wwPDB EM Validation Summary Report

Dec 26, 2024 – 01:31 PM EST

PDB ID	:	6Q9D
EMDB ID	:	EMD-4480
Title	:	CI Peripheral Arm focused refinement from Ovine respiratory SC I+III2
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-18
Resolution	:	3.80 Å(reported)
Based on initial model	:	1LNK

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 ⓘ 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 ⓘ) were used in the production of this report:

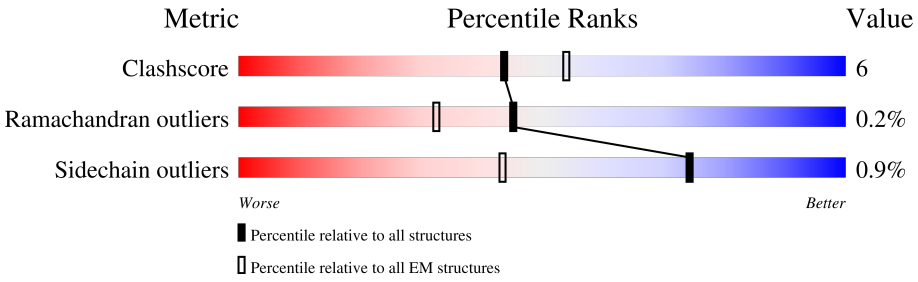
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	V1	445	6% 82% 15% •
2	V2	217	8% 75% 22% • •
3	S1	704	7% 77% 20% •
4	S2	430	12% 76% 12% 11%
5	S3	228	7% 78% 12% • 9%
6	S7	179	10% 72% 15% • 13%
7	S8	176	9% 81% 18% •
8	V3	75	• 40% 12% • 45%

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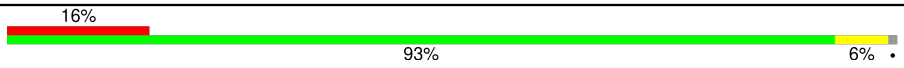
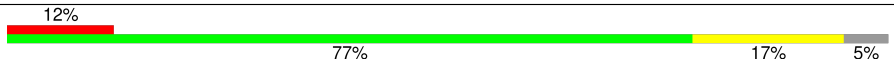
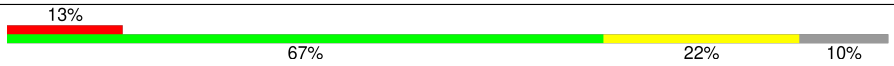
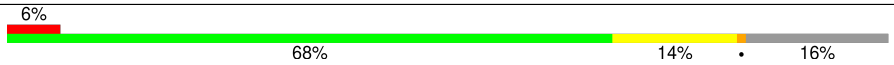
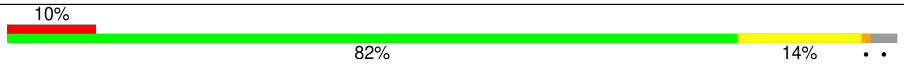
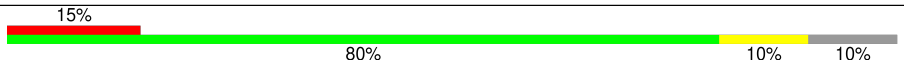
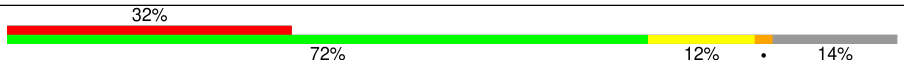
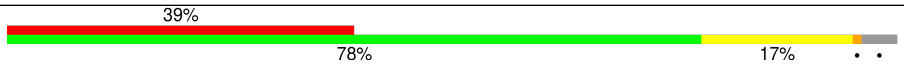
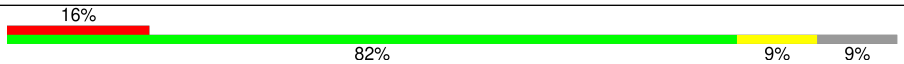
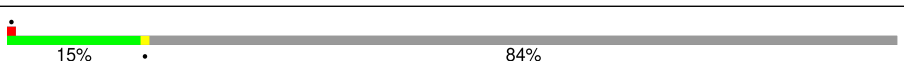
Mol	Chain	Length	Quality of chain
9	S6	96	
10	S4	133	
11	A9	338	
12	A2	98	
13	A5	115	
14	A6	127	
15	A7	112	
16	AL	145	
17	AA	88	
18	AM	143	

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 27662 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] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V2	212	1647	1052	277	308	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called NADH:ubiquinone oxidoreductase core subunit S2,NADH:ubiquinone oxidoreductase core subunit S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S2	383	3071	1957	529	561	24	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S3	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called NADH:ubiquinone oxidoreductase core subunit S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase core subunit S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	303	Total	C	N	O	S	0	0
			2402	1537	436	424	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	96	Total	C	N	O	S	0	0
			766	478	146	139	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	139	Total	C	N	O	S	0	0
			1160	746	209	201	4		

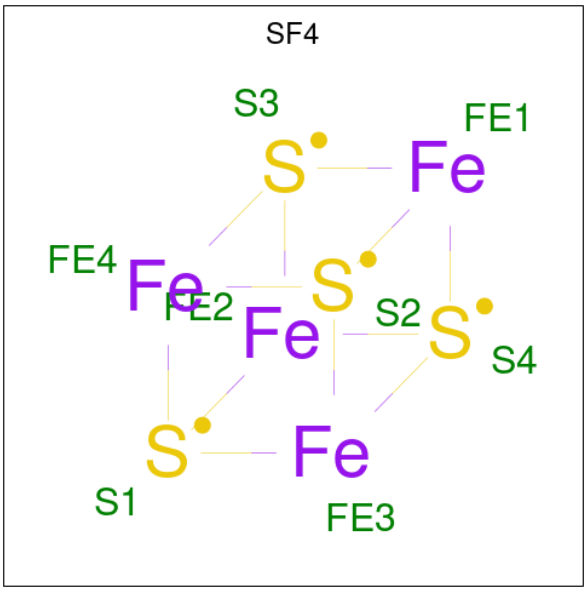
- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

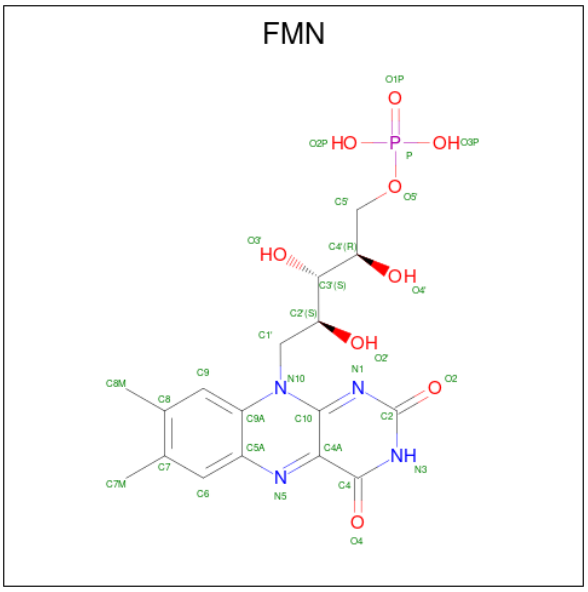
Mol	Chain	Residues	Atoms					AltConf	Trace
18	AM	23	Total	C	N	O	S	0	0
			186	118	36	31	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



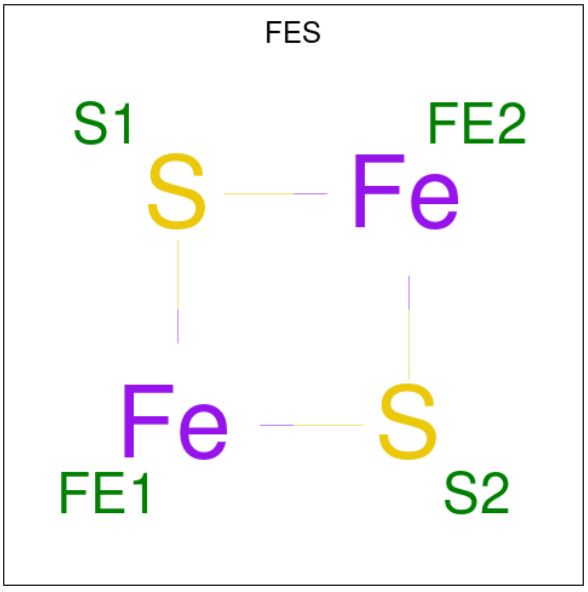
Mol	Chain	Residues	Atoms	AltConf
19	V1	1	Total Fe S 8 4 4	0
19	S1	1	Total Fe S 8 4 4	0
19	S1	1	Total Fe S 8 4 4	0
19	S7	1	Total Fe S 8 4 4	0
19	S8	1	Total Fe S 8 4 4	0
19	S8	1	Total Fe S 8 4 4	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
20	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

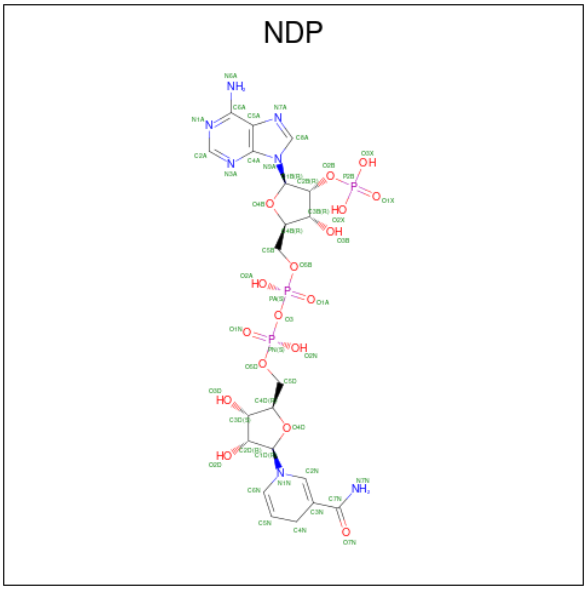


Mol	Chain	Residues	Atoms			AltConf
21	V2	1	Total	Fe	S	0
			4	2	2	
21	S1	1	Total	Fe	S	0
			4	2	2	

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

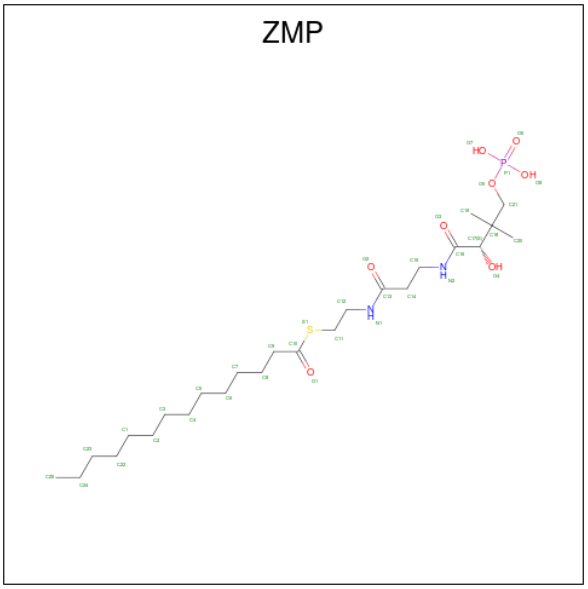
Mol	Chain	Residues	Atoms		AltConf
22	S6	1	Total	Zn	0
			1	1	

