



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:02 pm GMT

PDB ID : 6QCA  
EMDB ID : EMD-4502  
Title : Ovine respiratory complex I FRC open class 5  
Authors : Letts, J.A.; Sazanov, L.A.  
Deposited on : 2018-12-27  
Resolution : 6.20 Å (reported)  
Based on initial model : 5LNK

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

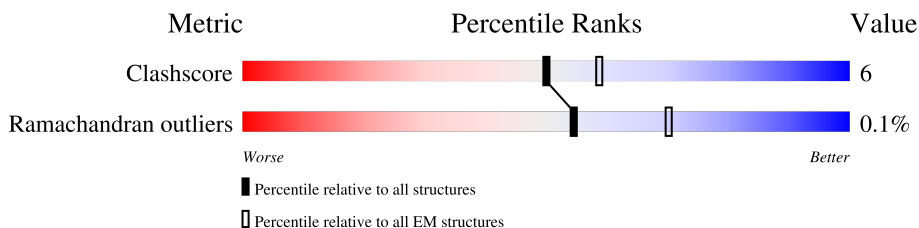
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 6.20 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	158937	4297
Ramachandran outliers	154571	4023

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

Mol	Chain	Length	Quality of chain
1	V1	445	
2	V2	217	
3	S1	704	
4	S2	430	
5	S3	228	
6	S7	179	
7	S8	176	
8	V3	75	
9	S6	96	

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Mol	Chain	Length	Quality of chain
10	S4	133	18% 91% 5%
11	A9	338	20% 81% 15%
12	A2	98	8% 80% 16%
13	A5	115	22% 92% ...
14	A6	127	9% 86% 10%
15	A7	112	41% 75% 10% 14%
16	AL	145	60% 91% 8%
17	AA	88	14% 90% 9%
17	AB	88	17% 98% ..
18	D3	115	29% 78% 22%
19	D1	318	30% 94% 5%
20	D6	175	46% 91% 6%
21	4L	98	31% 99% .
22	D5	606	24% 97% .
23	D4	459	22% 98% .
24	D2	347	25% 99% .
25	AK	140	39% 97% ..
26	B5	143	11% 97% .
27	A8	171	17% 95% 5%
28	BJ	175	17% 91% 7%
29	AJ	320	18% 94% 6%
30	S5	105	19% 93% 6%
31	A3	83	24% 88% 11%
32	B3	97	30% 67% 8% 25%
33	C2	120	19% 90% 8% ..

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Mol	Chain	Length	Quality of chain
34	B4	128	<p>21% 97%</p>
35	AM	143	<p>23% 94%</p>
36	B6	127	<p>20% 69% 6% 24%</p>
37	B7	136	<p>16% 82% 5% 12%</p>
38	B9	178	<p>11% 95%</p>
39	B2	72	<p>26% 81% 10% 10%</p>
40	B8	158	<p>25% 97%</p>
41	BK	125	<p>21% 81% 18%</p>
42	C1	49	<p>10% 92% 6%</p>
43	B1	57	<p>28% 89% 9%</p>
44	A1	70	<p>21% 94% 6%</p>

## 2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 40144 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		
1	V1	430	2099	1239	430	430	0	0

- Molecule 2 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	V2	212	1045	621	212	212	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	S1	688	3390	2014	688	688	0	0

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	S2	424	2090	1242	424	424	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	S3	208	1034	618	208	208	0	0

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	S7	156	769	457	156	156	0	0

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S8	176	871	519	176	176	0	0

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	V3	41	204	122	41	41	0	0

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	S6	95	462	272	95	95	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	S4	126	625	373	126	126	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	A9	287	1413	839	287	287	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	A2	82	406	242	82	82	0	0

- Molecule 13 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	A5	111	550	328	111	111	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	A6	114	567	339	114	114	0	0

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	A7	96	476	284	96	96	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	AL	144	708	420	144	144	0	0

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	AA	80	397	237	80	80	0	0
17	AB	87	432	258	87	87	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	D3	90	449	269	90	90	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	D1	303	1505	899	303	303	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	D6	171	829	487	171	171	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	4L	98	486	290	98	98	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	D5	606	3001	1789	606	606	0	0

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	D4	459	2277	1359	459	459	0	0

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	D2	347	1721	1027	347	347	0	0

- Molecule 25 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	AK	140	682	402	140	140	0	0

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	B5	139	687	409	139	139	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	A8	171	847	505	171	171	0	0

- Molecule 28 is a protein called NDUFB10.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	BJ	171	853	511	171	171	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	AJ	319	1575	937	319	319	0	0

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	S5	99	490	292	99	99	0	0

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	A3	74	367	219	74	74	0	0

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	B3	73	356	210	73	73	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	C2	119	589	351	119	119	0	0

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	B4	128	635	379	128	128	0	0

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	AM	139	Total	C	N	O	0	0
			681	403	139	139		

- Molecule 36 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	B6	96	Total	C	N	O	0	0
			477	285	96	96		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	B7	119	Total	C	N	O	0	0
			592	354	119	119		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	B9	176	Total	C	N	O	0	0
			874	522	176	176		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	B2	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	B8	157	Total	C	N	O	0	0
			775	461	157	157		

- Molecule 41 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BK	102	Total	C	N	O	0	0
			506	302	102	102		

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	C1	46	227	135	46	46	0	0

- Molecule 43 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	B1	52	258	154	52	52	0	0

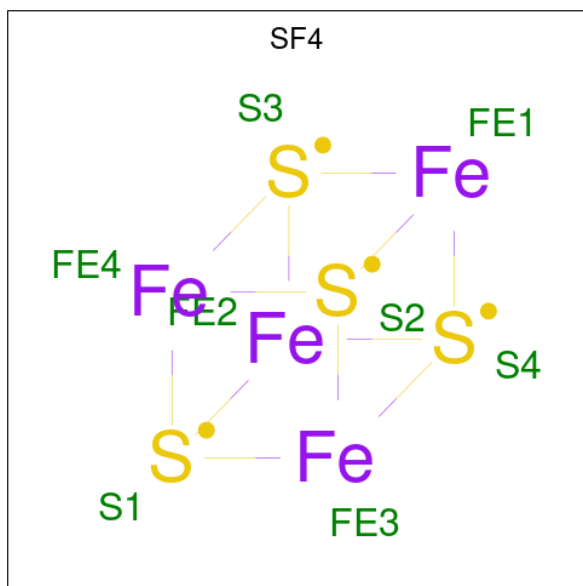
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	A1	70	343	203	70	70	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



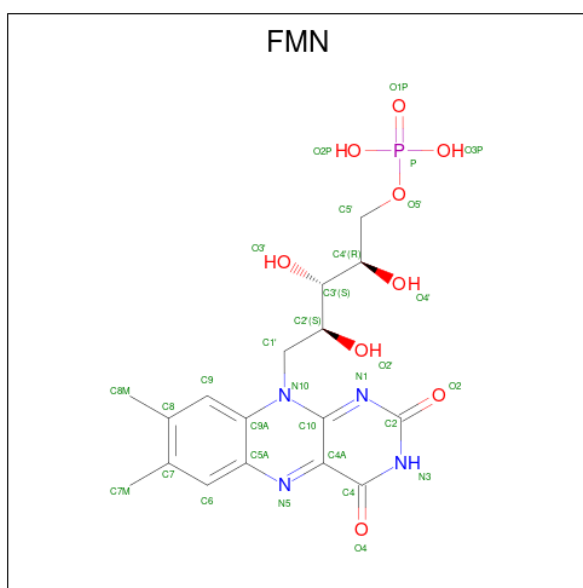
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	V1	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	S1	1	Total 16	Fe 8	S 8	0
45	S1	1	Total 16	Fe 8	S 8	0
45	S7	1	Total 8	Fe 4	S 4	0
45	S8	1	Total 16	Fe 8	S 8	0
45	S8	1	Total 16	Fe 8	S 8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

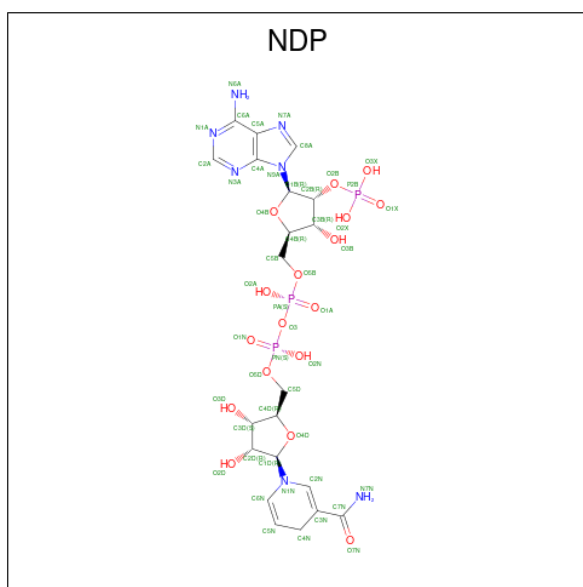


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	V2	1	4	2	2	0
47	S1	1	4	2	2	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

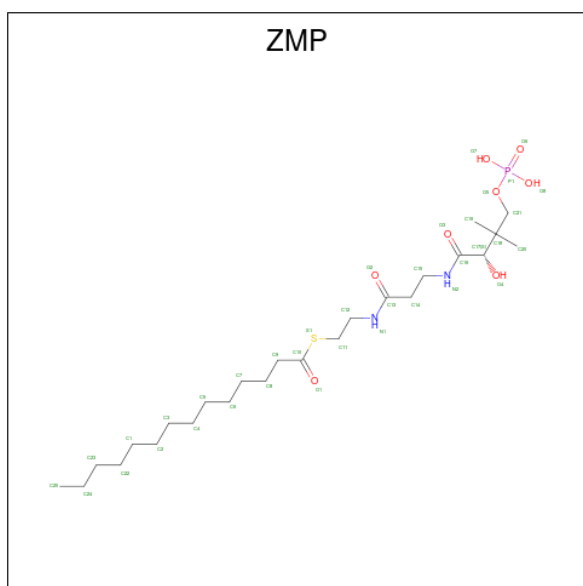
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	S6	1	1	1	0

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl})amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).

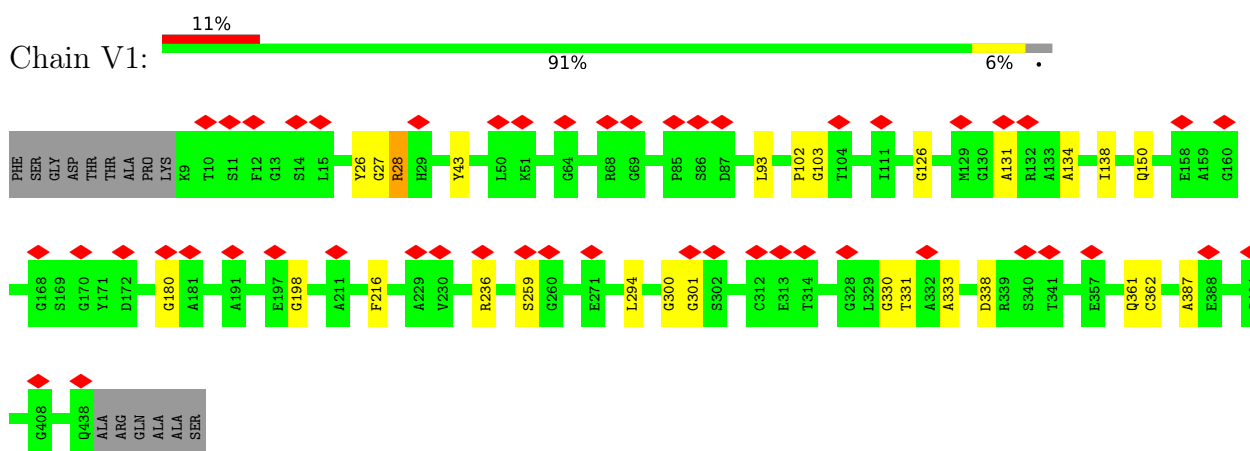


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
50	A6	1	34	23	2	7	1	1	0
50	AB	1	31	20	2	7	1	1	0

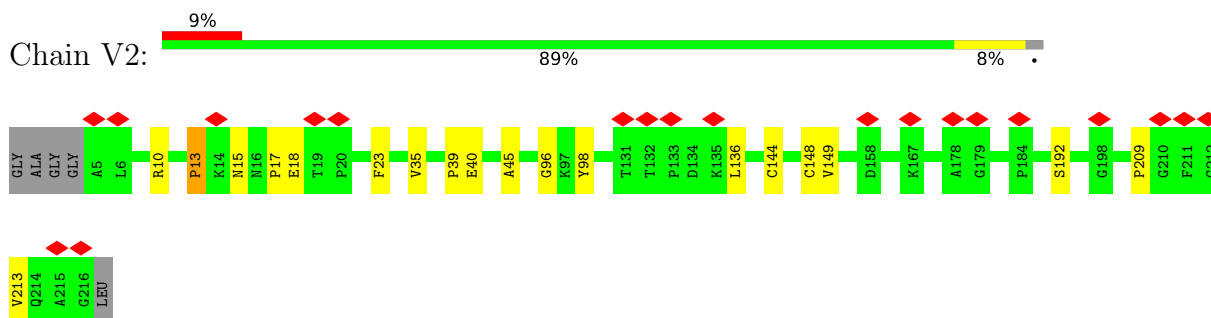
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

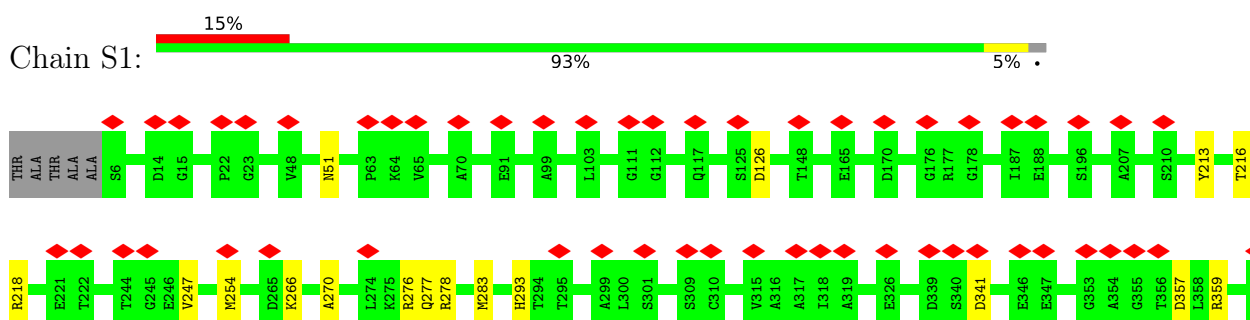
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

