1147 115 1147 115 1147 115 1157 113 1157 113 1157 113 1157 113 1157 113 1157 113 1157 113 1157 113 1151 134 1151 134 1151 136 1151 136 1151 151 151 154 151 154 151 154 151 154 151 154 151 154 153 154 154 154 155 155 156 156 156 156 157 157 157 1101 157 1101 157 1101 157 1130 156 1130 156 1130 156 1130 156 1130 156 1130 156 1130

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

Chain H:	89%		10%	·		
MET A2 K20 K21 F22 F22 R24 140 147	R84 R84 R84 V96 V115 M123 M123 M123 P116 P116 P116 P116					
• Molecule 9: D	• Molecule 9: DNA-directed RNA polymerase II subunit RPB9					
Chain I:	80%	13%	7%			



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:		86%		12% •
M1 L12 L12 L44 L44 L42 C43 C43 C43 C43 C43 C43 C43 C43 C43 C43	F58 Y61 K62 K62 E68 I 72 L100 L101	G115 ILE GLU		
• Molecule 12: RNA	A polymerase II	subunit K		
Chain L:	67%		9%	24%
MET ASP THR CLYS CLN VAL PRO PRO CLN CLN CLN CLN CLN	118 118 118 118 118 118 118 118 118 118	88		
• Molecule 13: Non-	-template DNA			
Chain N:	40%	15%	46%	
DC DC DT DT DT DC DC DC DC C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	20 20 20 20 20 20 20 20 20 20 20 20 20 2	UA 026 031 033 033 033 033 033 036 036		
		WORLE	DW IDE	

PDB

• Molecule 14:	RNA				
Chain P:	22%	7%		72%	
			•	**	
U D A A Q Q A A D D A A	A Q D Q Q D Q	C P P C C C C C C	A G G C C A A A C C C A A A C C C C A A A C C C C A A A C C C A A A C C C A A A C C C A A A C C C A A A C C C C A A A C C C C A A A C C C C A A A C C C C A A A C C C C A A A C C C C C A A A C C C C C A A A C C C C C A A A C C C C C A A A C C C C C A A A C C C C C A A A C C C C C A A A C C C C C C A A A C C C C C C A A A C C C C C C A A A C C C C C C A A A C C C C C C A A A C C C C C C C A A C C C C C C C C C A A C C C C C C C A A C C C C C C C C C A A C	A35 G36 G37 U46	
• Molecule 15:	Template	e DNA			
Chain T:	7%	56%		23%	21%
DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD	C22 C23 G24 T27 T34	C35 C37 C37 C37 C37 C39 C39 C39 C39 C39	C41 C41 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5		
• Molecule 16:	Transcrip	otion elong	ation factor	SPT6	
Chain S:	37%		10%	53%	
SER ASN ALA ALA MET SER PHE VAL CLU SER GLU	ALA GLU GLU GLU GLU GLU	TYR ASN ASP GLU GLV GLV VAL VAL	PRO ARG VAL THR LYS LYS PHE VAL	GLU GLU GLU GLU GLU GLU GLU GLU GLU	GLU GLU ASN ASP ASP GLN GLN GLN GLN CLU CLU GLY GLY GLY GLY GLY
ILE ASN ASP ASP ASP ASP GLU GLU GLU	GLU ASP GLU GLY SER ASP SER	GLY ASP SER GLU ASP ASP VAL CLY	HIS LYS LYS ARG LYS ARG THR SER	PHE ASP ASP ARG LEU GLU ASP ASP ASP PHE	LEU LEU GLU GLU GLU GLU GLU CLY VAL LYS CLY GLY GLY GLY
TYR ARG ARG VAL LYS LYS NET ASP ASP ASP CLU	ASP ASP ASP GLU GLU TYR	CLY CLU CLU CLU CLU CLU CLU CLU CLU	ALA ILE ALA GLU GLU PHE FHE GLN	ASP GLY GLU GLU GLU GLU GLU ALA	ALU ALA ALA ALA ALA ALA ALA ALU GLU GLU GLU GLU GLU GLU
GLU SER ASP TLE ASP ASP PHE TLE VAL ASP ASP	ASP GLY GLN PRO LEU LYS LYS	PRO LYS ARG LYS LYS LYS LEU PRO	GLY TYR ASP ALA ALA LEU GLN	GLU ALA GLN GLN GLN TLE PHE ASP PHE	TYR TYR ASP ASP ASP CLU TYR ASN TYR ASN CLU CLU CLU CLU CLU CLU CLU CLU
GLU GLU TYR GLU TYR GLU ALP ALP GLU	GLY GLU ILE ARG ARG ARG PRO	LYS LYS LYS THR LYS LYS ARG VAL	SER ARG SER TLE PHE GLU MET	TYR GLU PRO SER GLU LLU LLU CLU SER SER HIS	148.0 148.0 1284 13302 13303 13303 13303 13303 13303 13303 13303 133113 133111 133111 133111 133111 133111 133111 133111 133111 133111 133111 13
W319 R322 1329 1330 1333 1333 1333 1333 1333 1333 133	CYS ASP TYR LEU ASP ARG GLY	GLN PRO ALA SER SER PHE SER SER	LYS LYS GLY P353 P355 M365 R367 N368	4369 4370 7371 8372 7373 7374 7374 7378 7379	Contemporation Contem
0421 0427 1LE 1LE SER ALA ASP ASP ASP LYS PRO	LEU ALA ASP GLY TLE R441 A442	L443 D444 E445 E449 V454 0455	L460 R473 D474 K477	N480 ALA ALA LYS LYS ALA SER ARG LYS LYS LEU	ARG ARG ARG ARG ARG ALU ALU ALU ALU ALU ALU ALA ALA
GLU ASP ASP GLU GLU GLU FRU GLU FRU GLU FRU GLU	R520 M523 I526	L550 R551 D552 R556 V574	P581 R589 A597 (604 V605	Q608 1618 P644 E647 L658	L665 D668 K674 CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
F686 E687 K690 R695 N706 R707 Q708	1713 E714 L721 1742	K748 N751 W752 L753 R754 V755	R759 PR0 ASP GLN GLN GLU GLU	ASP ASP ASP ASP ASP PHE ASP GIU ASP ASN ASN ASV	LIVE LIVE SYB7 SYB7 SYB7 C796 C796 N800 B804 E804 L809
P812 PHE LYS LYS ARG ARG ALA ALA TRP	ARG GLU E824 L836 E853	A857 Q858 1861 E862 D863 V864	K865 R866 1867 886 8870 LEU ASP	GLN GLN GLN GLN GLN SER SER SER SER SER	903 903 1887 1887 1889 1889 1889 1889 1889 1890 1903 1915 1915 1915 1915 1916 1916 1916
R918 R919 1920 1921 1922 P923 1923 1925 1925 1926	L938 C939 L940 K941 F942 L954	L955 1963 N967 P980	0983 0984 1985 1985 0989 0991 1992	697 11004 N1008 N1018 N1014	11019 11019 11025 11026 11026 11027 11026 11033 1031 1033 1033 1033 1036 1103 1103
			PROTI	PDB EIN DATA BANK	





