Full wwPDB EM Validation Report ⓘ

Aug 24, 2026 – 08:24 pm BST

PDB ID	:	8A1W / pdb_00008a1w
EMDB ID	:	EMD-15091
Title	:	Sodium pumping NADH-quinone oxidoreductase with substrate Q1
Authors	:	Hau, J.-L.; Kaltwasser, S.; Vonck, J.; Fritz, G.; Steuber, J.
Deposited on	:	2022-06-02
Resolution	:	2.56 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:

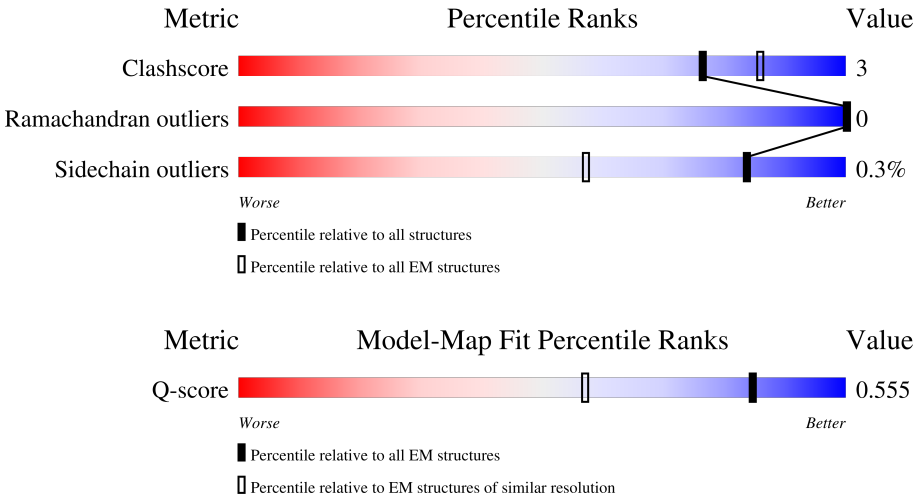
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.56 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.



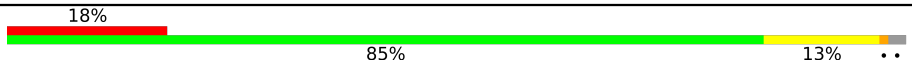
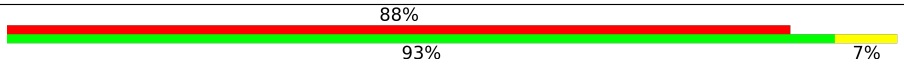
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7558 (2.06 - 3.06)

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	A	468	89% 6% 5%
2	B	415	6% 93% 7%
3	C	257	16% 88% 8%
4	D	210	5% 91%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	198	
6	F	408	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 30681 atoms, of which 15285 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
2	B	412	Total	C	H	N	O	S	0	0
			6346	2106	3164	518	536	22		

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

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

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

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

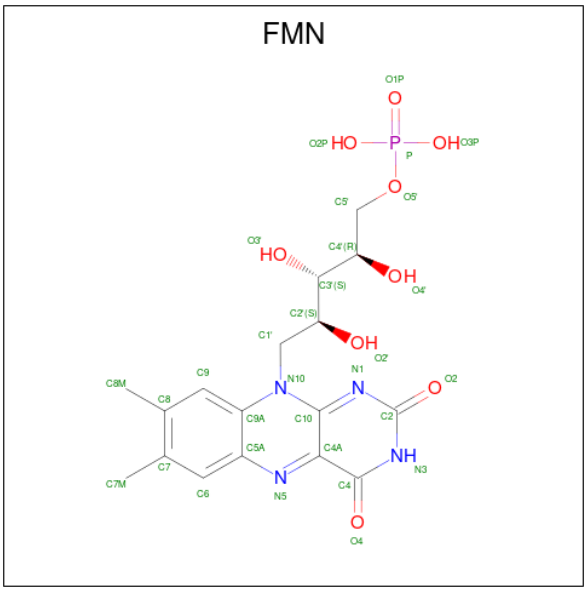
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	195	Total	C	H	N	O	S	0	0
			3041	997	1555	226	253	10		

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

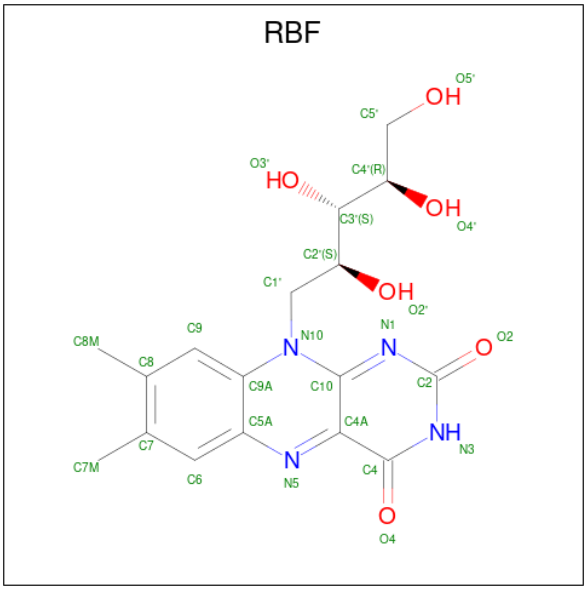
Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	406	Total	C	H	N	O	S	0	0
			6239	2020	3086	517	593	23		

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



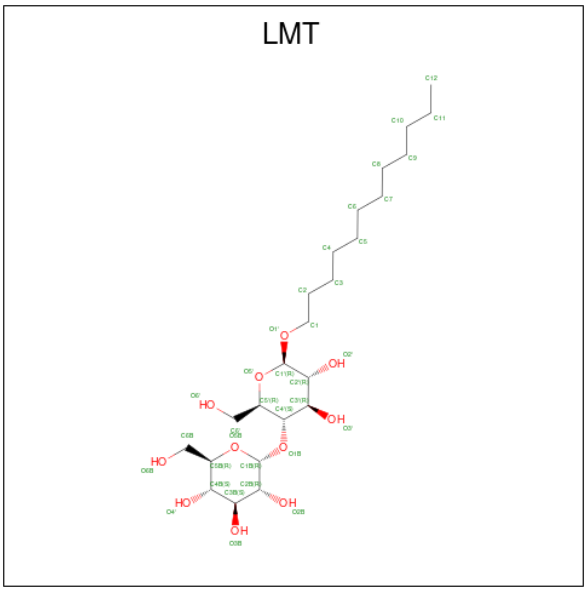
Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total	C	H	N	O	P	0
			49	17	19	4	8	1	
7	C	1	Total	C	H	N	O	P	0
			49	17	19	4	8	1	

- Molecule 8 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$).



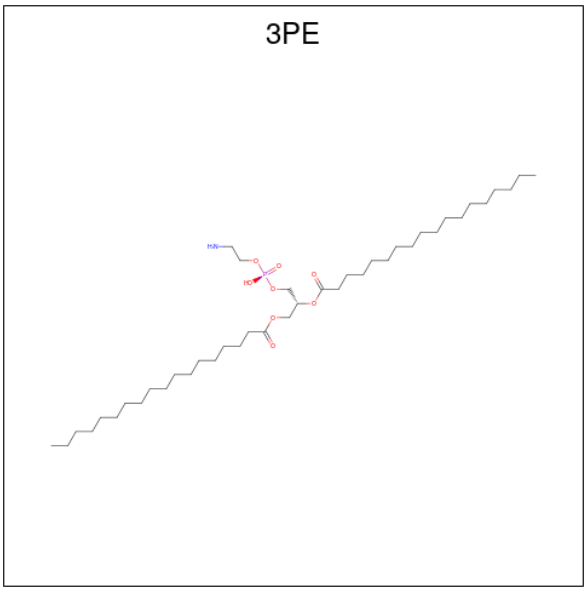
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	H	N	O	0
			46	17	19	4	6	

- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



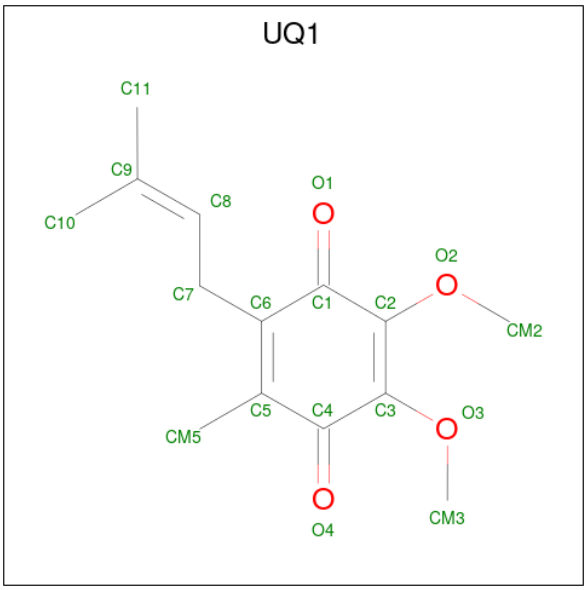
Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	H	O	0
			80	24	45	11	
9	B	1	Total	C	H	O	0
			81	24	46	11	
9	D	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
10	B	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
10	B	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
10	B	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
10	D	1	Total	C	H	N	O	P	0
			106	34	62	1	8	1	

- Molecule 11 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).

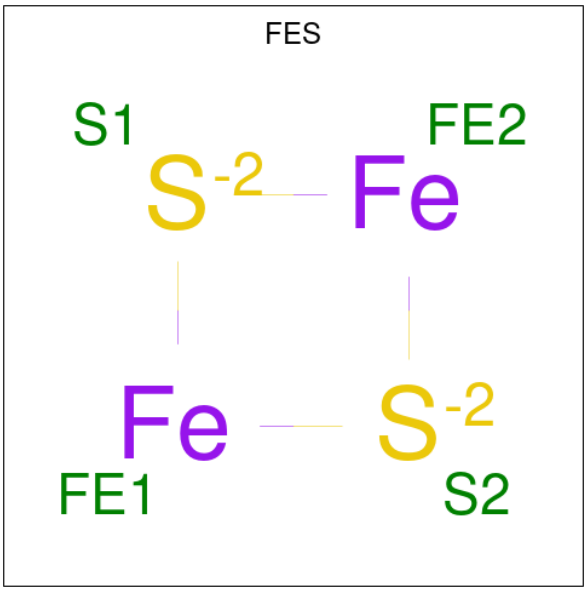


Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	H	O	0
			36	14	18	4	

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

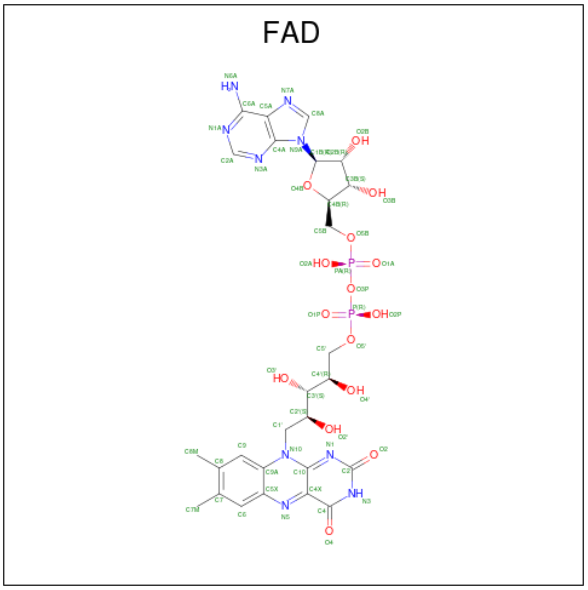
Mol	Chain	Residues	Atoms		AltConf
12	B	2	Total	Na	0
			2	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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 (CCD ID: 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	

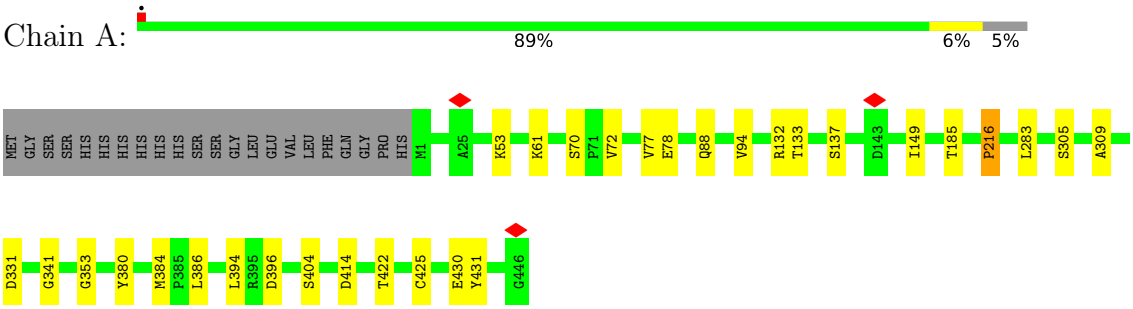
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	A	145	Total O 145 145	0
15	B	117	Total O 117 117	0
15	C	6	Total O 6 6	0
15	D	7	Total O 7 7	0
15	E	14	Total O 14 14	0

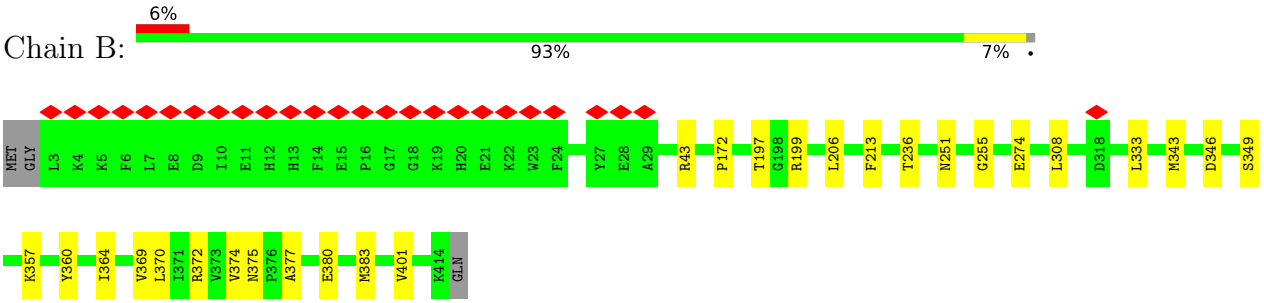
3 Residue-property plots (i)

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.

