

wwPDB EM Validation Summary Report (i)

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PDB ID	:	8W9Z
EMDB ID	:	EMD-37386
Title	:	The cryo-EM structure of the Nicotiana tabacum PEP-PAP
Authors	:	Wu, X.X.; Zhang, Y.
Deposited on	:	2023-09-06
Resolution	:	3.00 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)
:	1.9.13
:	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 3.00 Å.

Sidechain outliers

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.



154315

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.

3826

Mol	Chain	Length	Quality of chain	
1	А	337	87%	13%
1	a	337	94%	• 6%
2	В	1070	85%	15%
3	С	688	85%	• 14%
4	с	1388	84%	• 15%
5	D	892	72% •	28%
6	Е	860	• 81%	• 19%
7	F	682	79%	20%
8	G	266	81%	• 18%

Continued on next page...



Mol	Chain	Length	Quality of chain	
9	Н	531	49%	51%
10	Ι	486	77%	23%
11	i	648	58% •	41%
12	J	507	82%	• 17%
13	K	331	64% •	35%
14	L	303	75%	• 23%
15	М	178	65%	35%
15	m	178	61% •	39%
16	Ν	770	69%	30%
17	Ο	167	52% ·	47%
18	Р	143	73%	27%

Continued from previous page...



2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 60525 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 subunit alpha.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	293	Total 2202	C 1397	N 382	0 411	S 12	0	0
1	a	318	Total 2441	C 1555	N 424	0 452	S 10	0	0

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

Mol	Chain	Residues		Α	AltConf	Trace			
2	В	909	Total 6820	C 4328	N 1216	O 1253	S 23	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
3	С	592	Total 4431	C 2832	N 783	O 799	${ m S}$ 17	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta".

Mol	Chain	Residues		А	AltConf	Trace			
4	с	1174	Total 8086	C 5072	N 1482	O 1503	S 29	0	0

• Molecule 5 is a protein called PAP1(pTAC3).

Mol	Chain	Residues		At	AltConf	Trace			
5	D	645	Total 5088	C 3228	N 878	O 956	S 26	0	0

• Molecule 6 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplasticlike.



Mol	Chain	Residues		At	AltConf	Trace			
6	Е	700	Total 4534	C 2823	N 822	O 866	S 23	0	0

• Molecule 7 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

Mol	Chain	Residues		At	AltConf	Trace			
7	F	544	Total 4233	C 2678	N 756	O 780	S 19	0	0

• Molecule 8 is a protein called superoxide dismutase.

Mol	Chain	Residues		Ate	AltConf	Trace			
8	G	218	Total 1727	C 1122	N 291	O 309	$\frac{S}{5}$	0	0

• Molecule 9 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

Mol	Chain	Residues	Atoms			AltConf	Trace		
9	Н	260	Total 2110	C 1338	N 371	O 393	S 8	0	0

• Molecule 10 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace	
10	Ι	374	Total 2897	C 1856	N 512	0 517	S 12	0	0

• Molecule 11 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace	
11	i	383	Total 2983	C 1902	N 508	O 557	S 16	0	0

• Molecule 12 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
12	J	422	Total 3368	C 2157	N 578	O 612	S 21	0	0

• Molecule 13 is a protein called PAP8(pTAC6).



Mol	Chain	Residues	Atoms				AltConf	Trace	
13	К	214	Total 1779	C 1127	N 307	O 337	S 8	0	0

• Molecule 14 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms				AltConf	Trace	
14	L	234	Total 1475	C 943	N 261	O 270	S 1	0	0

• Molecule 15 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	М	116	Total 935	$\begin{array}{c} \mathrm{C} \\ 598 \end{array}$	N 150	0 180	${f S}{7}$	0	0
15	m	109	Total 851	$\begin{array}{c} \mathrm{C} \\ 545 \end{array}$	N 135	O 164	${ m S} 7$	0	0

• Molecule 16 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

Mol	Chain	Residues	Atoms			AltConf	Trace		
16	Ν	537	Total 2982	C 1814	N 579	O 583	S 6	0	0

• Molecule 17 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
17	Ο	88	Total 692	C 434	N 124	0 131	${ m S} { m 3}$	0	0

• Molecule 18 is a protein called PAP13(pTAC18).

