

wwPDB EM Validation Summary Report (i)

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PDB ID	:	8WA1
EMDB ID	:	EMD-37388
Title	:	The cryo-EM structure of the Nicotiana tabacum PEP-PAP-TEC2
Authors	:	Wu, X.X.; Zhang, Y.
Deposited on	:	2023-09-06
Resolution	:	2.80 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 2.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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 >=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	337	83%	• 15%
1	a	337	86%	• 10%
2	В	1070	90%	• 7%
3	С	688	90%	5% 5%
4	D	892	68% •	28%
5	Е	860	79%	19%
6	F	682	78%	20%
7	G	266	79% •	18%



Mol	Chain	Length	Quality of chai	n
8	Н	531	48% •	51%
9	Ι	486	75%	• 23%
10	J	507	79%	• 17%
11	Κ	331	61% .	38%
12	L	303	71%	5% 24%
13	М	178	65%	• 35%
13	m	178	59% •	39%
14	N	770	68%	• 30%
15	0	167	56% •	42%
16	Р	143	69%	• 29%
17	Q	24	17% 83%	
18	R	24	58%	42%
19	S	27	230/	67%
20	C C	1388	0.00	150/
20		1300	82%	• 15%
21	ì	648	57% •	42%



2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 62699 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	1 A	200	Total	С	Ν	Ο	\mathbf{S}	0	0
	200	2190	1392	378	409	11	0	0	
1	1 a	303	Total	С	Ν	Ο	\mathbf{S}	0	0
1			2358	1508	405	434	11	0	U

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

Mol	Chain	Residues		Α	AltConf	Trace			
2	В	998	Total 7604	C 4823	N 1367	O 1391	S 23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	653	Total 4899	C 3131	N 873	O 875	S 20	0	0

• Molecule 4 is a protein called PAP1(pTAC3).

Mol	Chain	Residues		At	AltConf	Trace			
4	D	645	Total 5063	C 3202	N 885	O 950	S 26	0	0

• Molecule 5 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplasticlike.

Mol	Chain	Residues		At	AltConf	Trace			
5	Е	700	Total 4563	C 2840	N 829	O 872	S 22	0	0

• Molecule 6 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.



Mol	Chain	Residues		At	AltConf	Trace			
6	F	544	Total 4259	C 2692	N 763	O 785	S 19	0	0

• Molecule 7 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total 1742	C 1134	N 291	0 310	${f S}{7}$	0	0

• Molecule 8 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

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

• Molecule 9 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues		At	AltConf	Trace			
9	Ι	376	Total 2946	C 1886	N 519	O 528	S 13	0	0

• Molecule 10 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	J	421	Total 3410	C 2184	N 577	O 627	S 22	0	0

• Molecule 11 is a protein called PAP8(pTAC6).

Mol	Chain	Residues		Ate	AltConf	Trace			
11	K	204	Total 1705	C 1077	N 298	O 322	S 8	0	0

• Molecule 12 is a protein called superoxide dismutase.

Mol	Chain	Residues		At	AltConf	Trace			
12	L	229	Total 1776	C 1141	N 306	0 324	${S \atop 5}$	0	0

• Molecule 13 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	М	116	Total 935	C 598	N 150	0 180	${ m S} 7$	0	0
13	m	109	Total 855	C 548	N 136	0 164	S 7	0	0

• Molecule 14 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6diaminopimelate ligase-like.

Mol	Chain	Residues		At	AltConf	Trace			
14	Ν	537	Total 2995	C 1825	N 582	0 582	S 6	0	0

• Molecule 15 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	О	97	Total 780	C 490	N 140	0 146	$\frac{S}{4}$	0	0

• Molecule 16 is a protein called PAP13(pTAC18).

