

# Full wwPDB EM Validation Report (i)

#### Feb 26, 2024 – 06:38 PM EST

PDB ID : 6VM1

EMDB ID : EMD-21235

Title: Chloroplast ATP synthase (C3, CF1FO)

Authors: Yang, J.-H.; Williams, D.; Kandiah, E.; Fromme, P.; Chiu, P.-L.

Deposited on : 2020-01-27

Resolution : 7.90 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:

EMDB validation analysis : 0.0.1.dev70

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $MapQ \quad : \quad 1.9.13$ 

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

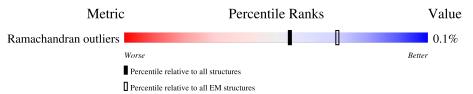
Validation Pipeline (wwPDB-VP) : 2.36

## 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 7.90 Å.

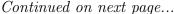
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023

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	A	507	95%	
1	В	507	96%	
1	С	507	96%	
2	D	498	94%	
2	Е	498	94%	
2	F	498	94%	
3	I	184	80%	20%
4	J	222	59% 41%	
5	a	247	90%	10%
6	d	257	68%	31%
7	e	134	96%	•





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Mol	Chain	Length	Quality of chain	
8	g	364	86%	• 13%
9	M	81	98%	
9	N	81	98%	
9	О	81	98%	
9	Р	81	98%	
9	Q	81	15% 98%	
9	R	81	98%	
9	S	81	7% 98%	
9	Т	81	98%	
9	U	81	7%	
9	V	81	98%	
9	W	81	98%	
9	X	81	98%	
9	Y	81	98%	
9	Z	81	98%	



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25331 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 ATP synthase subunit alpha, chloroplastic.

Mol	Chain	Residues		Ator	ns		AltConf	Trace
1	Λ	495	Total	С	N	О	0	0
1	Λ	490	2436	1446	495	495	0	0
1	В	498	Total	С	N	О	0	0
1	Б	490	2451	1455	498	498	U	U
1	C	501	Total	С	N	О	0	0
1	C	301	2466	1464	501	501	0	0

• Molecule 2 is a protein called ATP synthase subunit beta, chloroplastic.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	480	Total C N O 2353 1393 480 480	0	0
2	E	478	Total C N O 2343 1387 478 478	0	0
2	F	479	Total C N O 2348 1390 479 479	0	0

• Molecule 3 is a protein called ATP synthase subunit b, chloroplastic.

Mo	Chain	Residues	Atoms				AltConf	Trace
3	Т	148	Total	С	N	О	0	0
3	1	140	731	435	148	148	0	

• Molecule 4 is a protein called ATP synthase subunit b', chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	131	Total 651	C 389	N 131	O 131	0	0

• Molecule 5 is a protein called ATP synthase subunit a, chloroplastic.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	223	Total 1096	C 650	N 223	O 223	0	0

• Molecule 6 is a protein called ATP synthase delta chain, chloroplastic.

Mol (	Chain	Residues	${f Atoms}$				AltConf	Trace
6	d	177	Total	C	N 177	O 177	0	0

• Molecule 7 is a protein called ATP synthase epsilon chain, chloroplastic.

Mol	Chain	Residues	${f Atoms}$				AltConf	Trace
7	е	129	Total 637	C 379	N 129	O 129	0	0

• Molecule 8 is a protein called ATP synthase gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
Q	C.	316	Total	С	N	O	0	0
	g	310	1566	934	316	316		

• Molecule 9 is a protein called ATP synthase subunit c, chloroplastic.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
9	R	79	Total	С	N	О	0	0
9	π	19	384	226	79	79	0	U
9	Q	79	Total	С	N	О	0	0
9	Q	19	384	226	79	79	U	U
9	Р	79	Total	С	N	O	0	0
	1	19	384	226	79	79		0
9	О	79	Total	С	N	O	0	0
9		19	384	226	79	79	0	U
9	N	79	Total	С	N	О	0	0
9	11	19	384	226	79	79	U	U
9	M	79	Total	С	N	O	0	0
	101	19	384	226	79	79		0
9	Z	79	Total	С	N	О	0	0
9	L	19	384	226	79	79		U
9	Y	79	Total	С	N	О	0	0
9	1	19	384	226	79	79	U	
9	X	79	Total	С	N	О	0	0
	Λ	19	384	226	79	79	U	