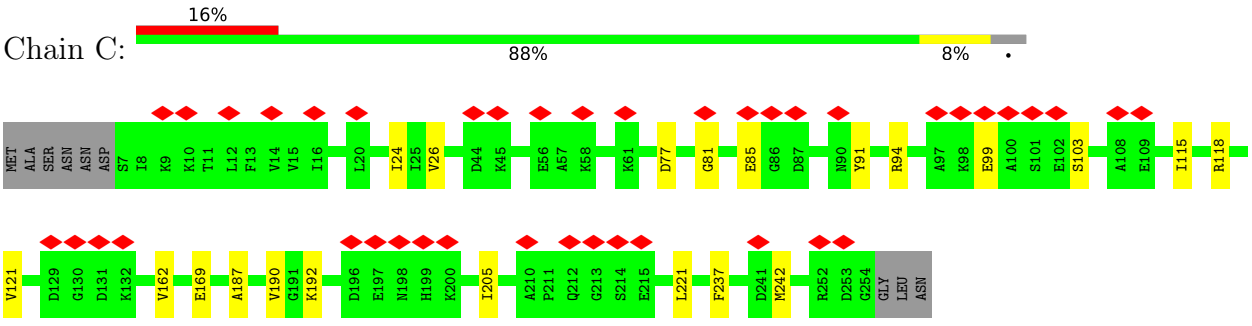
• Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



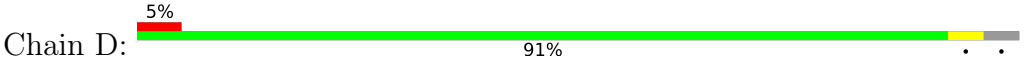
• Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

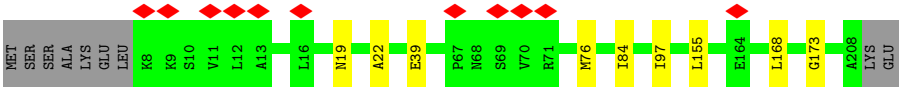


• Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C



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

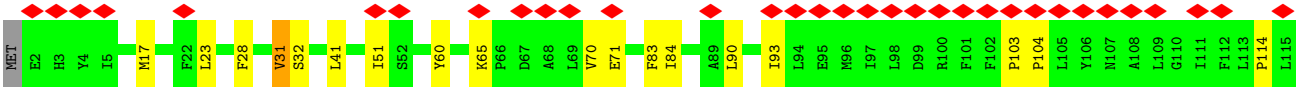


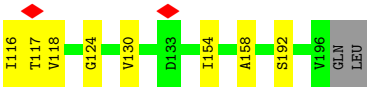


• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E

Chain E:

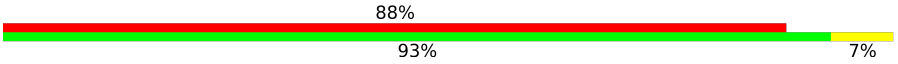


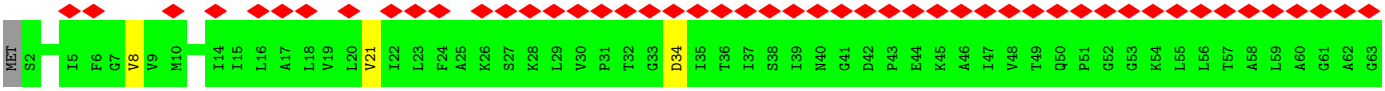


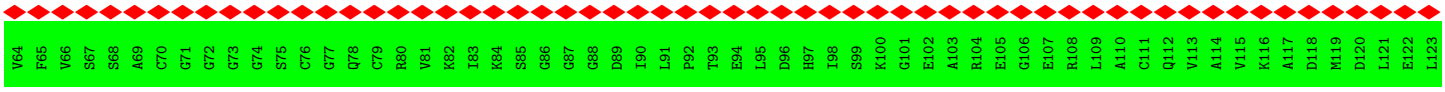


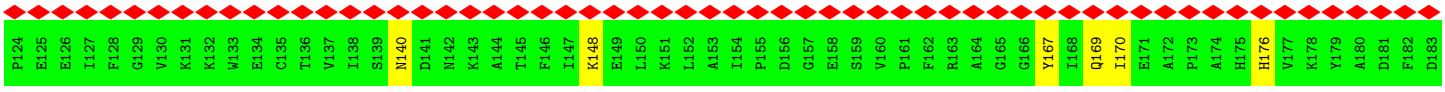
• Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F

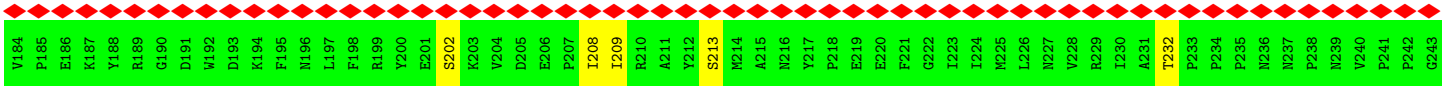
Chain F:



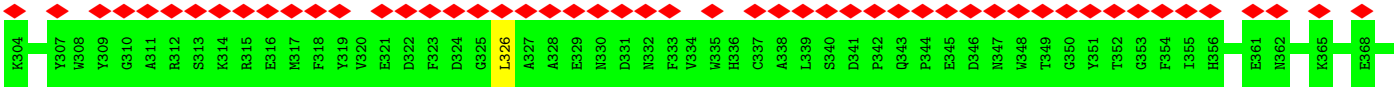


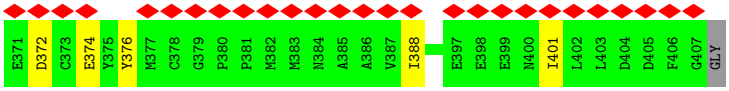












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.079	Depositor
Minimum map value	-0.041	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, LMT, UQ1, 3PE, RBF, FES, FMN, NA

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	0.18	0/3480	0.33	1/4715 (0.0%)
2	B	0.09	0/3280	0.24	0/4463
3	C	0.08	0/1914	0.20	0/2583
4	D	0.08	0/1568	0.22	0/2130
5	E	0.10	0/1519	0.22	0/2061
6	F	0.07	0/3231	0.18	0/4374
All	All	0.11	0/14992	0.25	1/20326 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	PRO	N-CA-CB	-5.22	96.86	102.60

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	3416	3461	3463	20	0
2	B	3182	3164	3164	20	0
3	C	1882	1892	1892	13	0
4	D	1536	1618	1618	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1486	1555	1555	17	0
6	F	3153	3086	3086	18	0
7	B	30	19	19	3	0
7	C	30	19	19	1	0
8	B	27	19	20	1	0
9	B	70	91	90	1	0
9	D	35	46	45	2	0
10	B	135	204	204	0	0
10	D	44	62	62	0	0
11	B	18	18	18	2	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	145	0	0	6	0
15	B	117	0	0	4	0
15	C	6	0	0	1	0
15	D	7	0	0	0	0
15	E	14	0	0	0	0
All	All	15396	15285	15286	91	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 (91) 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:305:SER:O	15:A:501:HOH:O	2.01	0.79
2:B:346:ASP:OD2	2:B:349:SER:OG	2.03	0.76
1:A:430:GLU:OE2	15:A:502:HOH:O	2.05	0.75
3:C:91:TYR:OH	3:C:121:VAL:O	2.02	0.74
1:A:61:LYS:NZ	6:F:372:ASP:OD1	2.21	0.74
2:B:172:PRO:O	15:B:601:HOH:O	2.05	0.74
1:A:88:GLN:OE1	15:A:503:HOH:O	2.05	0.74
6:F:140:ASN:O	6:F:148:LYS:NZ	2.22	0.72
6:F:244:GLN:NE2	14:F:1501:FAD:O1A	2.23	0.72
2:B:377:ALA:O	7:C:1000:FMN:O2'	2.11	0.69
9:B:504:LMT:O3'	9:B:504:LMT:O5B	2.13	0.67
1:A:414:ASP:OD2	15:A:505:HOH:O	2.16	0.63
3:C:162:VAL:HG12	3:C:192:LYS:O	2.01	0.61
3:C:77:ASP:O	3:C:81:GLY:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:388:ILE:HD13	6:F:401:ILE:HD13	1.83	0.59
4:D:168:LEU:O	4:D:173:GLY:N	2.36	0.58
5:E:41:LEU:HD11	5:E:116:ILE:HD11	1.85	0.58
5:E:84:ILE:HD11	5:E:118:VAL:HG12	1.83	0.58
1:A:394:LEU:HD22	1:A:431:TYR:CD1	2.39	0.58
3:C:26:VAL:HG13	4:D:84:ILE:HG21	1.87	0.56
11:B:506:UQ1:CM2	11:B:506:UQ1:O1	2.54	0.55
11:B:506:UQ1:CM3	11:B:506:UQ1:O4	2.55	0.55
6:F:169:GLN:HB3	6:F:209:ILE:HD11	1.90	0.54
4:D:39:GLU:HB3	4:D:97:ILE:HD11	1.89	0.54
6:F:232:THR:O	14:F:1501:FAD:O3B	2.25	0.54
2:B:274:GLU:OE1	7:B:501:FMN:HM83	2.08	0.53
1:A:77:VAL:HG23	1:A:78:GLU:HG2	1.91	0.52
3:C:24:ILE:HD13	6:F:8:VAL:HG21	1.90	0.52
5:E:51:ILE:HG22	5:E:90:LEU:HD13	1.92	0.52
3:C:99:GLU:O	3:C:103:SER:OG	2.24	0.51
2:B:370:LEU:O	2:B:374:VAL:HG22	2.10	0.51
3:C:94:ARG:NH2	3:C:169:GLU:OE1	2.40	0.51
2:B:380:GLU:O	7:B:501:FMN:N3	2.44	0.51
2:B:333:LEU:O	2:B:372:ARG:NH2	2.41	0.51
2:B:251:ASN:O	2:B:255:GLY:N	2.42	0.50
2:B:357:LYS:NZ	15:B:613:HOH:O	2.41	0.50
6:F:286:ALA:HB3	6:F:287:PRO:CD	2.42	0.49
1:A:341:GLY:O	1:A:353:GLY:N	2.46	0.49
2:B:213:PHE:CG	2:B:383:MET:HE1	2.47	0.49
2:B:308:LEU:HD21	2:B:370:LEU:HG	1.95	0.49
2:B:375:ASN:ND2	5:E:192:SER:O	2.45	0.49
5:E:31:VAL:HG21	5:E:41:LEU:HD22	1.95	0.49
1:A:149:ILE:HD12	1:A:185:THR:HB	1.95	0.49
6:F:167:TYR:N	6:F:264:PHE:O	2.42	0.49
6:F:170:ILE:O	6:F:209:ILE:HD12	2.13	0.49
3:C:187:ALA:O	3:C:190:VAL:HG22	2.13	0.48
5:E:60:TYR:O	5:E:65:LYS:N	2.47	0.48
2:B:360:TYR:CZ	2:B:364:ILE:HD11	2.48	0.48
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.96	0.47
1:A:422:THR:O	15:A:506:HOH:O	2.20	0.47
2:B:274:GLU:O	15:B:602:HOH:O	2.20	0.47
3:C:118:ARG:NH1	3:C:242:MET:O	2.45	0.47
6:F:374:GLU:OE1	6:F:376:TYR:OH	2.33	0.47
1:A:53:LYS:O	1:A:70:SER:O	2.32	0.47
6:F:293:PHE:CE1	6:F:326:LEU:HD11	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ARG:NE	15:B:623:HOH:O	2.48	0.46
9:D:302:LMT:O3'	9:D:302:LMT:O2B	2.28	0.46
2:B:308:LEU:HD23	2:B:369:VAL:HB	1.97	0.46
4:D:76:MET:SD	5:E:118:VAL:HG11	2.56	0.45
4:D:19:ASN:HB3	4:D:22:ALA:HB3	1.99	0.45
5:E:93:ILE:HD11	6:F:21:VAL:HG12	2.00	0.44
1:A:133:THR:O	1:A:137:SER:N	2.50	0.44
3:C:115:ILE:HD11	3:C:237:PHE:CE2	2.53	0.43
1:A:384:MET:HE1	1:A:386:LEU:HD12	2.00	0.43
5:E:41:LEU:CD1	5:E:116:ILE:HD11	2.48	0.43
2:B:197:THR:HG23	8:B:502:RBF:HC52	2.01	0.43
3:C:221:LEU:O	15:C:1101:HOH:O	2.21	0.43
4:D:155:LEU:HD22	9:D:302:LMT:H41	1.99	0.43
6:F:286:ALA:HB3	6:F:287:PRO:HD3	2.00	0.43
2:B:206:LEU:HD21	2:B:343:MET:SD	2.59	0.43
6:F:272:THR:O	6:F:303:ARG:NH1	2.52	0.42
5:E:23:LEU:HD13	5:E:124:GLY:HA3	2.01	0.42
1:A:331:ASP:OD1	1:A:331:ASP:N	2.49	0.42
1:A:380:TYR:OH	1:A:425:CYS:SG	2.72	0.42
1:A:396:ASP:OD2	1:A:404:SER:OG	2.33	0.42
2:B:236:THR:HG21	7:B:501:FMN:C5'	2.50	0.42
5:E:32:SER:O	5:E:158:ALA:HA	2.20	0.41
1:A:430:GLU:OE1	2:B:43:ARG:HG2	2.20	0.41
1:A:132:ARG:NH2	15:A:514:HOH:O	2.43	0.41
5:E:17:MET:CE	5:E:23:LEU:HD12	2.50	0.41
5:E:70:VAL:HG12	5:E:71:GLU:N	2.36	0.41
3:C:85:GLU:OE1	3:C:85:GLU:N	2.54	0.41
5:E:83:PHE:CZ	5:E:130:VAL:HG21	2.55	0.41
1:A:283:LEU:HD12	1:A:309:ALA:CB	2.50	0.41
5:E:103:PRO:N	5:E:104:PRO:HD2	2.36	0.41
6:F:34:ASP:OD1	6:F:34:ASP:N	2.54	0.41
5:E:28:PHE:HA	5:E:154:ILE:HD13	2.02	0.40
5:E:114:PRO:O	5:E:117:THR:OG1	2.25	0.40
3:C:205:ILE:N	3:C:205:ILE:HD12	2.36	0.40
6:F:176:HIS:ND1	6:F:202:SER:O	2.55	0.40
6:F:208:ILE:HD12	6:F:245:MET:HB2	2.04	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%)	439 (99%)	5 (1%)	0	100	100
2	B	410/415 (99%)	407 (99%)	3 (1%)	0	100	100
3	C	246/257 (96%)	244 (99%)	2 (1%)	0	100	100
4	D	199/210 (95%)	194 (98%)	5 (2%)	0	100	100
5	E	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
6	F	404/408 (99%)	400 (99%)	4 (1%)	0	100	100
All	All	1896/1956 (97%)	1875 (99%)	21 (1%)	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%)	375 (100%)	1 (0%)	86	91
2	B	318/320 (99%)	317 (100%)	1 (0%)	86	91
3	C	198/205 (97%)	198 (100%)	0	100	100
4	D	168/176 (96%)	168 (100%)	0	100	100
5	E	162/165 (98%)	161 (99%)	1 (1%)	78	85
6	F	336/337 (100%)	334 (99%)	2 (1%)	78	85
All	All	1558/1598 (98%)	1553 (100%)	5 (0%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	PRO
2	B	401	VAL
5	E	31	VAL
6	F	213	SER
6	F	244	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	114	ASN
1	A	170	GLN
1	A	249	GLN
1	A	322	GLN
2	B	240	GLN
3	C	46	GLN
3	C	143	ASN
3	C	216	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
10	3PE	D	301	-	43,43,50	0.53	0	46,48,55	0.63	2 (4%)
9	LMT	B	504	-	36,36,36	1.15	5 (13%)	47,47,47	1.01	3 (6%)
11	UQ1	B	506	-	18,18,18	0.95	1 (5%)	22,25,25	1.09	4 (18%)
10	3PE	B	507	-	50,50,50	0.52	0	53,55,55	0.53	1 (1%)
10	3PE	B	508	-	50,50,50	0.50	0	53,55,55	0.65	2 (3%)
7	FMN	B	501	2	29,32,33	1.11	2 (6%)	40,47,50	1.32	8 (20%)
13	FES	E	1001	4,5	0,4,4	-	-	-		
8	RBF	B	502	-	29,29,29	0.58	0	41,43,43	0.68	1 (2%)
9	LMT	D	302	-	36,36,36	1.17	6 (16%)	47,47,47	1.00	2 (4%)
7	FMN	C	1000	3	29,32,33	1.12	2 (6%)	40,47,50	1.28	7 (17%)
9	LMT	B	503	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	3 (6%)
14	FAD	F	1501	-	56,58,58	0.27	0	81,89,89	0.37	1 (1%)
10	3PE	B	505	-	32,32,50	0.63	0	35,37,55	0.64	1 (2%)
13	FES	F	1502	6	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
10	3PE	D	301	-	-	9/47/47/54	-
9	LMT	B	504	-	-	9/21/61/61	0/2/2/2
11	UQ1	B	506	-	-	4/9/33/33	0/1/1/1
10	3PE	B	507	-	-	19/54/54/54	-
10	3PE	B	508	-	-	13/54/54/54	-
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
13	FES	E	1001	4,5	-	-	0/1/1/1
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
9	LMT	D	302	-	-	8/21/61/61	0/2/2/2
7	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
9	LMT	B	503	-	-	8/21/61/61	0/2/2/2
14	FAD	F	1501	-	-	8/34/50/50	0/6/6/6
10	3PE	B	505	-	-	15/36/36/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FES	F	1502	6	-	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1000	FMN	C4A-N5	3.70	1.37	1.30
7	B	501	FMN	C4A-N5	3.69	1.37	1.30
9	B	504	LMT	O3'-C3'	-2.75	1.36	1.43
9	B	503	LMT	O3'-C3'	-2.72	1.36	1.43
9	D	302	LMT	O3'-C3'	-2.65	1.36	1.43
7	B	501	FMN	C10-N1	2.58	1.38	1.33
7	C	1000	FMN	C10-N1	2.56	1.38	1.33
9	B	503	LMT	O2B-C2B	-2.41	1.37	1.43
9	B	504	LMT	O2B-C2B	-2.36	1.37	1.43
9	D	302	LMT	O2B-C2B	-2.36	1.37	1.43
9	B	504	LMT	O2'-C2'	-2.34	1.37	1.43
9	D	302	LMT	O3B-C3B	-2.34	1.37	1.43
9	D	302	LMT	O2'-C2'	-2.32	1.37	1.43
9	B	503	LMT	O2'-C2'	-2.30	1.37	1.43
9	B	503	LMT	O3B-C3B	-2.29	1.37	1.43
9	B	504	LMT	O3B-C3B	-2.25	1.37	1.43
9	B	504	LMT	O4'-C4B	-2.12	1.38	1.43
9	B	503	LMT	O4'-C4B	-2.11	1.38	1.43
9	D	302	LMT	O4'-C4B	-2.10	1.38	1.43
9	D	302	LMT	O1'-C1'	-2.08	1.36	1.40
11	B	506	UQ1	C3-C4	-2.06	1.42	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	508	3PE	C2-O21-C21	3.18	125.61	117.79
7	C	1000	FMN	C4-N3-C2	-3.16	119.80	125.64
7	B	501	FMN	C4-N3-C2	-3.09	119.93	125.64
10	D	301	3PE	C2-O21-C21	2.71	124.45	117.79
7	C	1000	FMN	C4A-C10-N10	2.67	120.39	116.48
7	C	1000	FMN	C4A-C4-N3	2.65	119.92	113.19
7	B	501	FMN	C4A-C4-N3	2.61	119.81	113.19
14	F	1501	FAD	P-O3P-PA	-2.55	124.06	132.83
7	B	501	FMN	C10-C4A-N5	-2.55	119.45	124.86
9	D	302	LMT	C3'-C4'-C5'	-2.54	105.11	110.93
9	D	302	LMT	C1'-O5'-C5'	-2.51	108.76	113.69
7	B	501	FMN	C4A-C10-N10	2.49	120.12	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	506	UQ1	O3-C3-C4	2.44	124.82	116.56
9	B	504	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
11	B	506	UQ1	O2-C2-C1	2.42	124.76	116.56
7	C	1000	FMN	C4A-C10-N1	-2.40	119.16	124.73
9	B	503	LMT	C1'-O5'-C5'	-2.38	109.02	113.69
7	C	1000	FMN	O4-C4-C4A	-2.37	120.30	126.60
9	B	504	LMT	C3'-C4'-C5'	-2.37	105.50	110.93
7	B	501	FMN	C4A-C10-N1	-2.36	119.25	124.73
10	D	301	3PE	O12-P-O14	2.35	123.86	112.24
10	B	508	3PE	O12-P-O14	2.35	123.85	112.24
7	B	501	FMN	O4-C4-C4A	-2.32	120.43	126.60
7	C	1000	FMN	C10-C4A-N5	-2.32	119.93	124.86
10	B	505	3PE	O12-P-O14	2.32	123.70	112.24
10	B	507	3PE	O12-P-O14	2.32	123.69	112.24
7	B	501	FMN	C9A-C5A-N5	-2.29	119.94	122.43
11	B	506	UQ1	O2-C2-C3	-2.15	115.53	123.64
9	B	504	LMT	O5B-C5B-C4B	2.10	113.51	109.69
9	B	503	LMT	O5B-C5B-C4B	2.10	113.50	109.69
7	C	1000	FMN	C4-C4A-C10	2.07	120.26	116.79
11	B	506	UQ1	O3-C3-C2	-2.07	115.85	123.64
7	B	501	FMN	C4-C4A-C10	2.06	120.25	116.79
8	B	502	RBF	C4-N3-C2	-2.04	121.87	125.64
9	B	503	LMT	C3'-C4'-C5'	-2.04	106.25	110.93