Mol	Chain	Residues		At	oms		AltConf	Trace	
16	Р	102	Total 843	$\begin{array}{c} \mathrm{C} \\ 547 \end{array}$	N 142	0 151	${ m S} { m 3}$	0	0

• Molecule 17 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
17	Q	4	Total 82	C 40	N 11	O 27	Р 4	0	0

• Molecule 18 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues		Ate	AltConf	Trace			
18	R	14	Total 285	C 136	N 53	O 82	Р 14	0	0

• Molecule 19 is a RNA chain called RNA (27-mer).

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
19	S	9	Total 192	C 86	N 35	O 62	Р 9	0	0



• Molecule 20 is a protein called DNA-directed RNA polymerase subunit beta".

Mol	Chain	Residues		Α	toms			AltConf	Trace
20	с	1176	Total 8166	C 5119	N 1500	O 1517	S 30	0	0

• Molecule 21 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues		At	oms			AltConf	Trace
21	i	375	Total 2937	C 1873	N 500	0 548	S 16	0	0

• Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
22	В	1	Total Zn 1 1	0

• Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 24 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
24	G	1	Total Fe 1 1	0
24	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





MET ASN ASN ASN ASN PHE PHE SER ILE GLN ASP ASP GLY GLY CLY



• Molecule 4: PAP1(pTAC3)



Chain F.

U	na	III	E:													79	9%													•			19	9%								
MET	LEU	SER CYS	ASN SER	PHE	PRO	VAL PHE	THR	VAL	PRO	SER	HIS	ARG	LEU	PHE	AL.A	LYS	ILE	ASN	TYR	GLY	LEU	SER	PRO	HIS	ARG	LEU	LEU	THR	VAL	ALA VAL	ARG	ALA LYS	PRO	LYS	LEU	ILE LEU	GLY	ASN	THR	VAL		
_																													٠	ب	•				•	•		Þ	٠	•	•	•
THR	VAL GLU	CLY GLY	LYS TYR	SER	ASP	VAL GLU	THR	U I I E O	ASN	LEU	SER	SER	PRO	PRO	GLV	SER	ILE	ALA	CYS	LEU	ASP THR	PHE	LYS	LYS	LEU	LEU	THR	D102	F107	K108	E109	F110	TITA	A112	G114	D115		R118	R121	Y125		I130
	•	٠	•	•			•	•	•	•		٠	•		•	•	•	•																								
-	K133	1145 1446	G147	R148	E149	G150	V167	A168	R183	N184		K201	1 C U U	N.234 НО 35	F736	00	E270	A271		F392	E515	DEEO	8GGH	F580	K584	-	L599	E613	K600	-	E641	L676	K670		R684	V710	1 02.4	E/ 31 L732	F733	V747 V748	-	R788
L796	S801	SER	GLU PRO	SER	GLY	SER	LYS	ASP	ARG	ILE	PRO	LEU	ASN	SER	TLE	SER	LEU	CLV GLV	THR	GLN	THR SER	VAL	SER	ALA	LYS	SER	GLU	SER	ASN	ALA ASP	SER	ARG	SER	THR	SER	ASP SER	GLU	LEU MET	ALA	YIN		
SER	VAL																																									
•	M	ole	CII	le	6.	Р	roi	tei	'n	P	L	4.9	зт	ΤT)	T	R	AI	NS	30	'R	IF	г	יז <i>ר</i>	ЛС	JΔ	ΔT.	LN	Y	A	гг	עוי	JF		10	-li]	ke					

Chain F:

78%



20%

MET THR MET TTHR SERVELLEU SERVER SER ALA PHE LEU GLU ALA ALA PHE GLY LYS GLU LYS ASP SER ASP GLU VAL VAL VAL VAL VAL VAL VAL ASP ASP AL/ GLN GLN UAL VAL VAL ARC GLU GLU CLEU TYR ASP GGLU GGLU ASP ASP ASP ASP ASSERT • Molecule 7: superoxide dismutase Chain G: 79% 18% MET TRPACE SERNA S • Molecule 8: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like Chain H: 48% 51% MALLA ALLA LUCULUU ALLA MALLA ALLA MALLA ALAGA ARREAL ALA THR ARG SERA ARG ALA ARG ALA ARG ALA ARG GLU PRO GUN PRO FON P • Molecule 9: Fructokinase-like 1, chloroplastic Chain I: 75% 23% MET TILE SERVER SERVER

