Full wwPDB EM Validation Report ⓘ

Nov 14, 2023 – 01:28 pm GMT

PDB ID	:	8A1U
EMDB ID	:	EMD-15089
Title	:	Sodium pumping NADH-quinone oxidoreductase with substrates NADH and Q2
Authors	:	Hau, J.-L.; Kaltwasser, S.; Vonck, J.; Fritz, G.; Steuber, J.
Deposited on	:	2022-06-02
Resolution	:	2.86 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:

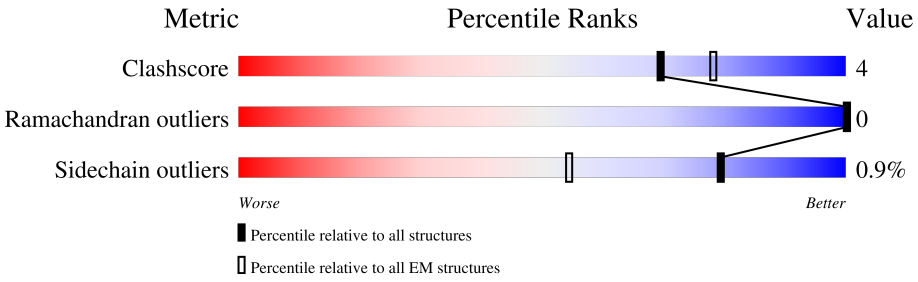
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	468	87% 8% ·
2	B	415	86% 9% 5%
3	C	257	9% 89% 8% ·
4	D	210	6% 91% 5% ·
5	E	198	11% 92% 8% ·
6	F	408	68% 88% 12% ·

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 30479 atoms, of which 15221 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	448	6907	2176	3475	588	651	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 Q9KPS1
A	-20	GLY	-	expression tag	UNP Q9KPS1
A	-19	SER	-	expression tag	UNP Q9KPS1
A	-18	SER	-	expression tag	UNP Q9KPS1
A	-17	HIS	-	expression tag	UNP Q9KPS1
A	-16	HIS	-	expression tag	UNP Q9KPS1
A	-15	HIS	-	expression tag	UNP Q9KPS1
A	-14	HIS	-	expression tag	UNP Q9KPS1
A	-13	HIS	-	expression tag	UNP Q9KPS1
A	-12	HIS	-	expression tag	UNP Q9KPS1
A	-11	SER	-	expression tag	UNP Q9KPS1
A	-10	SER	-	expression tag	UNP Q9KPS1
A	-9	GLY	-	expression tag	UNP Q9KPS1
A	-8	LEU	-	expression tag	UNP Q9KPS1
A	-7	GLU	-	expression tag	UNP Q9KPS1
A	-6	VAL	-	expression tag	UNP Q9KPS1
A	-5	LEU	-	expression tag	UNP Q9KPS1
A	-4	PHE	-	expression tag	UNP Q9KPS1
A	-3	GLN	-	expression tag	UNP Q9KPS1
A	-2	GLY	-	expression tag	UNP Q9KPS1
A	-1	PRO	-	expression tag	UNP Q9KPS1
A	0	HIS	-	expression tag	UNP Q9KPS1

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	395	Total	C	H	N	O	S	0	0
			6064	2012	3025	494	511	22		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	251	Total	C	H	N	O	S	0	0
			3814	1204	1912	328	366	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	202	Total	C	H	N	O	S	0	0
			3173	1026	1629	244	264	10		

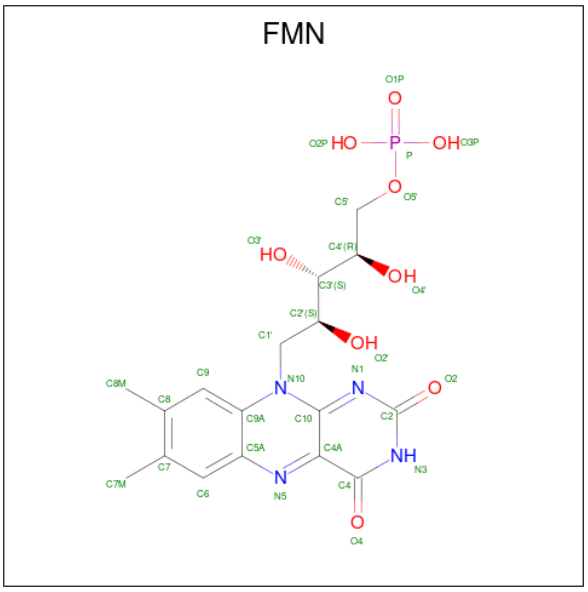
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	197	Total	C	H	N	O	S	0	0
			3078	1008	1574	229	257	10		

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

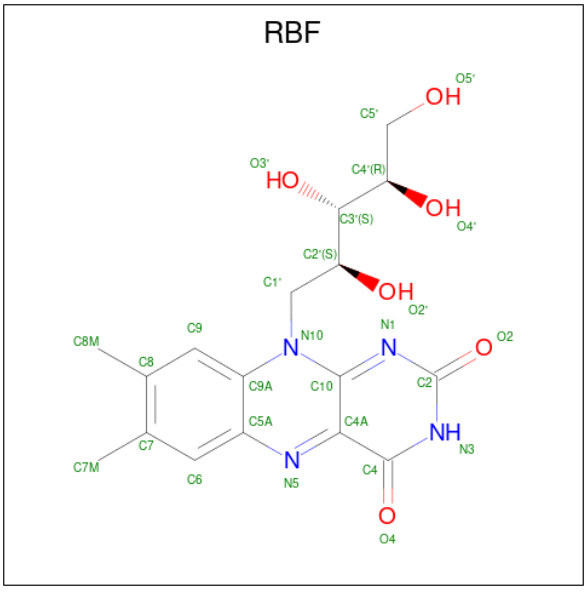
Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	405	Total	C	H	N	O	S	0	0
			6232	2018	3083	516	592	23		

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: 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	

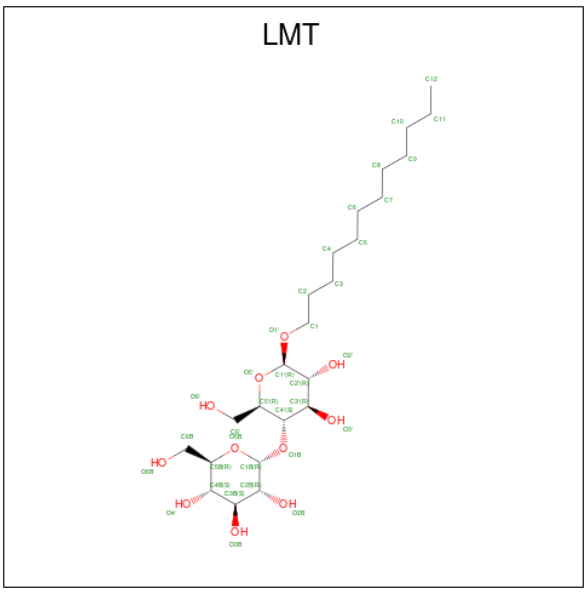
- Molecule 8 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



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

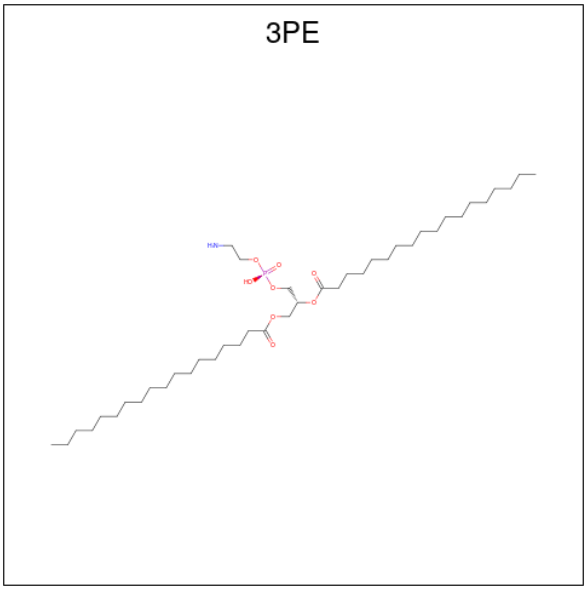
- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:

$C_{24}H_{46}O_{11}$).



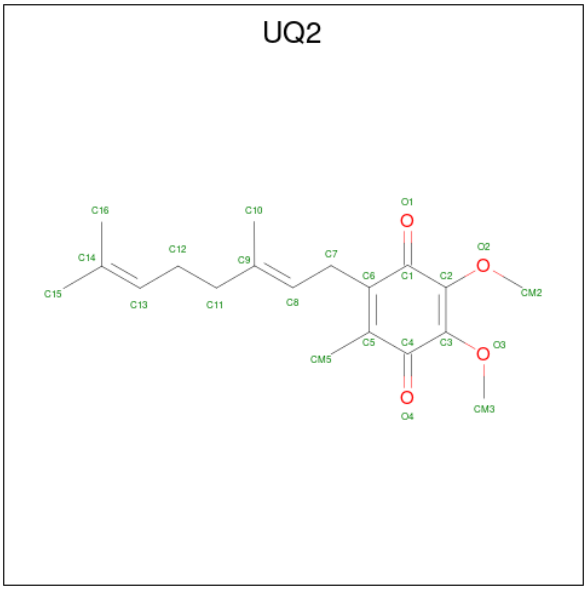
Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	H	O	0
			74	24	39	11	
9	B	1	Total	C	H	O	0
			74	24	39	11	
9	D	1	Total	C	H	O	0
			74	24	39	11	

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



Mol	Chain	Residues	Atoms						AltConf
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
			73	23	40	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-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).

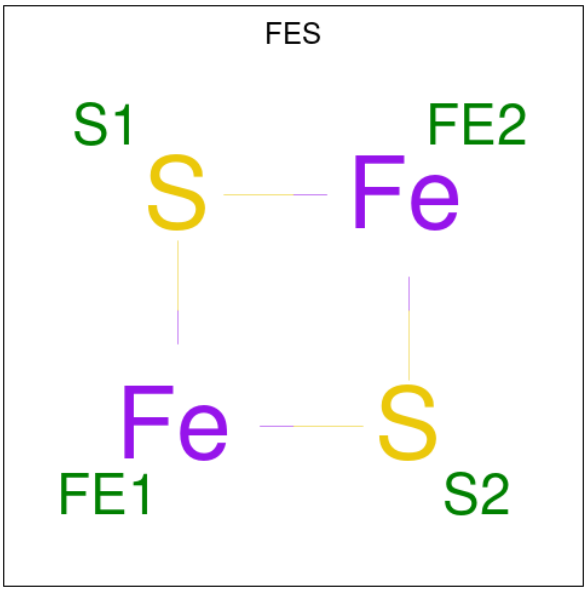


Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	H	O	0
			49	19	26	4	

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

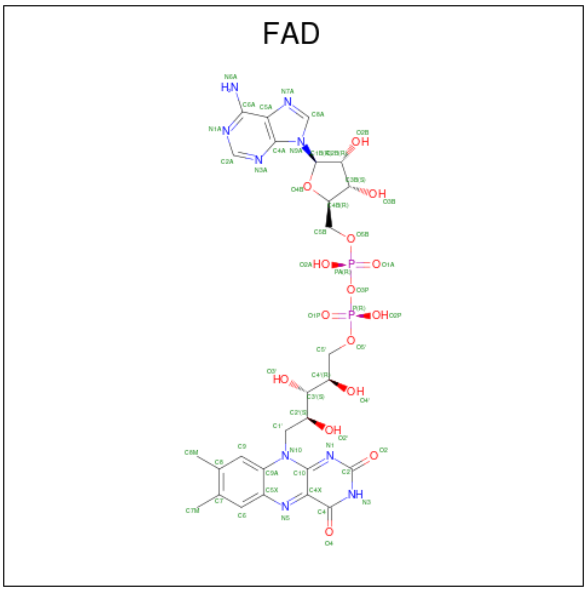
Mol	Chain	Residues	Atoms		AltConf
12	B	2	Total	Na	0
			2	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



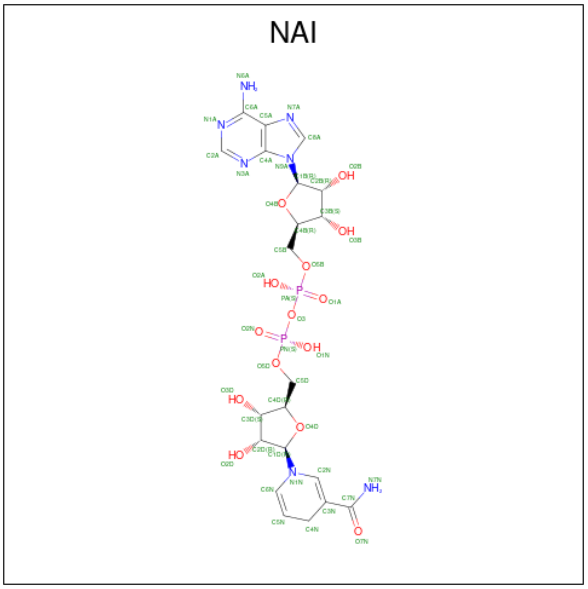
Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total	Fe	S	0
			4	2	2	
13	F	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is FLAVIN-ADENINE DINUCLEOTIDE (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
			83	27	30	9	15	2	

- Molecule 15 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
15	F	1	Total	C	H	N	O	P	0
			71	21	27	7	14	2	

- Molecule 16 is water.

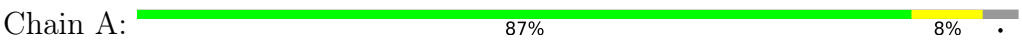
Mol	Chain	Residues	Atoms		AltConf
16	A	96	Total	O	0
			96	96	
16	B	73	Total	O	0
			73	73	
16	C	4	Total	O	0
			4	4	
16	D	4	Total	O	0
			4	4	
16	E	9	Total	O	0
			9	9	
16	F	1	Total	O	0
			1	1	

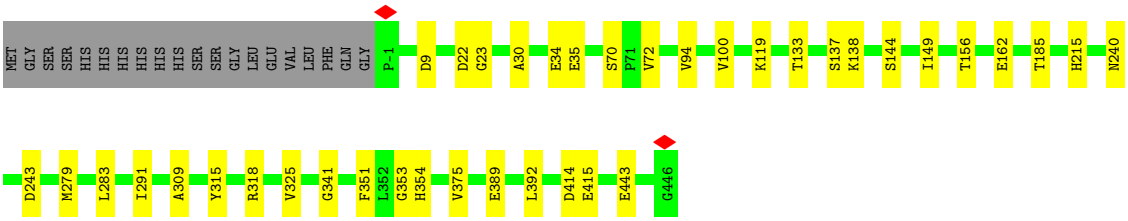
3 Residue-property plots (i)

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

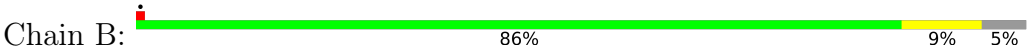
Chain A:

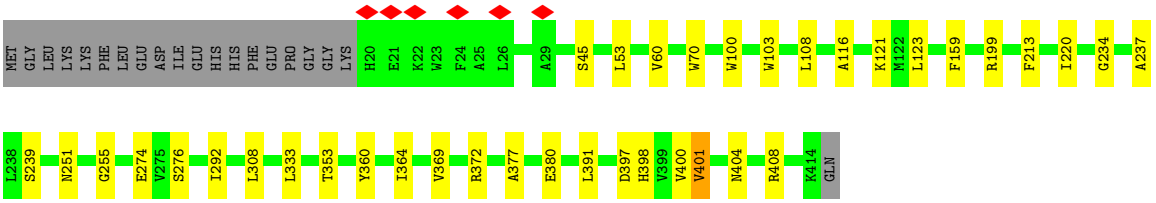




• Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

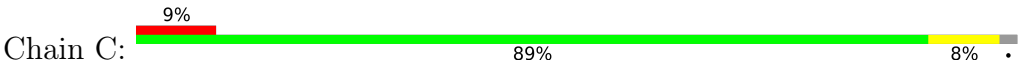
Chain B:

