

wwPDB EM Validation Summary Report (i)

Jan 28, 2023 - 02:04 PM EST

PDB ID	:	8EA3
EMDB ID	:	EMD-27971
Title	:	V-K CAST Transpososome from Scytonema hofmanni, major configuration
Authors	:	Rizo, A.N.; Park, JU.; Tsai, A.W.; Kellogg, E.H.
Deposited on	:	2022-08-27
Resolution	:	3.70 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:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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		Quality of	chain	
1	1	141	23%	45%	•	30%
2	3	71	30%	35%	6%	30%
3	7	265	48%		29%	10% • 13%
4	А	276	35%	75%		17% • 7%
4	В	276	9%	86%		7% 7%
4	С	276	-	80%		12% • 7%
4	D	276	-	81%		12% 7%



Mol	Chain	Length			Quality of cha	in
4	Ε	276	•		84%	9% 7%
4	F	276	6%		79%	14% 7%
4	G	276	6%		83%	9% · 7%
4	Н	276	5 0/		80%	13% • 7%
4	Ι	276	5%		79%	14% 7%
4	J	276	5%		79%	13% • 7%
4	Κ	276	•		76%	17% 7%
4	L	276	9%	E 20/	81%	12% • 7%
5	О	639		52%	79%	15% 6%
6	Q	167	100/		80%	17% ••
7	S	89	12%		81%	16% ••
8	W	584	13%		77%	10% • 12%
8	Х	584	22%	7	5%	10% • 13%
8	Y	584	22%	46%	5% •	48%
8	Ζ	584	23%	46%	5%	48%
8	W	584	•		98%	
8	х	584	÷		98%	
8	у	584			98%	
8	Z	584	•		98%	
9	2	51	25%		31%	43%
10	4	75	25%		36%	39%
11	5	50	12%	44%	_	44%
12	6	20	25%		40%	35%

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	MG	А	301	-	-	Х	-
13	MG	G	301	_	_	Х	-



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 55955 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 DNA chain called Target_LE.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
1	1	99	Total 2031	C 971	N 373	O 588	Р 99	0	0

• Molecule 2 is a DNA chain called Non-target_R.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
2	3	50	Total 1022	C 490	N 179	O 303	Р 50	0	0

• Molecule 3 is a RNA chain called sg_RNA.

Mol	Chain	Residues		Α	AltConf	Trace			
3	7	230	Total 4896	C 2187	N 863	0 1616	Р 230	0	0

• Molecule 4 is a protein called TnsC.

Mol	Chain	Residues		At	oms			AltConf	Trace
4	А	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	В	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	С	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	D	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	Е	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	F	257	Total 2066	C 1306	N 377	0 375	S 8	0	0
4	G	257	Total 2066	C 1306	N 377	0 375	S 8	0	0



Mol	Chain	Residues		Ate	\mathbf{oms}		AltConf	Trace	
4	п	257	Total	С	Ν	0	S	0	0
4	11	201	2066	1306	377	375	8	0	0
4	т	257	Total	С	Ν	0	S	0	0
4	1		2066	1306	377	375	8	0	0
4	Т	257	Total	С	Ν	Ο	\mathbf{S}	0	0
4	J		2066	1306	377	375	8	0	0
4	K	257	Total	С	Ν	0	\mathbf{S}	0	0
4	Γ	201	2066	1306	377	375	8	0	0
4	т	257	Total	С	Ν	0	\mathbf{S}	0	0
4		201	2066	1306	377	375	8		0

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• Molecule 5 is a protein called Cas12k.

Mol	Chain	Residues		At	AltConf	Trace			
5	0	601	Total 4865	C 3069	N 881	O 900	S 15	0	0

• Molecule 6 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	164	Total 1306	C 832	N 240	O 220	S 14	0	0

• Molecule 7 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	87	Total 702	C 433	N 140	0 128	S 1	0	0

• Molecule 8 is a protein called TnsB.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	W	14	Total C N O	0	0
0	vv	II	129 83 19 27	0	0
8	v	14	Total C N O	0	0
0	А	14	129 83 19 27	0	0
0	17	14	Total C N O	0	0
0	У	14	129 83 19 27	0	0
0	-	1.4	Total C N O	0	0
0	Z	14	129 83 19 27	0	0
0	117	514	Total C N O S	0	0
8	W	514	4122 2570 760 780 12	U	U



