

Oct 4, 2023 – 02:19 PM JST

PDB ID	:	7WVZ
EMDB ID	:	EMD-32863
Title	:	CalA3_modular PKS_KS-AT-DH-KR
Authors	:	Wang, J.; Wang, Z.
Deposited on	:	2022-02-12
Resolution	:	3.38 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.38 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
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	1738	93%	5%•
1	В	1738	93%	6% •



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 49889 atoms, of which 24824 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 Beta-ketoacyl-acyl-carrier-protein synthase I.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1 1	1710	Total	С	Η	Ν	Ο	S	0	0
	1719	25011	7824	12445	2332	2386	24	0	0	
1	1 D	1711	Total	С	Η	Ν	Ο	S	0	0
		24878	7783	12379	2322	2371	23		U	

Chain	Residue	Modelled	Actual	Comment	Reference
А	1728	ALA	-	expression tag	UNP A0A2N9BJK0
А	1729	ALA	-	expression tag	UNP A0A2N9BJK0
А	1730	ALA	-	expression tag	UNP A0A2N9BJK0
А	1731	LEU	-	expression tag	UNP A0A2N9BJK0
А	1732	GLU	-	expression tag	UNP A0A2N9BJK0
А	1733	HIS	-	expression tag	UNP A0A2N9BJK0
А	1734	HIS	-	expression tag	UNP A0A2N9BJK0
А	1735	HIS	-	expression tag	UNP A0A2N9BJK0
A	1736	HIS	-	expression tag	UNP A0A2N9BJK0
А	1737	HIS	-	expression tag	UNP A0A2N9BJK0
А	1738	HIS	-	expression tag	UNP A0A2N9BJK0
В	1728	ALA	-	expression tag	UNP A0A2N9BJK0
В	1729	ALA	-	expression tag	UNP A0A2N9BJK0
В	1730	ALA	-	expression tag	UNP A0A2N9BJK0
В	1731	LEU	-	expression tag	UNP A0A2N9BJK0
В	1732	GLU	-	expression tag	UNP A0A2N9BJK0
В	1733	HIS	-	expression tag	UNP A0A2N9BJK0
В	1734	HIS	-	expression tag	UNP A0A2N9BJK0
В	1735	HIS	-	expression tag	UNP A0A2N9BJK0
В	1736	HIS	-	expression tag	UNP A0A2N9BJK0
В	1737	HIS	-	expression tag	UNP A0A2N9BJK0
В	1738	HIS	-	expression tag	UNP A0A2N9BJK0

There are 22 discrepancies between the modelled and reference sequences:



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: Beta-ketoacyl-acyl-carrier-protein synthase I



Chain B:



6% •

93%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224991	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 $(e^-/\text{\AA}^2)$	48.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 ($6k \ge 4k$)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0185	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.63	0/12833	1.05	81/17517~(0.5%)	
1	В	0.63	0/12765	1.06	95/17426~(0.5%)	
All	All	0.63	0/25598	1.06	176/34943~(0.5%)	

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
1	В	0	3
All	All	0	5

There are no bond length outliers.

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	810	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	А	810	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	В	1569	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	В	845	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	А	1569	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	А	1460	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	В	1552	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	В	44	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	В	1460	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	В	735	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	В	1681	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	1194	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	В	271	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	44	ARG	NE-CZ-NH1	7.16	123.88	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Z} = \mathbf{Observed}(^{o})$	
1	А	1552	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	В	115	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	В	541	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	А	541	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	А	754	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	А	271	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	А	682	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	В	1059	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	В	754	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	А	821	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	В	779	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	В	682	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	В	998	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	В	1017	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	А	431	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	В	1025	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	А	1327	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	А	867	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	В	1486	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	А	238	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	В	1475	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	В	415	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	В	821	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	В	565	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	В	1434	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	А	779	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	А	179	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	А	1475	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	В	1418	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	В	1472	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	В	823	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	А	1054	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	В	1447	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	А	1059	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	А	998	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	678	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	В	745	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	393	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	А	1043	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	В	1552	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	В	1150	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	745	ARG	NE-CZ-NH1	6.11	123.36	120.30