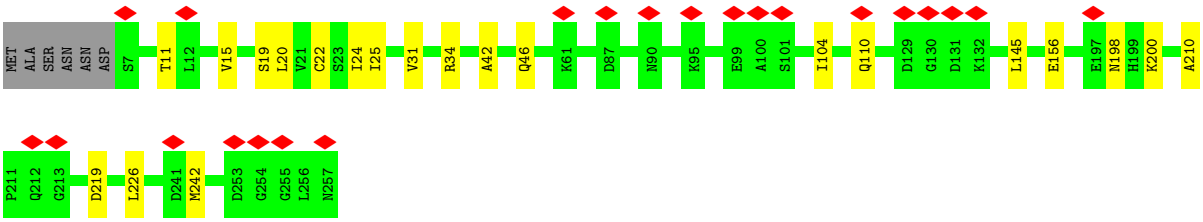




• Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C

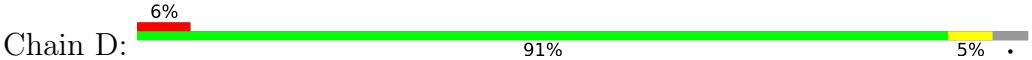
Chain C:



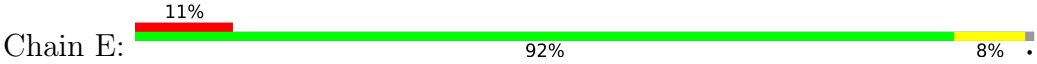


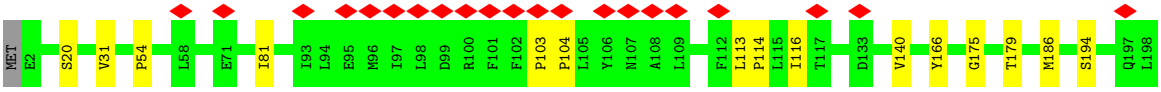
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

Chain D:

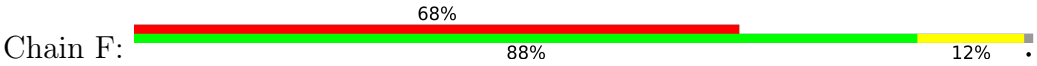


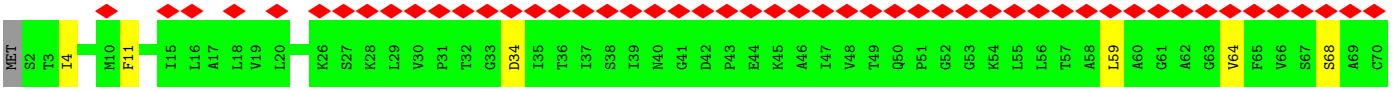
• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E

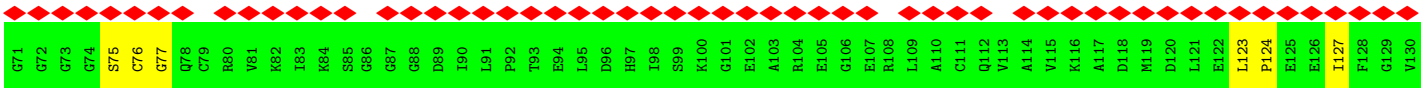


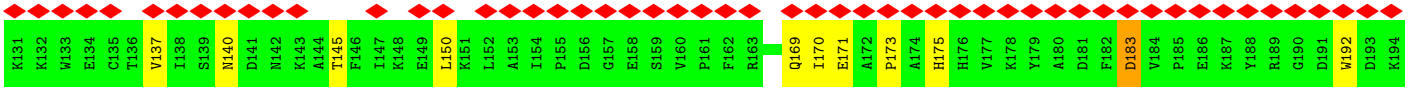


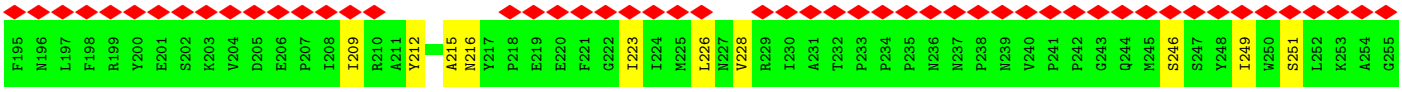
• Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F

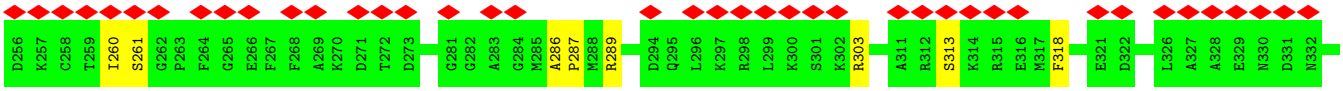


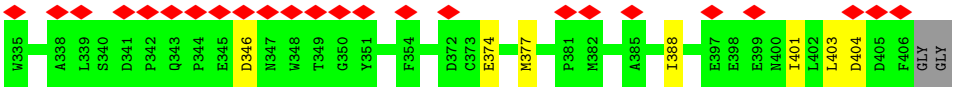












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	435715	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	244328	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0205	Depositor
Map size (Å)	229.14, 229.14, 229.14	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.273, 1.273, 1.273	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, NAI, 3PE, LMT, FMN, NA, FES, UQ2, RBF

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	0.24	0/3498	0.47	0/4741
2	B	0.25	0/3132	0.43	0/4266
3	C	0.25	0/1934	0.43	0/2610
4	D	0.25	0/1576	0.42	0/2141
5	E	0.25	0/1537	0.41	0/2084
6	F	0.24	0/3227	0.43	0/4369
All	All	0.24	0/14904	0.44	0/20211

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

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	3432	3475	3477	27	0
2	B	3039	3025	3025	27	0
3	C	1902	1912	1912	11	0
4	D	1544	1629	1629	5	0
5	E	1504	1574	1574	12	0
6	F	3149	3083	3083	32	0
7	B	30	19	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	30	19	19	1	0
8	B	27	19	20	2	0
9	B	70	78	90	1	0
9	D	35	39	45	1	0
10	B	135	204	204	0	0
10	D	44	62	62	0	0
11	B	23	26	26	4	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	30	31	1	0
15	F	44	27	27	0	0
16	A	96	0	0	7	0
16	B	73	0	0	1	0
16	C	4	0	0	0	0
16	D	4	0	0	0	0
16	E	9	0	0	0	0
16	F	1	0	0	0	0
All	All	15258	15221	15243	111	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 4.

All (111) 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)
2:B:353:THR:HG21	2:B:400:VAL:HG11	1.61	0.81
1:A:35:GLU:OE2	16:A:801:HOH:O	2.03	0.76
3:C:198:ASN:OD1	3:C:200:LYS:NZ	2.20	0.73
2:B:377:ALA:O	7:C:1000:FMN:O2'	2.07	0.72
1:A:100:VAL:O	16:A:802:HOH:O	2.07	0.71
1:A:279:MET:SD	1:A:318:ARG:NH1	2.64	0.70
1:A:138:LYS:NZ	1:A:443:GLU:OE2	2.22	0.70
2:B:234:GLY:O	16:B:601:HOH:O	2.11	0.69
1:A:243:ASP:OD2	16:A:804:HOH:O	2.14	0.66
6:F:216:ASN:ND2	6:F:223:ILE:O	2.29	0.66
1:A:34:GLU:OE2	16:A:803:HOH:O	2.13	0.66
1:A:185:THR:O	16:A:812:HOH:O	2.13	0.64
1:A:119:LYS:NZ	1:A:144:SER:O	2.28	0.62
2:B:274:GLU:OE2	7:B:501:FMN:O3'	2.14	0.61
6:F:173:PRO:O	6:F:175:HIS:ND1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:ASN:OD1	2:B:408:ARG:NH2	2.34	0.60
6:F:403:LEU:HD23	6:F:404:ASP:N	2.17	0.60
2:B:199:ARG:NH1	5:E:166:TYR:O	2.36	0.59
2:B:239:SER:N	7:B:501:FMN:O2P	2.35	0.59
1:A:162:GLU:OE1	16:A:806:HOH:O	2.17	0.58
6:F:137:VAL:HG13	6:F:150:LEU:HD11	1.85	0.58
6:F:171:GLU:N	6:F:171:GLU:OE1	2.37	0.58
2:B:116:ALA:O	2:B:121:LYS:NZ	2.37	0.57
1:A:9:ASP:OD1	1:A:215:HIS:N	2.39	0.56
6:F:170:ILE:O	6:F:209:ILE:HD12	2.06	0.56
11:B:507:UQ2:CM2	11:B:507:UQ2:O1	2.54	0.56
1:A:22:ASP:OD1	1:A:23:GLY:N	2.38	0.55
11:B:507:UQ2:CM3	11:B:507:UQ2:O4	2.55	0.54
1:A:389:GLU:OE1	2:B:353:THR:HG23	2.08	0.54
1:A:351:PHE:O	1:A:354:HIS:ND1	2.39	0.53
5:E:81:ILE:HD13	6:F:11:PHE:CZ	2.44	0.53
1:A:156:THR:OG1	1:A:215:HIS:O	2.14	0.53
9:B:503:LMT:O3'	9:B:503:LMT:O5B	2.26	0.53
2:B:159:PHE:CD2	11:B:507:UQ2:H5M3	2.45	0.52
2:B:308:LEU:HD23	2:B:369:VAL:HB	1.91	0.52
6:F:388:ILE:CD1	6:F:401:ILE:HG21	2.39	0.52
6:F:183:ASP:N	6:F:183:ASP:OD1	2.42	0.52
1:A:149:ILE:HD12	1:A:185:THR:HB	1.92	0.51
6:F:169:GLN:O	6:F:261:SER:N	2.43	0.51
6:F:123:LEU:HD23	6:F:127:ILE:HG21	1.93	0.51
3:C:110:GLN:NE2	3:C:242:MET:SD	2.83	0.51
3:C:156:GLU:N	3:C:156:GLU:OE1	2.43	0.51
5:E:81:ILE:HD13	6:F:11:PHE:CE2	2.46	0.51
6:F:215:ALA:HB2	6:F:286:ALA:HB1	1.92	0.50
3:C:31:VAL:HG21	6:F:4:ILE:HG13	1.93	0.50
3:C:20:LEU:O	3:C:24:ILE:HD13	2.12	0.49
1:A:291:ILE:HG12	1:A:325:VAL:HG11	1.95	0.49
6:F:68:SER:OG	6:F:169:GLN:NE2	2.46	0.48
2:B:108:LEU:HB2	2:B:123:LEU:HD21	1.94	0.48
2:B:380:GLU:O	7:B:501:FMN:N3	2.46	0.48
6:F:170:ILE:HG22	6:F:260:ILE:HG22	1.96	0.48
6:F:215:ALA:O	6:F:289:ARG:NH1	2.47	0.47
6:F:228:VAL:HG21	6:F:249:ILE:HG21	1.96	0.47
2:B:360:TYR:CZ	2:B:364:ILE:HD11	2.48	0.47
4:D:15:VAL:O	4:D:19:ASN:ND2	2.46	0.47
4:D:96:ASP:N	4:D:96:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ASN:HB3	4:D:22:ALA:HB3	1.97	0.47
5:E:54:PRO:HG3	5:E:140:VAL:HG22	1.97	0.47
5:E:175:GLY:O	5:E:179:THR:OG1	2.31	0.47
9:D:302:LMT:O3'	9:D:302:LMT:O2B	2.32	0.47
1:A:70:SER:OG	1:A:72:VAL:O	2.26	0.47
3:C:42:ALA:O	3:C:46:GLN:HG3	2.15	0.47
2:B:251:ASN:O	2:B:255:GLY:N	2.46	0.47
6:F:169:GLN:HG2	6:F:209:ILE:HD11	1.98	0.46
3:C:19:SER:HG	6:F:11:PHE:HD1	1.63	0.46
1:A:283:LEU:HD12	1:A:309:ALA:CB	2.46	0.46
2:B:333:LEU:O	2:B:372:ARG:NH2	2.46	0.46
2:B:292:ILE:HG22	8:B:502:RBF:HC71	1.98	0.45
2:B:397:ASP:OD1	2:B:398:HIS:N	2.48	0.45
6:F:124:PRO:O	6:F:127:ILE:HG22	2.16	0.45
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.98	0.45
6:F:388:ILE:HD13	6:F:401:ILE:HG21	1.97	0.45
5:E:31:VAL:HG12	5:E:31:VAL:O	2.17	0.45
6:F:140:ASN:HD22	6:F:150:LEU:HD13	1.81	0.45
5:E:54:PRO:CG	5:E:140:VAL:HG22	2.47	0.45
2:B:360:TYR:CE2	2:B:364:ILE:HD11	2.52	0.44
1:A:133:THR:O	1:A:137:SER:N	2.50	0.44
1:A:414:ASP:OD1	1:A:415:GLU:N	2.50	0.44
3:C:22:CYS:O	3:C:25:ILE:HG13	2.17	0.44
6:F:303:ARG:NH2	6:F:374:GLU:OE1	2.45	0.44
6:F:403:LEU:HD23	6:F:404:ASP:H	1.83	0.44
1:A:240:ASN:ND2	16:A:804:HOH:O	2.51	0.44
1:A:341:GLY:O	1:A:353:GLY:N	2.50	0.43
5:E:103:PRO:N	5:E:104:PRO:HD2	2.33	0.43
6:F:145:THR:O	6:F:192:TRP:NE1	2.48	0.43
3:C:210:ALA:N	3:C:219:ASP:OD1	2.51	0.43
5:E:113:LEU:N	5:E:114:PRO:HD2	2.33	0.43
2:B:100:TRP:HA	2:B:103:TRP:CD1	2.53	0.43
6:F:313:SER:OG	6:F:346:ASP:OD2	2.29	0.43
6:F:76:CYS:SG	6:F:77:GLY:N	2.91	0.43
6:F:377:MET:CE	6:F:401:ILE:HG23	2.49	0.42
2:B:237:ALA:HB3	2:B:333:LEU:HD22	2.02	0.42
6:F:212:TYR:HB3	6:F:226:LEU:HD11	2.01	0.42
2:B:391:LEU:HD22	5:E:186:MET:HG2	2.01	0.42
5:E:116:ILE:O	5:E:116:ILE:HG22	2.19	0.42
3:C:145:LEU:HD13	3:C:226:LEU:HD13	2.02	0.42
1:A:291:ILE:CG1	1:A:325:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HG21	8:B:502:RBF:HC82	2.02	0.41
14:F:1501:FAD:H51A	14:F:1501:FAD:O2P	2.21	0.41
1:A:375:VAL:HG21	2:B:53:LEU:HD11	2.02	0.41
6:F:286:ALA:HB3	6:F:287:PRO:CD	2.49	0.41
4:D:66:ILE:HG12	4:D:74:VAL:HG11	2.03	0.41
5:E:116:ILE:O	5:E:116:ILE:CG2	2.69	0.41
11:B:507:UQ2:H72	11:B:507:UQ2:H5M1	1.90	0.41
1:A:30:ALA:HB3	1:A:315:TYR:CG	2.56	0.40
2:B:213:PHE:HA	2:B:220:ILE:HG21	2.03	0.40
4:D:83:VAL:HG11	4:D:109:ILE:HG13	2.02	0.40
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.56	0.40
6:F:59:LEU:HD22	6:F:64:VAL:HG21	2.02	0.40
1:A:392:LEU:HD13	2:B:401:VAL:HG21	2.03	0.40
3:C:11:THR:O	3:C:15:VAL:HG22	2.22	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	446/468 (95%)	437 (98%)	9 (2%)	0	100	100
2	B	393/415 (95%)	389 (99%)	4 (1%)	0	100	100
3	C	249/257 (97%)	246 (99%)	3 (1%)	0	100	100
4	D	200/210 (95%)	191 (96%)	9 (4%)	0	100	100
5	E	195/198 (98%)	193 (99%)	2 (1%)	0	100	100
6	F	403/408 (99%)	398 (99%)	5 (1%)	0	100	100
All	All	1886/1956 (96%)	1854 (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	378/395 (96%)	378 (100%)	0	100	100
2	B	303/320 (95%)	301 (99%)	2 (1%)	84	94
3	C	200/205 (98%)	198 (99%)	2 (1%)	76	91
4	D	169/176 (96%)	167 (99%)	2 (1%)	71	89
5	E	164/165 (99%)	162 (99%)	2 (1%)	71	89
6	F	336/337 (100%)	330 (98%)	6 (2%)	59	82
All	All	1550/1598 (97%)	1536 (99%)	14 (1%)	79	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	45	SER
2	B	401	VAL
3	C	34	ARG
3	C	104	ILE
4	D	35	THR
4	D	157	SER
5	E	20	SER
5	E	194	SER
6	F	34	ASP
6	F	75	SER
6	F	183	ASP
6	F	246	SER
6	F	251	SER
6	F	318	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
14	FAD	F	1501	-	53,58,58	0.61	0	68,89,89	0.74	2 (2%)
10	3PE	B	504	-	50,50,50	0.52	0	53,55,55	0.53	1 (1%)
10	3PE	B	506	-	32,32,50	0.63	0	35,37,55	0.62	1 (2%)
13	FES	F	1502	6	0,4,4	-	-	-		
8	RBF	B	502	-	29,29,29	0.58	0	41,43,43	0.68	1 (2%)
9	LMT	B	503	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
11	UQ2	B	507	-	23,23,23	0.82	1 (4%)	28,31,31	1.00	4 (14%)
9	LMT	D	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	2 (4%)
7	FMN	C	1000	3	29,32,33	1.12	2 (6%)	40,47,50	1.30	7 (17%)
10	3PE	B	508	-	50,50,50	0.51	0	53,55,55	0.60	1 (1%)
10	3PE	D	301	-	43,43,50	0.54	0	46,48,55	0.62	2 (4%)
13	FES	E	1001	5,4	0,4,4	-	-	-		
15	NAI	F	1503	-	42,48,48	0.58	0	47,73,73	0.85	3 (6%)
9	LMT	B	505	-	36,36,36	1.17	6 (16%)	47,47,47	1.00	2 (4%)
7	FMN	B	501	2	29,32,33	1.12	2 (6%)	40,47,50	1.29	7 (17%)