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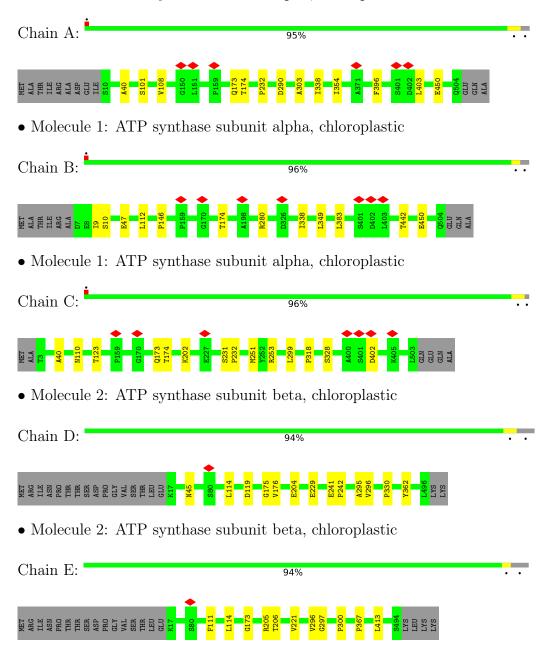
Mol	Chain	Residues		Aton	ıs		AltConf	Trace
9	W	79	Total	С	N	О	0	0
9	VV	19	384	226	79	79	0	U
9	V	79	Total	С	N	О	0	0
9	v	19	384	226	79	79	0	U
9	U	79	Total	С	N	О	0	0
9		19	384	226	79	79		U
9	Т	79	Total	С	N	О	0	0
9	1	19	384	226	79	79		U
9	S	79	Total	С	N	О	0	0
9	l B	19	384	226	79	79		U



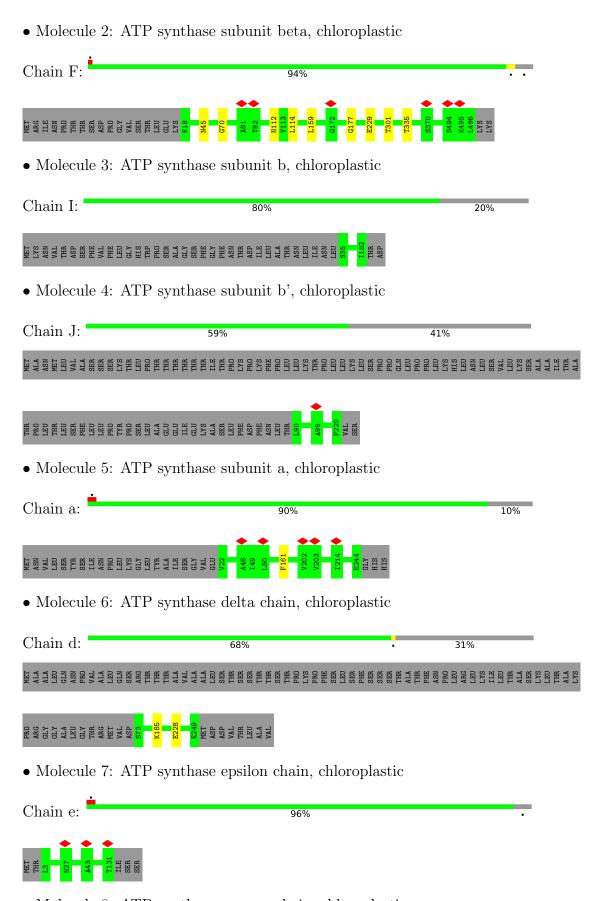
## 3 Residue-property plots (i)

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: ATP synthase subunit alpha, chloroplastic