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• Molecule 10: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2

79%

Chain J:

17%

MET VAL SER SER SER THR THR ILE LEU CLN GLN PRO	THR ASN LEU LEU HHE CLN CLN PRO CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	PAUA LEU GLN CLN CLN CLN CLN CLN CLN CLN CLN SER SER SER SER SER SER SER SER SER SER	ARG PRO LEU LEU ARG ARA ARA ASN ALA SSN ALA ASN ALA
ALA THR SER SER SER THR LEU GLU GLU GLU GLV SER SER	SER PRO PRO PRO SER SER PRO PRO LEU PRO SER PRO CIN CIN DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 86 DI 87 DI 8	V269 1287 1287 1300 1300 1300 1300 13362 13362 13362 13362 13370 13470	8402 8403 8404 8404 1416 1416 E444 H450
L453 1458 F507			
• Molecule 11:	PAP8(pTAC6)		
Chain K:	61%	• 38%	
MET SER ALA ALA ALA GLN CLN LEU PHE PHE PRO PRO	PRO LEU LEU THR PHE PHE PHE PHE PRO PRO PRO PRO CLN LEU LEU LEU LEU LEU LEU THR FHE FHE	VAL LYS PRO TLE SER SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	LYS ARG ARG ARG ARG ASP PHE ARG ARG ARG ARA ASP ASP
GLU ASP ALA ALA ASP GLY GLY FRO ASP ASP ASP	MSP MSP ASP ASP CLU ASP CLU CLU CLU CLU CLU SSP ASP ASP ASP ASP ASP ASP ASP ASP ASP	THSF THS LEU CLEU CLEU CLEU CLEU CLEU CLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA ASP SSP	ILE ALA ALA MET VAL HIS SER SER SER SER PHE VAL THR
GLN GLY TRP ASN SER GLU LVS LVS LVS LVS LVS K272	R312 V337 F331		
• Molecule 12:	superoxide dismutase		
Chain L:	71%	5%	24%
MET MET MET ALA ALA ALA SER THR THR LEU LLU THR	SER ALLA PHE PHE PHO PHE PHE PHE CLN CYS CYS CYS ARG CYS ARG CYS ARG CYS ARG CYS TRP TRP TRP TRP	HLS LLYS LLYS CLN PHE PHE ALA ALA PHC PRO CLY PRO CLY FRO PRO ALA ALA ALA	L51 M65 M65 F70 E71 H78 E100
L104 1105 1106 ASP ASP ASP ASP LEU LEU	F162 9169 9169 122 1225 1222 1222 1222 1222 1222 1232 123	GLY CULU VAL ARG CUU UAL TTRR VAL TTRR SER SER ASP ASP ASP ALA ALA	
• Molecule 13:	Thioredoxin-like protein CI	TRX1, chloroplastic	
Chain M:	65%	• 35	%
MET GLN ALA ALA ALA ALA LEU FLEU FRO PRO	ALA PRO PRO PRO PRO PRO PRO PRO ALA ALA ASER ASIR ASIR ASIR ASIR ASIR ASIR ASIR ASI	PHE SPHE TYR TYR CYS CYS CYS CYS PRO PRO PRO PRO FRO FRO SER THR THR THR THR	LEU SER ARG LYS SER ILYS PRO PRO PRO VAL
ALA THR G3 L144 L178			
• Molecule 13:	Thioredoxin-like protein CI	TRX1, chloroplastic	
Chain m:	59%	• 39%	
MET GLN GLN ALA ALA ALA ILEU PHE PHE PRO LEU	ALA PRO PRO CLN THR SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	PHE SER TYR TYR TYR CYS PRO PRO PRO PRO SER LEU LEU LEU LEU SER THR THR	LEU SER ARG LYS SER ILYS SER LYS PRO PRO ALA VAL