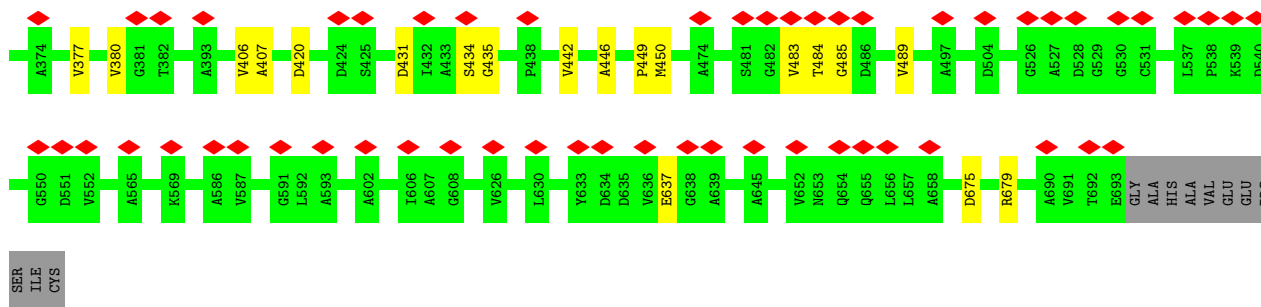


- Molecule 2: NDUFV2

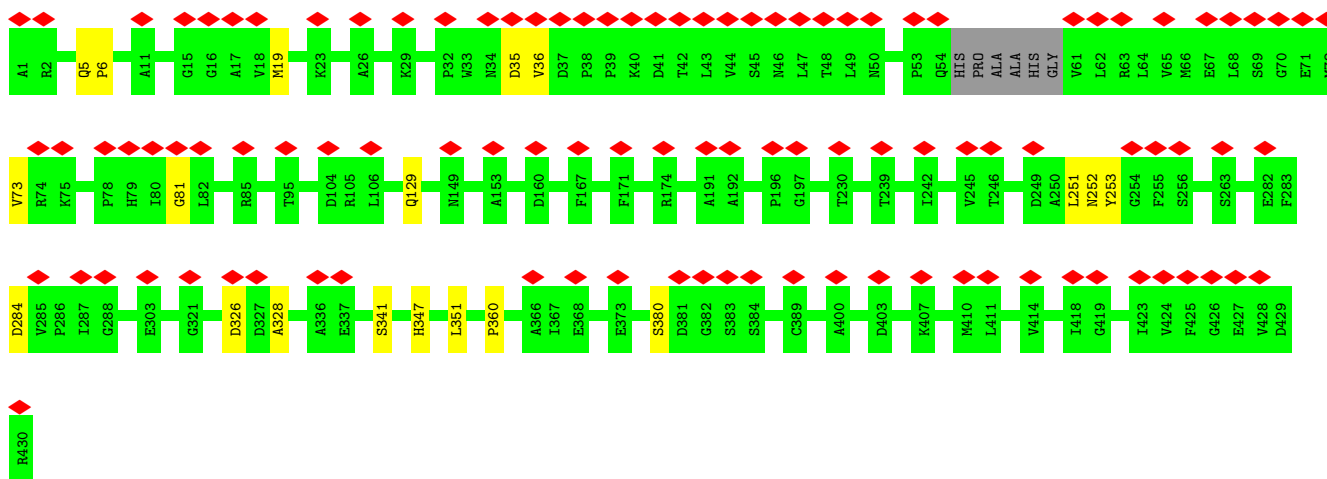


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

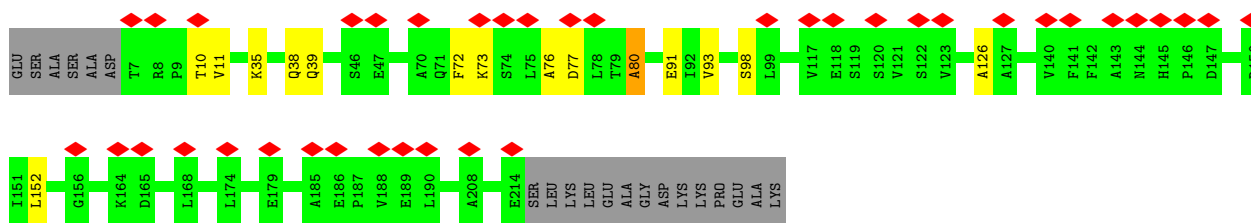
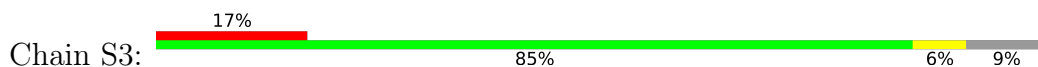




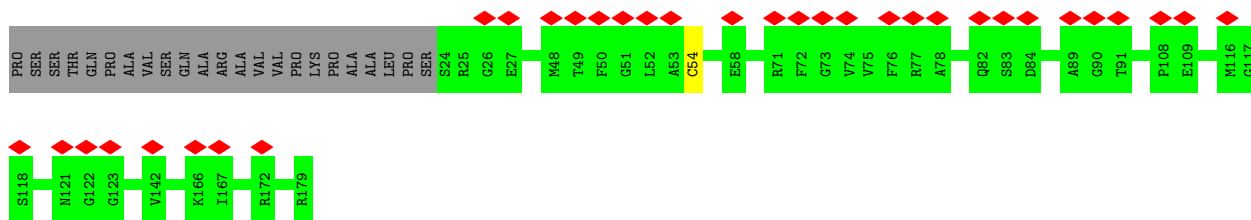
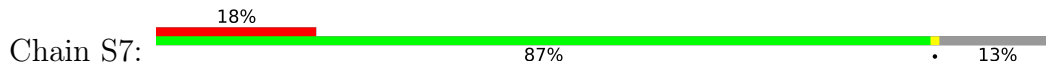
• Molecule 4: NDUFS2



• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

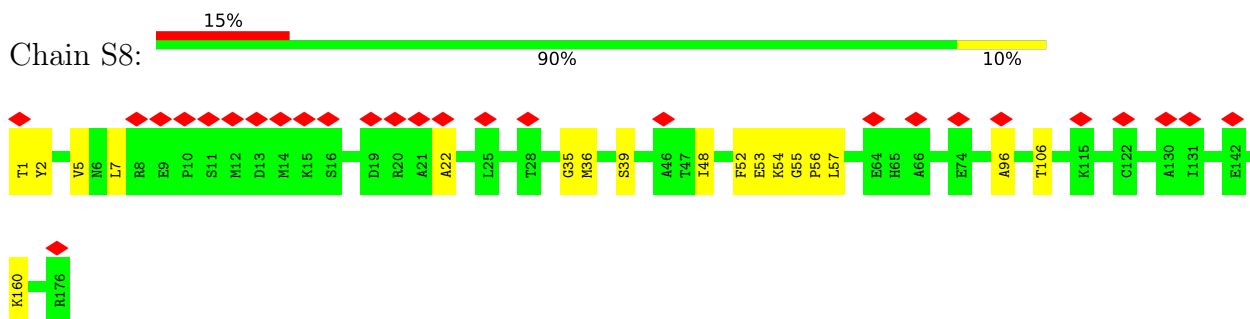


• Molecule 6: NDUFS7

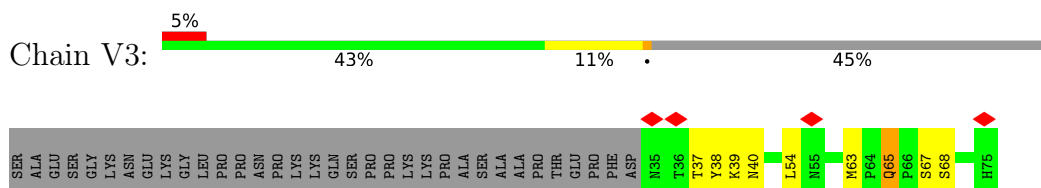




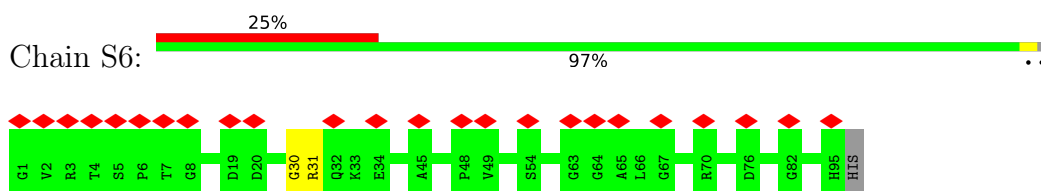
- Molecule 7: NDUFS8



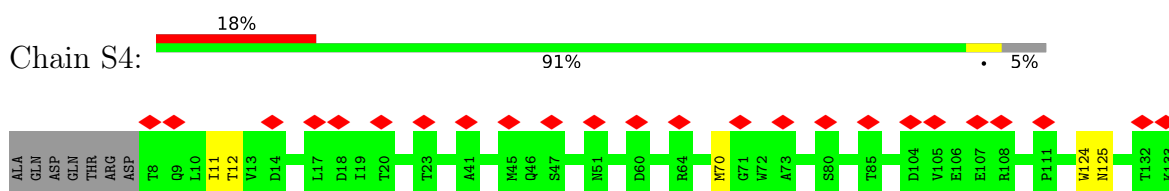
- Molecule 8: NDUFV3



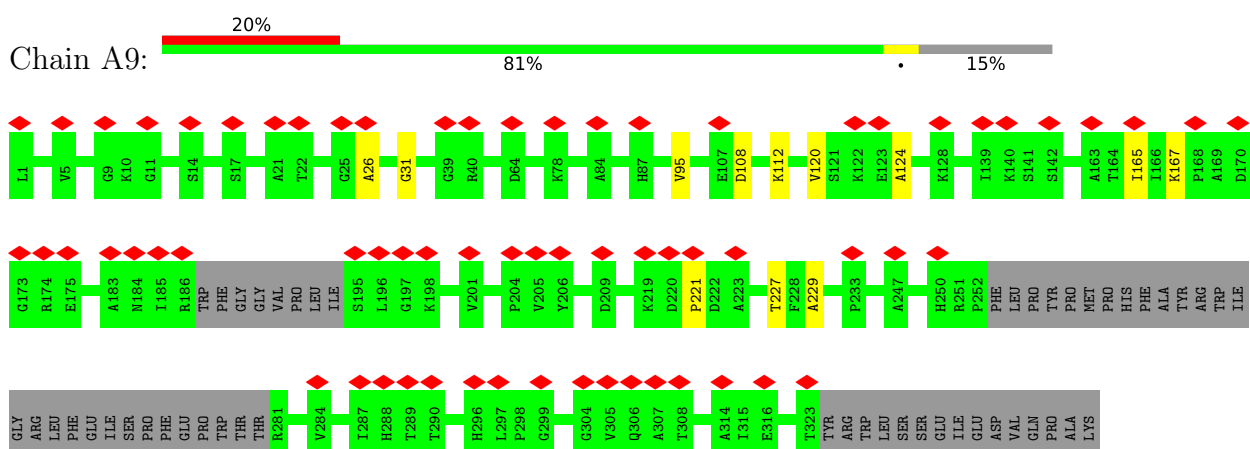
- Molecule 9: NDUFS6



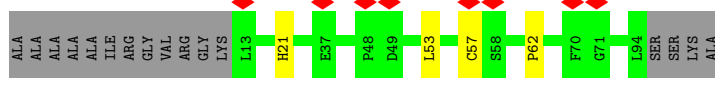
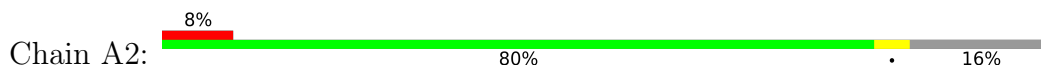
- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4



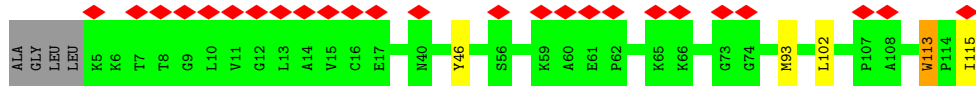
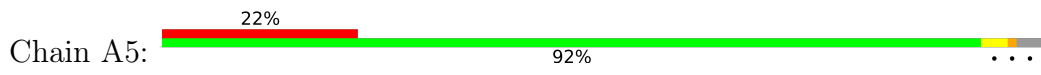
- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9



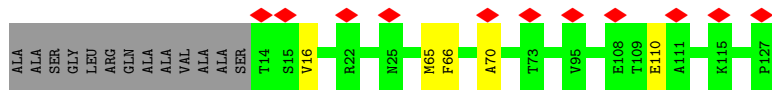
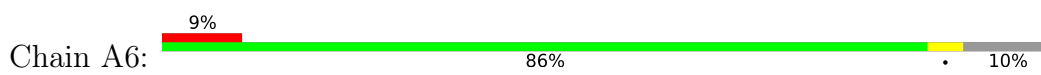
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



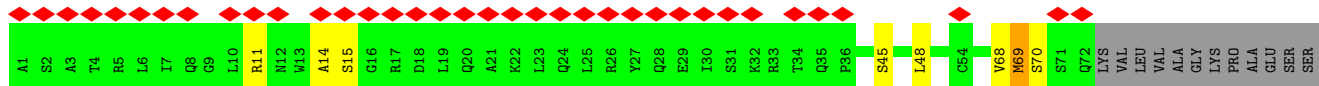
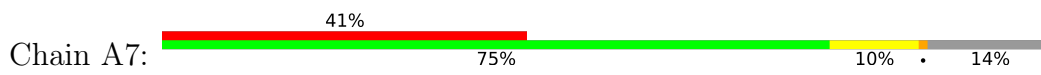
• Molecule 13: NDUFA5



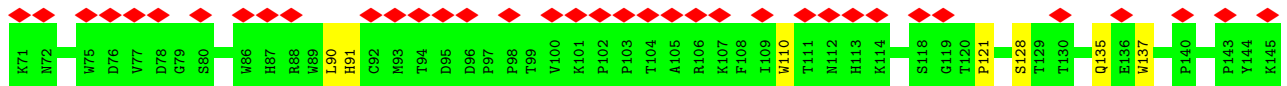
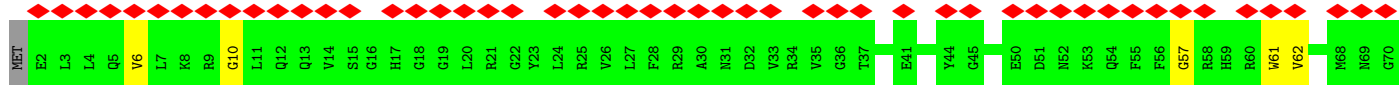
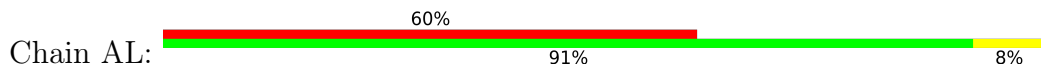
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6



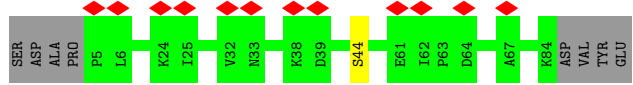
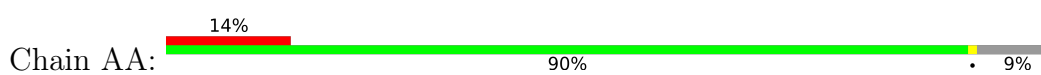
• Molecule 15: NDUFA7



