W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 11:16 PM JST

PDB ID	:	7VWL
EMDB ID	:	EMD-32155
Title	:	Membrane arm of deactive state CI from rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-11
Resolution	:	2.70 Å(reported)

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

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

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

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 Å.

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

Metric	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		0.3%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
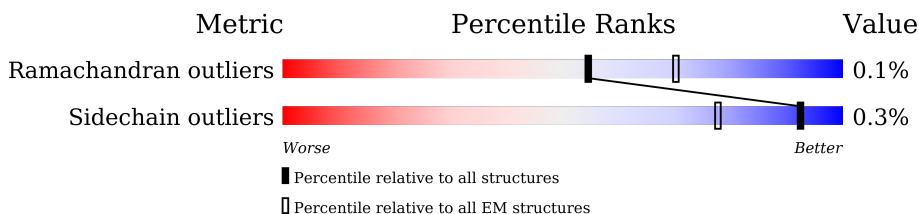
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	40	22% / 100%
2	S	70	• / 100%
3	U	83	6% / 100%
4	V	140	21% / 99% •
5	W	113	• / 100%
6	X	88	7% / 100%
7	Y	70	19% / 100%
8	Z	84	21% / 100%
9	a	140	• / 100%

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Mol	Chain	Length	Quality of chain
10	b	126	11% / 80% / 18%
11	c	156	5% / 100%
12	d	175	6% / 100%
13	e	107	12% / 100%
14	f	42	12% / 100%
15	g	121	100%
16	h	105	100%
17	i	347	100%
18	j	113	17% / 88% / 12%
19	k	98	5% / 100%
20	l	603	100%
21	m	175	8% / 74% / 26%
22	n	56	18% / 98%
23	o	128	5% / 100%
24	p	178	99%
25	r	459	100%
26	s	318	95% / 5%
27	u	171	100%
28	v	131	15% / 92% / 5%
29	w	320	9% / 100%

2   Entry composition ⓘ

There are 36 unique types of molecules in this entry. The entry contains 39049 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Q	40	333	217	56	59	1	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	70	567	364	104	94	5	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	83	643	417	110	115	1	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	V	140	1021	651	174	190	6	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	W	113	949	614	160	167	8	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total 702	C 452	N 103	O 142	S 5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	70	Total 600	C 393	N 98	O 108	S 1	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	84	Total 674	C 437	N 116	O 120	S 1	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	140	Total 1165	C 762	N 199	O 201	S 3	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total 879	C 573	N 158	O 147	S 1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total 1315	C 853	N 213	O 241	S 8	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			343	225	58	60		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	k	98	748	493	113	128	14	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	l	603	4773	3164	740	819	50	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	m	129	951	637	138	168	8	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	n	56	448	291	81	75	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	o	128	1062	691	182	189	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	p	178	1534	982	279	265	8	0	0

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	r	459	3631	2412	572	609	38	0	0

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	303	Total 2394	C 1607	N 369	O 397	S 21	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	171	Total 1398	C 887	N 250	O 251	S 10	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total 1032	C 644	N 195	O 184	S 9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total 2576	C 1640	N 435	O 491	S 10	0	0

- Molecule 30 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).
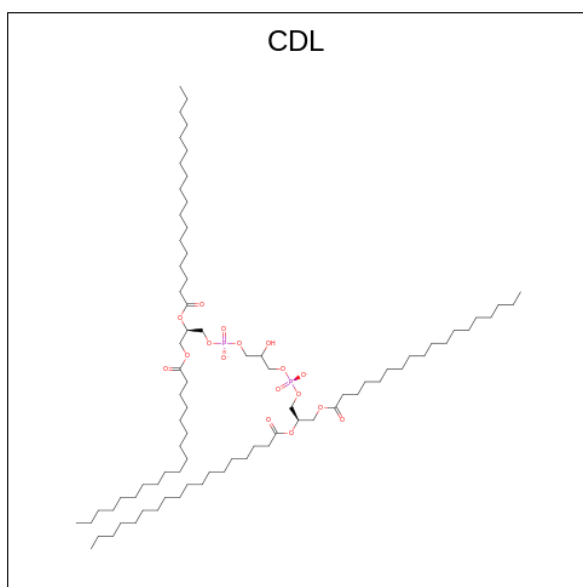
CDL

Mol	Chain	Residues	Atoms				AltConf
30	V	1	Total	C	O	P	0
			71	52	17	2	
30	a	1	Total	C	O	P	0
			91	72	17	2	
30	i	1	Total	C	O	P	0
			66	47	17	2	
30	l	1	Total	C	O	P	0
			65	46	17	2	
30	r	1	Total	C	O	P	0
			199	161	34	4	
30	r	1	Total	C	O	P	0
			199	161	34	4	
30	u	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 31 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).

8Q1
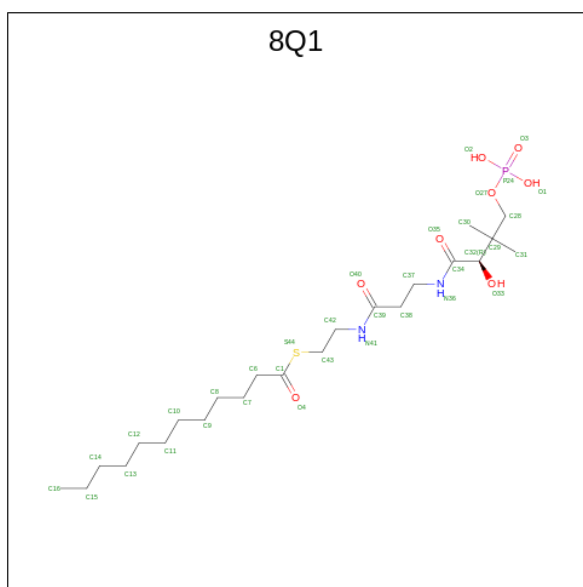
Mol	Chain	Residues	Atoms						AltConf
31	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 32 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DI METHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSA NE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).

PLX

Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
32	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 33 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).

