



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 09:45 AM JST

PDB ID : 5XTB
EMDB ID : EMD-6771
Title : Cryo-EM structure of human respiratory complex I matrix arm
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-18
Resolution : 3.40 Å(reported)

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

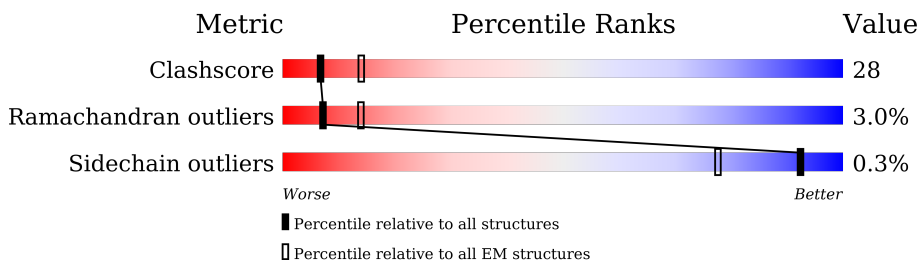
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.






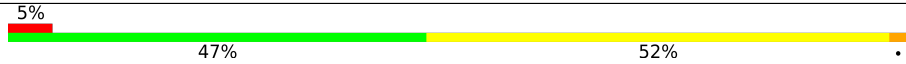
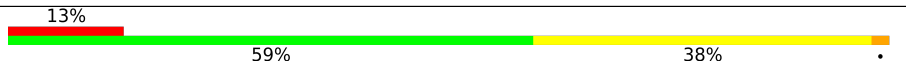
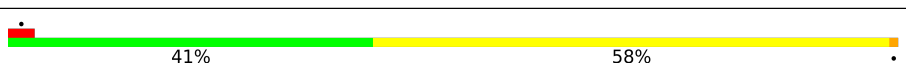

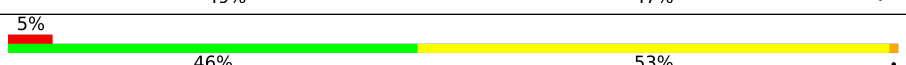

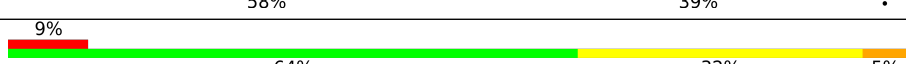
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	431	
2	B	176	
3	C	156	
4	E	113	
5	F	83	
6	G	85	
7	H	112	
8	I	110	

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Mol	Chain	Length	Quality of chain
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	385	
17	T	95	
18	W	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	A	501	-	-	X	-
19	SF4	B	302	-	-	X	-
19	SF4	M	801	-	-	X	-
20	FMN	A	502	-	-	X	-
22	NDP	J	401	-	-	X	-
23	FES	O	301	-	-	X	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 27962 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	A	431	3322	2096	594	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1420	893	243	271	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1249	794	227	214	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	968	623	178	162	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	83	670	422	124	122	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	85	672	434	99	134	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	922	593	157	169	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	95	769	483	146	138	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	337	2712	1759	482	463	8	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	274	173	47	53	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	964	608	173	179	4	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	5274	3310	917	1009	38	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	1195	770	210	212	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	212	1643	1047	276	310	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1730	1117	297	313	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	385	3087	1971	536	558	22	0	0

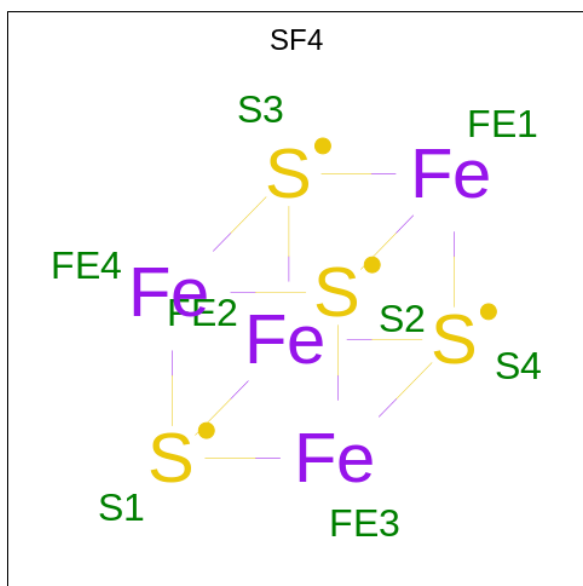
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	95	742	459	138	142	3	0	0

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

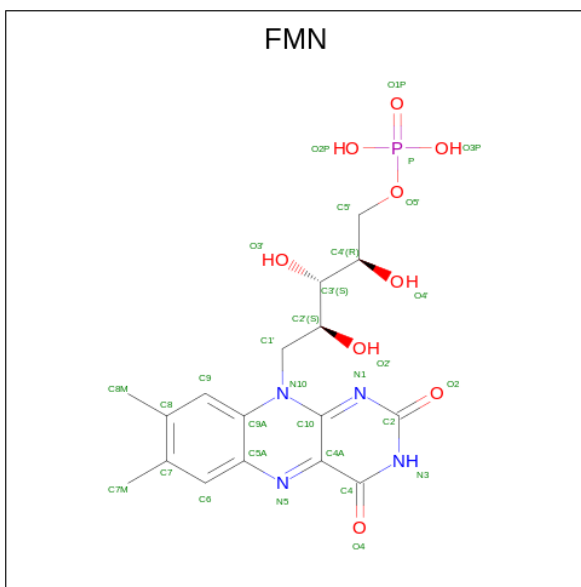
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	22	179	113	35	30	1	0	0

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



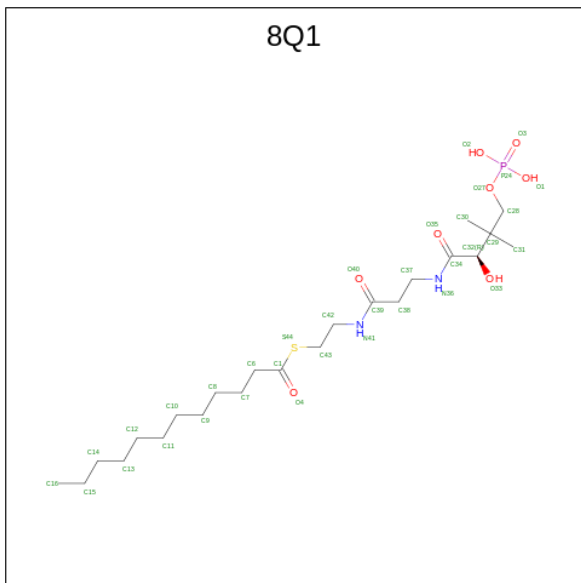
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	A	1	8	4	4	0
19	B	1	16	8	8	0
19	B	1	16	8	8	0
19	C	1	8	4	4	0
19	M	1	16	8	8	0
19	M	1	16	8	8	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



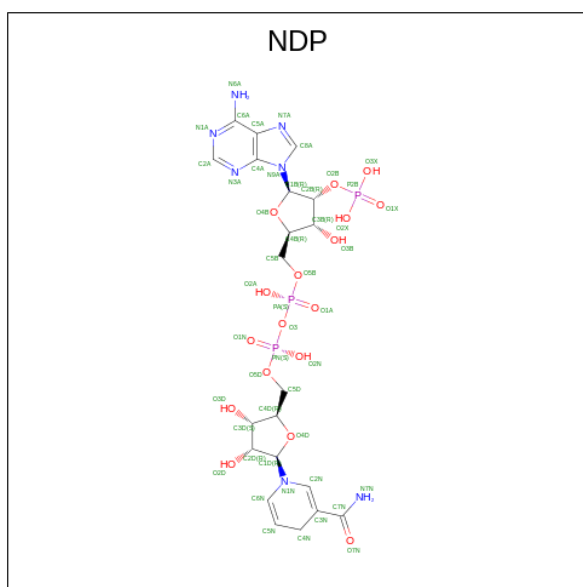
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	A	1	31	17	4	9	1	0

- Molecule 21 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



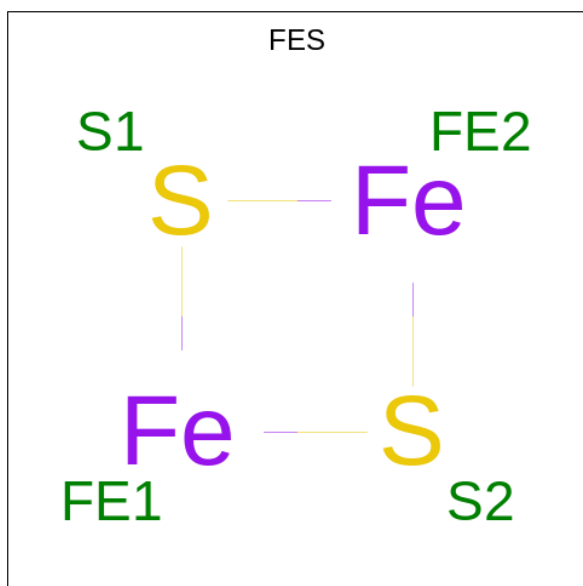
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
21	E	1	35	23	2	8	1	1	0