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	LMT	C2'-C1'-O1'-C1
9	B	503	LMT	O5'-C1'-O1'-C1
9	B	504	LMT	C2'-C1'-O1'-C1
9	B	504	LMT	O5'-C1'-O1'-C1
10	B	505	3PE	C1-O11-P-O12
10	B	505	3PE	C11-O13-P-O14
10	B	505	3PE	O13-C11-C12-N
10	B	507	3PE	C11-O13-P-O12
10	B	507	3PE	C2-C1-O11-P
10	B	507	3PE	C12-C11-O13-P
10	B	507	3PE	C22-C21-O21-C2
10	D	301	3PE	C11-O13-P-O11
10	D	301	3PE	C11-O13-P-O12
10	D	301	3PE	C3-C2-O21-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	F	1501	FAD	N10-C1'-C2'-O2'
14	F	1501	FAD	N10-C1'-C2'-C3'
10	B	508	3PE	O32-C31-O31-C3
9	B	504	LMT	C2B-C1B-O1B-C4'
10	D	301	3PE	O22-C21-O21-C2
10	B	508	3PE	C32-C31-O31-C3
10	D	301	3PE	C22-C21-O21-C2
10	B	507	3PE	O22-C21-O21-C2
9	D	302	LMT	C4'-C5'-C6'-O6'
14	F	1501	FAD	O4B-C4B-C5B-O5B
14	F	1501	FAD	C3B-C4B-C5B-O5B
9	D	302	LMT	O5'-C5'-C6'-O6'
9	B	503	LMT	O5B-C1B-O1B-C4'
14	F	1501	FAD	O4B-C1B-N9A-C4A
11	B	506	UQ1	C3-C2-O2-CM2
11	B	506	UQ1	C2-C3-O3-CM3
9	B	503	LMT	C5'-C4'-O1B-C1B
9	B	504	LMT	C5'-C4'-O1B-C1B
10	B	505	3PE	C1-O11-P-O13
10	B	505	3PE	C11-O13-P-O11
11	B	506	UQ1	C1-C2-O2-CM2
10	B	508	3PE	C26-C27-C28-C29
9	D	302	LMT	C6-C7-C8-C9
9	D	302	LMT	C2'-C1'-O1'-C1
9	B	503	LMT	C3'-C4'-O1B-C1B
10	B	507	3PE	C3D-C3E-C3F-C3G
14	F	1501	FAD	O4B-C1B-N9A-C8A
9	B	504	LMT	O5B-C1B-O1B-C4'
10	B	507	3PE	C38-C39-C3A-C3B
10	B	505	3PE	C31-C32-C33-C34
10	B	508	3PE	C31-C32-C33-C34
10	D	301	3PE	C32-C31-O31-C3
9	D	302	LMT	O5'-C1'-O1'-C1
9	D	302	LMT	C2-C3-C4-C5
10	B	508	3PE	C1-O11-P-O13
11	B	506	UQ1	C4-C3-O3-CM3
10	D	301	3PE	C32-C33-C34-C35
10	D	301	3PE	O32-C31-O31-C3
10	B	507	3PE	C3A-C3B-C3C-C3D
9	B	504	LMT	C3'-C4'-O1B-C1B
10	B	507	3PE	C3C-C3D-C3E-C3F
10	B	505	3PE	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

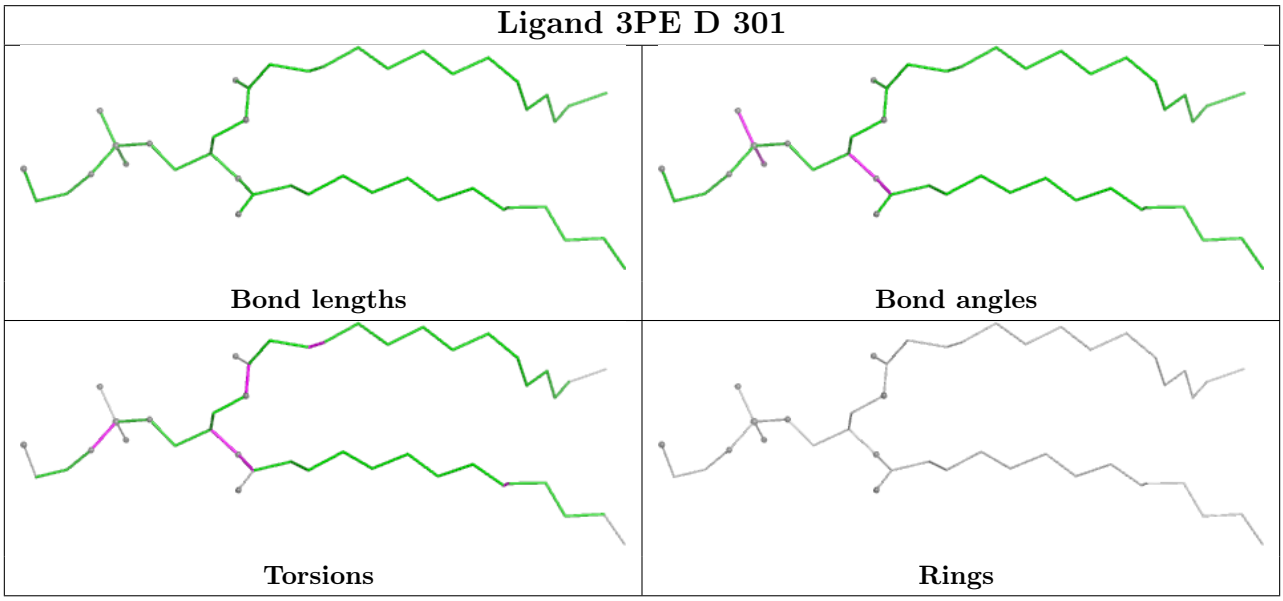
Mol	Chain	Res	Type	Atoms
10	B	505	3PE	C33-C34-C35-C36
10	B	508	3PE	C28-C29-C2A-C2B
10	D	301	3PE	C28-C29-C2A-C2B
10	B	505	3PE	C23-C24-C25-C26
9	B	504	LMT	C11-C10-C9-C8
14	F	1501	FAD	C5'-O5'-P-O3P
10	B	505	3PE	C11-O13-P-O12
10	B	508	3PE	C1-O11-P-O12
10	B	507	3PE	C2A-C2B-C2C-C2D
10	B	505	3PE	C12-C11-O13-P
10	B	505	3PE	O11-C1-C2-O21
9	B	503	LMT	C11-C10-C9-C8
10	B	507	3PE	C21-C22-C23-C24
7	B	501	FMN	C4'-C5'-O5'-P
10	B	507	3PE	C1-O11-P-O13
9	D	302	LMT	C7-C8-C9-C10
10	B	507	3PE	C23-C24-C25-C26
10	B	505	3PE	C1-C2-O21-C21
10	B	505	3PE	C3-C2-O21-C21
10	B	508	3PE	C3-C2-O21-C21
9	B	503	LMT	C3-C4-C5-C6
9	D	302	LMT	C5'-C4'-O1B-C1B
10	B	508	3PE	O21-C21-C22-C23
10	B	507	3PE	C2B-C2C-C2D-C2E
10	B	507	3PE	C39-C3A-C3B-C3C
10	B	507	3PE	C33-C34-C35-C36
10	B	505	3PE	C21-C22-C23-C24
14	F	1501	FAD	C2B-C1B-N9A-C8A
9	B	504	LMT	C5-C6-C7-C8
10	B	508	3PE	C2-C1-O11-P
10	B	507	3PE	C1-O11-P-O14
10	B	507	3PE	C11-O13-P-O14
10	B	508	3PE	O22-C21-C22-C23
10	B	508	3PE	C37-C38-C39-C3A
10	B	507	3PE	O13-C11-C12-N
9	B	503	LMT	C7-C8-C9-C10
10	B	508	3PE	C12-C11-O13-P
9	B	504	LMT	C2-C1-O1'-C1'

There are no ring outliers.

