



Full wwPDB EM Validation Report ⓘ

Nov 14, 2023 – 01:29 pm GMT

PDB ID : 8A1V
EMDB ID : EMD-15090
Title : Sodium pumping NADH-quinone oxidoreductase with substrate Q2
Authors : Hau, J.-L.; Kaltwasser, S.; Vonck, J.; Fritz, G.; Steuber, J.
Deposited on : 2022-06-02
Resolution : 2.73 Å (reported)
Based on initial model : 4P6V

This is a Full wwPDB EM Validation 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.dev70
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) : 2.36

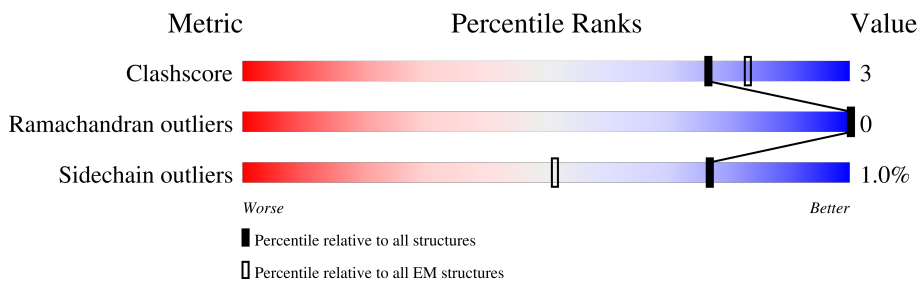
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	468	
2	B	415	
3	C	257	
4	D	210	
5	E	198	
6	F	408	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 30259 atoms, of which 14997 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 Na(+)-translocating NADH-quinone reductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	446	6877	2165	3461	584	650	17	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A655PZA5
A	-20	GLY	-	expression tag	UNP A0A655PZA5
A	-19	SER	-	expression tag	UNP A0A655PZA5
A	-18	SER	-	expression tag	UNP A0A655PZA5
A	-17	HIS	-	expression tag	UNP A0A655PZA5
A	-16	HIS	-	expression tag	UNP A0A655PZA5
A	-15	HIS	-	expression tag	UNP A0A655PZA5
A	-14	HIS	-	expression tag	UNP A0A655PZA5
A	-13	HIS	-	expression tag	UNP A0A655PZA5
A	-12	HIS	-	expression tag	UNP A0A655PZA5
A	-11	SER	-	expression tag	UNP A0A655PZA5
A	-10	SER	-	expression tag	UNP A0A655PZA5
A	-9	GLY	-	expression tag	UNP A0A655PZA5
A	-8	LEU	-	expression tag	UNP A0A655PZA5
A	-7	GLU	-	expression tag	UNP A0A655PZA5
A	-6	VAL	-	expression tag	UNP A0A655PZA5
A	-5	LEU	-	expression tag	UNP A0A655PZA5
A	-4	PHE	-	expression tag	UNP A0A655PZA5
A	-3	GLN	-	expression tag	UNP A0A655PZA5
A	-2	GLY	-	expression tag	UNP A0A655PZA5
A	-1	PRO	-	expression tag	UNP A0A655PZA5
A	0	HIS	-	expression tag	UNP A0A655PZA5

- Molecule 2 is a protein called Na(+)-translocating NADH-quinone reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	395	6063	2012	3024	494	511	22	0	0

- Molecule 3 is a protein called Na(+)-translocating NADH-quinone reductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	248	3774	1192	1892	324	362	4	0	0

- Molecule 4 is a protein called Na(+)-translocating NADH-quinone reductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	201	3154	1020	1618	243	263	10	0	0

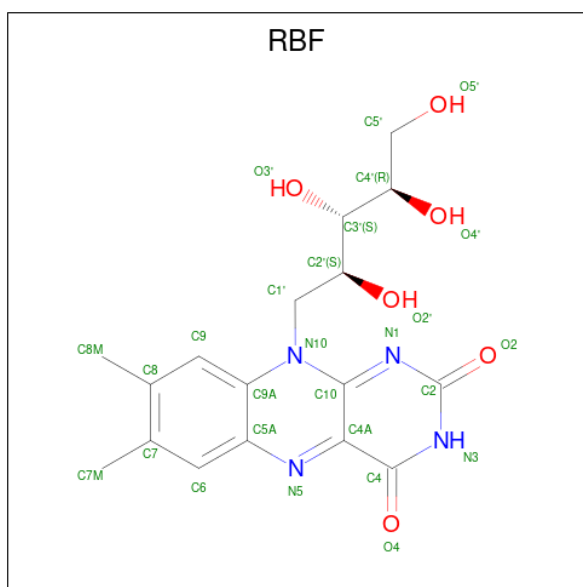
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	196	3058	1002	1563	228	255	10	0	0

- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

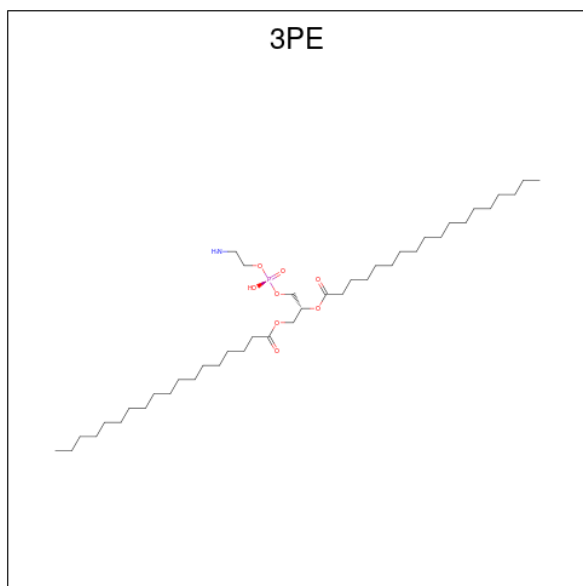
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	406	6239	2020	3086	517	593	23	0	0

- Molecule 7 is RIBOFLAVIN (three-letter code: RBF) (formula: C₁₇H₂₀N₄O₆).



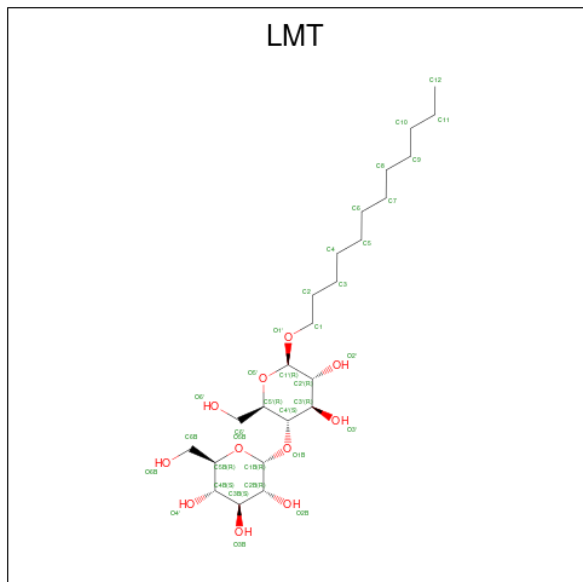
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
7	B	1	46	17	19	4	6	0

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



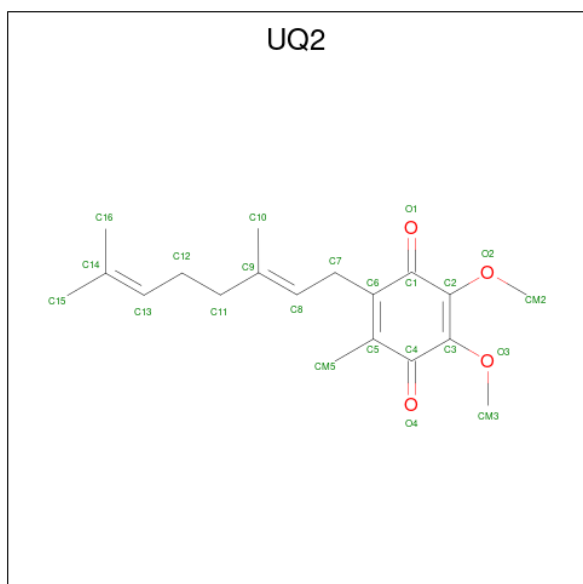
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
8	B	1	106	34	62	1	8	1	0
8	B	1	73	23	40	1	8	1	0

- Molecule 9 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



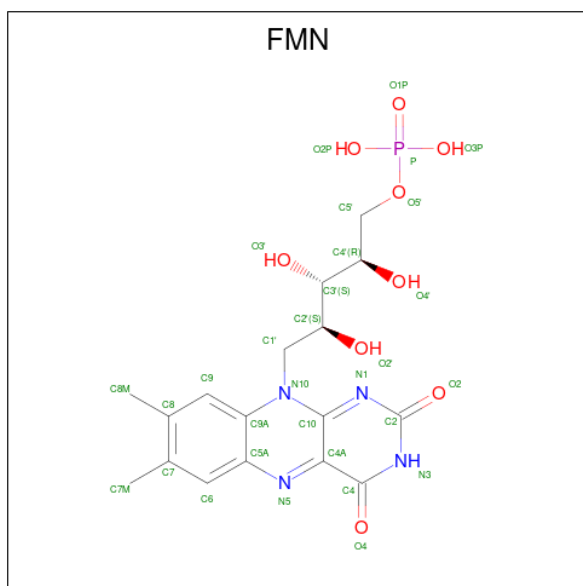
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	B	1	81	24	46	11	0
9	D	1	81	24	46	11	0
9	E	1	81	24	46	11	0

- Molecule 10 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
10	B	1	49	19	26	4	0

- Molecule 11 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

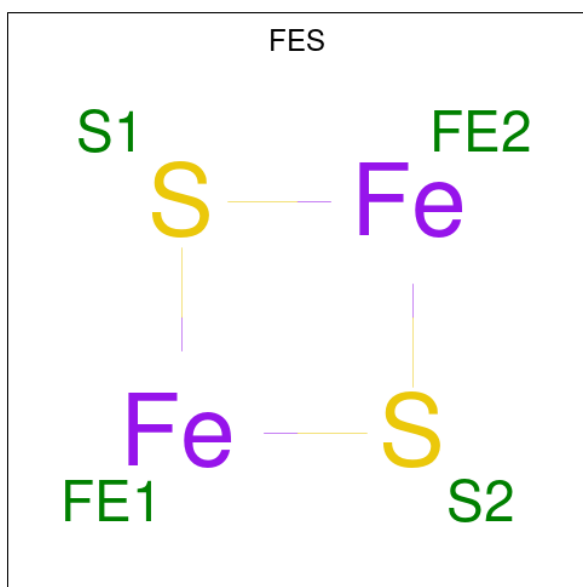


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
11	B	1	49	17	19	4	8	1	0
11	C	1	48	17	18	4	8	1	0

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

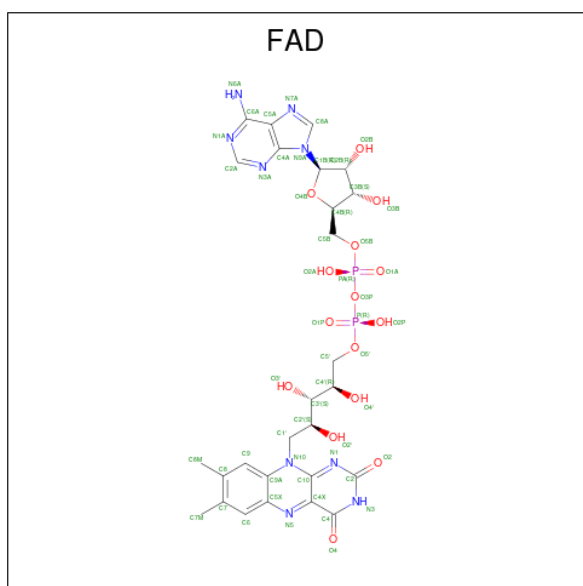
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
12	B	2	2	2	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total	Fe	S	0
			4	2	2	
13	F	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
14	F	1	Total	C	H	N	O	P	0
			84	27	31	9	15	2	

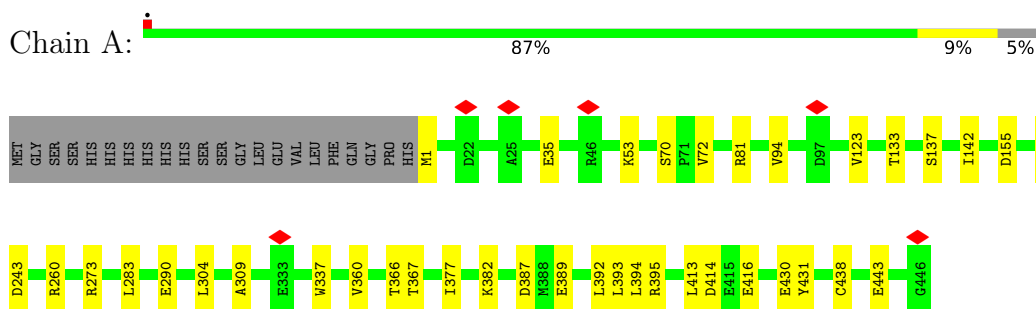
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	186	Total 186	O 186	0
15	B	140	Total 140	O 140	0
15	C	16	Total 16	O 16	0
15	D	13	Total 13	O 13	0
15	E	31	Total 31	O 31	0

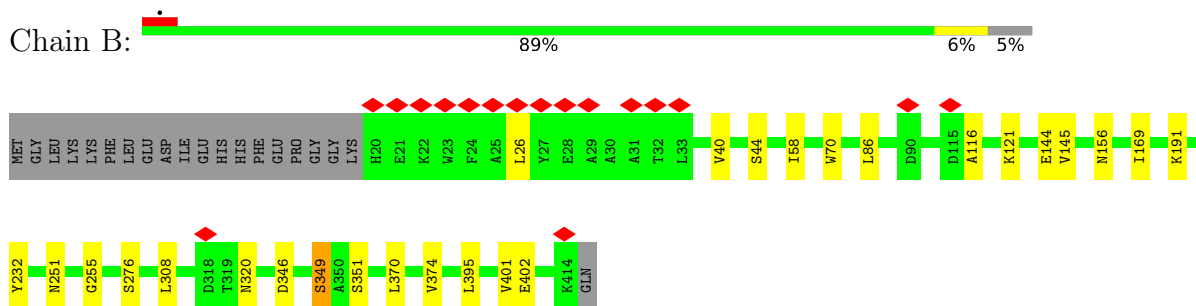
3 Residue-property plots [i](#)

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.