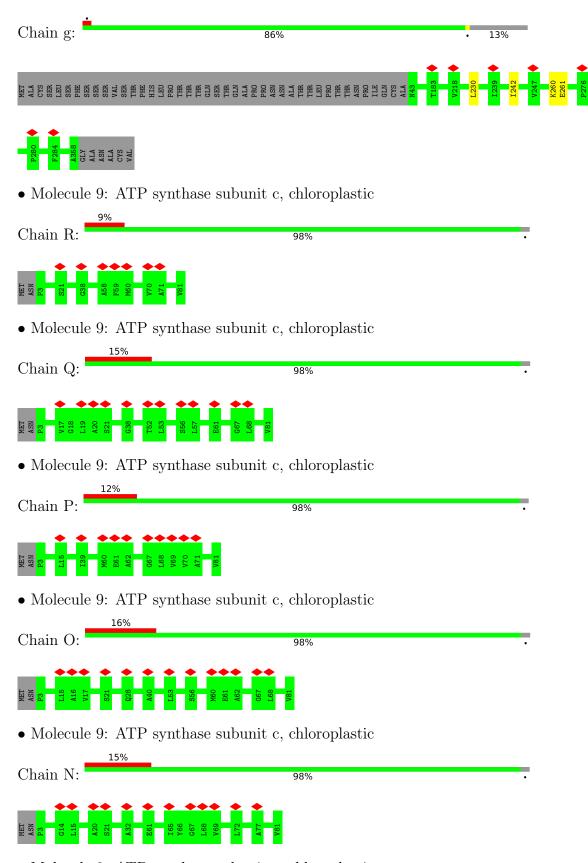






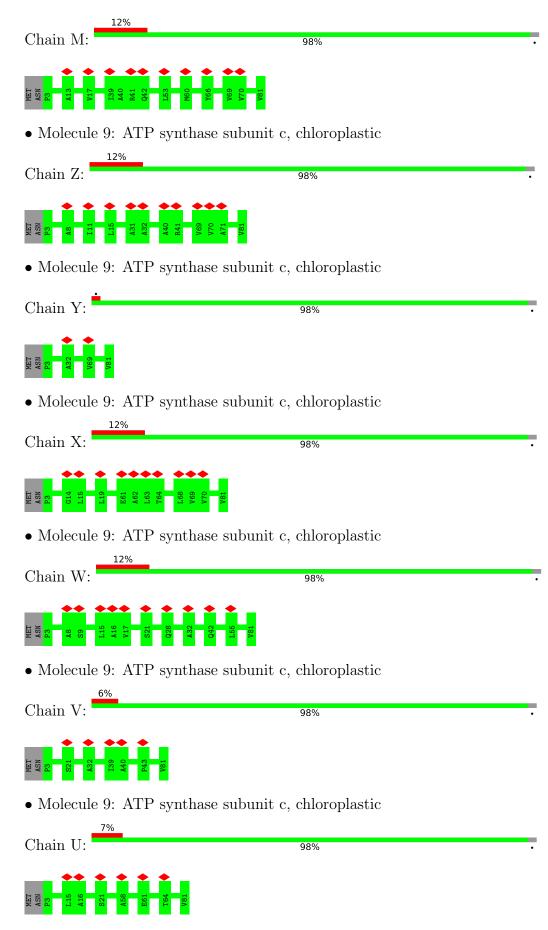
• Molecule 8: ATP synthase gamma chain, chloroplastic





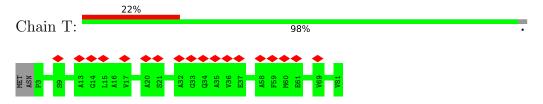
• Molecule 9: ATP synthase subunit c, chloroplastic







 $\bullet$  Molecule 9: ATP synthase subunit c, chloroplastic



 $\bullet$  Molecule 9: ATP synthase subunit c, chloroplastic





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13947	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 $(e^-/\text{Å}^2)$	43.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	48077	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00948	Depositor
Map size (Å)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	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	Во	nd lengths	Во	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	0.42	0/2435	0.57	0/3384
1	В	0.43	0/2450	0.61	0/3405
1	С	0.42	0/2465	0.62	0/3426
2	D	0.43	0/2352	0.62	1/3263 (0.0%)
2	Е	0.44	0/2342	0.61	0/3249
2	F	0.44	0/2347	0.59	0/3256
3	I	0.34	0/730	0.37	0/1015
4	J	0.33	0/650	0.44	0/906
5	a	0.34	0/1095	0.49	0/1520
6	d	0.41	0/876	0.51	0/1220
7	е	0.41	0/636	0.66	0/884
8	g	0.43	1/1565~(0.1%)	0.53	0/2181
9	M	0.32	0/383	0.41	0/528
9	N	0.32	0/383	0.41	0/528
9	О	0.32	0/383	0.42	0/528
9	P	0.32	0/383	0.41	0/528
9	Q	0.32	0/383	0.41	0/528
9	R	0.32	0/383	0.41	0/528
9	S	0.32	0/383	0.42	0/528
9	Т	0.32	0/383	0.41	0/528
9	U	0.32	0/383	0.41	0/528
9	V	0.32	0/383	0.41	0/528
9	W	0.32	0/383	0.42	0/528
9	X	0.32	0/383	0.41	0/528
9	Y	0.32	0/383	0.41	0/528
9	Z	0.32	0/383	0.41	0/528
All	All	0.40	1/25305~(0.0%)	0.55	1/35101 (0.0%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	В	0	12
1	С	0	14
2	D	0	10
2	Е	0	9
2	F	0	9
6	d	0	2
8	g	0	2
All	All	0	71

### All (1) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
8	g	230	LEU	C-N	-6.72	1.18	1.34

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	362	TYR	C-N-CA	5.54	145.27	122.00

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	SER	Peptide
1	A	108	VAL	Peptide
1	A	173	GLN	Peptide
1	A	174	THR	Peptide
1	A	232	PRO	Peptide
1	A	290	ASP	Peptide
1	A	303	ALA	Peptide
1	A	338	ILE	Peptide
1	A	354	ILE	Peptide
1	A	396	PHE	Peptide
1	A	40	ALA	Peptide
1	A	403	LEU	Peptide
1	A	450	GLU	Peptide
1	В	10	SER	Peptide
1	В	112	LEU	Peptide
1	В	146	PRO	Peptide
1	В	174	THR	Peptide
1	В	280	ARG	Peptide