- Molecule 22 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
			Total	C	N	O	P	
22	J	1	48	21	7	17	3	0

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

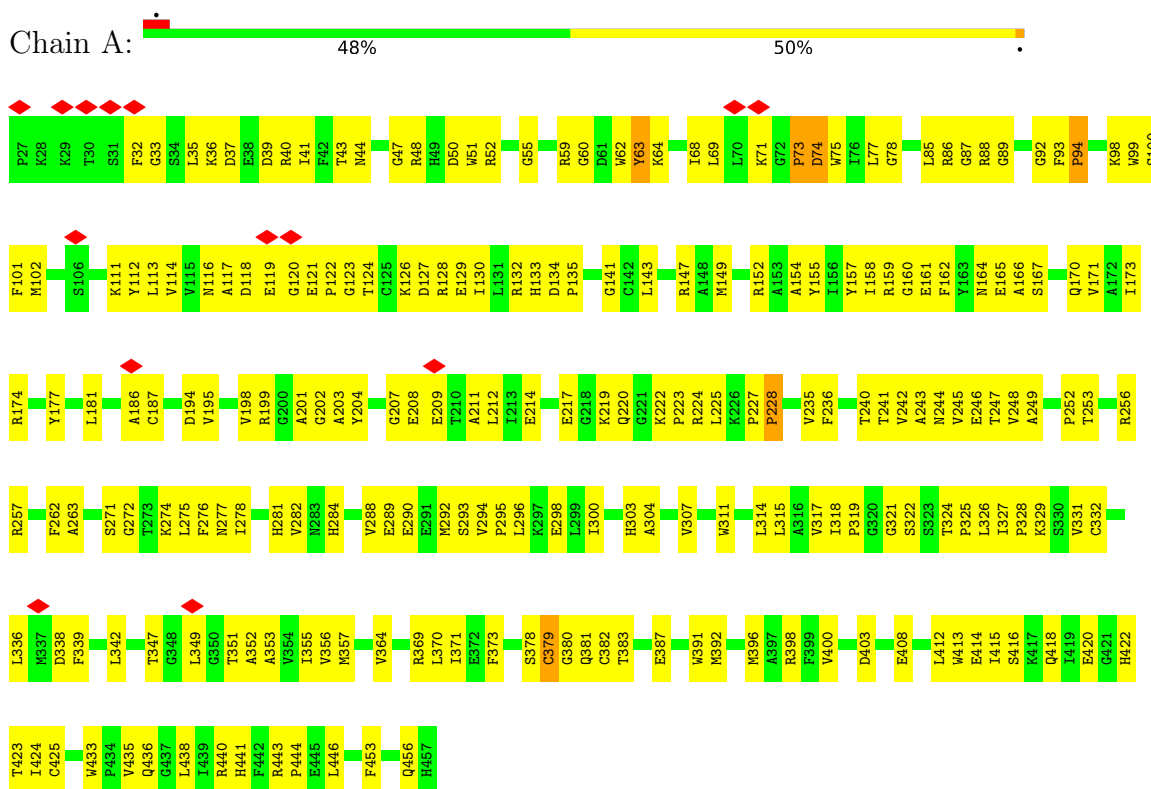


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	M	1	4	2	2	0
23	O	1	4	2	2	0

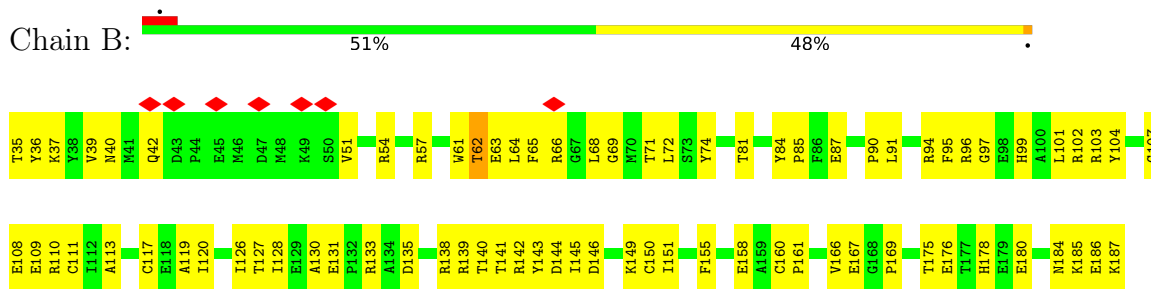
3 Residue-property plots [i](#)

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

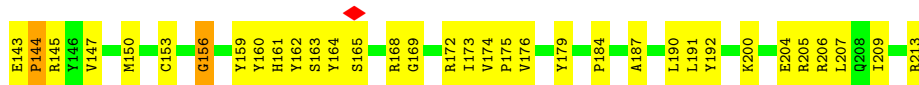
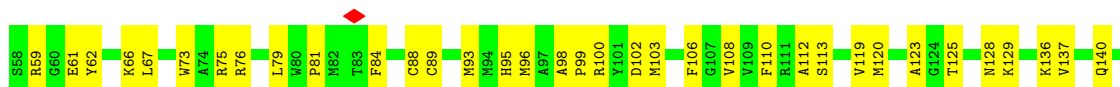


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

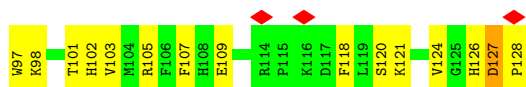
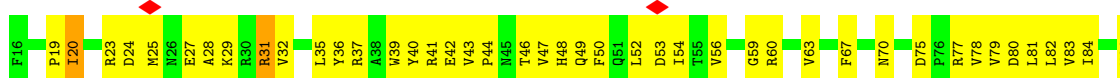




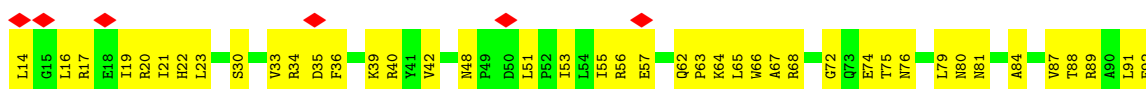
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



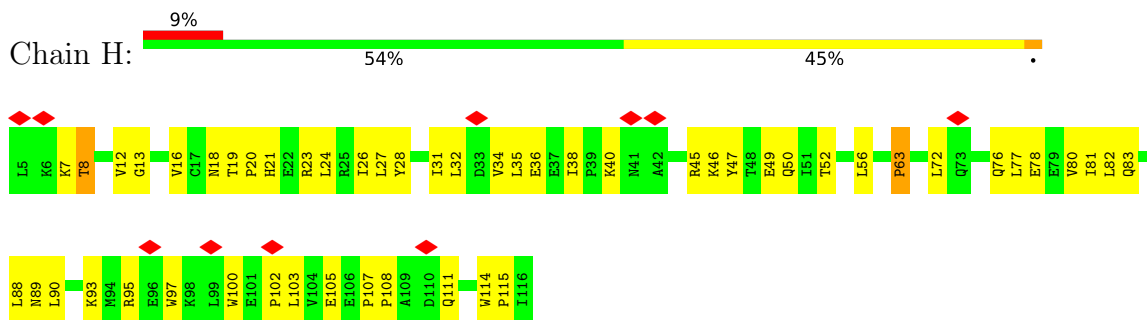
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



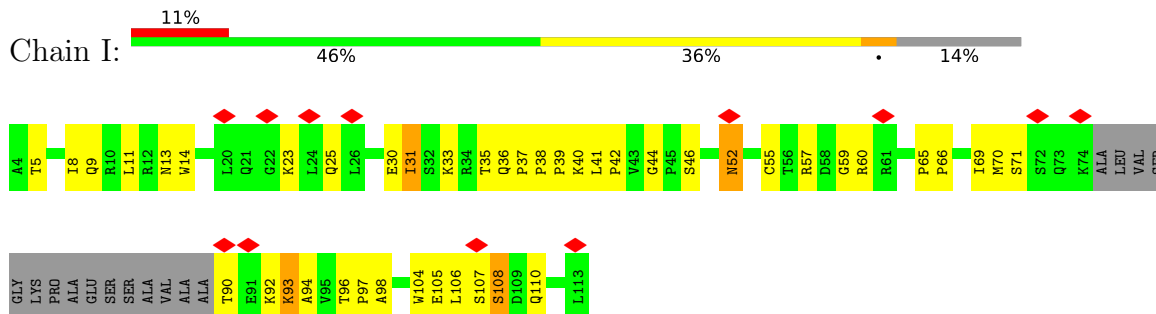
- Molecule 6: Acyl carrier protein, mitochondrial