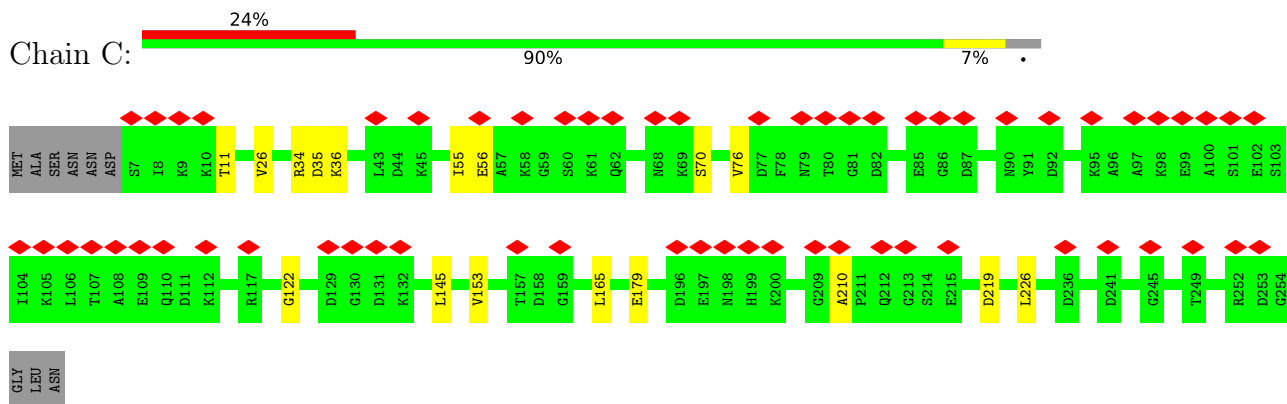
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



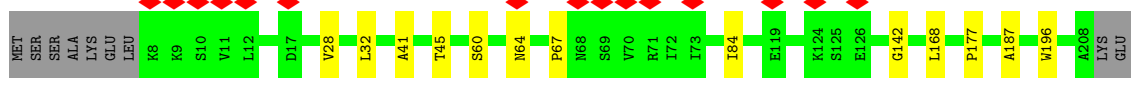
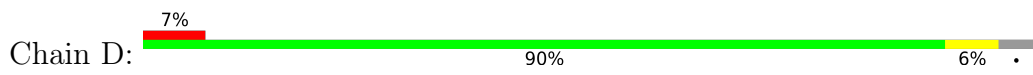
- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B



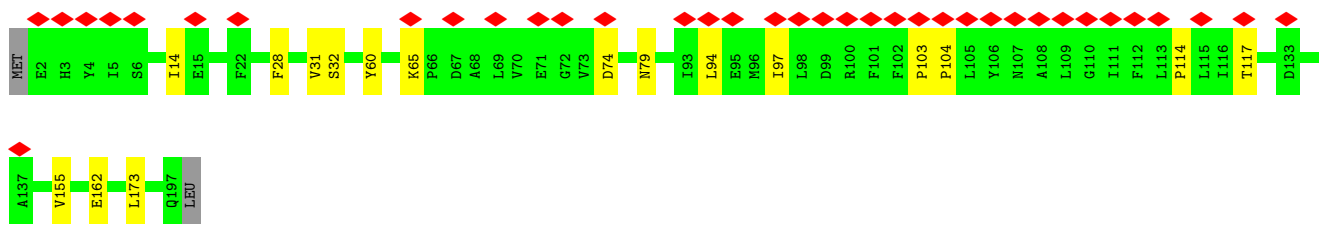
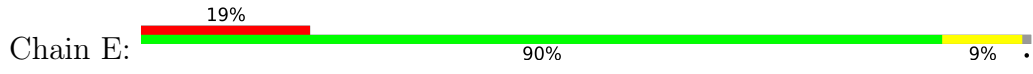
- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C



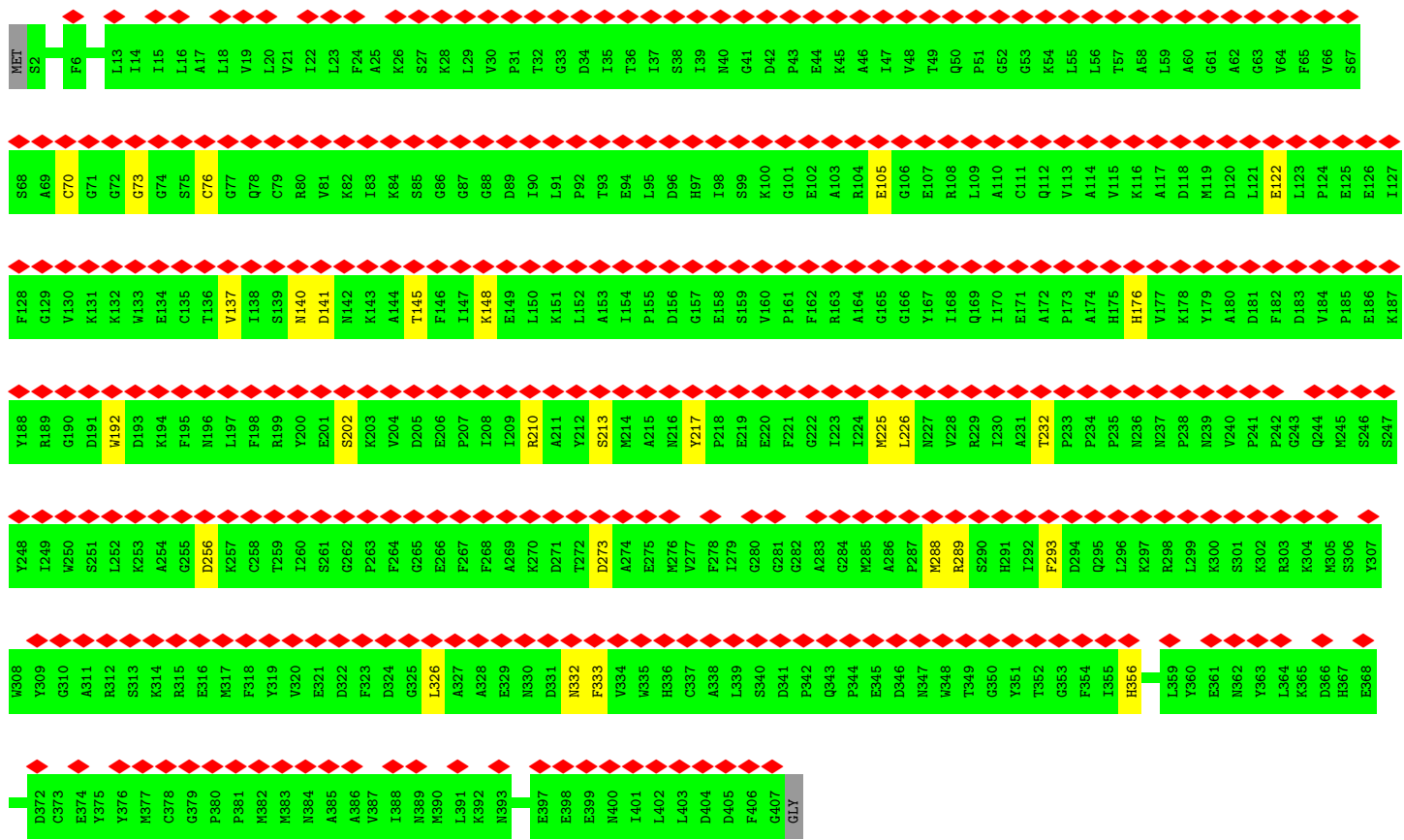
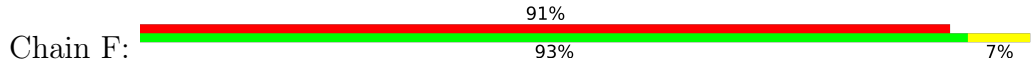
- Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D



• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



• Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226672	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	191781	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0133	Depositor
Map size (Å)	292.0, 292.0, 292.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9125, 0.9125, 0.9125	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: 3PE, FMN, NA, RBF, FAD, FES, UQ2, LMT

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	0.25	0/3480	0.48	0/4715
2	B	0.25	0/3132	0.43	0/4266
3	C	0.24	0/1914	0.43	0/2583
4	D	0.25	0/1568	0.42	0/2130
5	E	0.25	0/1528	0.41	0/2073
6	F	0.25	0/3231	0.44	0/4374
All	All	0.25	0/14853	0.44	0/20141

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	3416	3461	3463	29	0
2	B	3039	3024	3025	19	0
3	C	1882	1892	1892	11	0
4	D	1536	1618	1618	10	0
5	E	1495	1563	1563	11	0
6	F	3153	3086	3086	14	0
7	B	27	19	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	77	102	102	0	0
9	B	35	46	45	2	0
9	D	35	46	45	0	0
9	E	35	46	45	0	0
10	B	23	26	26	2	0
11	B	30	19	19	1	0
11	C	30	18	19	1	0
12	B	2	0	0	0	0
13	E	4	0	0	0	0
13	F	4	0	0	0	0
14	F	53	31	31	2	0
15	A	186	0	0	15	0
15	B	140	0	0	4	0
15	C	16	0	0	2	0
15	D	13	0	0	0	0
15	E	31	0	0	2	0
All	All	15262	14997	14999	90	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 3.

All (90) 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)
1:A:414:ASP:OD2	15:A:501:HOH:O	2.00	0.79
5:E:162:GLU:OE1	15:E:301:HOH:O	2.02	0.78
1:A:389:GLU:OE2	15:A:502:HOH:O	2.01	0.77
1:A:360:VAL:O	15:A:503:HOH:O	2.03	0.76
1:A:430:GLU:OE2	15:A:504:HOH:O	2.04	0.76
2:B:40:VAL:O	15:B:701:HOH:O	2.02	0.76
1:A:1:MET:N	15:A:513:HOH:O	2.20	0.75
1:A:366:THR:O	15:A:506:HOH:O	2.05	0.74
1:A:243:ASP:OD2	15:A:505:HOH:O	2.04	0.74
1:A:81:ARG:NH1	15:A:512:HOH:O	2.19	0.73
9:B:603:LMT:O3'	9:B:603:LMT:O5B	2.07	0.72
2:B:402:GLU:OE1	15:B:702:HOH:O	2.07	0.71
1:A:416:GLU:OE1	15:A:507:HOH:O	2.09	0.70
1:A:377:ILE:O	15:A:508:HOH:O	2.11	0.68
2:B:346:ASP:OD2	2:B:349:SER:OG	2.11	0.67
2:B:156:ASN:OD1	15:B:703:HOH:O	2.12	0.67
3:C:210:ALA:N	3:C:219:ASP:OD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:LEU:HD23	4:D:187:ALA:HB3	1.78	0.66
1:A:387:ASP:OD1	15:A:509:HOH:O	2.15	0.65
3:C:179:GLU:OE2	15:C:1101:HOH:O	2.14	0.63
1:A:367:THR:OG1	15:A:510:HOH:O	2.16	0.62
2:B:144:GLU:OE2	2:B:191:LYS:NZ	2.26	0.62
3:C:34:ARG:NH1	5:E:74:ASP:OD1	2.33	0.61
6:F:293:PHE:CE1	6:F:326:LEU:HD11	2.36	0.60
1:A:382:LYS:NZ	15:A:517:HOH:O	2.29	0.59
3:C:56:GLU:OE1	3:C:56:GLU:N	2.35	0.59
1:A:260:ARG:NH2	15:A:521:HOH:O	2.34	0.58
2:B:320:ASN:OD1	15:B:704:HOH:O	2.17	0.58
2:B:251:ASN:O	2:B:255:GLY:N	2.37	0.57
4:D:196:TRP:HB2	5:E:173:LEU:HD13	1.86	0.57
1:A:337:TRP:HZ3	2:B:58:ILE:HG21	1.70	0.56
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.88	0.55
4:D:32:LEU:HD23	4:D:187:ALA:CB	2.37	0.55
2:B:26:LEU:HD13	2:B:145:VAL:HG13	1.90	0.54
5:E:28:PHE:O	5:E:32:SER:OG	2.17	0.54
1:A:337:TRP:CZ3	2:B:58:ILE:HG21	2.44	0.53
6:F:140:ASN:O	6:F:148:LYS:NZ	2.25	0.53
1:A:123:VAL:HG21	1:A:142:ILE:HD12	1.90	0.53
4:D:41:ALA:O	4:D:45:THR:HG23	2.09	0.53
5:E:31:VAL:HG12	5:E:31:VAL:O	2.09	0.52
1:A:392:LEU:HD13	2:B:401:VAL:HG11	1.90	0.52
6:F:70:CYS:SG	6:F:73:GLY:N	2.83	0.51
3:C:35:ASP:OD1	3:C:36:LYS:N	2.43	0.51
2:B:116:ALA:O	2:B:121:LYS:NZ	2.45	0.50
1:A:394:LEU:HD22	1:A:431:TYR:CD1	2.47	0.50
1:A:194:LYS:NZ	15:A:533:HOH:O	2.46	0.49
5:E:60:TYR:O	5:E:65:LYS:N	2.47	0.48
6:F:225:MET:O	6:F:226:LEU:HD12	2.13	0.48
1:A:133:THR:O	1:A:137:SER:N	2.45	0.48
6:F:105:GLU:N	6:F:105:GLU:OE1	2.47	0.48
1:A:123:VAL:CG2	1:A:142:ILE:HD12	2.44	0.48
6:F:145:THR:O	6:F:192:TRP:NE1	2.46	0.48
3:C:26:VAL:HG13	4:D:84:ILE:HG21	1.97	0.47
5:E:14:ILE:O	15:E:302:HOH:O	2.20	0.46
6:F:232:THR:O	14:F:1501:FAD:O3B	2.32	0.46
3:C:76:VAL:N	3:C:122:GLY:O	2.48	0.46
3:C:153:VAL:HG22	3:C:165:LEU:HD13	1.98	0.45
5:E:94:LEU:HD23	5:E:97:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:1000:FMN:H6	15:C:1107:HOH:O	2.16	0.45
1:A:394:LEU:HD22	1:A:431:TYR:CG	2.52	0.45
6:F:332:ASN:OD1	6:F:333:PHE:N	2.50	0.45
1:A:53:LYS:O	1:A:70:SER:O	2.36	0.44
3:C:11:THR:HG22	4:D:67:PRO:HB3	1.99	0.44
2:B:370:LEU:O	2:B:374:VAL:HG22	2.18	0.44
1:A:273:ARG:NH2	1:A:290:GLU:OE2	2.41	0.44
6:F:176:HIS:ND1	6:F:202:SER:O	2.51	0.44
1:A:283:LEU:HD12	1:A:309:ALA:CB	2.49	0.43
4:D:168:LEU:HD22	4:D:177:PRO:HG3	2.00	0.43
5:E:114:PRO:O	5:E:117:THR:OG1	2.30	0.43
2:B:395:LEU:HD11	5:E:155:VAL:HG12	2.01	0.43
3:C:55:ILE:HD13	3:C:70:SER:OG	2.19	0.43
3:C:145:LEU:HD13	3:C:226:LEU:HD13	2.00	0.43
2:B:308:LEU:HD21	2:B:370:LEU:CD2	2.50	0.42
6:F:273:ASP:OD1	6:F:273:ASP:N	2.52	0.42
10:B:605:UQ2:H3M3	10:B:605:UQ2:H2M2	2.01	0.42
4:D:28:VAL:HG12	4:D:32:LEU:HD12	2.01	0.41
6:F:122:GLU:O	6:F:122:GLU:CG	2.68	0.41
2:B:169:ILE:HG22	11:B:606:FMN:HM83	2.03	0.41
4:D:45:THR:HG21	4:D:142:GLY:HA2	2.01	0.41
4:D:64:ASN:OD1	4:D:64:ASN:N	2.53	0.41
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.55	0.41
2:B:86:LEU:HD11	2:B:232:TYR:HA	2.02	0.41
5:E:103:PRO:N	5:E:104:PRO:HD2	2.36	0.41
6:F:141:ASP:N	6:F:141:ASP:OD1	2.54	0.41
1:A:393:LEU:HD21	1:A:413:LEU:HD11	2.03	0.41
1:A:304:LEU:O	2:B:44:SER:OG	2.29	0.40
10:B:605:UQ2:H5M1	10:B:605:UQ2:H72	1.84	0.40
6:F:210:ARG:NH2	14:F:1501:FAD:O1P	2.53	0.40
9:B:603:LMT:O5B	9:B:603:LMT:C3'	2.70	0.40
6:F:137:VAL:N	6:F:256:ASP:O	2.44	0.40