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Mol         Chain         Res         Type         Group           1         B         338         ILE         Peptide           1         B         349         LEU         Peptide           1         B         383         LEU         Peptide           1         B         442         THR         Peptide           1         B         47         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C <td< th=""><th>1         B         338         ILE         Peptic           1         B         349         LEU         Peptic           1         B         349         LEU         Peptic           1         B         383         LEU         Peptic           1         B         442         THR         Peptic           1         B         450         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         110         ASN         Peptic           1         C         173         GLN         Peptic           1         C         173         GLN         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         233         ARG         Peptic           1         C         253         ARG         Peptic           1         C         253         <t< th=""><th></th><th colspan="6">Continued from previous page</th></t<></th></td<>	1         B         338         ILE         Peptic           1         B         349         LEU         Peptic           1         B         349         LEU         Peptic           1         B         383         LEU         Peptic           1         B         442         THR         Peptic           1         B         450         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         110         ASN         Peptic           1         C         173         GLN         Peptic           1         C         173         GLN         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         233         ARG         Peptic           1         C         253         ARG         Peptic           1         C         253 <t< th=""><th></th><th colspan="6">Continued from previous page</th></t<>		Continued from previous page					
1         B         349         LEU         Peptide           1         B         383         LEU         Peptide           1         B         442         THR         Peptide           1         B         450         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         233         ARG         Peptide           1         C         253         ARG         Peptide           1         C         253	1         B         349         LEU         Peptic           1         B         383         LEU         Peptic           1         B         442         THR         Peptic           1         B         450         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           2         D         140 <t< th=""><th>Mol</th><th>Chain</th><th>Res</th><th>Type</th><th>Group</th></t<>	Mol	Chain	Res	Type	Group		
1         B         383         LEU         Peptide           1         B         442         THR         Peptide           1         B         450         GLU         Peptide           1         B         47         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         232         PRO         Peptide           1         C         253         ARG         Peptide           1         C         318<	1         B         383         LEU         Peptic           1         B         442         THR         Peptic           1         B         450         GLU         Peptic           1         B         47         GLU         Peptic           1         C         110         ASN         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         174         THR         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         318         PRO         Peptic           2         D         114         <					_		
1         B         442         THR         Peptide           1         B         450         GLU         Peptide           1         B         47         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         174         THR         Peptide           1         C         173         GLN         Peptide           1         C         202         LYS         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         253         ARG         Peptide           1         C         318         PRO         Peptide           2         D         114<	1         B         442         THR         Peptic           1         B         450         GLU         Peptic           1         B         47         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         174         THR         Peptic           1         C         174         THR         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         299         LEU         Peptic           1         C         328         SER         Peptic           2         D         114 <td< td=""><td></td><td></td><td></td><td></td><td></td></td<>							
1         B         450         GLU         Peptide           1         B         47         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         231         SER         Peptide           1         C         253         ARG         Peptide           1         C         253         ARG         Peptide           1         C         328         SER         Peptide           2         D         114<	1         B         450         GLU         Peptic           1         B         47         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         231         SER         Peptic           1         C         232         ARG         Peptic           1         C         233         ARG         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         117 <td< td=""><td></td><td></td><td></td><td></td><td></td></td<>							
1         B         47         GLU         Peptide           1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         232         PRO         Peptide           1         C         232         PRO         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           2         D         114<	1         B         47         GLU         Peptic           1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         231         SER         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         119 <td< td=""><td></td><td></td><td></td><td></td><td>-</td></td<>					-		
1         B         9         ILE         Peptide           1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         232         PRO         Peptide           1         C         253         ARG         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         175	1         B         9         ILE         Peptic           1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         175         GLY         Peptic           2         D         176 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>							
1         C         110         ASN         Peptide           1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         328         SER         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         1	1         C         110         ASN         Peptic           1         C         123         THR         Peptic           1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         253         ARG         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         175         GLY         Peptic           2         D         175         GLY         Peptic           2         D         204			47		_		
1         C         123         THR         Peptide           1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         231         MET         Peptide           1         C         253         ARG         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         328         SER         Peptide           2         D         114         LEU         Peptide           2         D         114         LEU         Peptide           2         D         175         GLY         Peptide           2         D         2	1         C         123         THR         Peptic           1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         251         MET         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         114         LEU         Peptic           2         D         175         GLY         Peptic           2         D         204         GLU         Peptic           2         D         241							
1         C         173         GLN         Peptide           1         C         174         THR         Peptide           1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         328         SER         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         2	1         C         173         GLN         Peptic           1         C         174         THR         Peptic           1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         330	1		110	ASN	Peptide		
1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         33	1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         251         MET         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           2         D         114         LEU         Peptic           2         D         114         LEU         Peptic           2         D         117         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         330         <	1	С			Peptide		
1         C         202         LYS         Peptide           1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         33	1         C         202         LYS         Peptic           1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         251         MET         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           2         D         114         LEU         Peptic           2         D         114         LEU         Peptic           2         D         175         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         330         <	1	С	173	GLN	Peptide		
1         C         231         SER         Peptide           1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         330         PRO         Peptide           2         E         11	1         C         231         SER         Peptic           1         C         232         PRO         Peptic           1         C         251         MET         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         176         VAL         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         E         111         <		С	174	THR	Peptide		