Mol	Chain	Residues	Atoms				AltConf	Trace	
18	Р	105	Total 887	C 576	N 148	0 158	${f S}{5}$	0	0

• Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
19	В	1	TotalZn11	0



• Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
20	С	1	Total Mg 1 1	0

• Molecule 21 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total Fe 1 1	0
21	L	1	Total Fe 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 subunit alpha









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# > 6 3 9 3 5 5 5 4 7 5 6			
E149 4199 E200 K201 H235 E236 C237	A271 1502 1502 1502 1503 1634 1634 1634 1634 1634 1634 1757 1757 1757 1757 1757 1757 1757 1754 1754 1754 1754 1754 1757 1632 1752 1632 1774 1774 1775 1774 1775	PRO SER SER SER SER GLY CLY ASP ASP ASP PLC LEU TLE PRO SER ASP SER ASP	PRO TILE SEER SEER LEU LEU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
LYS ARG SER GLU SER ALA ASN ASP ASP CSE ASP SER ARG SER	THR LYS SER ASP ASP CLU CLU LEU LEU MET AET SER SER VAL		
• Molecule 7: Pro	tein PLASTID TRANSC	RIPTIONALLY ACTIV	VE 10-like
Chain F:	79%		20%
MET GLN THR LEU GLN SER SER SER SER LEU PHE PHE	PRO SER SER THR LYS LUS LEU LEU LEU LVS PRO SER SER SER SER SER SER	PHE PRO SER SER SER LEU LYS PRO PRO PRO HIS HIS	SER SER ASP ASP PHE PRO GLU ASP ASP ASP
ALA PHE LEU LEU ALA PHE PHE PRO CLYS CLYS CLYS EY2	D206 1594 1594 1594 150 MET ALN ALL ALL ALL ALU ASP ASP	ASP SER SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	PHE TYR TYR SER SER LLU GLY PRO SER ALA
ASN VAL SER ASN ASN QLN PRO TYR ASN GLY THR GLU SER	ARG SER ASP ASP ASP ASP OLU CLU ASP ILV SER SER		
• Molecule 8: sup	eroxide dismutase		
Chain G:	81%		18%
MET TRP SER SER SER SER SER LEU CVS SER SER SER SER	SER ARG GLN CLEU CLEU VAL LEU ASP CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	LEU LEU VAL LYS ASN ASN LYS SER SER CYS GLY VAL VAS	E135 L174 A266
• Molecule 9: Pro	tein PLASTID TRANSC	RIPTIONALLY ACTIV	VE 12-like
Chain H:	49%	51%	
MET ALA SER VAL LEU LEU SER SER LEU TYR GIN ASP ARG	OLY LEU ARG THR MET WET VAL SER ASP OLY PHE PRO CYS CYS CYS	ARG LYS THR LYS THR THR THR THR THR THR THR THR THR THR	LEU VAL SER SER SER SER PRO PHE CIN LYS ALA PRO
LEU ALA PRO CYS CYS CYS CYS CYS GLU CYS GLU LYS GLU SSN ASN	GLN SER CLN CLN CLN CLN CLN SER PHE CLU VAL CLU CLU CLU CLU CLU TTR PHO CLU TTR SER TTR SER SER SER SER SER SER SER SER SER SE	TYR MET MET MET ARP SER SER GLV GLV GLV GLU PRU ALA ALA ALA ALA ALA	SER FRO GLY GLN GLU GLU FRP PRO GLU GLY GLY
THR ALA SER SER ARG VAL ARG ALA ALA ALA ALA ALA CUU	THR CLY THR SER THR CLY THR CLY CLY CLY CLY CLY CLY CLY SER ARG CLY SER ARG	LITS LITS LITS SER ALA ALA ALA ALA ALA CLU CLU TLE TLE TLE	SER ASP ASP ASP ASP SER ALA CLU SER PRO ASP ASN LEU
PRO GLU GLU PRO LIYS ASP ASP L187 N238 N238 N238 N238 B5446	ILE GLU VAL ALA ALA ALA ALA ALA ALA ALA ALA ALA	ASP ASP ASP GLU GLU GLU GLU VAL ASP GLU GLU GLU GLU GLU GLU	LLE THR ARG ASN SER VAL LFEU LFEU LFEU ASN
PRO GLU LLEU LYS SER LYS GLU CLYS CLU PRO LYS LYS LYS	ASP MET SER LEU LLEU CLU CLU CLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ARD PHE ASP GLU GLU GLU GLU	
• Molecule 10: Fr	uctokinase-like 1, chlorop	lastic	
Chain I:	77%	2	3%