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
14	FAD	F	1501	-	-	0/30/50/50	0/6/6/6
10	3PE	B	504	-	-	17/54/54/54	-
10	3PE	B	506	-	-	11/36/36/54	-
13	FES	F	1502	6	-	-	0/1/1/1
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
9	LMT	B	503	-	-	9/21/61/61	0/2/2/2
11	UQ2	B	507	-	-	7/15/39/39	0/1/1/1
9	LMT	D	302	-	-	11/21/61/61	0/2/2/2
7	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
10	3PE	B	508	-	-	24/54/54/54	-
10	3PE	D	301	-	-	15/47/47/54	-
13	FES	E	1001	5,4	-	-	0/1/1/1
15	NAI	F	1503	-	-	3/25/72/72	0/5/5/5
9	LMT	B	505	-	-	11/21/61/61	0/2/2/2
7	FMN	B	501	2	-	6/15/17/18	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	FMN	C4A-N5	3.76	1.38	1.30
7	C	1000	FMN	C4A-N5	3.72	1.38	1.30
9	D	302	LMT	O3'-C3'	-2.70	1.36	1.43
9	B	505	LMT	O3'-C3'	-2.70	1.36	1.43
9	B	503	LMT	O3'-C3'	-2.66	1.36	1.43
7	B	501	FMN	C10-N1	2.61	1.38	1.33
7	C	1000	FMN	C10-N1	2.56	1.38	1.33
9	B	505	LMT	O2B-C2B	-2.44	1.37	1.43
9	D	302	LMT	O2'-C2'	-2.37	1.37	1.43
9	D	302	LMT	O2B-C2B	-2.37	1.37	1.43
9	D	302	LMT	O3B-C3B	-2.37	1.37	1.43
9	B	503	LMT	O2'-C2'	-2.36	1.37	1.43
9	B	505	LMT	O3B-C3B	-2.34	1.37	1.43
9	B	503	LMT	O3B-C3B	-2.34	1.37	1.43
9	B	503	LMT	O2B-C2B	-2.28	1.37	1.43
9	B	505	LMT	O2'-C2'	-2.27	1.37	1.43
9	B	505	LMT	O4'-C4B	-2.25	1.37	1.43
9	B	503	LMT	O4'-C4B	-2.14	1.37	1.43
9	D	302	LMT	O4'-C4B	-2.12	1.38	1.43
11	B	507	UQ2	C3-C4	-2.02	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	LMT	O1'-C1'	-2.01	1.36	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1000	FMN	C4-N3-C2	-3.15	119.81	125.64
7	B	501	FMN	C4-N3-C2	-3.04	120.02	125.64
15	F	1503	NAI	O4B-C1B-C2B	-2.79	102.84	106.93
7	C	1000	FMN	C4A-C10-N10	2.77	120.53	116.48
7	C	1000	FMN	C4A-C4-N3	2.71	120.07	113.19
7	B	501	FMN	C4A-C4-N3	2.67	119.98	113.19
7	B	501	FMN	C4A-C10-N10	2.59	120.27	116.48
7	C	1000	FMN	O4-C4-C4A	-2.46	120.07	126.60
11	B	507	UQ2	O3-C3-C4	2.45	124.83	116.56
9	B	505	LMT	C1'-O5'-C5'	-2.43	108.93	113.69
7	B	501	FMN	O4-C4-C4A	-2.42	120.18	126.60
9	D	302	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
7	C	1000	FMN	C4A-C10-N1	-2.40	119.17	124.73
10	D	301	3PE	O12-P-O14	2.37	123.94	112.24
11	B	507	UQ2	O2-C2-C1	2.36	124.55	116.56
9	B	503	LMT	C1'-O5'-C5'	-2.35	109.07	113.69
10	B	506	3PE	O12-P-O14	2.32	123.71	112.24
10	B	508	3PE	O12-P-O14	2.32	123.69	112.24
10	D	301	3PE	C2-O21-C21	2.31	123.48	117.79
10	B	504	3PE	O12-P-O14	2.31	123.64	112.24
9	B	503	LMT	C3'-C4'-C5'	-2.30	105.64	110.93
7	B	501	FMN	C10-C4A-N5	-2.30	119.99	124.86
7	B	501	FMN	C4A-C10-N1	-2.29	119.41	124.73
7	C	1000	FMN	C10-C4A-N5	-2.28	120.02	124.86
14	F	1501	FAD	C5A-C6A-N6A	2.27	123.80	120.35
15	F	1503	NAI	C5A-C6A-N6A	2.26	123.78	120.35
9	B	505	LMT	C3'-C4'-C5'	-2.19	105.90	110.93
11	B	507	UQ2	O2-C2-C3	-2.12	115.64	123.64
7	B	501	FMN	C9A-C5A-N5	-2.05	120.21	122.43
9	D	302	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
14	F	1501	FAD	C4-N3-C2	-2.04	121.88	125.64
11	B	507	UQ2	O3-C3-C2	-2.03	115.98	123.64
8	B	502	RBF	C4-N3-C2	-2.03	121.89	125.64
15	F	1503	NAI	C3N-C7N-N7N	2.02	121.25	117.67
7	C	1000	FMN	C4-C4A-C10	2.01	120.18	116.79

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	501	FMN	C3'-C4'-C5'-O5'
7	B	501	FMN	O4'-C4'-C5'-O5'
9	D	302	LMT	C2'-C1'-O1'-C1
9	D	302	LMT	O5'-C1'-O1'-C1
10	B	504	3PE	O13-C11-C12-N
10	B	504	3PE	C22-C21-O21-C2
10	B	506	3PE	O13-C11-C12-N
10	B	506	3PE	C22-C21-O21-C2
10	B	508	3PE	C1-O11-P-O14
10	B	508	3PE	O13-C11-C12-N
10	B	508	3PE	C2-C3-O31-C31
15	F	1503	NAI	O4D-C1D-N1N-C2N
9	B	503	LMT	O5B-C1B-O1B-C4'
10	B	508	3PE	O32-C31-O31-C3
10	D	301	3PE	O32-C31-O31-C3
9	B	505	LMT	O5B-C1B-O1B-C4'
10	B	504	3PE	O22-C21-O21-C2
10	B	506	3PE	O22-C21-O21-C2
10	D	301	3PE	O22-C21-O21-C2
10	B	508	3PE	C32-C31-O31-C3
10	D	301	3PE	C32-C31-O31-C3
10	D	301	3PE	C22-C21-O21-C2
9	B	505	LMT	C2B-C1B-O1B-C4'
9	B	505	LMT	O5'-C5'-C6'-O6'
11	B	507	UQ2	C12-C11-C9-C10
11	B	507	UQ2	C12-C11-C9-C8
9	D	302	LMT	O5B-C5B-C6B-O6B
11	B	507	UQ2	C3-C2-O2-CM2
11	B	507	UQ2	C2-C3-O3-CM3
9	B	503	LMT	C4'-C5'-C6'-O6'
7	B	501	FMN	O3'-C3'-C4'-C5'
7	B	501	FMN	C2'-C3'-C4'-C5'
9	B	505	LMT	C4'-C5'-C6'-O6'
10	B	508	3PE	C1-O11-P-O13
11	B	507	UQ2	C1-C2-O2-CM2
9	B	503	LMT	C5'-C4'-O1B-C1B
9	B	503	LMT	C3'-C4'-O1B-C1B
7	B	501	FMN	C2'-C3'-C4'-O4'
9	B	505	LMT	O5B-C5B-C6B-O6B
10	D	301	3PE	C27-C28-C29-C2A
10	B	504	3PE	C28-C29-C2A-C2B
10	B	508	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
10	B	508	3PE	C3E-C3F-C3G-C3H
10	B	504	3PE	C32-C31-O31-C3
9	B	503	LMT	C4-C5-C6-C7
10	B	508	3PE	C37-C38-C39-C3A
10	B	508	3PE	C21-C22-C23-C24
10	B	504	3PE	O32-C31-O31-C3
10	B	508	3PE	C2D-C2E-C2F-C2G
10	B	508	3PE	C35-C36-C37-C38
10	B	508	3PE	C28-C29-C2A-C2B
10	B	504	3PE	C2C-C2D-C2E-C2F
9	D	302	LMT	O5'-C5'-C6'-O6'
7	B	501	FMN	O3'-C3'-C4'-O4'
10	B	504	3PE	C2-C1-O11-P
9	D	302	LMT	C3-C4-C5-C6
10	B	504	3PE	C3C-C3D-C3E-C3F
11	B	507	UQ2	C4-C3-O3-CM3
9	B	503	LMT	O5B-C5B-C6B-O6B
10	B	508	3PE	C29-C2A-C2B-C2C
10	B	508	3PE	C1-C2-C3-O31
9	D	302	LMT	C11-C10-C9-C8
10	B	508	3PE	C2B-C2C-C2D-C2E
10	B	508	3PE	C3B-C3C-C3D-C3E
10	D	301	3PE	C26-C27-C28-C29
10	B	506	3PE	O11-C1-C2-O21
10	D	301	3PE	C38-C39-C3A-C3B
10	B	504	3PE	O21-C2-C3-O31
10	B	506	3PE	C2-C1-O11-P
9	D	302	LMT	O1'-C1-C2-C3
9	D	302	LMT	C5-C6-C7-C8
9	B	505	LMT	C3-C4-C5-C6
9	B	503	LMT	O5'-C5'-C6'-O6'
10	B	504	3PE	C21-C22-C23-C24
10	B	504	3PE	C1-C2-C3-O31
10	D	301	3PE	C1-C2-C3-O31
9	B	503	LMT	C11-C10-C9-C8
9	D	302	LMT	C1-C2-C3-C4
10	B	504	3PE	C12-C11-O13-P
10	B	506	3PE	C12-C11-O13-P
10	D	301	3PE	C12-C11-O13-P
10	B	506	3PE	O21-C2-C3-O31
10	B	508	3PE	O21-C2-C3-O31
9	B	505	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	D	301	3PE	O21-C2-C3-O31
10	B	504	3PE	C1-O11-P-O13
10	D	301	3PE	C11-O13-P-O11
10	D	301	3PE	C25-C26-C27-C28
11	B	507	UQ2	C11-C12-C13-C14
10	D	301	3PE	C2-C1-O11-P
10	B	508	3PE	C25-C26-C27-C28
15	F	1503	NAI	O4D-C4D-C5D-O5D
10	D	301	3PE	C3-C2-O21-C21
9	D	302	LMT	C2B-C1B-O1B-C4'
9	B	503	LMT	C7-C8-C9-C10
10	B	506	3PE	O21-C21-C22-C23
10	B	508	3PE	C1-C2-O21-C21
10	B	508	3PE	C3-C2-O21-C21
10	D	301	3PE	C1-C2-O21-C21
9	D	302	LMT	O5B-C1B-O1B-C4'
10	B	508	3PE	C3F-C3G-C3H-C3I
10	B	506	3PE	C1-C2-C3-O31
10	B	508	3PE	C39-C3A-C3B-C3C
9	B	505	LMT	C6-C7-C8-C9
9	B	505	LMT	C4-C5-C6-C7
9	B	505	LMT	C7-C8-C9-C10
9	B	505	LMT	O5'-C1'-O1'-C1
10	B	506	3PE	O22-C21-C22-C23
10	B	504	3PE	C1-O11-P-O14
15	F	1503	NAI	C2N-C3N-C7N-N7N
10	B	504	3PE	O11-C1-C2-C3
10	B	506	3PE	O11-C1-C2-C3
10	B	504	3PE	C3B-C3C-C3D-C3E
10	B	508	3PE	C2E-C2F-C2G-C2H

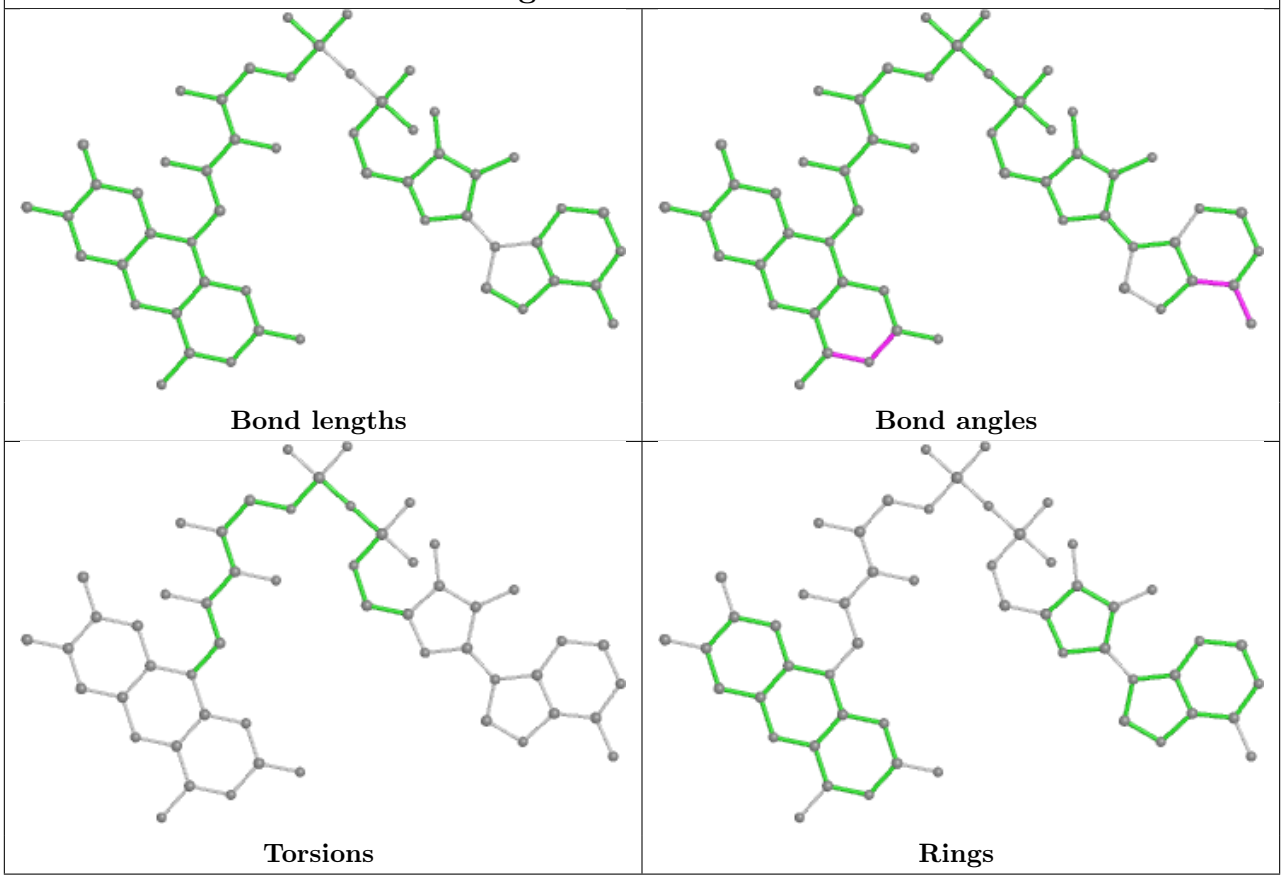
There are no ring outliers.