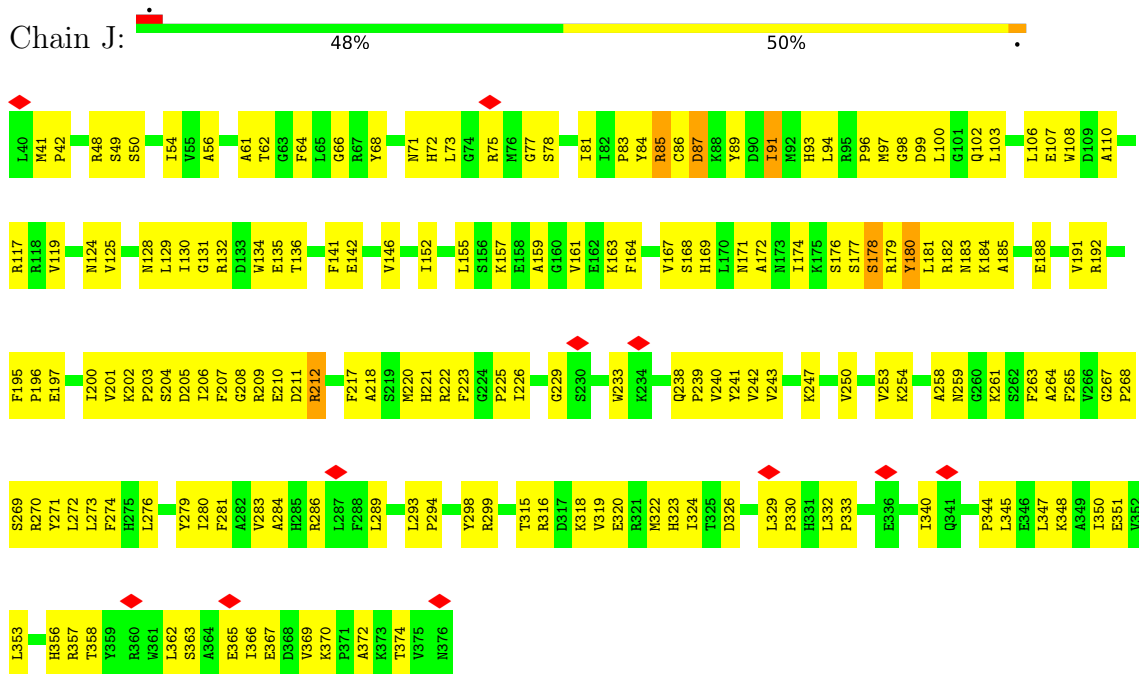
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



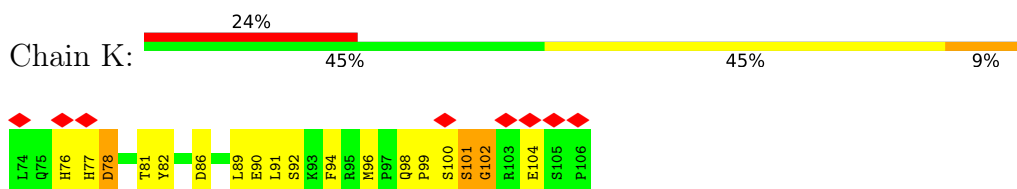
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



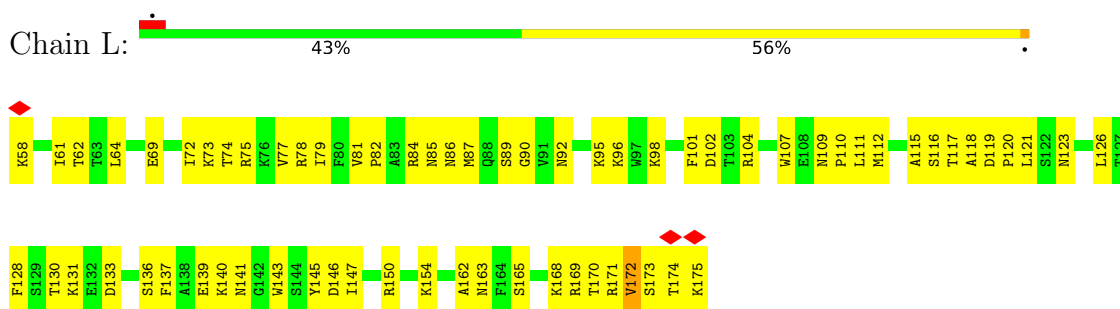
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



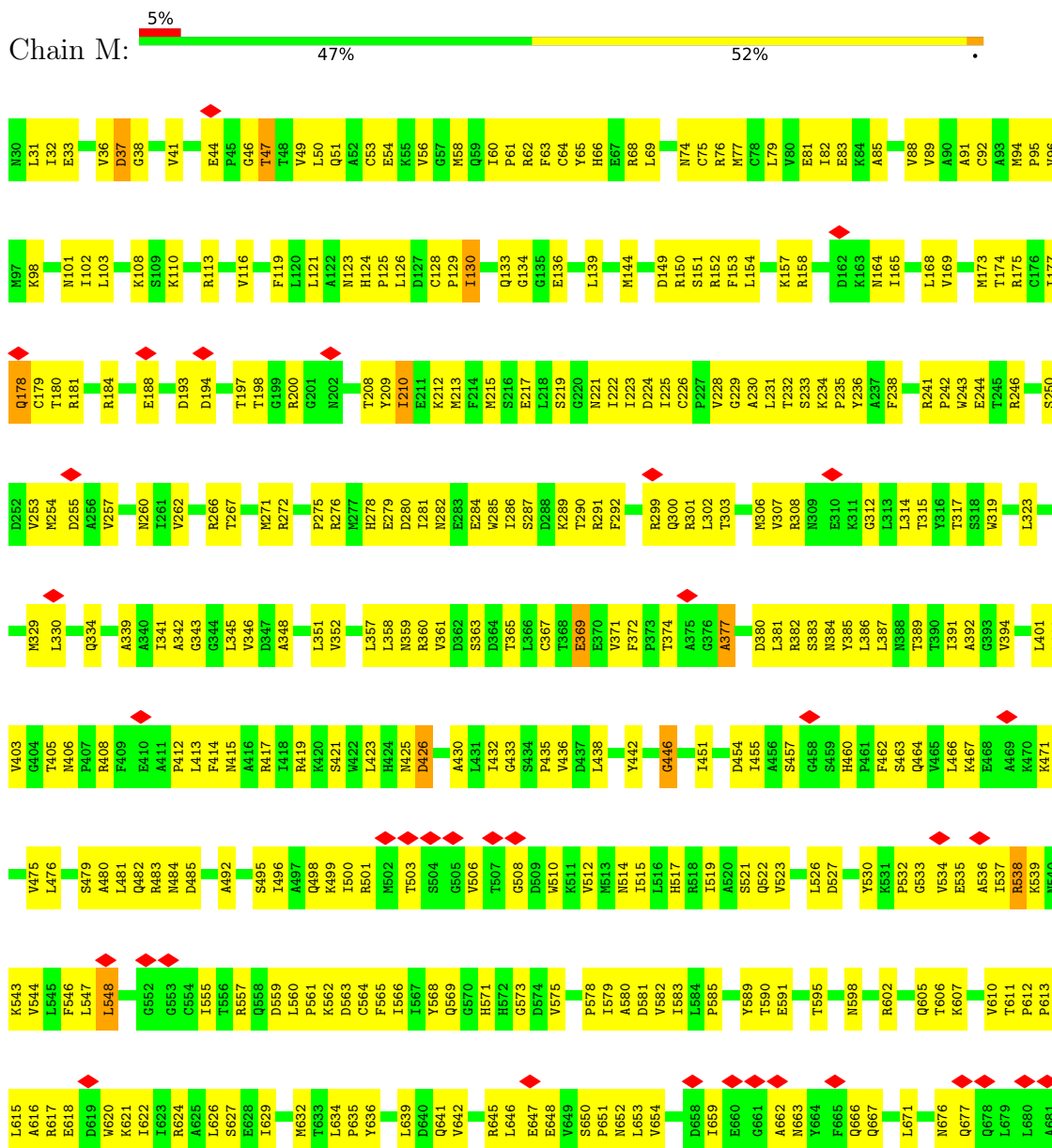
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