PEE

Mol	Chain	Residues	Atoms					AltConf
33	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
33	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
33	l	1	Total	C	N	O	P	0
			92	72	2	16	2	
33	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
33	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).
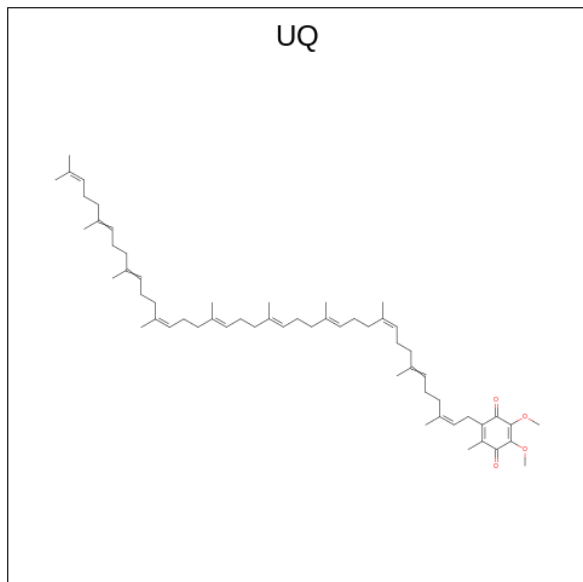
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	s	1	28	24	4	0

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).
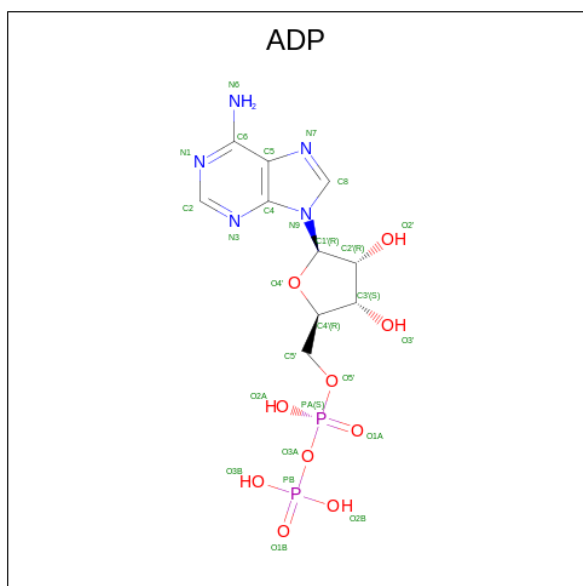
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	w	1	27	10	5	10	2	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	Q	6	Total 6	O 6	0
36	S	1	Total 1	O 1	0
36	U	3	Total 3	O 3	0
36	V	2	Total 2	O 2	0
36	a	4	Total 4	O 4	0
36	b	1	Total 1	O 1	0
36	c	5	Total 5	O 5	0
36	d	2	Total 2	O 2	0
36	e	2	Total 2	O 2	0
36	h	4	Total 4	O 4	0
36	i	62	Total 62	O 62	0
36	j	14	Total 14	O 14	0
36	k	15	Total 15	O 15	0
36	l	53	Total 53	O 53	0
36	m	14	Total 14	O 14	0
36	n	2	Total 2	O 2	0
36	p	2	Total 2	O 2	0
36	r	84	Total 84	O 84	0
36	s	65	Total 65	O 65	0
36	u	1	Total 1	O 1	0
36	w	3	Total 3	O 3	0

3   Residue-property plots ⓘ

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: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:
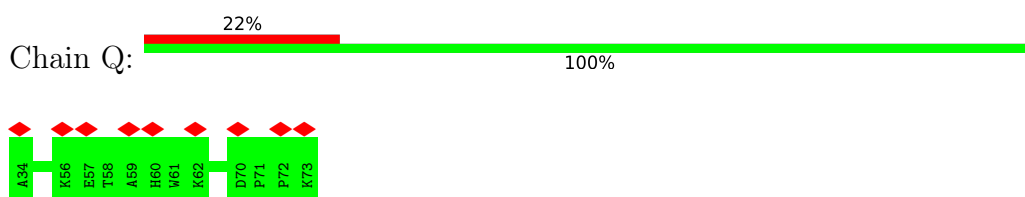
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:
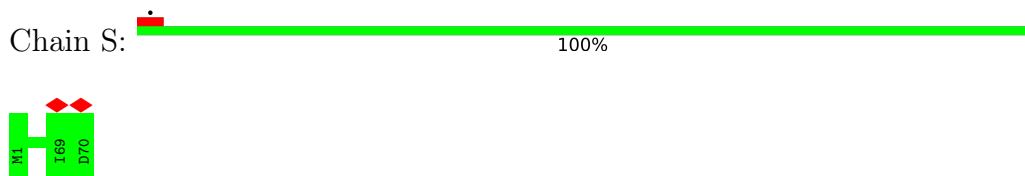
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:
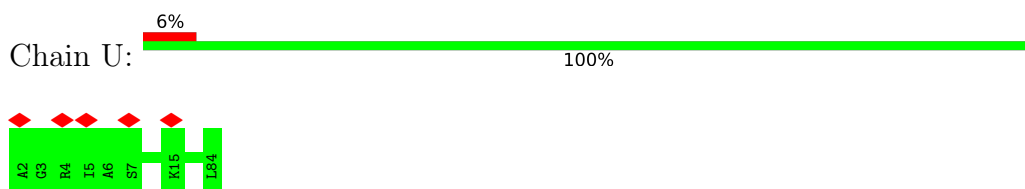
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:
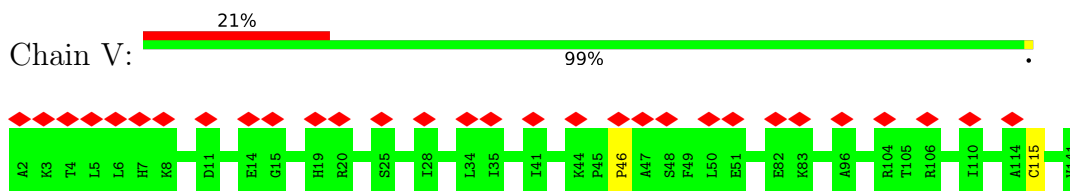
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:

• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:

7%

100%

S69 D70 A71 P72 E96 M105 E156

• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:

19%

100%

G36 G37 V38 H39 I40 E41 E59 Q91 E95 L100 P101 D102 D103 E104 D105

• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:

21%

100%

E8 H9 G10 H11 S12 K13 M14 E15 E25 N59 N60 A81 E85 Y86 Y87 L88 E89 S90 Q91

• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:

100%

H50 G51 K52 N189

• Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:

11%

80%

18%

S2 P37 R38 R39 V40 TRP PRO MET GLU GLN PHE TRP ASN LYS PHE LEU GLN ASP GLY ALA PRO TRP LYS ASN VAL ILE TYR LYS T64 Y65 R66 H67 E122 F123 P124 D125 Q126 H127

• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:

5%

100%

H31 V32 T33 K34 D35 E177 P178 E179 Y184 E185 I186

• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:

6%

100%

• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:
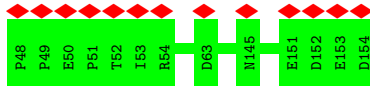
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial
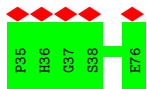
Chain f:

• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:

• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5
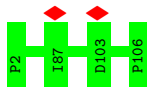
Chain h:

• Molecule 17: NADH-ubiquinone oxidoreductase chain 2
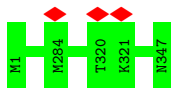
Chain i:

• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:

• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

Chain k:

• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:

• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m:

• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:

• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:

• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:

• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain r:

100%

M1 K86 L126 V127 Y459

• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s:

95%   5%

M1 L61 R62 P63 A64 T65 S66 S67 M70 P90 M91 N124 T201 GLU GLY GLU SER GLU LEU VAL SER GLY PHE ASN VAL GLU TYR ALA A217 S318
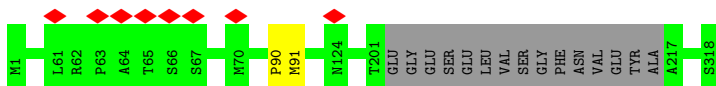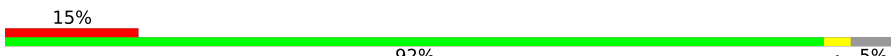
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:

100%

P2 H99 E109 D134 E139 E153 A154 E155 M172
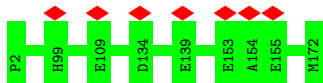
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

15%

Chain v:

92%   5%

MYR G2 R8 A13 D28 P32 E33 R34 K35 E36 R37 E38 N76 F77 L78 Q110 R115 E116 Q117 R118 E119 A120 E121 M122 A123 R124 G125 GLN GLY PRO GLY GLU VAL
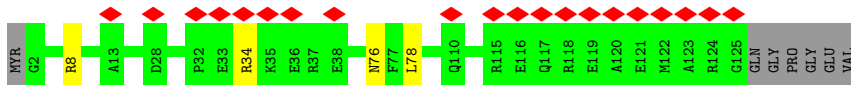
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

9%

Chain w:

100%

L36 Q37 E47 E55 C67 S68 G69 E79 R175 E213 I214 M227 L246 P247 E248 M249 S250 E251 K252 C253 E254 R261 D265 A266 E267 E271 Y275 L276 K277 C278 D279 K280 G281 P284 D285 D288 D346 K355
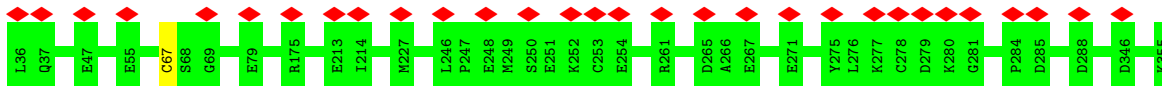
4   Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169835	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	257.808, 257.808, 257.808	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UQ, PLX, PEE, ADP, CDL, 8Q1

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

Mol	Chain	Bond lengths RMSZ	Bond lengths #$|Z|$ >5	Bond angles RMSZ	Bond angles #$|Z|$ >5
1	Q	0.25	0/350	0.45	0/483
2	S	0.27	0/582	0.48	0/783
3	U	0.26	0/664	0.44	0/912
4	V	0.26	0/1042	0.45	0/1411
5	W	0.28	0/973	0.49	0/1312
6	X	0.27	0/714	0.45	0/967
7	Y	0.26	0/626	0.47	0/857
8	Z	0.25	0/695	0.44	0/939
9	a	0.28	0/1199	0.49	0/1623
10	b	0.27	0/906	0.54	0/1232
11	c	0.27	0/1371	0.46	0/1875
12	d	0.26	0/1494	0.50	0/2015
13	e	0.27	0/916	0.50	0/1246
14	f	0.29	0/351	0.46	0/474
15	g	0.29	0/1031	0.50	0/1394
16	h	0.25	0/889	0.49	0/1190
17	i	0.26	0/2773	0.46	0/3768
18	j	0.26	0/819	0.47	0/1117
19	k	0.31	0/759	0.51	0/1029
20	l	0.27	0/4901	0.47	0/6667
21	m	0.30	0/973	0.50	0/1320
22	n	0.24	0/459	0.54	0/621
23	o	0.27	0/1092	0.53	0/1481
24	p	0.27	0/1590	0.51	0/2155
25	r	0.27	0/3723	0.47	0/5078
26	s	0.27	0/2464	0.48	0/3369
27	u	0.25	0/1436	0.49	0/1938
28	v	0.25	0/1056	0.55	0/1416
29	w	0.27	0/2636	0.50	0/3573
All	All	0.27	0/38484	0.48	0/52245

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	s	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	s	91	MET	Peptide

5.2　Too-close contacts　ⓘ

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

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

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	Percentiles	
1	Q	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
4	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	46
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Z	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
9	a	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	b	99/126 (79%)	92 (93%)	7 (7%)	0	100	100
11	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
12	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
13	e	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
14	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
15	g	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
16	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
19	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
20	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
21	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
24	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	25	50
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	41	66
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/131 (93%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	303 (95%)	14 (4%)	1 (0%)	41	66
All	All	4586/4757 (96%)	4399 (96%)	183 (4%)	4 (0%)	54	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	w	67	CYS
4	V	46	PRO
26	s	90	PRO
24	p	174	PRO

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	58 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	100 (99%)	1 (1%)	76	91
5	W	99/99 (100%)	99 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	Y	63/63 (100%)	63 (100%)	0	100	100
8	Z	65/65 (100%)	65 (100%)	0	100	100
9	a	122/122 (100%)	122 (100%)	0	100	100
10	b	98/119 (82%)	96 (98%)	2 (2%)	55	81
11	c	141/141 (100%)	141 (100%)	0	100	100
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	99/99 (100%)	99 (100%)	0	100	100
14	f	36/38 (95%)	36 (100%)	0	100	100
15	g	108/108 (100%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	311 (100%)	0	100	100
18	j	88/99 (89%)	88 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	534/537 (99%)	531 (99%)	3 (1%)	86	95
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	44/53 (83%)	43 (98%)	1 (2%)	50	78
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	263 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	105/115 (91%)	101 (96%)	4 (4%)	33	62
29	w	280/283 (99%)	280 (100%)	0	100	100
All	All	4063/4179 (97%)	4052 (100%)	11 (0%)	92	98