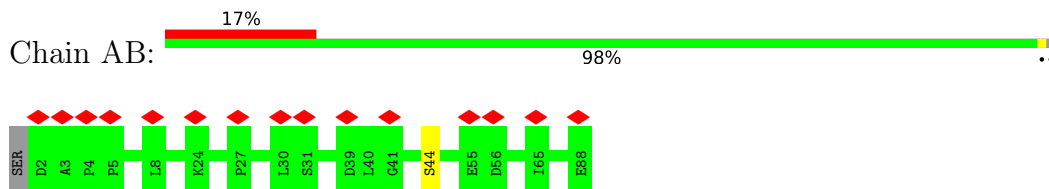
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



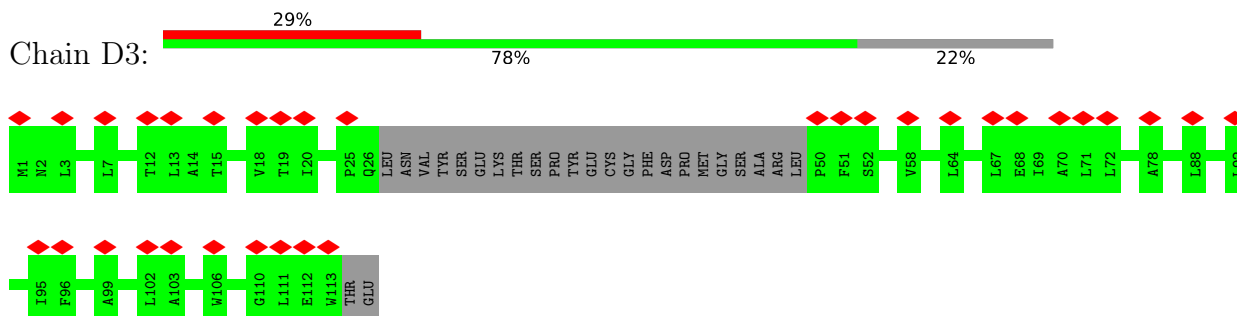
• Molecule 17: Acyl carrier protein



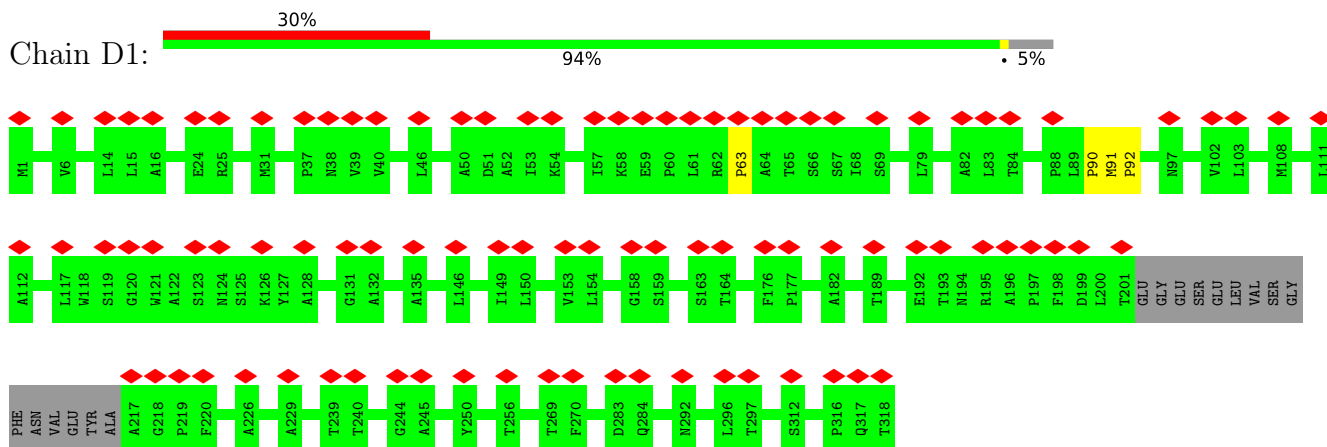
- Molecule 17: Acyl carrier protein



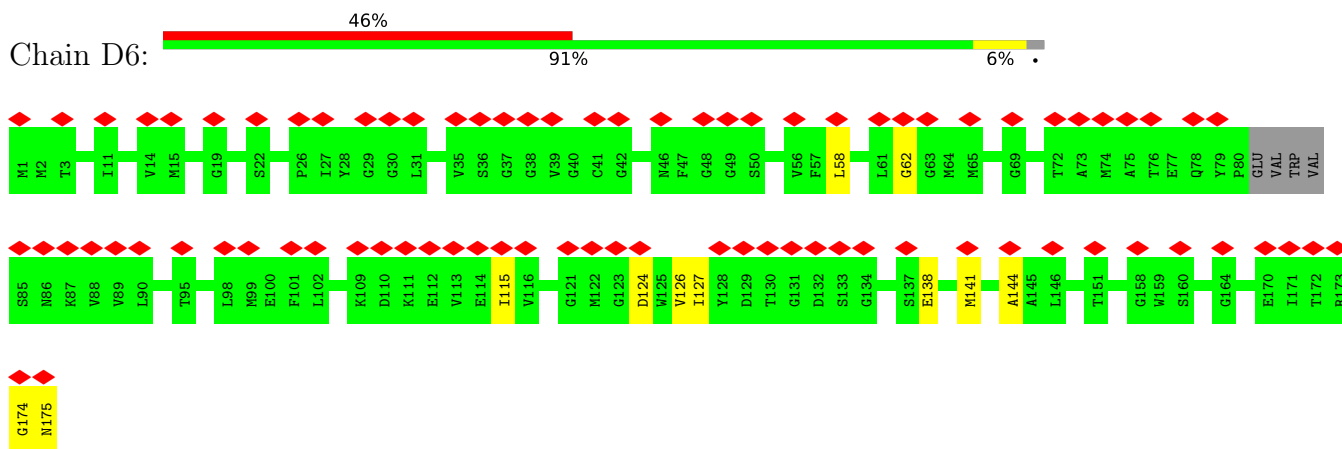
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



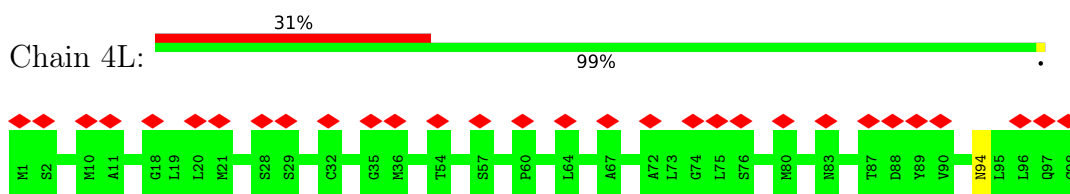
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



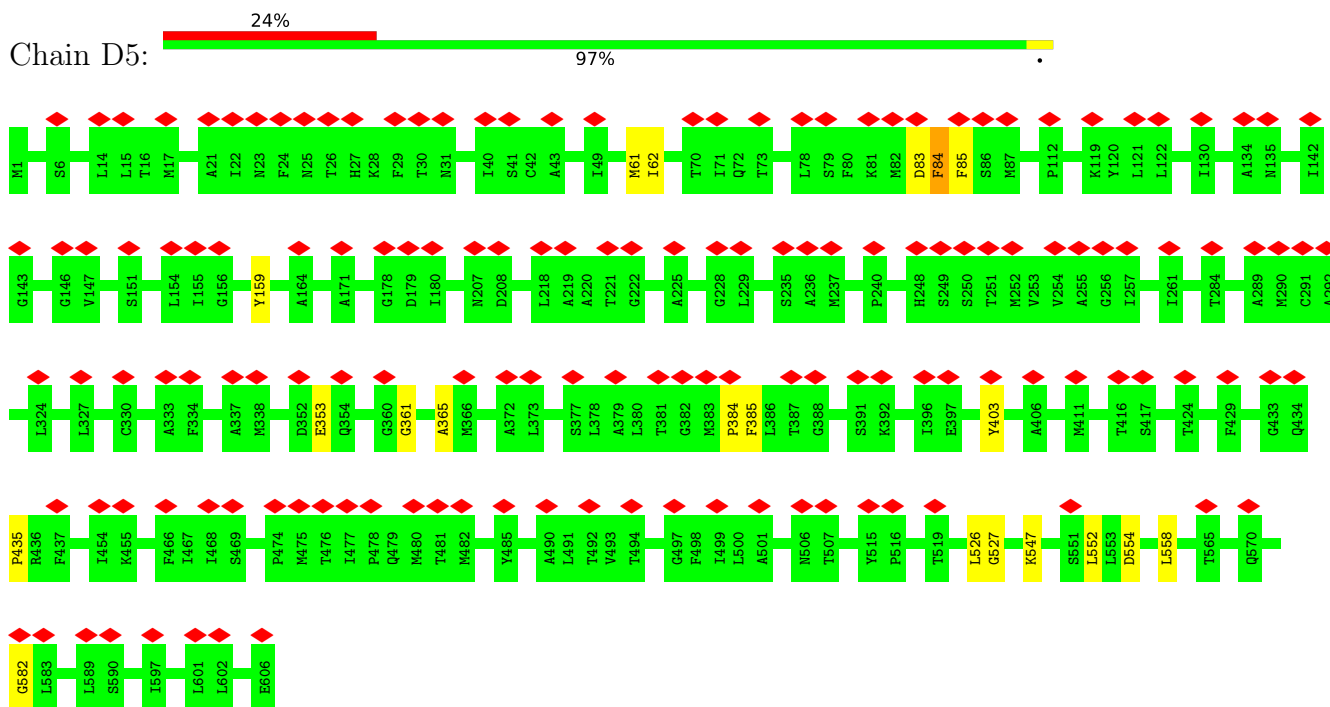
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



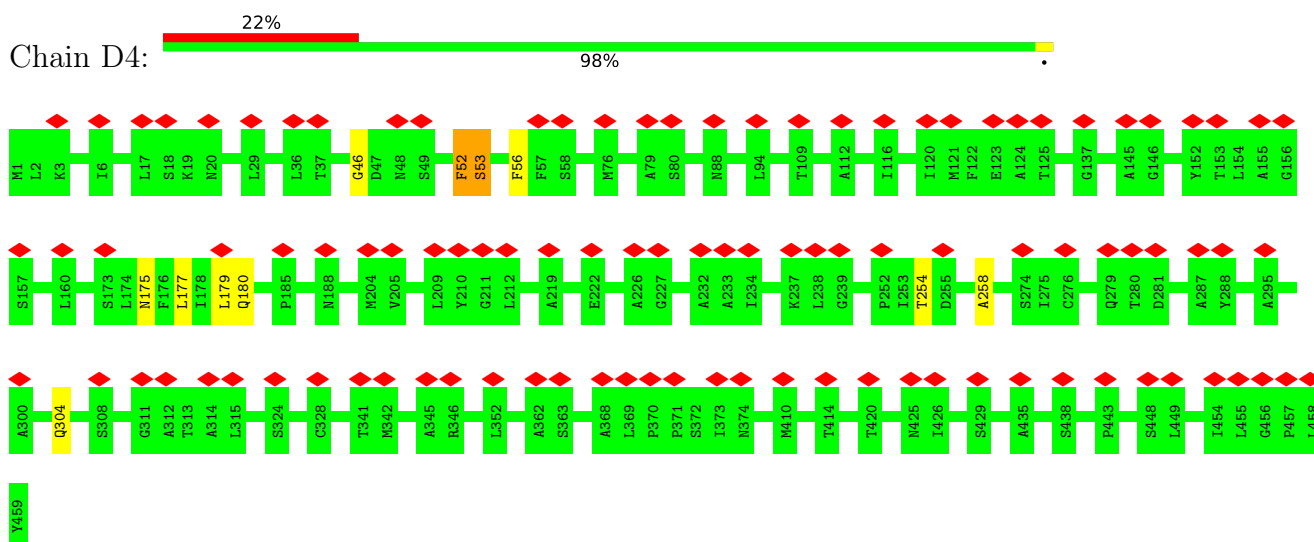
- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

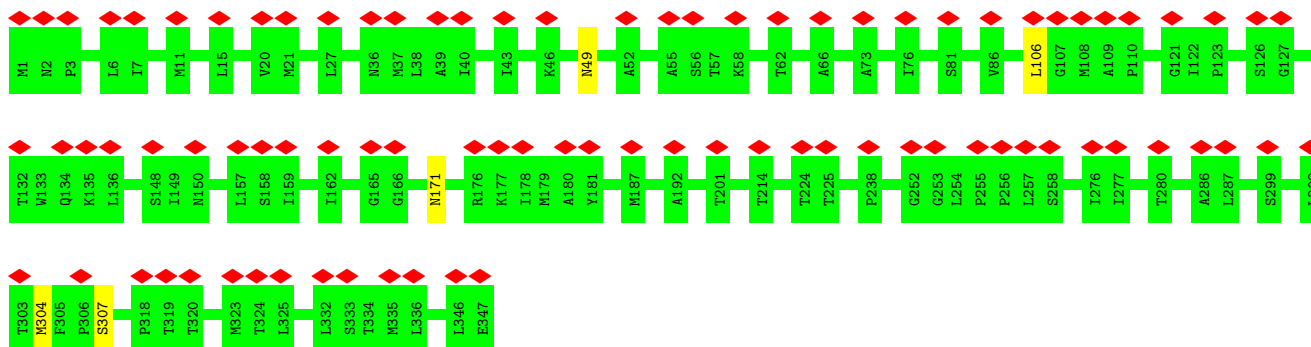


- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

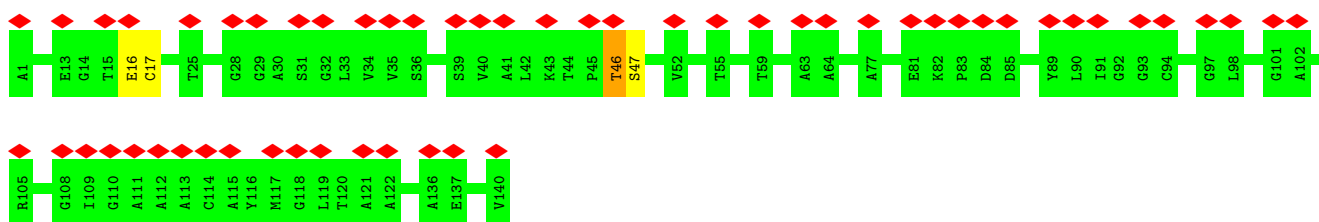
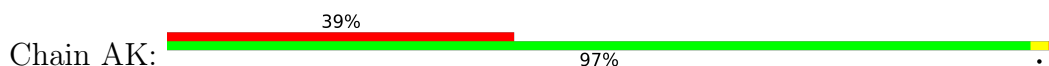