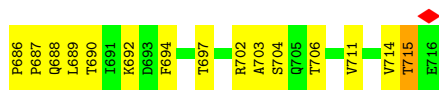


• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

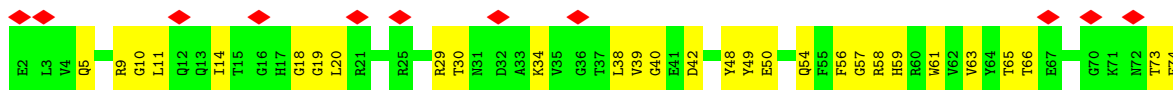


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

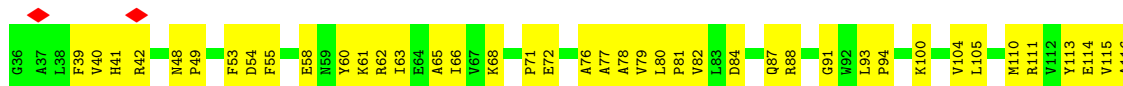




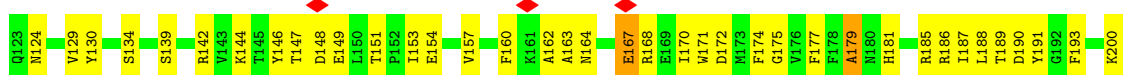
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

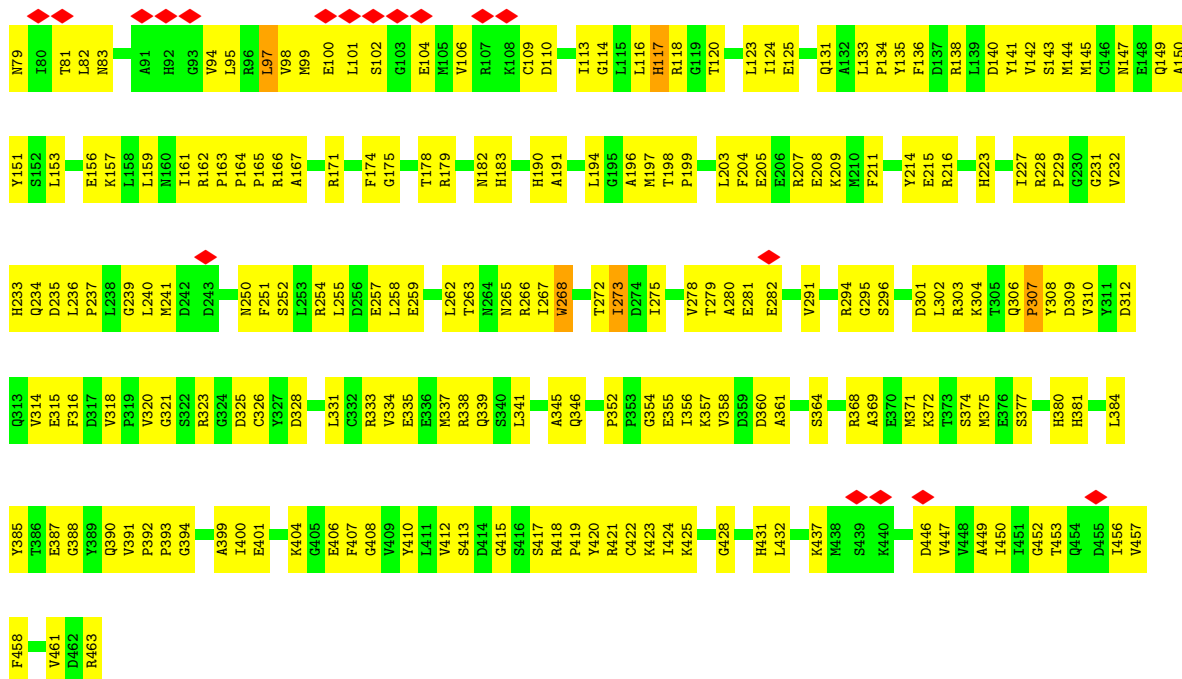


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

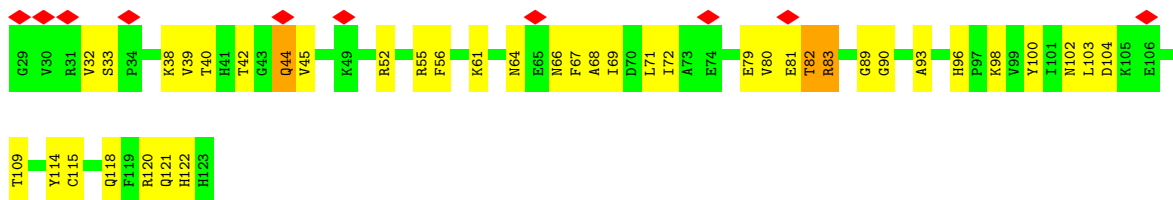


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	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	0.616	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0516	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	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: SF4, FMN, 8Q1, FES, 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	A	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.53	0/1335
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.44	0/3161	0.60	1/4275 (0.0%)
17	T	0.31	0/755	0.47	0/1017
18	W	0.34	0/185	0.65	0/249
All	All	0.36	0/28433	0.54	1/38494 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	97	LEU	CA-CB-CG	5.67	128.34	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	3322	0	3289	209	0
2	B	1420	0	1371	99	0
3	C	1249	0	1253	65	0
4	E	968	0	982	62	0
5	F	670	0	679	37	0
6	G	672	0	650	32	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	227	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	329	0
13	N	1195	0	1155	47	0
14	O	1643	0	1646	111	0
15	P	1730	0	1685	114	0
16	Q	3087	0	3069	223	0
17	T	742	0	723	37	0
18	W	179	0	179	11	0
19	A	8	0	0	6	0
19	B	16	0	0	3	0
19	C	8	0	0	1	0
19	M	16	0	0	4	0
20	A	31	0	19	17	0
21	E	35	0	0	4	0
22	J	48	0	26	26	0
23	M	4	0	0	1	0
23	O	4	0	0	2	0
All	All	27962	0	27752	1536	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 28.

The worst 5 of 1536 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)
9:J:130:ILE:HG23	22:J:401:NDP:C8A	1.45	1.46
12:M:134:GLY:HA2	19:M:801:SF4:S3	1.57	1.42
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
9:J:206:ILE:HA	9:J:240:VAL:O	1.35	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.24

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	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7	30
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25	57
3	C	154/156 (99%)	137 (89%)	12 (8%)	5 (3%)	4	22
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8	32
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	28
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	16
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	8
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	30
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	4
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	21
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	21
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	14
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	22
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	13
16	Q	383/385 (100%)	355 (93%)	23 (6%)	5 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	17
18	W	20/22 (91%)	16 (80%)	1 (5%)	3 (15%)	0	0
All	All	3453/3506 (98%)	3119 (90%)	230 (7%)	104 (3%)	7	23

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

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	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	78	90
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	67	83
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	92	97
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	331/331 (100%)	329 (99%)	2 (1%)	86	94
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	19/19 (100%)	19 (100%)	0	100	100
All	All	3006/3021 (100%)	2997 (100%)	9 (0%)	92	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Q	268	TRP
16	Q	273	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
16	Q	234	GLN
16	Q	431	HIS
9	J	102	GLN
9	J	71	ASN
16	Q	442	HIS

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

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	SF4	B	302	2	0,12,12	-	-	-		
21	8Q1	E	201	-	31,34,34	1.65	6 (19%)	40,43,43	1.38	7 (17%)
23	FES	O	301	14	0,4,4	-	-	-		
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	B	301	2	0,12,12	-	-	-		
23	FES	M	803	-	0,4,4	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
19	SF4	A	501	1	0,12,12	-	-	-		
19	SF4	M	801	12	0,12,12	-	-	-		
22	NDP	J	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.32	4 (7%)

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	B	302	2	-	-	0/6/5/5
21	8Q1	E	201	-	-	18/41/41/41	-
23	FES	O	301	14	-	-	0/1/1/1
19	SF4	C	301	3	-	-	0/6/5/5
19	SF4	B	301	2	-	-	0/6/5/5
23	FES	M	803	-	-	-	0/1/1/1
20	FMN	A	502	-	-	7/18/18/18	0/3/3/3
19	SF4	M	802	12	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	M	801	12	-	-	0/6/5/5
22	NDP	J	401	-	-	15/30/77/77	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	201	8Q1	C34-N36	5.24	1.45	1.33
21	E	201	8Q1	C39-N41	4.94	1.44	1.33
20	A	502	FMN	C9A-C5A	4.43	1.48	1.41
22	J	401	NDP	C6N-C5N	3.08	1.38	1.33
20	A	502	FMN	C8-C7	3.07	1.48	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	401	NDP	PN-O3-PA	-5.21	114.95	132.83
21	E	201	8Q1	C6-C1-S44	4.52	118.72	113.46
22	J	401	NDP	N3A-C2A-N1A	-3.78	122.77	128.68
20	A	502	FMN	C4-C4A-N5	2.84	122.27	118.23
21	E	201	8Q1	C43-S44-C1	2.79	110.57	101.87