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	v	8	ARG
28	v	34	ARG
28	v	78	LEU
28	v	76	ASN
20	l	541	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
27	u	95	GLN
27	u	99	HIS
28	v	76	ASN
28	v	4	HIS
22	n	14	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
34	UQ	s	402	-	28,28,63	3.27	7 (25%)	34,37,79	2.77	11 (32%)
30	CDL	V	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.12	5 (6%)
30	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.10	5 (5%)
32	PLX	e	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.62	1 (1%)
33	PEE	s	401	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
33	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
33	PEE	l	702	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
32	PLX	i	402	-	51,51,51	1.15	3 (5%)	55,59,59	0.61	1 (1%)
30	CDL	u	201	-	62,62,99	1.14	4 (6%)	68,74,111	1.17	4 (5%)
32	PLX	j	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
33	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
32	PLX	a	202	-	51,51,51	0.62	0	55,59,59	0.69	0
30	CDL	r	504	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
30	CDL	l	701	-	64,64,99	1.28	9 (14%)	70,76,111	1.00	4 (5%)
32	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.63	1 (1%)
30	CDL	r	503	-	98,98,99	1.09	9 (9%)	104,110,111	0.89	4 (3%)
33	PEE	i	403	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
33	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
33	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
35	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.43	5 (17%)
30	CDL	i	401	-	65,65,99	1.13	4 (6%)	71,77,111	1.22	7 (9%)
31	8Q1	X	201	-	31,34,34	2.06	6 (19%)	40,43,43	1.80	10 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	UQ	s	402	-	-	9/21/45/87	0/1/1/1
30	CDL	V	201	-	-	29/81/81/110	-
30	CDL	a	201	-	-	28/101/101/110	-
32	PLX	e	201	-	-	32/55/55/55	-
33	PEE	s	401	-	-	26/54/54/54	-
33	PEE	m	201	-	-	17/44/44/54	-
33	PEE	l	702	-	-	19/49/49/54	-
32	PLX	i	402	-	-	28/55/55/55	-
30	CDL	u	201	-	-	21/73/73/110	-
32	PLX	j	202	-	-	30/55/55/55	-
33	PEE	j	201	-	-	22/54/54/54	-
32	PLX	a	202	-	-	13/55/55/55	-
30	CDL	r	504	-	-	67/110/110/110	-
30	CDL	l	701	-	-	38/75/75/110	-
32	PLX	r	502	-	-	21/55/55/55	-
30	CDL	r	503	-	-	56/109/109/110	-
33	PEE	i	403	-	-	21/50/50/54	-
33	PEE	r	501	-	-	23/54/54/54	-
33	PEE	l	703	-	-	24/49/49/54	-
35	ADP	w	401	-	-	3/12/32/32	0/3/3/3
30	CDL	i	401	-	-	30/76/76/110	-
31	8Q1	X	201	-	-	19/41/41/41	-

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C13-C14	9.32	1.55	1.33
34	s	402	UQ	C8-C9	8.96	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.87	1.30	1.53
34	s	402	UQ	C18-C19	8.24	1.56	1.32
35	w	401	ADP	O4'-C4'	7.72	1.62	1.45

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	s	402	UQ	C7-C8-C9	-9.19	111.49	126.79
34	s	402	UQ	C12-C13-C14	-5.76	113.80	127.66
31	X	201	8Q1	C6-C1-S44	5.68	120.07	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	401	CDL	OA6-CA5-C11	4.52	121.24	111.50
34	s	402	UQ	C11-C9-C8	-4.49	112.03	121.12

There are no chirality outliers.

5 of 576 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	V	201	CDL	CA2-OA2-PA1-OA5
30	V	201	CDL	CB2-OB2-PB2-OB4
30	V	201	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	CA2-OA2-PA1-OA3
30	i	401	CDL	CA3-OA5-PA1-OA4

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand UQ s 402

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL V 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL a 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PLX e 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE s 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE m 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE l 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PLX i 402

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL u 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PLX j 202

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE j 201

Bond lengths

Bond angles

Torsions

Rings

Ligand PLX a 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL r 504

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL l 701

Bond lengths

Bond angles

Torsions

Rings

Ligand PLX r 502

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL r 503	
Bond lengths	Bond angles
Torsions	Rings

Ligand PEE i 403	
Bond lengths	Bond angles
Torsions	Rings

Ligand PEE r 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand PEE l 703

Bond lengths	Bond angles
Torsions	Rings

Ligand ADP w 401

Bond lengths	Bond angles
Torsions	Rings

Ligand CDL i 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 8Q1 X 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32155. 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 ⓘ

