wwPDB EM Validation Summary Report

Sep 22, 2022 – 04:15 am BST

PDB ID	:	7Z7R
EMDB ID	:	EMD-14535
Title	:	Complex I from E. coli, LMNG-purified, Apo, Open-ready state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-16
Resolution	:	3.36 Å(reported)
Based on initial models	:	3RKO, 4HEA

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

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

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

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

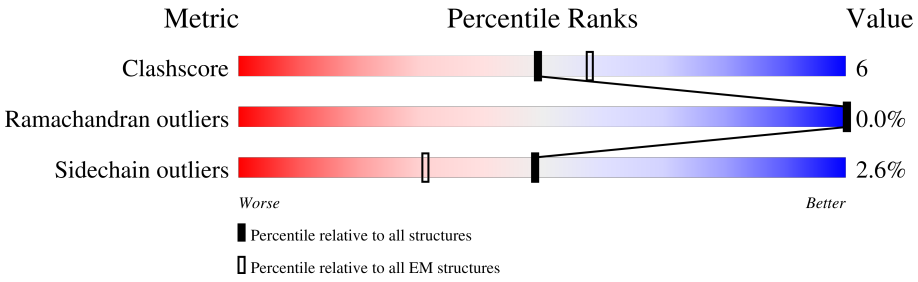
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.36 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 <=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	F	445	85% 13% •
2	E	166	81% 13% 6%
3	G	908	85% 15%
4	C	596	82% 16% • •
5	B	220	75% 18% • 5%
6	I	180	87% 13%
7	H	325	83% 16% •
8	A	147	62% 15% 23%

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Mol	Chain	Length	Quality of chain
9	L	613	
10	M	509	
11	N	485	
12	K	100	
13	J	184	

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
14	SF4	G	1001	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 37252 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-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	439	3407	2162	596	629	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase I subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	156	1220	768	215	229	8	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	905	7027	4392	1269	1329	37	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	586	4736	3036	825	851	24	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	208	1656	1051	288	301	16	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	180	1436	915	242	264	15	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	322	Total	C	N	O	S	0	0
			2529	1696	398	417	18		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	113	Total	C	N	O	S	0	0
			894	606	143	141	4		

- Molecule 9 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	605	Total	C	N	O	S	0	0
			4627	3076	740	779	32		

- Molecule 10 is a protein called NADH dehydrogenase I subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	504	Total	C	N	O	S	0	0
			3953	2661	617	646	29		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	470	Total	C	N	O	S	0	0
			3563	2382	563	598	20		

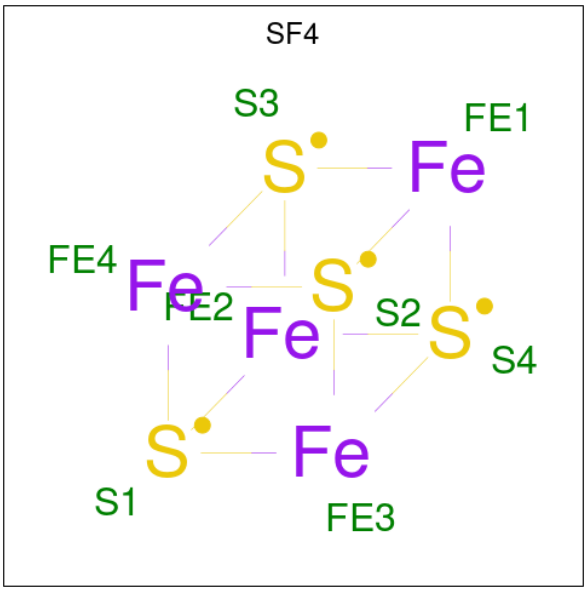
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit J.

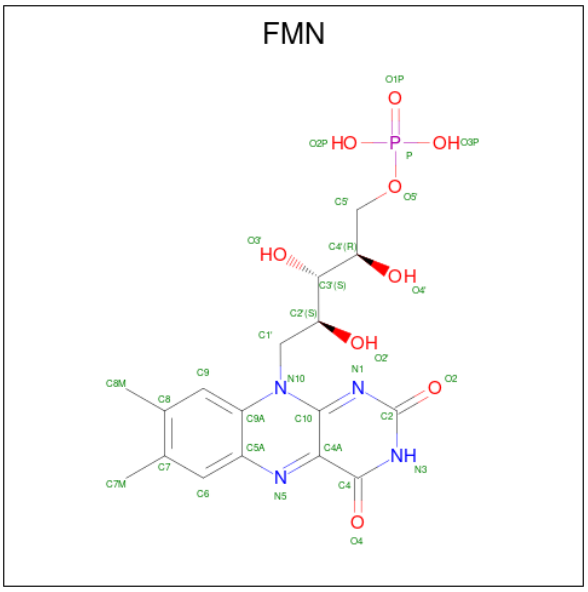
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



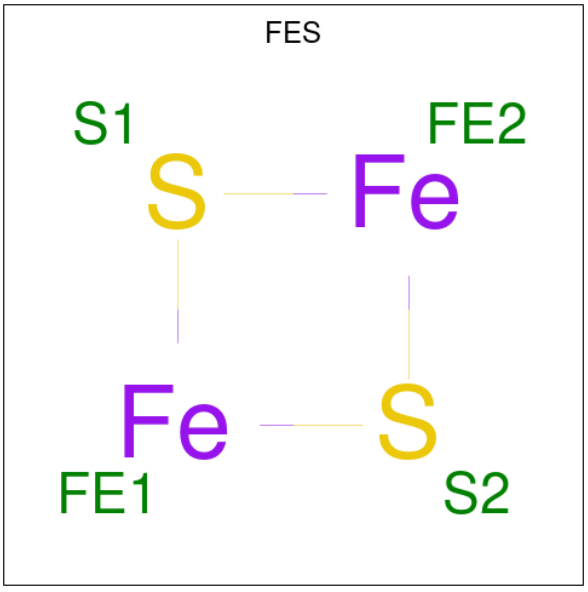
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

- Molecule 15 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

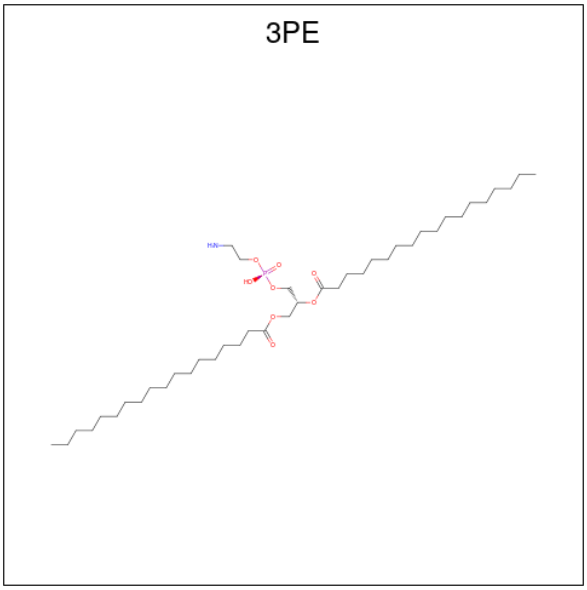


Mol	Chain	Residues	Atoms				AltConf
16	E	1	Total	Fe	S		0
			4	2	2		
16	G	1	Total	Fe	S		0
			4	2	2		

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca).