- Molecule 23 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
23	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 24 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



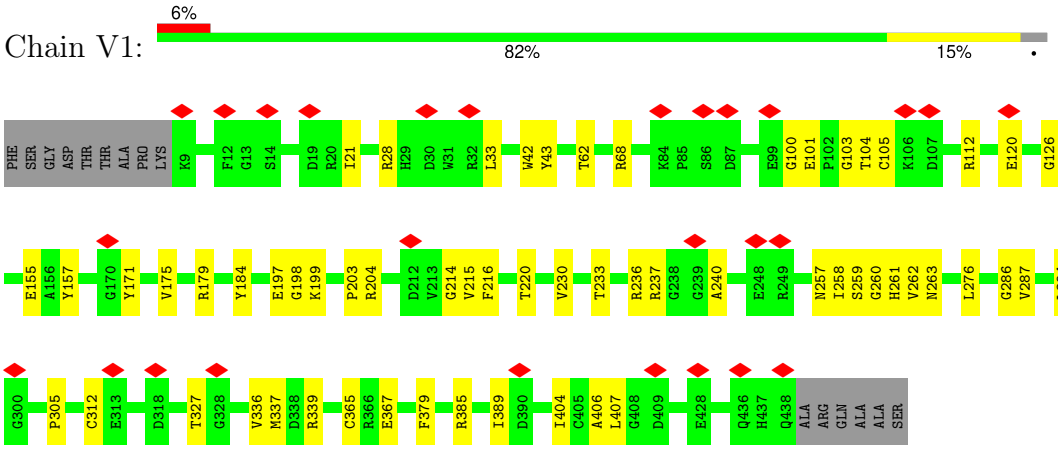
Mol	Chain	Residues	Atoms						AltConf
24	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

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.

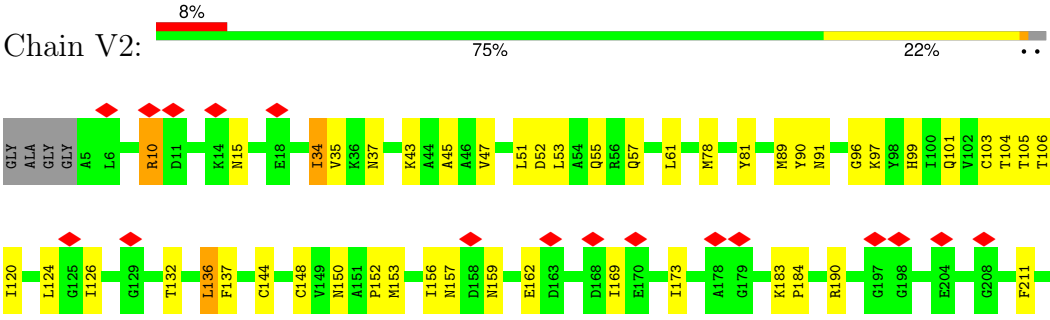
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



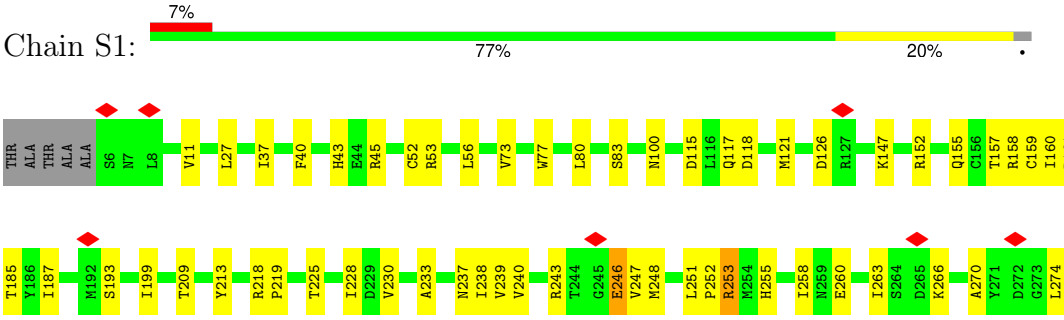
• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

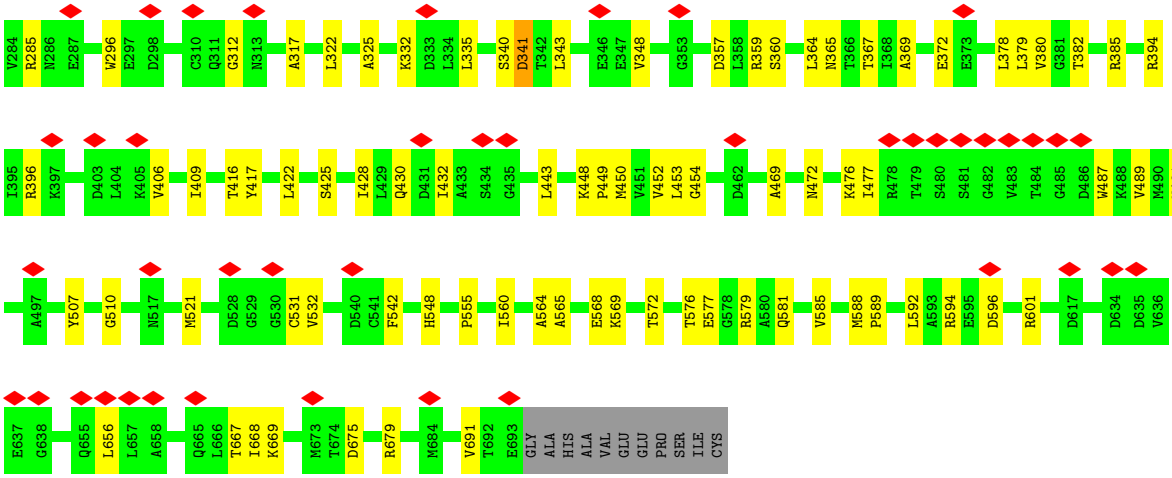
Chain V2:



• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

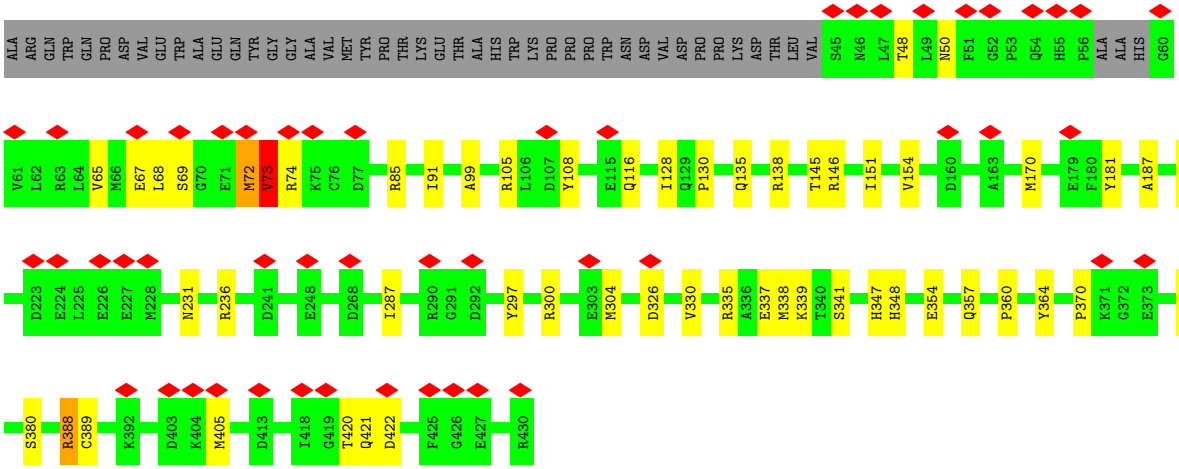
Chain S1:





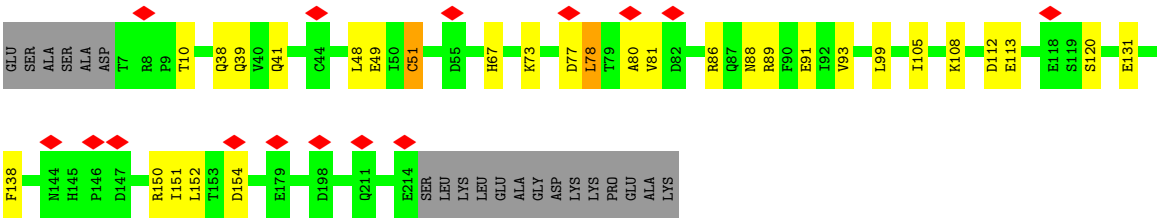
• Molecule 4: NADH:ubiquinone oxidoreductase core subunit S2,NADH:ubiquinone oxidoreductase core subunit S2

Chain S2:



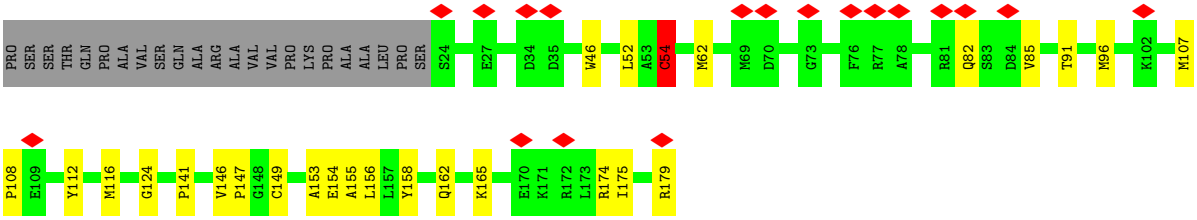
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:

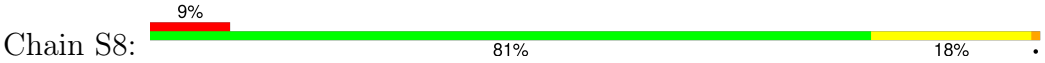


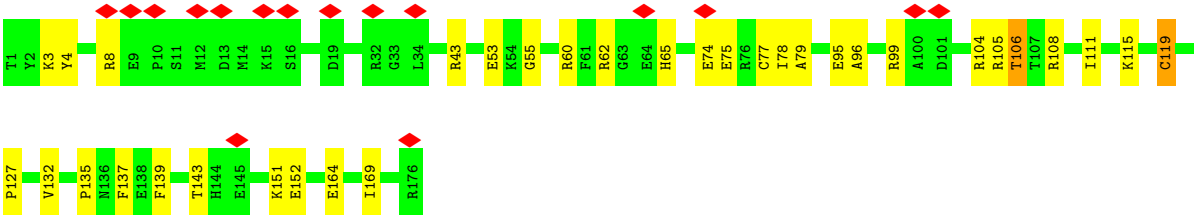
• Molecule 6: NADH:ubiquinone oxidoreductase core subunit S7

Chain S7:

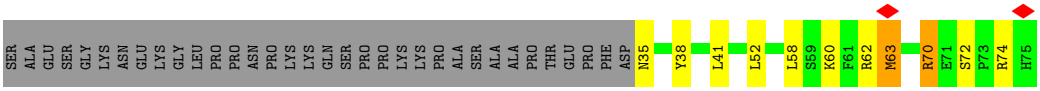


• Molecule 7: NADH:ubiquinone oxidoreductase core subunit S8

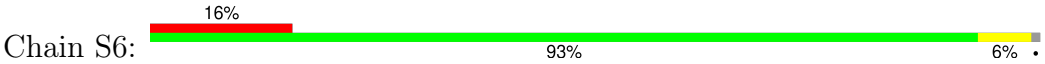




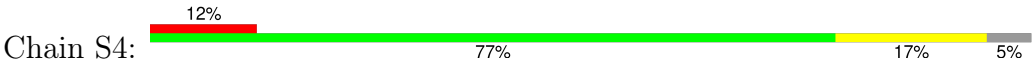
• Molecule 8: NADH:ubiquinone oxidoreductase subunit V3



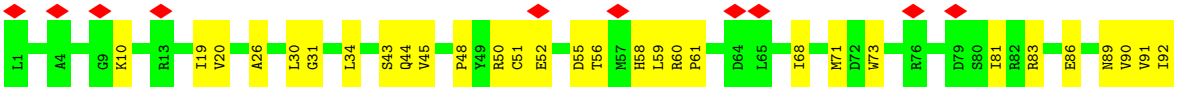
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

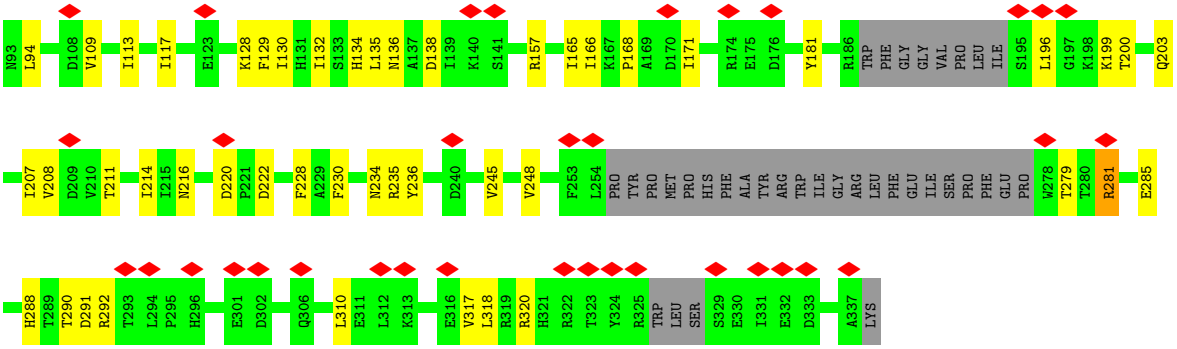


• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4



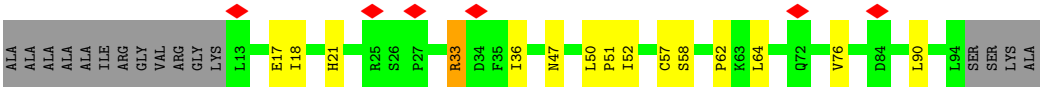
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9





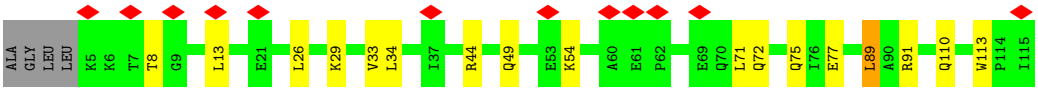
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



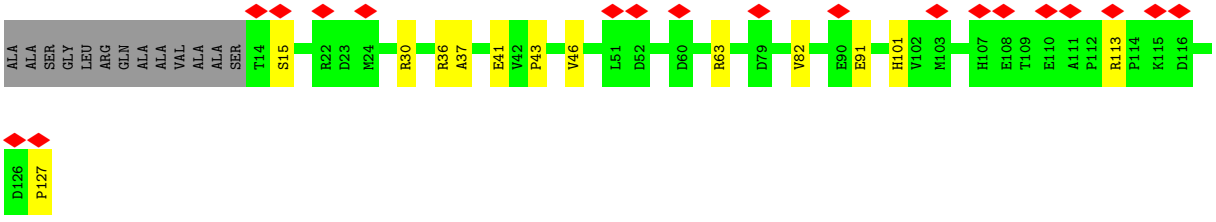
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:



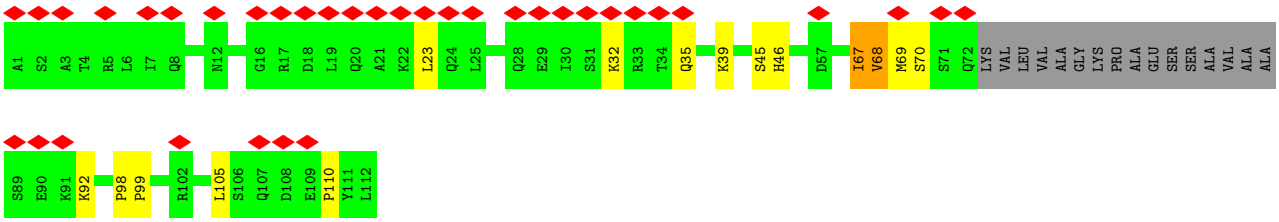
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



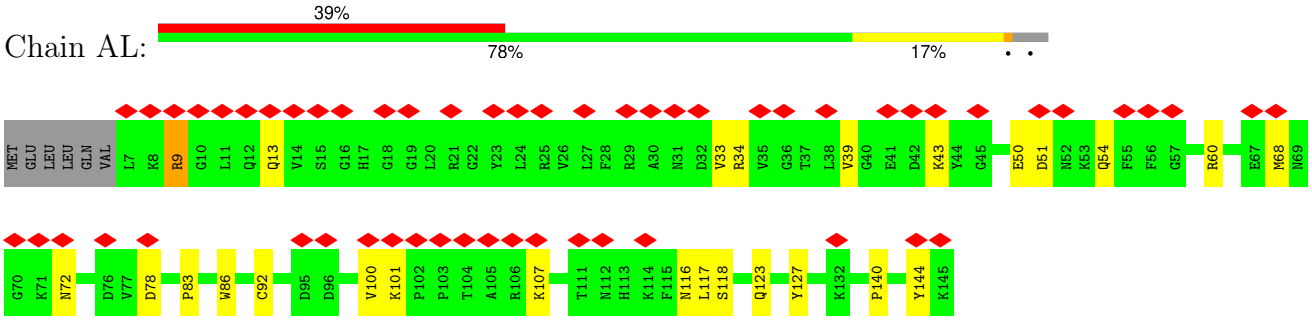
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7:



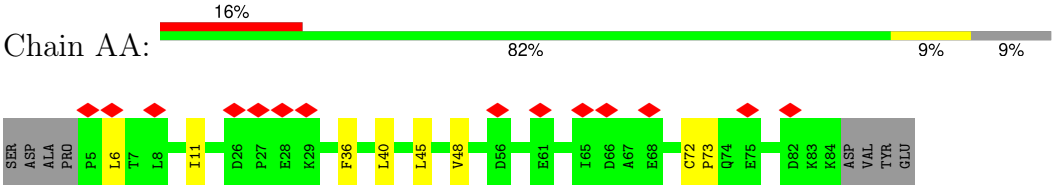
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:



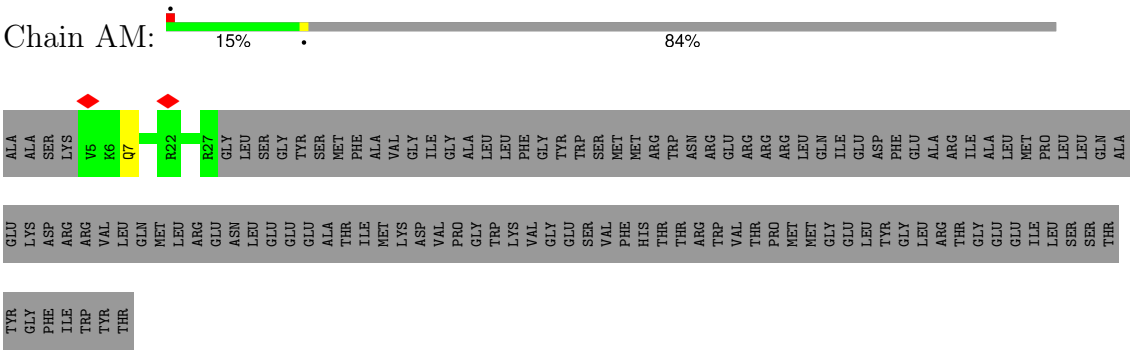
• Molecule 17: Acyl carrier protein

Chain AA:



• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AM:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178121	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.429	Depositor
Minimum map value	-0.368	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, SF4, NDP, FMN, ZN, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	V1	0.38	0/3386	0.61	0/4575
2	V2	0.36	0/1687	0.68	1/2295 (0.0%)
3	S1	0.35	0/5362	0.61	2/7266 (0.0%)
4	S2	0.39	0/3143	0.63	1/4246 (0.0%)
5	S3	0.37	0/1776	0.62	0/2417
6	S7	0.38	0/1278	0.57	0/1728
7	S8	0.43	1/1445 (0.1%)	0.61	0/1956
8	V3	0.31	0/355	0.67	1/480 (0.2%)
9	S6	0.34	0/749	0.57	0/1009
10	S4	0.32	0/1047	0.57	0/1415
11	A9	0.35	0/2455	0.67	1/3319 (0.0%)
12	A2	0.33	0/676	0.62	0/911
13	A5	0.32	0/921	0.66	2/1249 (0.2%)
14	A6	0.31	0/993	0.52	0/1336
15	A7	0.31	0/784	0.63	0/1060
16	AL	0.33	0/1201	0.62	0/1632
17	AA	0.30	0/655	0.64	0/881
18	AM	0.30	0/191	0.51	0/257
All	All	0.36	1/28104 (0.0%)	0.62	8/38032 (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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V2	0	1
3	S1	0	2
4	S2	0	1
5	S3	0	1
7	S8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	A9	0	1
13	A5	0	1
15	A7	0	4
16	AL	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S8	119	CYS	CB-SG	-5.91	1.72	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A5	89	LEU	CA-CB-CG	7.91	133.49	115.30
2	V2	136	LEU	CA-CB-CG	7.13	131.69	115.30
11	A9	222	ASP	CB-CG-OD1	6.89	124.50	118.30
4	S2	72	MET	C-N-CA	6.52	137.99	121.70
8	V3	41	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S1	213	TYR	Peptide
3	S1	341	ASP	Peptide
4	S2	73	VAL	Mainchain
5	S3	51	CYS	Peptide
2	V2	10	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V1	3312	0	3266	46	0
2	V2	1647	0	1657	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S1	5275	0	5300	86	0
4	S2	3071	0	3041	42	0
5	S3	1726	0	1676	27	0
6	S7	1247	0	1256	20	0
7	S8	1414	0	1371	25	0
8	V3	345	0	323	10	0
9	S6	737	0	710	4	0
10	S4	1024	0	1023	16	0
11	A9	2402	0	2400	43	0
12	A2	665	0	678	8	0
13	A5	901	0	936	10	0
14	A6	969	0	980	10	0
15	A7	766	0	779	15	0
16	AL	1160	0	1125	15	0
17	AA	645	0	649	5	0
18	AM	186	0	190	1	0
19	S1	16	0	0	1	0
19	S7	8	0	0	1	0
19	S8	16	0	0	0	0
19	V1	8	0	0	0	0
20	V1	31	0	19	2	0
21	S1	4	0	0	0	0
21	V2	4	0	0	0	0
22	S6	1	0	0	0	0
23	A9	48	0	26	0	0
24	AA	34	0	40	0	0
All	All	27662	0	27445	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 347 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.20	1.37
5:S3:38:GLN:O	15:A7:70:SER:HA	1.40	1.22
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.11	0.99
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.65	0.95
5:S3:38:GLN:O	15:A7:70:SER:CA	2.16	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V1	428/445 (96%)	394 (92%)	34 (8%)	0	100	100
2	V2	210/217 (97%)	178 (85%)	31 (15%)	1 (0%)	25	58
3	S1	686/704 (97%)	618 (90%)	66 (10%)	2 (0%)	37	69
4	S2	379/430 (88%)	341 (90%)	37 (10%)	1 (0%)	37	69
5	S3	206/228 (90%)	176 (85%)	30 (15%)	0	100	100
6	S7	154/179 (86%)	139 (90%)	14 (9%)	1 (1%)	22	55
7	S8	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
8	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	111 (90%)	13 (10%)	0	100	100
11	A9	295/338 (87%)	261 (88%)	34 (12%)	0	100	100
12	A2	80/98 (82%)	70 (88%)	10 (12%)	0	100	100
13	A5	109/115 (95%)	99 (91%)	10 (9%)	0	100	100
14	A6	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
15	A7	92/112 (82%)	78 (85%)	13 (14%)	1 (1%)	12	42
16	AL	137/145 (94%)	115 (84%)	21 (15%)	1 (1%)	19	52
17	AA	78/88 (89%)	64 (82%)	14 (18%)	0	100	100
18	AM	21/143 (15%)	19 (90%)	2 (10%)	0	100	100
All	All	3417/3849 (89%)	3042 (89%)	368 (11%)	7 (0%)	45	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	247	VAL
16	AL	107	LYS
3	S1	359	ARG
6	S7	54	CYS