6.1.1　Primary map

| X | Y | Z |
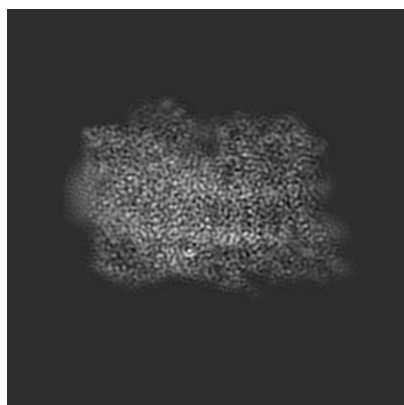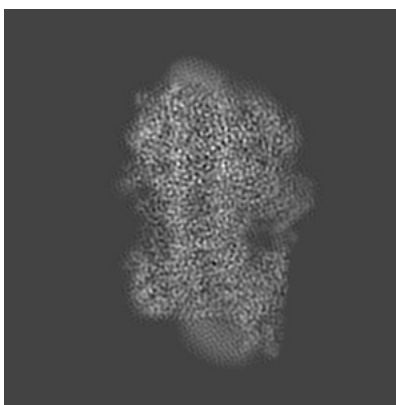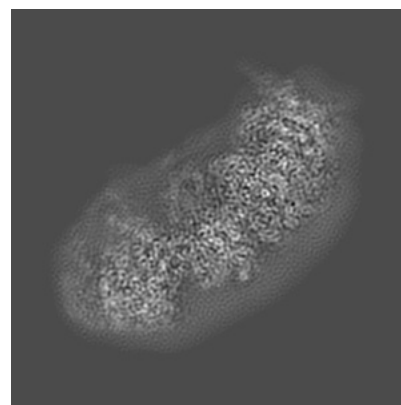
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
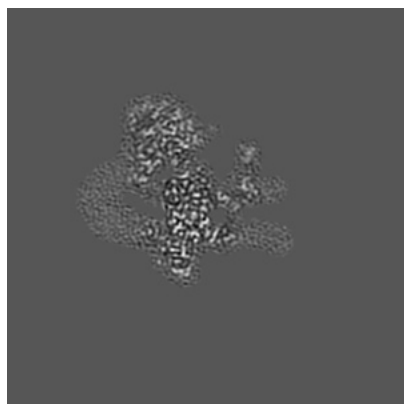
6.2.1　Primary map
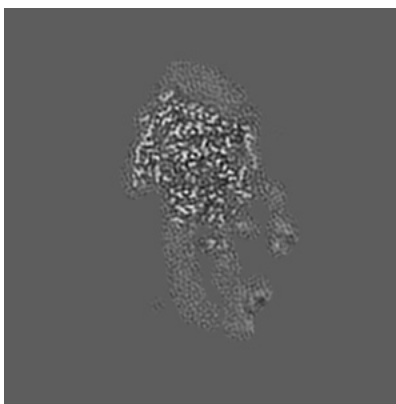
| X Index: 240 | Y Index: 240 | Z Index: 240 |
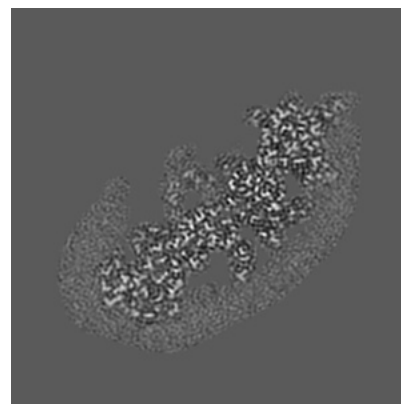
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
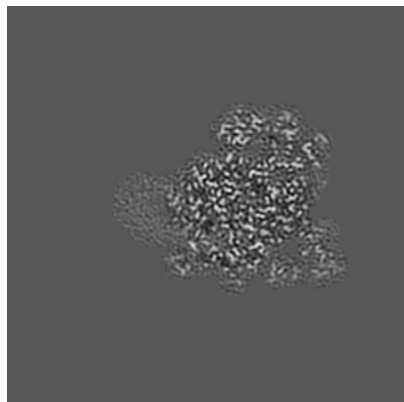
6.3.1   Primary map
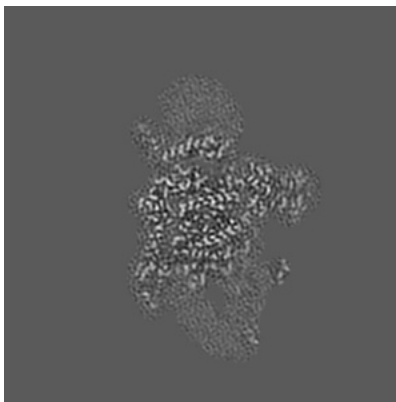
| X Index: 321 | Y Index: 202 | Z Index: 258 |
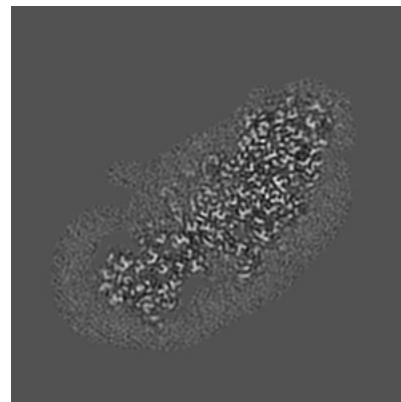
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ
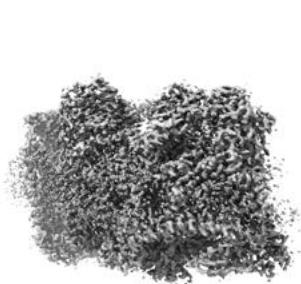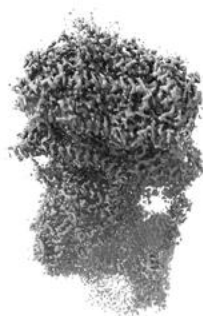
6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation (i)