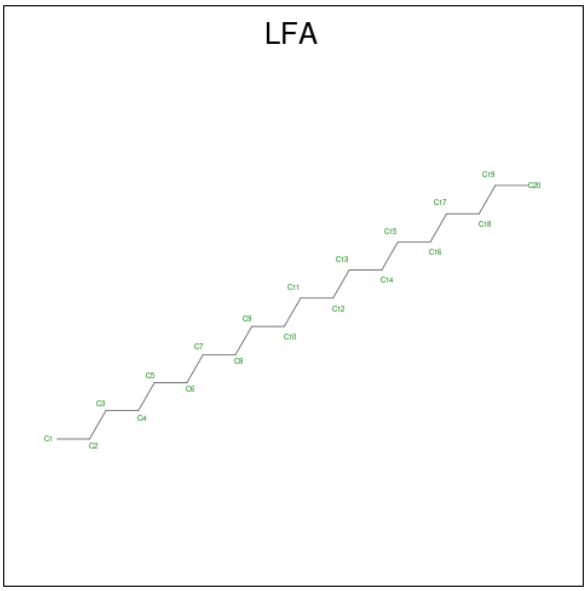
Mol	Chain	Residues	Atoms		AltConf
17	G	1	Total	Ca	0
			1	1	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	L	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 19 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



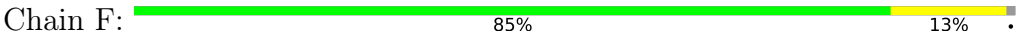
Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C 20 20	0

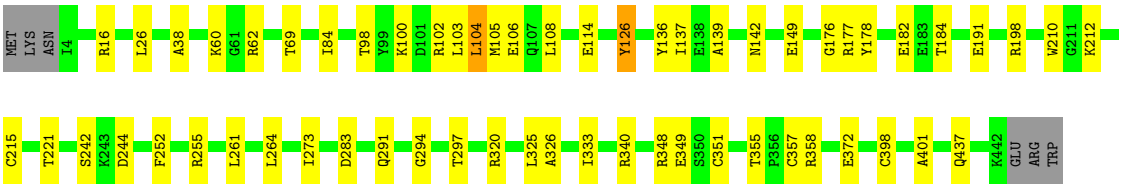
3 Residue-property plots (i)

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-quinone oxidoreductase subunit F

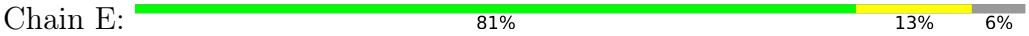
Chain F:

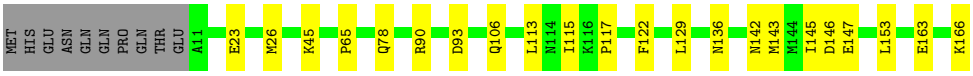




• Molecule 2: NADH dehydrogenase I subunit E

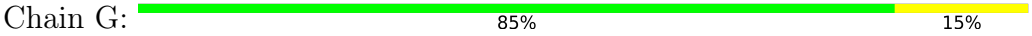
Chain E:

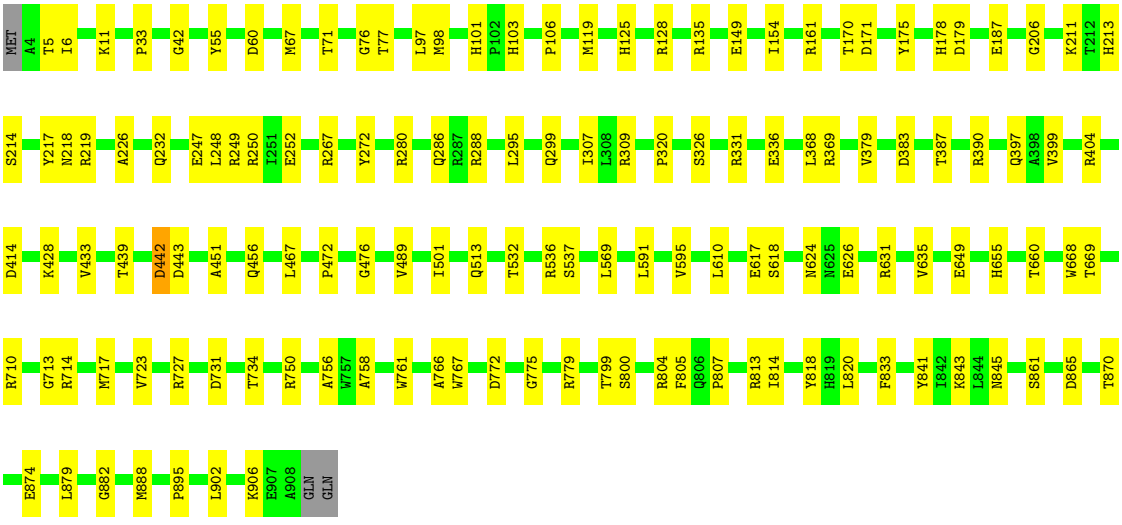




• Molecule 3: NADH-quinone oxidoreductase

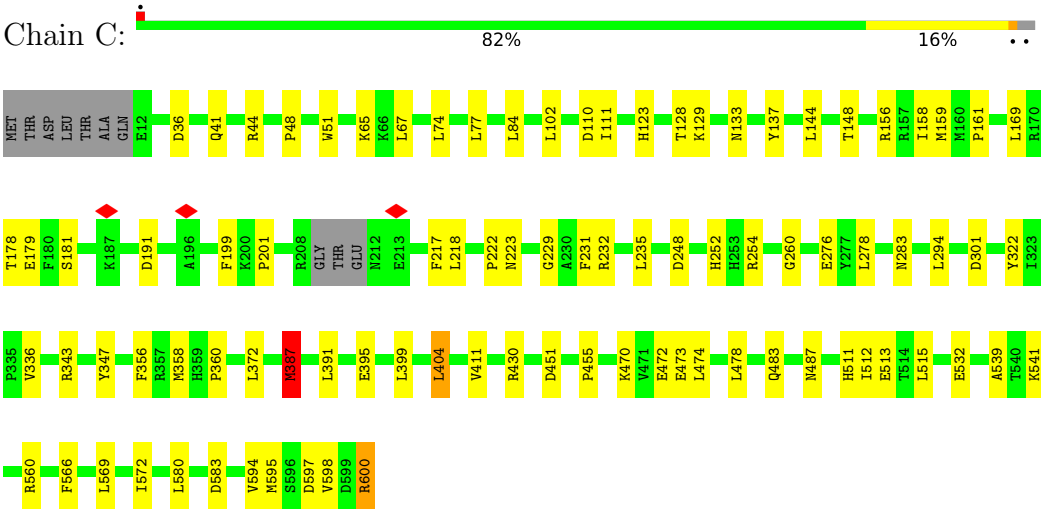
Chain G:





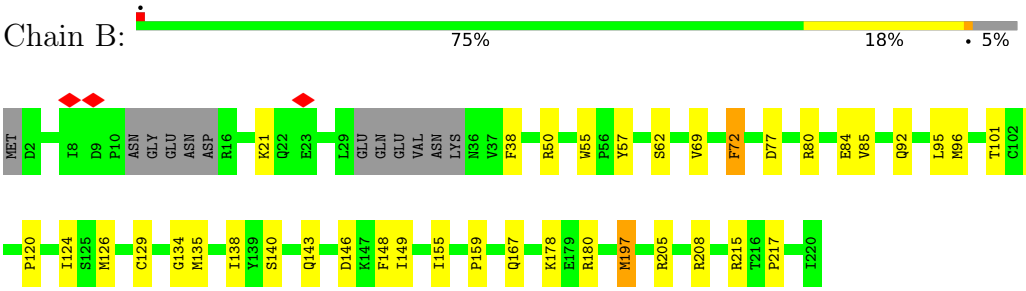
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