Mol	Chain	Residues		At	AltConf	Trace			
0	v	507	Total	С	Ν	0	S	0	0
0	Λ	507	4068	2537	748	771	12	0	0
0	V	204	Total	С	Ν	0	S	0	0
0	I	304	2453	1537	449	457	10	0	0
0	7	201	Total	С	Ν	0	S	0	0
8	L	Z 301	2426	1522	442	452	10	0	0

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• Molecule 9 is a DNA chain called LE_R.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
9	2	29	Total 593	C 285	N 105	0 175	Р 28	0	0

• Molecule 10 is a DNA chain called RE_F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	46	Total 941	C 449	N 175	0 271	Р 46	0	0

• Molecule 11 is a DNA chain called RE_R1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	28	Total 573	C 277	N 98	0 171	Р 27	0	0

• Molecule 12 is a DNA chain called RE_R2.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
12	6	13	Total 263	C 125	N 46	O 79	Р 13	0	0

• Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
13	А	1	Total Mg 1 1	0
13	В	1	Total Mg 1 1	0
13	С	1	Total Mg 1 1	0
13	D	1	Total Mg 1 1	0



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Mol	Chain	Residues	Atoms	AltConf
13	Е	1	Total Mg 1 1	0
13	F	1	Total Mg 1 1	0
13	G	1	Total Mg 1 1	0
13	Н	1	Total Mg 1 1	0
13	Ι	1	Total Mg 1 1	0
13	J	1	Total Mg 1 1	0
13	K	1	Total Mg 1 1	0
13	L	1	Total Mg 1 1	0
13	W	1	Total Mg 1 1	0
13	Х	1	Total Mg 1 1	0

• Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues		Atoms				
14	Λ	1	Total	С	Ν	Ο	Р	0
14	A	1	31	10	5	13	3	0



Mol	Chain	Residues		Ate	oms			AltConf
14	D	1	Total	С	Ν	0	Р	0
14	D	1	31	10	5	13	3	0
14	С	1	Total	С	Ν	0	Р	0
14	C	1	31	10	5	13	3	0
14	Л	1	Total	С	Ν	Ο	Р	0
14	D	1	31	10	5	13	3	0
14	F	1	Total	С	Ν	Ο	Р	0
14	Ľ	1	31	10	5	13	3	0
14	F	1	Total	С	Ν	Ο	Р	0
14	Г	1	31	10	5	13	3	0
14	С	1	Total	С	Ν	Ο	Р	0
14	G	1	31	10	5	13	3	0
14	Ц	1	Total	С	Ν	Ο	Р	0
14	11	1	31	10	5	13	3	0
14	Т	1	Total	С	Ν	Ο	Р	0
14	I	T	31	10	5	13	3	0
14	T	1	Total	С	Ν	Ο	Р	0
14	0	1	31	10	5	13	3	0
14	K	1	Total	С	Ν	Ο	Р	0
14	IX	L	31	10	5	13	3	U
14	т	1	Total	С	Ν	Ο	Р	0
14			31	10	5	13	3	U

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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: Target_LE