• Molecule 14: UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like

Chair	n N:		68%	•	30%	
MET PRO PHE THR	LEU PHE SER LEU PRO PRO PHE	PRO SER LEU LEU HIS ASN PRO PRO PRO LEU	GLN PHE LYS PRO PRO FRA SER HIS HIS LEU	ARG LEU LYS TYR PRO PRO THR LEU THR THR	VAL SER ALA ALA GLY ALA ASP GLY CYS TYR TYR PRO	ASN PRO SER ASP ASP
ASP PRO GLU	ALA PRO GLU ASP SER MET HIS	GLY VAL ASN ASN LYS PHE GLN GLN GLN GLN GLN GLN	ALA ALA LYS LYS ALA ALA CYS GLU GLU GLU CEU	PHE LYS LYS GLU GLU GLN SER TLE PHE PHE ASN	ALA LEU ALA ASP VAL GLU ASP ASP ASP ASP PRO	ALA LEU ASN ASP ASN
ASP ASN SER GLY	ASP ASP LEU PHE GLY GLU ILE	ASP LYS ALA ALA ALA LEU LEU LYS ARG CLU GLU	VAL LYS GLY GLY LEU LEU LEU PRO PRO PRO	LYS ASN ASN THR THR LEU VAL CLU SER SER VAL	GLU ASN VAL ASP GLU GLU GLU GLU GLU VAL VAL	ASP LEU GLU GLU ILE
ASP GLY LEU SER	GLY LEU ALA GLU GLU GLU	SER ASP GLU GLU CLYS SER ASP ASP CLU CLU VAL SER	ASP ASP ASP ASP CLY CLY SLR SBR SBR ASP ASP ASP ASP	SER SER PHE ASP ILE ASP ASP CUU PHE	GLY LYS LYS THR LYS LYS PRO ARG ILE VAL E232 P471	K506 5507 7588 7588
H596 V608	1633 N651 T654 M672	L687 T759 F762 E768 SER HIS				
• Mo	lecule 15:	Protein PLAS	FID TRANSCI	RIPTIONALL	Y ACTIVE 7-lik	xe isoform X1
Chair	n O:	56%		•	42%	
MET ALA ALA SER	THR LEU THR PHE SER GLY PHE	SER THR LEU GLN THR PHE PRO LYS ILE ALA ALA	VAL GLU ASN THR LYS ASN VAL ASN PHE SER SER ILE	ARG SER GLN SER ALA SER ASN LYS ASN	GLU SER ARG GLY GLY ARG TLE TLE TRP ARG ARG	LYS LEU LYS LYS
ASP GLU THR LEU	ASP ALA LYS MET GLU R54	R78 E102 K147 L150 LEU				
• Mo	lecule 16:	PAP13(pTAC1	8)			
Chair	n P:		69%	·	29%	-
MET ALA SER PHE	ILE THR MET PRO ALA LEU SER	TYR LEU SER THR ASN SER SER SER CLU GLU	THR ASN PHE ARG PRO SER SER ARG GLY GLN	GLY VAL ARG ALA MET ARG THR E41 E45	174 191 895 818 858 858	
• Mo	lecule 17:	DNA (24-mer)				
Chair	n Q: 1	7%		83%		
DC DT DT	DA DT DT DC DC DC	DA DT DA DG DC DC DT T17	120			
• Mo	lecule 18:	DNA (24-mer)				
Chair	n R:	58%			42%	
A-4 C9 DG	DT DG DA DA DA	bc				