7 monomers are involved in 13 short contacts:

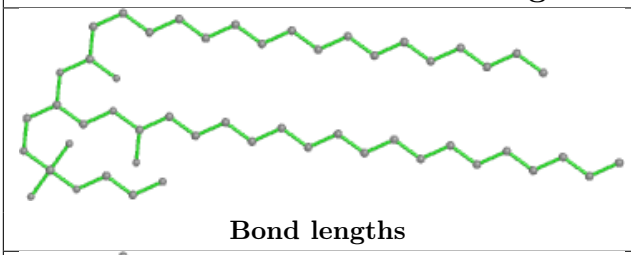
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	1501	FAD	1	0
8	B	502	RBF	2	0
9	B	503	LMT	1	0
11	B	507	UQ2	4	0
9	D	302	LMT	1	0
7	C	1000	FMN	1	0
7	B	501	FMN	3	0

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.

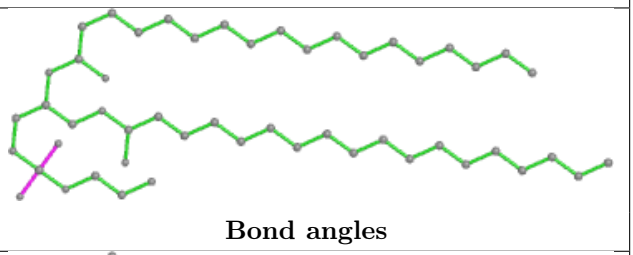
Ligand FAD F 1501



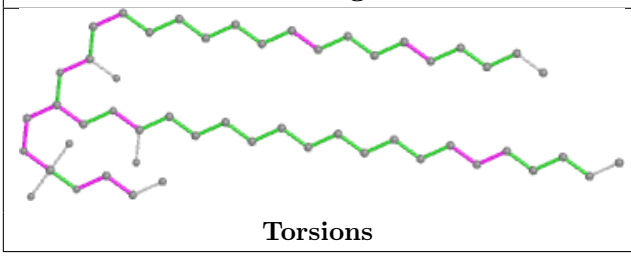
Ligand 3PE B 504



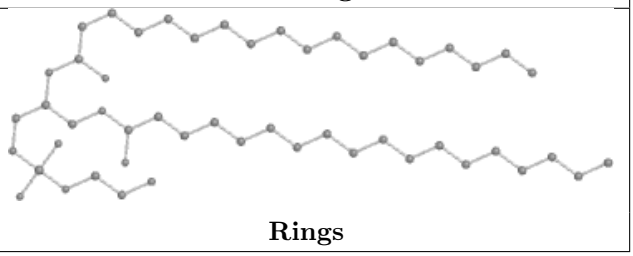
Bond lengths



Bond angles

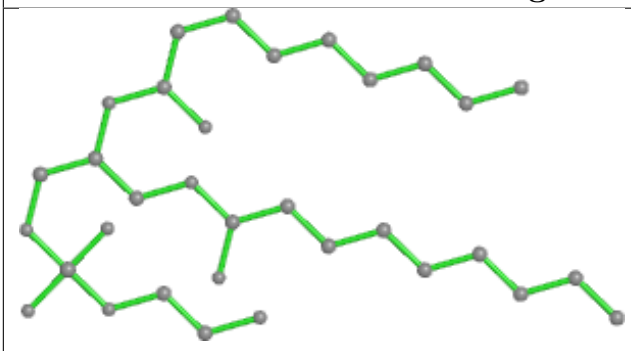


Torsions

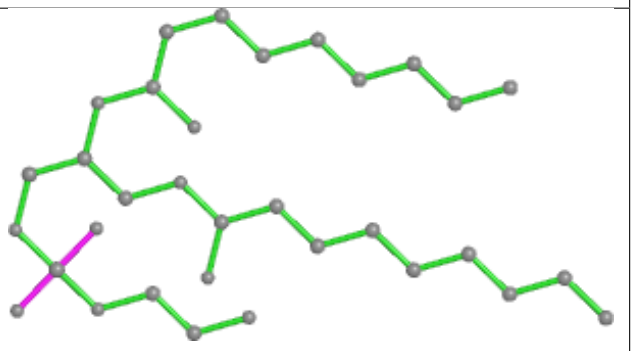


Rings

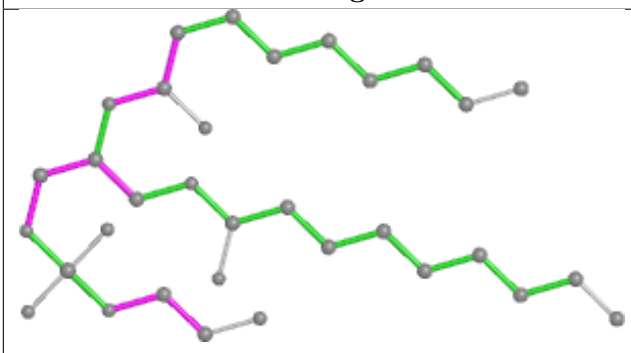
Ligand 3PE B 506



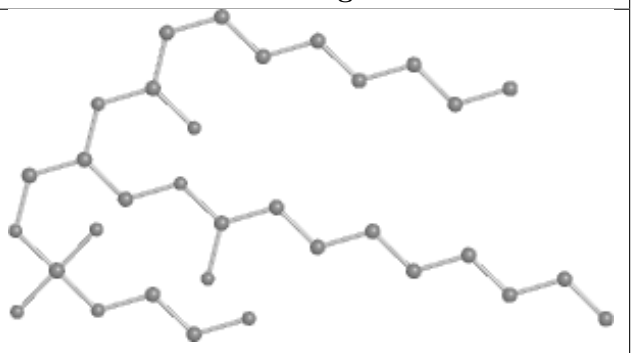
Bond lengths



Bond angles

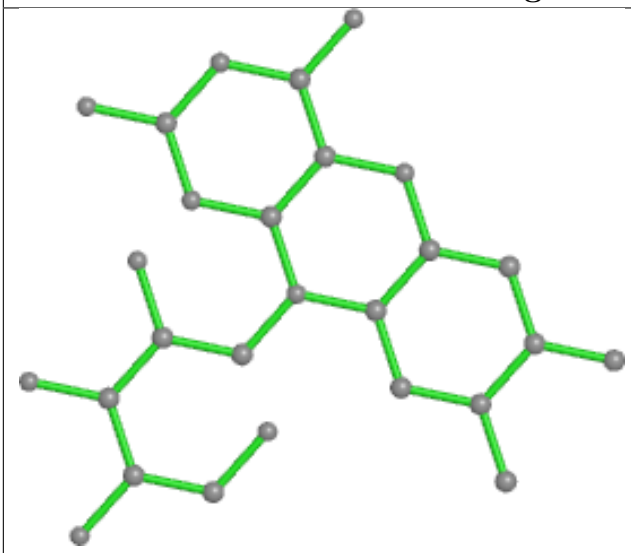


Torsions

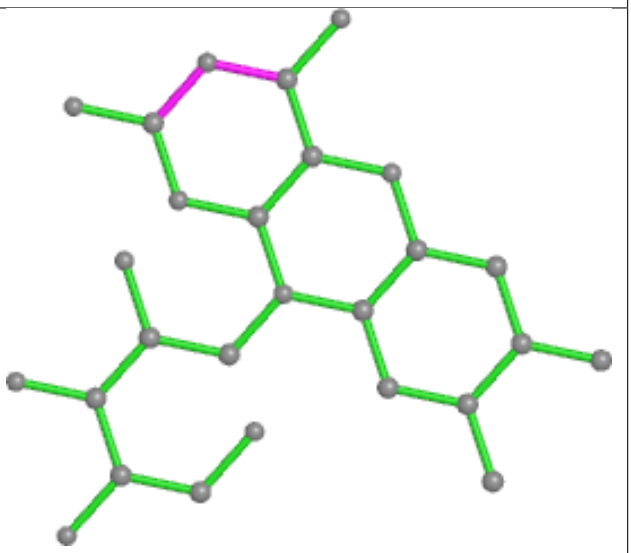


Rings

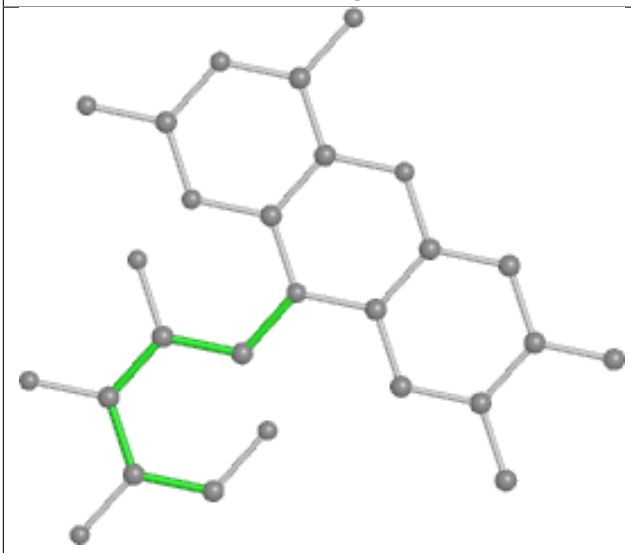
Ligand RBF B 502



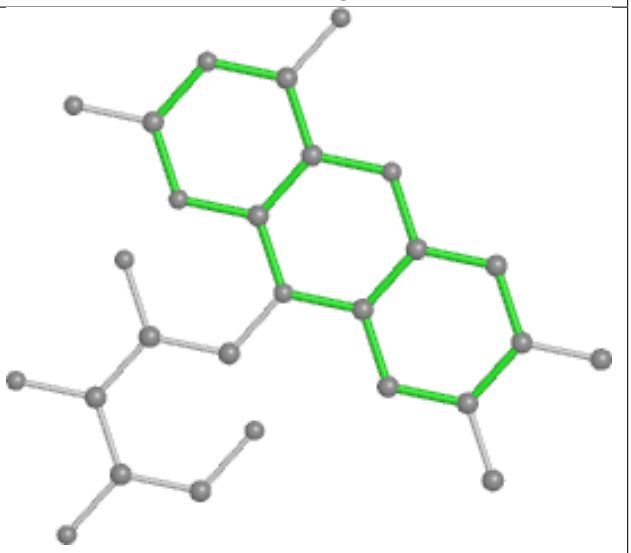
Bond lengths



Bond angles

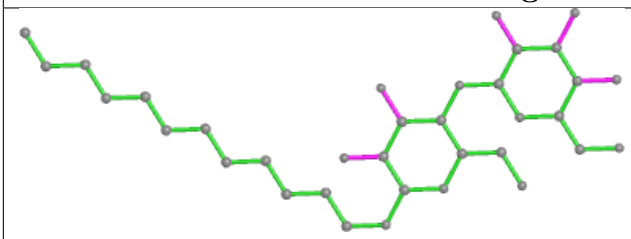


Torsions

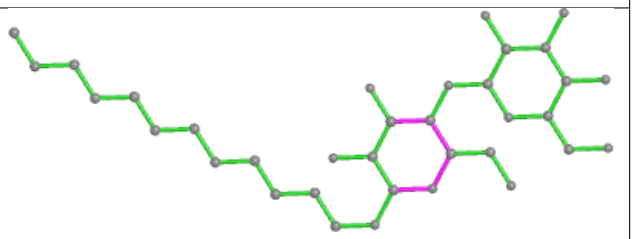


Rings

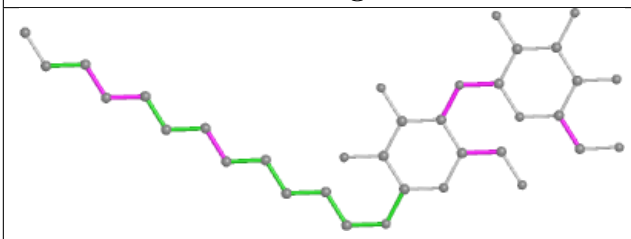
Ligand LMT B 503



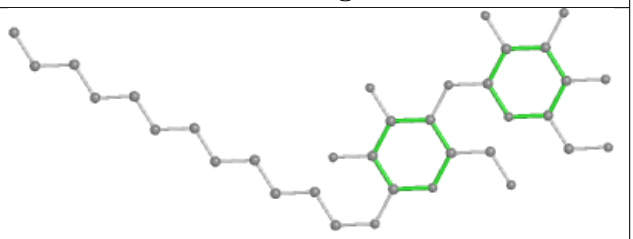
Bond lengths



Bond angles

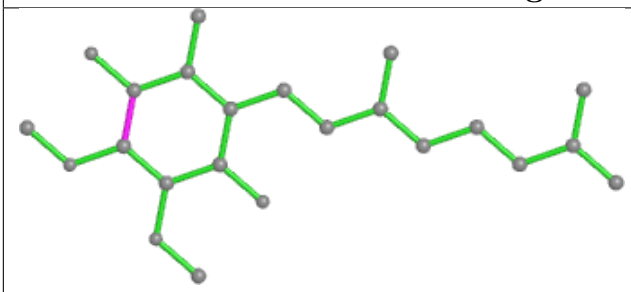


Torsions

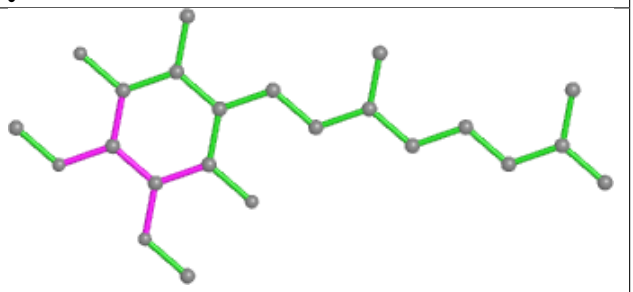


Rings

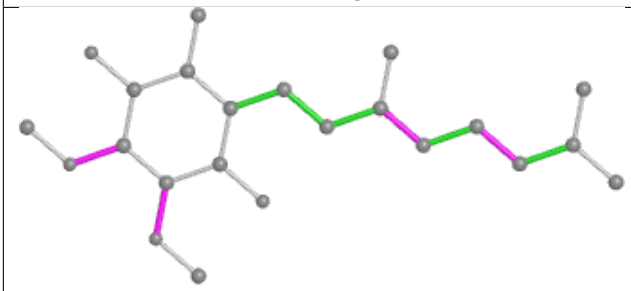
Ligand UQ2 B 507



Bond lengths



Bond angles



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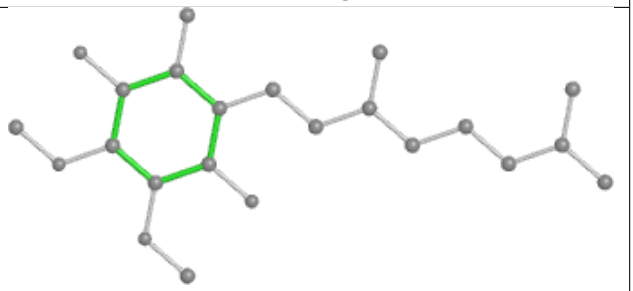
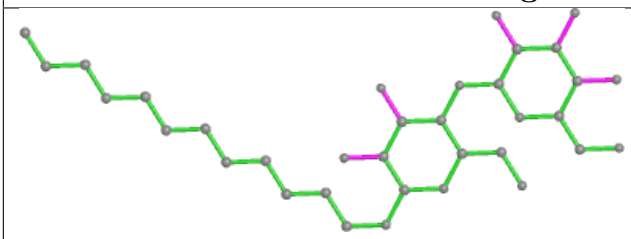