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	444/468 (95%)	436 (98%)	8 (2%)	0	100	100
2	B	393/415 (95%)	385 (98%)	8 (2%)	0	100	100
3	C	246/257 (96%)	244 (99%)	2 (1%)	0	100	100
4	D	199/210 (95%)	191 (96%)	8 (4%)	0	100	100
5	E	194/198 (98%)	192 (99%)	2 (1%)	0	100	100
6	F	404/408 (99%)	400 (99%)	4 (1%)	0	100	100
All	All	1880/1956 (96%)	1848 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	376/395 (95%)	370 (98%)	6 (2%)	62	78
2	B	303/320 (95%)	301 (99%)	2 (1%)	84	90
3	C	198/205 (97%)	198 (100%)	0	100	100
4	D	168/176 (96%)	167 (99%)	1 (1%)	86	91
5	E	163/165 (99%)	162 (99%)	1 (1%)	86	91
6	F	336/337 (100%)	330 (98%)	6 (2%)	59	75
All	All	1544/1598 (97%)	1528 (99%)	16 (1%)	77	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	155	ASP
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	395	ARG
1	A	438	CYS
1	A	443	GLU
2	B	349	SER
2	B	351	SER
4	D	60	SER
5	E	79	ASN
6	F	76	CYS
6	F	213	SER
6	F	217	TYR
6	F	288	MET
6	F	289	ARG
6	F	356	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	252	ASN
4	D	176	GLN
6	F	244	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, 2 are 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
9	LMT	D	301	-	36,36,36	1.17	5 (13%)	47,47,47	1.02	3 (6%)
10	UQ2	B	605	-	23,23,23	0.54	0	28,31,31	0.64	0
11	FMN	C	1000	3	29,32,33	1.11	2 (6%)	40,47,50	1.31	7 (17%)
8	3PE	B	602	-	43,43,50	0.54	0	46,48,55	0.61	2 (4%)
7	RBF	B	601	-	29,29,29	0.59	0	41,43,43	0.69	1 (2%)
11	FMN	B	606	2	29,32,33	1.10	2 (6%)	40,47,50	1.34	8 (20%)
13	FES	F	1502	6	0,4,4	-	-	-	-	-
9	LMT	B	603	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	2 (4%)
8	3PE	B	604	-	32,32,50	0.63	0	35,37,55	0.60	1 (2%)
9	LMT	E	201	-	36,36,36	1.17	6 (16%)	47,47,47	0.94	2 (4%)
14	FAD	F	1501	-	53,58,58	0.46	0	68,89,89	0.52	2 (2%)
13	FES	E	202	5,4	0,4,4	-	-	-	-	-

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
9	LMT	D	301	-	-	10/21/61/61	0/2/2/2
10	UQ2	B	605	-	-	7/15/39/39	0/1/1/1
11	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
8	3PE	B	602	-	-	23/47/47/54	-
7	RBF	B	601	-	-	0/14/14/14	0/3/3/3
11	FMN	B	606	2	-	3/15/17/18	0/3/3/3
13	FES	F	1502	6	-	-	0/1/1/1
9	LMT	B	603	-	-	10/21/61/61	0/2/2/2
8	3PE	B	604	-	-	8/36/36/54	-
9	LMT	E	201	-	-	13/21/61/61	0/2/2/2
14	FAD	F	1501	-	-	10/30/50/50	0/6/6/6
13	FES	E	202	5,4	-	-	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1000	FMN	C4A-N5	3.68	1.37	1.30
11	B	606	FMN	C4A-N5	3.58	1.37	1.30
9	B	603	LMT	O3'-C3'	-2.84	1.36	1.43
9	D	301	LMT	O3'-C3'	-2.71	1.36	1.43
9	E	201	LMT	O3'-C3'	-2.71	1.36	1.43
11	C	1000	FMN	C10-N1	2.58	1.38	1.33
11	B	606	FMN	C10-N1	2.52	1.38	1.33
9	B	603	LMT	O2B-C2B	-2.49	1.37	1.43
9	D	301	LMT	O2'-C2'	-2.41	1.37	1.43
9	B	603	LMT	O2'-C2'	-2.38	1.37	1.43
9	D	301	LMT	O2B-C2B	-2.32	1.37	1.43
9	E	201	LMT	O2B-C2B	-2.31	1.37	1.43
9	E	201	LMT	O3B-C3B	-2.30	1.37	1.43
9	E	201	LMT	O2'-C2'	-2.28	1.37	1.43
9	D	301	LMT	O3B-C3B	-2.26	1.37	1.43
9	B	603	LMT	O3B-C3B	-2.24	1.37	1.43
9	D	301	LMT	O4'-C4B	-2.13	1.38	1.43
9	E	201	LMT	O4'-C4B	-2.09	1.38	1.43
9	B	603	LMT	O4'-C4B	-2.07	1.38	1.43
9	E	201	LMT	O1'-C1'	-2.06	1.36	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1000	FMN	C4-N3-C2	-3.20	119.73	125.64
11	B	606	FMN	C4-N3-C2	-3.07	119.97	125.64
11	C	1000	FMN	C4A-C10-N10	2.95	120.79	116.48
9	D	301	LMT	C3'-C4'-C5'	-2.80	104.50	110.93
11	C	1000	FMN	C4A-C4-N3	2.70	120.04	113.19
14	F	1501	FAD	P-O3P-PA	-2.59	123.95	132.83
11	B	606	FMN	C10-C4A-N5	-2.57	119.40	124.86
11	B	606	FMN	C4A-C4-N3	2.57	119.71	113.19
11	B	606	FMN	C4A-C10-N10	2.52	120.17	116.48
9	B	603	LMT	C3'-C4'-C5'	-2.48	105.25	110.93
9	E	201	LMT	C3'-C4'-C5'	-2.42	105.38	110.93
11	C	1000	FMN	C4A-C10-N1	-2.42	119.12	124.73
9	B	603	LMT	C1'-O5'-C5'	-2.40	108.98	113.69
11	B	606	FMN	C4A-C10-N1	-2.35	119.27	124.73
11	C	1000	FMN	O4-C4-C4A	-2.35	120.37	126.60
8	B	604	3PE	O12-P-O14	2.32	123.73	112.24
11	B	606	FMN	O4-C4-C4A	-2.30	120.49	126.60
9	D	301	LMT	O5B-C5B-C4B	2.29	113.85	109.69
11	C	1000	FMN	C10-C4A-N5	-2.27	120.03	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	1501	FAD	C5A-C6A-N6A	2.27	123.80	120.35
9	D	301	LMT	C1'-O5'-C5'	-2.27	109.24	113.69
11	B	606	FMN	C9A-C5A-N5	-2.25	119.99	122.43
8	B	602	3PE	O12-P-O14	2.25	123.35	112.24
9	E	201	LMT	C1'-O5'-C5'	-2.20	109.37	113.69
8	B	602	3PE	C2-O21-C21	2.11	122.99	117.79
11	B	606	FMN	C4-C4A-C10	2.10	120.32	116.79
11	C	1000	FMN	C4-C4A-C10	2.01	120.17	116.79
7	B	601	RBF	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	602	3PE	C1-O11-P-O12
8	B	604	3PE	C1-O11-P-O14
8	B	604	3PE	O13-C11-C12-N
9	B	603	LMT	C2'-C1'-O1'-C1
9	B	603	LMT	O5'-C1'-O1'-C1
9	D	301	LMT	O5'-C1'-O1'-C1
9	D	301	LMT	C2-C1-O1'-C1'
9	E	201	LMT	C2'-C1'-O1'-C1
9	E	201	LMT	O5'-C1'-O1'-C1
10	B	605	UQ2	C12-C11-C9-C8
10	B	605	UQ2	C12-C11-C9-C10
11	B	606	FMN	C3'-C4'-C5'-O5'
11	B	606	FMN	O4'-C4'-C5'-O5'
14	F	1501	FAD	C5B-O5B-PA-O3P
14	F	1501	FAD	N10-C1'-C2'-O2'
14	F	1501	FAD	N10-C1'-C2'-C3'
14	F	1501	FAD	C5'-O5'-P-O1P
14	F	1501	FAD	C5'-O5'-P-O2P
14	F	1501	FAD	C5'-O5'-P-O3P
9	B	603	LMT	C2B-C1B-O1B-C4'
9	E	201	LMT	O5'-C5'-C6'-O6'
9	B	603	LMT	C4'-C5'-C6'-O6'
9	E	201	LMT	O5B-C5B-C6B-O6B
9	E	201	LMT	C4'-C5'-C6'-O6'
9	B	603	LMT	C5'-C4'-O1B-C1B
9	B	603	LMT	O5'-C5'-C6'-O6'
9	D	301	LMT	C2'-C1'-O1'-C1
9	E	201	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	F	1501	FAD	O4B-C4B-C5B-O5B
14	F	1501	FAD	C3B-C4B-C5B-O5B
9	D	301	LMT	C5'-C4'-O1B-C1B
8	B	602	3PE	C1-O11-P-O13
8	B	602	3PE	C11-O13-P-O11
8	B	602	3PE	C32-C31-O31-C3
8	B	602	3PE	C32-C33-C34-C35
9	E	201	LMT	C11-C10-C9-C8
8	B	602	3PE	C39-C3A-C3B-C3C
9	E	201	LMT	C2-C3-C4-C5
9	B	603	LMT	O5B-C1B-O1B-C4'
9	E	201	LMT	C4B-C5B-C6B-O6B
8	B	602	3PE	O32-C31-O31-C3
8	B	602	3PE	C29-C2A-C2B-C2C
9	B	603	LMT	C3'-C4'-O1B-C1B
9	E	201	LMT	C4-C5-C6-C7
9	B	603	LMT	C6-C7-C8-C9
9	D	301	LMT	O5'-C5'-C6'-O6'
9	D	301	LMT	C3'-C4'-O1B-C1B
8	B	602	3PE	C22-C21-O21-C2
8	B	602	3PE	O11-C1-C2-C3
8	B	602	3PE	C21-C22-C23-C24
8	B	602	3PE	C34-C35-C36-C37
8	B	602	3PE	C26-C27-C28-C29
9	E	201	LMT	C5'-C4'-O1B-C1B
8	B	602	3PE	O22-C21-O21-C2
8	B	602	3PE	C24-C25-C26-C27
8	B	602	3PE	O11-C1-C2-O21
8	B	602	3PE	C27-C28-C29-C2A
9	B	603	LMT	C11-C10-C9-C8
8	B	604	3PE	C1-O11-P-O13
8	B	602	3PE	C1-O11-P-O14
8	B	602	3PE	C11-O13-P-O14
14	F	1501	FAD	C5B-O5B-PA-O2A
8	B	604	3PE	C12-C11-O13-P
8	B	604	3PE	O11-C1-C2-O21
10	B	605	UQ2	C4-C3-O3-CM3
8	B	604	3PE	O11-C1-C2-C3
11	B	606	FMN	C4'-C5'-O5'-P
8	B	602	3PE	C3-C2-O21-C21
10	B	605	UQ2	C2-C3-O3-CM3
8	B	602	3PE	C25-C26-C27-C28