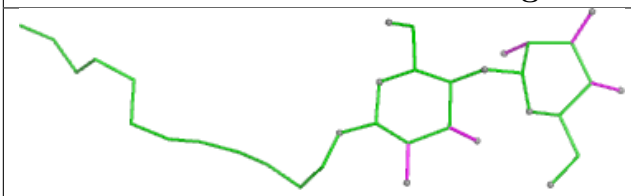
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	LMT	1	0
11	B	506	UQ1	2	0
7	B	501	FMN	3	0
8	B	502	RBF	1	0
9	D	302	LMT	2	0
7	C	1000	FMN	1	0
14	F	1501	FAD	2	0

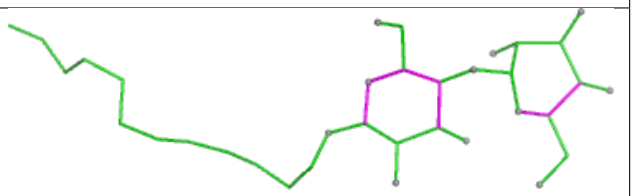
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



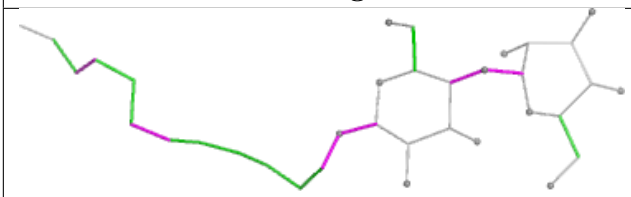
Ligand LMT B 504



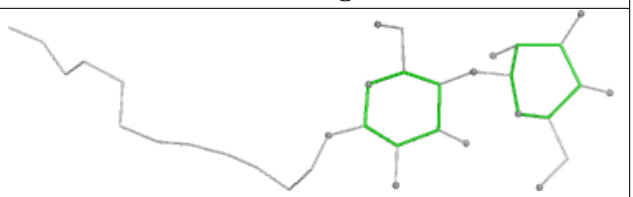
Bond lengths



Bond angles

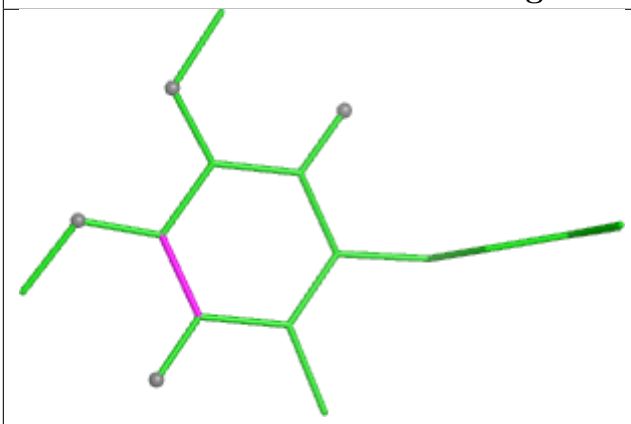


Torsions

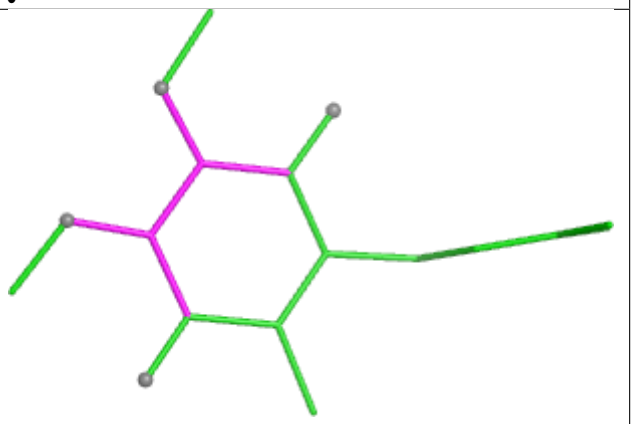


Rings

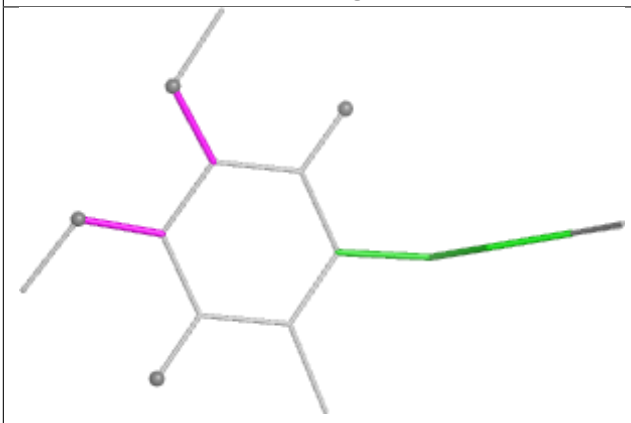
Ligand UQ1 B 506



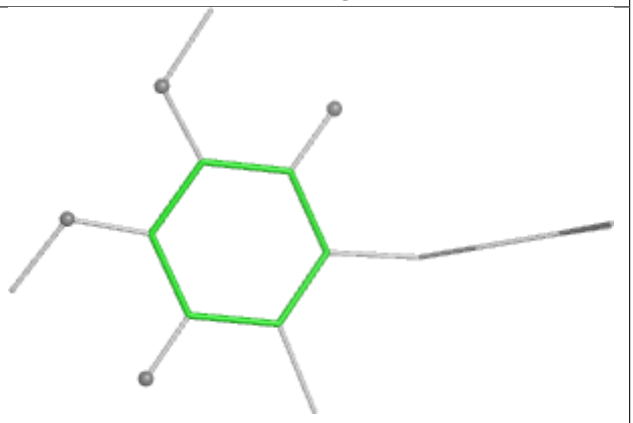
Bond lengths



Bond angles

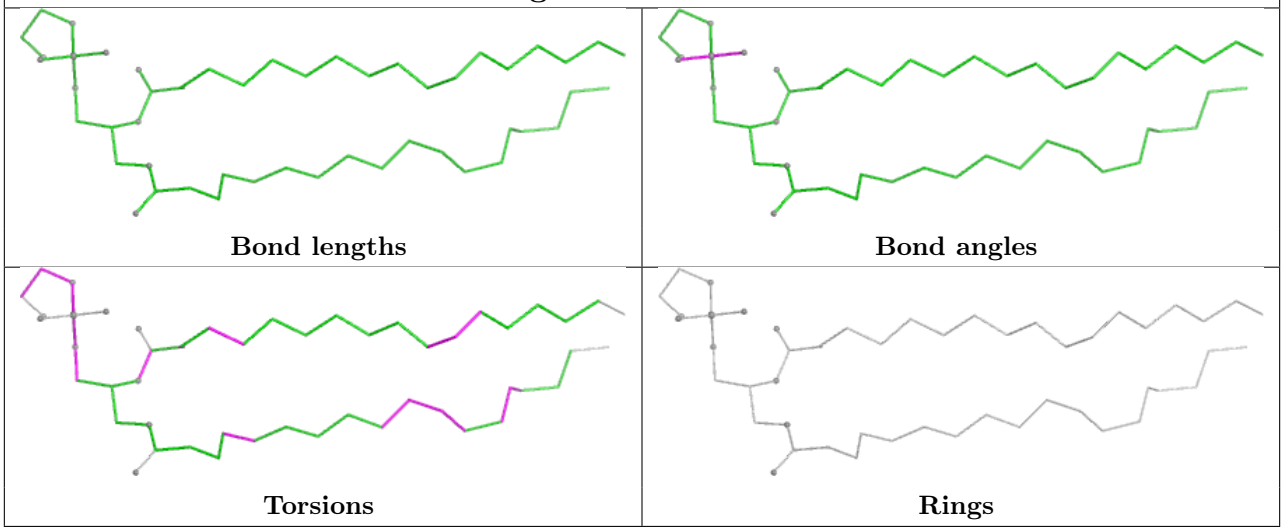


Torsions

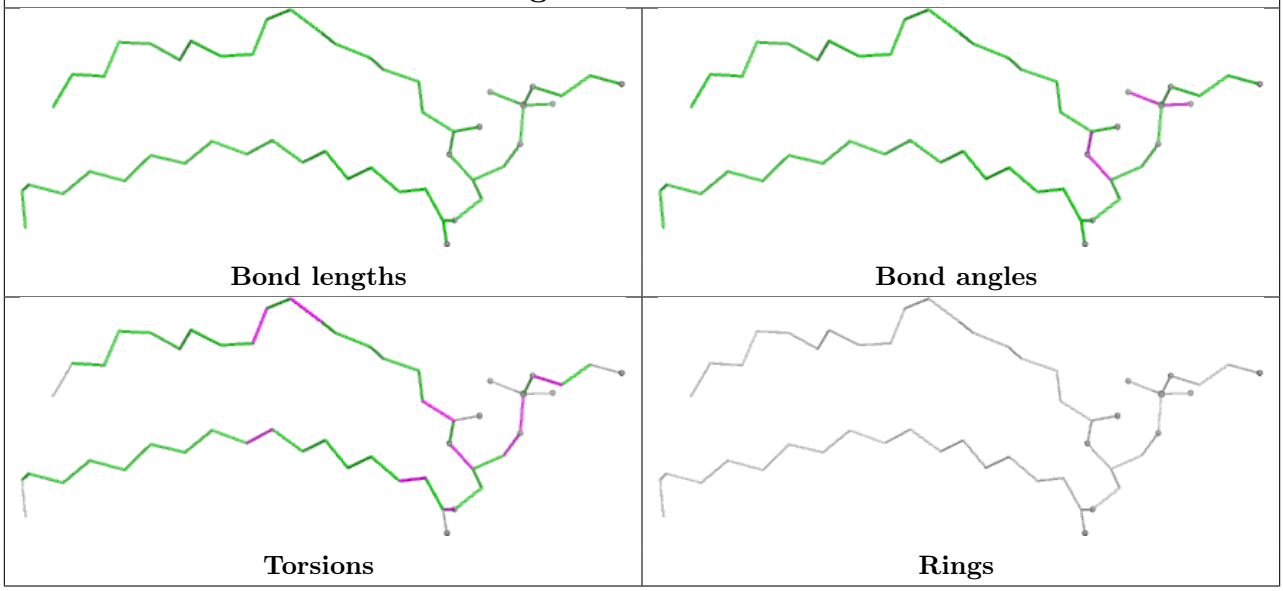


Rings

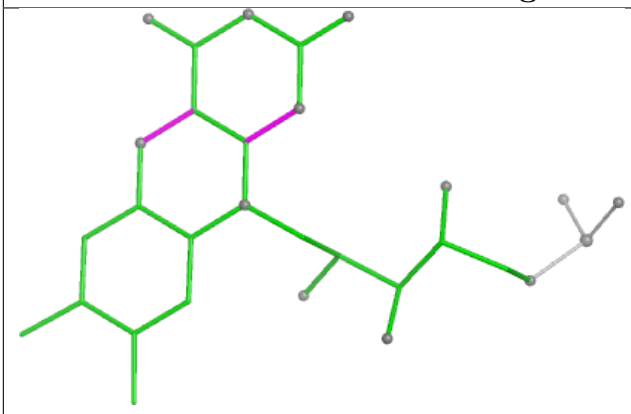
Ligand 3PE B 507



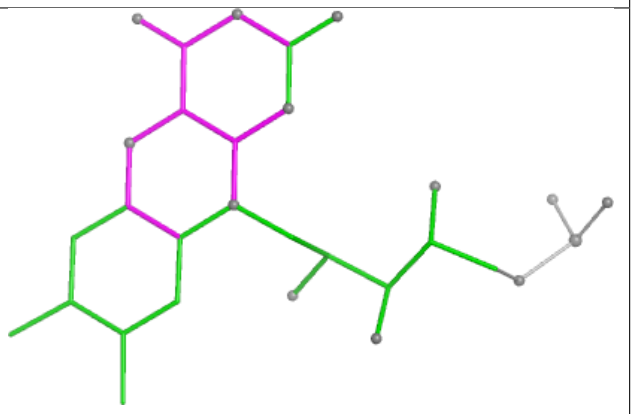
Ligand 3PE B 508