Rings

Ligand LMT D 302



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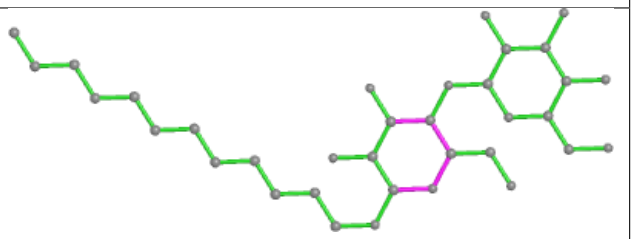
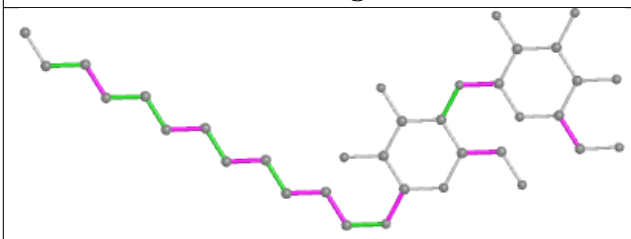


Bond angles



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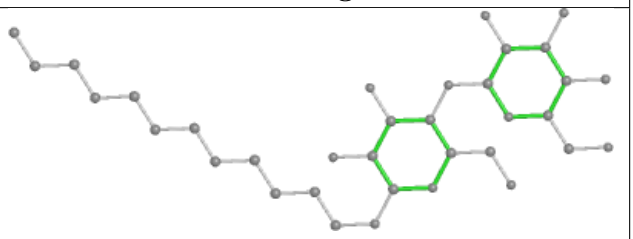
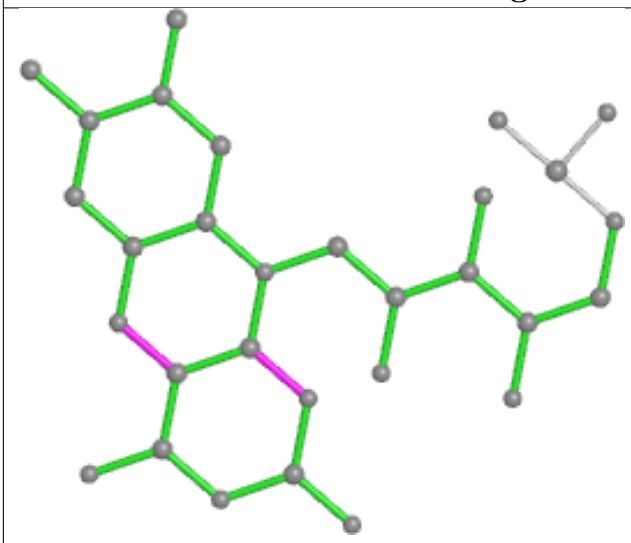


Rings

Ligand FMN C 1000



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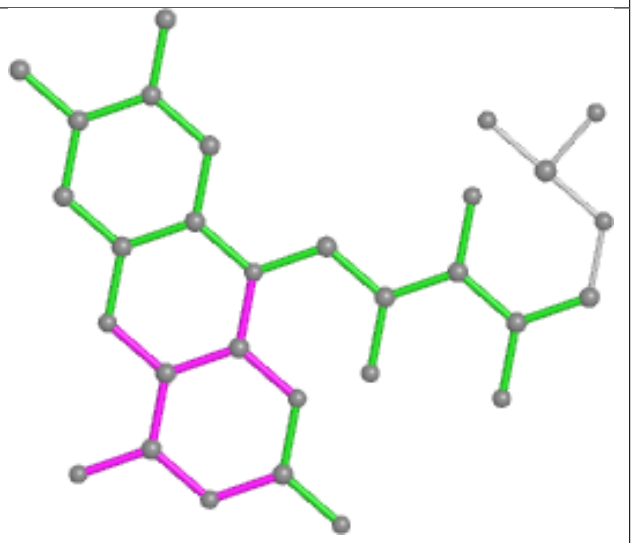
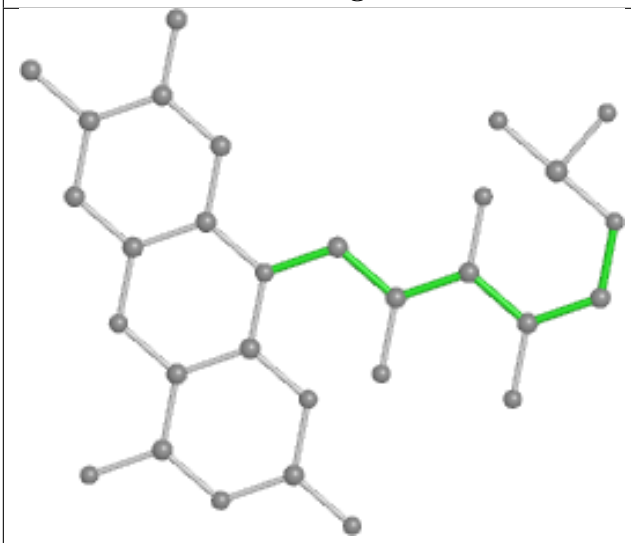


Bond angles



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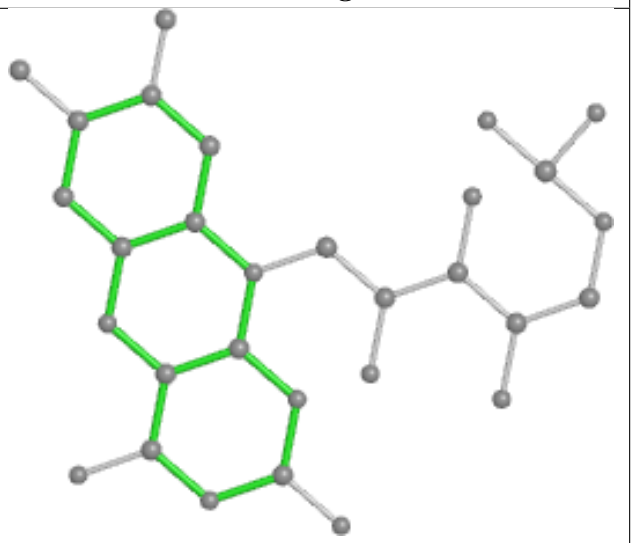
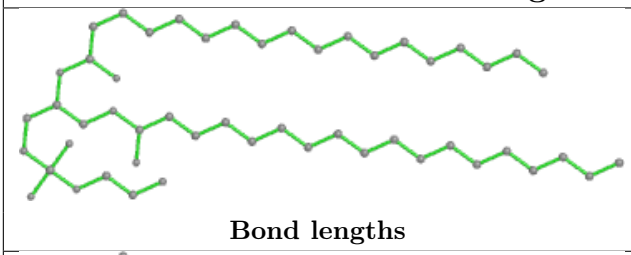


Rings

Ligand 3PE B 508



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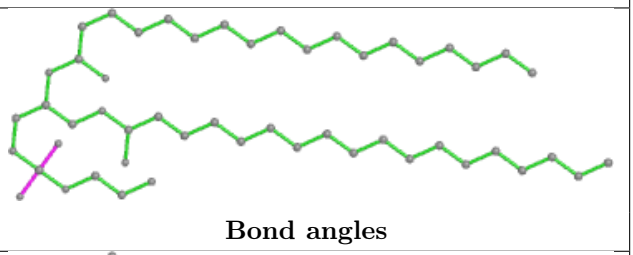
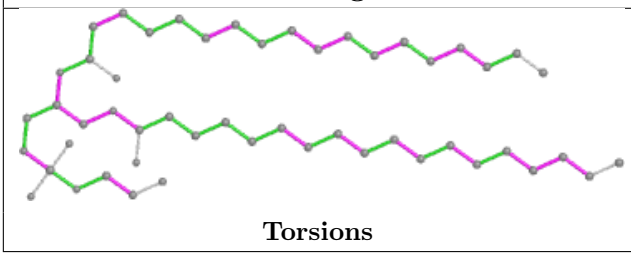


Bond angles



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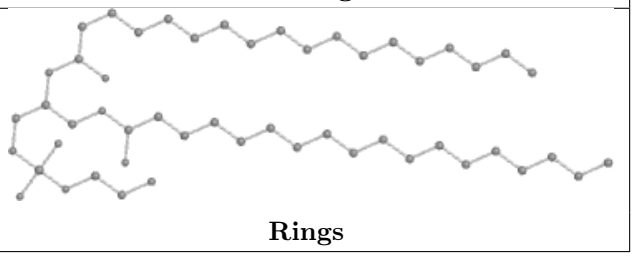
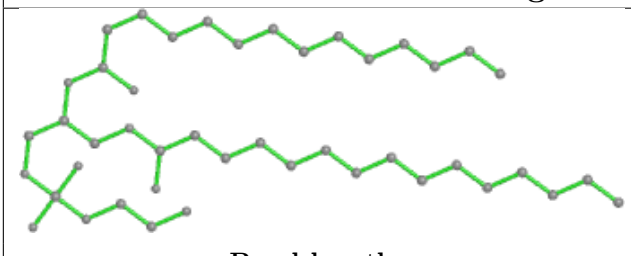
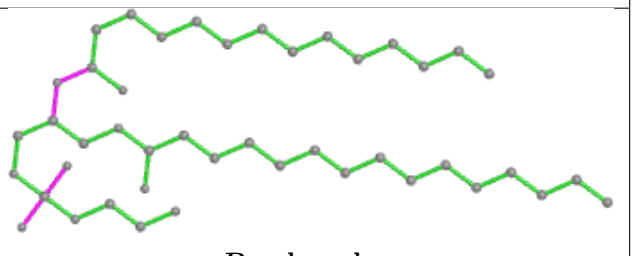