D W I D E DATA BANK

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• Molecule 11: Fructokinase-like 2, chloroplastic

Chain i:	58%	•	41%	
MET ALA ALA LEU LEU SER SER LEU LEU SER SER SER	LEU PRO ARG CLN CLN CLN CLN CLN ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	LEU GLN GLN GLN GLV GLY CLEU CYS LEU CYS CLYS CNAL	VAL SER LYS CLV GLV PRO GLU ALA ILE LYS	GLU LEU SER LYS THR
GLU VAL PHE GLY GLY GLY CLYS LYS LYS THR YAL ARG	TLE SER SER LYS ARG ARG ARG ARG ARG LYS LYS UAL VAL VAL CTRR	SEA ASP ASP PRO PRO VAL ASN GLU GLU GLU ASN THR STHR	GLY SER THR GLU GLU GLU LYS LYS CLN GLN ARG	THR ARG LYS LYS LYS
GLU ILE SER SER SER PHE GLY ASP SER SER ILE	SER ASP ASP ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER SER LYS LYS LYS LYS LYS LYS LYS LYS LYS LYS	GLU THR VAL VAL SER FHR FHR GLU SER SER SER LEU	ASP VAL GLU GLY ASN
VAL THR ASP ASP GLU GLU VAL LEU PRO THR SER SER	SER SER GLY GLY GLY SER VAL CLU CLY SER TLE ARG TLE ARG TLS SER CLY SER ALA	SER SER SER SER SER SER SER LVS CLU CLU CLU CLN THR VAL	ARG ARG ARG ARG LYS LYS LYS LYS ASN ASN LEU CGLU	GLU GLY SER GLN THR
GLU LEU SER ASP ASP ASP GLU GLU CLU CLU VAL	ALA ALA ASN ALA ASP ASP ASP ASP GSU VB31 VB31 VB31 T58 H584	T587 E638 E638 ILE LEU VAL VAL VAL SER		
• Molecule 12:	Protein PLASTID TRA	ANSCRIPTIONALI	Y ACTIVE 14-1	ike isoform X2
Chain J:	82%		• 17%	
MET VAL SER SER SER THR THR TLEU LEU LLEU CLN GLN	THR LEU PHE PHE PHIS GLN GLU TRP GLN GLN GLN GLN COU	ALA ALA ALA PRO LEU CLN CLN CLN CLN TLE TLE TLE TLE TLE TLE SER SER	ASN LYS GLY GLY ARG PRO PRO LEU LEU ARG ARG	SER ALA ASN GLY ALA
ALA THR SER SER SER LEU GLU GLU ASP SEP	SER THR THR PRO PRO PRO PRO PHE PHE PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	R1 19 245 245 245 267 8400 8400 8400 8400 8400		
• Molecule 13:	PAP8(pTAC6)			
Chain K:	64%		35%	
MET SER ALA ALA ALA GLN CLEU PHE PHE PHE PHE PHE PRO	PRO LEU LEU SER SER FHR THR THR PHE SER SER SER SER SER SER SER SER SER SE	ALLA PHE ALA LYS LYS THR THR SER SER ASN SER ASN SER VAL VYS	GLN SER LEU THR THR LYS ARG ARG ARG ARG ARG	VAL PHE ALA ASP ASP
GLY ASP ASP ASP ASP GLY GLY FRO ASP ASP ASP ASP	ASP MET ASP ASP ASP GLU CVAL CVAL GLU GLU GLU GLU GLU CVAL CVAL CVAL CVAL CVAL CVAL CVAL CVAL	ASP ASP TYR ASP ASP LEU LEU CLY GLY GLY SER SER SER SER ALA	ALA THR GLY GLY ASP ASP ASP MET MET MET MET SER SER SER	SER PHE V118 T173
P298				
• Molecule 14:	superoxide dismutase			

Chain L:

75%



• Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

$\alpha_1 \cdot \mathbf{M}$		
Chain M:	65%	35%



• Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

Chain m:	6	1%	•	39%	
MET GLN ALA ALA ALA LEU SER SER	PRO PRO PRO PRO PRO GLN GLN SER ALA ALA CYS	SER SER AASN GGLN TYR SER LLYS SER LEU FHE SER SER CYS	THR PRO PRO PRO SER LEU LEU SER	THR GGLN SER LVS SER SER TLE CVS CVS	PRO ALA VAL