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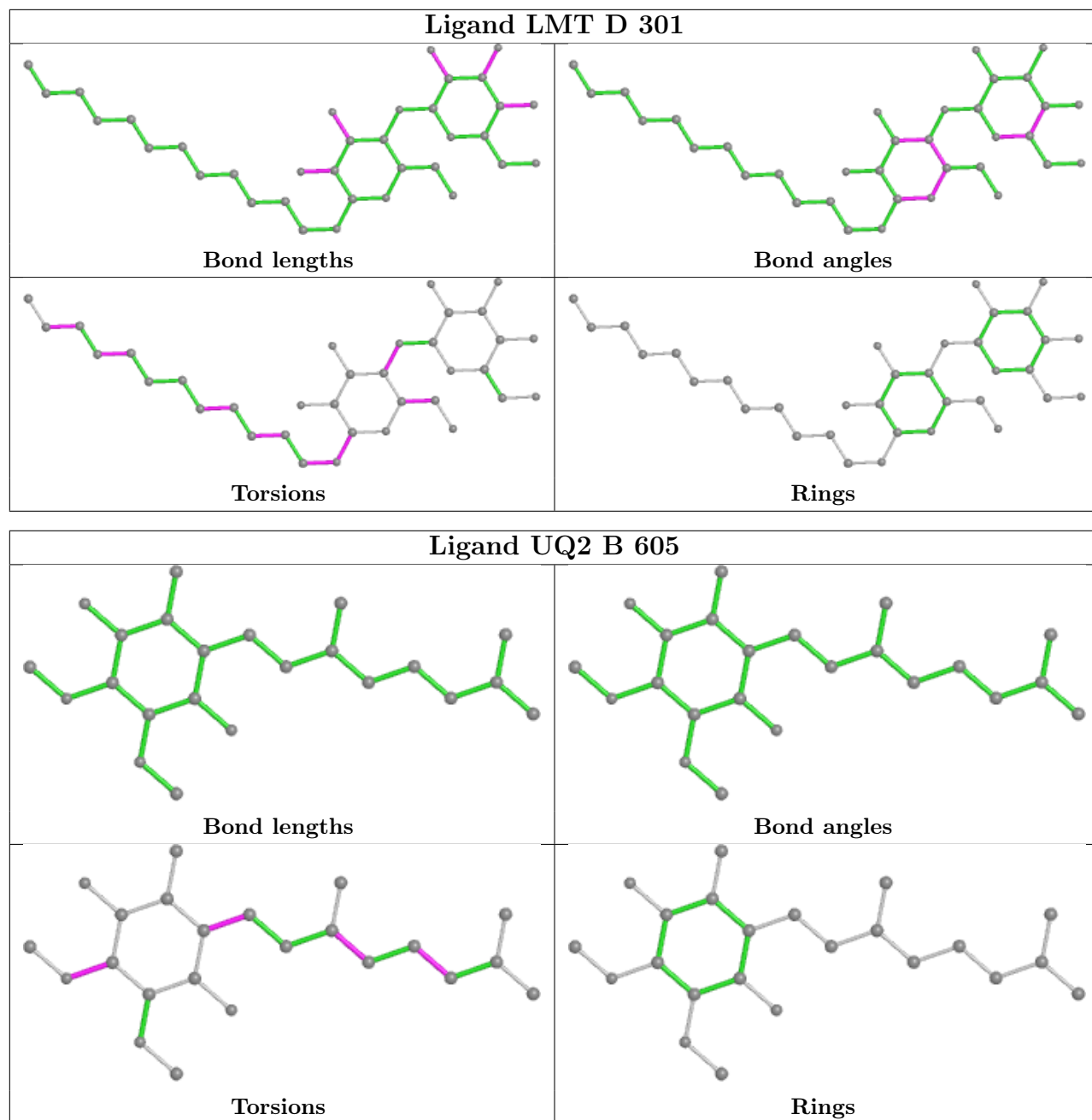
Mol	Chain	Res	Type	Atoms
9	E	201	LMT	C3'-C4'-O1B-C1B
8	B	604	3PE	C23-C24-C25-C26
9	D	301	LMT	C9-C10-C11-C12
10	B	605	UQ2	C5-C6-C7-C8
9	D	301	LMT	C1-C2-C3-C4
10	B	605	UQ2	C1-C6-C7-C8
8	B	602	3PE	C1-C2-O21-C21
10	B	605	UQ2	C11-C12-C13-C14
14	F	1501	FAD	PA-O3P-P-O2P
8	B	602	3PE	C3C-C3D-C3E-C3F
8	B	604	3PE	C35-C36-C37-C38
9	D	301	LMT	C7-C8-C9-C10
9	E	201	LMT	C6-C7-C8-C9
9	D	301	LMT	C3-C4-C5-C6

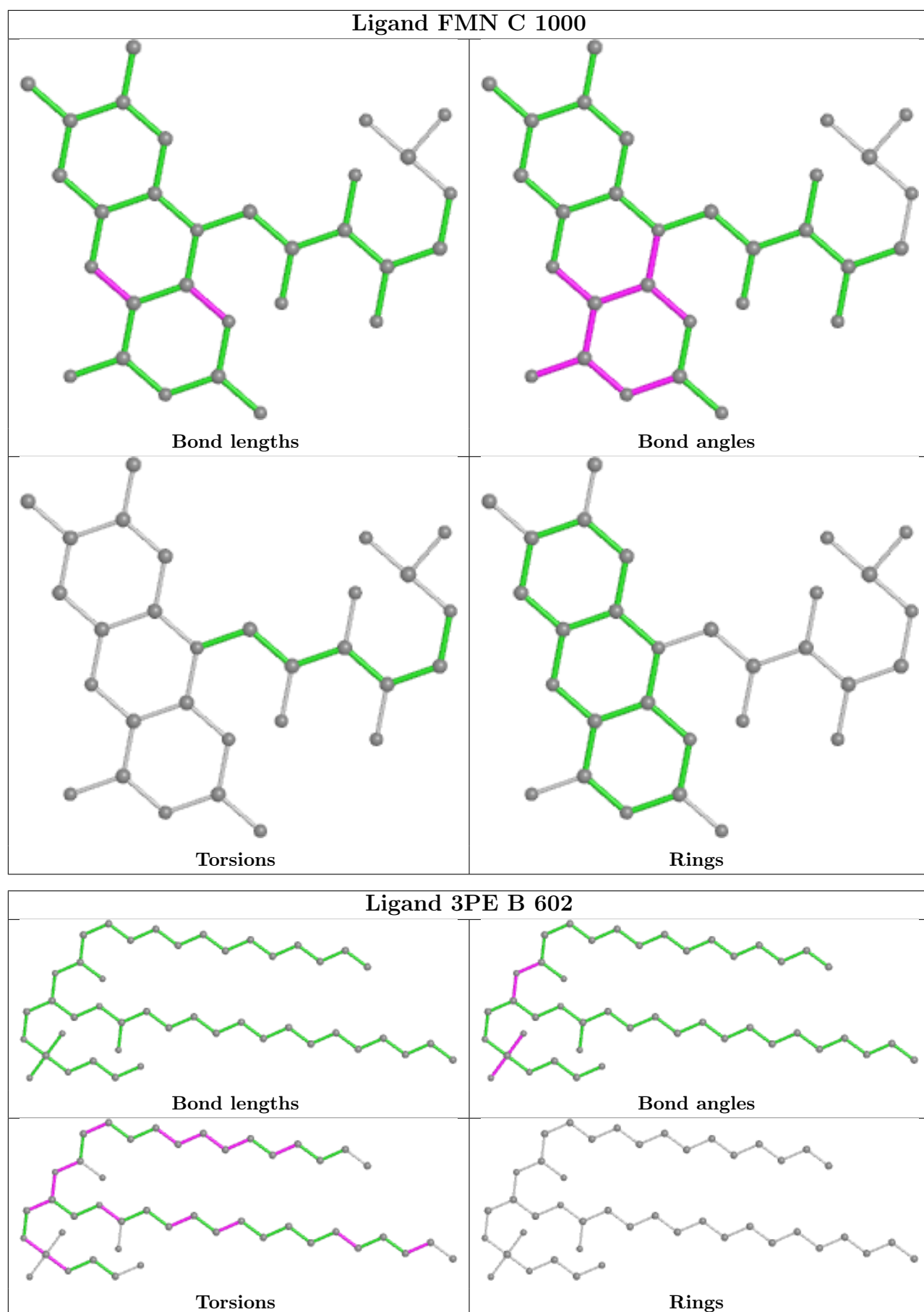
There are no ring outliers.

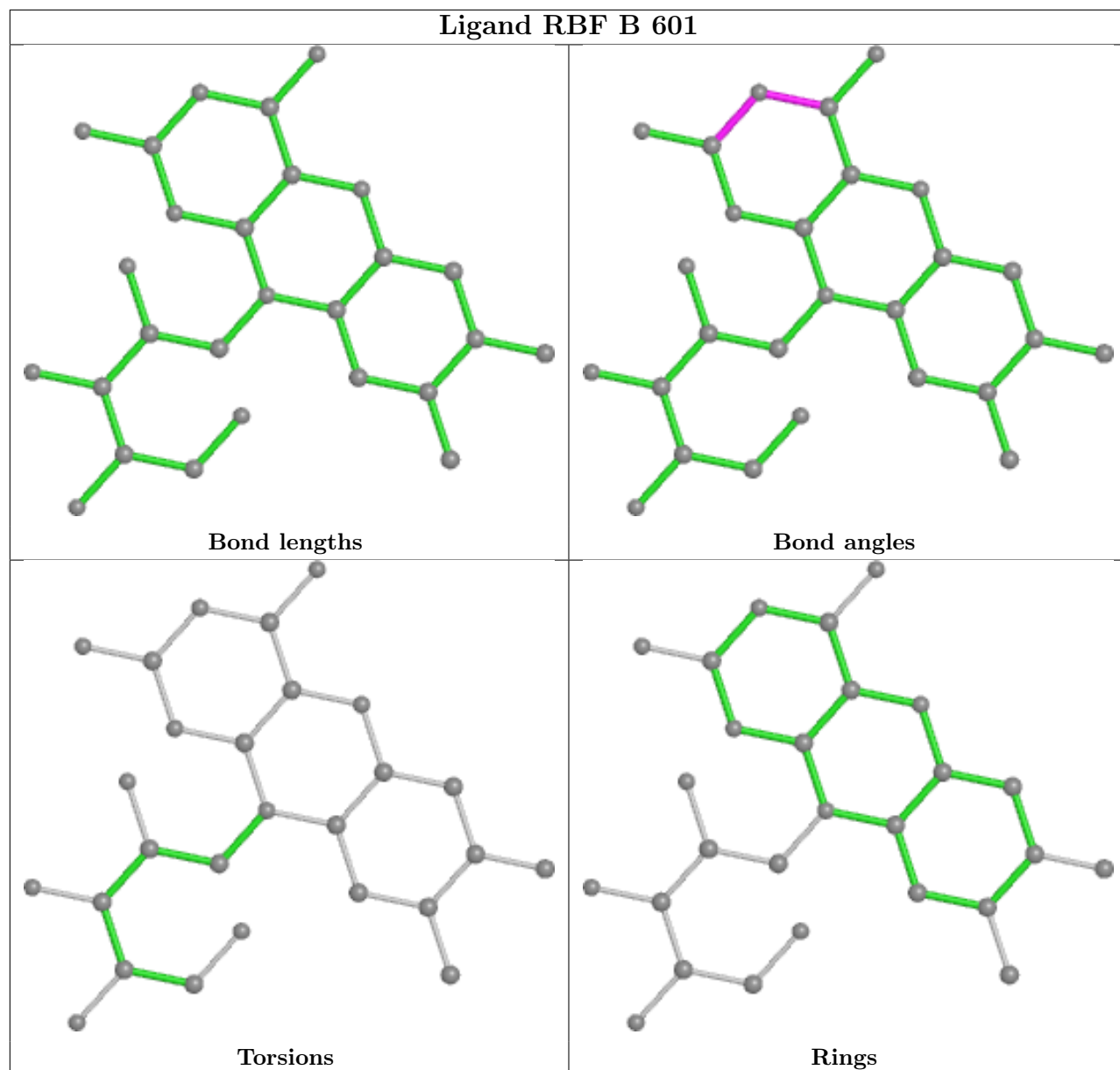
5 monomers are involved in 8 short contacts:

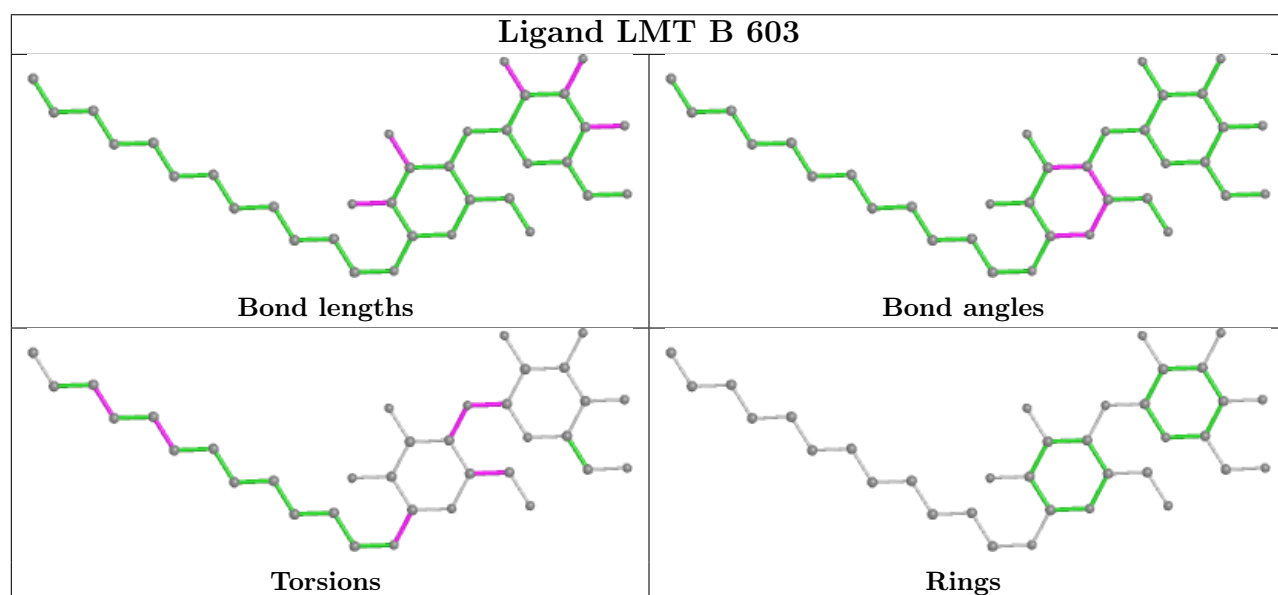
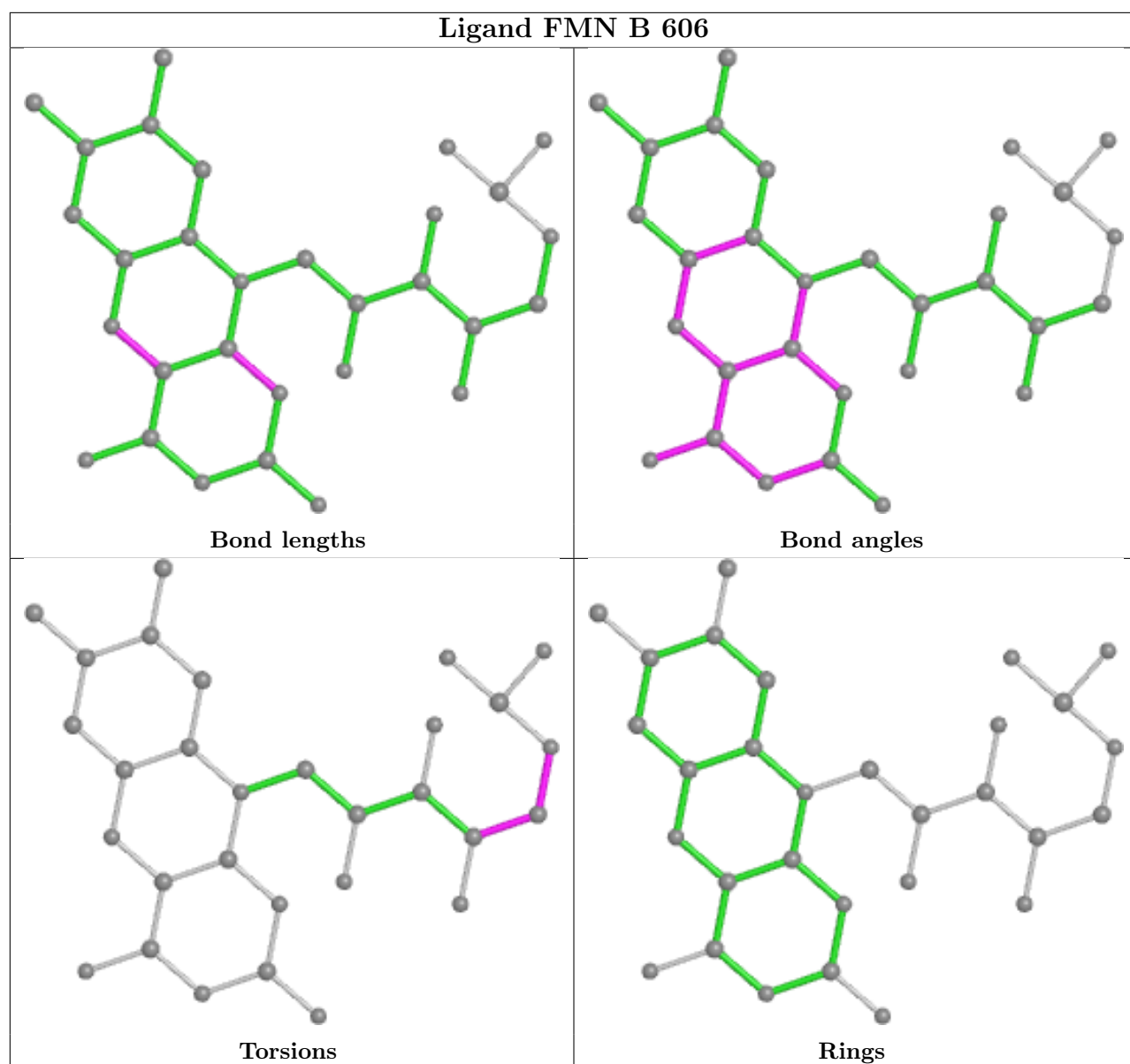
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	605	UQ2	2	0
11	C	1000	FMN	1	0
11	B	606	FMN	1	0
9	B	603	LMT	2	0
14	F	1501	FAD	2	0

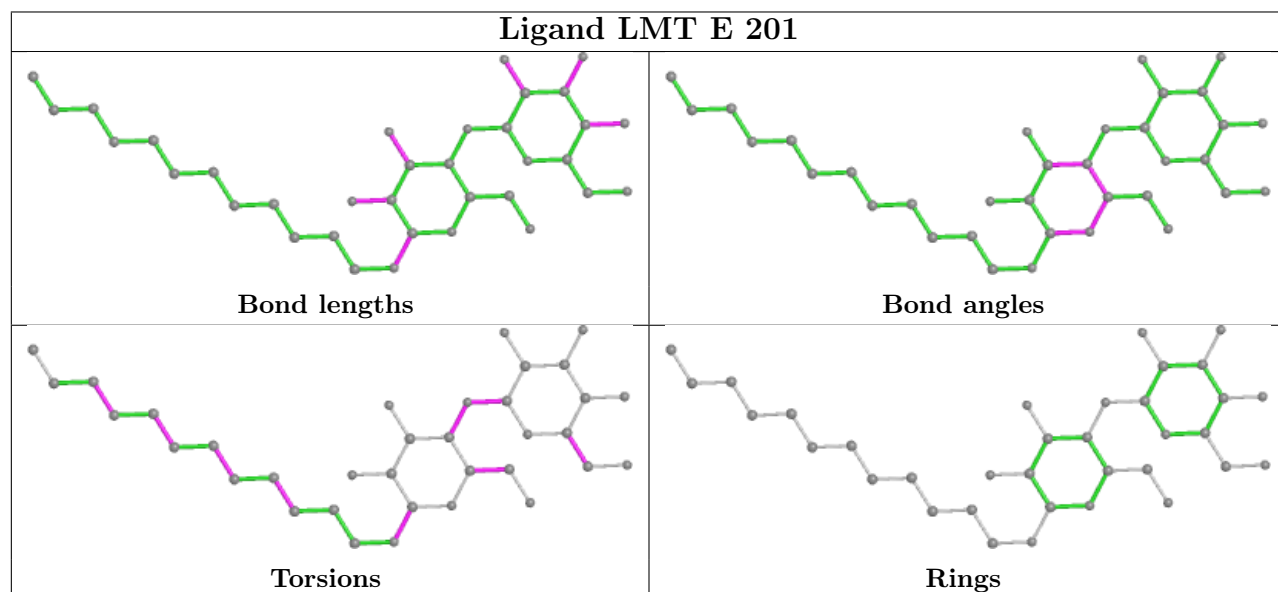
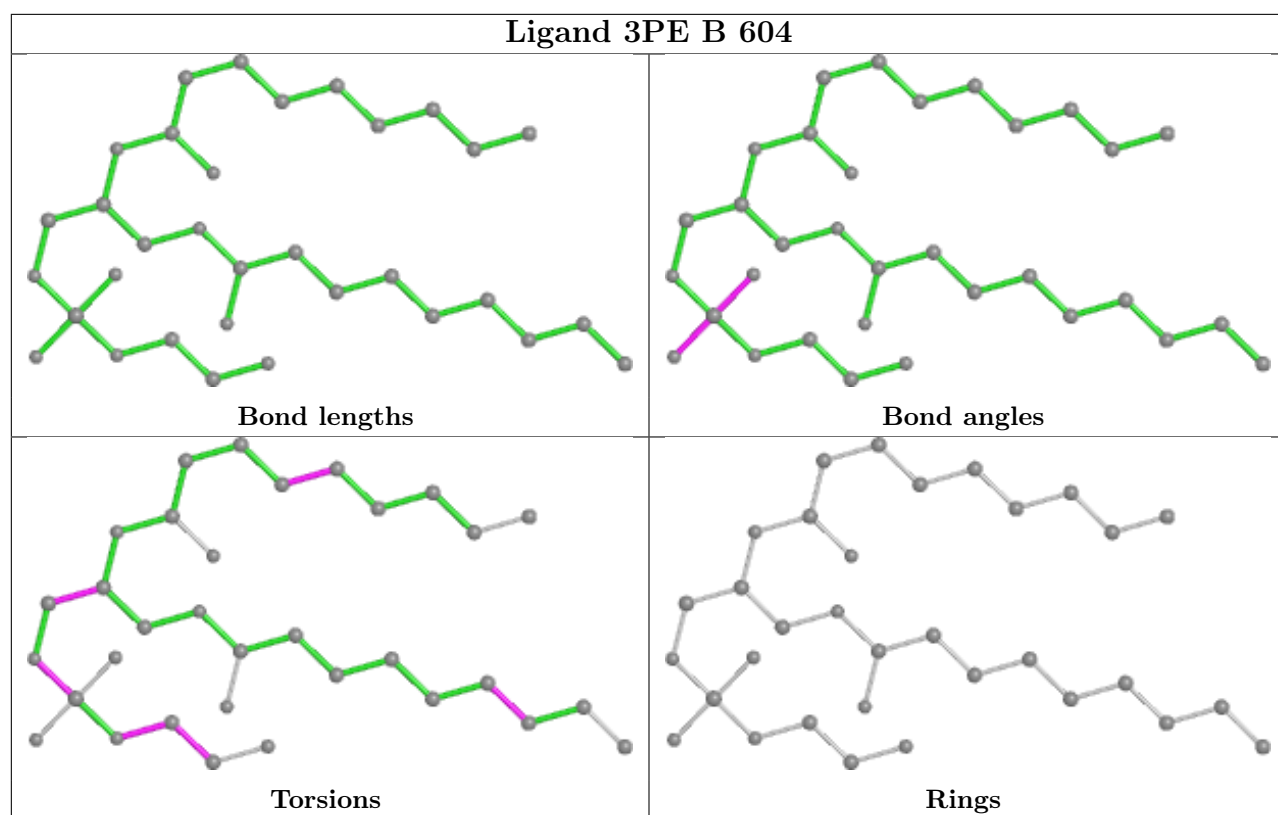
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