Rings

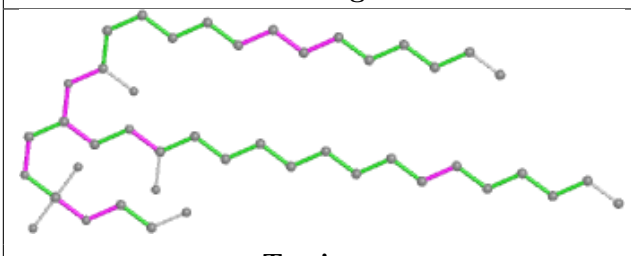
Ligand 3PE D 301



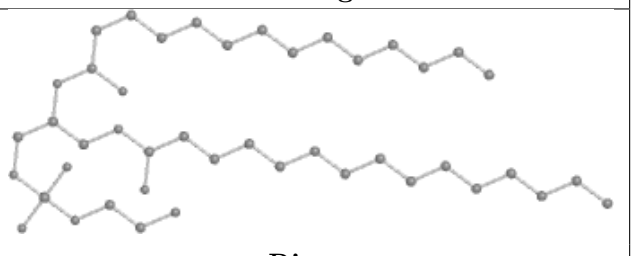
Bond lengths



Bond angles

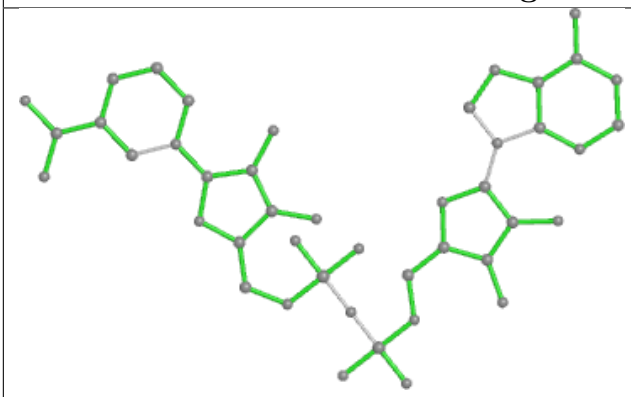


Torsions

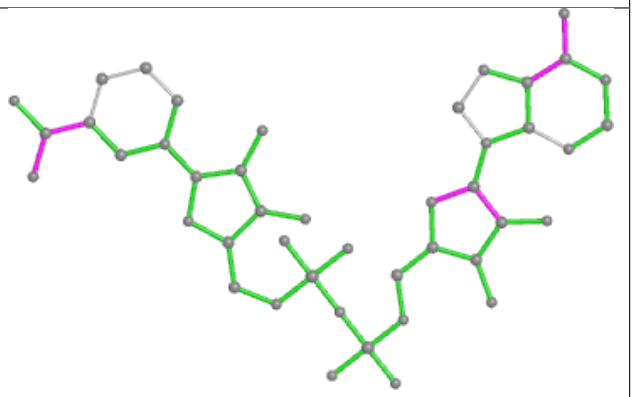


Rings

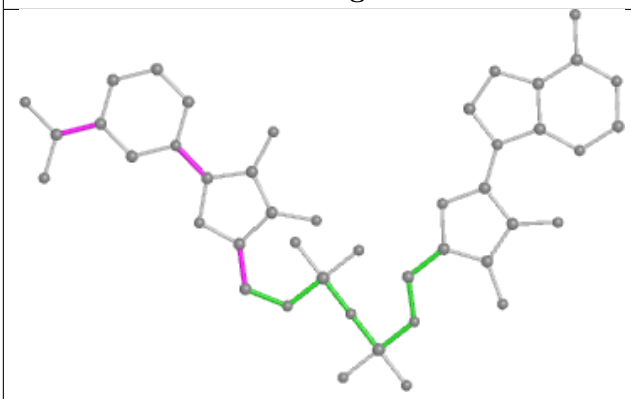
Ligand NAI F 1503



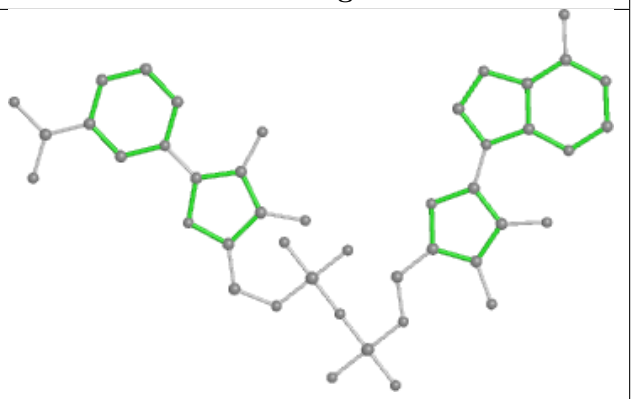
Bond lengths



Bond angles

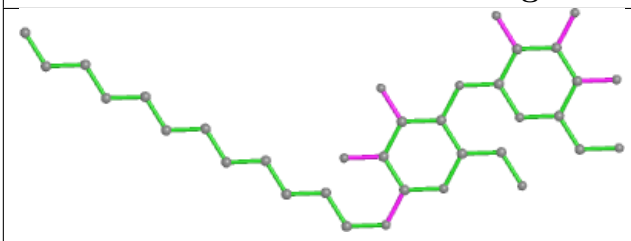


Torsions

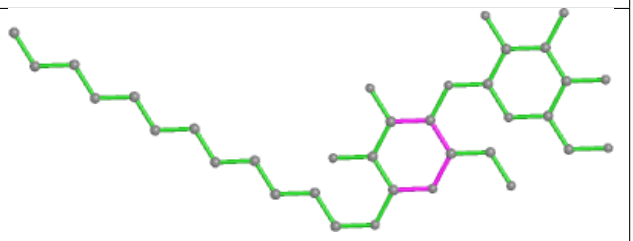


Rings

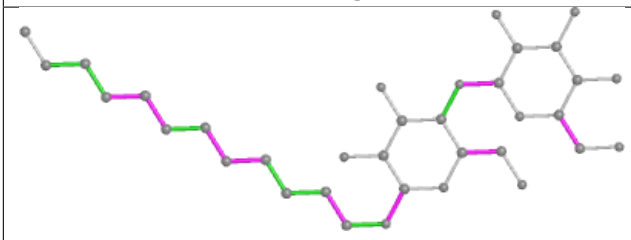
Ligand LMT B 505



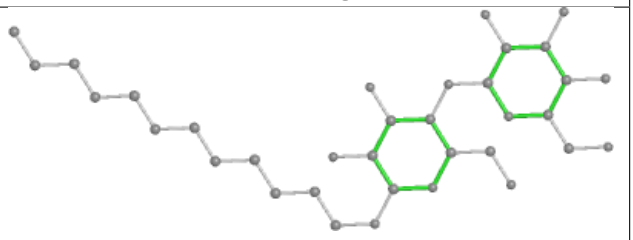
Bond lengths



Bond angles

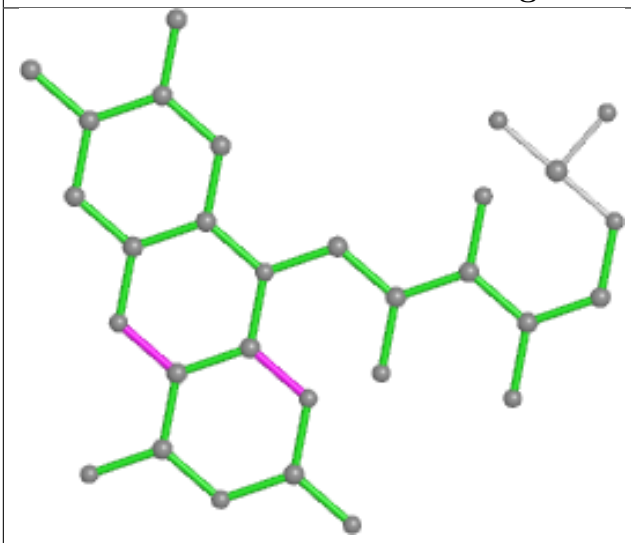


Torsions

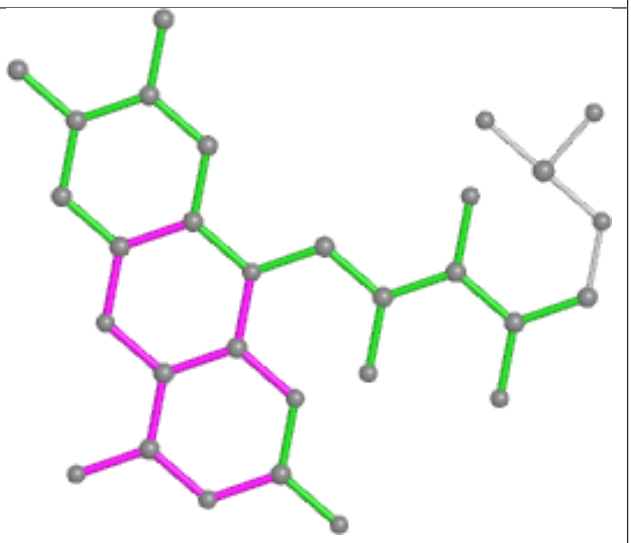


Rings

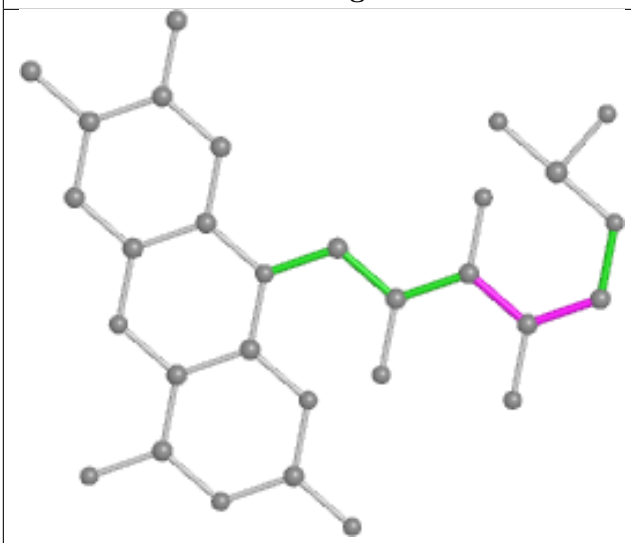
Ligand FMN B 501



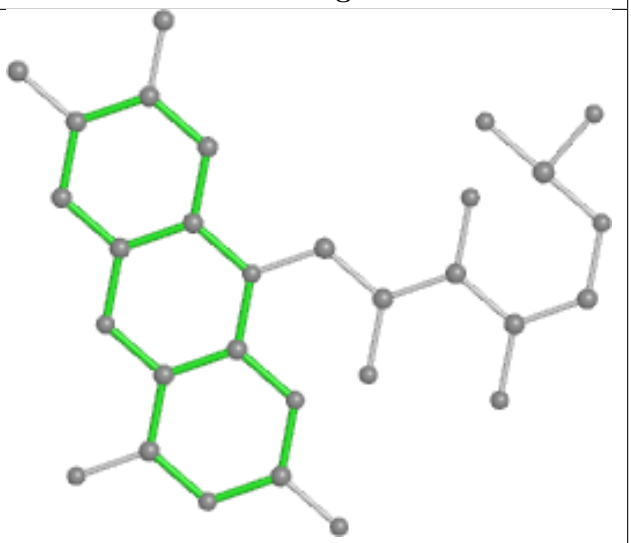
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

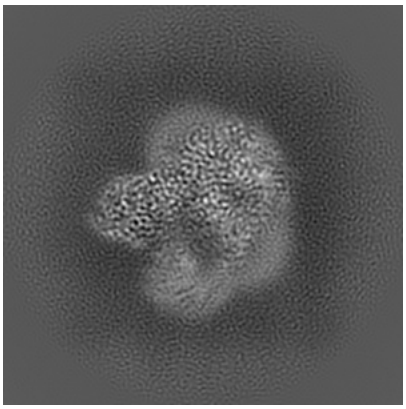
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15089. These allow visual inspection of the internal detail of the map and identification of artifacts.

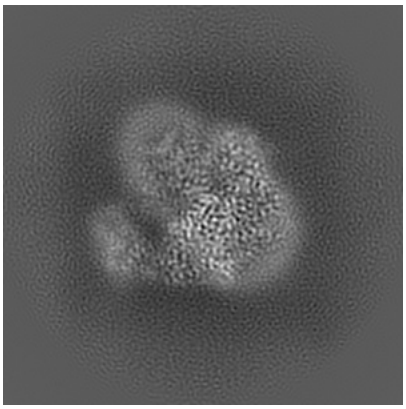
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

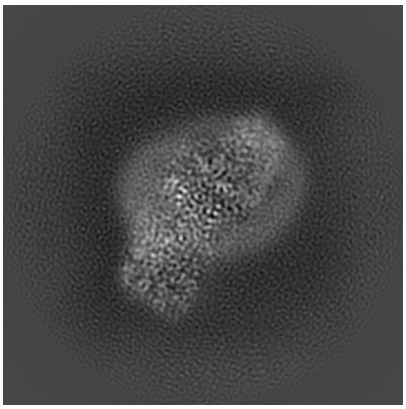
6.1.1 Primary map



X

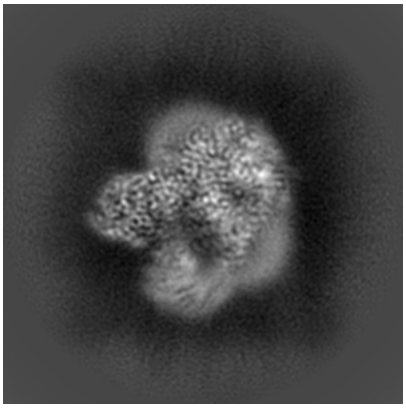


Y

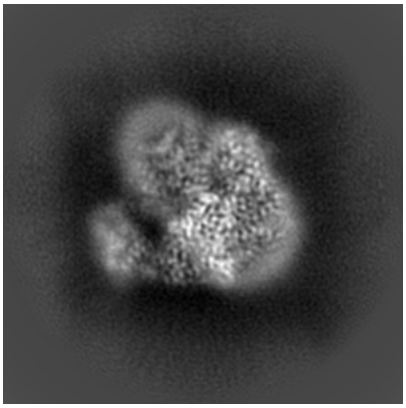


Z

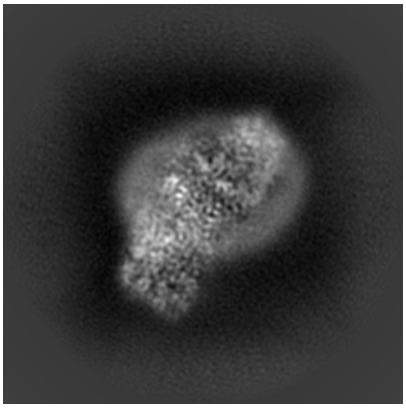
6.1.2 Raw map



X



Y

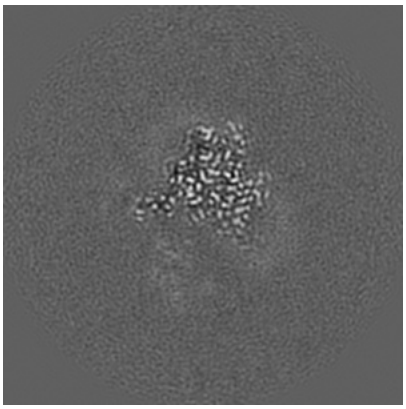


Z

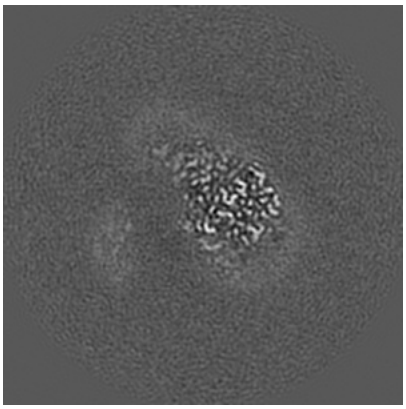
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

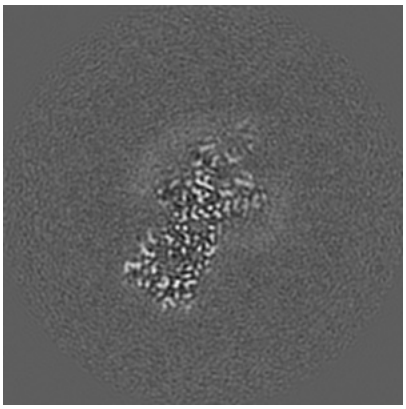
6.2.1 Primary map



X Index: 90

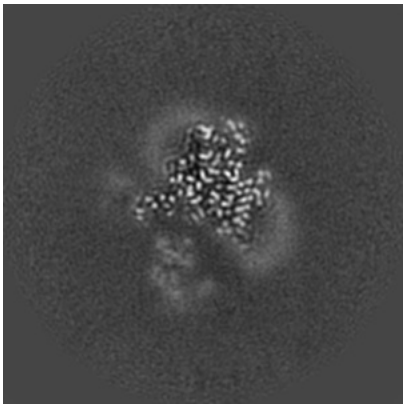


Y Index: 90

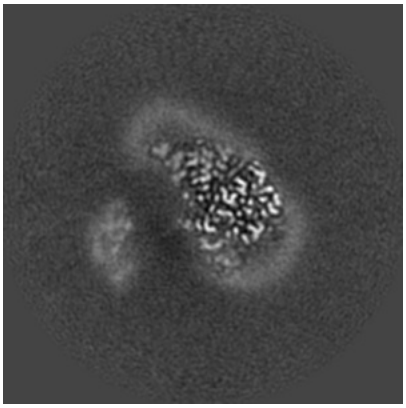


Z Index: 90

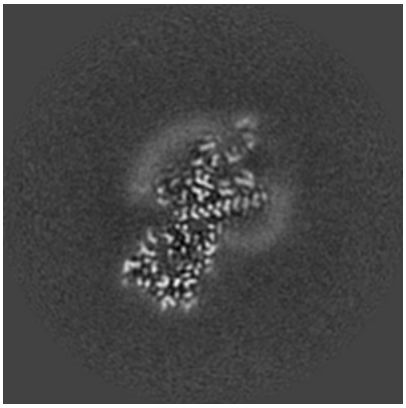
6.2.2 Raw map



X Index: 90



Y Index: 90

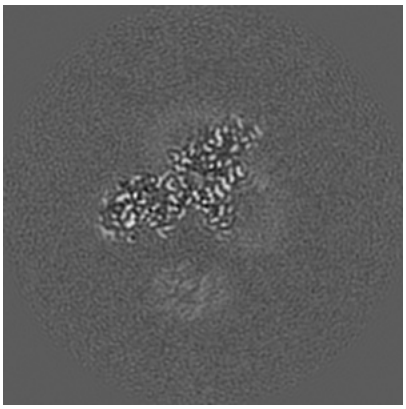


Z Index: 90

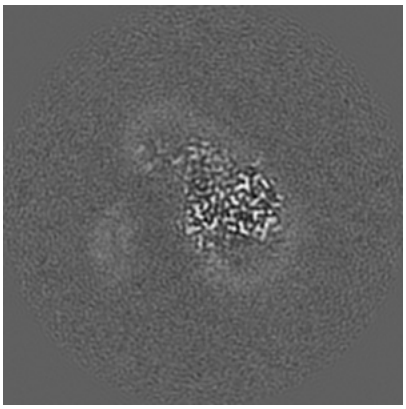
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

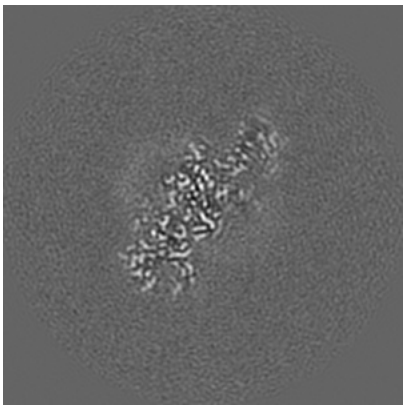
6.3.1 Primary map



X Index: 80

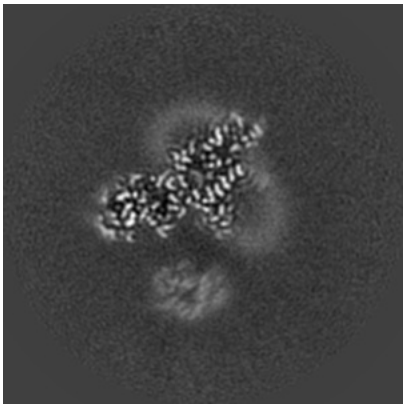


Y Index: 93

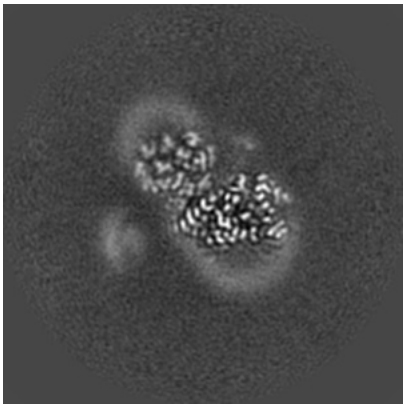


Z Index: 101

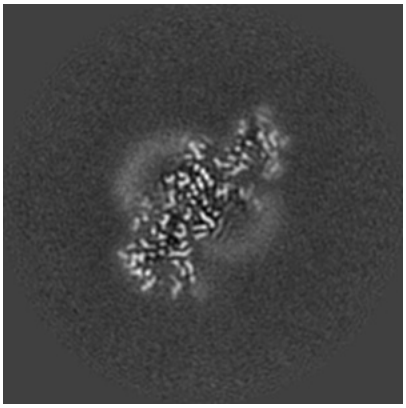
6.3.2 Raw map



X Index: 80



Y Index: 99

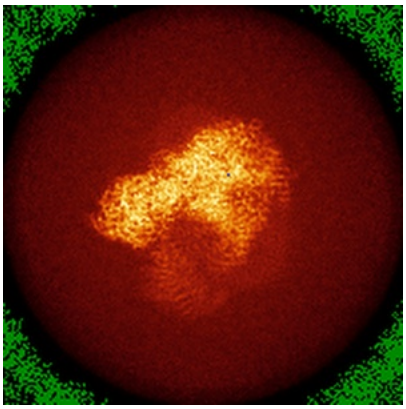


Z Index: 101

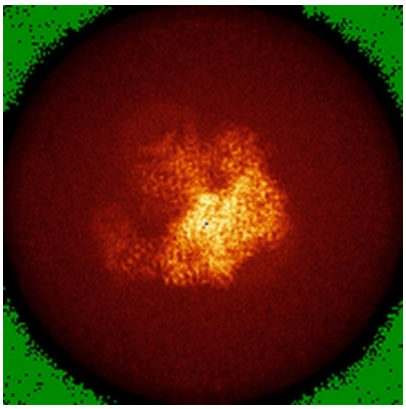
The images above show the largest variance slices of the map in three orthogonal directions.