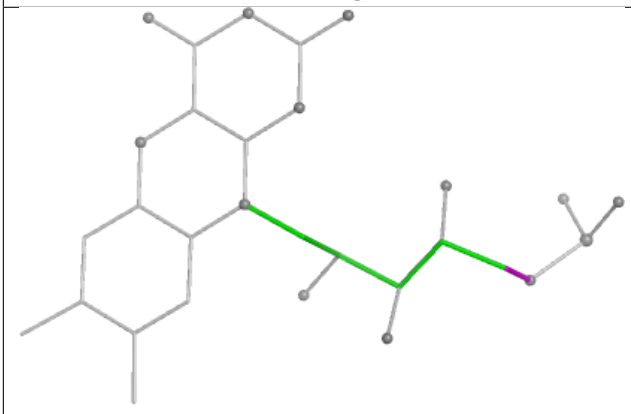
Ligand FMN B 501



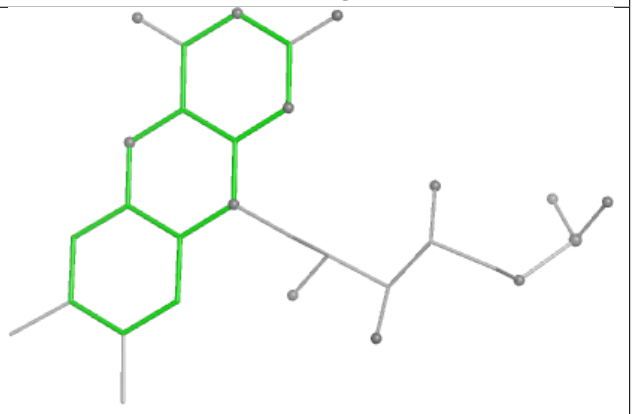
Bond lengths



Bond angles

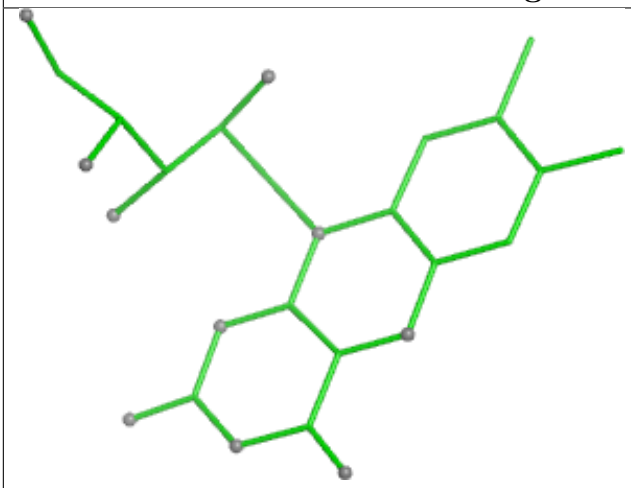


Torsions

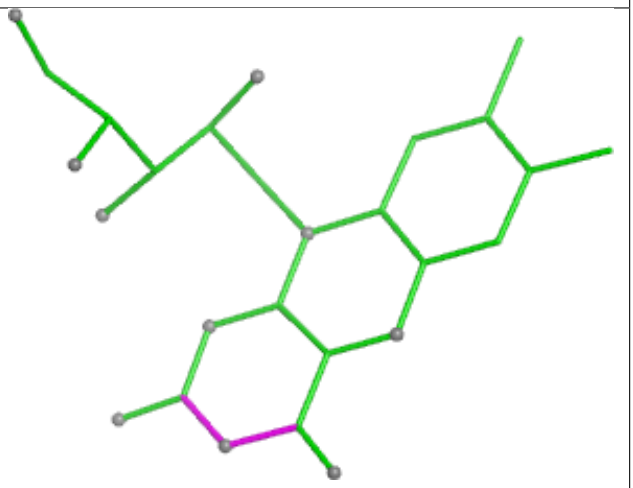


Rings

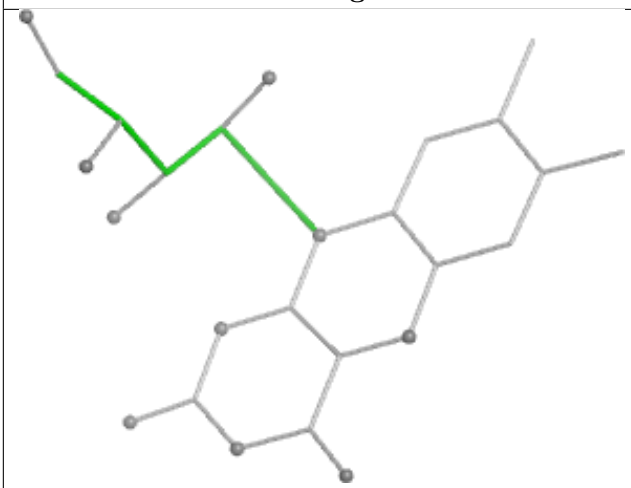
Ligand RBF B 502



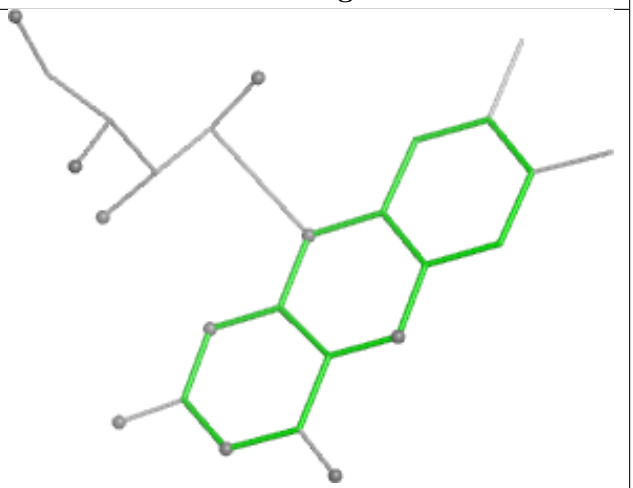
Bond lengths



Bond angles

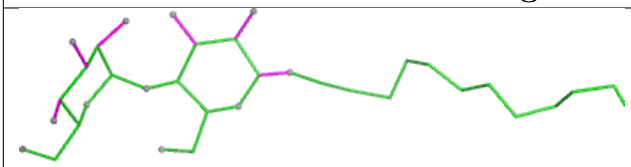


Torsions

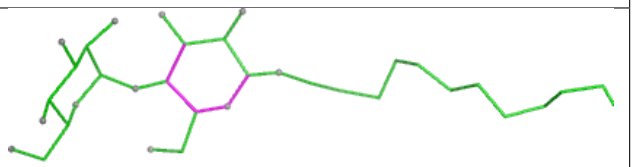


Rings

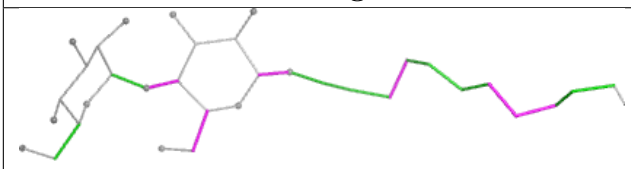
Ligand LMT D 302



Bond lengths



Bond angles

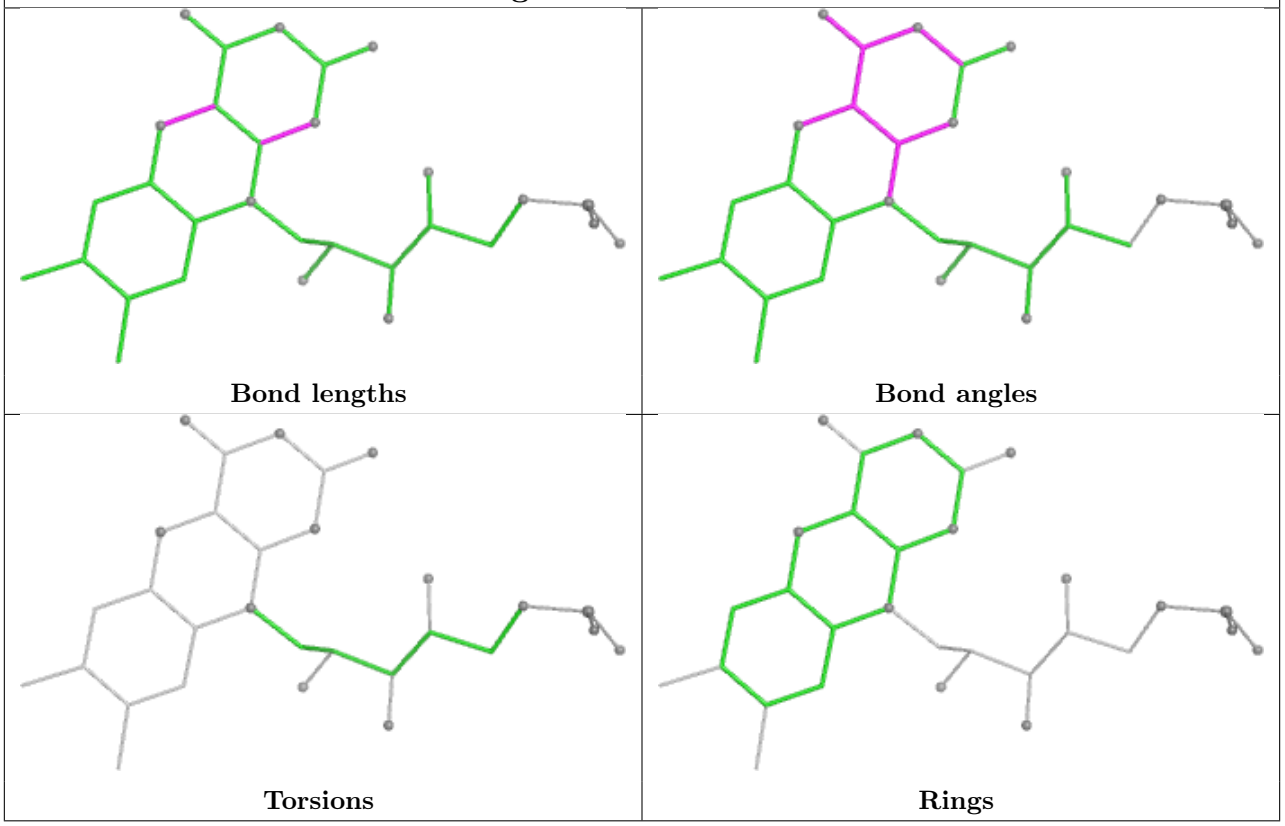


Torsions

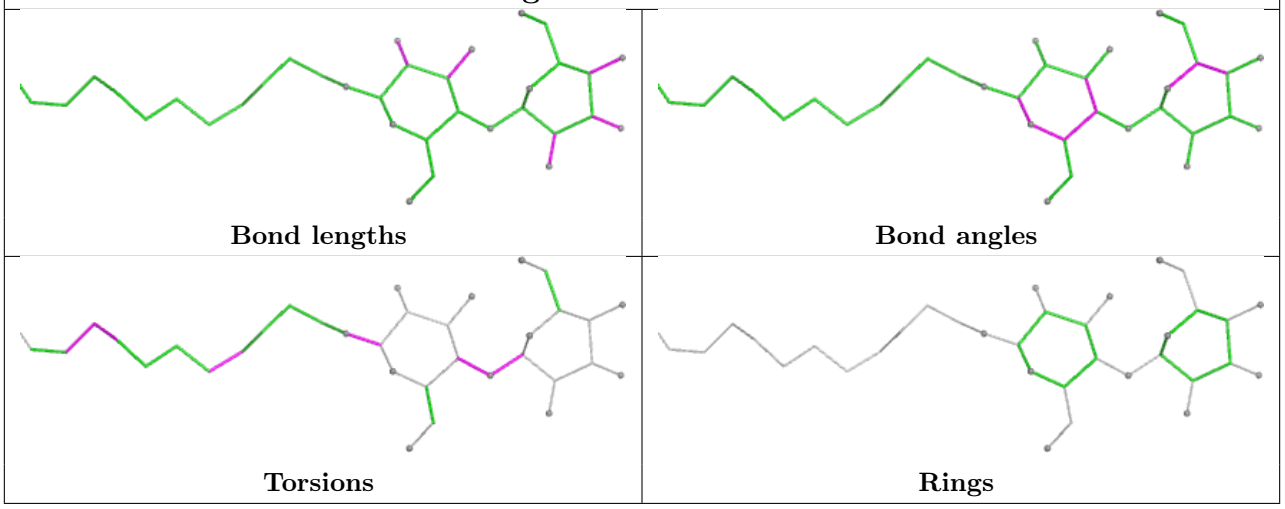


Rings

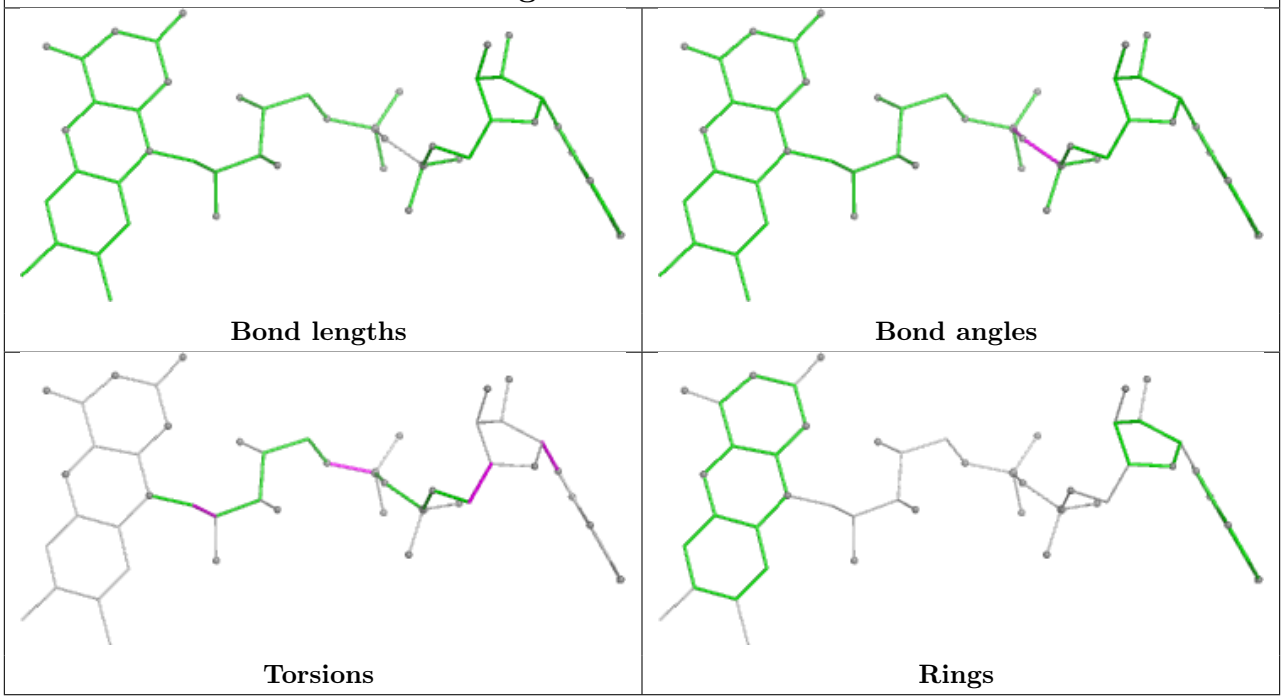
Ligand FMN C 1000



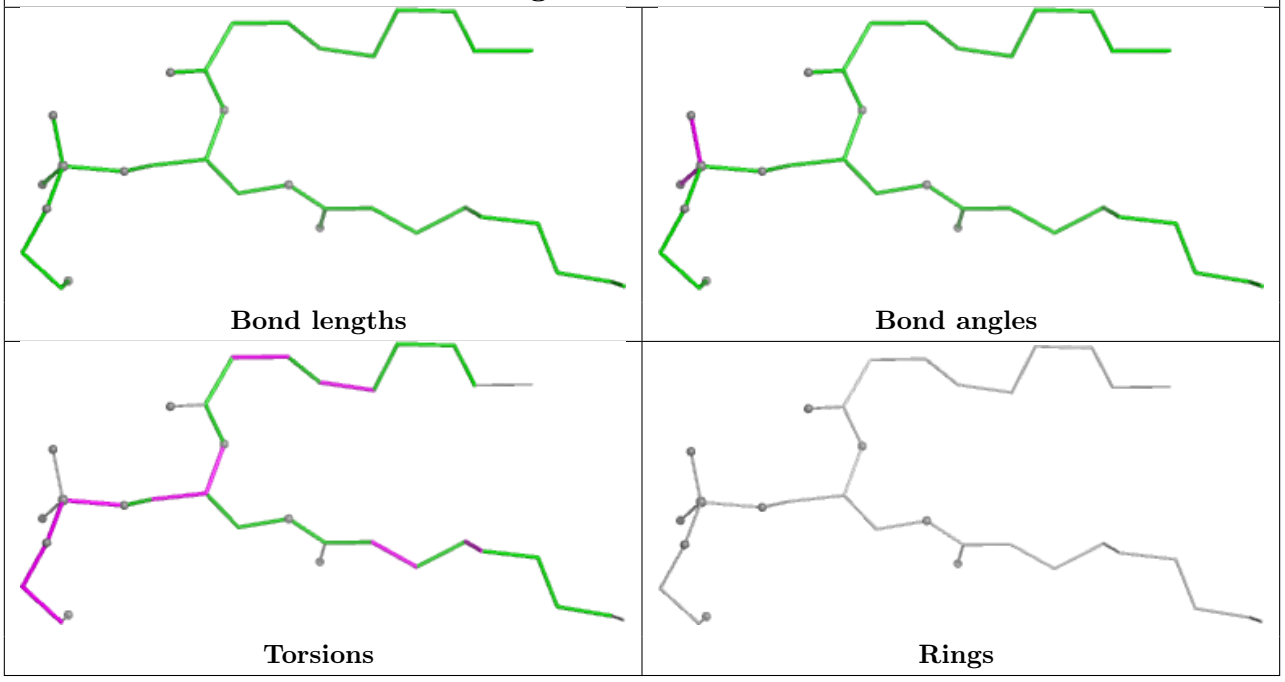
Ligand LMT B 503



Ligand FAD F 1501



Ligand 3PE B 505



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.