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Mol	Chain	Res	Type
2	V2	15	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	V1	344/354 (97%)	340 (99%)	4 (1%)	67 77
2	V2	182/183 (100%)	179 (98%)	3 (2%)	58 73
3	S1	578/588 (98%)	574 (99%)	4 (1%)	81 86
4	S2	332/371 (90%)	331 (100%)	1 (0%)	91 92
5	S3	189/204 (93%)	188 (100%)	1 (0%)	86 90
6	S7	132/150 (88%)	130 (98%)	2 (2%)	60 74
7	S8	151/151 (100%)	150 (99%)	1 (1%)	81 86
8	V3	40/68 (59%)	37 (92%)	3 (8%)	11 35
9	S6	79/80 (99%)	79 (100%)	0	100 100
10	S4	113/119 (95%)	112 (99%)	1 (1%)	75 82
11	A9	252/292 (86%)	249 (99%)	3 (1%)	67 77
12	A2	73/81 (90%)	72 (99%)	1 (1%)	62 75
13	A5	99/101 (98%)	99 (100%)	0	100 100
14	A6	107/113 (95%)	107 (100%)	0	100 100
15	A7	84/94 (89%)	84 (100%)	0	100 100
16	AL	125/131 (95%)	122 (98%)	3 (2%)	44 62
17	AA	74/81 (91%)	74 (100%)	0	100 100
18	AM	20/121 (16%)	20 (100%)	0	100 100
All	All	2974/3282 (91%)	2947 (99%)	27 (1%)	74 82

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S7	174	ARG

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Mol	Chain	Res	Type
8	V3	63	MET
16	AL	9	ARG
8	V3	60	LYS
8	V3	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
9	S6	16	GLN
11	A9	288	HIS
16	AL	72	ASN
11	A9	89	ASN
13	A5	49	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\|>2$
19	SF4	S1	801	3	0,12,12	-	-	-		
19	SF4	S1	802	3	0,12,12	-	-	-		
21	FES	S1	803	3	0,4,4	-	-	-		
19	SF4	S8	201	7	0,12,12	-	-	-		
19	SF4	S8	202	7	0,12,12	-	-	-		
19	SF4	V1	500	1	0,12,12	-	-	-		
24	ZMP	AA	101	17	28,33,36	0.66	1 (3%)	32,40,45	1.15	3 (9%)
21	FES	V2	300	2	0,4,4	-	-	-		
23	NDP	A9	401	-	47,52,52	0.62	0	61,80,80	0.71	2 (3%)
20	FMN	V1	501	-	33,33,33	0.28	0	48,50,50	0.40	0
19	SF4	S7	300	6	0,12,12	-	-	-		

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
19	SF4	S1	801	3	-	-	0/6/5/5
19	SF4	S1	802	3	-	-	0/6/5/5
21	FES	S1	803	3	-	-	0/1/1/1
19	SF4	S8	201	7	-	-	0/6/5/5
19	SF4	S8	202	7	-	-	0/6/5/5
24	ZMP	AA	101	17	-	10/38/40/43	-
19	SF4	V1	500	1	-	-	0/6/5/5
21	FES	V2	300	2	-	-	0/1/1/1
23	NDP	A9	401	-	-	15/30/77/77	0/5/5/5
20	FMN	V1	501	-	-	9/18/18/18	0/3/3/3
19	SF4	S7	300	6	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	101	ZMP	C9-C10	2.43	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	101	ZMP	O1-C10-C9	-2.79	120.75	123.98
23	A9	401	NDP	P2B-O2B-C2B	2.64	130.49	123.43
24	AA	101	ZMP	C15-C14-C13	-2.61	108.05	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A9	401	NDP	C5A-C6A-N6A	2.29	123.79	120.31
24	AA	101	ZMP	C11-C12-N1	-2.10	108.03	112.41

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	V1	501	FMN	N10-C1'-C2'-O2'
20	V1	501	FMN	N10-C1'-C2'-C3'
20	V1	501	FMN	C1'-C2'-C3'-C4'
23	A9	401	NDP	C5B-O5B-PA-O1A
23	A9	401	NDP	C5B-O5B-PA-O2A

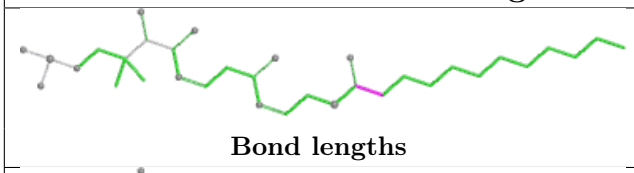
There are no ring outliers.

3 monomers are involved in 4 short contacts:

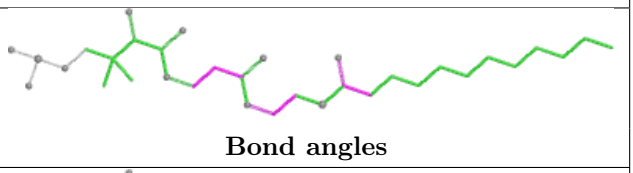
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S1	801	SF4	1	0
20	V1	501	FMN	2	0
19	S7	300	SF4	1	0

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.