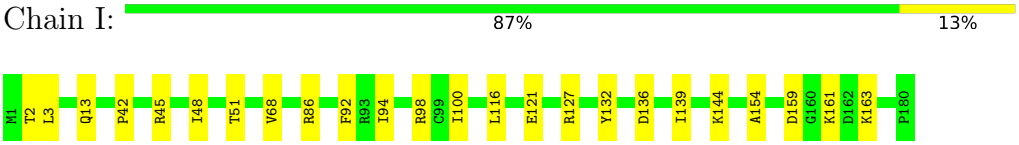
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



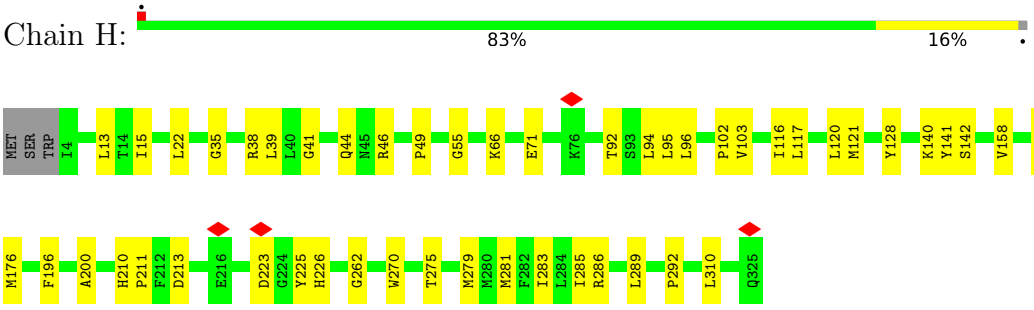
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:

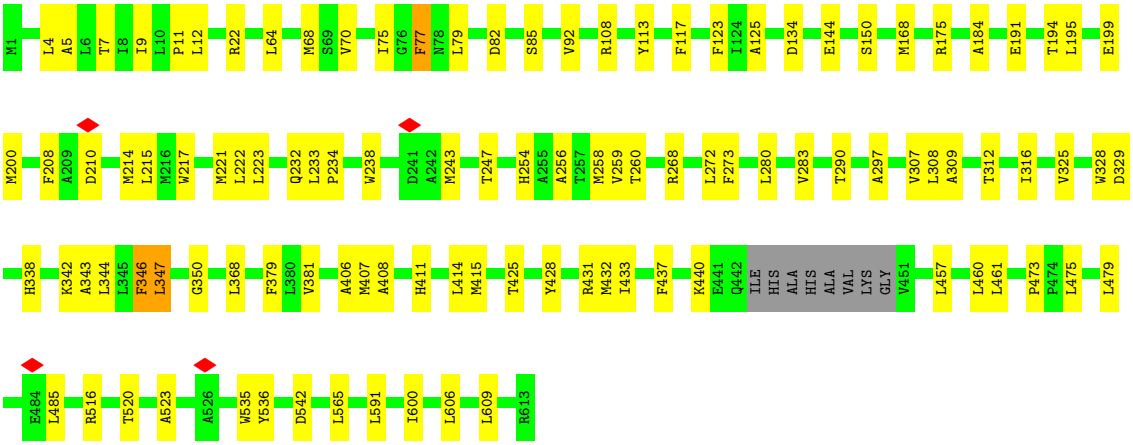


• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:

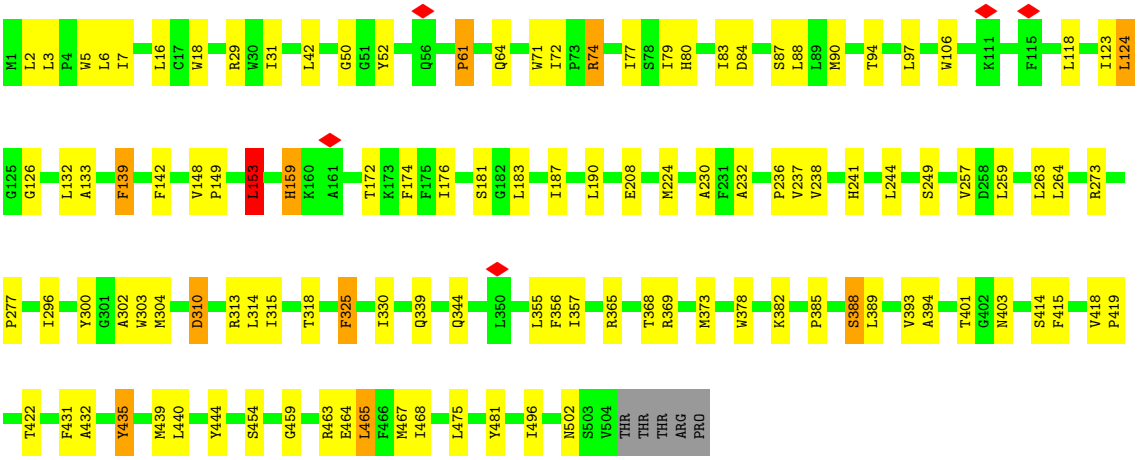
• Molecule 9: NADH dehydrogenase subunit L

Chain L:



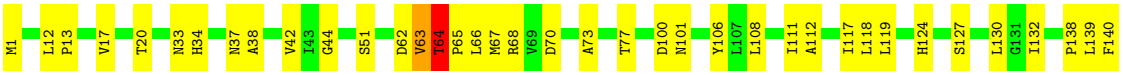
• Molecule 10: NADH dehydrogenase I subunit M

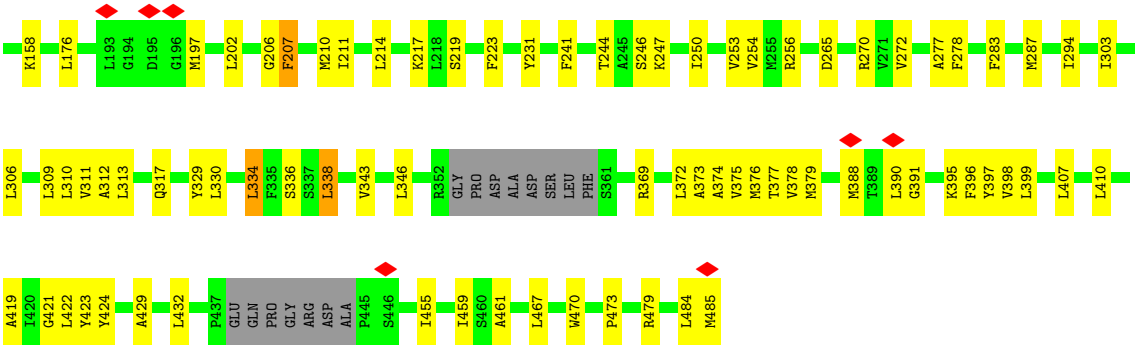
Chain M:



• Molecule 11: NADH-quinone oxidoreductase subunit N

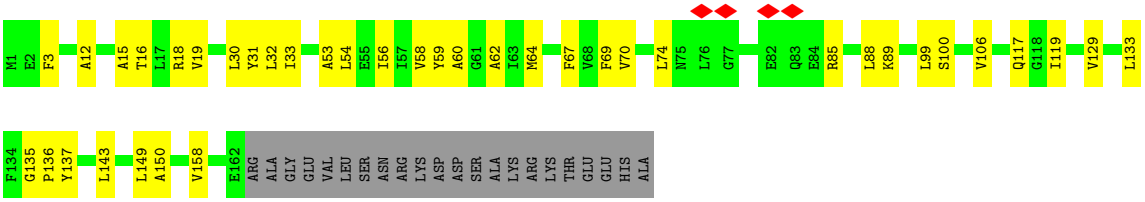
Chain N:





• Molecule 12: NADH-quinone oxidoreductase subunit K

• Molecule 13: NADH-quinone oxidoreductase subunit J



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108991	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	74	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	154.88, 215.38, 237.16	wwPDB
Map dimensions	128, 178, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 3PE, LFA, SF4, FMN, CA

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	F	0.27	0/3486	0.54	1/4713 (0.0%)
2	E	0.25	0/1248	0.50	0/1691
3	G	0.26	0/7178	0.52	0/9733
4	C	0.27	0/4866	0.55	1/6602 (0.0%)
5	B	0.28	0/1692	0.60	1/2292 (0.0%)
6	I	0.27	0/1470	0.53	0/1985
7	H	0.31	0/2603	0.60	1/3540 (0.0%)
8	A	0.29	0/921	0.64	3/1251 (0.2%)
9	L	0.28	0/4745	0.57	4/6465 (0.1%)
10	M	0.30	0/4074	0.61	6/5546 (0.1%)
11	N	0.30	0/3649	0.61	3/4977 (0.1%)
12	K	0.30	0/769	0.67	1/1040 (0.1%)
13	J	0.31	0/1252	0.59	1/1708 (0.1%)
All	All	0.28	0/37953	0.57	22/51543 (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
3	G	0	1
11	N	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	61	PRO	CA-N-CD	-7.12	101.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	210	ASP	CB-CG-OD2	7.03	124.63	118.30
1	F	104	LEU	CA-CB-CG	6.71	130.72	115.30
9	L	368	LEU	CA-CB-CG	6.64	130.58	115.30
9	L	347	LEU	CA-CB-CG	6.61	130.49	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	668	TRP	Peptide
11	N	63	VAL	Peptide
11	N	64	THR	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	F	3407	0	3374	33	0
2	E	1220	0	1187	14	0
3	G	7027	0	6829	74	0
4	C	4736	0	4656	59	0
5	B	1656	0	1644	29	0
6	I	1436	0	1415	18	0
7	H	2529	0	2581	33	0
8	A	894	0	904	13	0
9	L	4627	0	4770	63	0
10	M	3953	0	4053	65	0
11	N	3563	0	3741	71	0
12	K	760	0	817	21	0
13	J	1226	0	1297	30	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	3	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	E	4	0	0	1	0
16	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1	0	0	0	0
18	C	51	0	82	2	0
18	L	51	0	82	2	0
19	H	20	0	42	1	0
All	All	37252	0	37493	459	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 459 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)
11:N:375:VAL:HG23	11:N:461:ALA:HB2	1.70	0.74
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.68
10:M:181:SER:HB2	10:M:230:ALA:HA	1.75	0.68
4:C:276:GLU:O	4:C:283:ASN:ND2	2.26	0.68
7:H:116:ILE:HB	7:H:164:LEU:HD21	1.75	0.67

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	F	437/445 (98%)	428 (98%)	9 (2%)	0	100	100
2	E	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
3	G	903/908 (99%)	870 (96%)	33 (4%)	0	100	100
4	C	582/596 (98%)	567 (97%)	15 (3%)	0	100	100
5	B	202/220 (92%)	195 (96%)	7 (4%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	320/325 (98%)	313 (98%)	7 (2%)	0	100	100
8	A	109/147 (74%)	109 (100%)	0	0	100	100
9	L	601/613 (98%)	583 (97%)	18 (3%)	0	100	100
10	M	502/509 (99%)	485 (97%)	17 (3%)	0	100	100
11	N	464/485 (96%)	455 (98%)	8 (2%)	1 (0%)	47	78
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/184 (87%)	156 (98%)	4 (2%)	0	100	100
All	All	4710/4878 (97%)	4581 (97%)	128 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR

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	F	353/359 (98%)	346 (98%)	7 (2%)	55	78
2	E	129/139 (93%)	127 (98%)	2 (2%)	62	81
3	G	733/736 (100%)	721 (98%)	12 (2%)	62	81
4	C	506/515 (98%)	493 (97%)	13 (3%)	46	73
5	B	181/192 (94%)	177 (98%)	4 (2%)	52	76
6	I	154/154 (100%)	152 (99%)	2 (1%)	69	84
7	H	266/269 (99%)	260 (98%)	6 (2%)	50	75
8	A	89/119 (75%)	86 (97%)	3 (3%)	37	66
9	L	480/485 (99%)	467 (97%)	13 (3%)	44	72
10	M	413/418 (99%)	394 (95%)	19 (5%)	27	59
11	N	374/385 (97%)	362 (97%)	12 (3%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	79/79 (100%)	76 (96%)	3 (4%)	33 63
13	J	128/146 (88%)	124 (97%)	4 (3%)	40 69
All	All	3885/3996 (97%)	3785 (97%)	100 (3%)	49 73

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	379	PHE
10	M	310	ASP
13	J	69	PHE
9	L	440	LYS
10	M	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	845	ASN
10	M	344	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
16	FES	E	201	2	0,4,4	-	-	-		
19	LFA	H	601	-	19,19,19	0.16	0	18,18,18	0.12	0
14	SF4	B	301	5	0,12,12	-	-	-		
14	SF4	G	1002	3	0,12,12	-	-	-		
15	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.22	6 (12%)
16	FES	G	1004	3	0,4,4	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
18	3PE	C	701	-	50,50,50	0.30	0	53,55,55	0.29	0
14	SF4	I	202	6	0,12,12	-	-	-		
18	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.29	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	H	601	-	-	1/17/17/17	-
16	FES	E	201	2	-	-	0/1/1/1
14	SF4	B	301	5	-	-	0/6/5/5
14	SF4	G	1002	3	-	-	0/6/5/5
16	FES	G	1004	3	-	-	0/1/1/1
14	SF4	G	1003	3	-	-	0/6/5/5
18	3PE	C	701	-	-	11/54/54/54	-
14	SF4	I	202	6	-	-	0/6/5/5
18	3PE	L	801	-	-	6/54/54/54	-
15	FMN	F	502	-	-	9/18/18/18	0/3/3/3
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
14	SF4	I	201	6	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.70	1.37	1.30
15	F	502	FMN	C10-N1	2.29	1.37	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.18	119.77	125.64
15	F	502	FMN	C4A-C10-N10	2.86	120.66	116.48
15	F	502	FMN	C4A-C4-N3	2.64	119.89	113.19
15	F	502	FMN	O4-C4-C4A	-2.49	119.98	126.60
15	F	502	FMN	C10-C4A-N5	-2.27	120.04	124.86

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
15	F	502	FMN	C1'-C2'-C3'-C4'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P

There are no ring outliers.