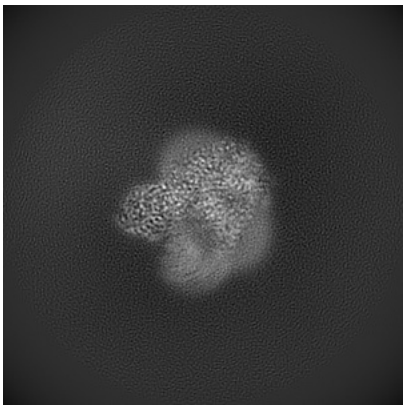
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15091. These allow visual inspection of the internal detail of the map and identification of artifacts.

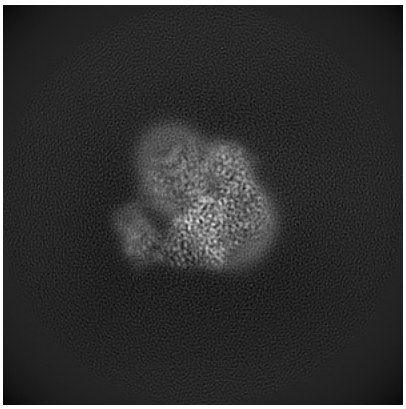
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

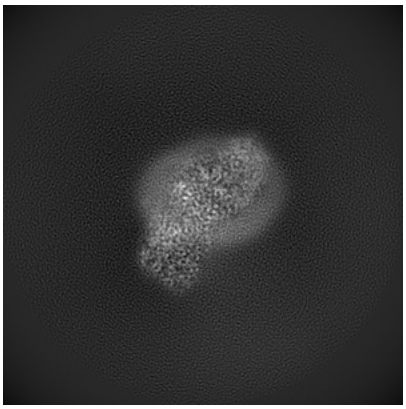
6.1.1 Primary map



X

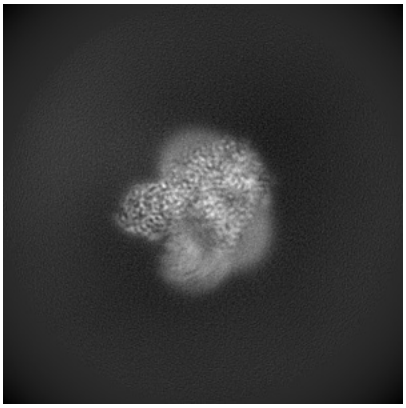


Y

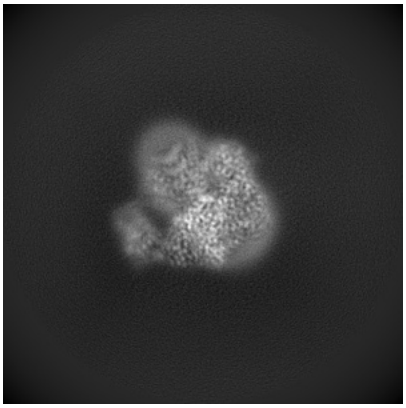


Z

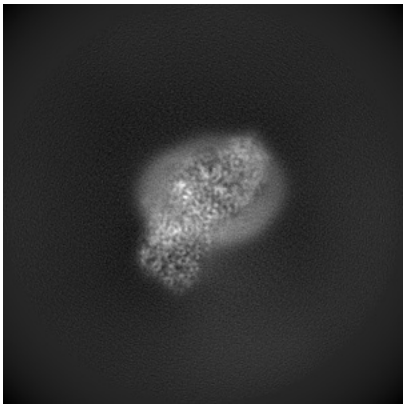
6.1.2 Raw map



X



Y

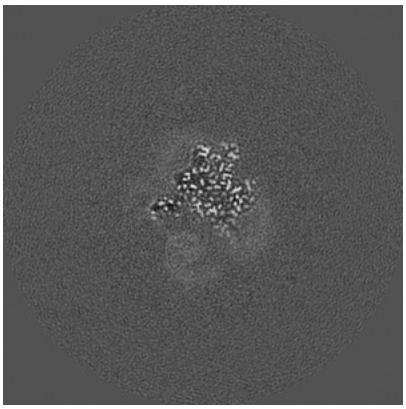


Z

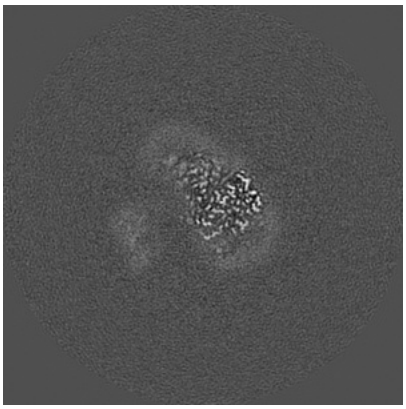
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

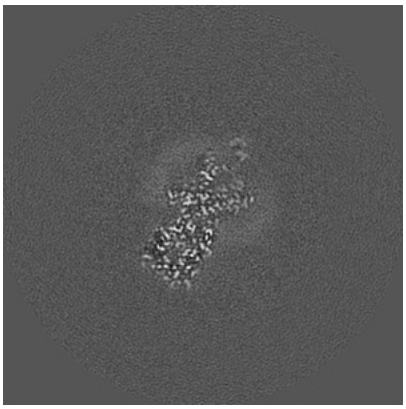
6.2.1 Primary map



X Index: 160

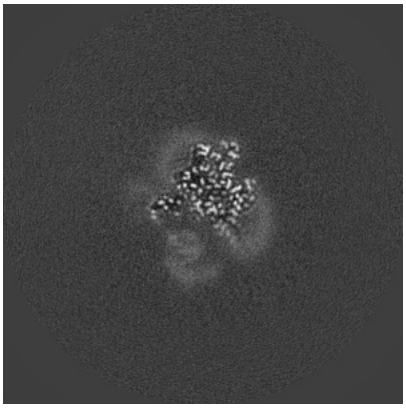


Y Index: 160

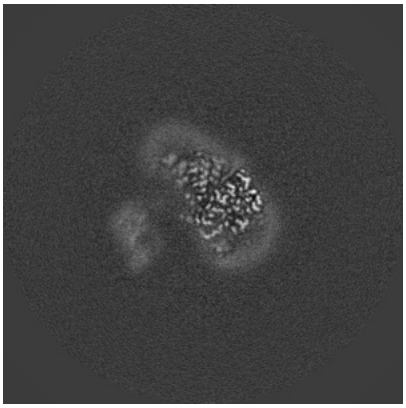


Z Index: 160

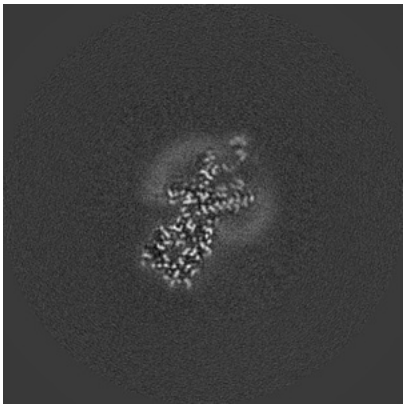
6.2.2 Raw map



X Index: 160



Y Index: 160

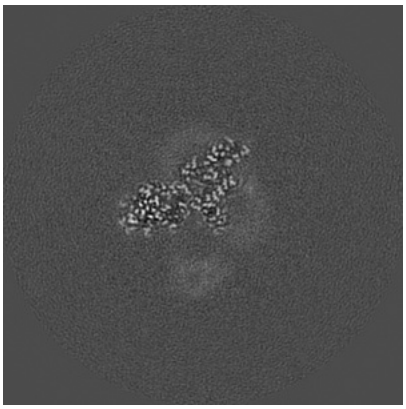


Z Index: 160

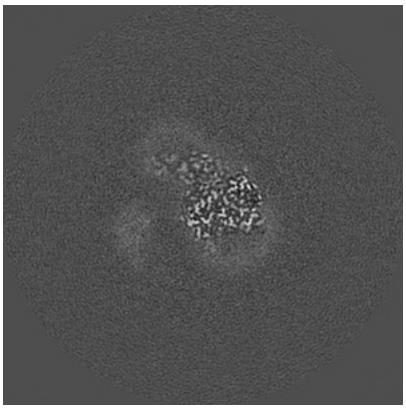
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

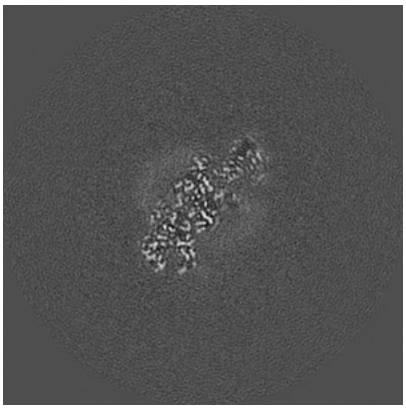
6.3.1 Primary map



X Index: 148

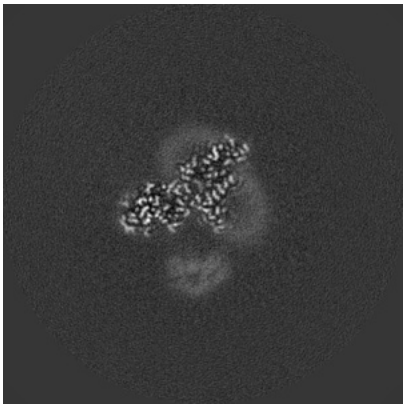


Y Index: 165

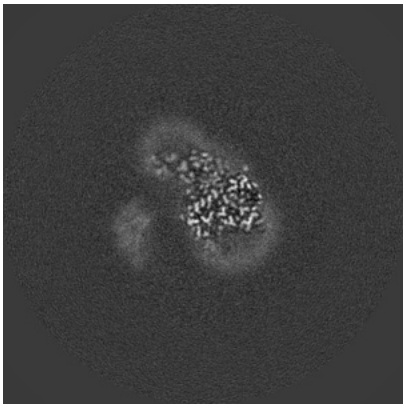


Z Index: 174

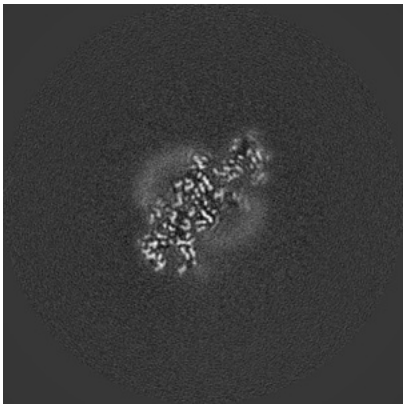
6.3.2 Raw map



X Index: 147



Y Index: 165

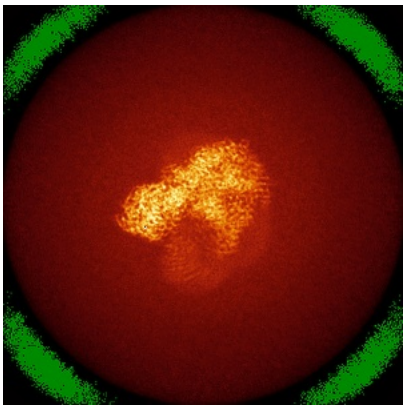


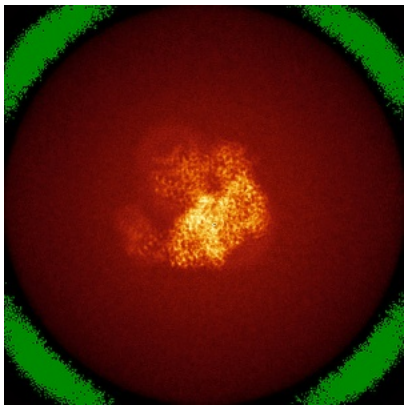
Z Index: 174

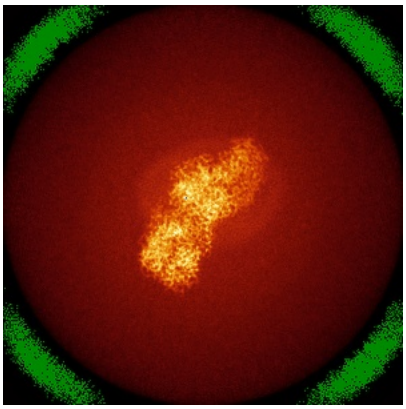
The images above show the largest variance slices of the map in three orthogonal directions.