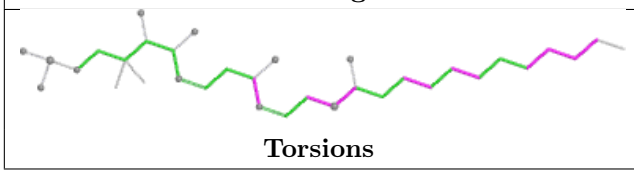
Ligand ZMP AA 101



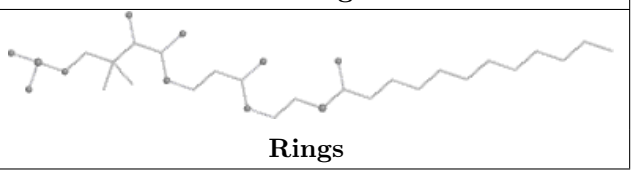
Bond lengths



Bond angles

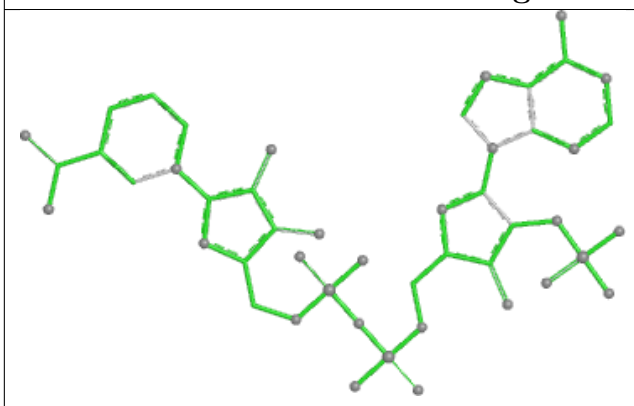


Torsions

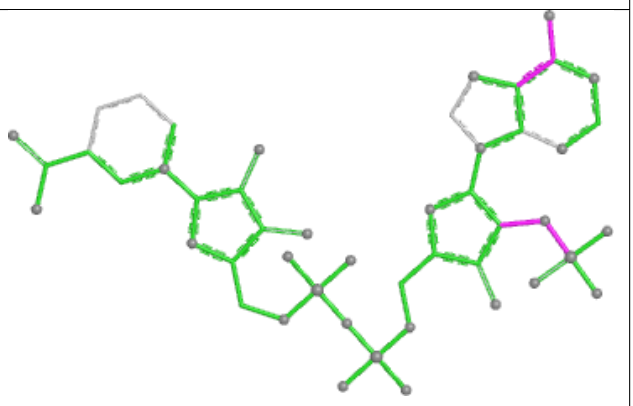


Rings

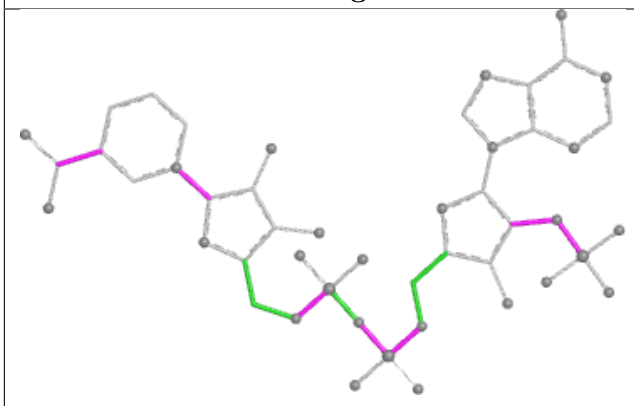
Ligand NDP A9 401



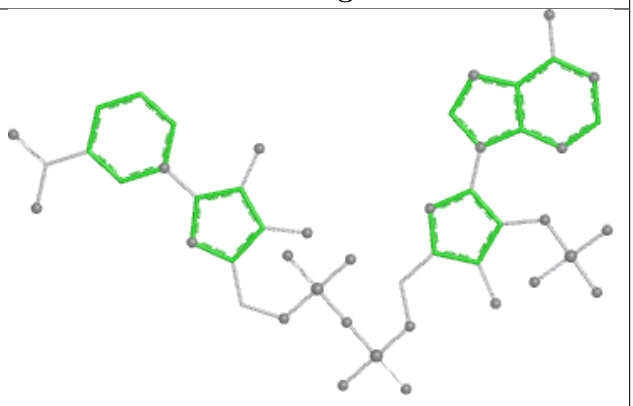
Bond lengths



Bond angles

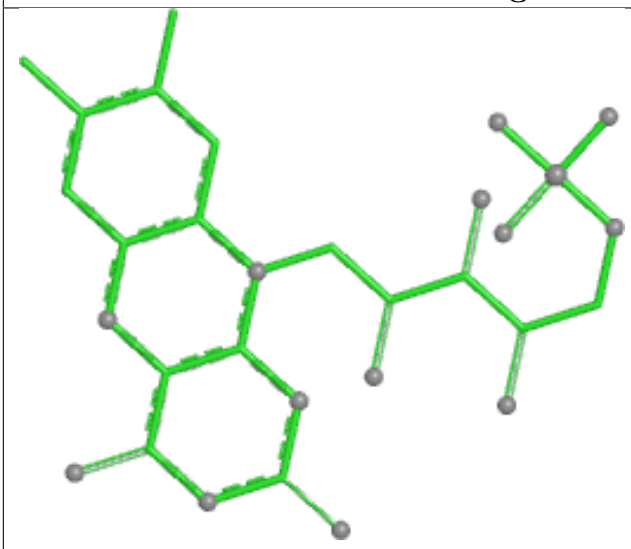


Torsions

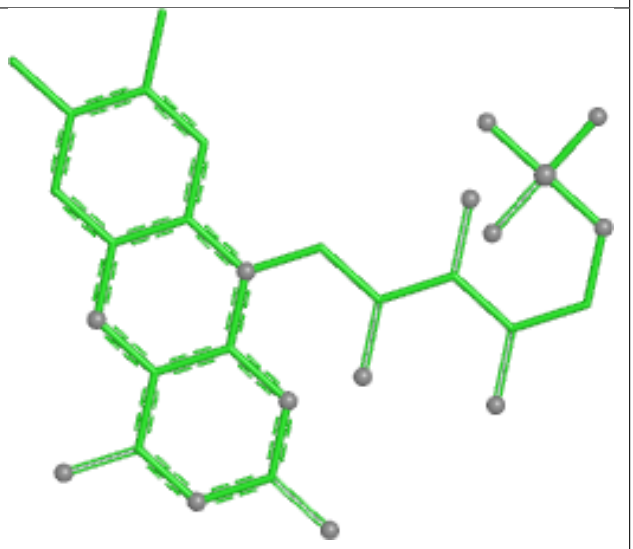


Rings

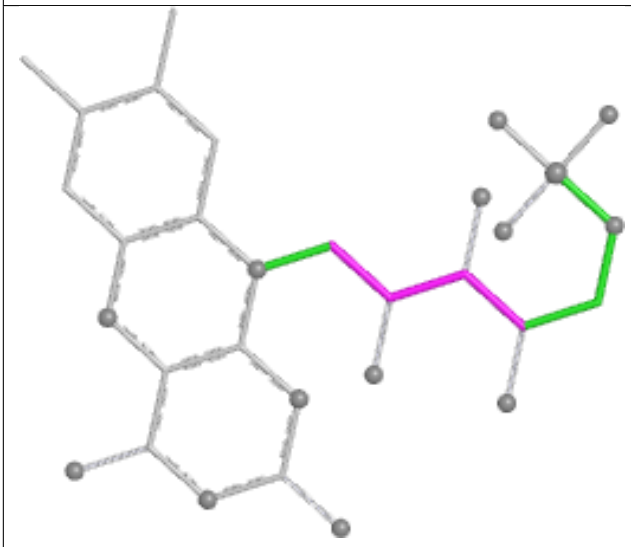
Ligand FMN V1 501



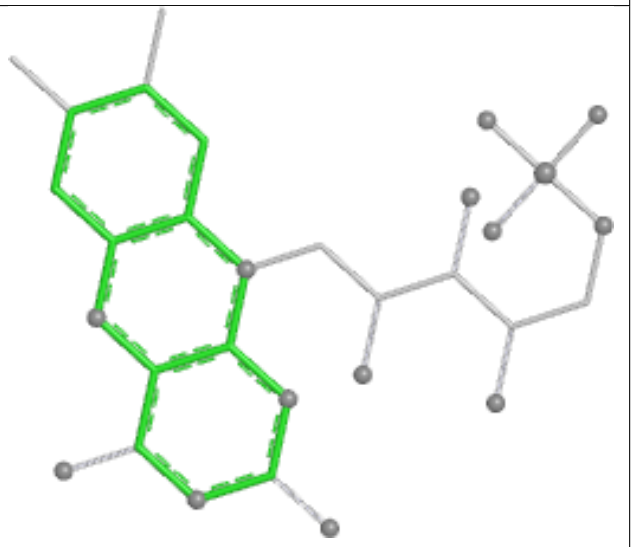
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

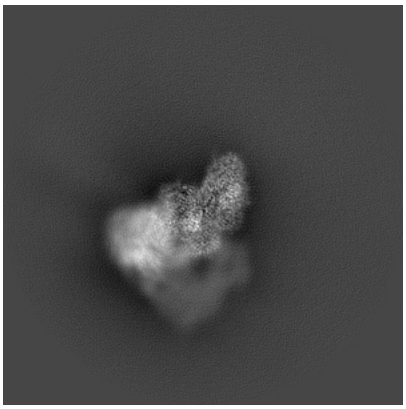
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4480. These allow visual inspection of the internal detail of the map and identification of artifacts.

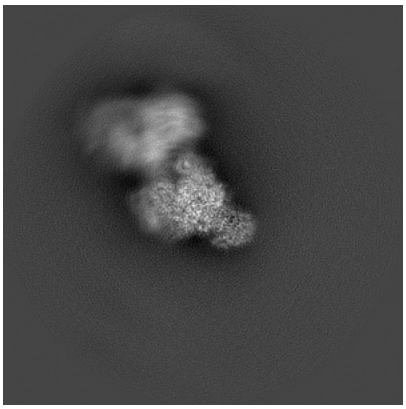
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

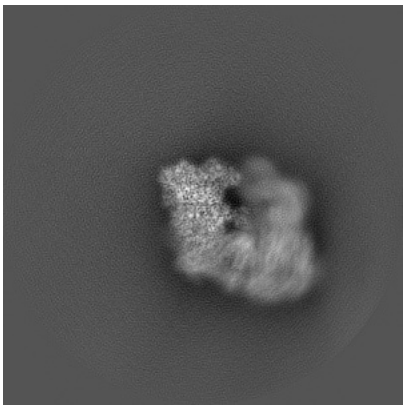
6.1.1 Primary map



X

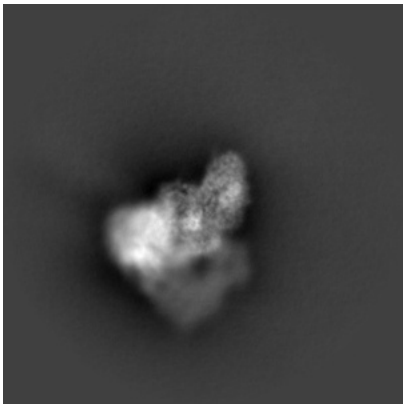


Y

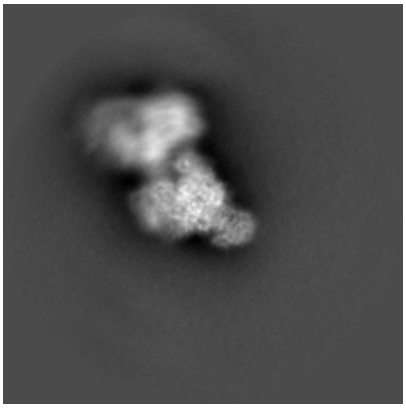


Z

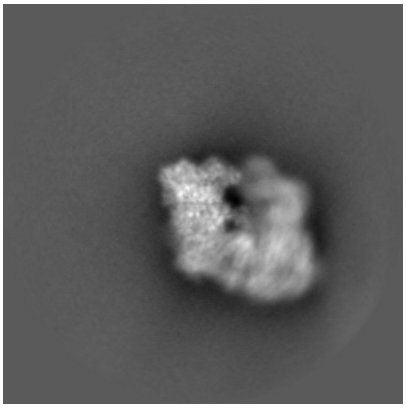
6.1.2 Raw map



X



Y

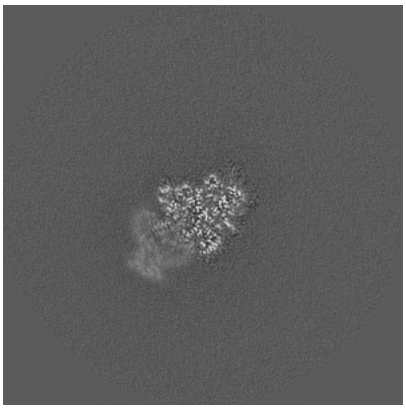


Z

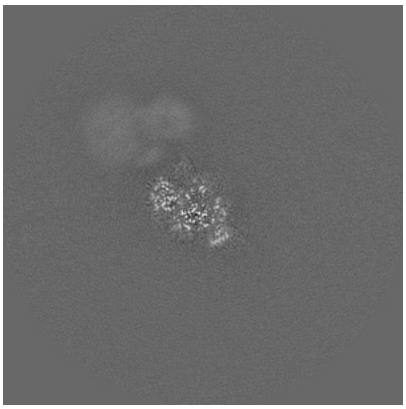
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



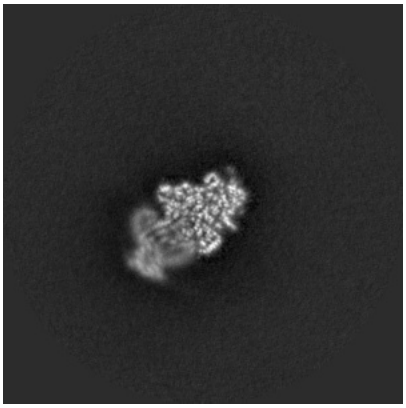
X Index: 200



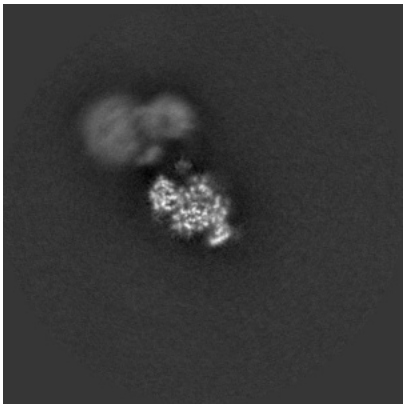
Y Index: 200

Z Index: 200

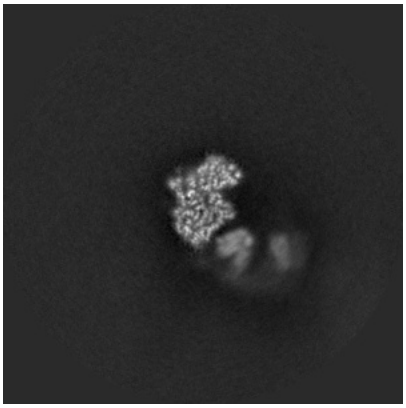
6.2.2 Raw map



X Index: 200



Y Index: 200

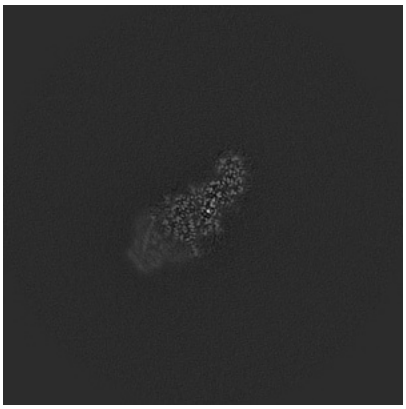


Z Index: 200

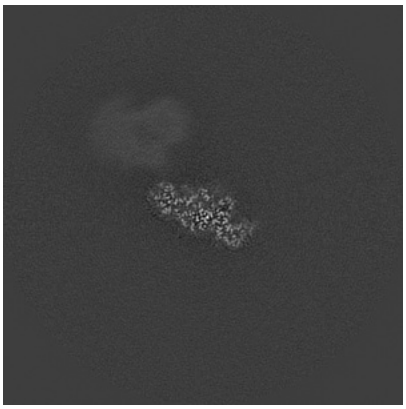
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