 \bullet Molecule 16: UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like

Chain N:		69%	30%	-
MET PRO THR LEU PHE SER LEU PRO	PRO PHE PRO SER LEU LEU HIS HIS ASN PRO PRO PRO CLU	PHE LYS PRO PRO PHE THR SER HIS HIS HIS LEU LEU LEU LEU LYS	PRO THR THR THR LEU THR THR VAL SER ALA ALA ALA ALA ALA ALA TYR TYR	TYR PRO ASN SER ASP ASP
ASP PRO GLU GLU GLU ASP SER	MET HIS GLY GLY VAL ASN LYS PHE GLN GLN GLN GLN GLN GLN	ALA LYS LYS LYS LYS GLN GLN GLU CLU LEU LYS LYS CLY	GLN SER TLE PHE VAL ASN ASN ASP GLU ASP ASP ASP ASP ASP ASP	ASN PRO ALA LEU ASP ASN ASP
ASP ASN SER GLY ASP ASP LEU PHE GLY	GLU TLE ASP ASP ASP ASP ASP ALA ALA LVS CLU CVS GLU VAL	LYS GLY GLY LEU LEU LYS PRO PRO PRO PRO PRO FR	LEU VAL VAL SER GLU GLU ASN ASN ASN ASN CLU CLU CLU CLU CLU CLU	VAL VAL ASP ASP CLU GLU GLU ILE
ASP GLY LEU SER GLY LEU ALA GLU ILE	GLU SER SER ASP ASP CLU CLU CLU CLU SER SER SER SER SER SER SER SER SER	ASP MET QLY CLY CLY CLY SSR SSR SSR SSR SSR SSR SSR SSR SSR SS	11.E ASP ASP PHE GUV CUV PHE CUV CVV ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	L661 T759 E768 SER HIS
• Molecule 1	17: Protein PLAST	ID TRANSCRIPT	IONALLY ACTIVE 7	-like isoform X1
Chain O:	52%	•	47%	_
MET ALA ALA SER THR LEU PHE SER	GLY PHE SER THR LEU CLEU CLEU FHR PHE PRO TLK ALA VAL	GLU ASN THR LYS LYS ASN ARG SER SER SER SER	ALA SER ASN ASN CLVS ASR ASN GLU GLV GLY GLY TRP ARG ARG ARG	ARG LYS LEU THR LYS LYS
ASP GLU THR LEU ASP ALA MET GLU GLU	R54 P141 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	LEU		



• Molecule 18: PAP13(pTAC18)

Chain P: 73%

27%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410910	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 $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 ($6k \ge 4k$)	Depositor
Maximum map value	1.856	Depositor
Minimum map value	-0.729	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	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)

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

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/2237	0.44	0/3034	
1	a	0.31	0/2487	0.44	0/3374	
2	В	0.27	0/6945	0.43	0/9418	
3	С	0.25	0/4518	0.42	0/6148	
4	с	0.32	0/8213	0.46	0/11205	
5	D	0.29	0/5191	0.43	0/7029	
6	Е	0.38	0/4604	0.49	0/6285	
7	F	0.33	0/4339	0.45	0/5885	
8	G	0.41	0/1777	0.46	0/2417	
9	Н	0.28	0/2167	0.40	0/2942	
10	Ι	0.34	0/2970	0.42	0/4026	
11	i	0.33	0/3056	0.44	0/4141	
12	J	0.30	0/3454	0.42	0/4689	
13	К	0.26	0/1824	0.41	0/2468	
14	L	0.69	0/1514	0.76	1/2100~(0.0%)	
15	М	0.45	0/951	0.52	0/1286	
15	m	0.41	0/865	0.55	0/1175	
16	N	0.23	0/3011	0.41	0/4163	
17	0	0.24	0/702	0.36	0/945	
18	Р	0.24	0/915	0.42	0/1241	
All	All	0.32	0/61740	0.45	1/83971~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	\mathbf{L}	152	PHE	N-CA-C	-6.93	92.30	111.00

There are no chirality outliers.

There are no planarity outliers.