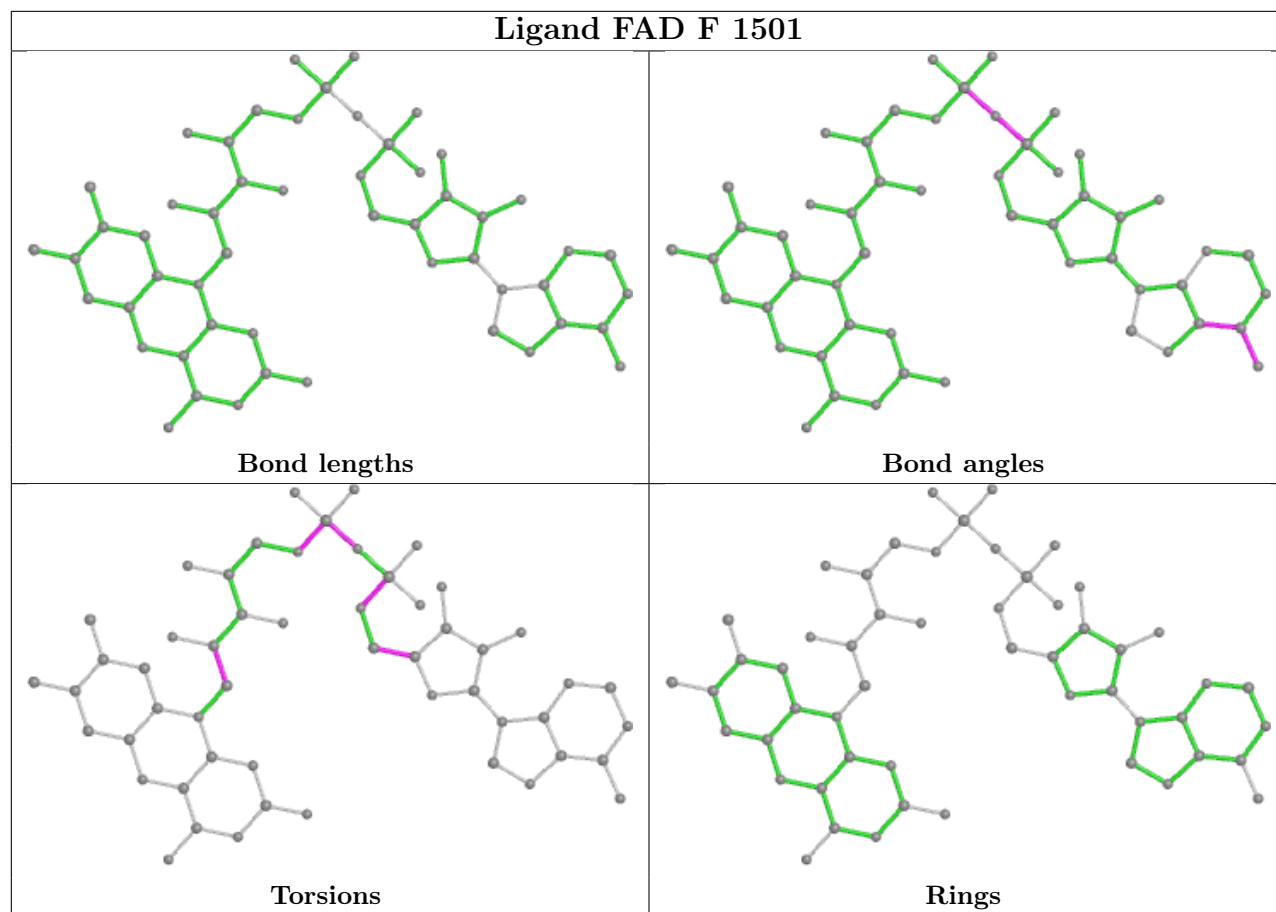












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

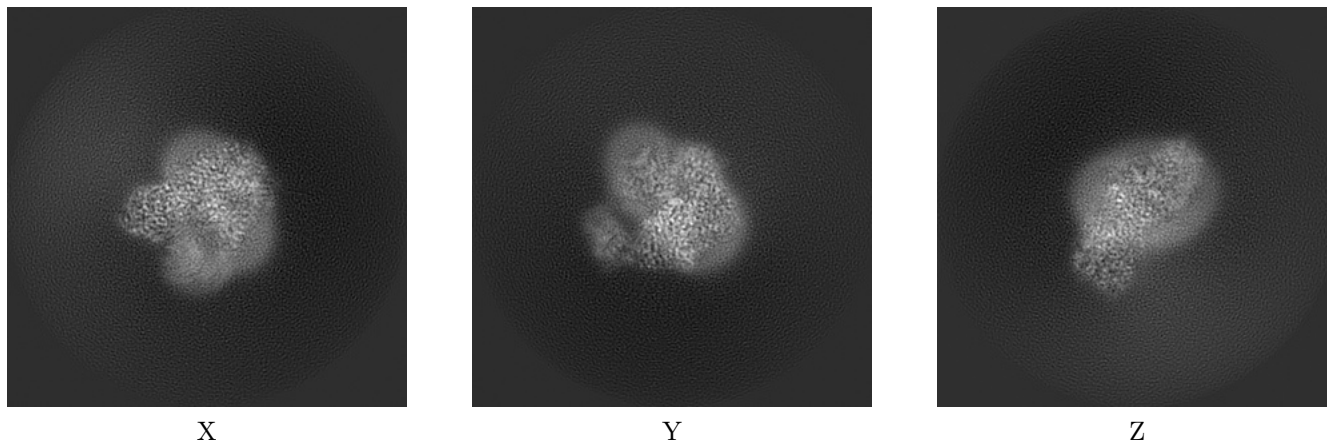
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15090. These allow visual inspection of the internal detail of the map and identification of artifacts.

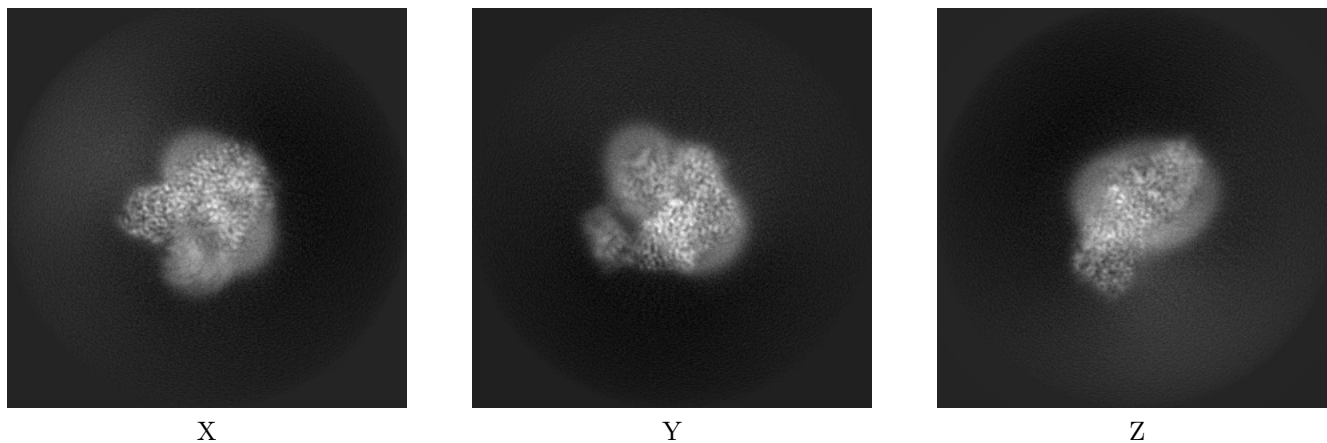
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



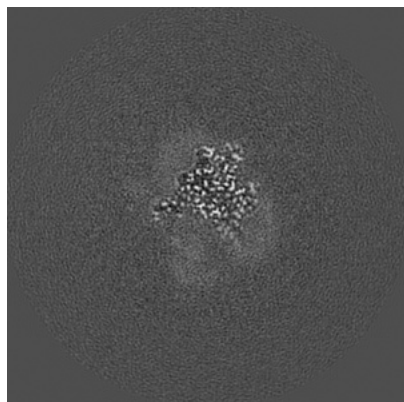
6.1.2 Raw map



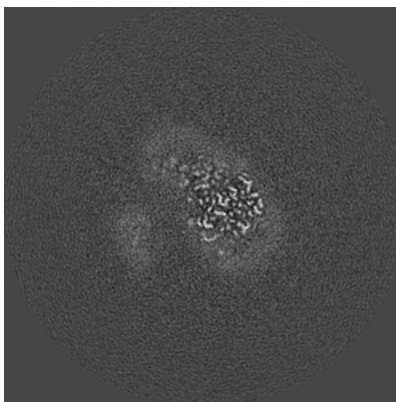
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

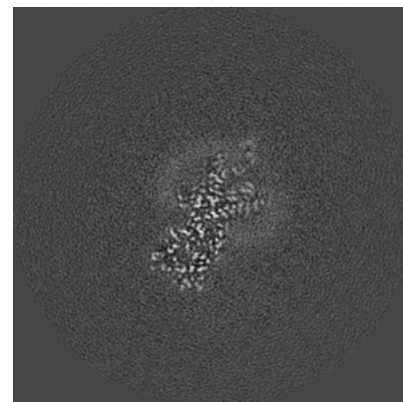
6.2.1 Primary map



X Index: 160

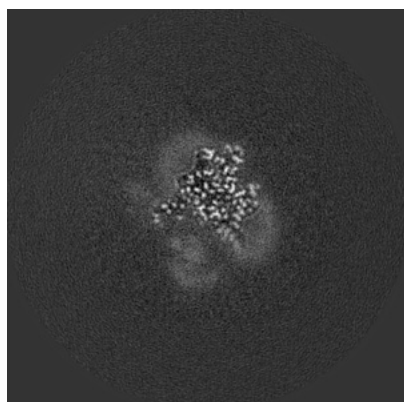


Y Index: 160

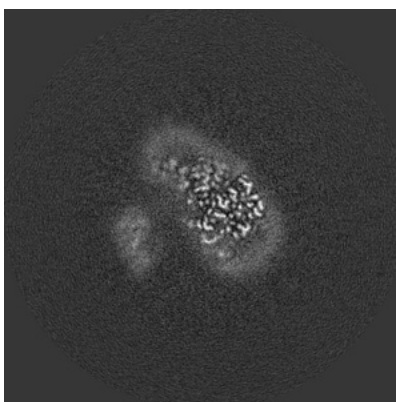


Z Index: 160

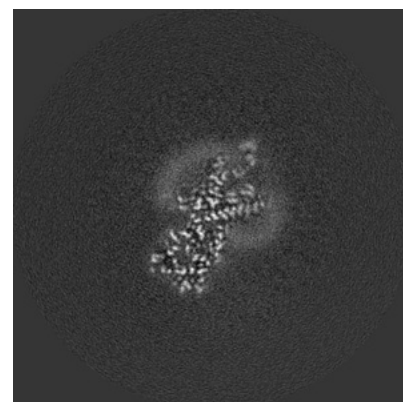
6.2.2 Raw map



X Index: 160



Y Index: 160

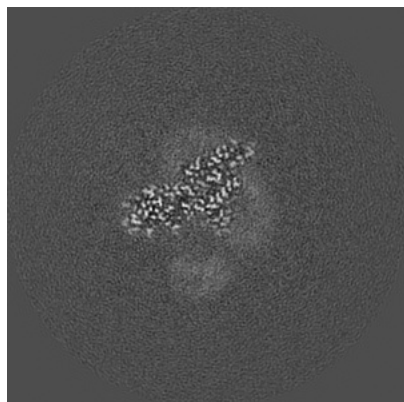


Z Index: 160

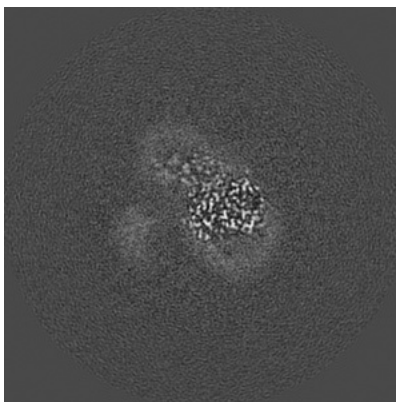
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

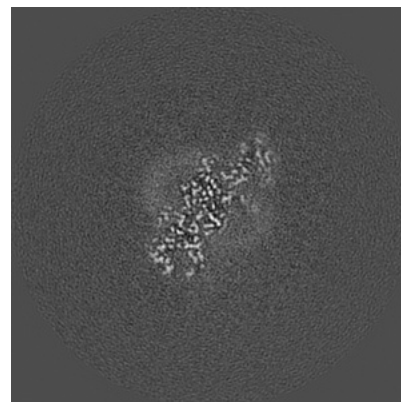
6.3.1 Primary map



X Index: 148

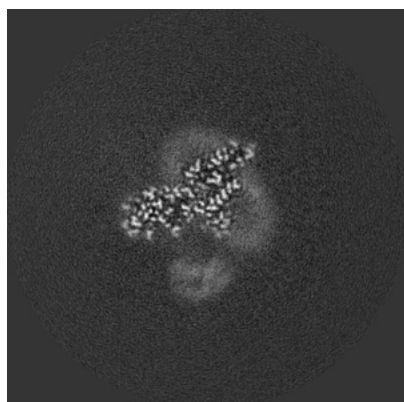


Y Index: 165

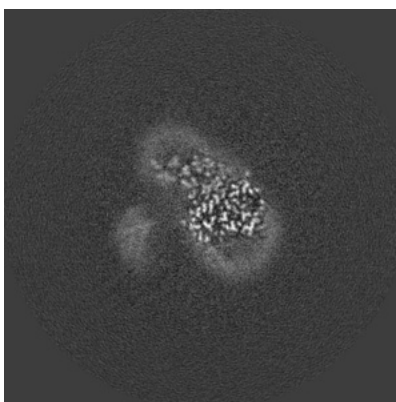


Z Index: 175

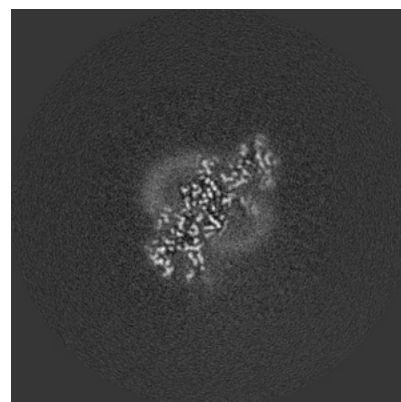
6.3.2 Raw map



X Index: 148



Y Index: 165

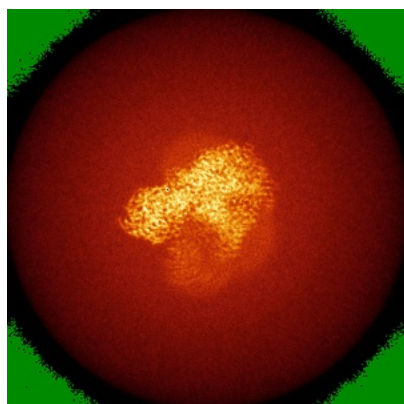


Z Index: 175

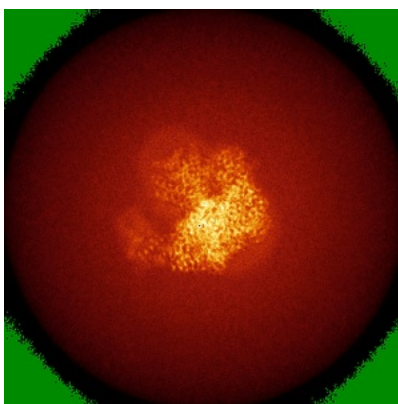
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