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	C1'-C2'-C3'-O3'
20	A	502	FMN	C1'-C2'-C3'-C4'
20	A	502	FMN	C3'-C4'-C5'-O5'
20	A	502	FMN	O4'-C4'-C5'-O5'
21	E	201	8Q1	C1-C6-C7-C8

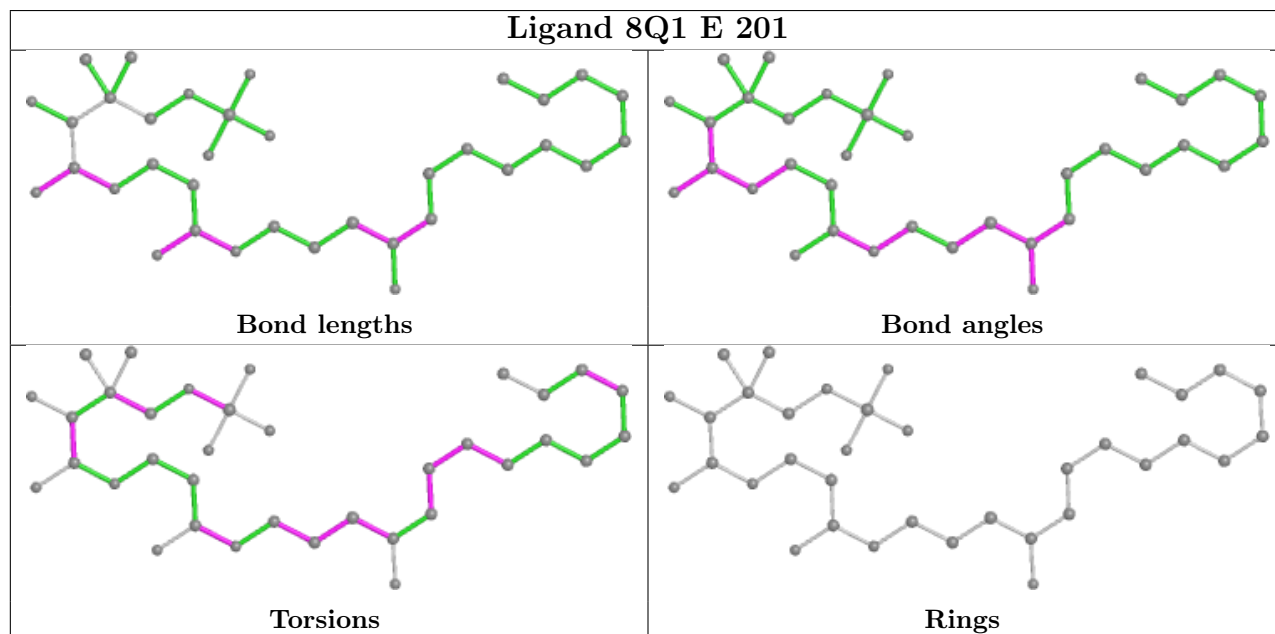
There are no ring outliers.

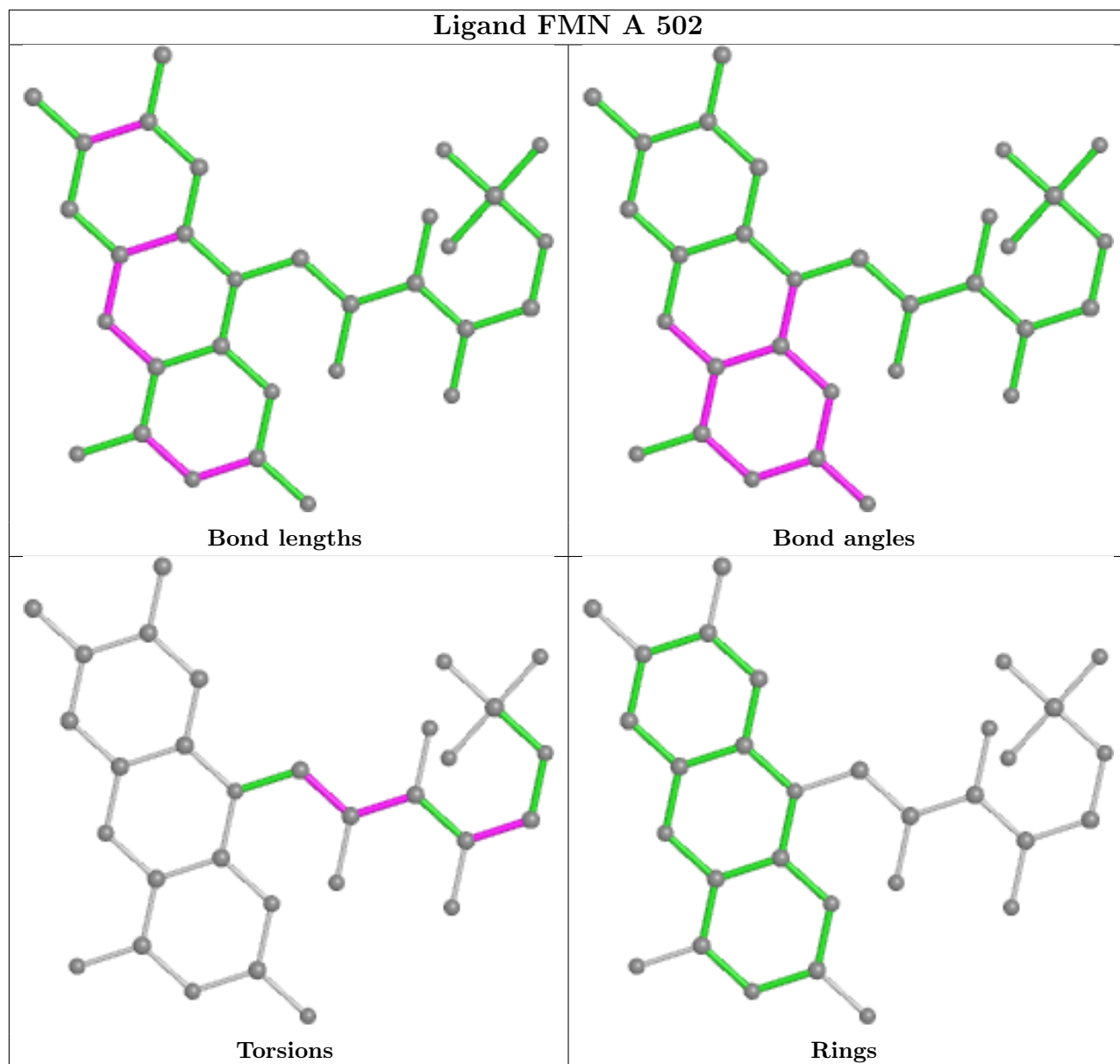
10 monomers are involved in 64 short contacts:

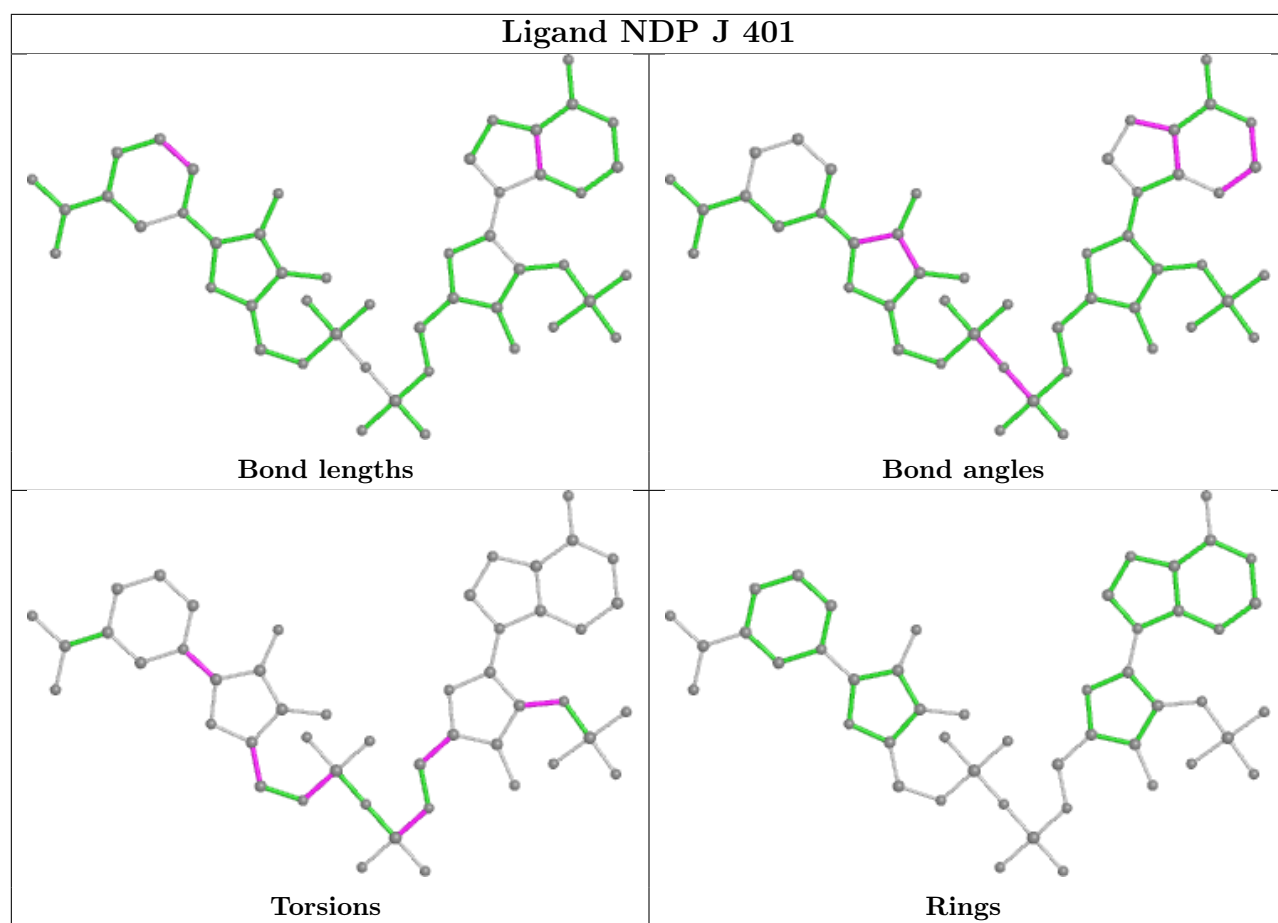
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	302	SF4	2	0
21	E	201	8Q1	4	0
23	O	301	FES	2	0
19	C	301	SF4	1	0
19	B	301	SF4	1	0
23	M	803	FES	1	0
20	A	502	FMN	17	0
19	A	501	SF4	6	0
19	M	801	SF4	4	0
22	J	401	NDP	26	0

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 [i](#)

There are no chain breaks in this entry.

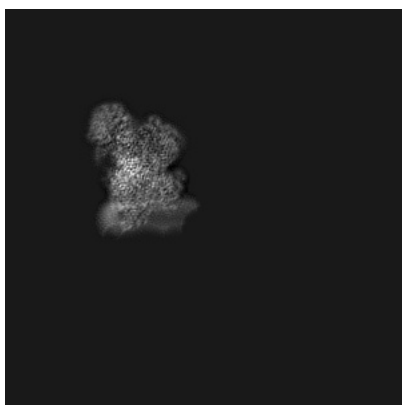
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6771. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

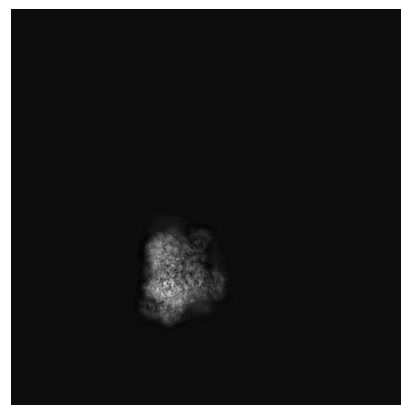
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

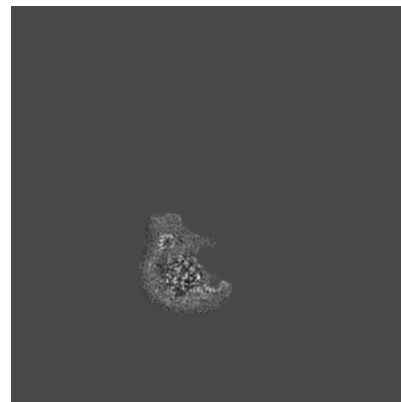
6.2.1 Primary map



X Index: 240



Y Index: 240

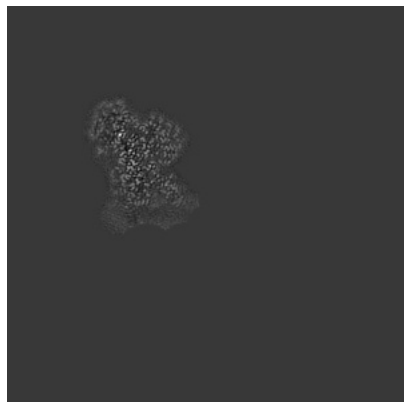


Z Index: 240

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 147



Z Index: 281

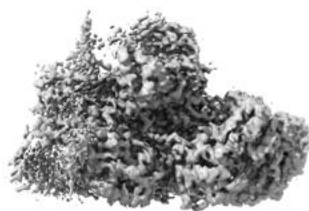
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0516. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