• Molecule 19: RM	NA (27-mer)			
Chain S:	33%	6	57%	
い コ < < コ < < こ < ひ < ひ o	ج ں ہے تو م م م			
• Molecule 20: DI	NA-directed RNA	polymerase sub	unit beta"	
Chain c:	8	2%	• 15%	
MET GLU GLU ARG NG NG NG NG NG NG NG NG NG NG	165 V94 E102 E114 Q157 Q151 Q191	v312 1320 LEU LEU ARG ARG PHE	HIS THR GLY GLY VAL PHE THR GLY GLY GLY THR THR THR	N397 E422 R480 N498 ALA
HIS HHE LEU SER SER CYS CYY ARG TYR THR ASR ASN LEU	VAL VAL THR ASN ASN ASN GLN GLN CLA CLA FHC FHC FHC	ASP ASP PHE CLYS CLYS CLYS CLY ARC ARC ARC TLC PRO	ASP TYR SER ASP ASP ASP ASP TLE CYS CYS GLY GLY TCE	ASN ASN LEU TYR S55 K569 K569 R570
R571 R571 R580 SER. SER. CLN GLN GLU ASN ASN LEU LEU LEU MET	PR0 CYS SCYS SCYS SCYS CLY ISS CLY TYR CLY TYR CLY CLY CLY THR CLU	HIS SER VAL LYS LYS LYS CLU ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ARG GLY VAL LYS CLU CLU PRO CLU CLYS CLYS VAL	D661 R747 N748 S749 K750 K843
K944 K955 K955 K955 K955 K178 K18 K18 K18 K18 K18 K18 K18 K18 K18 K1	SER ILYS LYS LYS LYS PRO PRO TLE TLE TLE ASR ASR ASR ASY	q1010 K1022 D1038 11067 T1128 L1128	K1136 SER SER ARC SER ARC ARC ARC ARC ARC ARC ARC ARC ARC AR	N1173 1182 1182 1182 1182 1233 V1270
F1290 G1330 LEU VAL HIS PRO SER LYS PRO SER LYS CIN HIS ASN ASN	ILE PRO LEU CLEU GLU GLV LVS LVS LVS ASN ASN PHE GLV GLV	GLU MET ASP ASP ILE LEU HIS HIS LYS LYS LYS LEU	PHE ASP ASP CYS CYS CYS LEU LEU LEU ASN PHE PHE HIE TILE TILE	GLN SER PHE ILE GLY PHE ASN ASP
SER				
• Molecule 21: Fr	uctokinase-like 2,	chloroplastic		
Chain i:	57%	·	42%	_
MET ALA ALA LEU SER PHE SER LEU CLEU CLEU CLEU PRO	ARG GLN HIS LEU HIS LEU HIS ASN PHE PRO ASN MET MET	VAL MET GLN GLN GLN GLY CLEU CLEU LEU LYS ASN LYS	TRP VAL LEU MET ALA VAL ALA CLY GLU FRO GLU GLU	TLE ALA CLYS CLVS CLU CLVS SER LYS THR
GLU VAL PHE CPHE GLY ALA ALA ALA CLYS LLYS LLYS LLYS THR THR THR THR SER	LYS ARG ALA PPRO PRO ALA ALA ARG ARG LYS LYS VAL VAL	GLU THR SER ASP ASP PRO PRO VAL VAL VAL CLU GLU	ALA ALA GLU ASN THR SER SER SER CLU CLU PRO CLU CLY STU	GLN GLN ARG ARG ARG LYS LYS LYS LYS
GLU TLE VAL GLU SER SER PHE GLY ASP SER TLE SER SER	ALA GLU GLU GLU ASN VAL TLE ASP GLU ALA GLU GLU GLU	PRO GLU SER SER SER ALA LYS PRO PRO LYS THR THR ARG	THR ARG LYS LYS LYS LYS CLU CYS GLU VAL VAL YAL SER THR THR CIU	SER THR LEU ASP VAL GLU GLU ASN
VAL THR ASP ASP CLU CLU CLU CLU PRO FRO SER SER SER SER	0.LU 0.LV 7.GL 7.LV 0.LU 1.LE 1.LY STR 1.LYS LYS	ALA SER SER SER SER SER CLU CLU CLU CLU PRO	THR CIAN CIAN CIAN CIAN VAL ARG ARG CIAN CIAN ARG CIAN	LEU GLU ASP GLU GLV GLV GLN THR
GLU LEU SER SER ASP ILEU CLU CLU CLU CLU CLU CLU CLU CLU ALA ASN	ALA ASP ALA ASP ASP ASP GLU GLU GLU CGLU ASP PHE ASP CLY	GLY GLY R3 08 R3 08 R3 08 M5 61 L5 61 L5 96	R642 LLEU LLEU VAL PRO VAL SER	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88607	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 $(e^-/\text{\AA}^2)$	57.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \times 4k)$	Depositor
Maximum map value	1.362	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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).