- Molecule 24: NADH-ubiquinone oxidoreductase chain 2

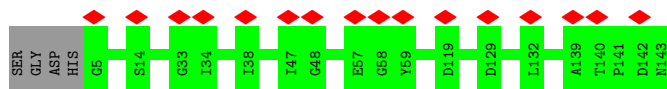




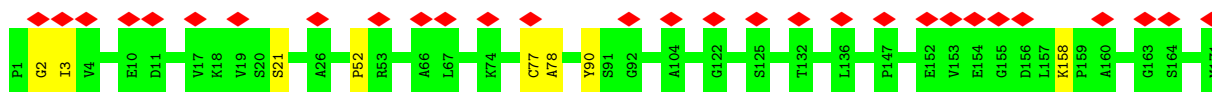
- Molecule 25: NDUFA11



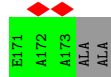
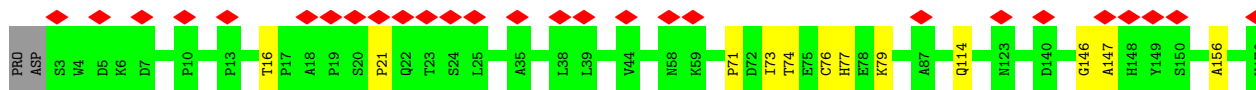
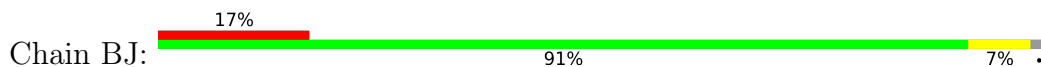
- Molecule 26: NADH:ubiquinone oxidoreductase subunit B5



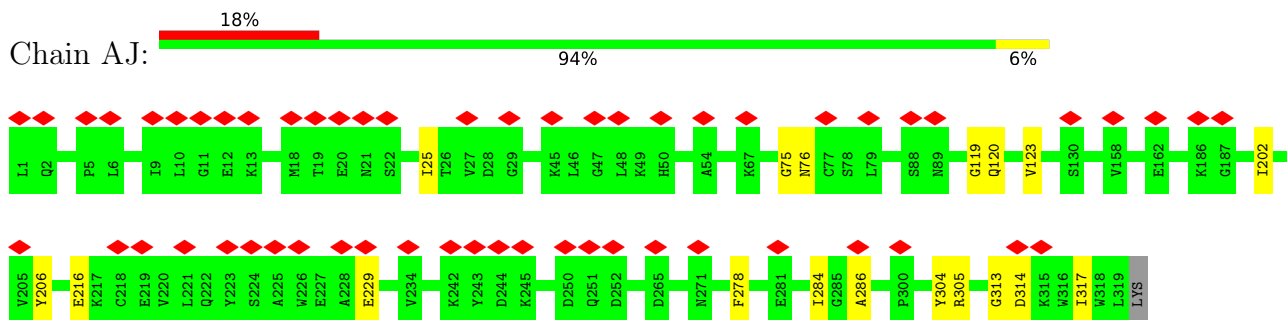
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



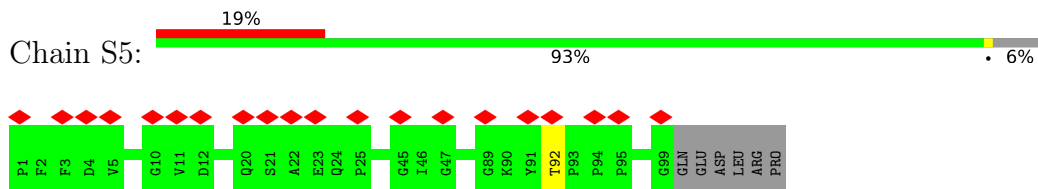
- Molecule 28: NDUFB10



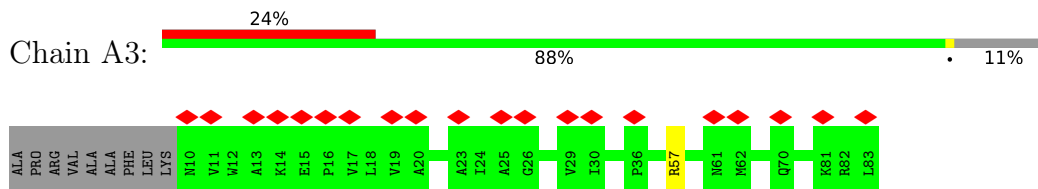
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



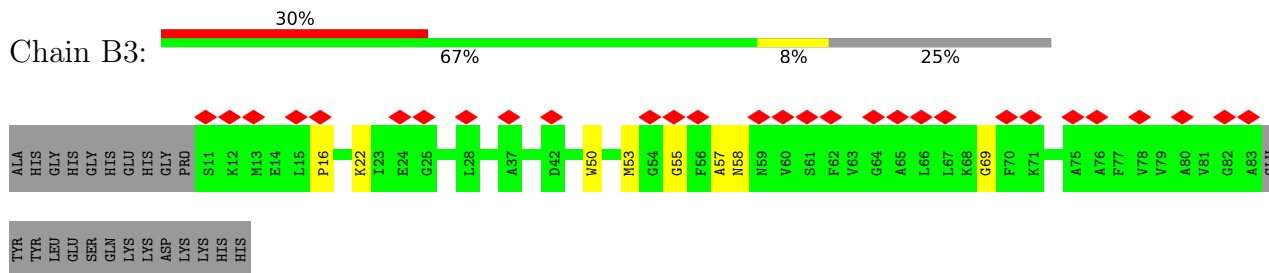
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



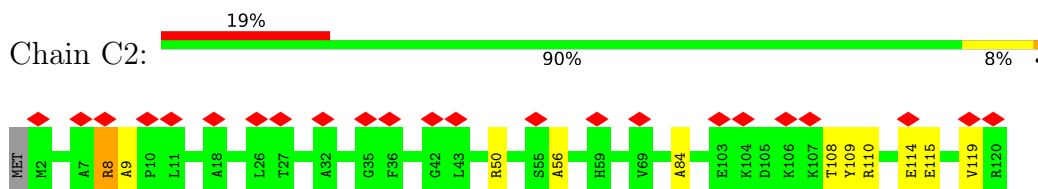
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



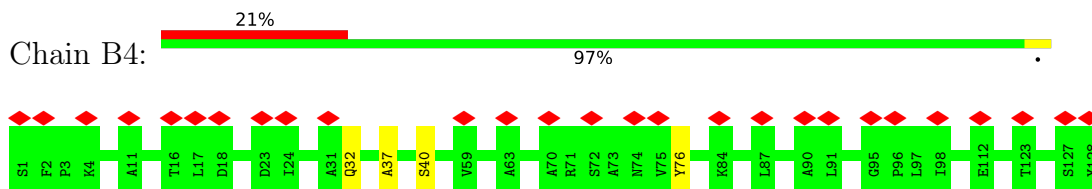
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



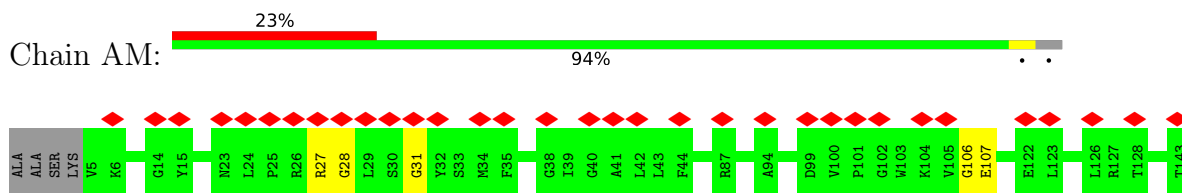
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



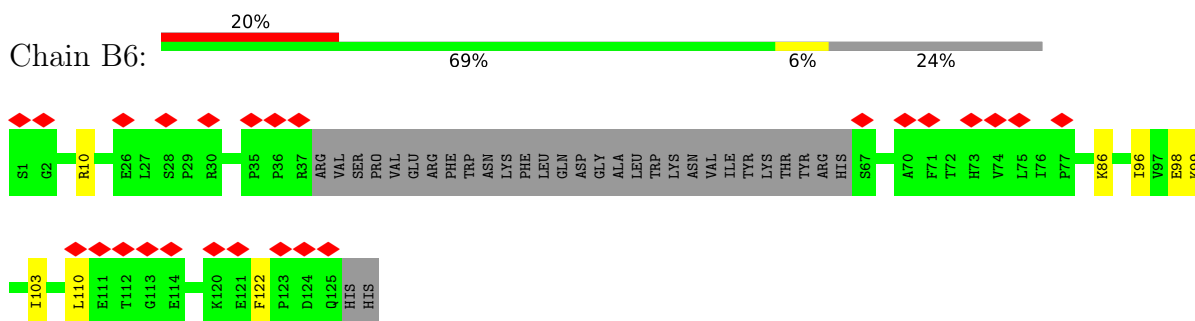
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



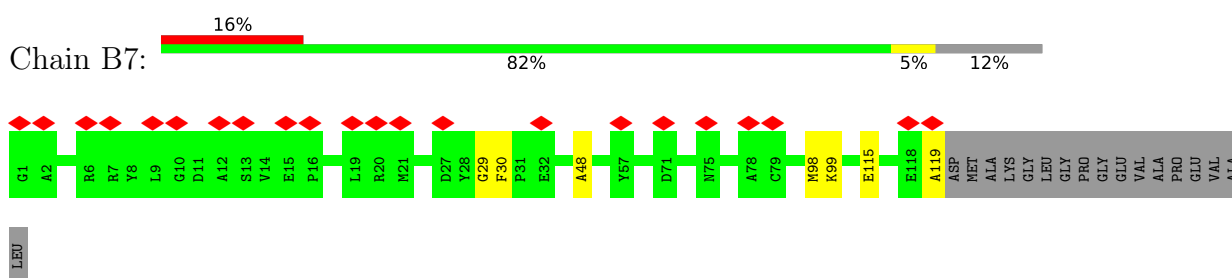
- Molecule 35: NDUFA13



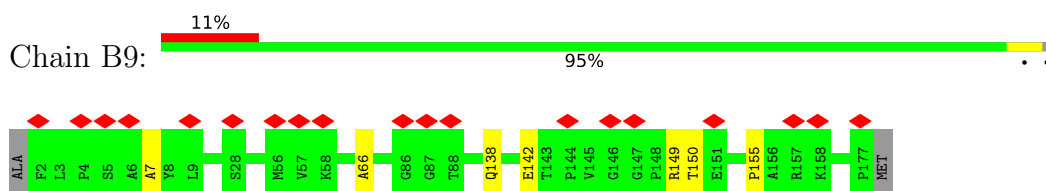
- Molecule 36: NDUFB6



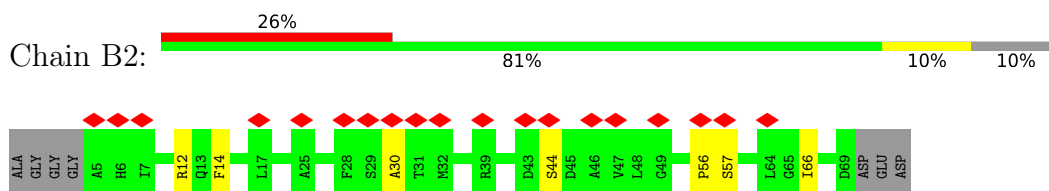
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

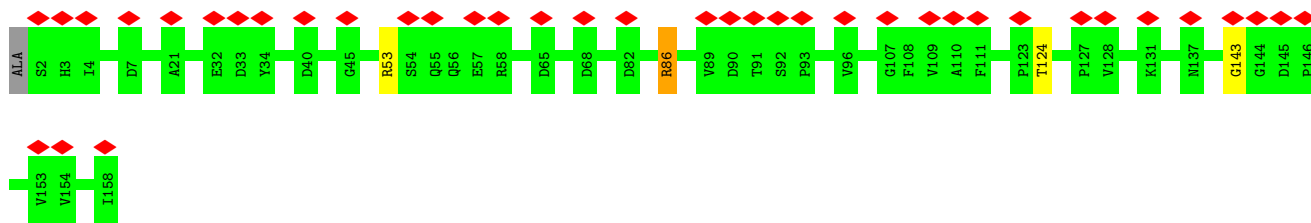


- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

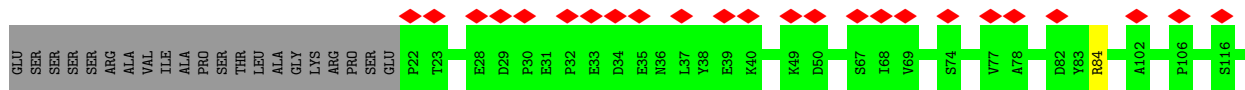
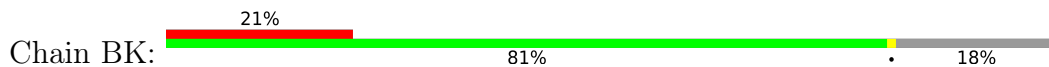


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

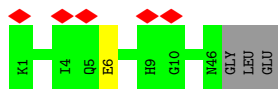
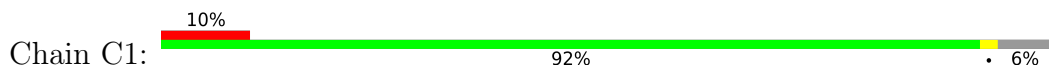




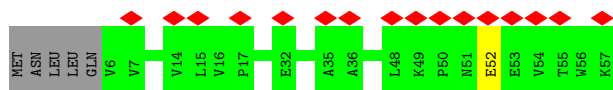
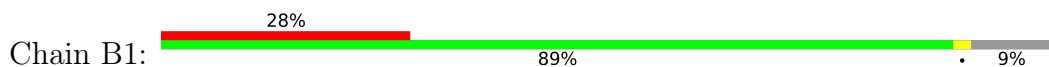
• Molecule 41: NDUFB1