1         C         232         PRO         Peptide           1         C         251         MET         Peptide           1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           2         D         114         LEU         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         11	1         C         232         PRO         Peptic           1         C         251         MET         Peptic           1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         176         VAL         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         <	1		202	LYS	Peptide		
1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114	1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         <	1	С	231				
1         C         253         ARG         Peptide           1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114	1         C         253         ARG         Peptic           1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         <	1	С	232	PRO	Peptide		
1         C         299         LEU         Peptide           1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         241         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         20	1         C         299         LEU         Peptic           1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         119         ASP         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         <	1	С	251	MET	Peptide		
1         C         318         PRO         Peptide           1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         E         11	1         C         318         PRO         Peptic           1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         204         GLU         Peptic           2         D         229         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         <	1		253	ARG	Peptide		
1         C         328         SER         Peptide           1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         114         LEU         Peptide           2         E         205         ARG         Peptide           2         E         20	1         C         328         SER         Peptic           1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         204         GLU         Peptic           2         D         229         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         296         <	1		299	LEU	Peptide		
1         C         40         ALA         Peptide           1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         22	1         C         40         ALA         Peptic           1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         204         GLU         Peptic           2         D         229         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         296         <	1	С	318	PRO	Peptide		
1         C         402         ASP         Peptide           2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         22	1         C         402         ASP         Peptic           2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413	1	С	328	SER	Peptide		
2         D         114         LEU         Peptide           2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         114         LEU         Peptic           2         D         119         ASP         Peptic           2         D         175         GLY         Peptic           2         D         176         VAL         Peptic           2         D         204         GLU         Peptic           2         D         229         GLU         Peptic           2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413	1	С	40	ALA	Peptide		
2         D         119         ASP         Peptide           2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         119         ASP         Peption           2         D         175         GLY         Peption           2         D         176         VAL         Peption           2         D         204         GLU         Peption           2         D         229         GLU         Peption           2         D         241         GLU         Peption           2         D         242         PRO         Peption           2         D         330         PRO         Peption           2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         1	1	С	402	ASP	Peptide		
2         D         175         GLY         Peptide           2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         175         GLY         Peption           2         D         176         VAL         Peption           2         D         204         GLU         Peption           2         D         229         GLU         Peption           2         D         241         GLU         Peption           2         D         242         PRO         Peption           2         D         330         PRO         Peption           2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         173         GLY         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	114	LEU	Peptide		
2         D         176         VAL         Peptide           2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         176         VAL         Peption           2         D         204         GLU         Peption           2         D         229         GLU         Peption           2         D         241         GLU         Peption           2         D         242         PRO         Peption           2         D         330         PRO         Peption           2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	119	ASP	Peptide		
2         D         204         GLU         Peptide           2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         204         GLU         Peption           2         D         229         GLU         Peption           2         D         241         GLU         Peption           2         D         242         PRO         Peption           2         D         330         PRO         Peption           2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         173         GLY         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	175	GLY	Peptide		
2         D         229         GLU         Peptide           2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         229         GLU         Peption           2         D         241         GLU         Peption           2         D         242         PRO         Peption           2         D         330         PRO         Peption           2         D         45         ASN         Peption           2         E         111         PHE         Peption           2         E         173         GLY         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	176	VAL	Peptide		
2         D         241         GLU         Peptide           2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         241         GLU         Peptic           2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         D         45         ASN         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic	2	D	204	GLU	Peptide		
2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         D         45         ASN         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic	2	D	229	GLU	Peptide		
2         D         242         PRO         Peptide           2         D         330         PRO         Peptide           2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         242         PRO         Peptic           2         D         330         PRO         Peptic           2         D         45         ASN         Peptic           2         E         111         PHE         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic	2	D	241	GLU	Peptide		
2         D         45         ASN         Peptide           2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         D         45         ASN         Peptic           2         E         111         PHE         Peptic           2         E         114         LEU         Peptic           2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic		D	242	PRO	Peptide		
2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         173         GLY         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	330	PRO	Peptide		
2         E         111         PHE         Peptide           2         E         114         LEU         Peptide           2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         111         PHE         Peption           2         E         114         LEU         Peption           2         E         173         GLY         Peption           2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	D	45	ASN			
2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic	2	Е	111	PHE			
2         E         173         GLY         Peptide           2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         173         GLY         Peptic           2         E         205         ARG         Peptic           2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic	2	Е	114	LEU	Peptide		
2         E         205         ARG         Peptide           2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         205         ARG         Peption           2         E         206         THR         Peption           2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption		Е	173	GLY			
2         E         206         THR         Peptide           2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         206         THR         Peptic           2         E         221         VAL         Peptic           2         E         296         VAL         Peptic           2         E         297         GLY         Peptic           2         E         413         LEU         Peptic           2         F         112         ASN         Peptic		Е	205	ARG			
2         E         221         VAL         Peptide           2         E         296         VAL         Peptide	2         E         221         VAL         Peption           2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption	2	Е	206	THR			
2 E 296 VAL Peptide	2         E         296         VAL         Peption           2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption		Е	221	VAL			
	2         E         297         GLY         Peption           2         E         413         LEU         Peption           2         F         112         ASN         Peption		Е		VAL			
	2         E         413         LEU         Peptid           2         F         112         ASN         Peptid				GLY			
	2 F 112 ASN Peptid		Е					
	2   F   114   LEU   Peptic	2	F	114	LEU	Peptide		