PROTEIN DATA BANK

• Molecu	ile 8: T	hsB					
Chain y:		_			98%		
MET ASN SER GLN GLN ASN PRO	ASP ASP LEU ALA VAL	ALS PRO LEU ALA TLE PRO	MET GLY LEU LEU CLY	GLU SER ALA THR THR LEU GLU	LYS ASN VAL TLE ALA THR GLN LEU SER	GLU GLU GLU VAL LYS CLU GLU TLE CLU GLU GLU	SER LEU LEU PRO CYS ASP ARG THR THR
TYR GLY GLN LYS LEU ARG	ALA ALA GLU LYS	LEU ASN VAL SER LEU ARG	THR VAL GLN ARG LEU VAL	LYS ASN TRP GLU GLU ASP GLY	LEU VAL GLY GLY LEU THR THR SER SER	ALA ASP LYS GLY LYS HIS ANG TLE GLY GLY PHE	TRP GLU ASN PHE TLE THR LYS TYR LYS LYS
GLU GLY ASN LYS GLY SER SER	ARG MET THR PRO	LTS GLN VAL ALA LEU ARG	VAL GLU ALA LYS ALA ALA ARG	GLU LEU LYS ASP SER LYS PRO	PRO ASN TYR LYS THR VAL LEU ARG	LEU ALA PRO TLE LEU GLU GLN GLN ALA ALA	LYS SER ILE ARG SER PRO GLY ARC GLY GLY
THR THR LEU SER VAL LYS THR	ARG GLU GLY LYS	ASF LEU SER VAL ASP TYR	SER ASN HIS VAL TRP GLN	CYS ASP HIS THR ARG VAL ASP	VAL LEU LEU VAL ASP GLN HIS GLY GLY	LLE LEU SER ARG PRO TRP LEU THR THR THR THR THR TLE	ASP THR TYR SER ARG CYS ILE MET GLY ILE
ASN LEU GLY PHE ASP ALA PRO	SER SER GLY VAL	VAL ALA LEU ALA LEU ARG	HIS ALA ILE LEU PRO LYS	ARG TYR GLY SER GLU TYR LYS	LEU HIS CYS CYS GLU TRP GLY THR TYR GLY	LYS PRO GLU HIS PHE TYR TYR ASP GLY CLY	ASP PHE ARG SER ASN HIS SER CLN ILE
GLY ALA GLN LEU GLY PHE VAT	CYS CYS HIS LEU ARG	ASF ARG PRO SER GLU GLV	GLY VAL VAL GLU ARG PRO	PHE LYS THR LEU ASN ASP GLN	LEU PHE SER THR LEU PRO GLY THR THR	GLY SER ASN VAL CLN GLN GLU PRO GLU ASP ALA	GLU LYS ASP ASP ALA ARG LEU LEU LEU ARG GLU
LEU GLU GLN LEU VAL ABG	TYR TLE VAL ASP	ANG TYR ASN GLN SER TLE	ASP ALA ARG MET GLY ASP	GLN THR ARG PHE GLU ARG TRP	GLU ALA GLY LEU PRO THR VAL VAL	PRU TILE PRO GLU ASP ASP LEU ASP ILEU CYS LEU	MET LYS GLN SER ARG ARG ARG THR VAL CLN ARG
GLY CYS CYS GLN PHE CI N	ASN LEU MET TYR	ARG GLY GLU TYR LEU ALA	GLY TYR ALA GLV GLU THR	VAL ASN LEU ARG ARG ASP PRO	ARG ASP ASP ILE THR THR ILE VAL TYR	ARG GLN GLU GLU ASN ASN GLN GLN CLU CLU PHE LEU THR	ARG ALA HIS ALA ALA GLV CLY CLV CLV CLU CLU
GLN LEU LEU LEU GLU GLU	GLU GLU ALA SER SER	ARG ARG LEU ARG ALA	GLY LYS THR ILE SER ASN	GLN SER LEU LEU GLN VAL	VAL ASP ARG ASP ALA ALA VAL ALA THR	LYS LYS SER ARG LYS GLU ARG GLU LEU LEU	GLN THR VAL LEU ARG SER ALA ALA ALA ALA ASP
				•	• • ••	** *	
GLU SER ASN ARG GLU SER	PRO SER GLN ILE	VAL GLU PRO ASP GLU VAL	GLU GLU SER THR GLU THR VAL	HIS SER GLN TYR GLU ASP	E571 E571 D574 D576 E576 Q577 L578 L578 R579	E580 E581 Y582 G583 PHE	
• Molecu	ile 8: T	nsB					
Chain z:					98%		
MET ASN SER GLN GLN ASN PRO	ASP ASP LEU ALA VAL	PRO LEU ALA TLE PRO	MET GLY LEU LEU CLY CLY	GLU SER ALA THR THR LEU GLU	LYS ASN VAL ILE ALA ALA THR GLN LEU SER	GLU GLU GLN ALA GLN VAL LYS LYS CLU CLU CLU CLU CLN GLN	SER LEU LEU CYS ASP ASP ARG THR THR
TYR GLY GLN LYS LEU ARG GTU	ALA ALA GLU LYS	LEU VAL SER LEU ARG	THR VAL GLN ARG LEU VAL	LYS ASN TRP GLU GLU ASP GLY	LEU VAL GLY LEU THR GLN SER SER	ALA ASP LYS GLY CLYS HIS ARG CLY GLU PHE	TRP GLU ASN PHE ILE THR LYS TYR LYS
GLU GLY ASN LYS GLY SER YS	ARG MET THR PRO	LTS GLN VAL ALA LEU ARG	VAL GLU ALA LYS ALA ALA ARG	GLU LEU LYS ASP SER LYS PRO	PRO ASN TYR LYS LYS THR VAL LEU ARG VAL	LEU ALA PRO TLE LEU GLU GLU GLN GLN ALA	LYS SER ILE ARG SER PRO GLY GLY
THR THR LEU SER VAL LYS THR	ARG GLV GLY LYS	ASP LEU SER VAL ASP TYR	SER ASN HIS VAL TRP GLN	CYS ASP HIS THR ARG VAL ASP	VAL LEU LEU VAL ASP GLN HIS GLV GLV	LLE LEU SER ARG PRO TRP LLEU THR VAL THR VAL	ASP THR TYR SER ARG CYS ILE MET GLY ILE
ASN LEU GLY PHE ASP ALA PRO	SER SER GLY VAL	VAL ALA LEU ALA LEU ARG	HIS ALA ILE LEU PRO LYS	ARG TYR GLY SER GLU TYR LYS	LEU HIS CYS CYS GLU TRP GLY THR TYR GLY	LYS PRO GLU HIS PHE TYR THR ASP GLY GLY LYS	ASP PHE ARG SER ASN HIS LEU SER CLN ILE
GLY ALA GLN LEU GLY PHE VAT	CYS HIS LEU ARG	ASF ARG PRO SER GLU GLY	GLY VAL VAL GLU ARG PRO	PHE LYS THR LEU ASN GLN	LEU PHE SER THR LEU PRO GLY TYR THR	GLY SER ASN VAL GLN GLN ARG GLU GLU ASP ALA	GLU LYS ASP ASP ARG ARG LEU LEU LEU ARG GLU
LEU GLU GLN LEU VAL ARG	TYR TLE VAL ASP	ANG TYR ASN GLN SER ILE	ASP ALA ARG MET GLY ASP	GLN THR ARG PHE GLU TRP	GLU ALA GLY CLEU PRO PRO PRO	PRU TLE GLU GLU ASP ASP TLEU TLEU LEU LEU	MET LYS GLN SER ARG ARG THR VAL GLN ARG