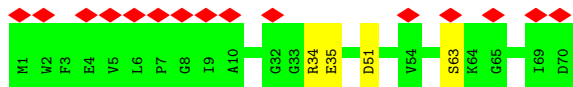
• Molecule 42: NDUFC1



• Molecule 43: NDUFB1



• Molecule 44: NDUFA1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12244	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 ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.574	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.4, 1.4, 1.4	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.30	0/2098	0.58	0/2905
2	V2	0.33	0/1044	0.71	1/1451 (0.1%)
3	S1	0.30	0/3389	0.59	1/4713 (0.0%)
4	S2	0.33	0/2088	0.59	0/2902
5	S3	0.32	0/1033	0.65	0/1441
6	S7	0.33	0/768	0.56	0/1067
7	S8	0.34	0/870	0.60	0/1211
8	V3	0.31	0/203	0.65	0/282
9	S6	0.29	0/461	0.54	0/636
10	S4	0.29	0/624	0.61	0/869
11	A9	0.31	0/1410	0.60	1/1956 (0.1%)
12	A2	0.28	0/405	0.58	0/563
13	A5	0.28	0/549	0.57	0/764
14	A6	0.31	0/566	0.56	1/789 (0.1%)
15	A7	0.31	0/474	0.65	0/658
16	AL	0.29	0/707	0.61	0/981
17	AA	0.27	0/396	0.60	0/551
17	AB	0.28	0/431	0.57	0/600
18	D3	0.29	0/447	0.54	0/622
19	D1	0.32	0/1503	0.62	1/2095 (0.0%)
20	D6	0.29	0/827	0.61	0/1139
21	4L	0.32	0/485	0.57	0/675
22	D5	0.32	0/3000	0.63	0/4181
23	D4	0.33	0/2276	0.60	0/3174
24	D2	0.32	0/1720	0.68	2/2398 (0.1%)
25	AK	0.31	0/681	0.59	1/941 (0.1%)
26	B5	0.32	0/686	0.52	0/954
27	A8	0.30	0/846	0.63	0/1178
28	BJ	0.32	0/852	0.57	1/1190 (0.1%)
29	AJ	0.30	0/1574	0.62	1/2190 (0.0%)
30	S5	0.32	0/489	0.59	0/680
31	A3	0.29	0/366	0.64	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	B3	0.30	0/355	0.67	0/490
33	C2	0.34	0/588	0.64	0/818
34	B4	0.29	0/634	0.54	0/883
35	AM	0.32	0/680	0.58	0/942
36	B6	0.33	0/475	0.67	0/660
37	B7	0.31	0/591	0.56	0/824
38	B9	0.31	0/873	0.57	0/1217
39	B2	0.33	0/322	0.69	1/448 (0.2%)
40	B8	0.33	0/774	0.73	1/1076 (0.1%)
41	BK	0.30	0/505	0.64	0/703
42	C1	0.30	0/226	0.57	0/313
43	B1	0.27	0/257	0.56	0/357
44	A1	0.29	0/342	0.58	0/473
All	All	0.31	0/39890	0.61	12/55469 (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
1	V1	0	2
2	V2	0	3
3	S1	0	6
4	S2	0	2
5	S3	0	2
7	S8	0	1
8	V3	0	2
10	S4	0	1
13	A5	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	2
22	D5	0	5
23	D4	0	2
25	AK	0	2
27	A8	0	1
28	BJ	0	1
29	AJ	0	2
30	S5	0	1
31	A3	0	1
32	B3	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	56

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D2	106	LEU	CB-CA-C	-13.30	84.94	110.20
24	D2	106	LEU	N-CA-C	12.96	146.01	111.00
2	V2	23	PHE	C-N-CA	7.40	140.21	121.70
28	BJ	21	PRO	C-N-CA	5.51	135.47	121.70
29	AJ	229	GLU	C-N-CA	5.47	135.38	121.70

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	35	VAL	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	2099	0	994	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V2	1045	0	462	22	0
3	S1	3390	0	1573	24	0
4	S2	2090	0	930	32	0
5	S3	1034	0	445	27	0
6	S7	769	0	351	0	0
7	S8	871	0	401	67	0
8	V3	204	0	78	23	0
9	S6	462	0	211	5	0
10	S4	625	0	274	11	0
11	A9	1413	0	639	6	0
12	A2	406	0	178	3	0
13	A5	550	0	239	4	0
14	A6	567	0	236	13	0
15	A7	476	0	210	53	0
16	AL	708	0	294	25	0
17	AA	397	0	168	2	0
17	AB	432	0	183	2	0
18	D3	449	0	203	0	0
19	D1	1505	0	676	0	0
20	D6	829	0	381	5	0
21	4L	486	0	222	1	0
22	D5	3001	0	1331	9	0
23	D4	2277	0	1004	8	0
24	D2	1721	0	744	8	0
25	AK	682	0	358	1	0
26	B5	687	0	302	0	0
27	A8	847	0	364	8	0
28	BJ	853	0	375	27	0
29	AJ	1575	0	694	36	0
30	S5	490	0	215	0	0
31	A3	367	0	157	0	0
32	B3	356	0	178	7	0
33	C2	589	0	254	50	0
34	B4	635	0	281	19	0
35	AM	681	0	302	8	0
36	B6	477	0	187	9	0
37	B7	592	0	260	13	0
38	B9	874	0	374	26	0
39	B2	323	0	136	16	0
40	B8	775	0	318	1	0
41	BK	506	0	214	1	0
42	C1	227	0	97	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	B1	258	0	109	0	0
44	A1	343	0	159	3	0
45	S1	16	0	0	0	0
45	S7	8	0	0	0	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	1	0
50	A6	34	0	40	10	0
50	AB	31	0	34	8	0
All	All	40144	0	17880	349	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 349 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)
37:B7:99:LYS:HA	39:B2:57:SER:CB	1.22	1.60
7:S8:35:GLY:CA	15:A7:14:ALA:HB1	1.29	1.56
7:S8:35:GLY:C	15:A7:14:ALA:HB1	1.30	1.46
7:S8:35:GLY:O	15:A7:14:ALA:CB	1.67	1.39
29:AJ:317:ILE:CA	33:C2:56:ALA:HA	1.54	1.34

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%)	381 (89%)	47 (11%)	0	100	100
2	V2	210/217 (97%)	167 (80%)	43 (20%)	0	100	100
3	S1	686/704 (97%)	614 (90%)	71 (10%)	1 (0%)	51	85
4	S2	420/430 (98%)	379 (90%)	41 (10%)	0	100	100
5	S3	206/228 (90%)	180 (87%)	26 (13%)	0	100	100
6	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	25	66
7	S8	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
8	V3	39/75 (52%)	32 (82%)	7 (18%)	0	100	100
9	S6	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
10	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100
12	A2	80/98 (82%)	72 (90%)	8 (10%)	0	100	100
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
15	A7	92/112 (82%)	77 (84%)	15 (16%)	0	100	100
16	AL	142/145 (98%)	119 (84%)	23 (16%)	0	100	100
17	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
19	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	41	76
20	D6	167/175 (95%)	145 (87%)	21 (13%)	1 (1%)	25	66
21	4L	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
22	D5	604/606 (100%)	532 (88%)	70 (12%)	2 (0%)	41	76
23	D4	457/459 (100%)	411 (90%)	45 (10%)	1 (0%)	47	81
24	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
25	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
26	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
27	A8	169/171 (99%)	136 (80%)	33 (20%)	0	100	100
28	BJ	169/175 (97%)	151 (89%)	17 (10%)	1 (1%)	25	66
29	AJ	317/320 (99%)	277 (87%)	40 (13%)	0	100	100
30	S5	97/105 (92%)	80 (82%)	17 (18%)	0	100	100
31	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B3	71/97 (73%)	58 (82%)	13 (18%)	0	100	100
33	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
34	B4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
35	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
36	B6	92/127 (72%)	79 (86%)	13 (14%)	0	100	100
37	B7	117/136 (86%)	100 (86%)	17 (14%)	0	100	100
38	B9	174/178 (98%)	148 (85%)	26 (15%)	0	100	100
39	B2	63/72 (88%)	54 (86%)	9 (14%)	0	100	100
40	B8	155/158 (98%)	117 (76%)	37 (24%)	1 (1%)	25	66
41	BK	100/125 (80%)	81 (81%)	19 (19%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7980/8509 (94%)	7032 (88%)	939 (12%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D5	84	PHE
23	D4	53	SER
3	S1	359	ARG
6	S7	54	CYS
22	D5	527	GLY

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
45	SF4	S1	801	-	0,12,12	-	-	-		
47	FES	V2	300	-	0,4,4	-	-	-		
47	FES	S1	803	-	0,4,4	-	-	-		
50	ZMP	A6	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.00	1 (3%)
49	NDP	A9	401	-	45,52,52	0.60	1 (2%)	53,80,80	0.64	1 (1%)
45	SF4	S8	201	-	0,12,12	-	-	-		
45	SF4	V1	500	-	0,12,12	-	-	-		
45	SF4	S8	202	-	0,12,12	-	-	-		
45	SF4	S7	300	-	0,12,12	-	-	-		
45	SF4	S1	802	-	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.27	0	48,50,50	0.42	0
50	ZMP	AB	101	-	24,30,36	0.76	1 (4%)	29,37,45	1.30	3 (10%)

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
45	SF4	S1	801	-	-	-	0/6/5/5
47	FES	V2	300	-	-	-	0/1/1/1
47	FES	S1	803	-	-	-	0/1/1/1
50	ZMP	A6	201	-	-	15/38/40/43	-
49	NDP	A9	401	-	-	13/30/77/77	0/5/5/5
45	SF4	S8	201	-	-	-	0/6/5/5
45	SF4	V1	500	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	S8	202	-	-	-	0/6/5/5
45	SF4	S7	300	-	-	-	0/6/5/5
45	SF4	S1	802	-	-	-	0/6/5/5
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
50	ZMP	AB	101	-	-	16/35/37/43	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.25	1.53	1.50
49	A9	401	NDP	P2B-O2B	2.24	1.63	1.59
50	A6	201	ZMP	C9-C10	2.14	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	AB	101	ZMP	O1-C10-C9	-3.39	119.98	123.99
50	A6	201	ZMP	O1-C10-C9	-2.59	120.92	123.99
50	AB	101	ZMP	C11-C12-N1	-2.52	107.11	112.42
50	AB	101	ZMP	C15-C14-C13	-2.47	108.24	112.36
49	A9	401	NDP	C5A-C6A-N6A	2.41	124.02	120.35

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	C2'-C3'-C4'-C5'
46	V1	501	FMN	O3'-C3'-C4'-C5'
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P

There are no ring outliers.

5 monomers are involved in 21 short contacts:

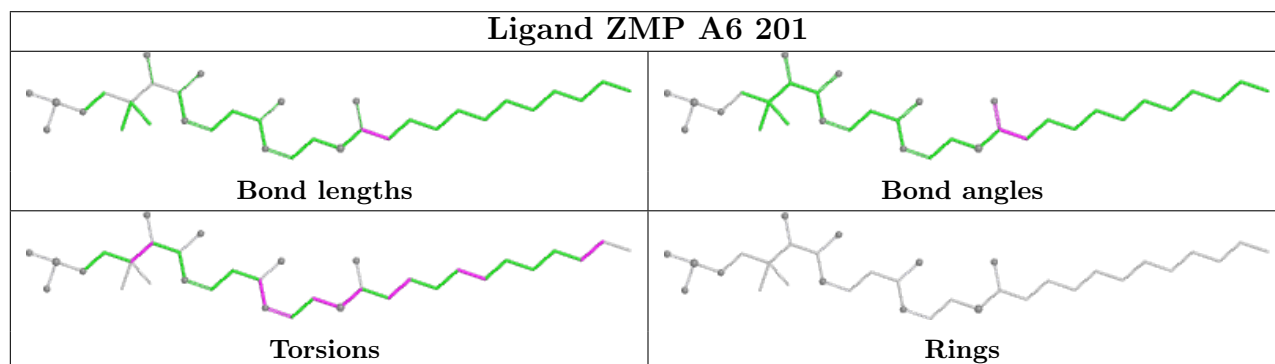
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	A6	201	ZMP	10	0
49	A9	401	NDP	1	0
45	V1	500	SF4	1	0
46	V1	501	FMN	1	0

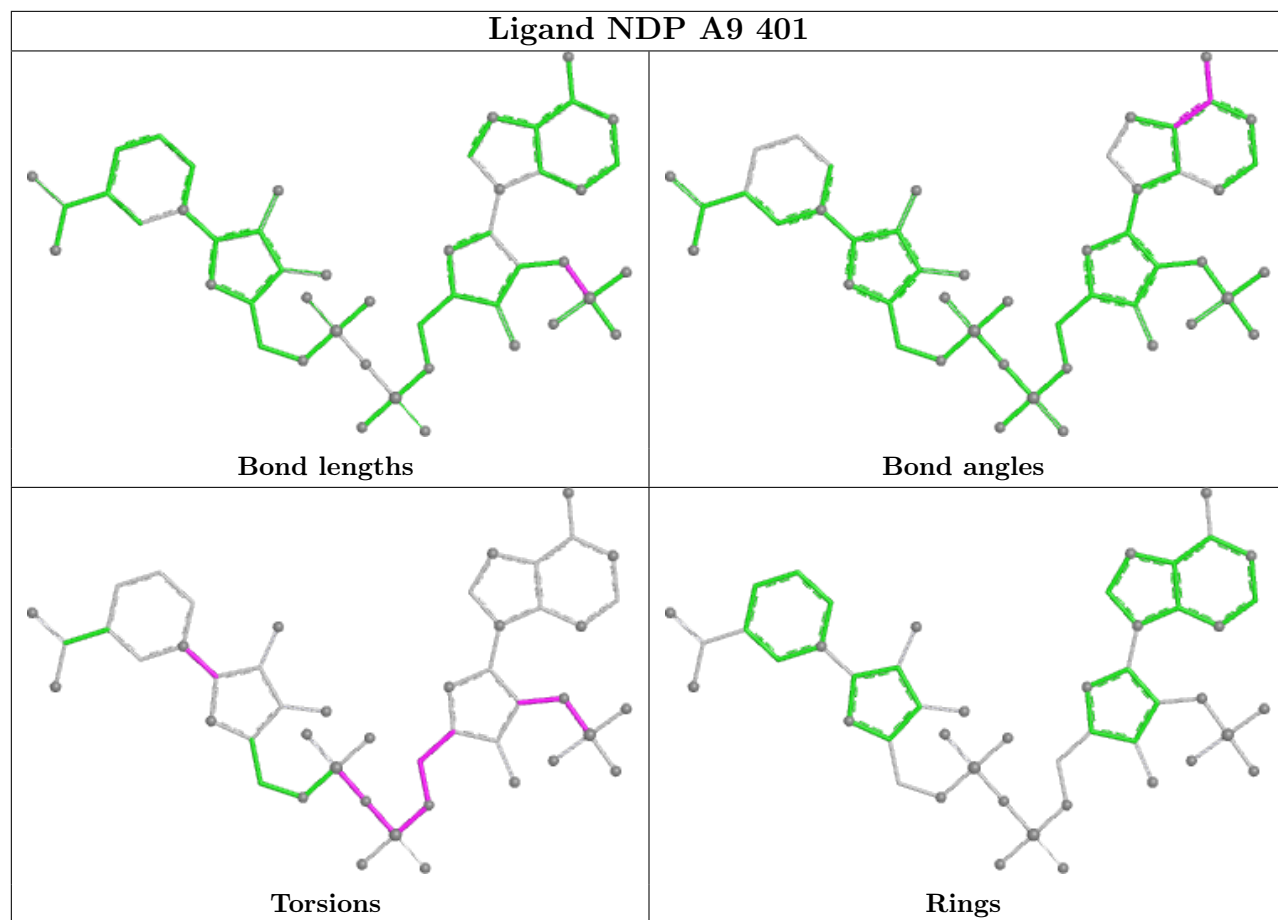
Continued on next page...