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

7   Map analysis   ⓘ

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

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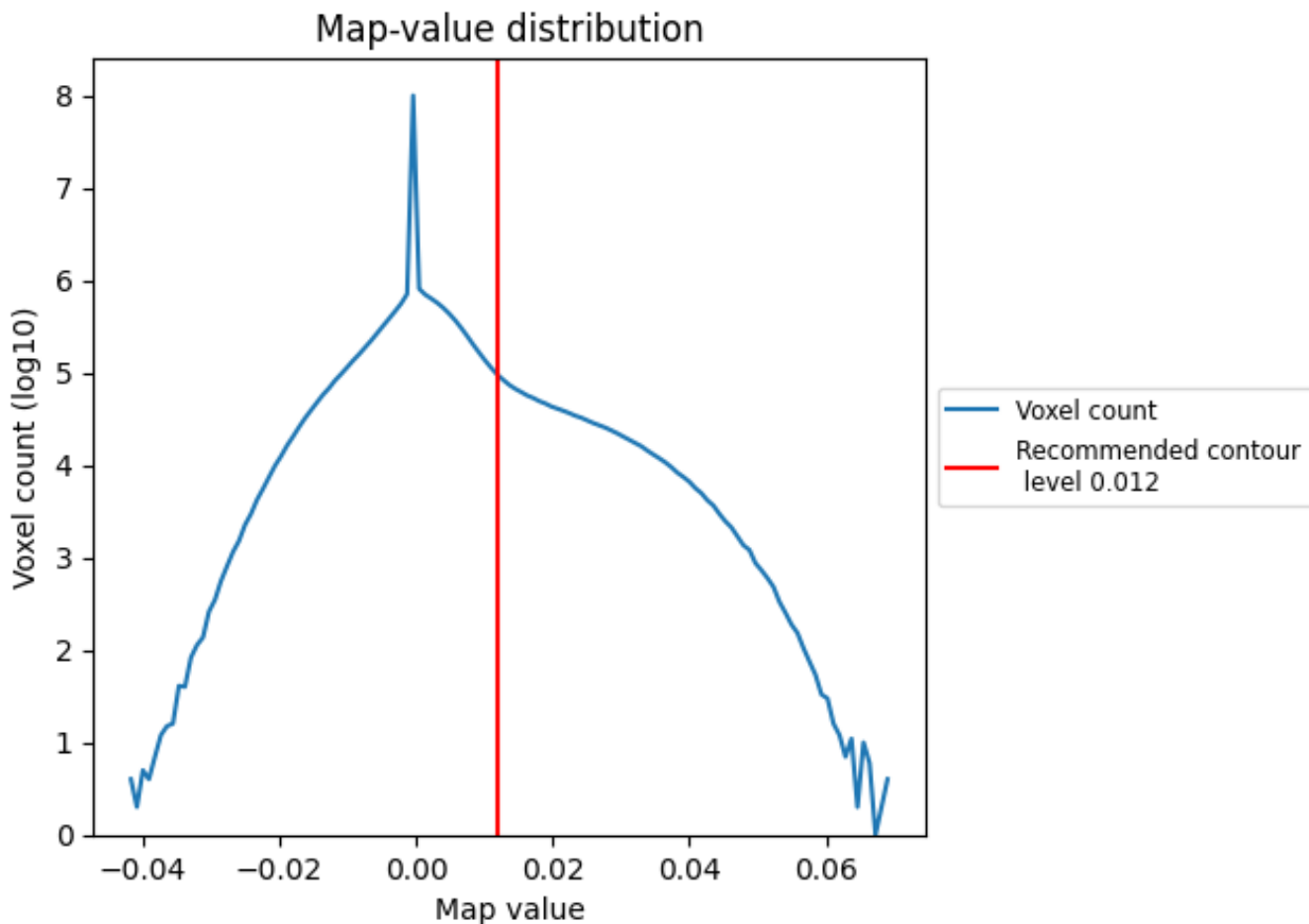
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
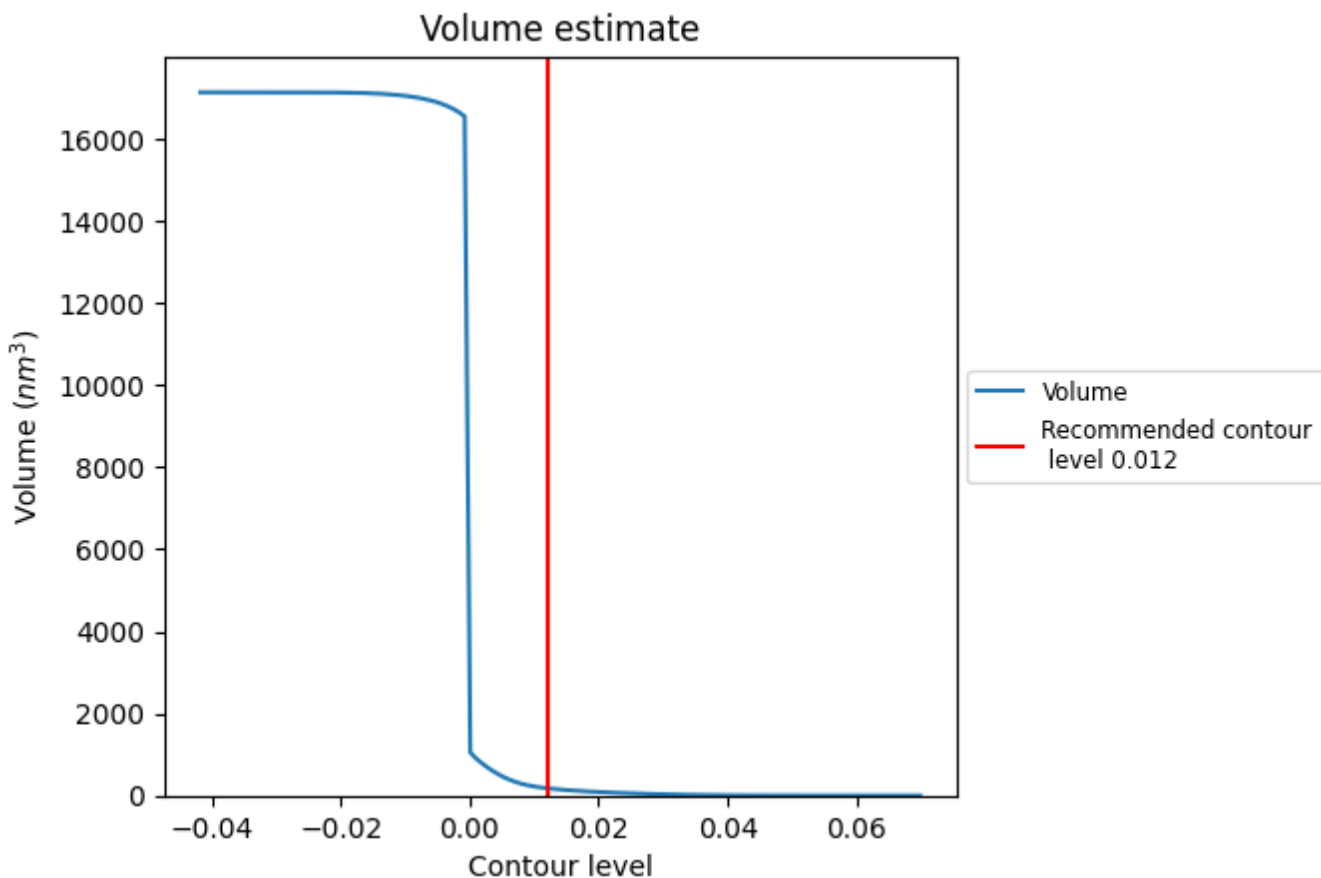
The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 161 kDa.