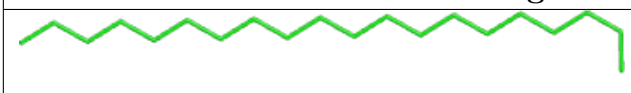
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	E	201	FES	1	0
19	H	601	LFA	1	0
14	G	1003	SF4	1	0
18	C	701	3PE	2	0
18	L	801	3PE	2	0
14	G	1001	SF4	2	0

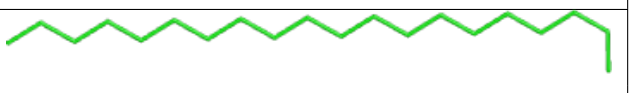
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

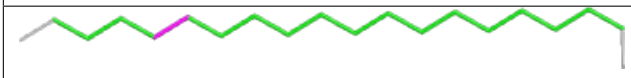
Ligand LFA H 601



Bond lengths



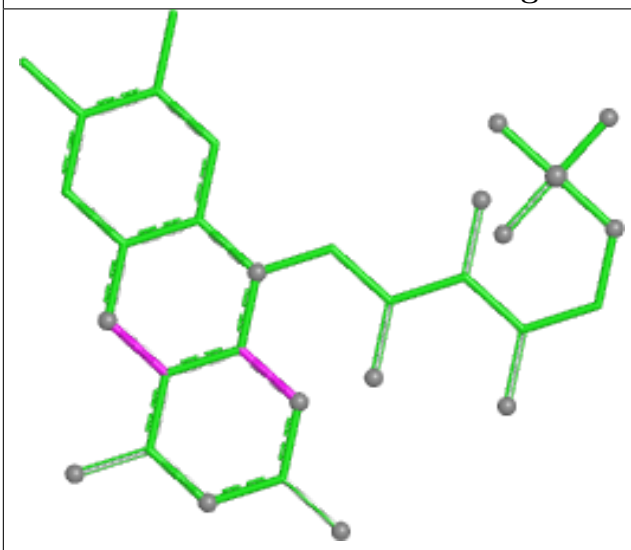
Bond angles



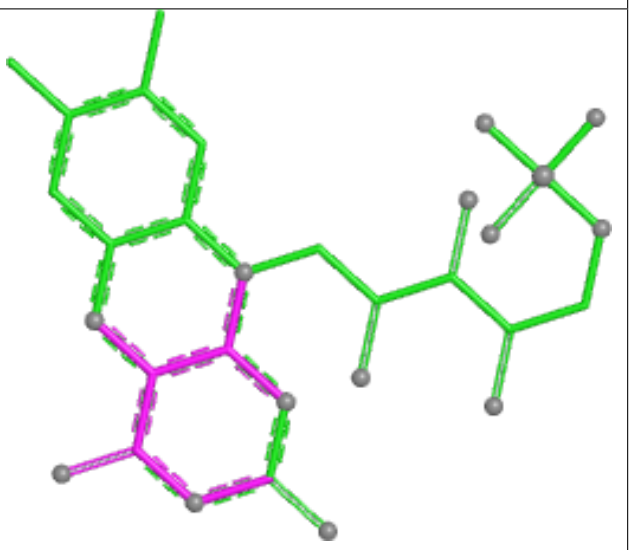
Torsions

Rings

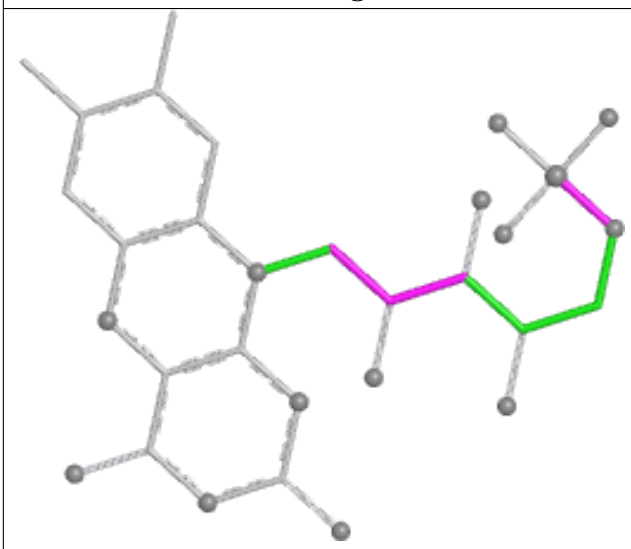
Ligand FMN F 502



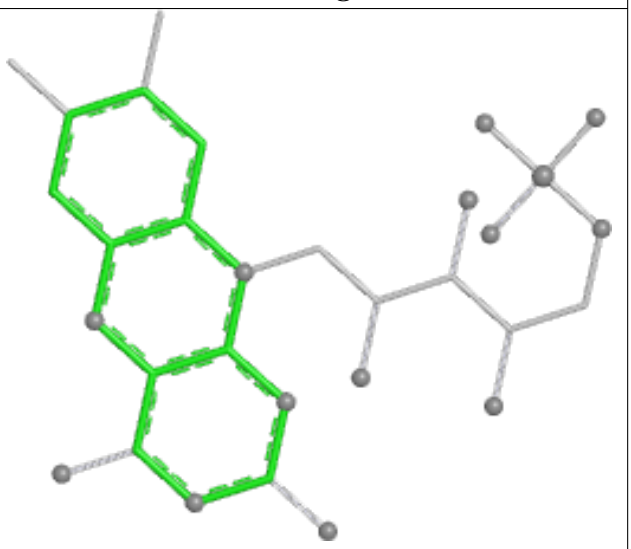
Bond lengths



Bond angles

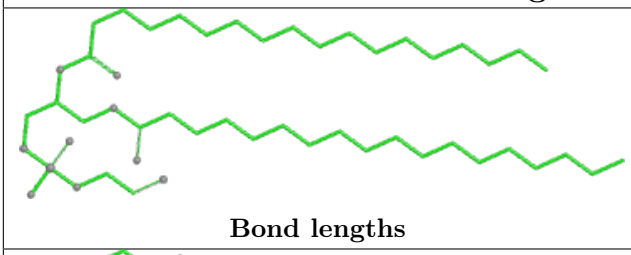


Torsions

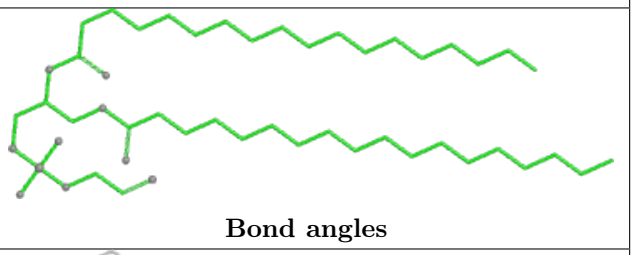


Rings

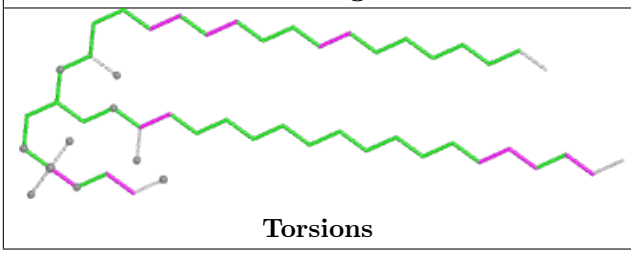
Ligand 3PE C 701



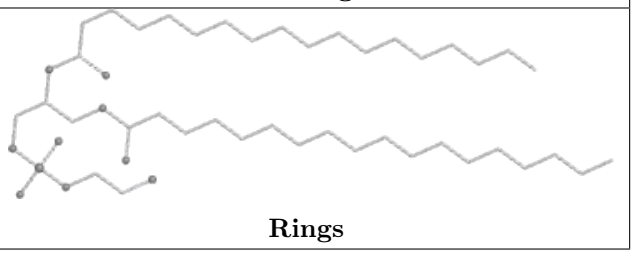
Bond lengths



Bond angles

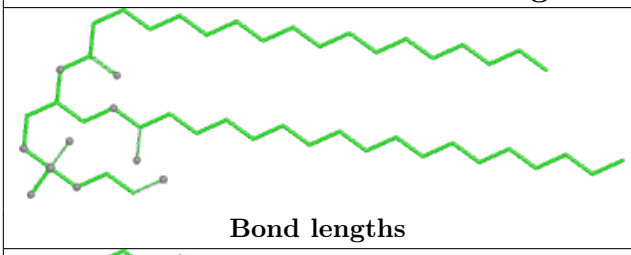


Torsions

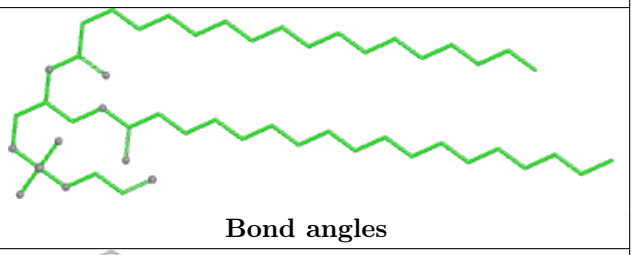


Rings

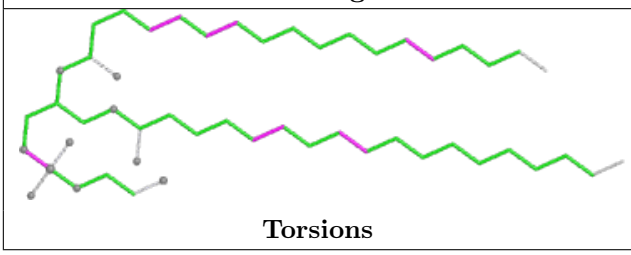
Ligand 3PE L 801