Mal	Chain	Bond	lengths	Bo	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/2227	0.43	0/3019
1	a	0.24	0/2403	0.41	0/3256
2	В	0.40	0/7751	0.51	3/10510~(0.0%)
3	С	0.32	0/4998	0.45	1/6792~(0.0%)
4	D	0.26	0/5161	0.42	0/6986
5	Е	0.24	0/4633	0.39	0/6321
6	F	0.26	0/4366	0.40	0/5918
7	G	0.38	0/1793	0.50	0/2437
8	Н	0.29	0/2167	0.38	0/2942
9	Ι	0.26	0/3021	0.41	0/4092
10	J	0.26	0/3498	0.40	0/4742
11	К	0.25	0/1747	0.40	0/2362
12	L	0.41	0/1828	0.55	0/2488
13	М	0.41	0/951	0.50	0/1286
13	m	0.34	0/869	0.45	0/1179
14	N	0.26	0/3024	0.45	0/4180
15	0	0.25	0/793	0.36	0/1065
16	Р	0.23	0/870	0.40	0/1182
17	Q	0.32	0/90	0.73	0/137
18	R	0.35	0/319	0.70	0/489
19	S	0.27	0/214	0.65	0/331
20	с	0.29	0/8294	0.44	0/11306
21	i	0.26	0/3009	0.44	0/4078
All	All	0.30	0/64026	0.44	4/87098~(0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

2 B 964 GLY N-CA-C 9.52 136.91 113.10	Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
	2	В	964	GLY	N-CA-C	9.52	136.91	113.10



0 0	iraca ji cii	e proces	rage				
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	911	THR	N-CA-C	-7.00	92.10	111.00
3	С	394	GLY	N-CA-C	-6.14	97.75	113.10
2	В	450	LEU	CA-CB-CG	5.19	127.23	115.30

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	entiles
1	А	284/337~(84%)	276 (97%)	8(3%)	0	100	100
1	a	299/337~(89%)	291 (97%)	8 (3%)	0	100	100
2	В	992/1070~(93%)	973~(98%)	19 (2%)	0	100	100
3	С	647/688~(94%)	629~(97%)	18 (3%)	0	100	100
4	D	639/892~(72%)	627 (98%)	12 (2%)	0	100	100
5	Е	698/860~(81%)	691 (99%)	7 (1%)	0	100	100
6	F	542/682~(80%)	532 (98%)	10 (2%)	0	100	100
7	G	216/266~(81%)	207 (96%)	9 (4%)	0	100	100
8	Н	258/531~(49%)	256 (99%)	2 (1%)	0	100	100
9	Ι	374/486~(77%)	365~(98%)	9 (2%)	0	100	100
10	J	419/507~(83%)	412 (98%)	6 (1%)	1 (0%)	47	78
11	K	202/331~(61%)	200 (99%)	2 (1%)	0	100	100
12	L	225/303~(74%)	215 (96%)	10 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
13	М	114/178~(64%)	112 (98%)	2(2%)	0	100	100
13	m	107/178~(60%)	107~(100%)	0	0	100	100
14	Ν	535/770~(70%)	523~(98%)	12 (2%)	0	100	100
15	Ο	95/167~(57%)	93~(98%)	2(2%)	0	100	100
16	Р	100/143~(70%)	100 (100%)	0	0	100	100
20	с	1162/1388~(84%)	1129 (97%)	33~(3%)	0	100	100
21	i	373/648~(58%)	360 (96%)	13(4%)	0	100	100
All	All	8281/10762 (77%)	8098 (98%)	182 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	408	GLY