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 ($6k \ge 4k$)	Depositor
Maximum map value	2.956	Depositor
Minimum map value	-1.515	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	576.18, 576.18, 576.18	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	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, ATP

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		Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	1	0.54	0/2280	0.99	4/3516~(0.1%)	
2	3	0.56	0/1143	1.10	6/1759~(0.3%)	
3	7	0.25	0/5470	0.76	7/8517~(0.1%)	
4	А	0.85	0/2097	0.92	4/2817~(0.1%)	
4	В	0.85	0/2097	0.99	9/2817~(0.3%)	
4	С	0.87	0/2097	0.95	7/2817~(0.2%)	
4	D	0.75	0/2097	1.06	16/2817~(0.6%)	
4	Е	0.81	0/2097	1.01	10/2817~(0.4%)	
4	F	0.86	0/2097	0.94	7/2817~(0.2%)	
4	G	0.78	0/2097	1.03	10/2817~(0.4%)	
4	Н	0.84	0/2097	1.01	10/2817~(0.4%)	
4	Ι	0.81	0/2097	0.99	6/2817~(0.2%)	
4	J	0.86	0/2097	1.03	9/2817~(0.3%)	
4	Κ	0.86	0/2097	1.03	10/2817~(0.4%)	
4	L	0.85	0/2097	0.96	6/2817~(0.2%)	
5	0	0.67	1/4952~(0.0%)	0.93	15/6677~(0.2%)	
6	Q	0.69	0/1345	1.04	5/1819~(0.3%)	
7	S	0.74	0/710	1.02	3/950~(0.3%)	
8	W	0.72	0/4192	0.95	15/5659~(0.3%)	
8	Х	0.72	0/4137	1.01	16/5585~(0.3%)	
8	Y	0.73	0/2499	0.90	7/3379~(0.2%)	
8	Ζ	0.72	1/2472~(0.0%)	0.95	9/3345~(0.3%)	
8	W	0.80	0/132	1.29	2/178~(1.1%)	
8	Х	1.21	0/132	1.17	2/178~(1.1%)	
8	У	0.95	0/132	1.29	2/178~(1.1%)	
8	Z	0.81	0/132	1.14	0/178	
9	2	0.49	0/664	0.93	0/1024	
10	4	0.50	0/1056	0.88	0/1626	
11	5	0.48	0/641	0.98	0/989	
12	6	0.47	0/293	0.87	0/449	
All	All	0.72	2/57546~(0.0%)	0.96	$19\overline{7}/\overline{79810}~(0.2\%)$	