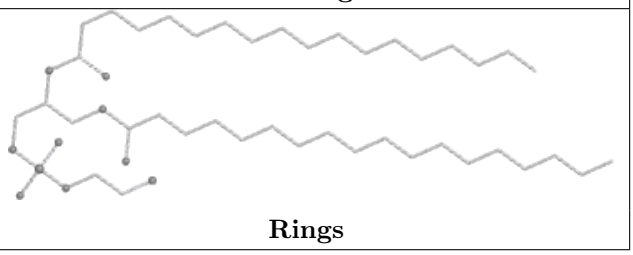
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

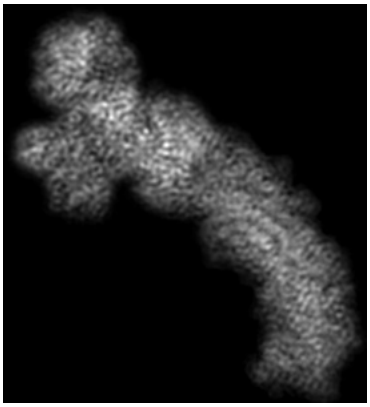
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14535. These allow visual inspection of the internal detail of the map and identification of artifacts.

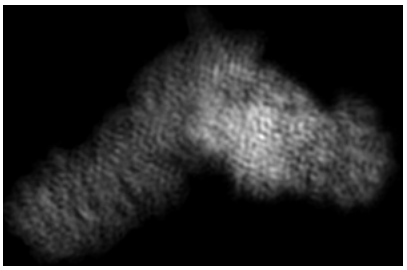
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

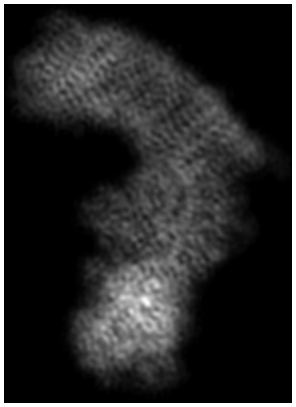
6.1.1 Primary map



X



Y

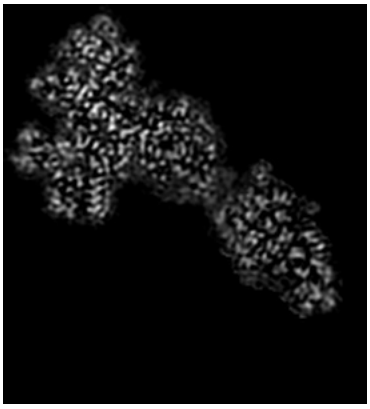


Z

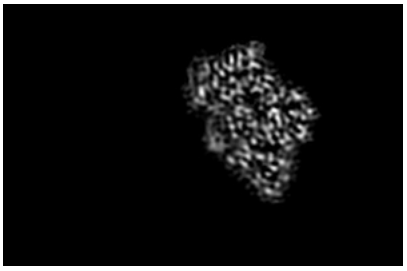
The images above show the map projected in three orthogonal directions.

6.2 Central slices

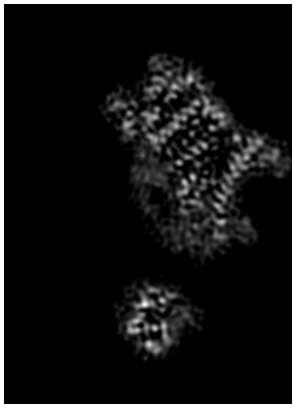
6.2.1 Primary map



X Index: 64



Y Index: 89



Z Index: 98

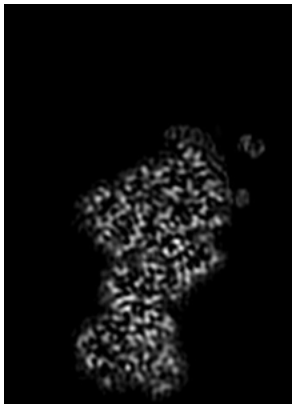
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 63

Y Index: 45



Z Index: 127

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

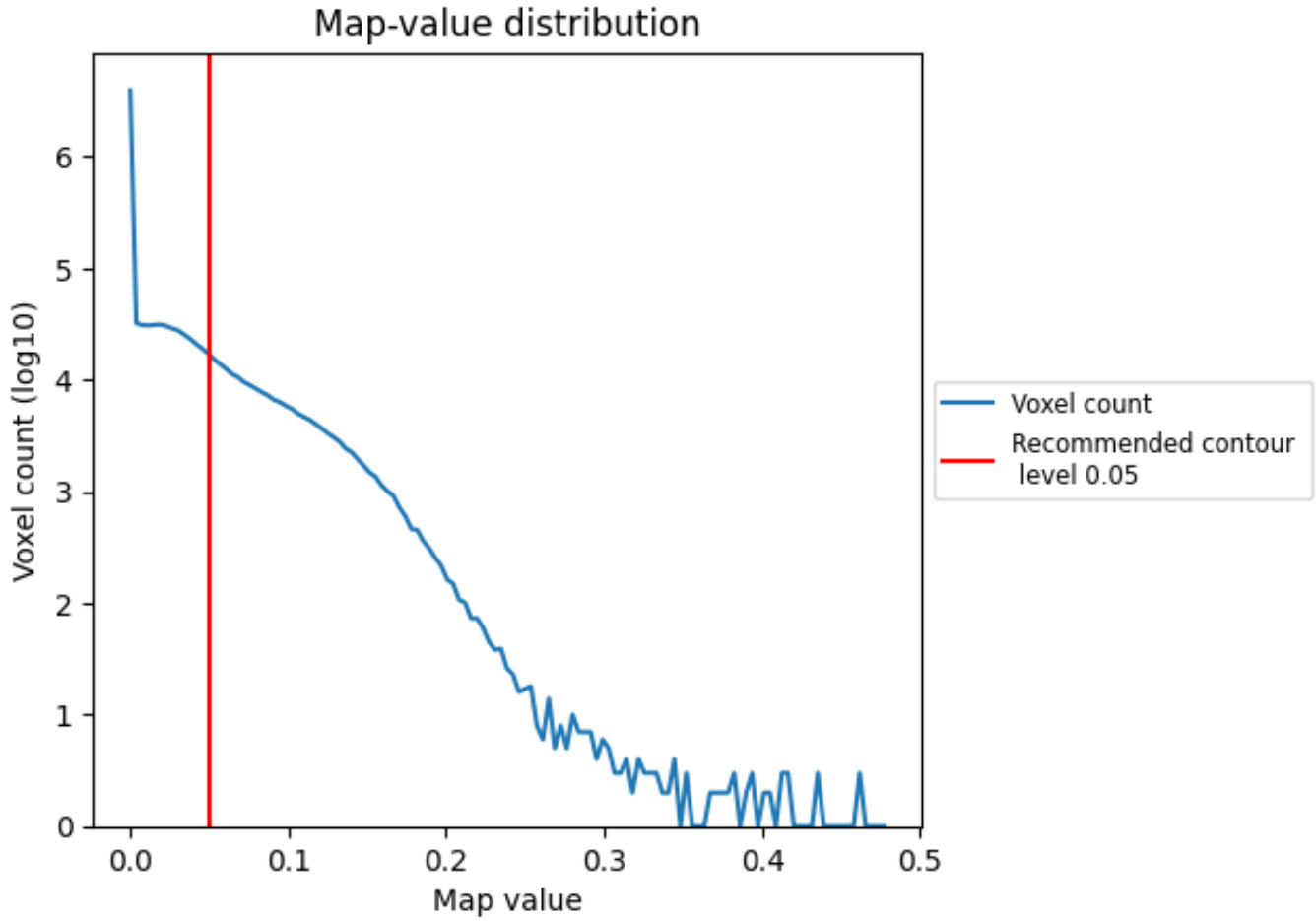
6.5 Mask visualisation (i)