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 ⓘ
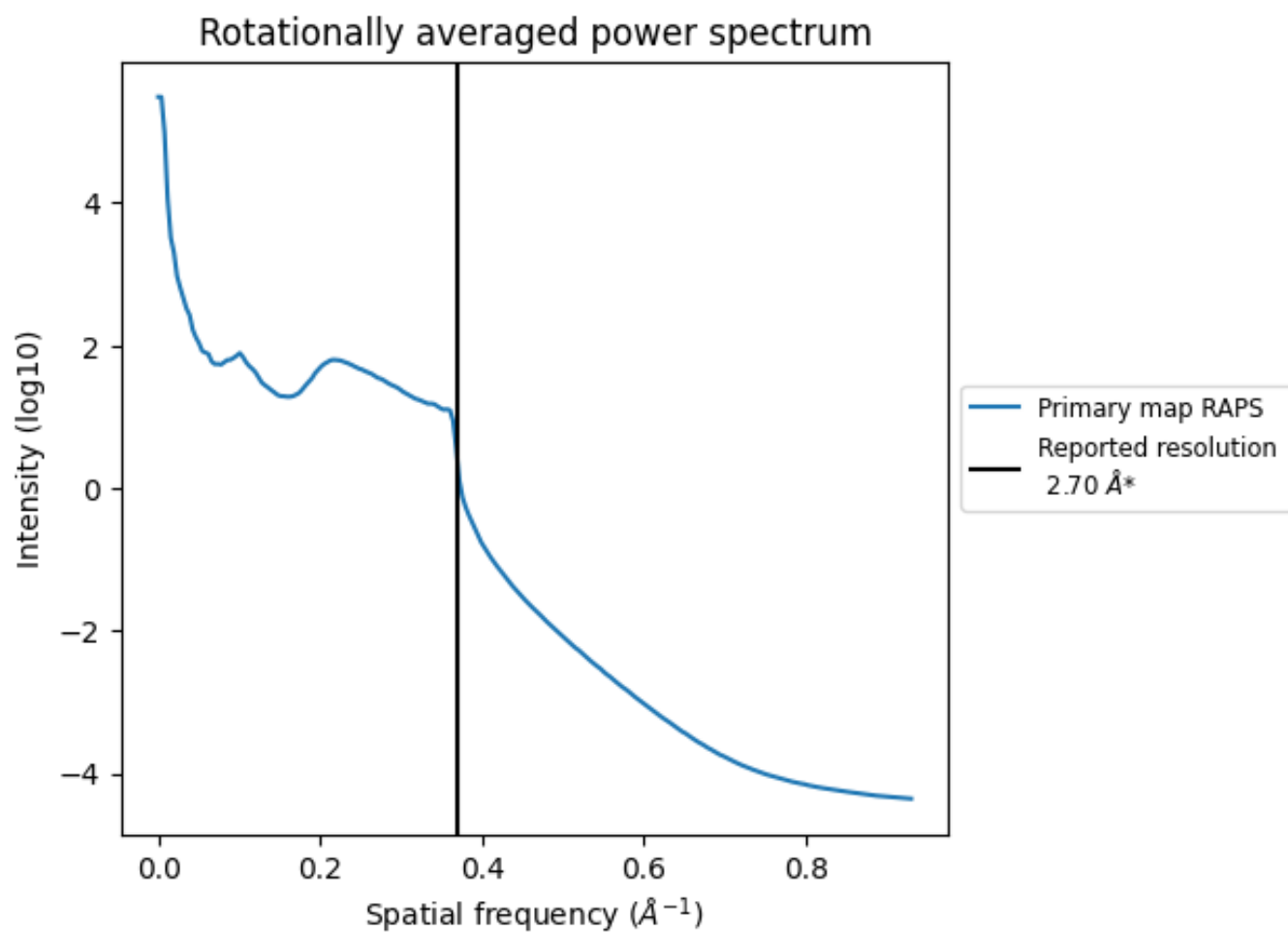
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32155 and PDB model 7VWL. Per-residue inclusion information can be found in section 3 on page 14.