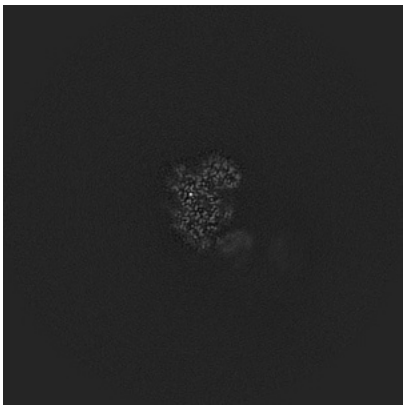
6.3.1 Primary map



X Index: 186

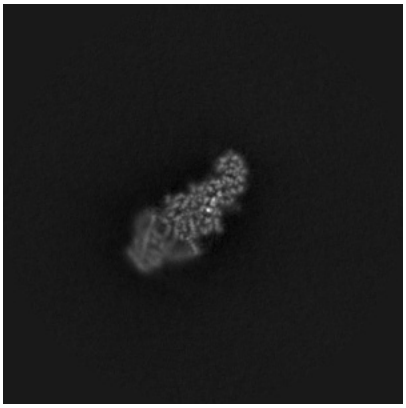


Y Index: 209

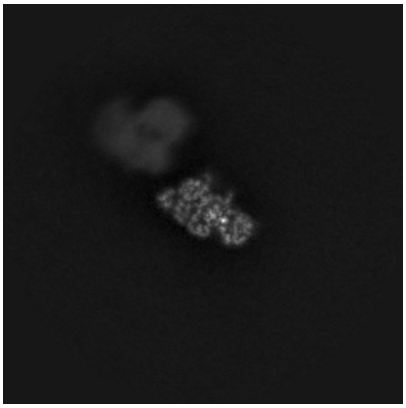


Z Index: 204

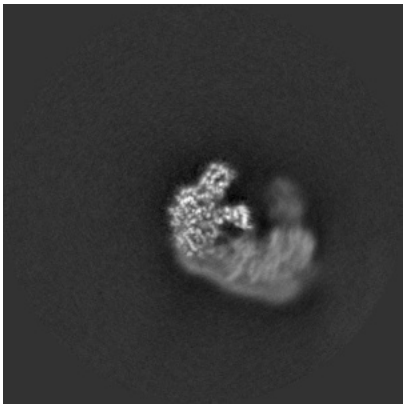
6.3.2 Raw map



X Index: 186



Y Index: 216

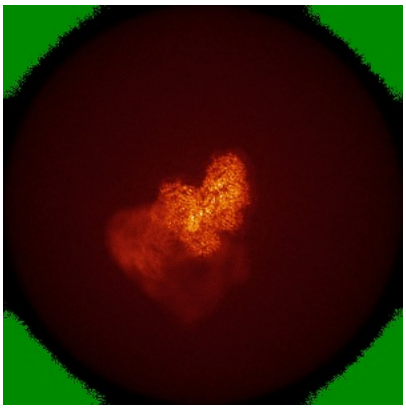


Z Index: 183

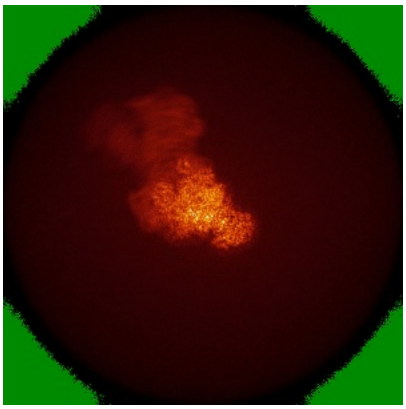
The images above show the largest variance slices of the map in three orthogonal directions.

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

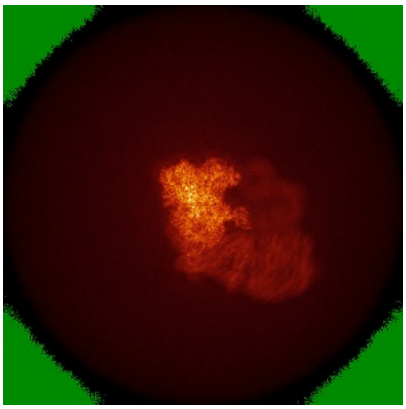
6.4.1 Primary map



X

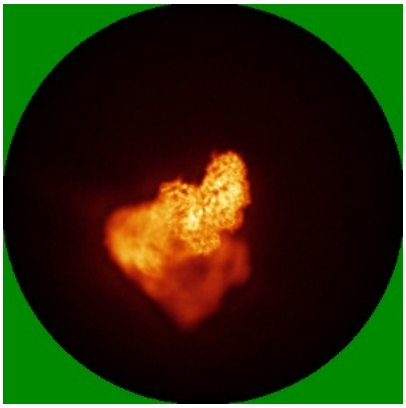


Y

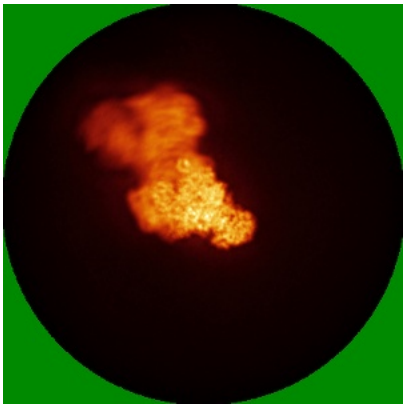


Z

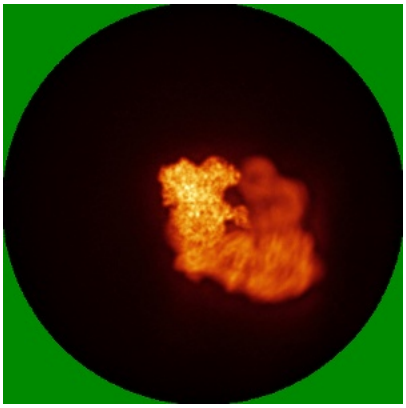
6.4.2 Raw map



X



Y



Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

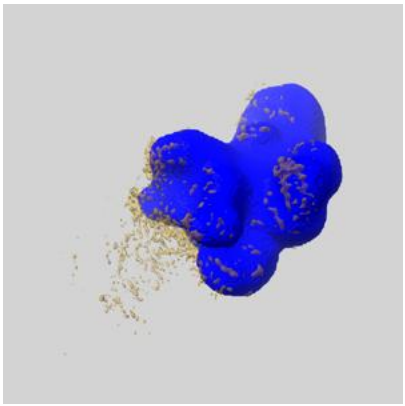
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

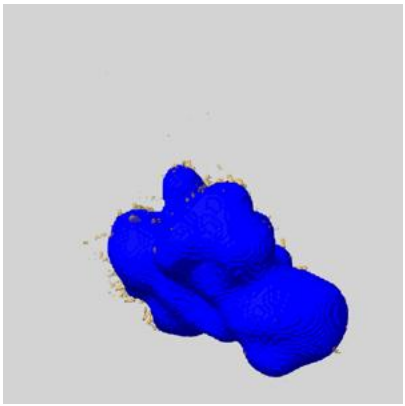
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

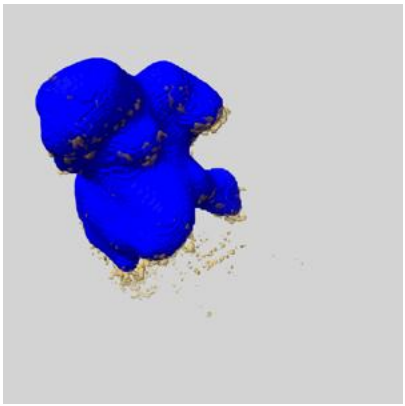
6.6.1 emd_4480_msk_1.map (i)