5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	289/337~(86%)	277~(96%)	12 (4%)	0	100	100
1	a	314/337~(93%)	303 (96%)	11 (4%)	0	100	100
2	В	897/1070~(84%)	862 (96%)	35~(4%)	0	100	100
3	С	584/688~(85%)	555~(95%)	29~(5%)	0	100	100
4	с	1160/1388~(84%)	1124 (97%)	36 (3%)	0	100	100
5	D	639/892~(72%)	620 (97%)	19 (3%)	0	100	100
6	Е	698/860~(81%)	680 (97%)	18 (3%)	0	100	100
7	F	542/682~(80%)	529 (98%)	13 (2%)	0	100	100
8	G	216/266~(81%)	211 (98%)	5 (2%)	0	100	100
9	Н	258/531~(49%)	254 (98%)	4 (2%)	0	100	100
10	Ι	372/486~(76%)	349 (94%)	23~(6%)	0	100	100
11	i	381/648~(59%)	365 (96%)	16 (4%)	0	100	100
12	J	420/507~(83%)	404 (96%)	16 (4%)	0	100	100
13	К	212/331~(64%)	207 (98%)	5 (2%)	0	100	100
14	L	230/303~(76%)	220 (96%)	9 (4%)	1 (0%)	34	72
15	М	114/178~(64%)	112 (98%)	2(2%)	0	100	100
15	m	107/178~(60%)	100 (94%)	7 (6%)	0	100	100
16	Ν	535/770~(70%)	521 (97%)	14 (3%)	0	100	100
17	Ο	86/167~(52%)	84 (98%)	2 (2%)	0	100	100
18	Р	103/143~(72%)	99 (96%)	4 (4%)	0	100	100
All	All	8157/10762 (76%)	7876 (97%)	280 (3%)	1 (0%)	100	100



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	134	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
1	А	223/308~(72%)	223 (100%)	0	100	100
1	a	257/308~(83%)	255~(99%)	2(1%)	81	93
2	В	667/924~(72%)	663~(99%)	4 (1%)	86	95
3	С	429/612~(70%)	424 (99%)	5 (1%)	71	90
4	с	679/1238~(55%)	671 (99%)	8 (1%)	71	90
5	D	528/770~(69%)	521 (99%)	7 (1%)	69	89
6	Е	300/741~(40%)	294 (98%)	6 (2%)	55	83
7	F	395/615~(64%)	393 (100%)	2 (0%)	88	96
8	G	172/232~(74%)	170 (99%)	2 (1%)	71	90
9	Н	212/472~(45%)	210 (99%)	2 (1%)	78	92
10	Ι	287/437~(66%)	286 (100%)	1 (0%)	92	97
11	i	316/567~(56%)	310~(98%)	6 (2%)	57	84
12	J	352/449~(78%)	346~(98%)	6 (2%)	60	85
13	Κ	199/300~(66%)	197~(99%)	2(1%)	76	91
14	L	83/258~(32%)	77~(93%)	6~(7%)	14	45
15	М	103/160~(64%)	103 (100%)	0	100	100
15	m	92/160~(58%)	91~(99%)	1 (1%)	73	90
16	Ν	95/659~(14%)	93~(98%)	2(2%)	53	82
17	Ο	69/144 (48%)	68 (99%)	1 (1%)	67	88
18	Р	91/129 (70%)	91 (100%)	0	100	100
All	All	5549/9483 (58%)	5486 (99%)	63 (1%)	74	90

5 of 63 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
6	Ε	634	ILE
14	L	145	LEU
8	G	174	LEU
14	L	144	LEU
15	m	101	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
12	J	180	ASN
12	J	281	GLN
17	0	99	GLN
4	с	77	GLN
4	с	73	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)

Of 4 ligands modelled in this entry, 4 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-37386. 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: 200



Y Index: 200



Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200

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: 250



Y Index: 223



Z Index: 184

6.3.2 Raw map



X Index: 250

Y Index: 223

Z Index: 184

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 0.1. 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 1962 nm^3 ; this corresponds to an approximate mass of 1772 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 0.333 ${\rm \AA^{-1}}$



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 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.41	3.08
Unmasked-calculated*	3.65	4.20	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37386 and PDB model 8W9Z. 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 0.1 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 (0.1).



9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.4050
А	0.9810	0.4340
В	0.9900	0.4720
С	0.9950	0.3800
D	0.9950	0.3680
E	0.9750	0.1700
F	0.9960	0.4270
G	0.9940	0.4700
Н	0.9920	0.5000
Ι	0.9930	0.5180
J	0.9940	0.4570
K	0.9910	0.4560
L	1.0000	0.4250
М	0.9900	0.5070
N	1.0000	0.1620
0	0.9930	0.4450
Р	0.9930	0.4410
a	0.9910	0.4690
С	0.9910	0.4090
i	0.9950	0.4700
m	0.9950	0.4400