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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	С	0	1
4	D	0	1
4	F	0	1
4	G	0	2
4	Н	0	1
4	Κ	0	1
4	L	0	1
8	W	0	3
8	Х	0	3
8	Y	0	3
8	Ζ	0	1
8	Х	0	1
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	0	12	SER	CA-CB	-5.69	1.44	1.52
8	Ζ	463	ASN	C-N	-5.04	1.22	1.34

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	3	34	DC	P-O3'-C3'	-11.67	105.69	119.70
3	7	230	G	P-O3'-C3'	-9.58	108.21	119.70
8	Х	495	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	1	30	DC	P-O3'-C3'	-9.21	108.64	119.70
4	Е	254	ARG	NE-CZ-NH1	9.13	124.87	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	С	254	ARG	Sidechain
4	D	128	ARG	Sidechain
4	F	182	ARG	Sidechain
4	G	189	ARG	Sidechain
4	G	240	TYR	Sidechain



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	1	2031	0	1118	148	0
2	3	1022	0	569	59	0
3	7	4896	0	2471	98	0
4	А	2066	0	2155	66	0
4	В	2066	0	2154	32	0
4	С	2066	0	2157	66	0
4	D	2066	0	2157	34	0
4	Е	2066	0	2157	25	0
4	F	2066	0	2158	59	0
4	G	2066	0	2158	25	0
4	Н	2066	0	2157	42	0
4	Ι	2066	0	2157	81	0
4	J	2066	0	2156	70	0
4	K	2066	0	2154	80	0
4	L	2066	0	2155	61	0
5	0	4865	0	4926	190	0
6	Q	1306	0	1290	47	0
7	S	702	0	721	18	0
8	W	4122	0	4147	114	0
8	Х	4068	0	4077	120	0
8	Y	2453	0	2421	44	0
8	Ζ	2426	0	2388	19	0
8	W	129	0	110	0	0
8	Х	129	0	110	0	0
8	у	129	0	110	0	0
8	Z	129	0	110	0	0
9	2	593	0	331	43	0
10	4	941	0	518	60	0
11	5	573	0	322	38	0
12	6	263	0	146	27	0
13	А	1	0	0	2	0
13	В	1	0	0	0	0
13	С	1	0	0	0	0
13	D	1	0	0	0	0
13	Е	1	0	0	0	0
13	F	1	0	0	1	0
13	G	1	0	0	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	Н	1	0	0	0	0
13	Ι	1	0	0	0	0
13	J	1	0	0	0	0
13	K	1	0	0	0	0
13	L	1	0	0	0	0
13	W	1	0	0	0	0
13	Х	1	0	0	0	0
14	А	31	0	12	3	0
14	В	31	0	12	8	0
14	С	31	0	12	3	0
14	D	31	0	12	5	0
14	Е	31	0	12	2	0
14	F	31	0	12	3	0
14	G	31	0	12	1	0
14	Н	31	0	12	3	0
14	Ι	31	0	12	3	0
14	J	31	0	12	1	0
14	Κ	31	0	12	1	0
14	L	31	0	12	8	0
All	All	55955	0	51904	1184	0

Continued from previous page...

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 11.

The worst 5 of 1184 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)
5:O:412:SER:CB	5:O:415:GLN:CD	1.75	1.53
3:7:86:G:H1	5:O:300:ARG:NH2	1.09	1.51
4:F:218:LEU:CD2	4:F:256:LEU:HD11	1.43	1.49
4:I:191:ARG:CZ	4:J:243:ARG:NH2	1.73	1.47
1:1:-24:DC:C6	8:W:77:ARG:NH2	1.88	1.41