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	Percentiles
1	А	226/308~(73%)	219~(97%)	7 (3%)	40 74
1	a	256/308~(83%)	242 (94%)	14 (6%)	21 52
2	В	767/924~(83%)	735~(96%)	32~(4%)	30 63
3	С	465/612~(76%)	432 (93%)	33~(7%)	14 39
4	D	523/770~(68%)	488 (93%)	35~(7%)	16 43
5	Ε	308/741~(42%)	289 (94%)	19 (6%)	18 47
6	F	401/615~(65%)	391~(98%)	10 (2%)	47 80
7	G	176/232~(76%)	168 (96%)	8 (4%)	27 60
8	Н	212/472~(45%)	205~(97%)	7 (3%)	38 72
9	Ι	298/437~(68%)	286 (96%)	12 (4%)	31 65
10	J	368/449~(82%)	$350 \ (95\%)$	18(5%)	25 57



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Κ	192/301~(64%)	189~(98%)	3(2%)	62 88
12	L	167/258~(65%)	153~(92%)	14 (8%)	11 31
13	М	103/160~(64%)	102~(99%)	1 (1%)	76 93
13	m	93/160~(58%)	89~(96%)	4 (4%)	29 62
14	Ν	99/659~(15%)	89~(90%)	10 (10%)	7 22
15	Ο	79/144~(55%)	75~(95%)	4(5%)	24 55
16	Р	82/129~(64%)	78~(95%)	4(5%)	25 57
20	с	697/1238~(56%)	666~(96%)	31 (4%)	28 61
21	i	316/567~(56%)	311 (98%)	5 (2%)	62 88
All	All	5828/9484~(62%)	5557 (95%)	271 (5%)	31 60

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
20	с	8	VAL
20	с	157	GLN
20	с	1270	VAL
4	D	758	ASP
4	D	496	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such side chains are listed below:

Mol	Chain	Res	Type
15	0	120	ASN
21	i	546	ASN
1	a	187	HIS
20	с	449	HIS
4	D	778	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	8/27 (29%)	0	0

There are no RNA backbone outliers to report.

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 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-37388. 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: 280



Y Index: 280



Z Index: 280

6.2.2 Raw map



X Index: 280

Y Index: 280

Z Index: 280

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: 274



Y Index: 307



Z Index: 256

6.3.2 Raw map



X Index: 274

Y Index: 307

Z Index: 256

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.



Mask visualisation (i) 6.6

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_37388_msk_1.map (i) 6.6.1





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 2097 $\rm nm^3;$ this corresponds to an approximate mass of 1894 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 0.357 ${\rm \AA^{-1}}$



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 0.357 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	2.80	-	-	
Author-provided FSC curve	2.81	3.25	2.85	
Unmasked-calculated*	3.83	7.59	3.94	

*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 3.83 differs from the reported value 2.8 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37388 and PDB model 8WA1. 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, 99% 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	0.9920	0.4140
А	0.9940	0.4720
В	0.9960	0.4970
С	0.9920	0.4530
D	0.9880	0.3930
Е	0.9600	0.1560
F	0.9970	0.3910
G	0.9950	0.3960
Н	0.9970	0.5150
I	0.9980	0.5290
J	0.9940	0.4810
K	0.9940	0.4900
L	0.9990	0.2920
М	0.9980	0.5330
N	0.9890	0.1520
0	0.9960	0.5040
Р	0.9990	0.3830
Q	1.0000	0.2810
R	1.0000	0.3110
S	1.0000	0.3220
a	0.9970	0.4980
С	0.9920	0.4130
i	0.9970	0.4850
m	0.9950	0.4610