4 Experimental information (i)

Property	Value	Source		
EM reconstruction method	SINGLE PARTICLE	Depositor		
Imposed symmetry	POINT, Not provided			
Number of particles used	174029	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 $(e^-/\text{\AA}^2)$	40.09	Depositor		
Minimum defocus (nm)	350	Depositor		
Maximum defocus (nm)	7500	Depositor		
Magnification	Not provided			
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor		
Maximum map value	59.731	Depositor		
Minimum map value	-28.119	Depositor		
Average map value	0.011	Depositor		
Map value standard deviation	1.105	Depositor		
Recommended contour level	3.5	Depositor		
Map size (Å)	461.99997, 461.99997, 461.99997			
Map dimensions	440, 440, 440	wwPDB		
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB		
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor		



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.32	0/11360	0.52	2/15328~(0.0%)	
2	В	0.35	0/9227	0.53	2/12454~(0.0%)	
3	С	0.36	0/2115	0.49	0/2873	
4	D	0.36	0/979	0.71	1/1312~(0.1%)	
5	Е	0.32	0/1752	0.52	0/2366	
6	F	0.35	0/636	0.55	0/859	
7	G	0.46	0/1378	0.67	1/1870~(0.1%)	
8	Н	0.33	0/1207	0.52	0/1628	
9	Ι	0.32	0/954	0.54	0/1293	
10	J	0.36	0/533	0.51	0/719	
11	K	0.33	0/939	0.54	1/1271~(0.1%)	
12	L	0.35	0/372	0.57	0/493	
13	N	0.50	0/619	0.74	0/954	
14	Р	0.33	0/313	0.79	0/486	
15	Т	0.57	0/857	0.95	0/1319	
16	S	0.36	0/6826	0.57	0/9194	
All	All	0.35	0/40067	0.56	7/54419~(0.0%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	2
7	G	0	1
16	S	0	1
All	All	0	4

There are no bond length outliers.