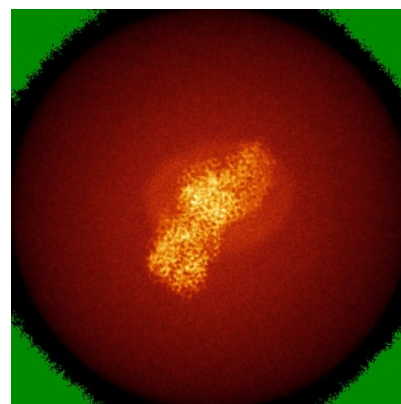
6.4.1 Primary map



X

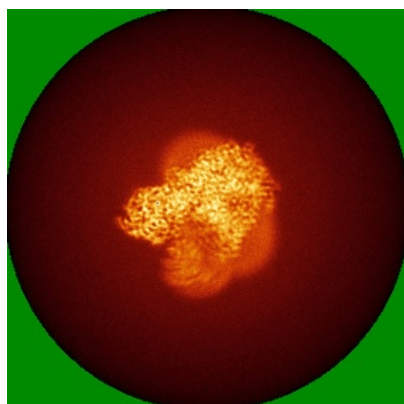


Y

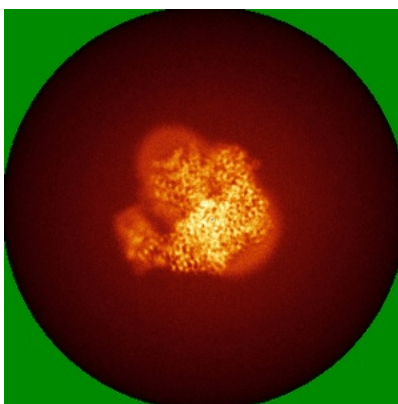


Z

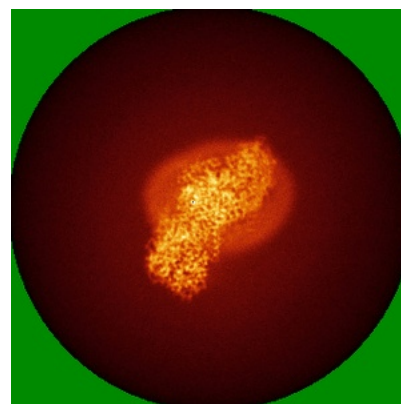
6.4.2 Raw map



X



Y

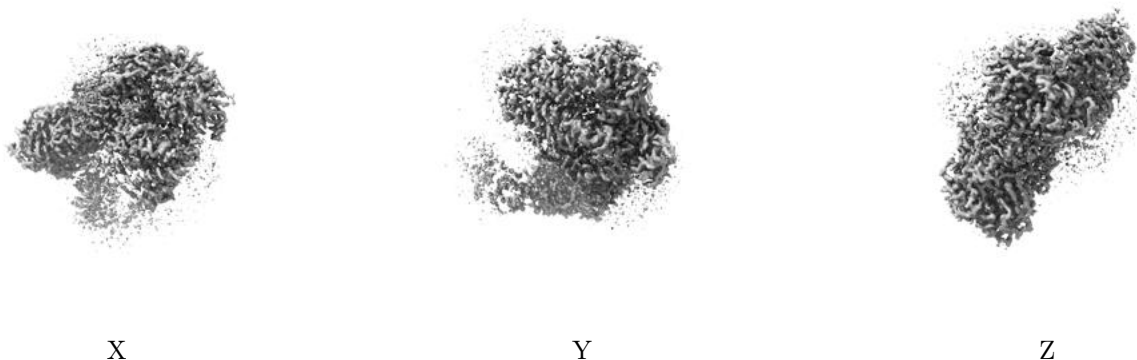


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0133. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

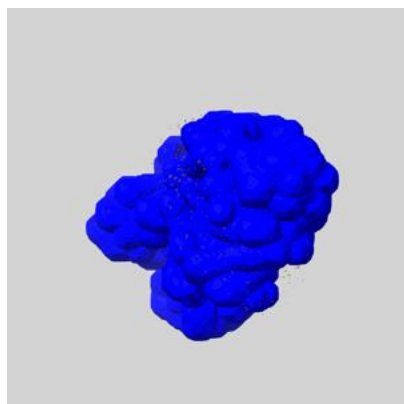
6.6 Mask visualisation [i](#)

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

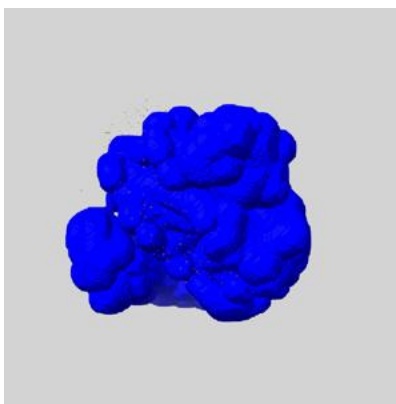
A mask typically either:

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

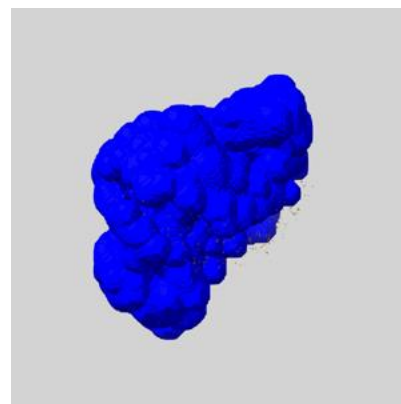
6.6.1 emd_15090_msk_1.map [i](#)



X



Y

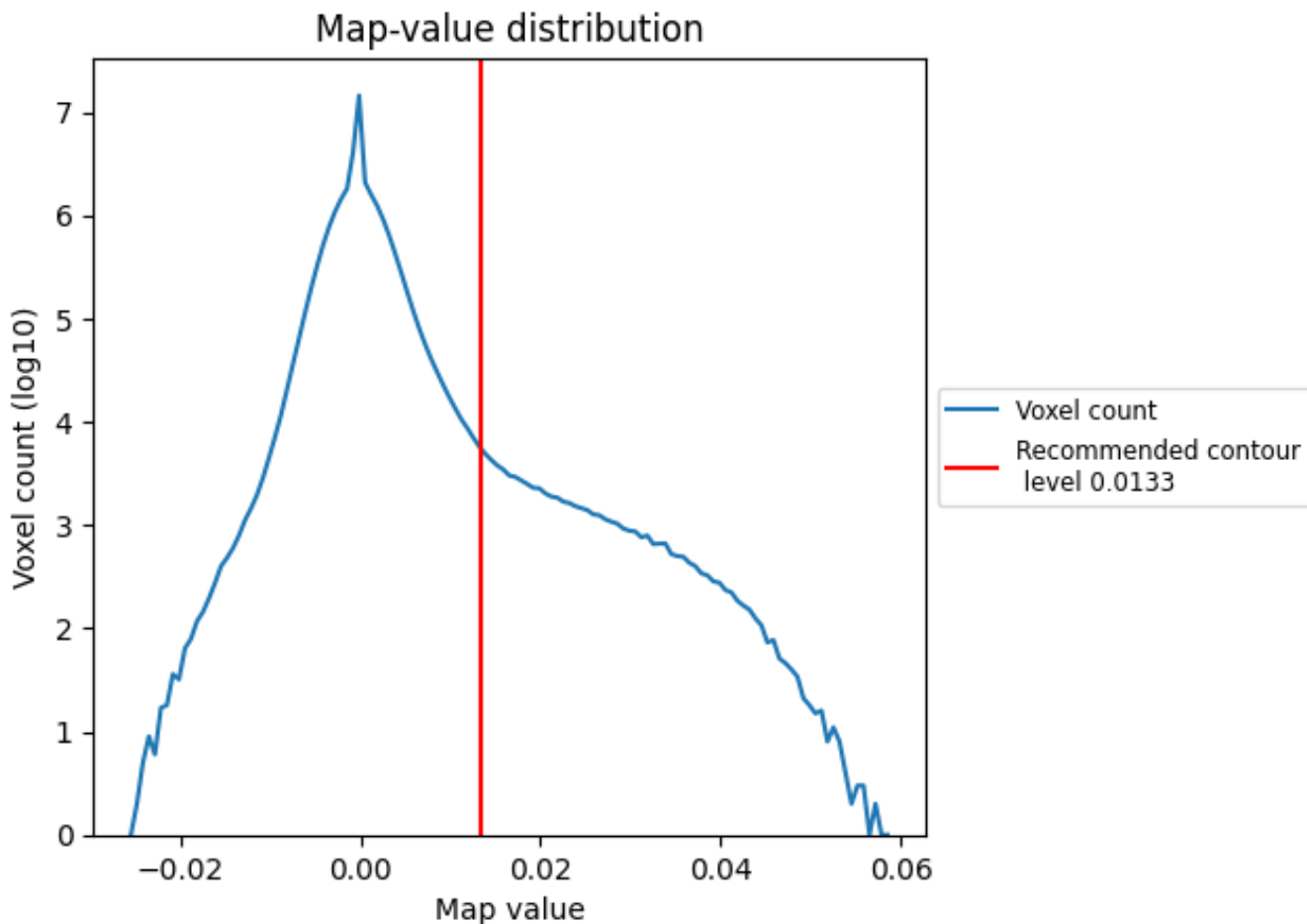


Z

7 Map analysis [i](#)

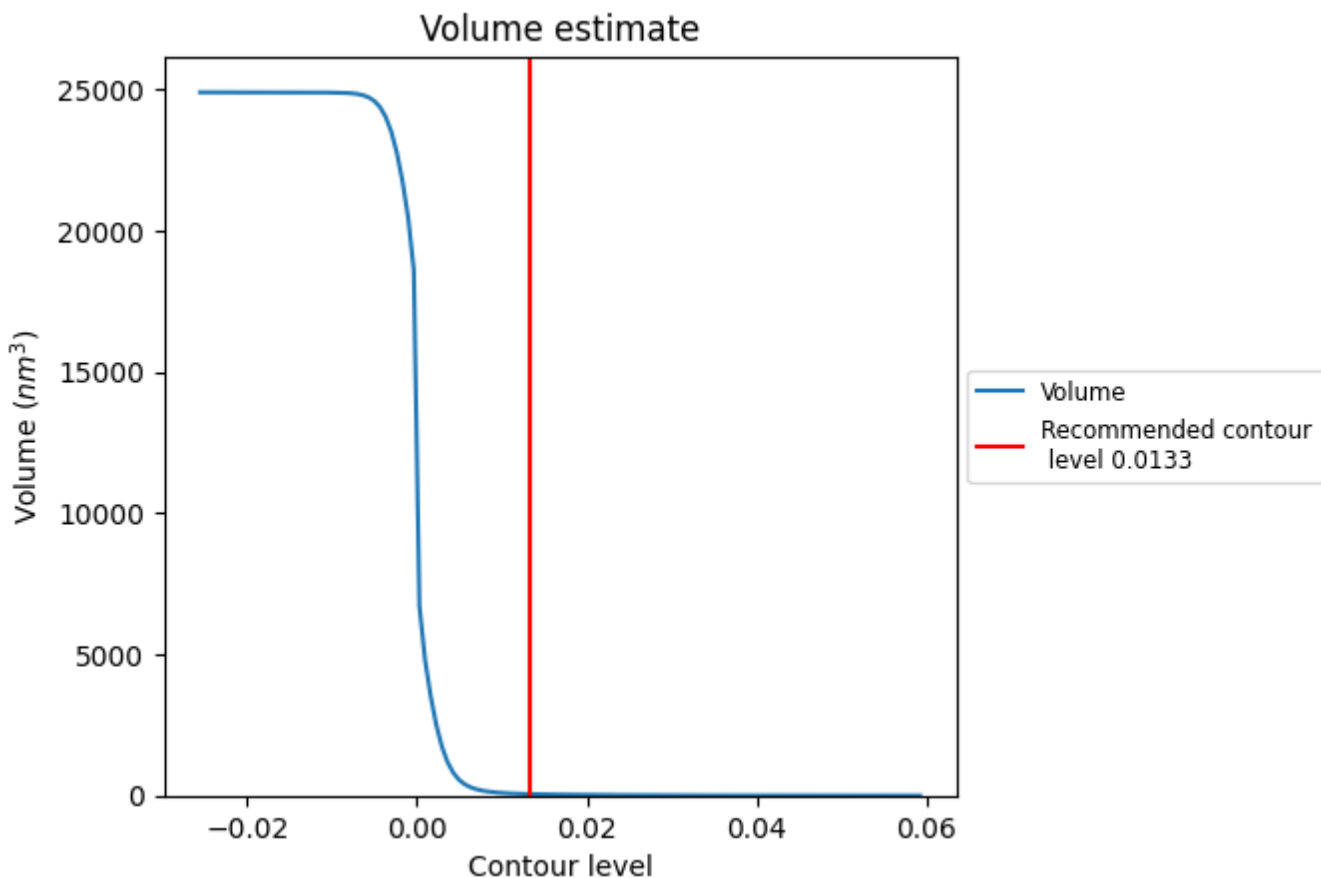
This section contains the results of statistical analysis of the map.

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.