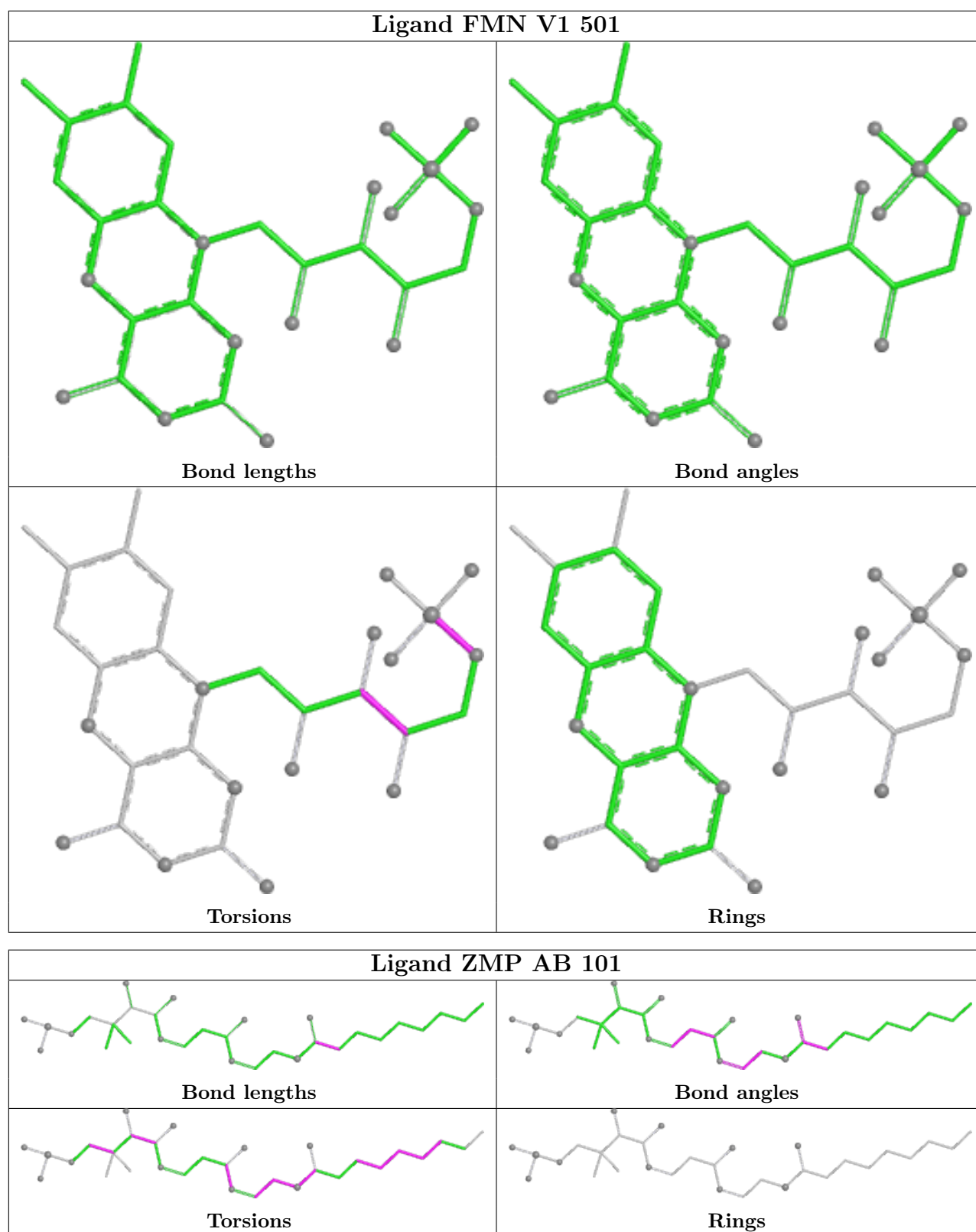
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	AB	101	ZMP	8	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 than 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.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

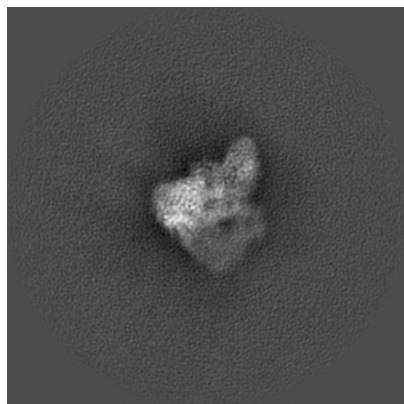
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4502. These allow visual inspection of the internal detail of the map and identification of artifacts.

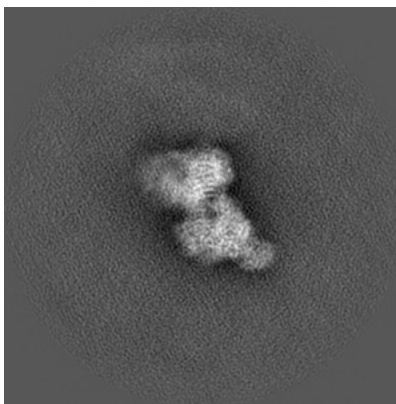
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

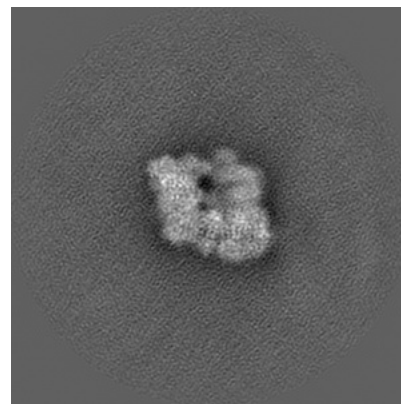
#### 6.1.1 Primary map



X

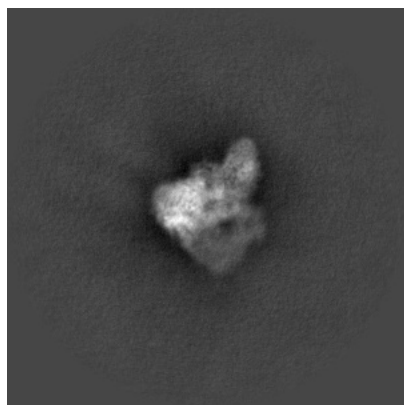


Y

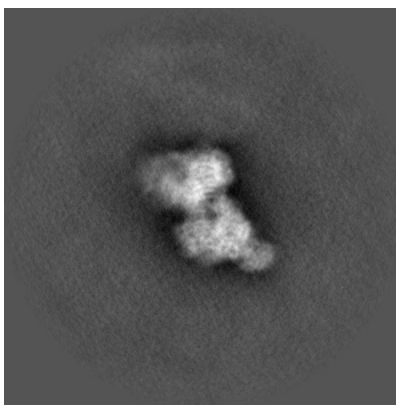


Z

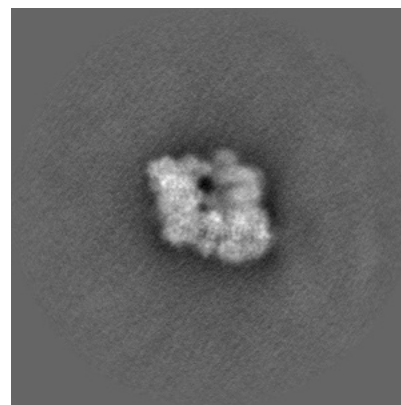
#### 6.1.2 Raw map



X



Y

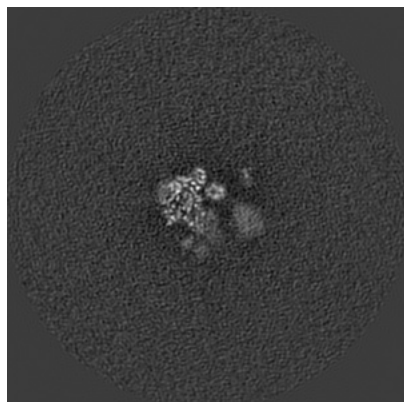


Z

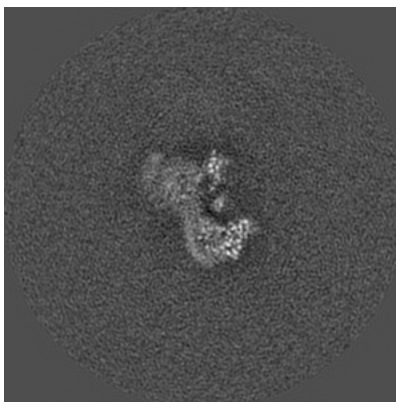
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

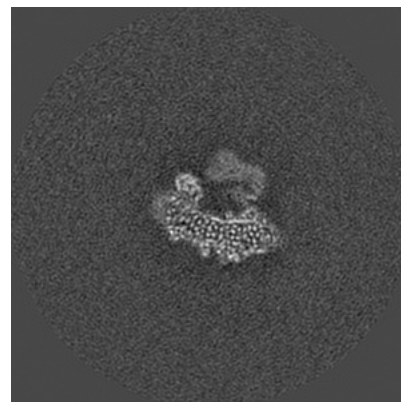
### 6.2.1 Primary map



X Index: 256

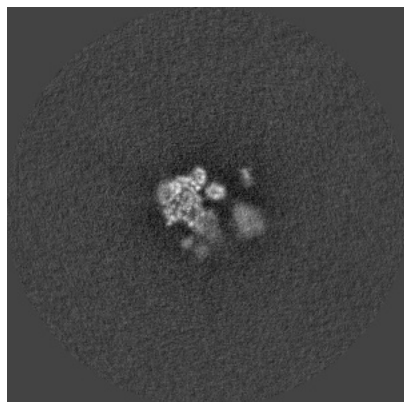


Y Index: 256

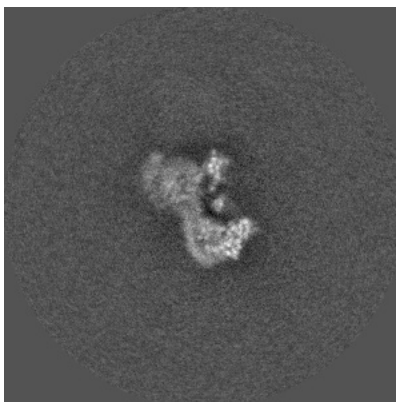


Z Index: 256

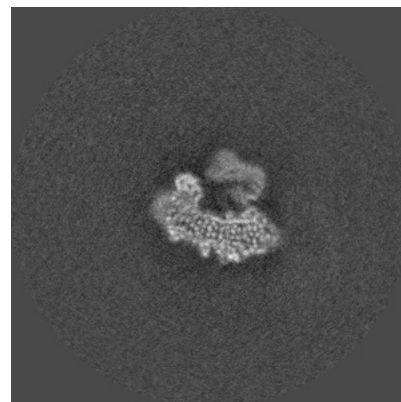
### 6.2.2 Raw map



X Index: 256



Y Index: 256



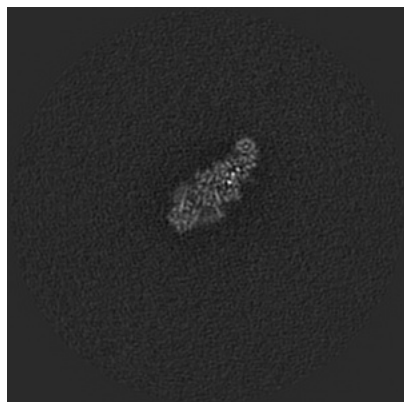
Z Index: 256

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

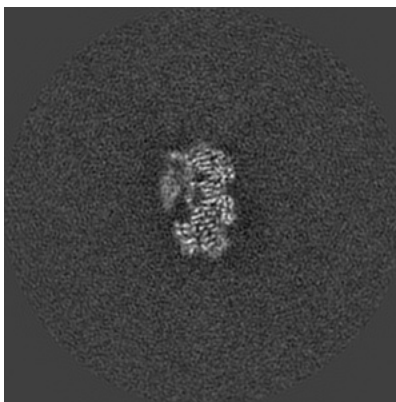


## 6.3 Largest variance slices [i](#)

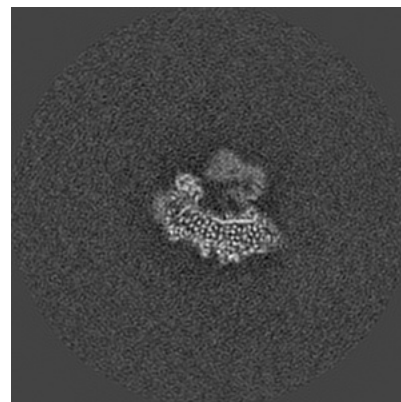
### 6.3.1 Primary map



X Index: 205

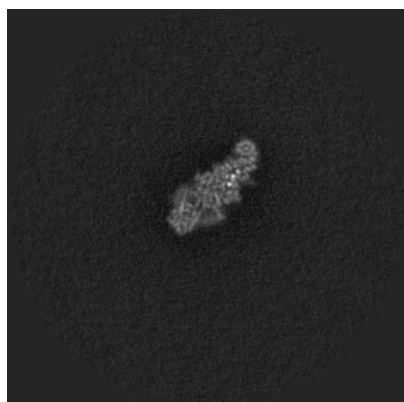


Y Index: 230

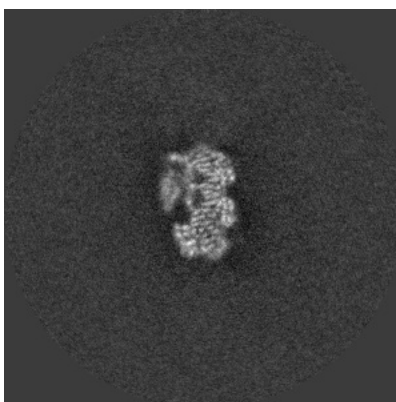


Z Index: 255

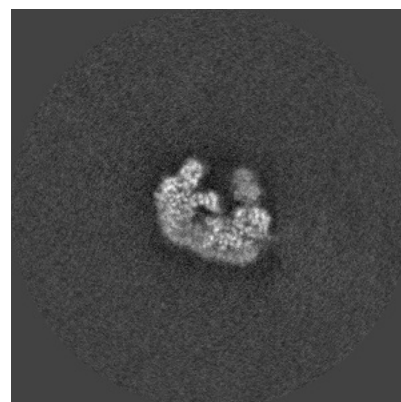
### 6.3.2 Raw map



X Index: 205



Y Index: 230

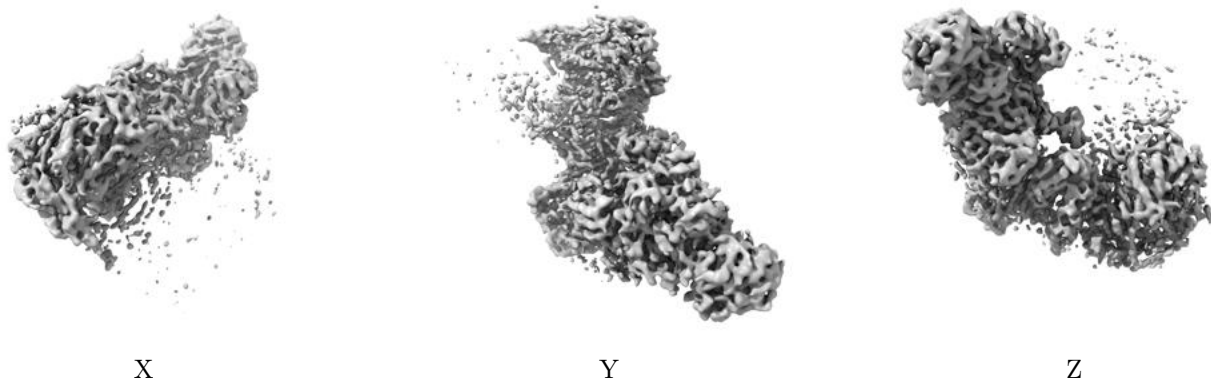


Z Index: 276

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

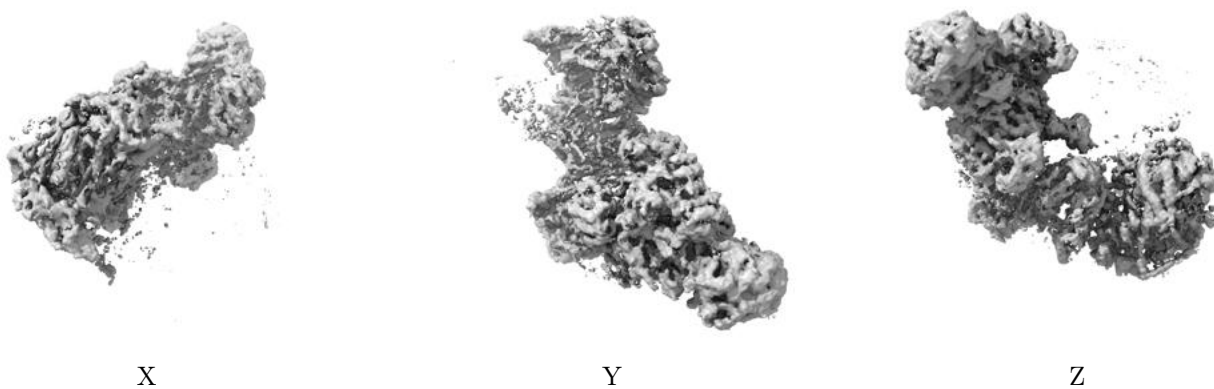
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