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

7 Map analysis

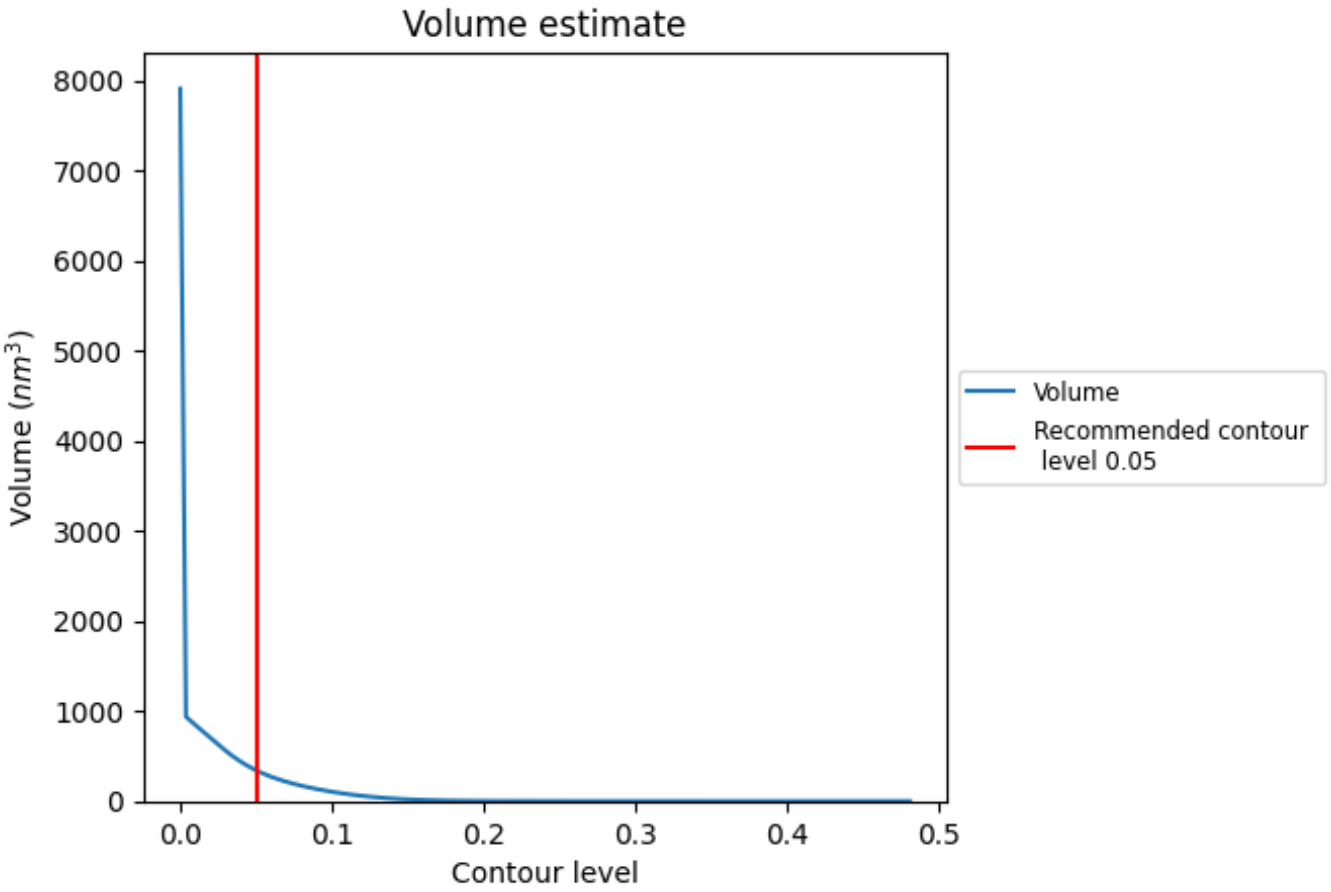
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 342 nm^3; this corresponds to an approximate mass of 309 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.

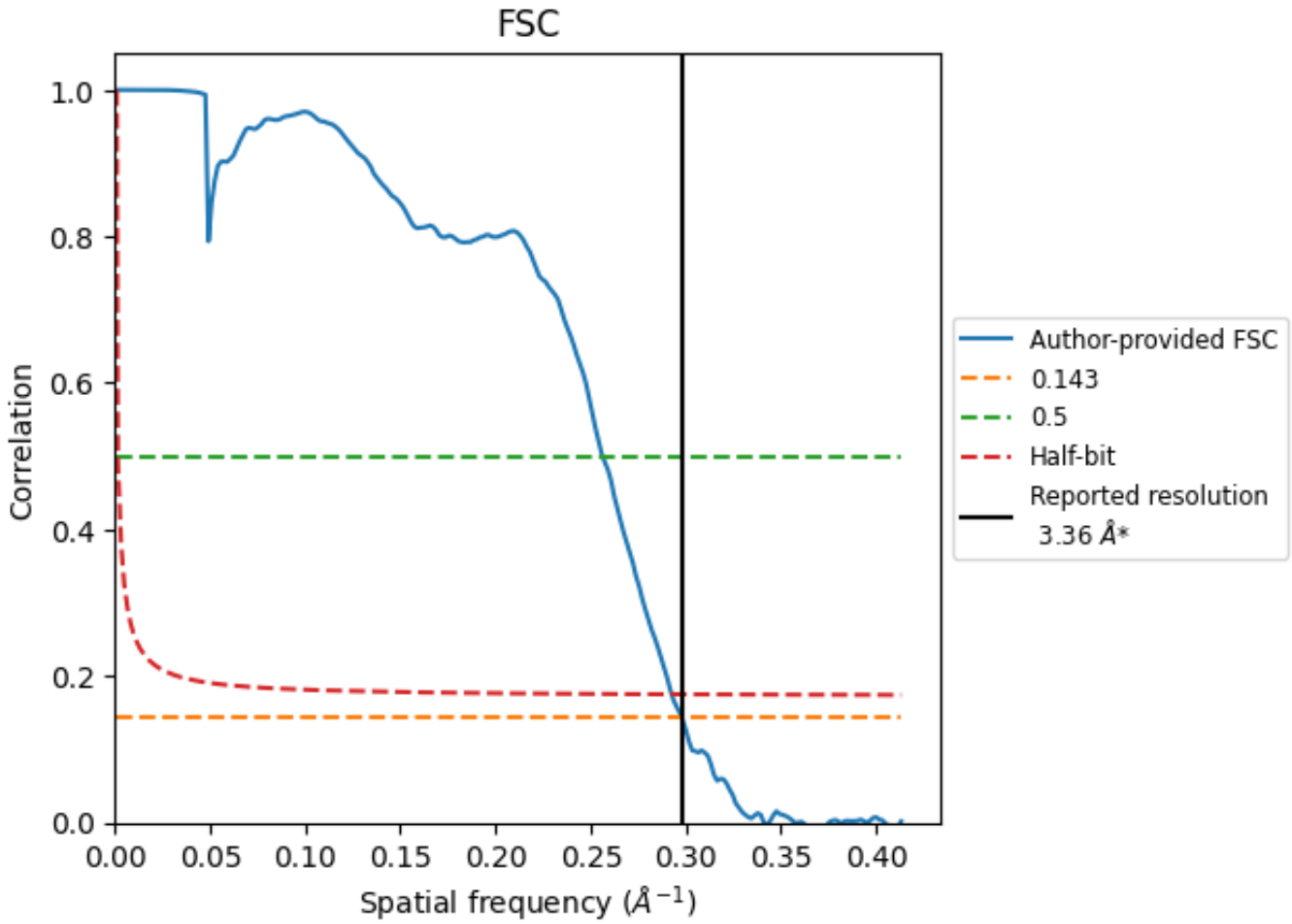
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