X



Y

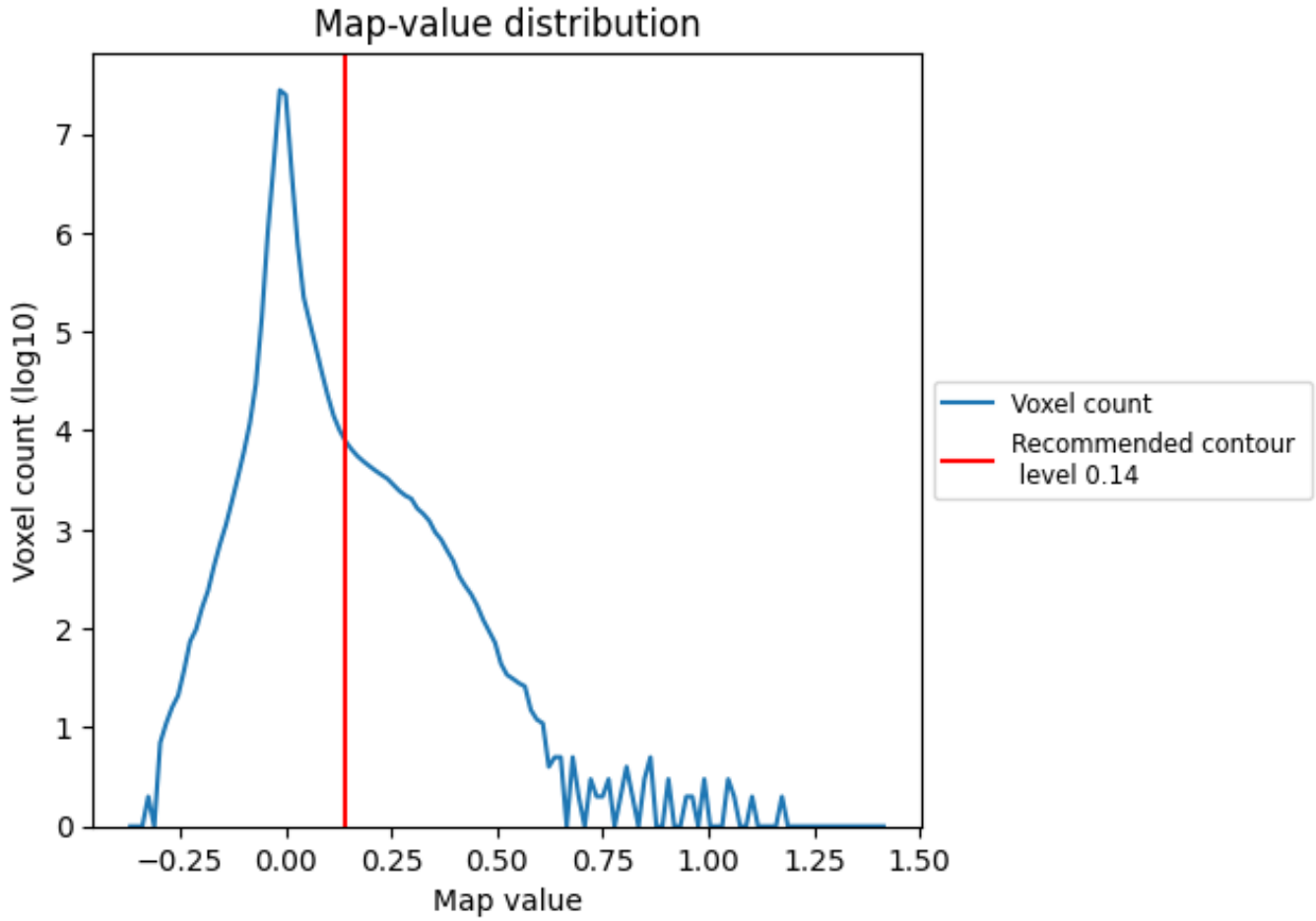


Z

7 Map analysis

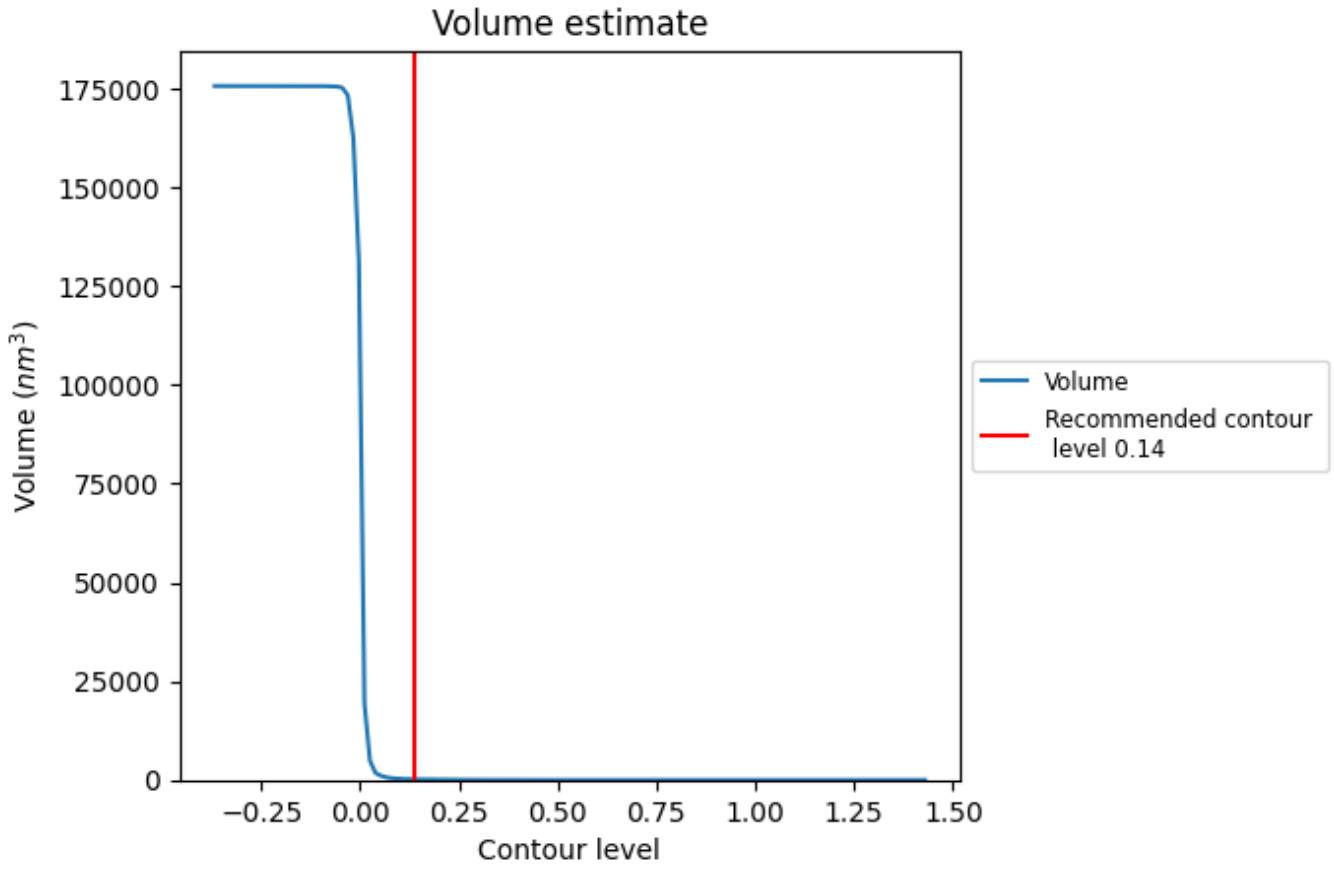
This section contains the results of statistical analysis of the map.

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.

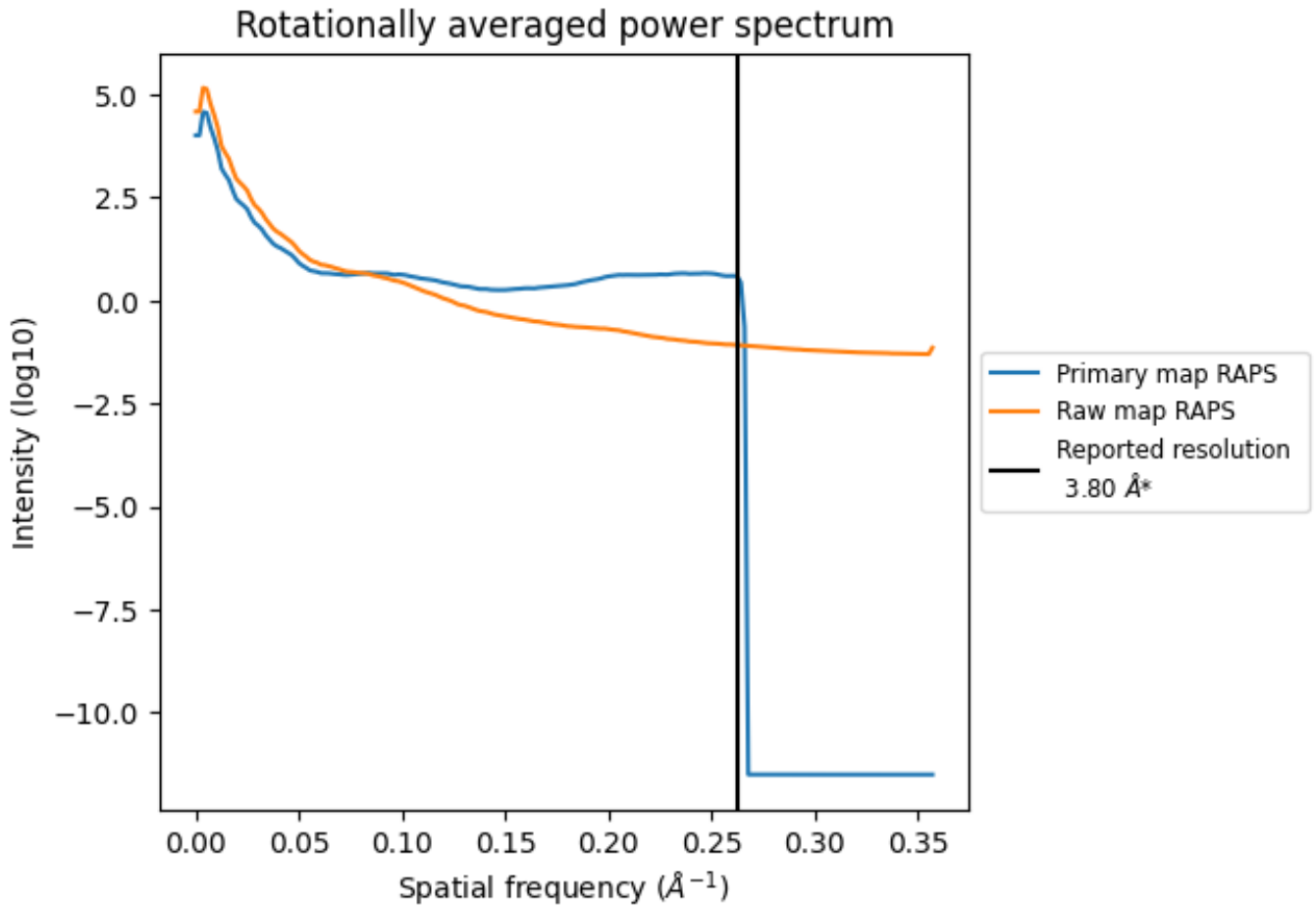
7.2 Volume estimate (i)



The volume at the recommended contour level is 162 nm^3; this corresponds to an approximate mass of 147 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