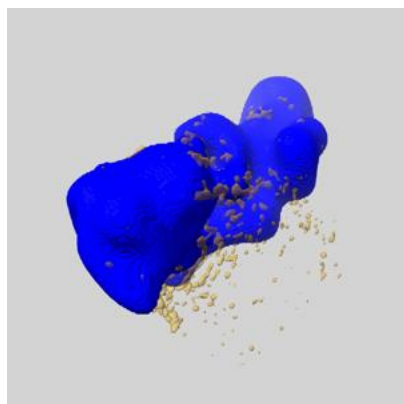
## 6.5 Mask visualisation [i](#)

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

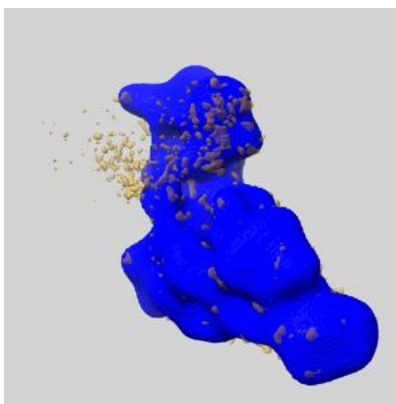
A mask typically either:

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

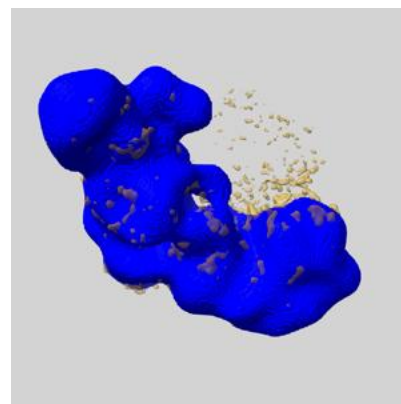
### 6.5.1 emd\_4502\_msk\_1.map [i](#)



X



Y

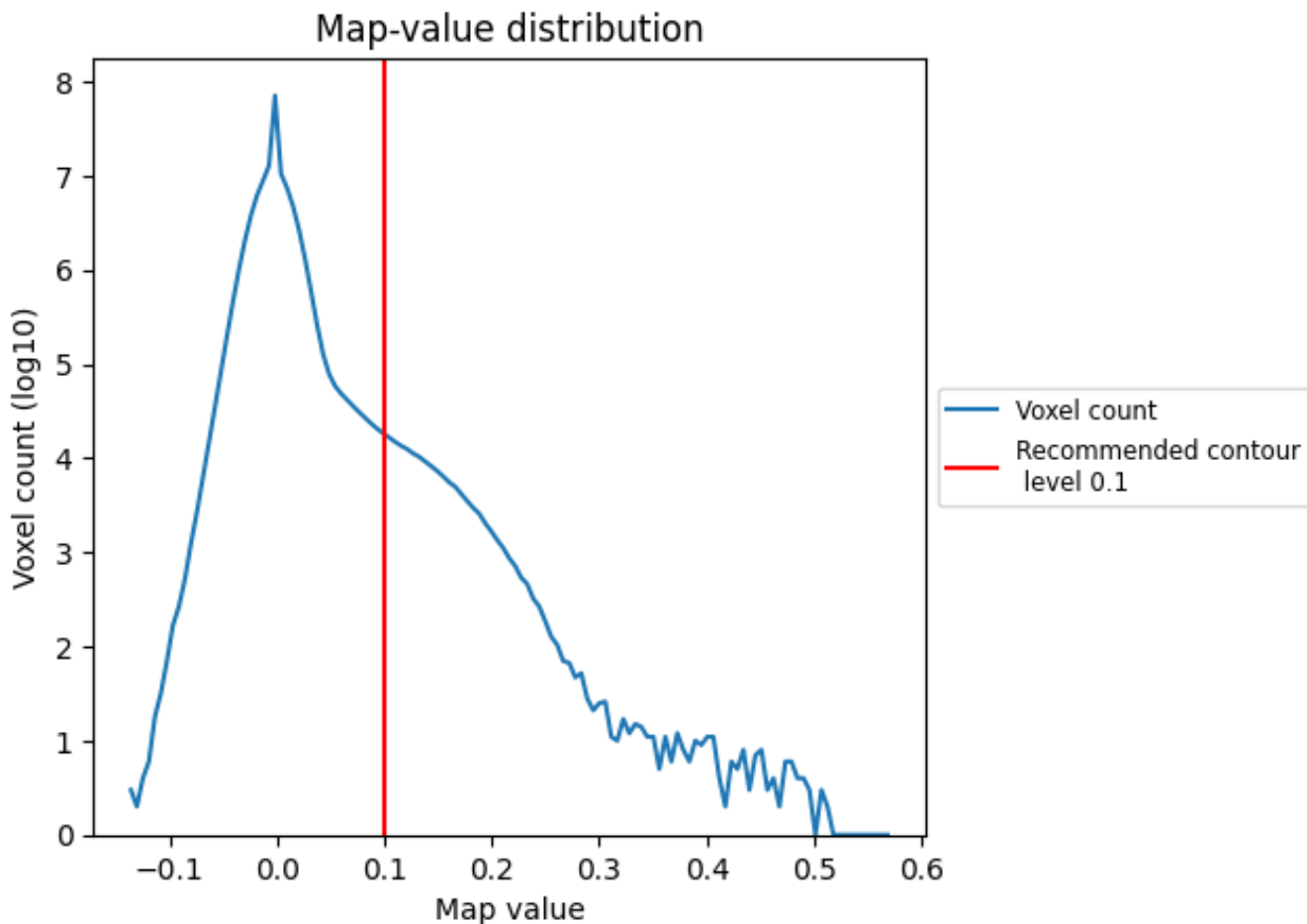


Z

## 7 Map analysis [i](#)

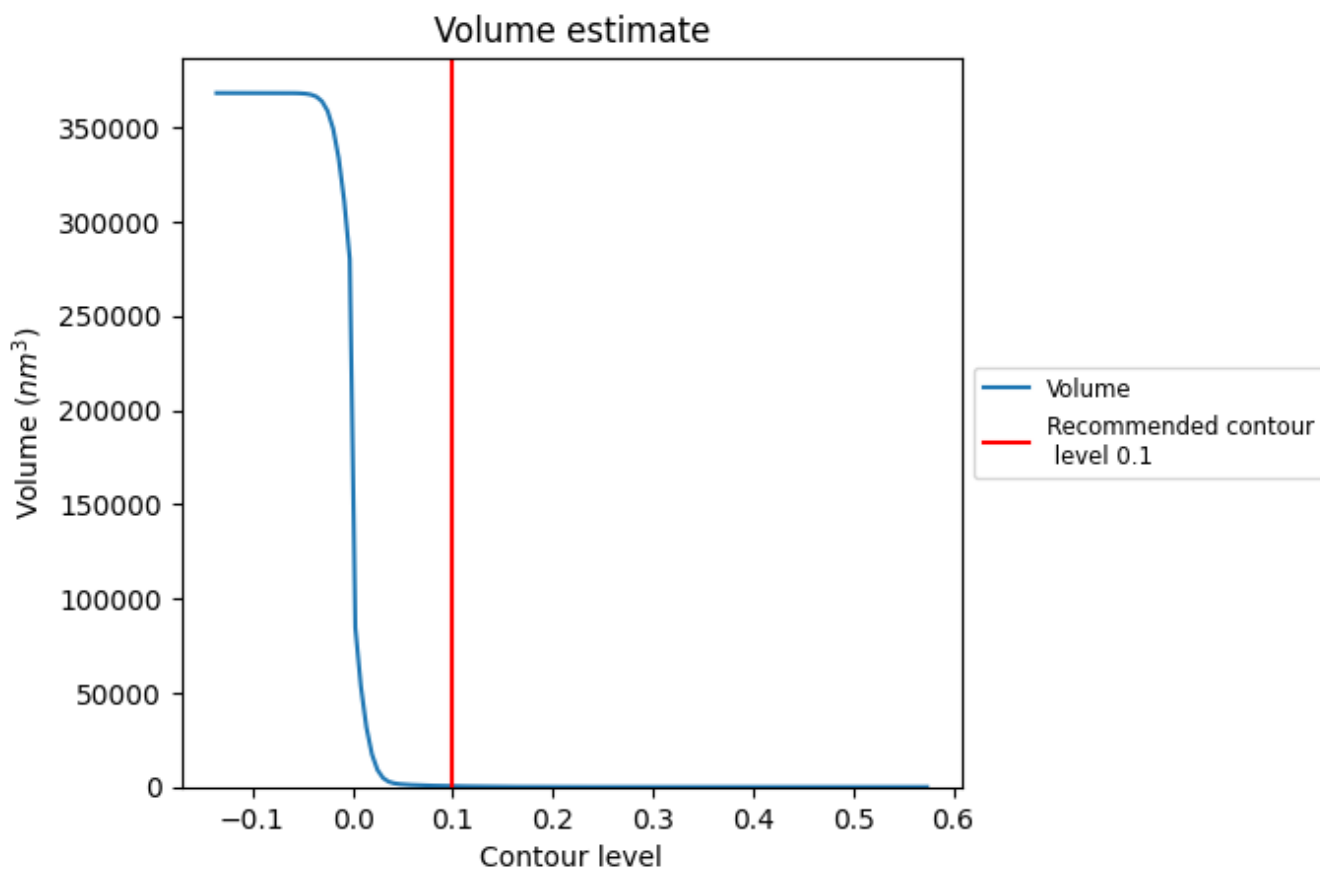
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

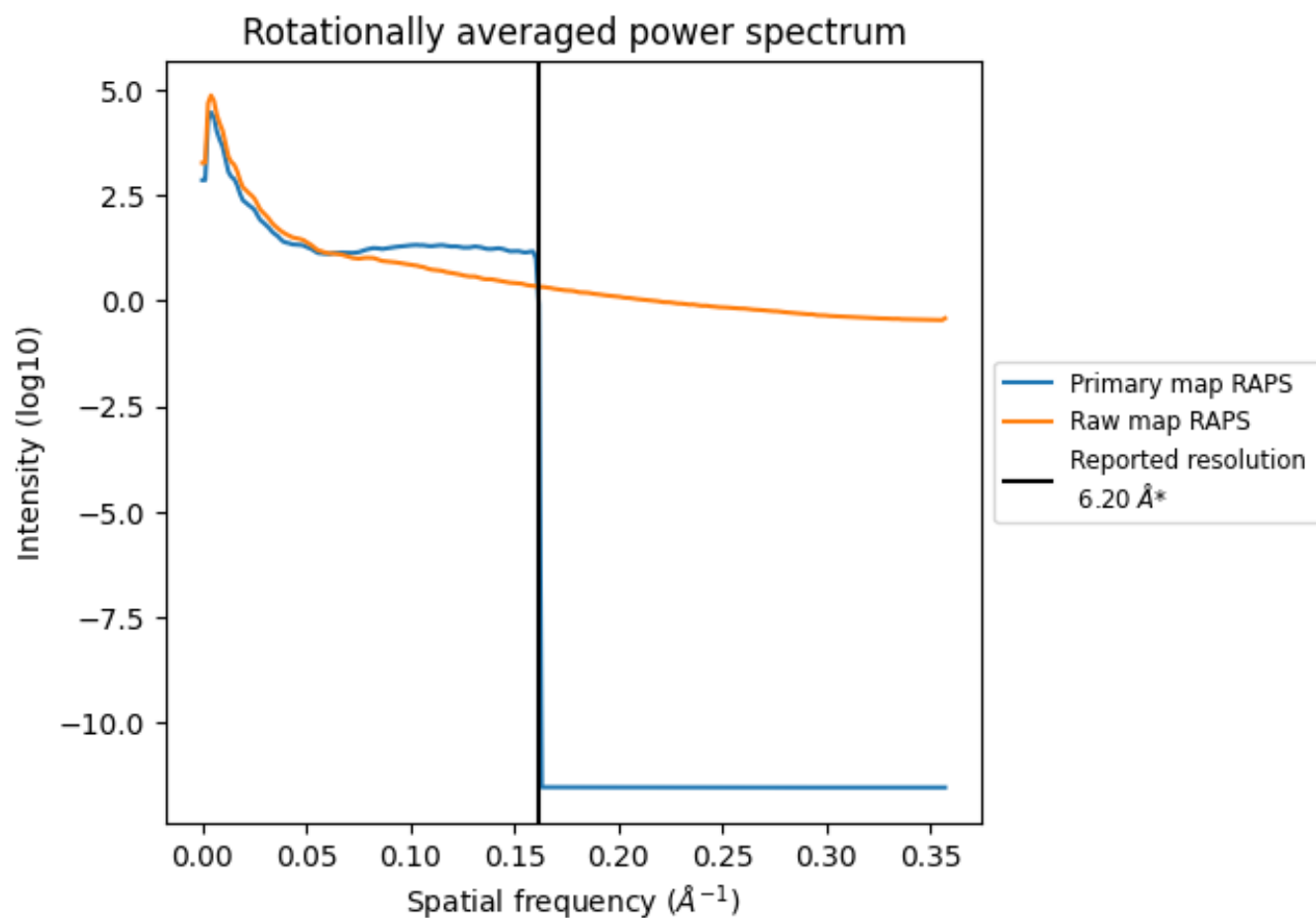
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 436  $\text{nm}^3$ ; this corresponds to an approximate mass of 394 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](#)