9.1   Map-model overlay ⓘ

| X | Y | Z |
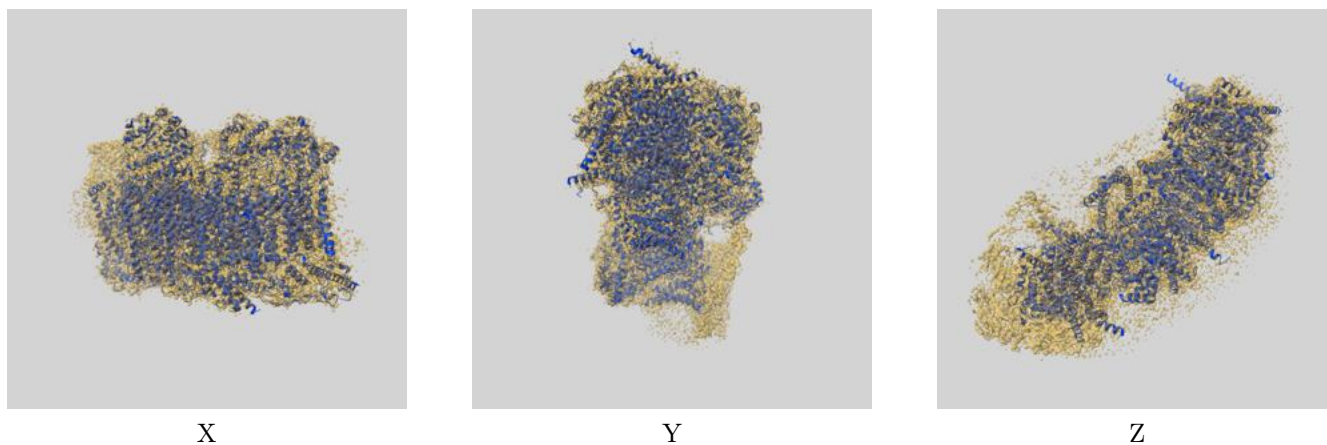
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
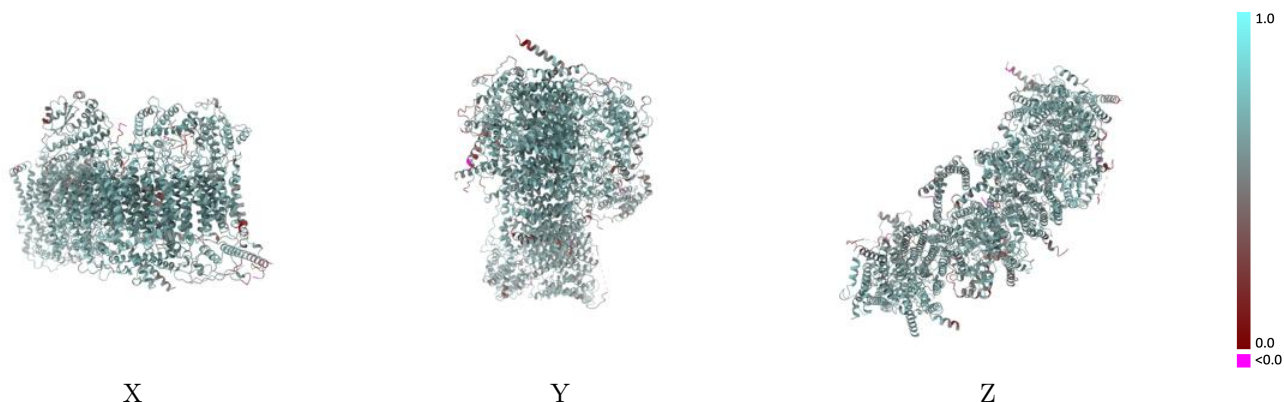
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
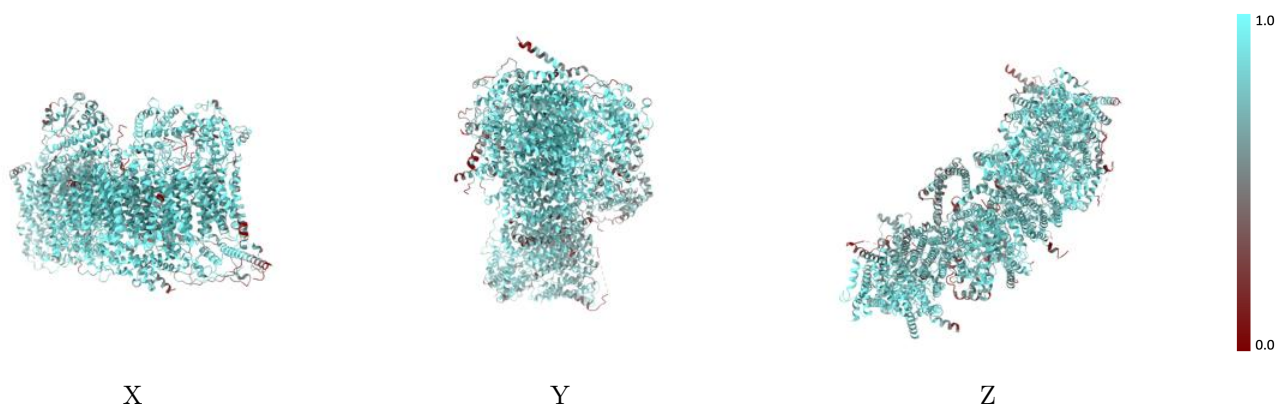
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4   Atom inclusion ⓘ
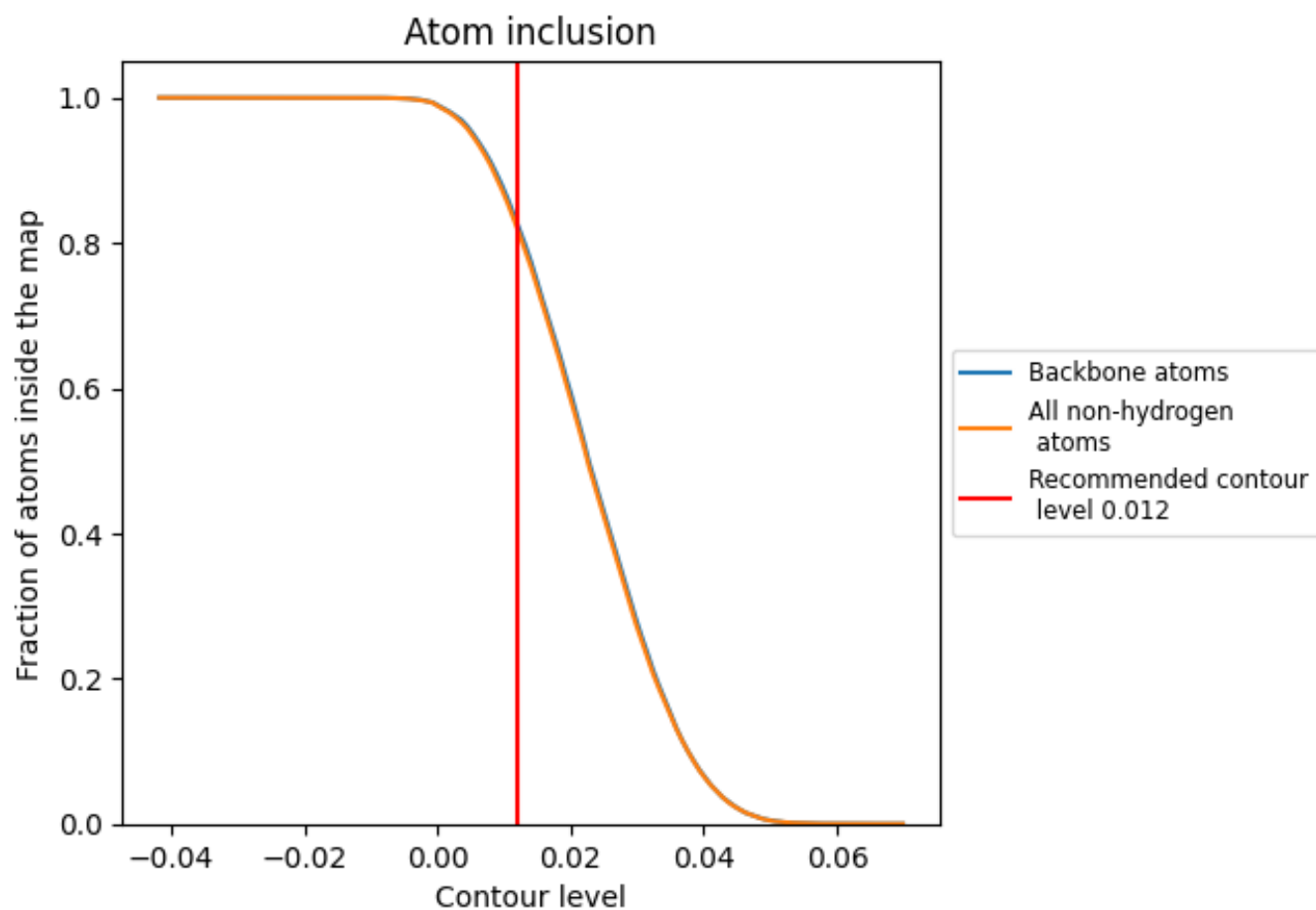
At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8195	0.5990
Q	0.6411	0.5390
S	0.8608	0.6060
U	0.8076	0.5850
V	0.5989	0.5300
W	0.8575	0.6160
X	0.7798	0.5690
Y	0.6872	0.5400
Z	0.6459	0.5100
a	0.8690	0.6300
b	0.7161	0.5440
c	0.8413	0.6040
d	0.8318	0.6060
e	0.7611	0.5650
f	0.7343	0.5530
g	0.9030	0.6290
h	0.8605	0.6100
i	0.9084	0.6370
j	0.6849	0.5540
k	0.8140	0.5920
l	0.8829	0.6320
m	0.7564	0.5640
n	0.7471	0.5730
o	0.8309	0.5990
p	0.8443	0.6100
r	0.9078	0.6360
s	0.8560	0.6100
u	0.8146	0.5960
v	0.7151	0.5410
w	0.7402	0.5620

1.0

0.0
<0.0