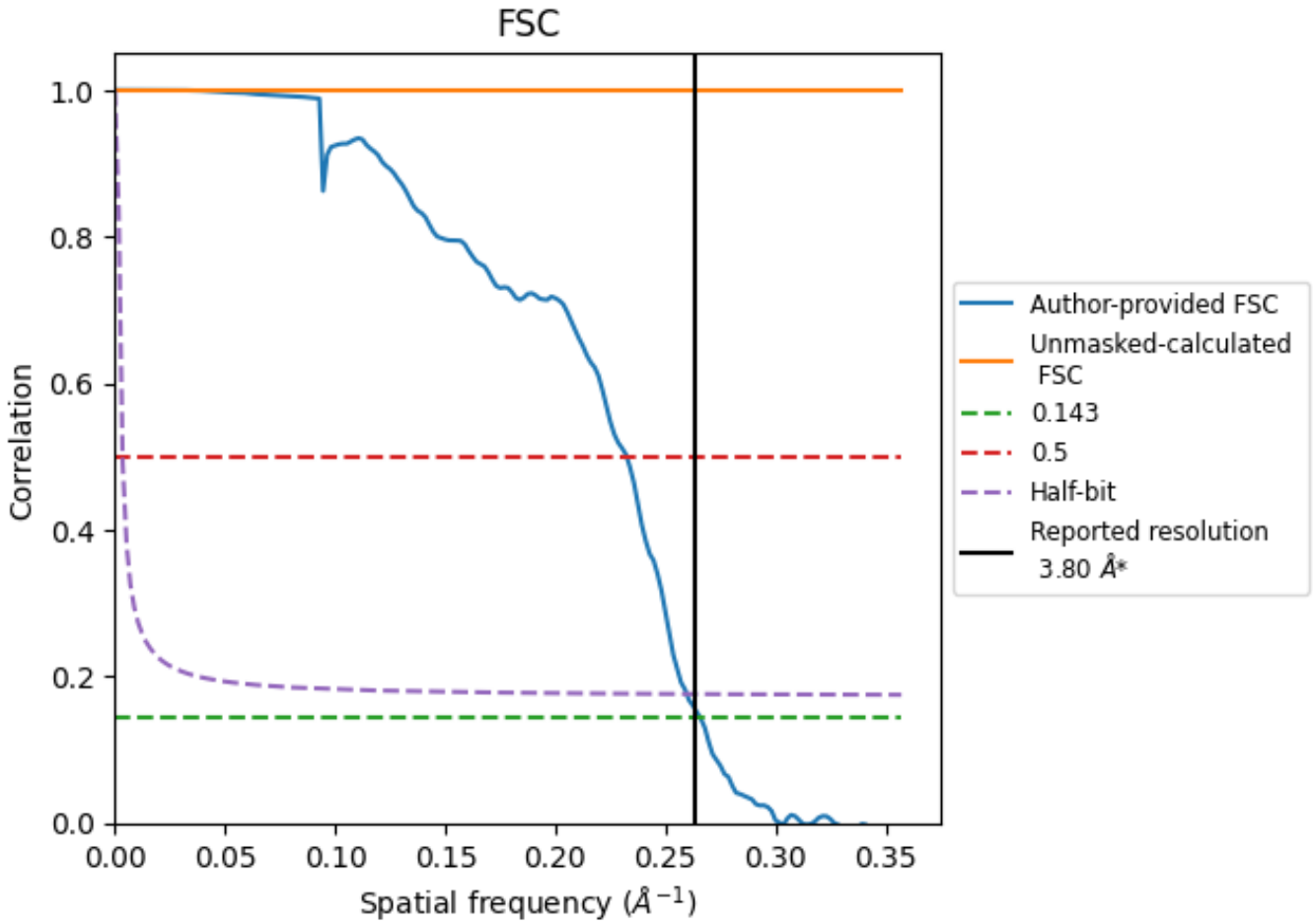


*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

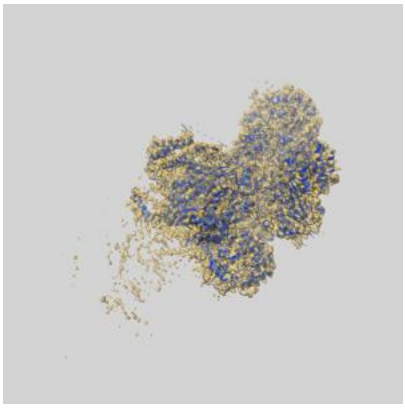
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.30	3.85
Unmasked-calculated*	-	-	-

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

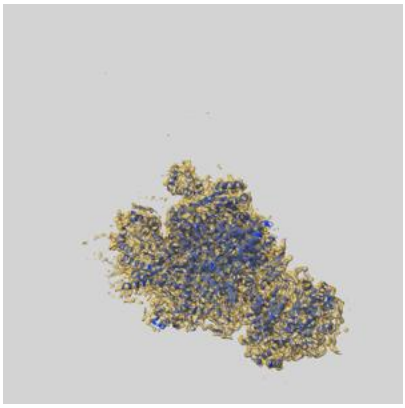
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4480 and PDB model 6Q9D. Per-residue inclusion information can be found in section 3 on page 11.

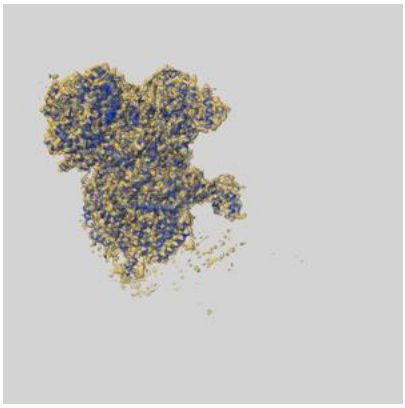
9.1 Map-model overlay



X



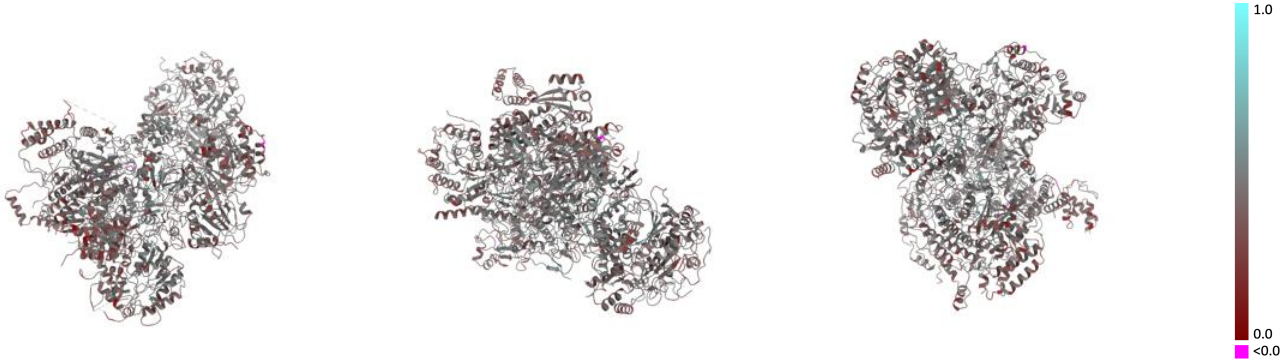
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

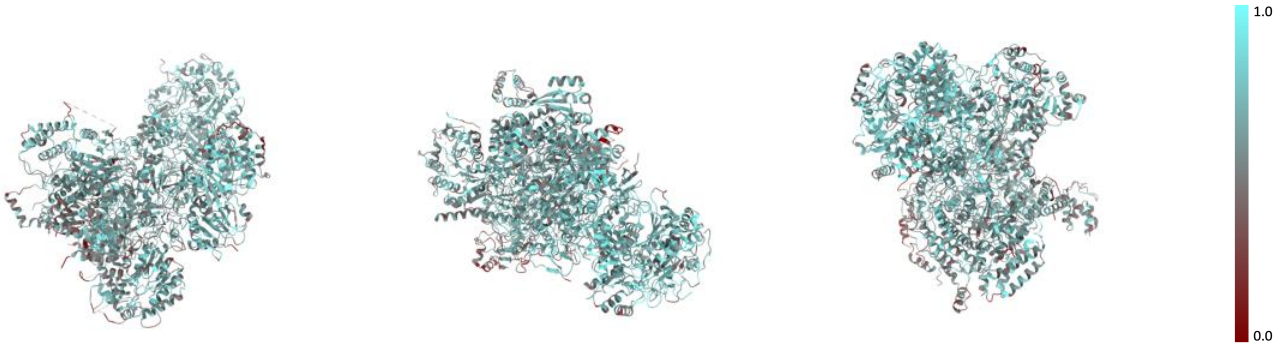
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

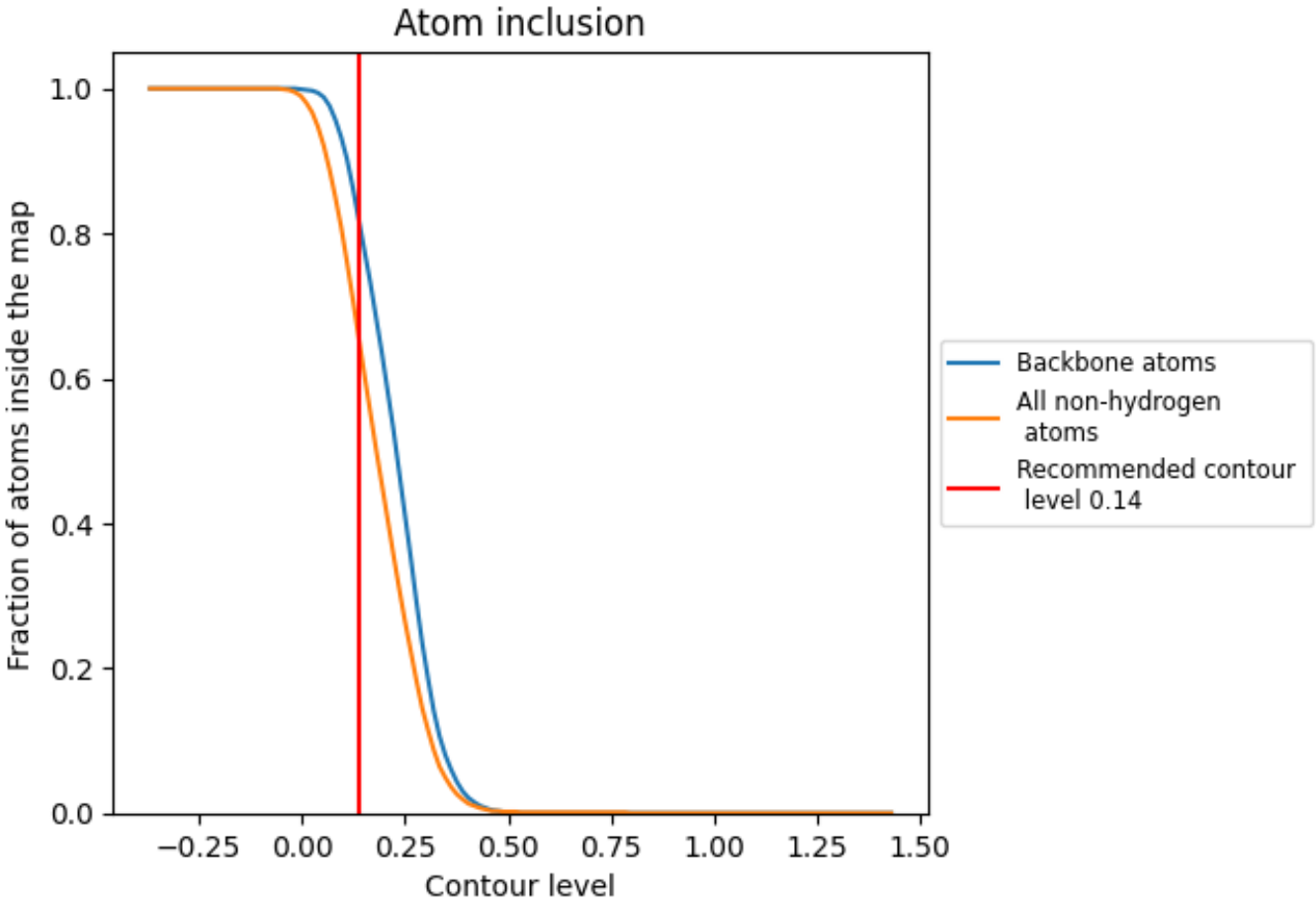
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.4240
A2	0.6940	0.4050
A5	0.6340	0.3890
A6	0.6020	0.4210
A7	0.5110	0.4050
A9	0.6200	0.4120
AA	0.5390	0.3350
AL	0.5020	0.4070
AM	0.5620	0.4220
S1	0.6790	0.4390
S2	0.6370	0.4270
S3	0.6690	0.4440
S4	0.6170	0.4300
S6	0.6550	0.4390
S7	0.6510	0.4340
S8	0.6770	0.4350
V1	0.7010	0.4300
V2	0.6890	0.4180
V3	0.7080	0.4160