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
4	А	255/276~(92%)	248~(97%)	6~(2%)	1 (0%)	34	69
4	В	255/276~(92%)	254 (100%)	1 (0%)	0	100	100
4	С	255/276~(92%)	247 (97%)	8(3%)	0	100	100
4	D	255/276~(92%)	248~(97%)	7 (3%)	0	100	100
4	Ε	255/276~(92%)	252 (99%)	3~(1%)	0	100	100
4	F	255/276~(92%)	250~(98%)	5(2%)	0	100	100
4	G	255/276~(92%)	250 (98%)	5(2%)	0	100	100
4	Н	255/276~(92%)	252~(99%)	2(1%)	1 (0%)	34	69
4	Ι	255/276~(92%)	254 (100%)	1 (0%)	0	100	100
4	J	255/276~(92%)	250 (98%)	5(2%)	0	100	100
4	Κ	255/276~(92%)	250~(98%)	5(2%)	0	100	100
4	L	255/276~(92%)	249 (98%)	6(2%)	0	100	100
5	Ο	595/639~(93%)	580 (98%)	14 (2%)	1 (0%)	47	78
6	Q	162/167~(97%)	151 (93%)	10 (6%)	1 (1%)	25	62
7	S	85/89~(96%)	83~(98%)	1 (1%)	1 (1%)	13	48
8	W	512/584~(88%)	493 (96%)	19 (4%)	0	100	100
8	Х	503/584~(86%)	484 (96%)	17 (3%)	2~(0%)	34	69
8	Y	296/584~(51%)	284 (96%)	12~(4%)	0	100	100
8	Z	293/584~(50%)	282 (96%)	9~(3%)	2(1%)	22	59
8	W	12/584~(2%)	12 (100%)	0	0	100	100
8	х	12/584 (2%)	12 (100%)	0	0	100	100
8	У	12/584~(2%)	12 (100%)	0	0	100	100
8	Z	12/584~(2%)	12 (100%)	0	0	100	100
All	All	5554/8879~(63%)	5409 (97%)	136 (2%)	9~(0%)	50	78



5 of 9 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
4	Н	61	GLU
5	0	413	ASP
8	Х	176	PRO
4	А	50	ARG
8	Ζ	323	PRO

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
4	А	224/238~(94%)	220 (98%)	4 (2%)	59	77
4	В	224/238~(94%)	224 (100%)	0	100	100
4	С	224/238~(94%)	221 (99%)	3 (1%)	69	83
4	D	224/238~(94%)	224 (100%)	0	100	100
4	Ε	224/238~(94%)	224 (100%)	0	100	100
4	F	224/238~(94%)	224 (100%)	0	100	100
4	G	224/238~(94%)	221 (99%)	3 (1%)	69	83
4	Н	224/238~(94%)	222 (99%)	2 (1%)	78	88
4	Ι	224/238~(94%)	224 (100%)	0	100	100
4	J	224/238~(94%)	222 (99%)	2 (1%)	78	88
4	K	224/238~(94%)	222 (99%)	2 (1%)	78	88
4	L	224/238~(94%)	221 (99%)	3 (1%)	69	83
5	Ο	529/564~(94%)	529 (100%)	0	100	100
6	Q	136/139~(98%)	136 (100%)	0	100	100
7	S	75/77~(97%)	75~(100%)	0	100	100
8	W	448/512~(88%)	446 (100%)	2 (0%)	91	95
8	Х	442/512~(86%)	441 (100%)	1 (0%)	93	97
8	Y	264/512 (52%)	261 (99%)	3 (1%)	73	85
8	Z	261/512~(51%)	261 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
8	W	13/512~(2%)	13~(100%)	0	100	100
8	х	13/512~(2%)	13 (100%)	0	100	100
8	У	13/512~(2%)	13 (100%)	0	100	100
8	Z	13/512~(2%)	13 (100%)	0	100	100
All	All	4895/7732~(63%)	4870 (100%)	25~(0%)	89	94

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 $5~{\rm of}~25$ residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
4	Κ	153	THR
4	L	150	LYS
8	Y	380	ARG
4	L	85	ARG
4	L	211	TRP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
8	W	217	HIS
8	Ζ	463	ASN
8	Y	473	HIS
4	Κ	185	GLN
7	S	42	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	7	227/265~(85%)	55 (24%)	5(2%)

5 of 55 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	7	9	А
3	7	15	G
3	7	18	А
3	7	22	А
3	7	24	G



All (5) RNA pucker outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
3	7	48	U
3	7	49	U
3	7	50	А
3	7	130	А
3	7	173	U

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 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	les
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
14	ATP	L	302	-	26,33,33	0.79	0	31,52,52	1.11	4 (12%)
14	ATP	F	302	13	26,33,33	0.83	0	31,52,52	1.37	3 (9%)
14	ATP	G	302	13	26,33,33	0.92	0	31,52,52	1.15	3 (9%)
14	ATP	Н	302	13	26,33,33	0.85	0	31,52,52	1.09	3 (9%)
14	ATP	Ι	302	13	26,33,33	0.86	0	31,52,52	1.18	3 (9%)
14	ATP	В	302	13	26,33,33	0.90	0	31,52,52	1.40	3 (9%)
14	ATP	D	302	13	26,33,33	0.87	0	31,52,52	1.25	3 (9%)
14	ATP	А	302	13	26,33,33	0.75	0	31,52,52	1.12	3 (9%)
14	ATP	J	302	13	26,33,33	0.84	0	31,52,52	1.32	3 (9%)
14	ATP	Е	302	13	26,33,33	0.94	0	31,52,52	1.48	3 (9%)



Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	В	ond ang	gles
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	ATP	К	302	13	26,33,33	0.80	0	$31,\!52,\!52$	1.24	4 (12%)
14	ATP	С	302	13	26,33,33	0.88	0	31,52,52	1.38	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	L	302	-	-	3/18/38/38	0/3/3/3
14	ATP	F	302	13	-	1/18/38/38	0/3/3/3
14	ATP	G	302	13	-	4/18/38/38	0/3/3/3
14	ATP	Н	302	13	-	5/18/38/38	0/3/3/3
14	ATP	Ι	302	13	-	7/18/38/38	0/3/3/3
14	ATP	В	302	13	-	1/18/38/38	0/3/3/3
14	ATP	D	302	13	-	3/18/38/38	0/3/3/3
14	ATP	А	302	13	-	5/18/38/38	0/3/3/3
14	ATP	J	302	13	-	2/18/38/38	0/3/3/3
14	ATP	Е	302	13	-	1/18/38/38	0/3/3/3
14	ATP	K	302	13	-	1/18/38/38	0/3/3/3
14	ATP	С	302	13	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	В	302	ATP	PB-O3B-PG	-5.65	113.42	132.83
14	Е	302	ATP	PB-O3B-PG	-5.26	114.76	132.83
14	F	302	ATP	PB-O3B-PG	-5.12	115.25	132.83
14	J	302	ATP	PA-O3A-PB	-4.50	117.39	132.83
14	С	302	ATP	PA-O3A-PB	-4.28	118.15	132.83

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	А	302	ATP	C5'-O5'-PA-O1A
14	А	302	ATP	C5'-O5'-PA-O2A
14	А	302	ATP	O4'-C4'-C5'-O5'



Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	А	302	ATP	C3'-C4'-C5'-O5'
14	Ι	302	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
14	L	302	ATP	8	0
14	F	302	ATP	3	0
14	G	302	ATP	1	0
14	Н	302	ATP	3	0
14	Ι	302	ATP	3	0
14	В	302	ATP	8	0
14	D	302	ATP	5	0
14	А	302	ATP	3	0
14	J	302	ATP	1	0
14	Е	302	ATP	2	0
14	Κ	302	ATP	1	0
14	С	302	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















































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-27971. 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: 270





Z Index: 270

6.2.2 Raw map



X Index: 270

Y Index: 270



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: 264



Y Index: 278



Z Index: 277

6.3.2 Raw map



X Index: 0





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 0.5. 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.



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_27971_msk_1.map (i) 6.5.1





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 338 $\rm nm^3;$ this corresponds to an approximate mass of 305 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 0.270 \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 0.270 ${\rm \AA^{-1}}$



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	3.70	-	-
Author-provided FSC curve	3.51	3.94	3.56
Unmasked-calculated*	6.88	8.73	7.10

*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 6.88 differs from the reported value 3.7 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27971 and PDB model 8EA3. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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 (0.5).



9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.



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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.3560
1	0.7494	0.3400
2	0.6239	0.2730
3	0.7847	0.3670
4	0.7662	0.3160
5	0.7766	0.3190
6	0.6578	0.2370
7	0.6458	0.2510
А	0.5044	0.3410
В	0.6608	0.3940
С	0.7520	0.4260
D	0.7676	0.4460
Е	0.7637	0.4410
F	0.7123	0.4120
G	0.7103	0.4080
Н	0.7074	0.4230
Ι	0.7157	0.4220
J	0.7275	0.4350
K	0.7779	0.4540
L	0.6667	0.4160
0	0.3838	0.2080
Q	0.7802	0.4330
\mathbf{S}	0.6088	0.3230
W	0.6697	0.4100
Х	0.5677	0.3530
Y	0.4412	0.2620
Z	0.4412	0.2690
W	0.4839	0.3620
X	0.3065	0.2780
У	0.3952	0.3500
Z	0.3065	0.2850