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

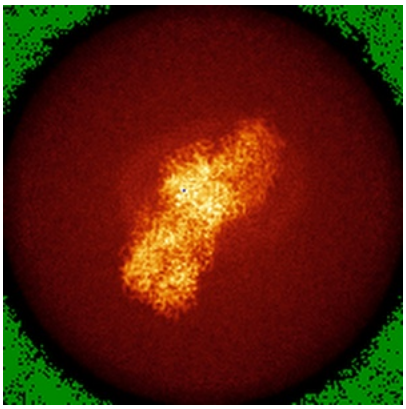
6.4.1 Primary map



X

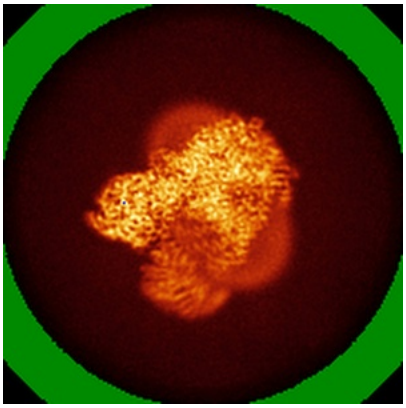


Y

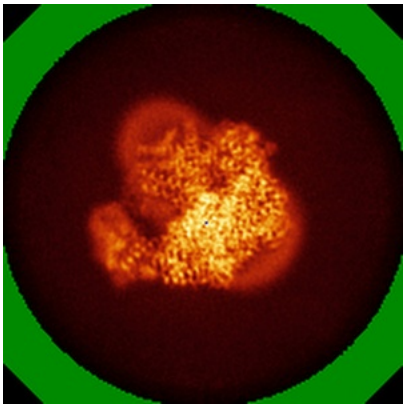


Z

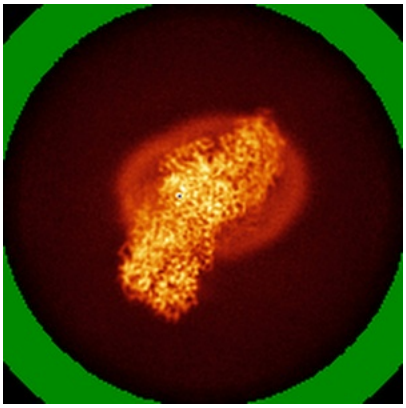
6.4.2 Raw map



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.

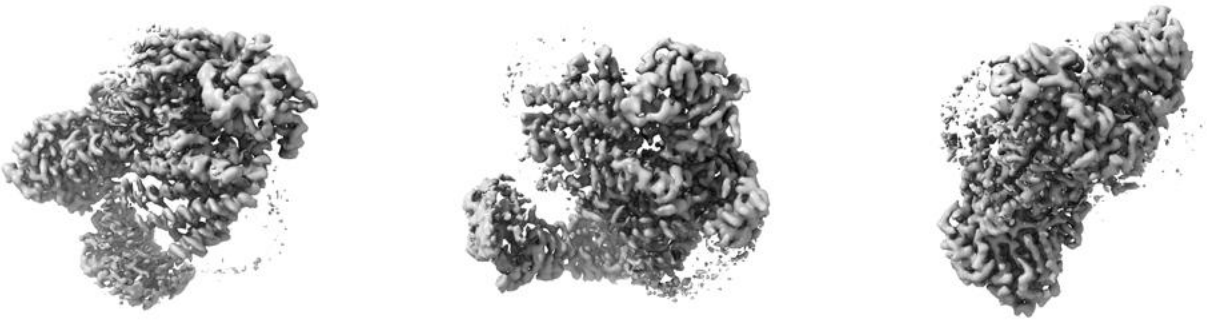
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0205. 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.

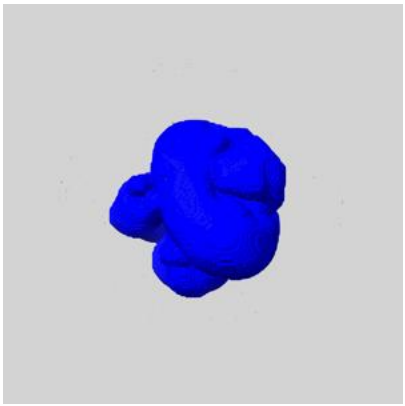
6.6 Mask visualisation (i)

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

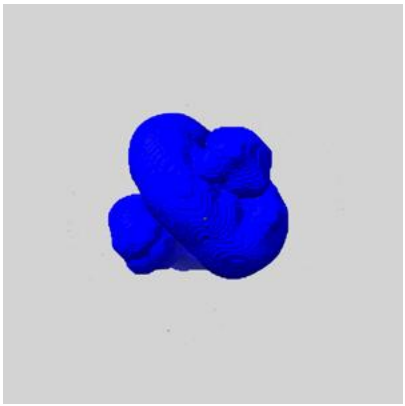
A mask typically either:

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

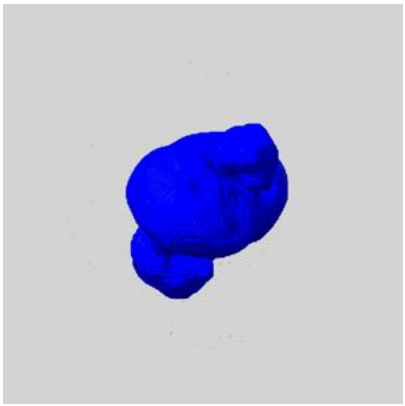
6.6.1 emd_15089_msk_1.map (i)



X



Y

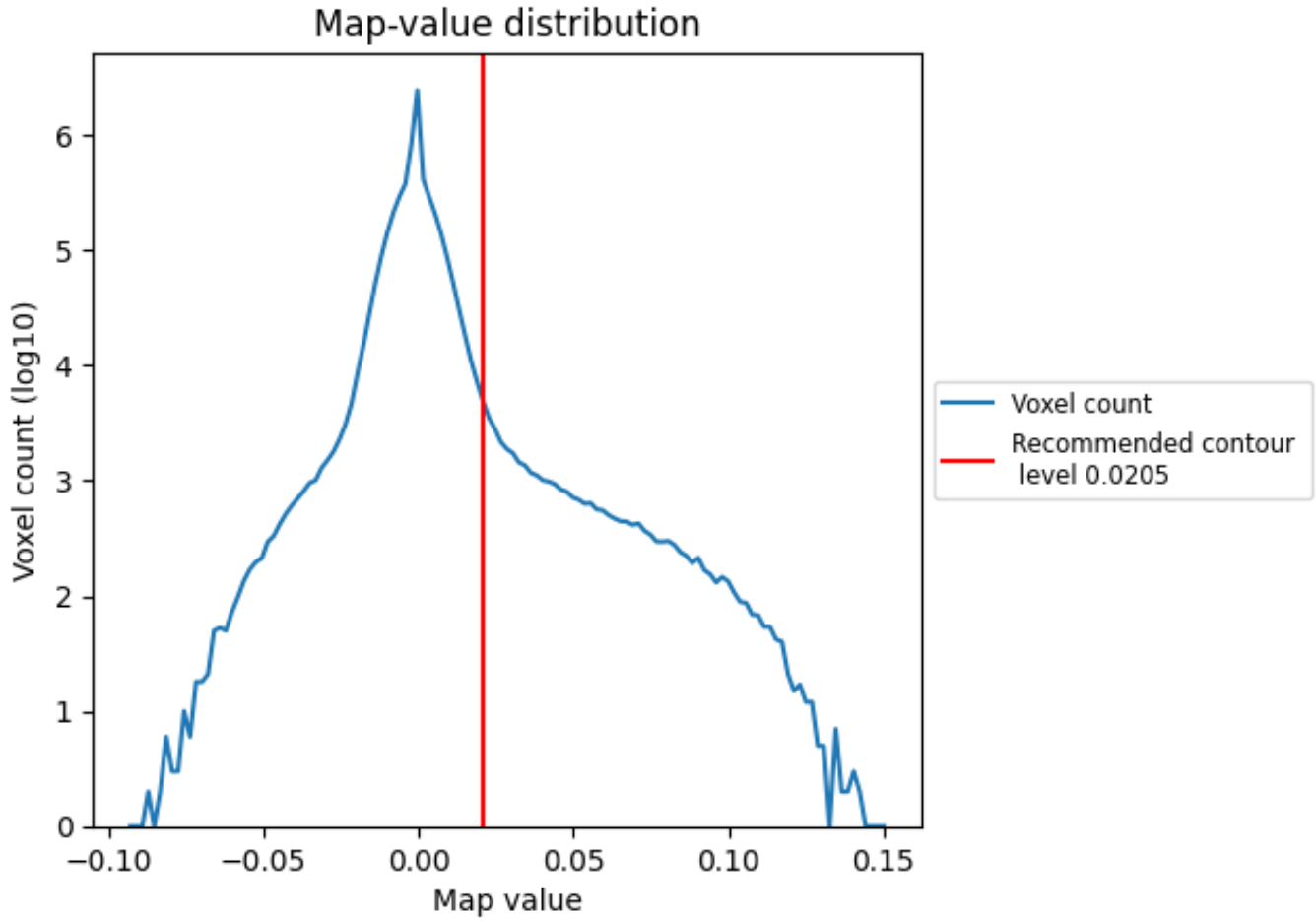


Z

7 Map analysis

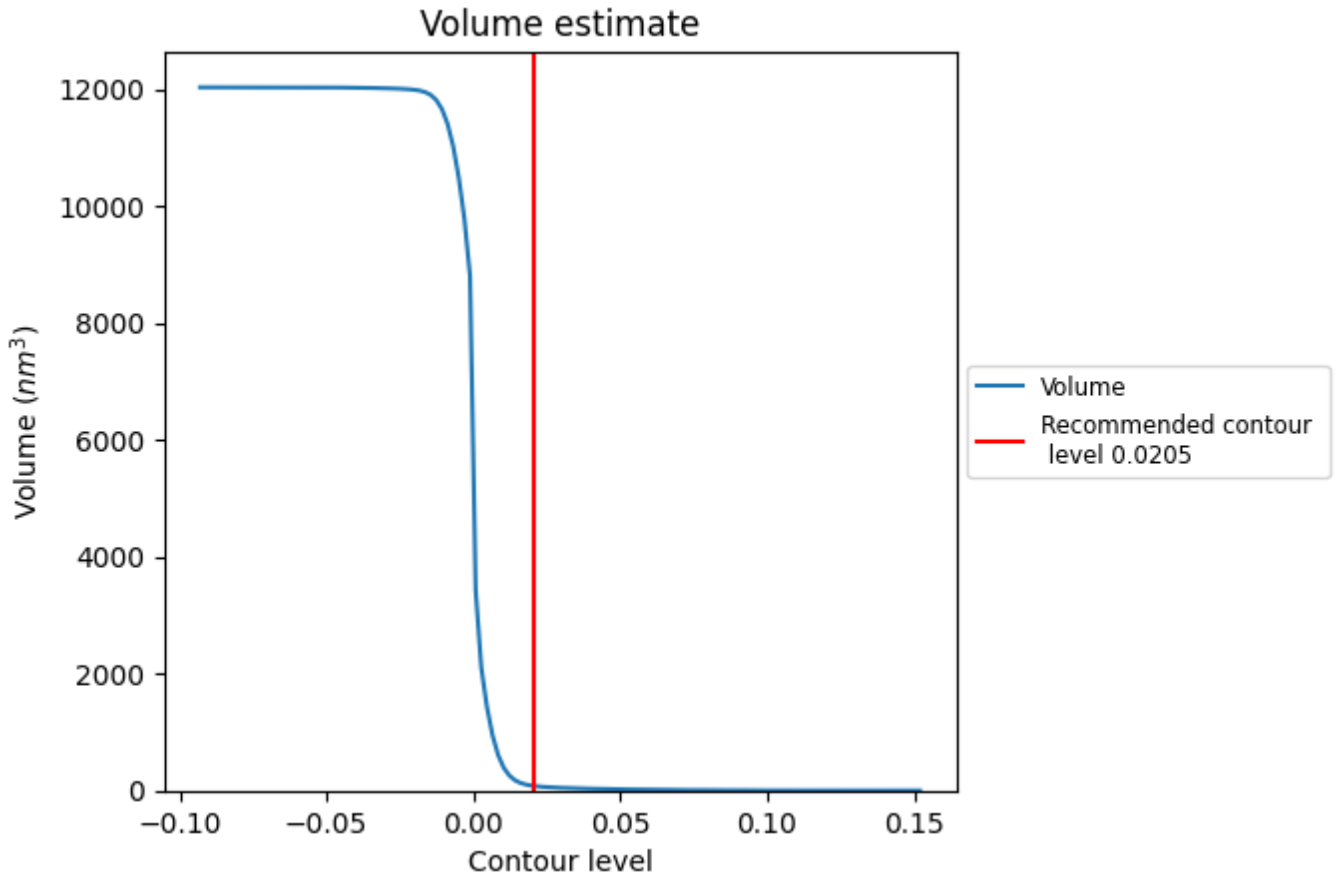
This section contains the results of statistical analysis of the map.

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.