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Mol	Chain	Res	Type	Group
2	F	159	LEU	Peptide
2	F	177	GLY	Peptide
2	F	229	GLU	Peptide
2	F	301	THR	Peptide
2	F	335	THR	Peptide
2	F	45	ASN	Peptide
2	F	70	GLY	Peptide
6	d	185	LYS	Peptide
6	d	228	GLU	Peptide
8	g	242	ILE	Peptide
8	g	260	LYS	Peptide

## 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	A	493/507~(97%)	411 (83%)	82 (17%)	0	100	100
1	В	496/507~(98%)	404 (82%)	92 (18%)	0	100	100
1	С	499/507 (98%)	400 (80%)	99 (20%)	0	100	100
2	D	478/498 (96%)	400 (84%)	76 (16%)	2 (0%)	34	72
2	Е	476/498 (96%)	379 (80%)	95 (20%)	2 (0%)	34	72
2	F	$477/498 \ (96\%)$	390 (82%)	87 (18%)	0	100	100
3	I	146/184 (79%)	144 (99%)	2 (1%)	0	100	100
4	J	129/222~(58%)	122 (95%)	7 (5%)	0	100	100
5	a	221/247 (90%)	185 (84%)	35 (16%)	1 (0%)	29	69
6	d	175/257 (68%)	149 (85%)	26 (15%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
7	e	127/134 (95%)	91 (72%)	36 (28%)	0	100	100
8	g	314/364 (86%)	260 (83%)	53 (17%)	1 (0%)	41	77
9	M	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	N	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	О	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Р	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Q	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	R	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	S	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Т	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	U	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	V	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	W	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	X	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Y	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Z	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
All	All	5109/5557 (92%)	4315 (84%)	788 (15%)	6 (0%)	54	86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	296	VAL
8	g	261	GLU
2	D	295	ALA
5	a	161	PHE
2	Е	367	PRO
2	Ε	300	PRO

### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	230:LEU	C	231:LEU	N	1.18



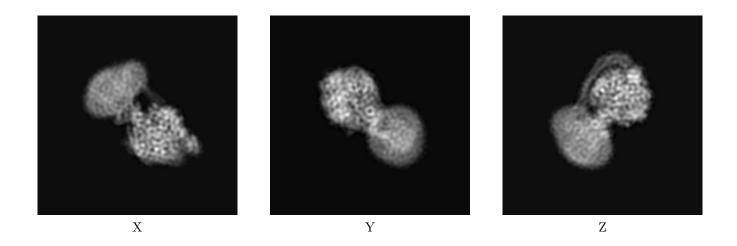
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21235. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

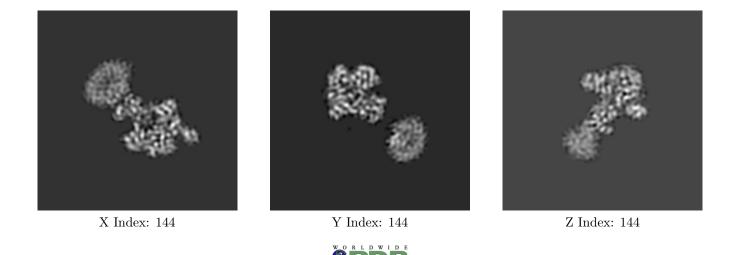
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

#### 6.2.1 Primary map



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

### 6.3 Largest variance slices (i)

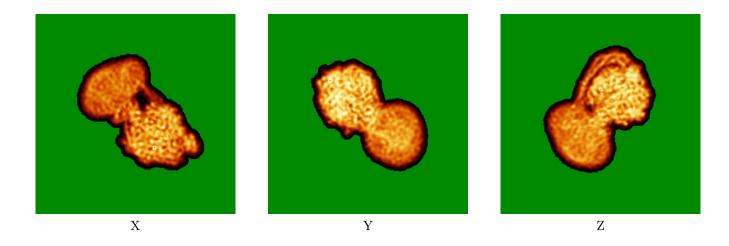
#### 6.3.1 Primary map



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

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

#### 6.4.1 Primary map

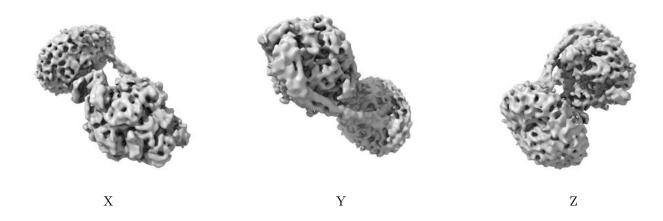


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00948. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.6 Mask visualisation (i)