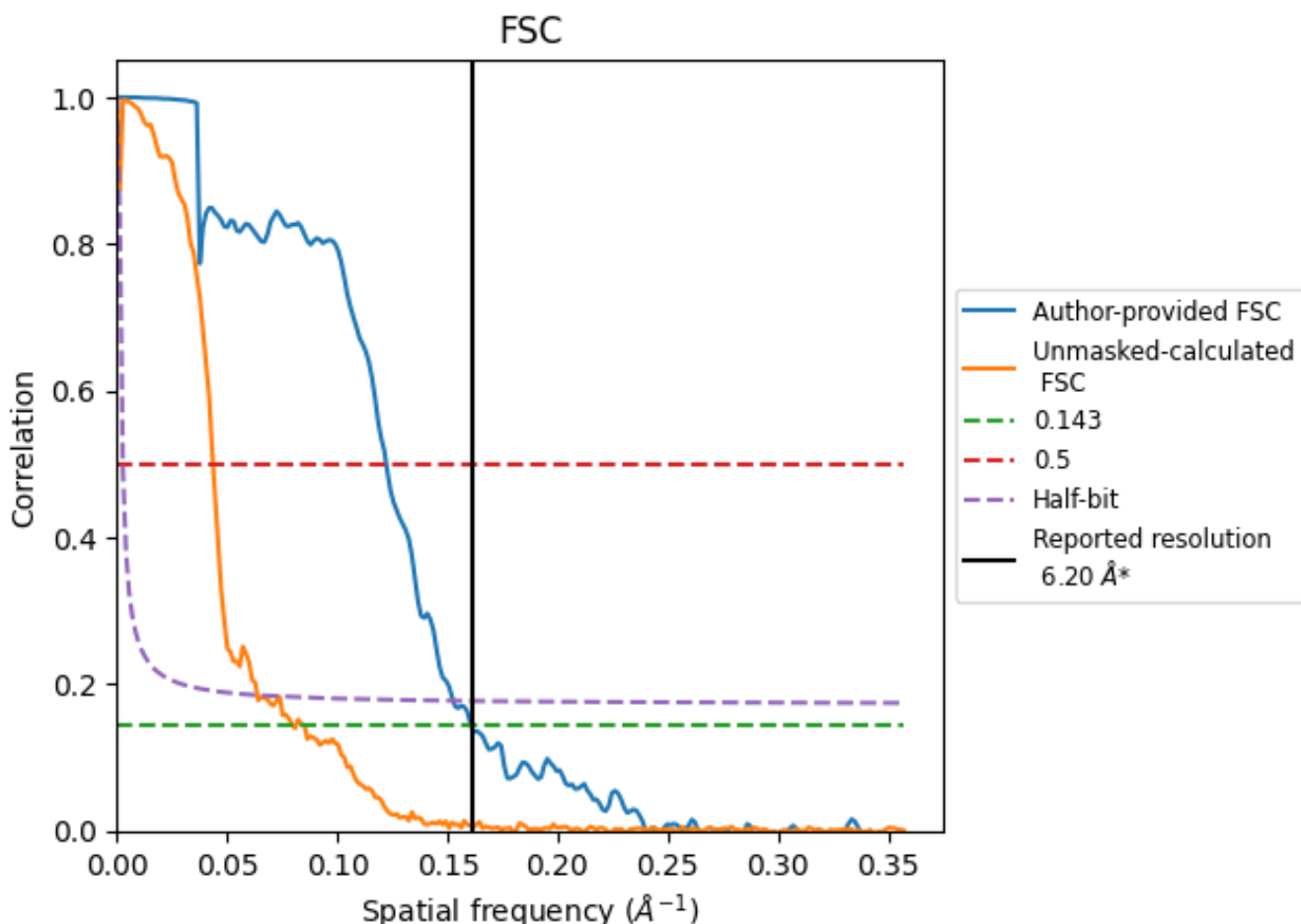


\*Reported resolution corresponds to spatial frequency of 0.161 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.161 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.22	8.18	6.55
Unmasked-calculated*	12.50	22.88	15.67

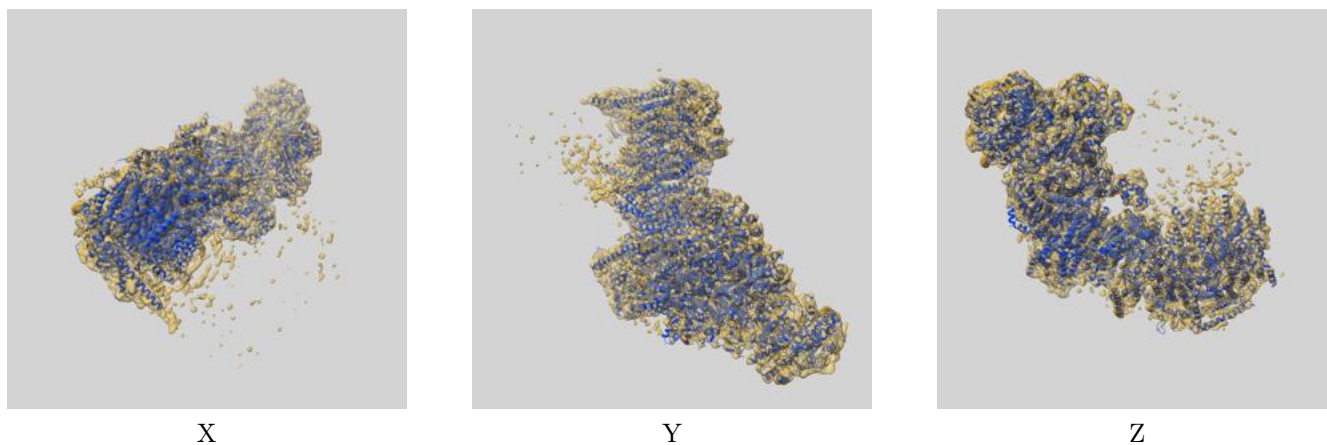
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.50 differs from the reported value 6.2 by more than 10 %



## 9 Map-model fit [i](#)

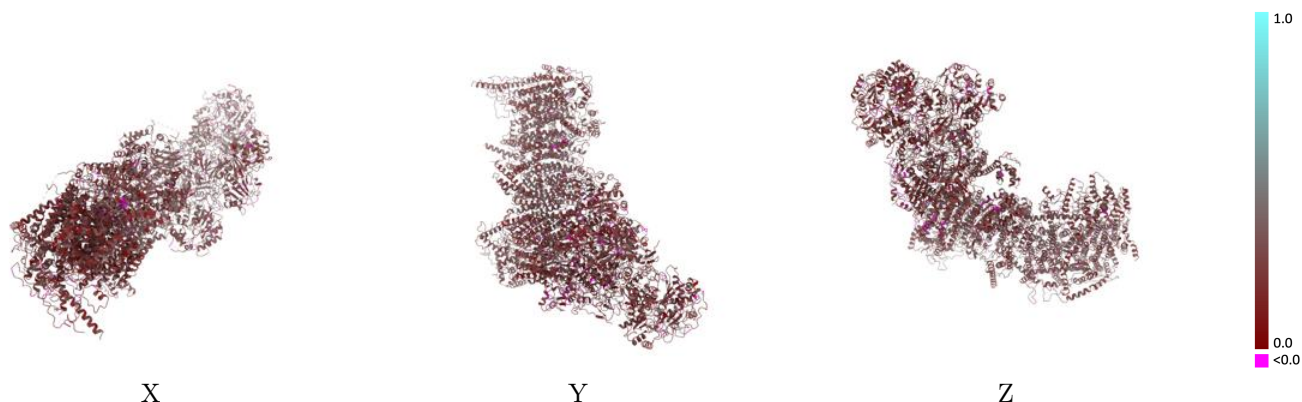
This section contains information regarding the fit between EMDB map EMD-4502 and PDB model 6QCA. Per-residue inclusion information can be found in section [3](#) on page [15](#).

### 9.1 Map-model overlay [i](#)



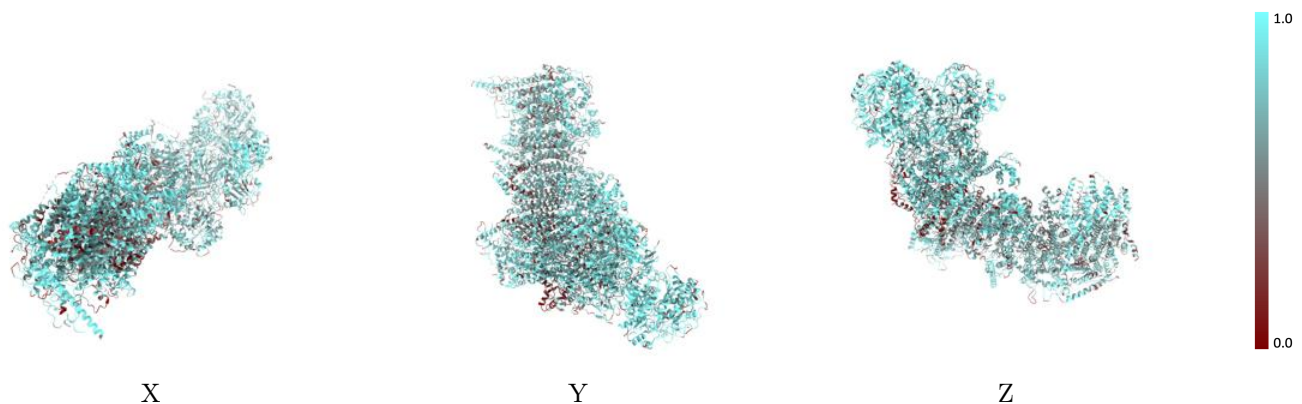
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



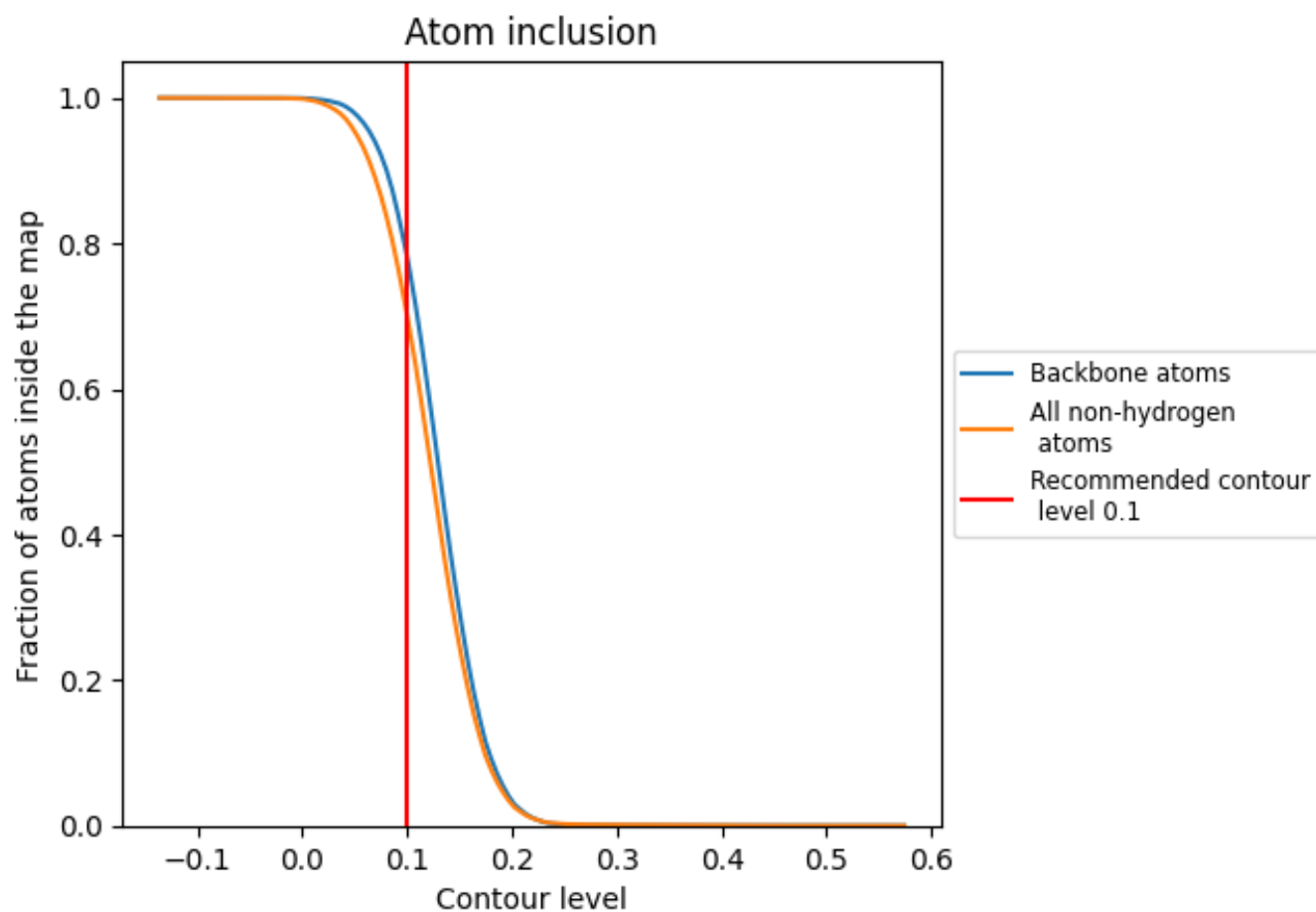
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7009	 0.2480
4L	 0.5967	 0.2520
A1	 0.7230	 0.2520
A2	 0.8276	 0.2330
A3	 0.6485	 0.2540
A5	 0.7109	 0.2560
A6	 0.7537	 0.2660
A7	 0.4706	 0.2030
A8	 0.7757	 0.2750
A9	 0.7070	 0.2440
AA	 0.7733	 0.2390
AB	 0.7235	 0.2450
AJ	 0.7410	 0.2550
AK	 0.5528	 0.2510
AL	 0.3771	 0.2010
AM	 0.7225	 0.2370
B1	 0.6434	 0.2480
B2	 0.6533	 0.2270
B3	 0.5927	 0.2350
B4	 0.7213	 0.2440
B5	 0.7918	 0.2570
B6	 0.7002	 0.2530
B7	 0.7601	 0.2430
B8	 0.6735	 0.2590
B9	 0.8078	 0.2710
BJ	 0.7773	 0.2620
BK	 0.6917	 0.2660
C1	 0.7885	 0.2580
C2	 0.7165	 0.2470
D1	 0.6047	 0.2490
D2	 0.6432	 0.2560
D3	 0.5635	 0.2670
D4	 0.6755	 0.2540
D5	 0.6658	 0.2470
D6	 0.5103	 0.2450



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Chain	Atom inclusion	Q-score
S1	 0.7636	 0.2410
S2	 0.6722	 0.2430
S3	 0.7282	 0.2560
S4	 0.7264	 0.2630
S5	 0.7490	 0.2430
S6	 0.6976	 0.2600
S7	 0.6924	 0.2490
S8	 0.7384	 0.2300
V1	 0.8143	 0.2360
V2	 0.8303	 0.2480
V3	 0.8186	 0.2580