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	678	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	В	1080	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	В	1224	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	А	390	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	А	1079	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	В	355	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	В	1294	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	А	1418	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	А	1531	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	А	820	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	В	1531	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	В	390	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	А	428	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	А	485	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	А	1434	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	В	156	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	А	1718	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	В	431	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	А	1486	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	В	179	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	А	1150	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	В	821	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	В	393	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	А	1027	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	В	1054	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	В	487	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	А	1447	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	А	1294	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	В	1430	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	В	1270	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	В	1693	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	А	829	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	А	1194	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	А	821	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	В	1327	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	А	845	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	В	1681	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	В	428	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	В	1569	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	635	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	А	900	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	А	694	ARG	NE-CZ-NH1	5.66	123.13	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	В	1502	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	В	1211	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	А	899	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	В	800	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	А	1502	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	А	23	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	А	24	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	В	1043	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	А	1518	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	В	867	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	А	1552	ARG	CD-NE-CZ	5.57	131.40	123.60
1	В	1079	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	В	485	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	А	814	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	А	1312	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	В	751	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	А	1443	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	В	510	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	В	1552	ARG	CD-NE-CZ	5.47	131.26	123.60
1	В	573	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	А	1025	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	В	1096	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	В	1083	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	А	823	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	В	635	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	А	573	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	А	1337	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	В	1027	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	В	1686	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	В	520	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	В	576	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	В	277	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	А	430	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	А	1296	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	В	678	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	1164	ARG	NE-CZ-NH1	$5.3\overline{7}$	122.98	120.30
1	A	545	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	А	355	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	В	276	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	735	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	В	424	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	В	694	ARG	NE-CZ-NH1	5.31	122.95	120.30



 $(^{o})$

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°
1	А	277	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	А	1083	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	А	1192	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	А	212	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	А	1486	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	В	899	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	В	1211	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	А	678	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	В	814	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	А	1211	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	А	751	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	В	506	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	А	127	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	В	1199	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	А	1569	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	В	1123	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	В	1443	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	В	430	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	В	1425	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	А	1096	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	В	1123	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	А	1270	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	В	855	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	В	1595	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	А	609	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	А	1184	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	А	565	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	В	770	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	В	271	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	В	605	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	В	1349	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	А	1422	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	В	127	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	В	22	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	А	480	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	1552	ARG	NE-CZ-NH2	-5.00	117.80	120.30

Continued from previous page...

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	115	ARG	Sidechain
Continued on next nage				



	5	1	1 5	
Mol	Chain	Res	Type	Group
1	А	1430	ARG	Sidechain
1	В	1294	ARG	Sidechain
1	В	1430	ARG	Sidechain
1	В	659	TYR	Sidechain

Continued from previous page...

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	12566	12445	12445	1	0
1	В	12499	12379	12378	1	0
All	All	25065	24824	24823	1	0

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 0.

All (1) 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)
1:A:852:GLU:HA	1:B:1229:GLY:HA2	2.03	0.41

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	ntile	\mathbf{s}
1	А	1717/1738~(99%)	1650 (96%)	64 (4%)	3~(0%)	47	78	



Conti	naca fron	i previous page						
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntile	\mathbf{s}
1	В	1709/1738~(98%)	1622 (95%)	85~(5%)	2(0%)	51	82	
All	All	3426/3476~(99%)	3272 (96%)	149 (4%)	5 (0%)	54	82	

Continued from previous page

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1499	GLY
1	В	1499	GLY
1	А	1695	LEU
1	А	711	VAL
1	В	1694	PRO

5.3.2Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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	Percer	ntiles
1	А	1237/1250~(99%)	1219~(98%)	18 (2%)	65	82
1	В	1229/1250~(98%)	1218 (99%)	11 (1%)	78	89
All	All	2466/2500~(99%)	2437 (99%)	29 (1%)	72	85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	ASP
1	А	198	THR
1	А	268	LEU
1	А	479	LEU
1	А	609	ARG
1	А	636	LEU
1	А	710	GLN
1	А	763	GLN
1	А	780	GLU
1	А	785	LEU
1	А	850	PHE



Mol	Chain	Res	Type
1	А	1054	ARG
1	А	1189	GLN
1	А	1271	ASP
1	А	1304	LEU
1	А	1323	ASP
1	А	1637	SER
1	A	1693	ARG
1	В	462	ASN
1	В	479	LEU
1	В	636	LEU
1	В	780	GLU
1	В	834	ASP
1	В	1054	ARG
1	В	1266	ASP
1	В	1485	GLU
1	В	1547	GLU
1	В	1637	SER
1	В	1692	HIS

Continued from previous page...

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	909	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32863. 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: 120



Y Index: 120



Z Index: 120

6.2.2 Raw map



X Index: 120

Y Index: 120

Z Index: 120

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: 108





Z Index: 122

6.3.2 Raw map



X Index: 113

Y Index: 112



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



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

6.4.1 Primary map



6.4.2 Raw map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 183 nm^3 ; this corresponds to an approximate mass of 166 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 0.296 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.296 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.37	3.75	3.42
Unmasked-calculated*	3.66	4.08	3.71

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32863 and PDB model 7WVZ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0185 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 (0.0185).



9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0185) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.4600
А	0.7640	0.4560
В	0.7720	0.4630