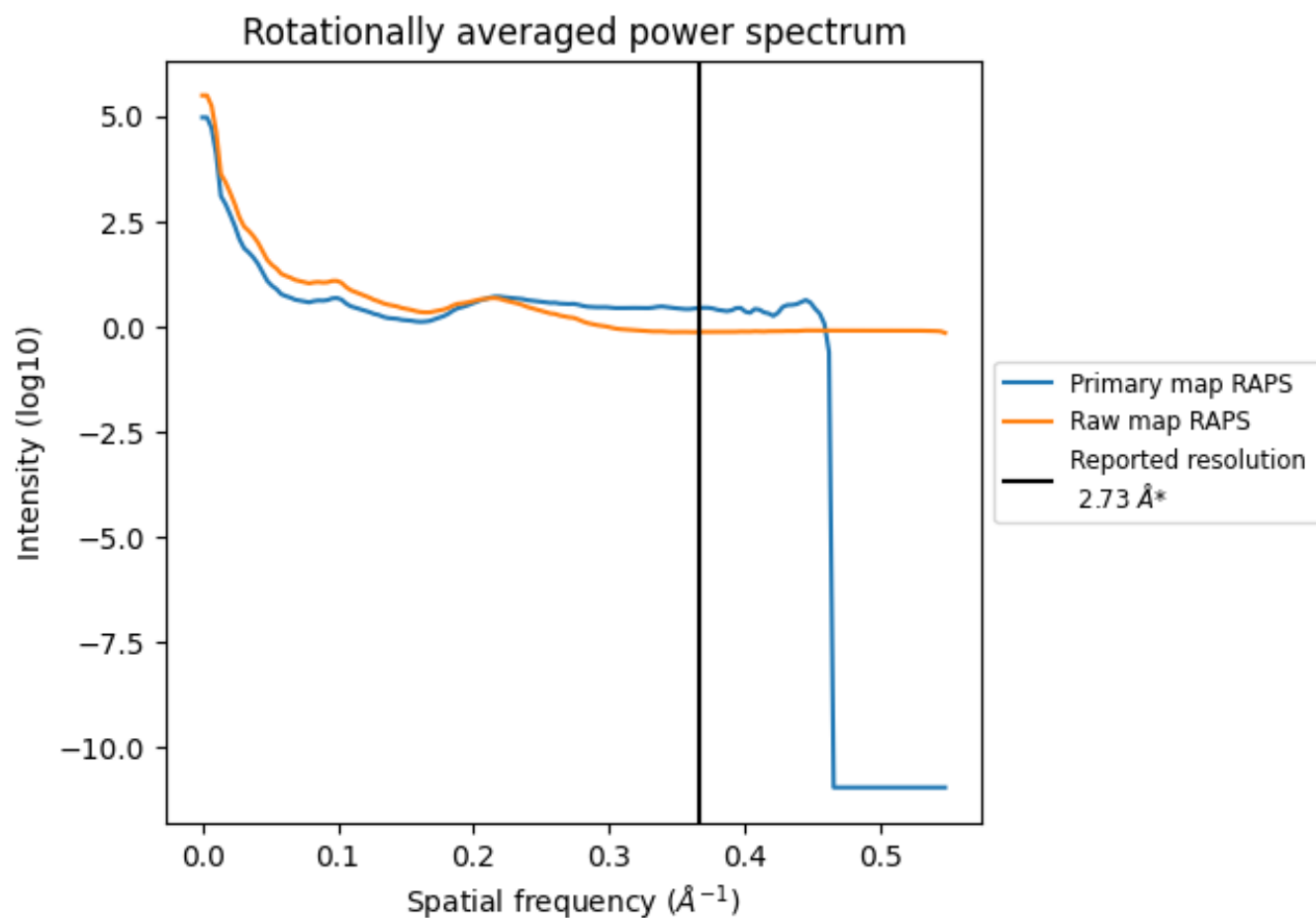
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm³; this corresponds to an approximate mass of 46 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](#)

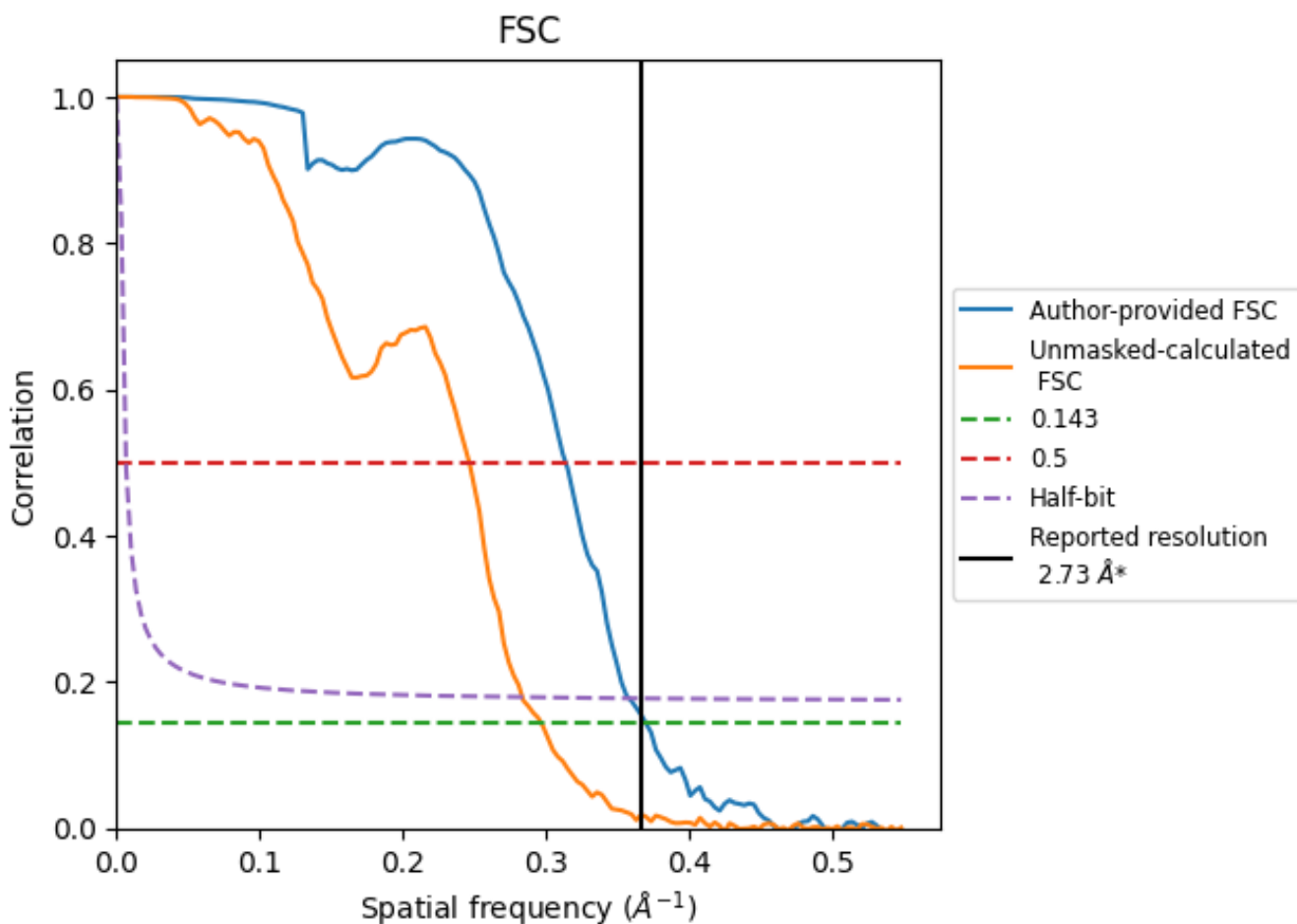


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 Å⁻¹

8.2 Resolution estimates

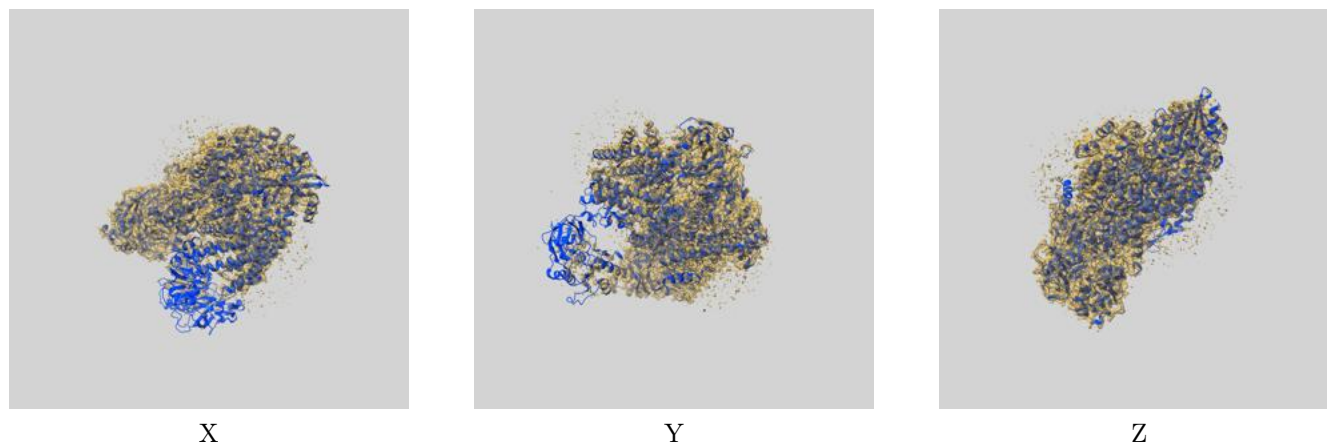
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.70	3.19	2.79
Unmasked-calculated*	3.37	4.06	3.53

*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 3.37 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15090 and PDB model 8A1V. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



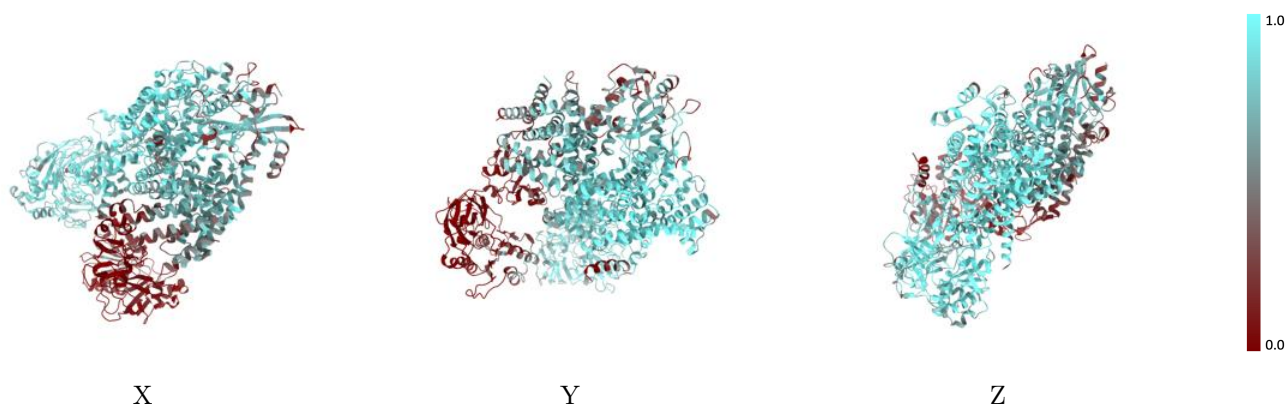
The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



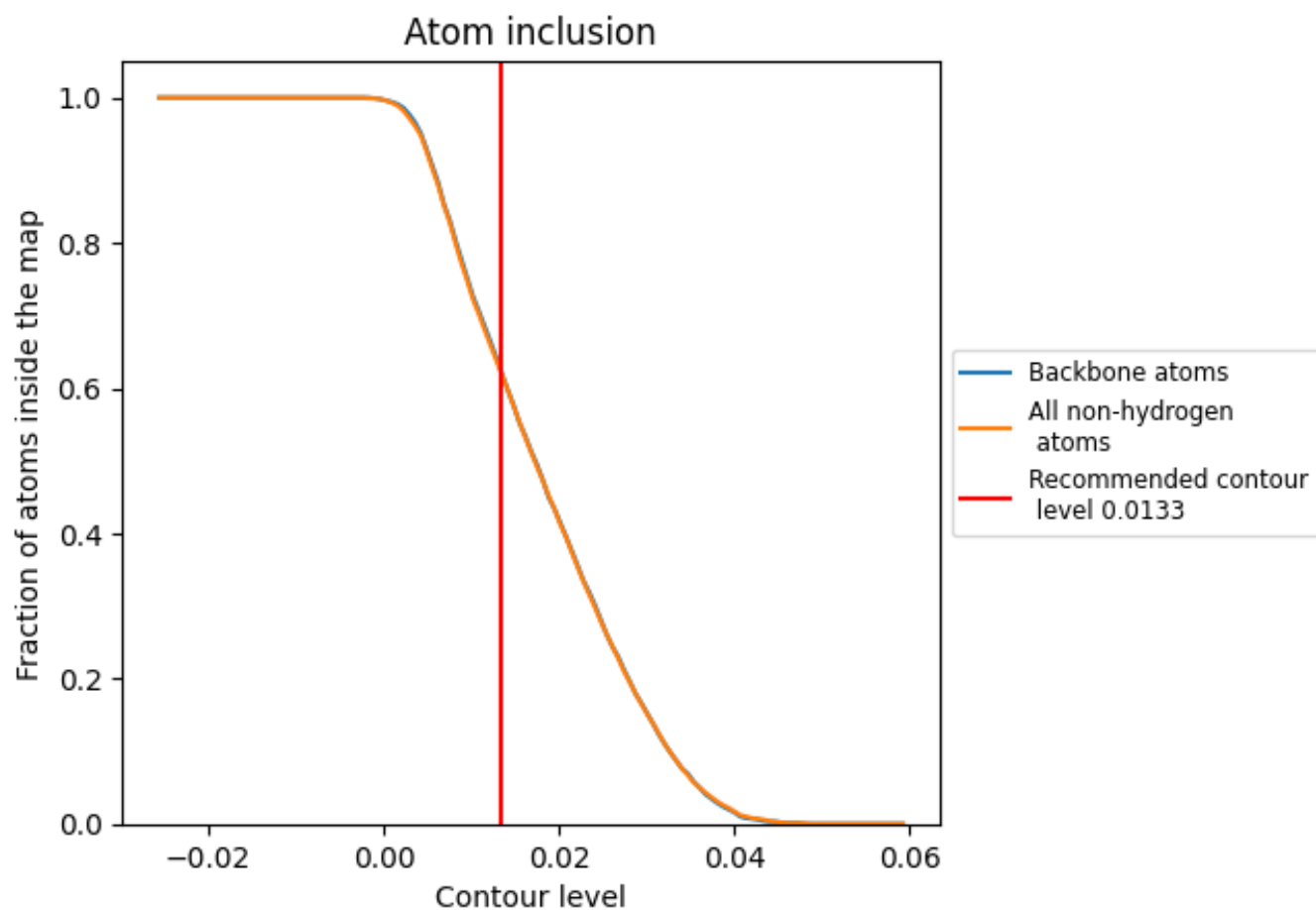
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0133).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.5400
A	0.8570	0.6510
B	0.8640	0.6480
C	0.6040	0.5500
D	0.7160	0.5900
E	0.6540	0.5640
F	0.1010	0.2720