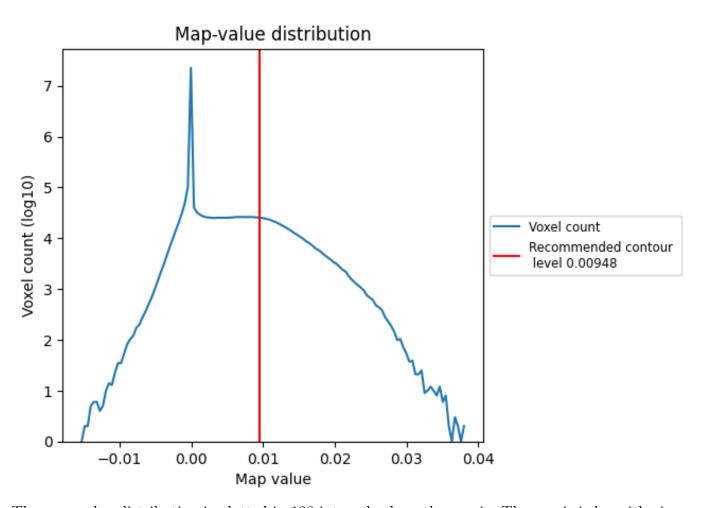
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

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

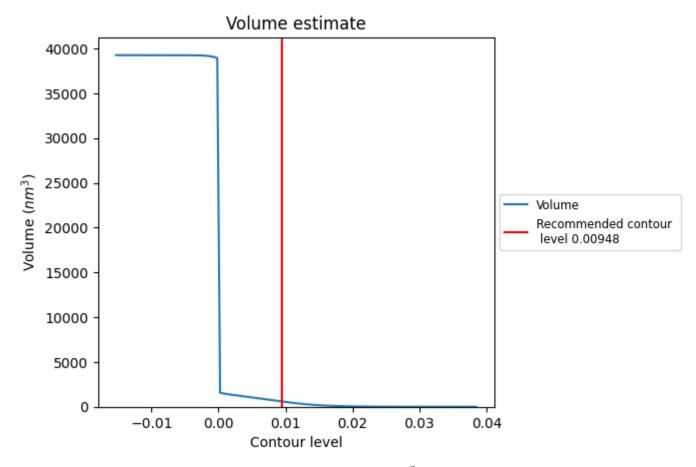
## 7.1 Map-value distribution (i)



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



## 7.2 Volume estimate (i)

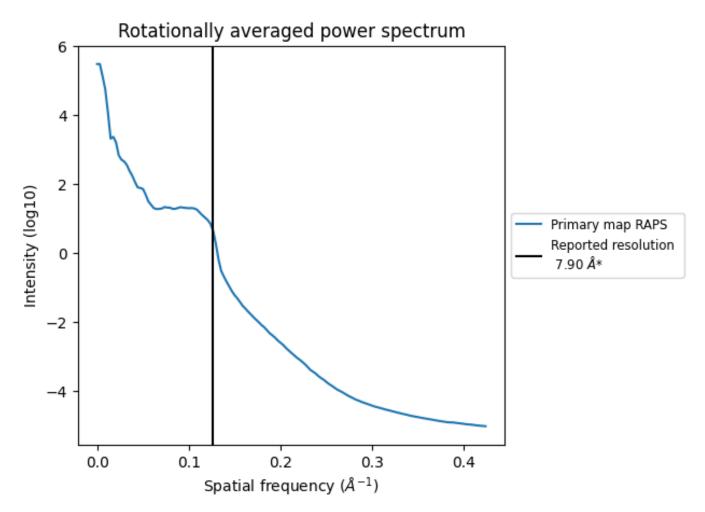


The volume at the recommended contour level is  $591~\mathrm{nm}^3$ ; this corresponds to an approximate mass of  $534~\mathrm{kDa}$ .