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

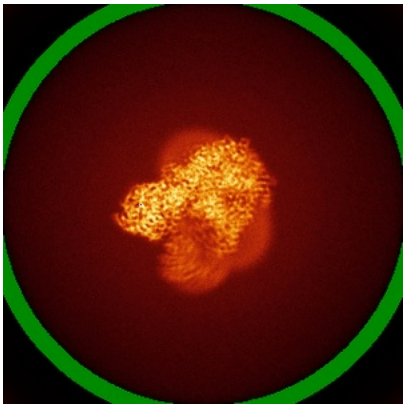
6.4.1 Primary map

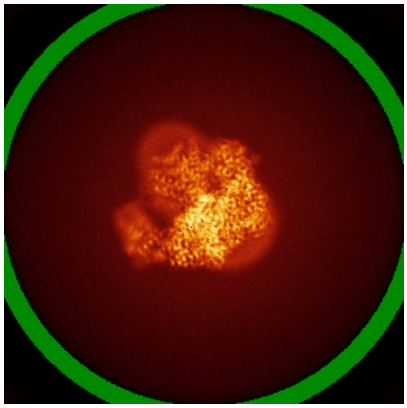

X

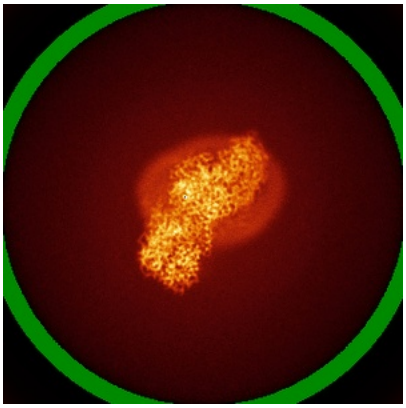

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

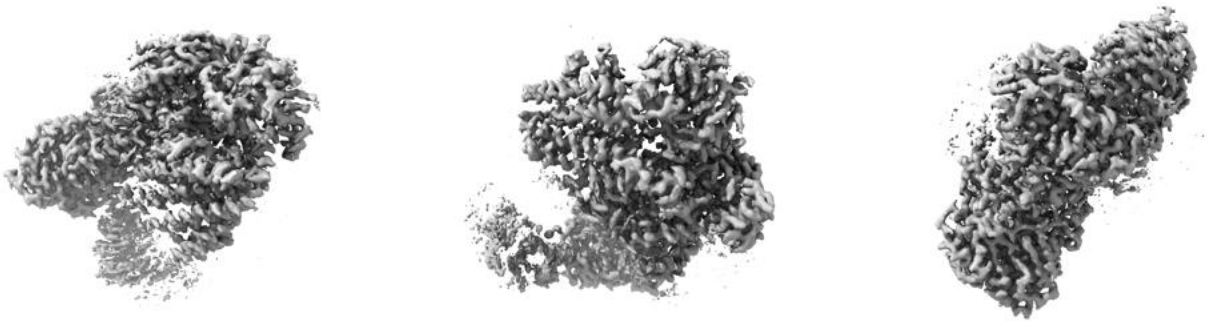
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

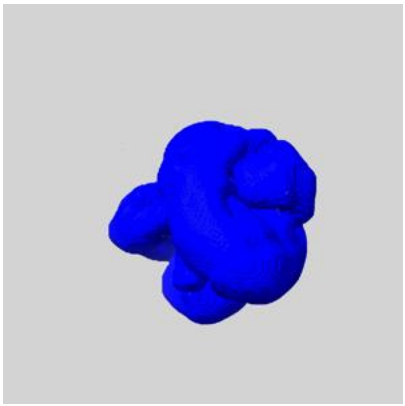
6.6 Mask visualisation

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

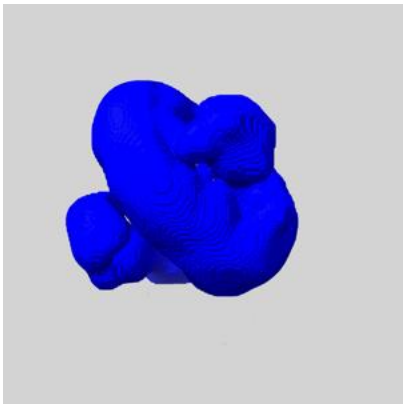
A mask typically either:

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

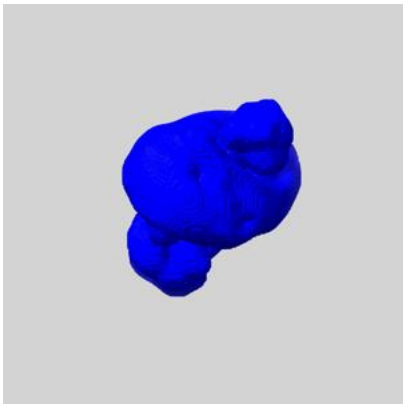
6.6.1 emd_15091_msk_1.map



X



Y

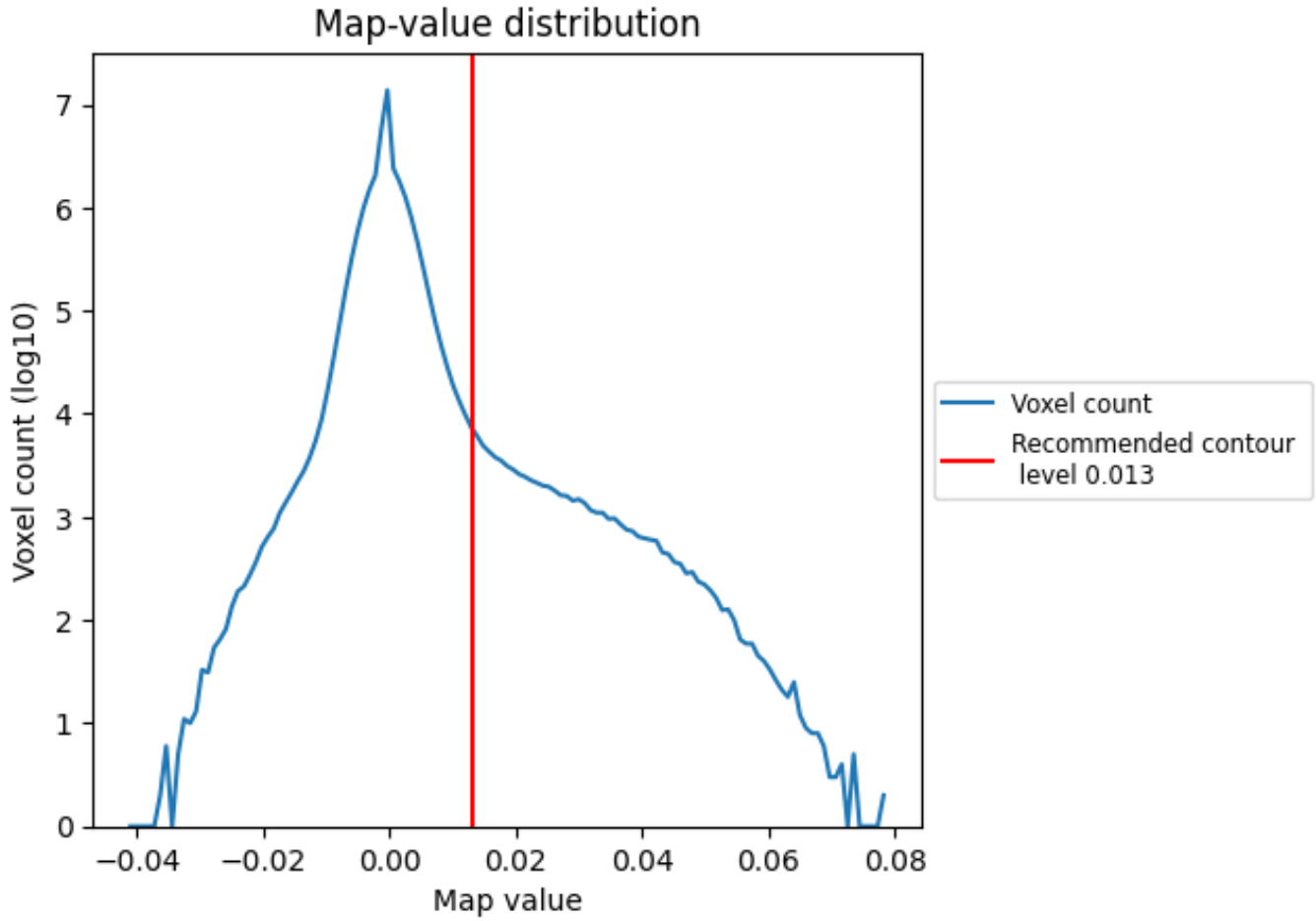


Z

7 Map analysis

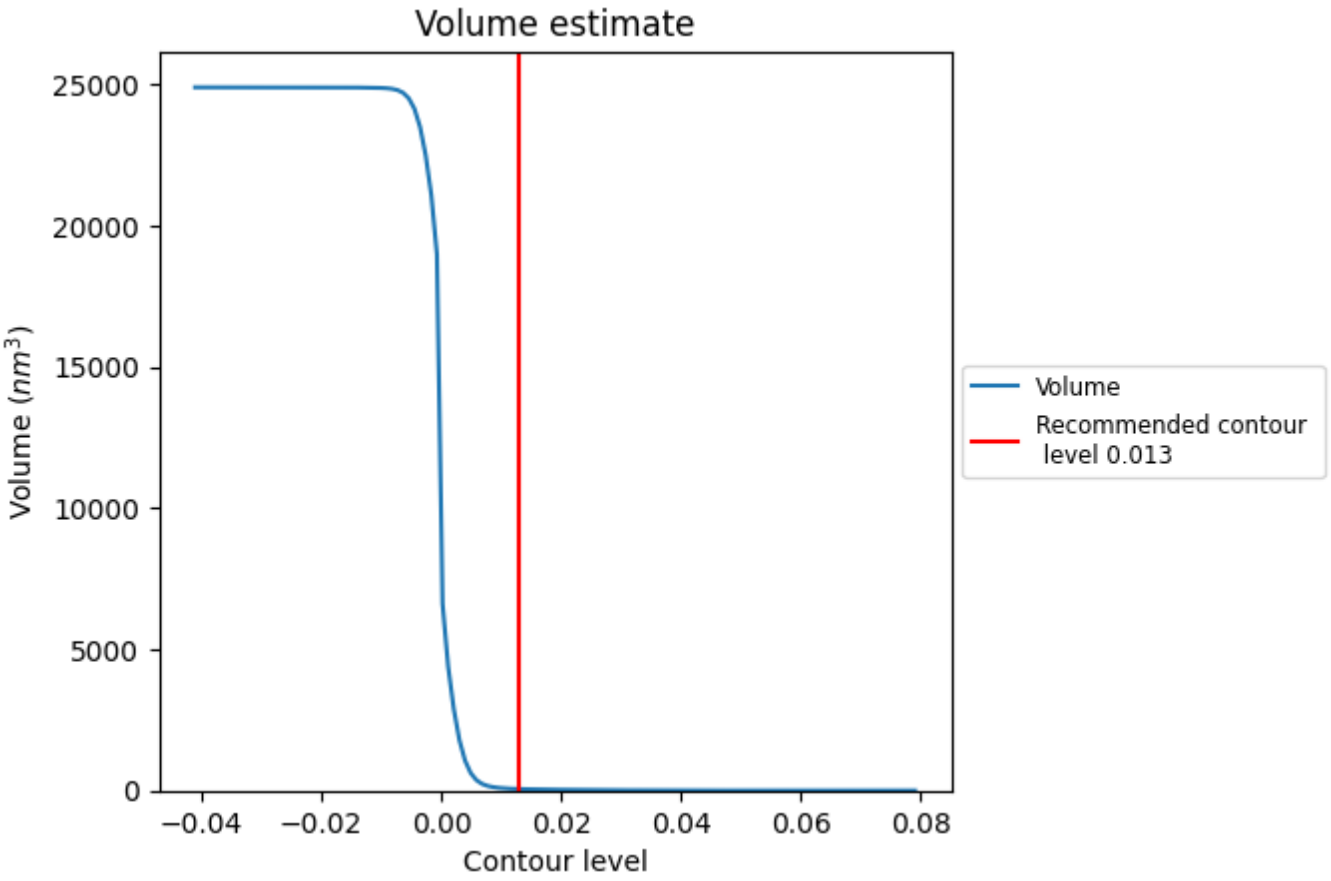
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

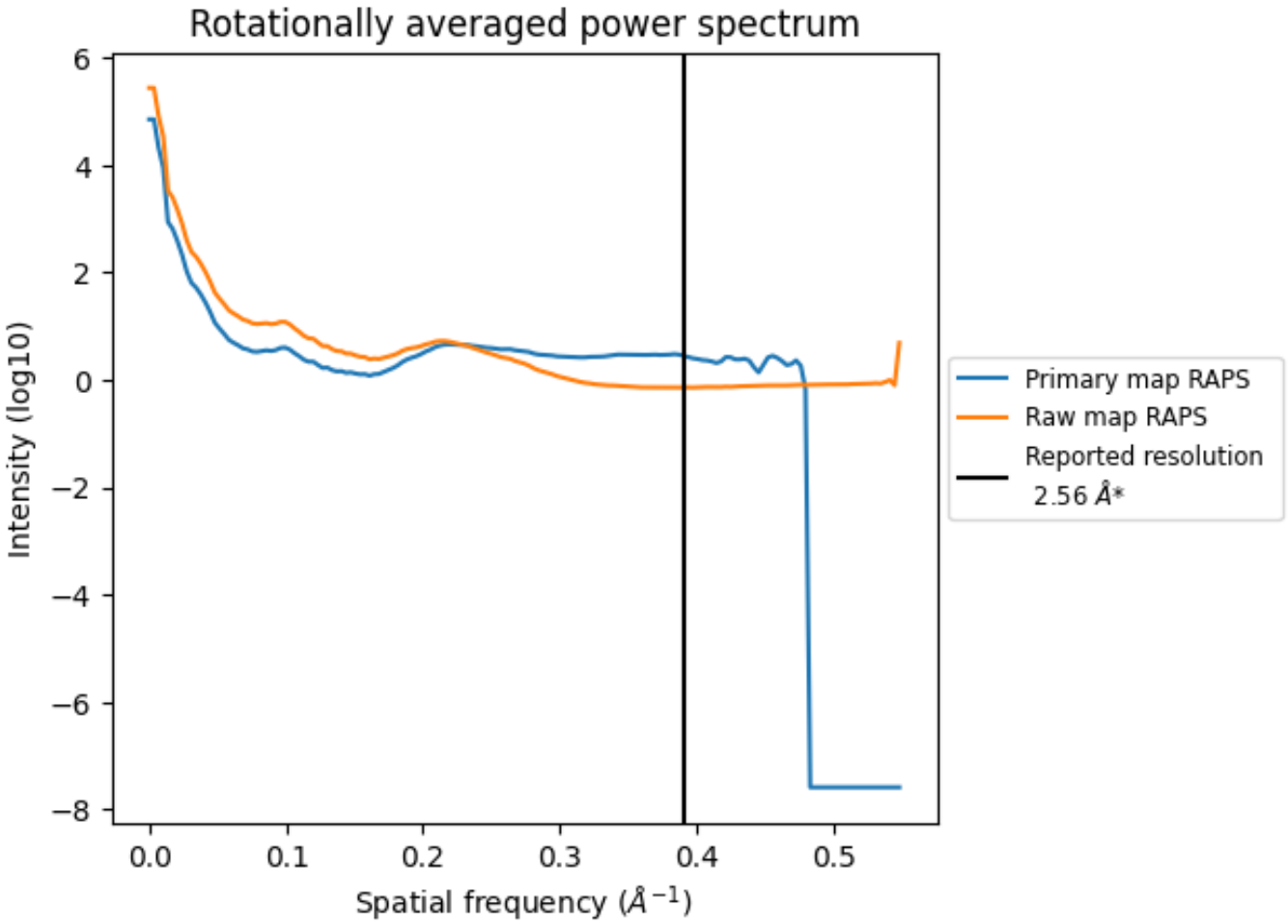
7.2 Volume estimate



The volume at the recommended contour level is 55 nm^3; this corresponds to an approximate mass of 49 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)