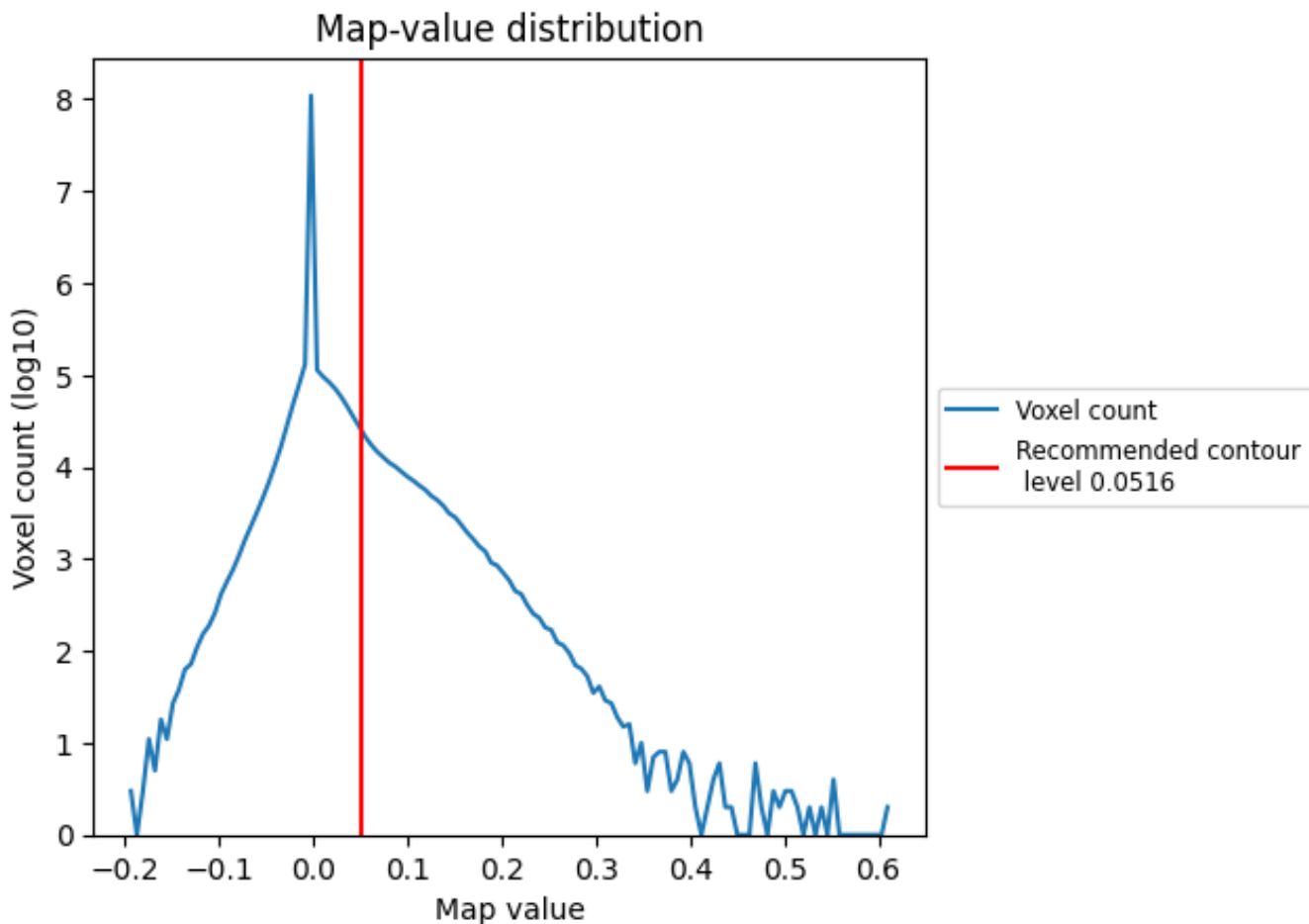
6.5 Mask visualisation

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

7 Map analysis [i](#)

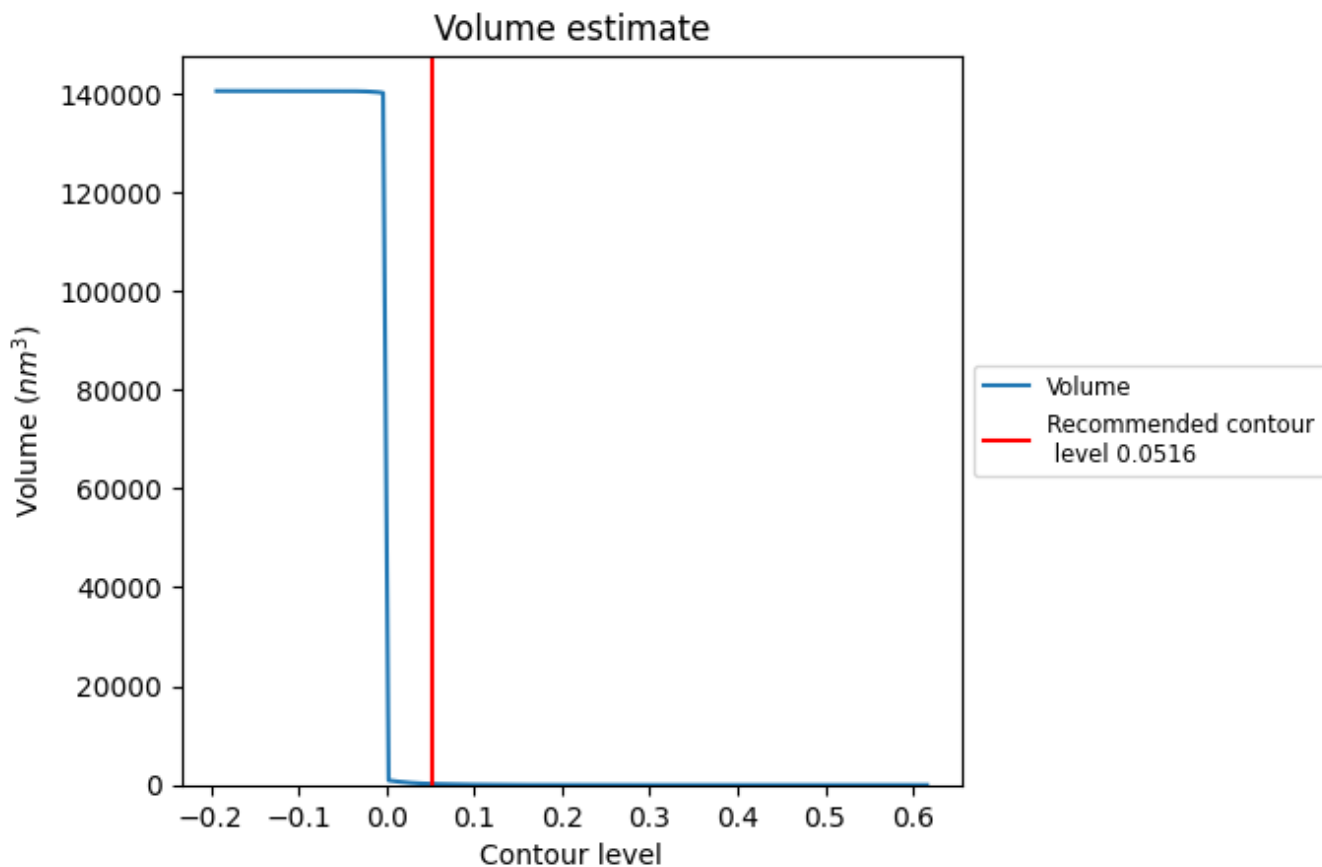
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

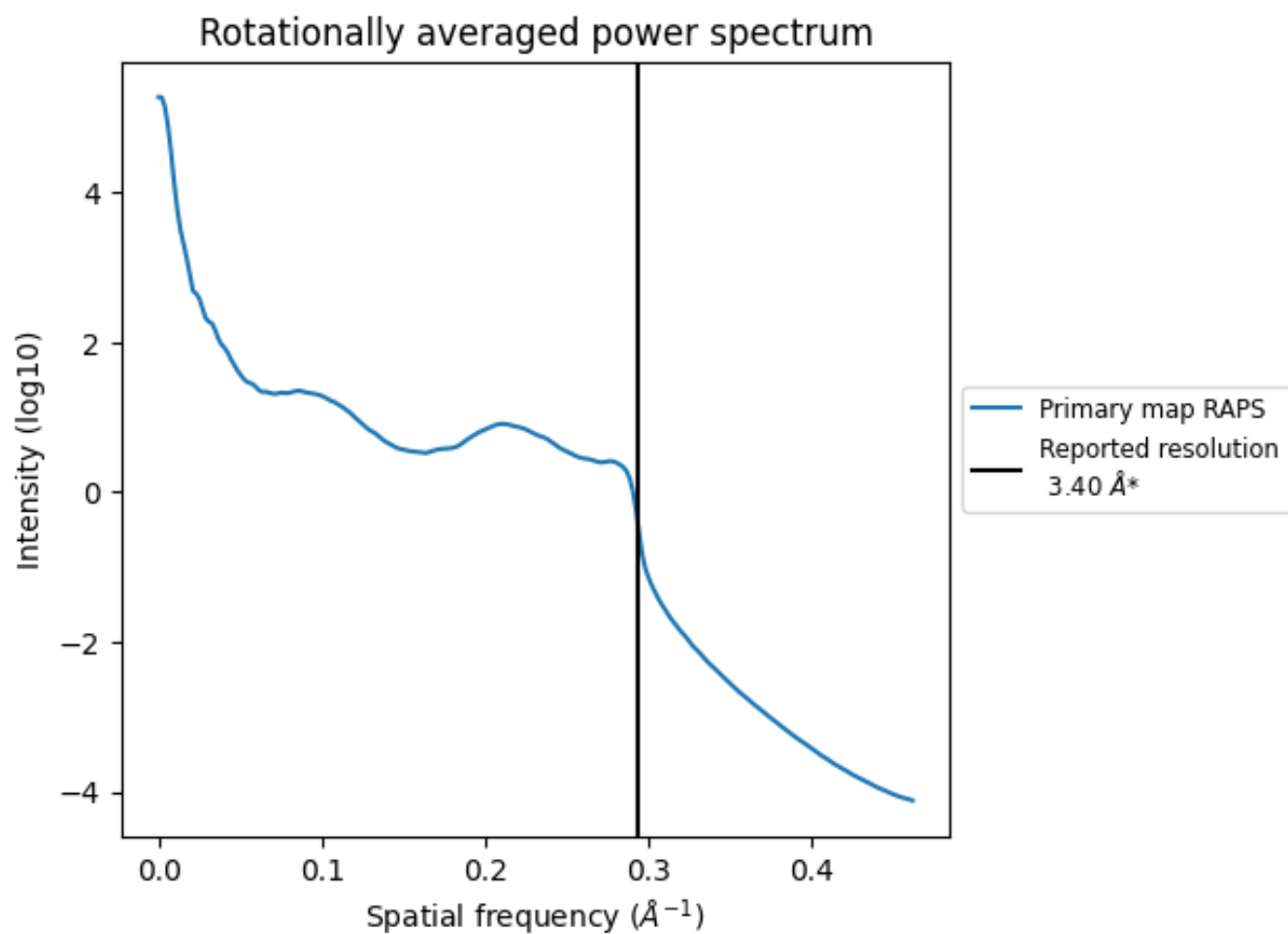
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 0.294 Å⁻¹

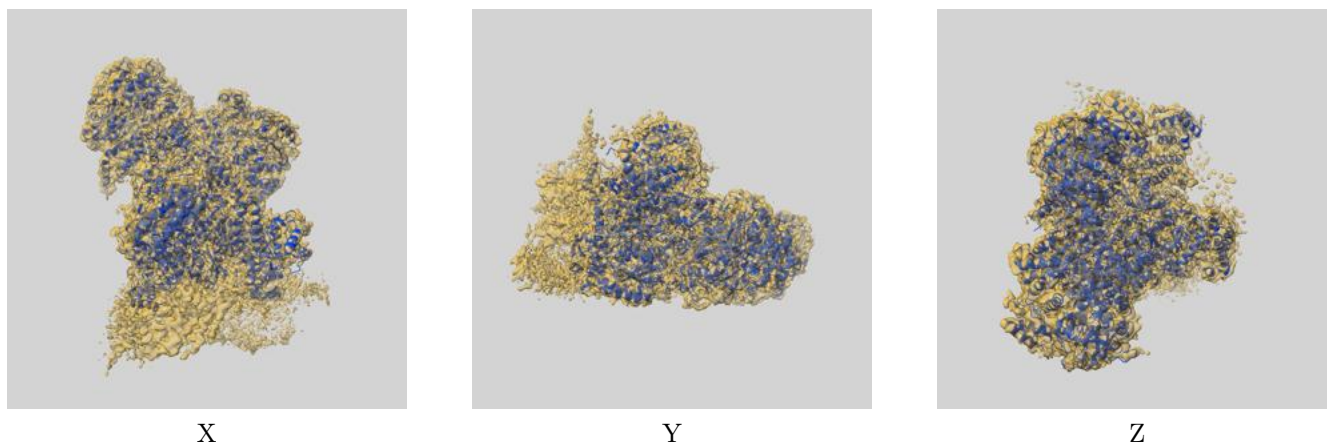
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