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)



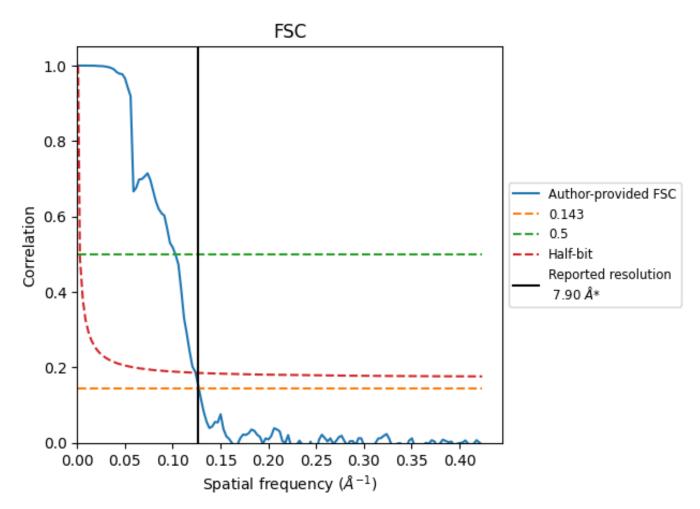
<sup>\*</sup>Reported resolution corresponds to spatial frequency of 0.127  ${\rm \AA}^{-1}$ 



## 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 0.127  $\rm \mathring{A}^{-1}$ 



## 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.85	9.74	8.08
Unmasked-calculated*	-	-	-

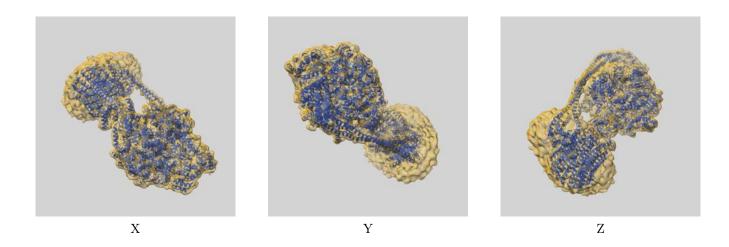
<sup>\*</sup>Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21235 and PDB model 6VM1. Per-residue inclusion information can be found in section 3 on page 7.

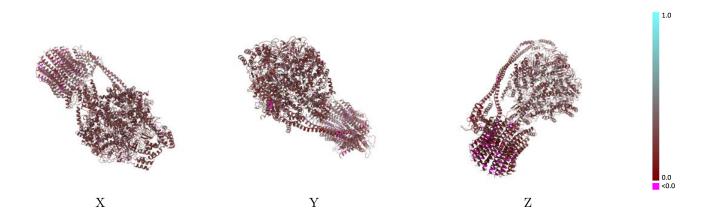
## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.00948 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.

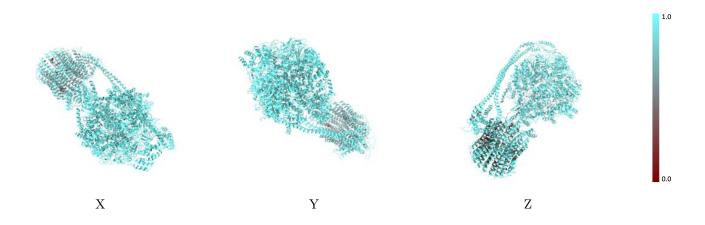


## 9.2 Q-score mapped to coordinate model (i)



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.

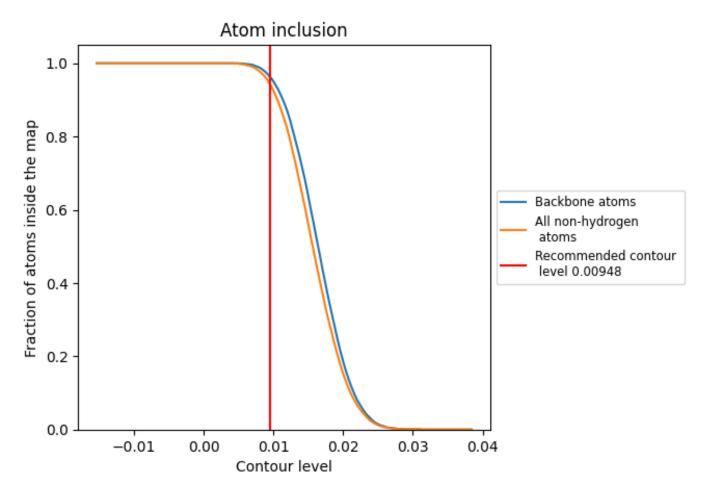
## 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00948).



## 9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.00948) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9440	0.2580
A	0.9760	0.2940
В	0.9710	0.2790
С	0.9700	0.2870
D	0.9820	0.2800
Е	0.9820	0.2910
F	0.9700	0.2860
I	0.9880	0.2480
J	0.9750	0.2430
M	0.8310	0.1760
N	0.8020	0.1800
О	0.7810	0.1550
Р	0.8440	0.1610
Q	0.8200	0.1740
R	0.8750	0.1920
S	0.8750	0.1900
T	0.7920	0.1490
U	0.8780	0.1850
V	0.8750	0.1680
W	0.8540	0.1780
X	0.8590	0.1690
Y	0.9190	0.2010
Z	0.8410	0.1650
a	0.9540	0.2370
d	0.9980	0.2850
e	0.9390	0.2810
g	0.9310	0.2830