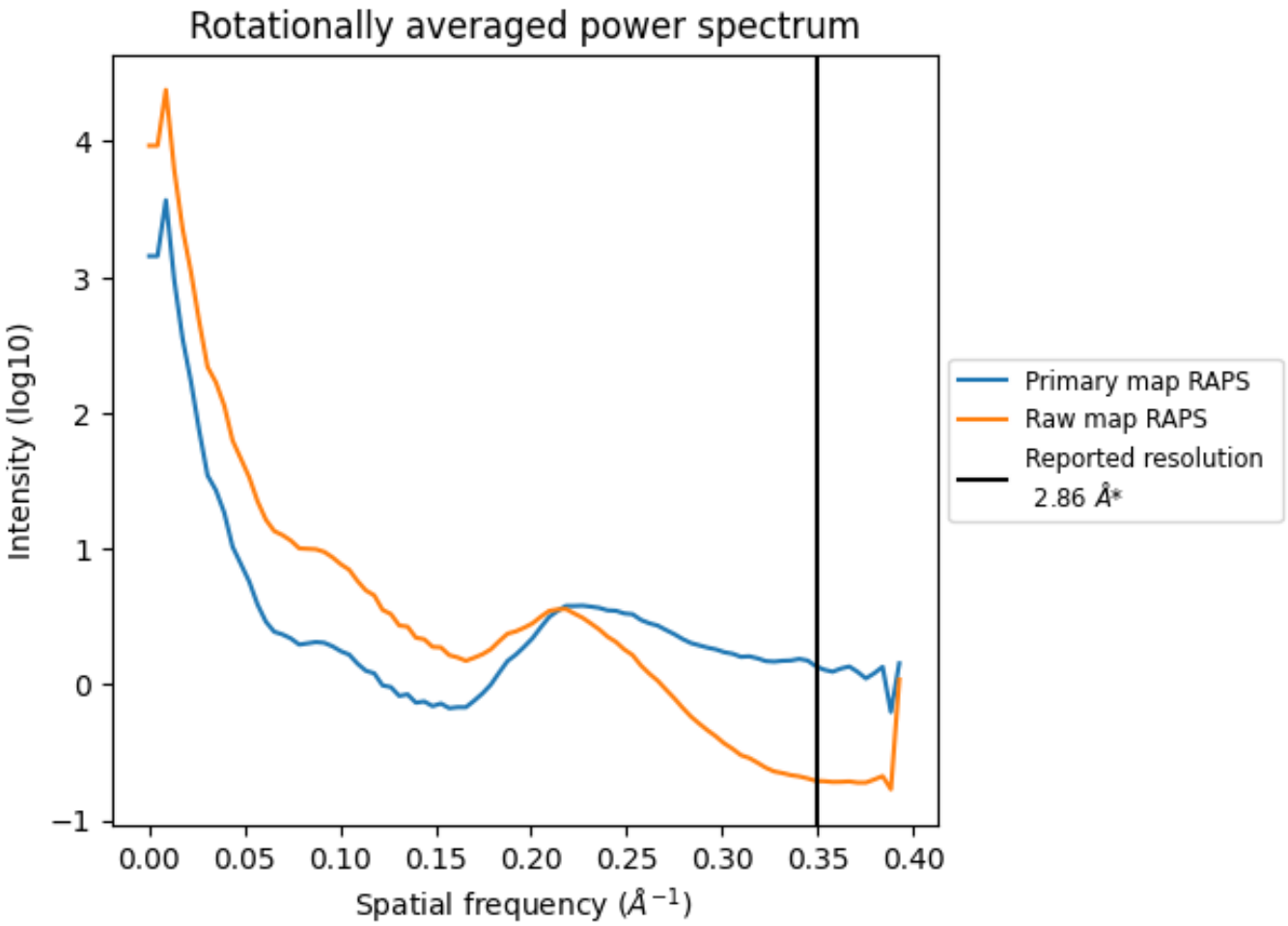
7.2 Volume estimate (i)



The volume at the recommended contour level is 80 nm^3; this corresponds to an approximate mass of 72 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)

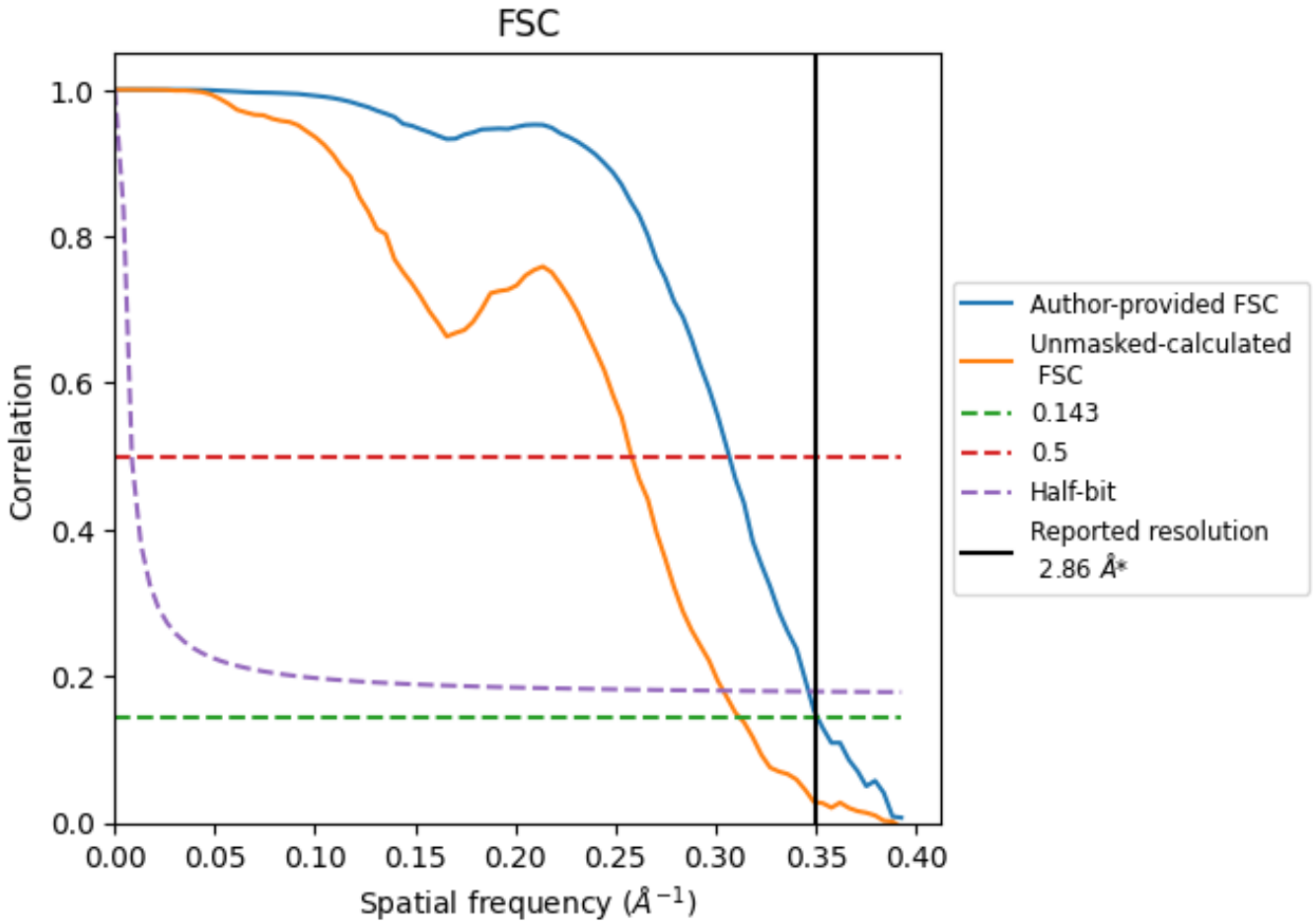


*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

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 0.350 Å^{-1}

8.2 Resolution estimates (i)

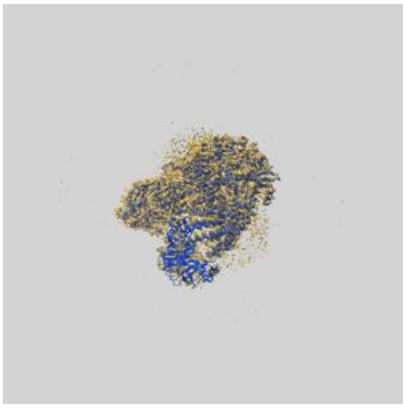
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.85	3.26	2.89
Unmasked-calculated*	3.20	3.87	3.29

*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 3.20 differs from the reported value 2.86 by more than 10 %

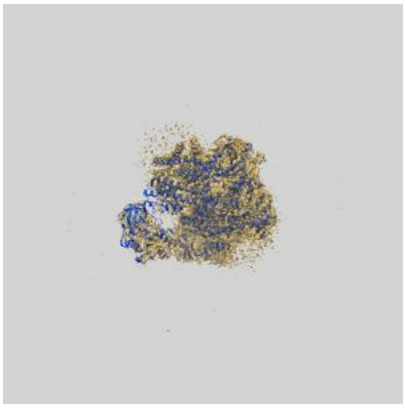
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15089 and PDB model 8A1U. Per-residue inclusion information can be found in section 3 on page 10.

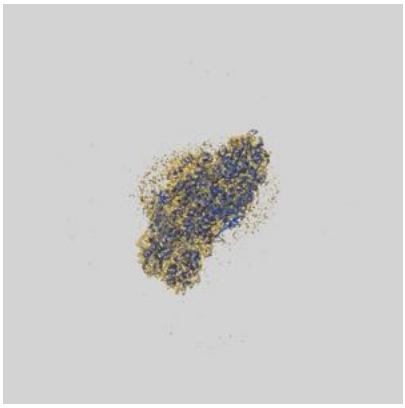
9.1 Map-model overlay



X



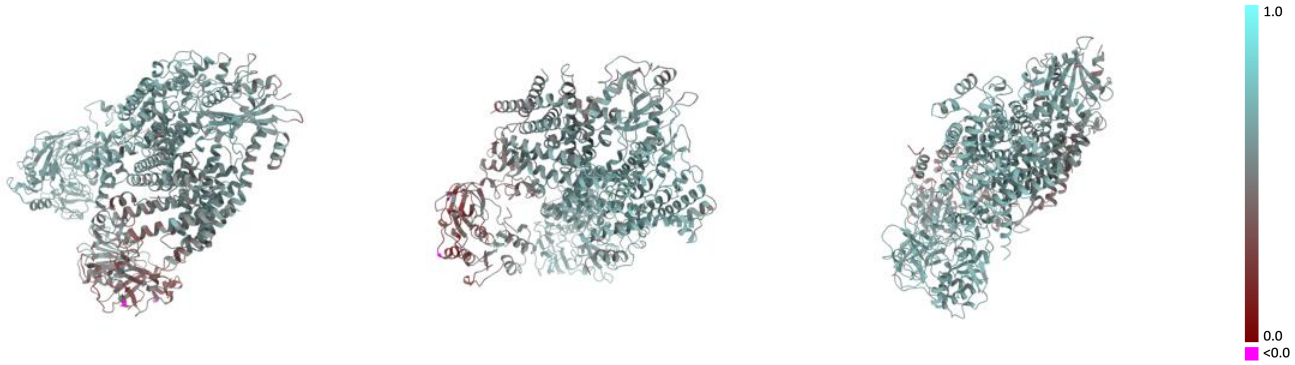
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0205 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.

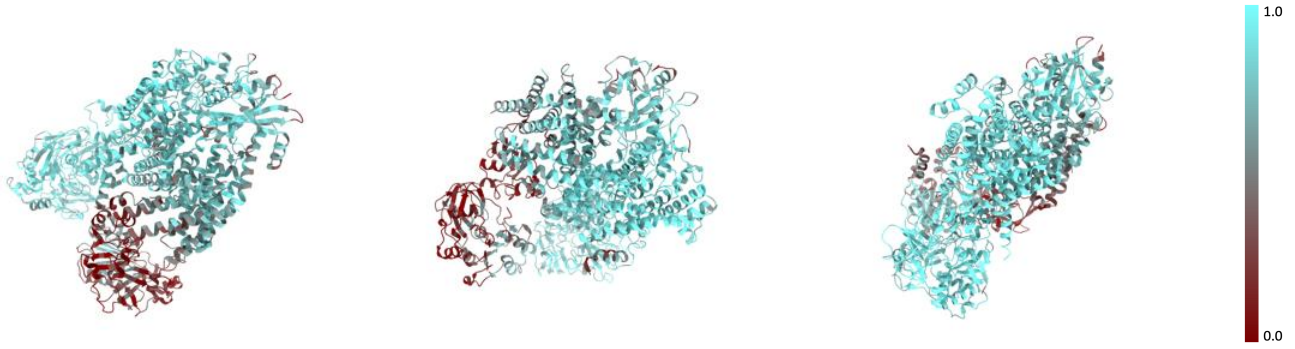
9.2 Q-score mapped to coordinate model (i)



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.

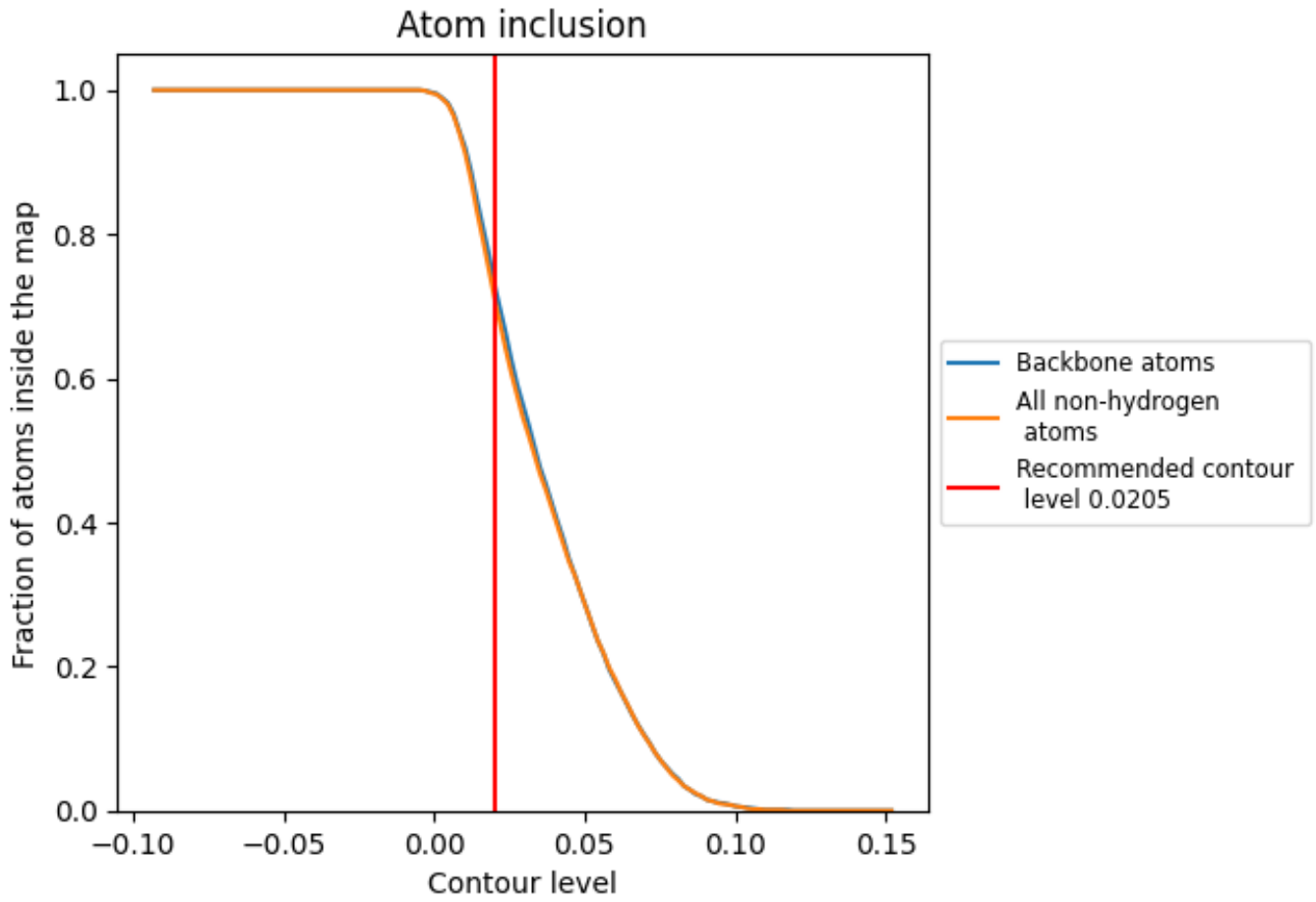
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0205).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.0205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.5580
A	0.8950	0.6270
B	0.8760	0.6180
C	0.7260	0.5600
D	0.7700	0.5800
E	0.7120	0.5540
F	0.2920	0.4150