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	483	ARG	CG-CD-NE	7.76	128.09	111.80
1	А	883	ILE	CG1-CB-CG2	-6.33	97.47	111.40
11	Κ	53	ASP	CB-CG-OD1	5.66	123.40	118.30
2	В	141	PRO	CA-N-CD	-5.16	104.28	111.50
4	D	130	LEU	CB-CG-CD1	5.11	119.69	111.00

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

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	538	VAL	Peptide
1	А	539	GLN	Peptide
7	G	124	ASN	Peptide
16	S	1156	GLU	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	А	11159	0	11304	130	0
2	В	9047	0	9080	126	0
3	С	2072	0	2019	36	0
4	D	967	0	973	19	0
5	Е	1721	0	1737	23	0
6	F	626	0	657	5	0
7	G	1347	0	1347	29	0
8	Н	1186	0	1147	10	0
9	Ι	932	0	856	14	0
10	J	524	0	540	7	0
11	K	920	0	942	9	0
12	L	367	0	367	5	0
13	Ν	549	0	289	5	0
14	Р	280	0	142	1	0
15	Т	769	0	429	10	0
16	S	6703	0	6683	120	0
17	A	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	А	2	0	0	0	0
18	В	1	0	0	0	0
18	С	1	0	0	0	0
18	Ι	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	39178	0	38512	490	0

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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 6.

The worst 5 of 490 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:836:LEU:HD12	16:S:867:ILE:CD1	1.85	1.05
16:S:836:LEU:CD1	16:S:867:ILE:CD1	2.52	0.87
5:E:115:LYS:NZ	5:E:129:GLN:OE1	2.07	0.86
16:S:836:LEU:HD12	16:S:867:ILE:HD13	1.56	0.85
16:S:836:LEU:CD1	16:S:867:ILE:HD13	2.11	0.78

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	А	1395/1970~(71%)	1362 (98%)	33~(2%)	0	100	100
2	В	1123/1251~(90%)	1090 (97%)	33~(3%)	0	100	100
3	С	254/275~(92%)	252 (99%)	2(1%)	0	100	100
4	D	114/184~(62%)	109 (96%)	5 (4%)	0	100	100
5	Ε	207/210~(99%)	202 (98%)	5 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
6	F	76/127~(60%)	75~(99%)	1 (1%)	0	100	100
7	G	169/172~(98%)	148 (88%)	21 (12%)	0	100	100
8	Н	146/150~(97%)	144 (99%)	2(1%)	0	100	100
9	Ι	114/125~(91%)	111 (97%)	3~(3%)	0	100	100
10	J	64/67~(96%)	63~(98%)	1 (2%)	0	100	100
11	K	113/117~(97%)	110~(97%)	3~(3%)	0	100	100
12	L	42/58~(72%)	41 (98%)	1 (2%)	0	100	100
16	S	795/1729~(46%)	756~(95%)	39~(5%)	0	100	100
All	All	4612/6435~(72%)	4463 (97%)	149 (3%)	0	100	100

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There are no Ramachandran outliers to report.

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	1239/1749~(71%)	1239 (100%)	0	100	100
2	В	991/1084 (91%)	989 (100%)	2 (0%)	93	98
3	С	235/252~(93%)	235~(100%)	0	100	100
4	D	109/160~(68%)	109 (100%)	0	100	100
5	Ε	191/192~(100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153~(99%)	151 (100%)	0	100	100
8	Н	129/131~(98%)	129 (100%)	0	100	100
9	Ι	102/112~(91%)	102 (100%)	0	100	100
10	J	55/56~(98%)	55~(100%)	0	100	100
11	Κ	104/106~(98%)	104 (100%)	0	100	100
12	L	40/55~(73%)	40 (100%)	0	100	100
16	S	726/1524~(48%)	725 (100%)	1 (0%)	93	98



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4140/5685~(73%)	4137 (100%)	3~(0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	762	LYS
2	В	764	VAL
16	S	869	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1445	HIS
2	В	538	GLN
2	В	902	GLN
2	В	990	GLN
16	S	608	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	Р	12/46~(26%)	2~(16%)	0

All (2) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16835. 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



X Index: 220

Y Index: 220



Z Index: 220 $\,$

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 240

Y Index: 241

Z Index: 148

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

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

6.4.1 Primary map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 516 $\rm nm^3;$ this corresponds to an approximate mass of 466 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 0.329 $\mathrm{\AA^{-1}}$



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-16835 and PDB model 80EU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



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



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).



9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score	
All	0.9160	0.5260	
А	0.8980	0.5530	
В	0.9080	0.5640	1 0
С	0.9510	0.6010	1.0
D	0.9620	0.4280	
Е	0.9120	0.5260	
F	0.9390	0.5780	
G	0.9610	0.4980	
Н	0.9430	0.5860	
I	0.8530	0.4750	
J	0.9570	0.6030	
K	0.9550	0.6010	0.0
L	0.8890	0.5220	<0.0
N	0.6140	0.2890	
P	0.7890	0.5060	
S	0.9800	0.4350	
Т	0.7060	0.4170	