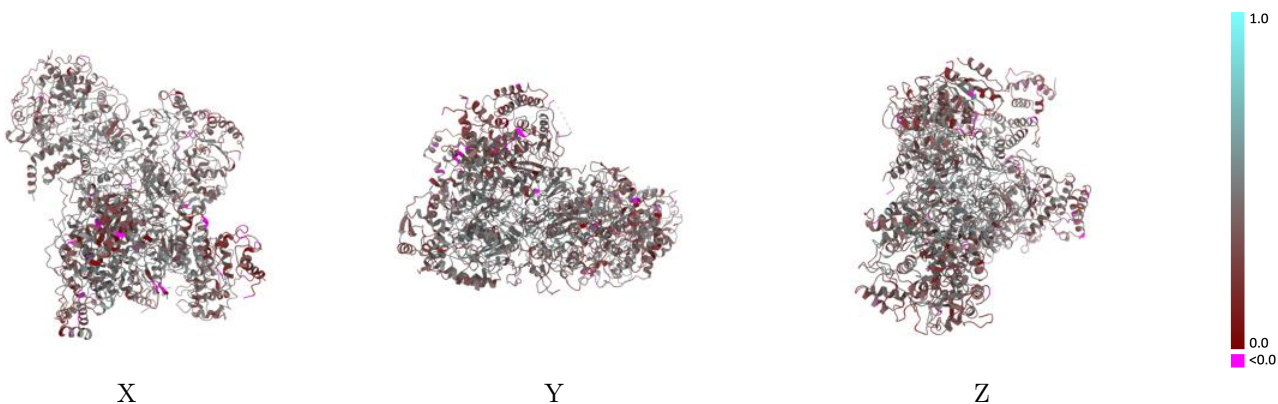
This section contains information regarding the fit between EMDB map EMD-6771 and PDB model 5XTB. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



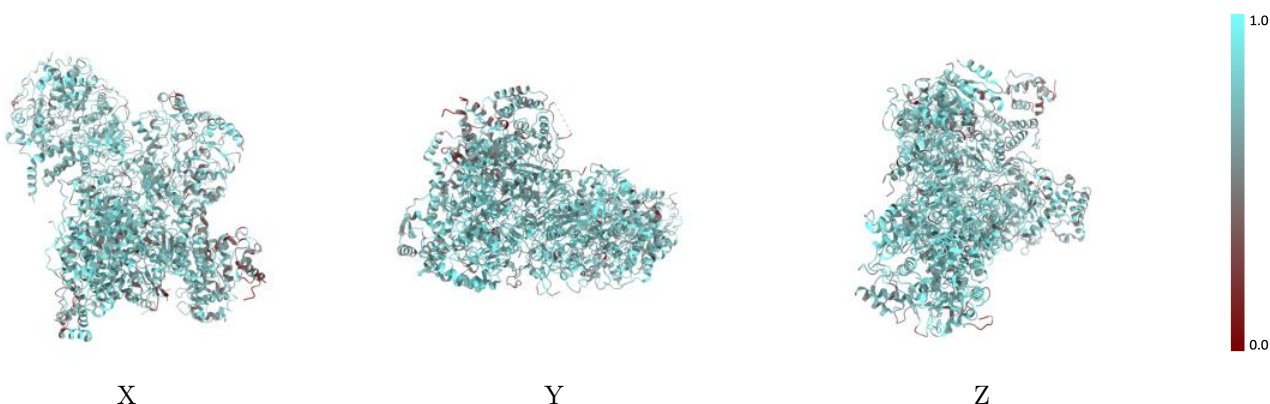
The images above show the 3D surface view of the map at the recommended contour level 0.0516 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



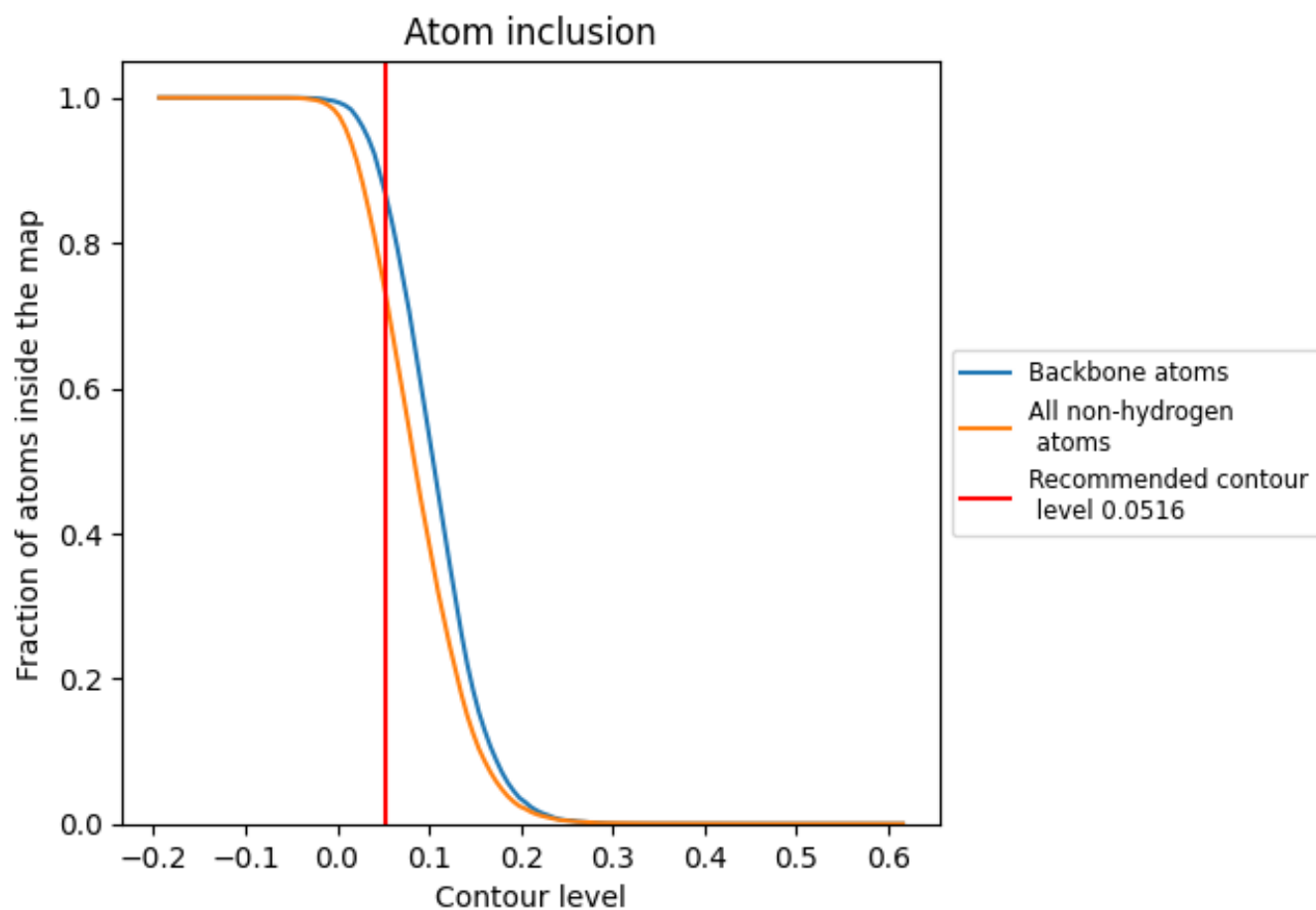
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0516).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.0516) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7368	 0.3890
A	 0.7467	 0.3790
B	 0.8259	 0.4490
C	 0.8321	 0.4710
E	 0.7084	 0.3800
F	 0.7389	 0.3330
G	 0.5150	 0.2360
H	 0.6729	 0.2830
I	 0.6255	 0.3560
J	 0.7499	 0.4070
K	 0.6791	 0.3400
L	 0.7428	 0.4100
M	 0.7461	 0.3910
N	 0.6793	 0.3760
O	 0.7256	 0.3710
P	 0.7328	 0.3860
Q	 0.7645	 0.4220
T	 0.7058	 0.3980
W	 0.7368	 0.3580