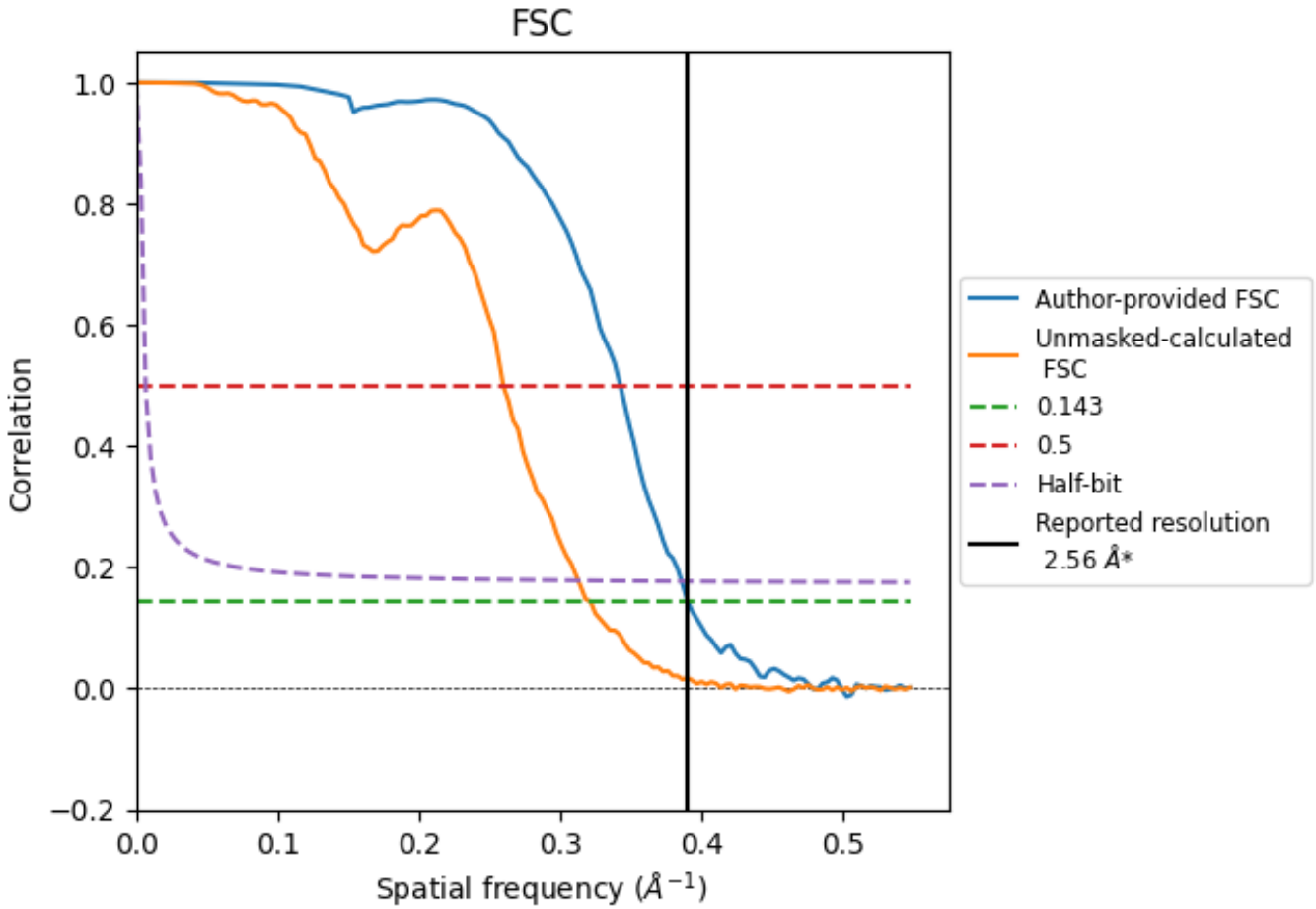


*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8.2 Resolution estimates (i)

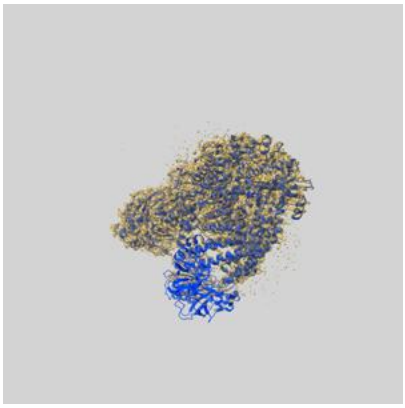
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	2.92	2.59
Unmasked-calculated*	3.11	3.84	3.19

*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 3.11 differs from the reported value 2.56 by more than 10 %

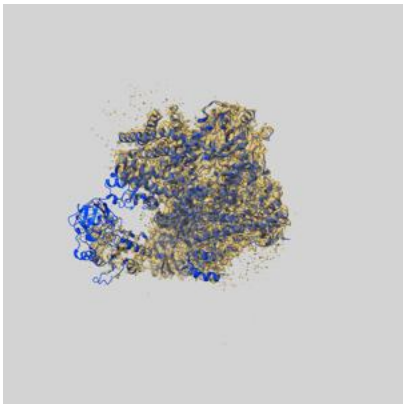
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15091 and PDB model 8A1W. Per-residue inclusion information can be found in section 3 on page 11.

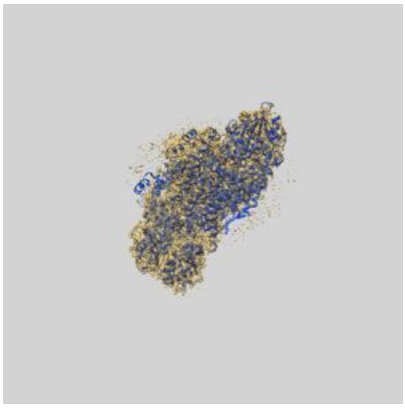
9.1 Map-model overlay



X



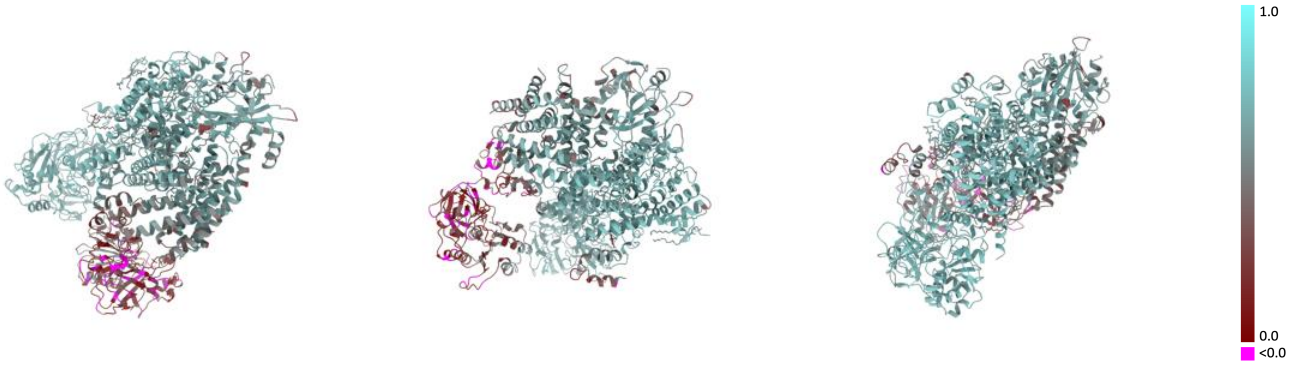
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

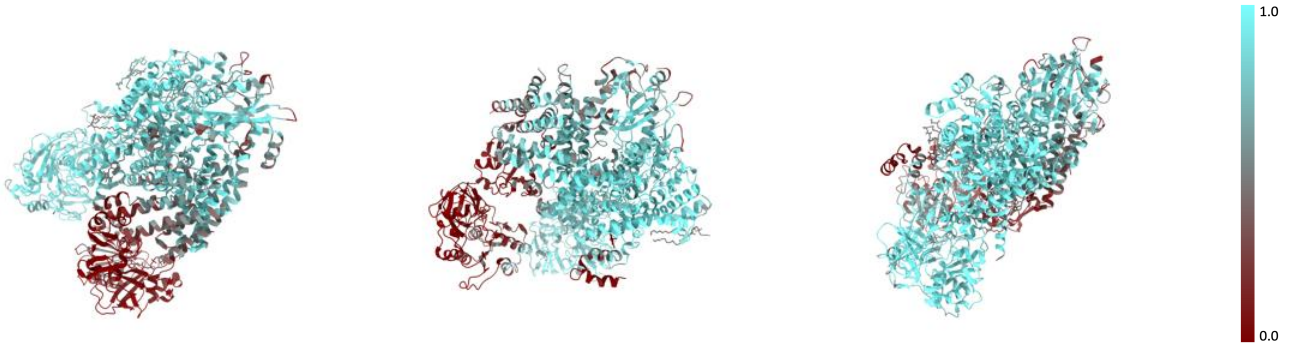
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

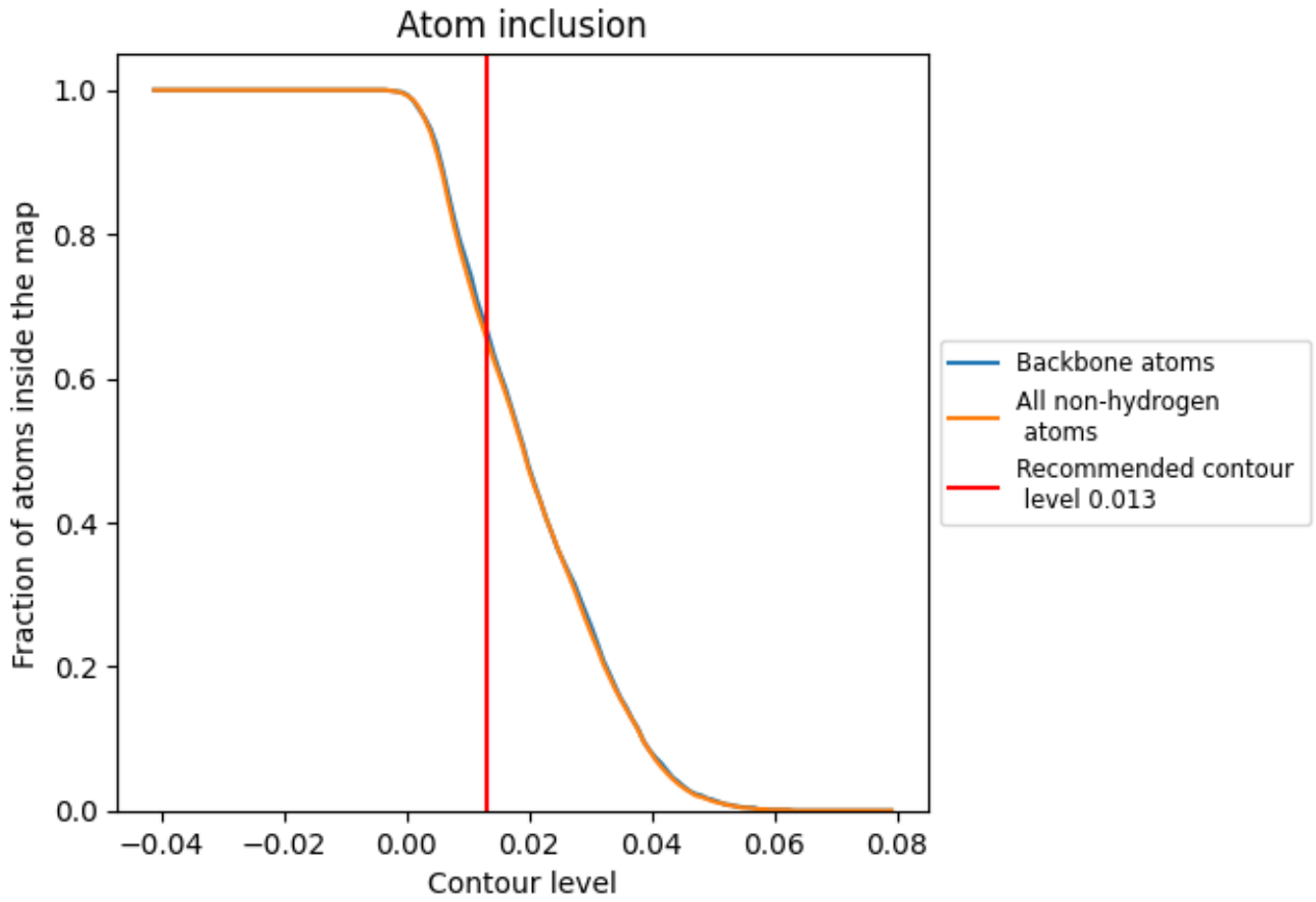
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.5550
A	0.9070	0.6770
B	0.8530	0.6580
C	0.6810	0.5730
D	0.7730	0.6170
E	0.6840	0.5870
F	0.1180	0.2590