8.2 Resolution estimates (i)

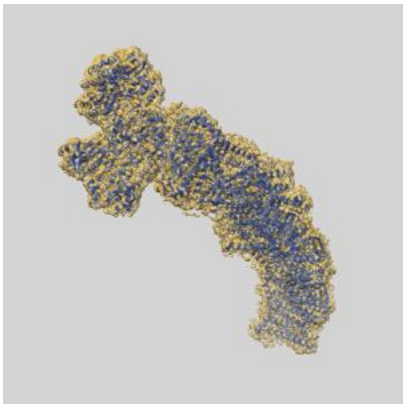
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.36	3.90	3.42
Unmasked-calculated*	-	-	-

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

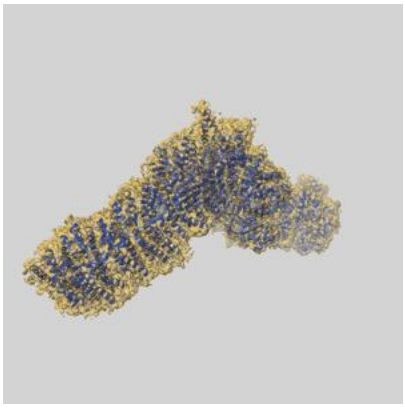
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14535 and PDB model 7Z7R. Per-residue inclusion information can be found in section 3 on page 10.

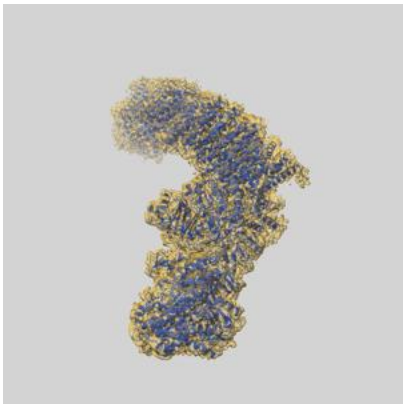
9.1 Map-model overlay



X



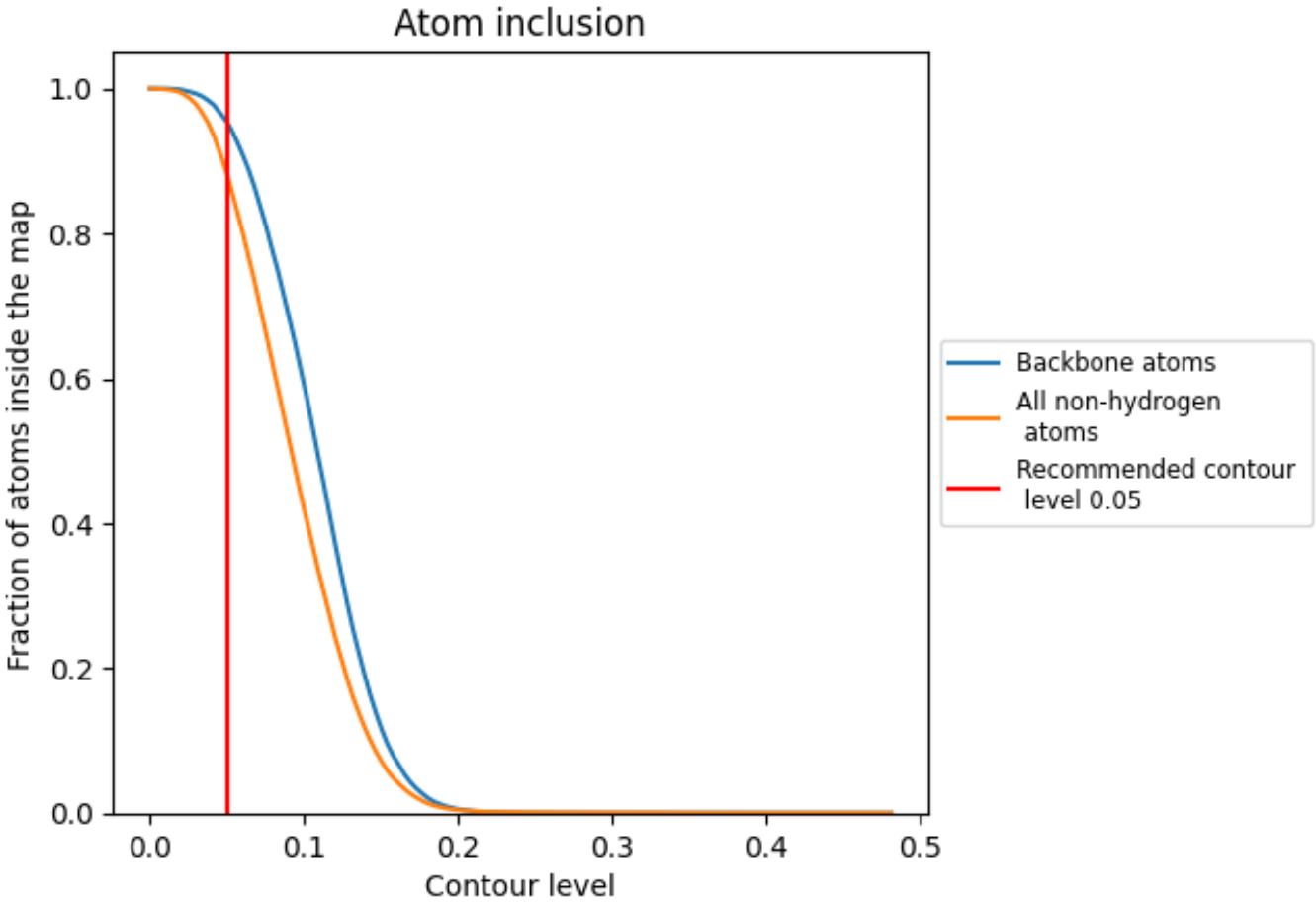
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.