



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:44 PM JST

PDB ID : 7XK7 / pdb_00007xk7
EMDB ID : EMD-33246
Title : Cryo-EM structure of Na⁺-pumping NADH-ubiquinone oxidoreductase from *Vibrio cholerae*, with korormicin
Authors : Kishikawa, J.; Ishikawa, M.; Masuya, T.; Murai, M.; Barquera, B.; Miyoshi, H.
Deposited on : 2022-04-19
Resolution : 2.90 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 : 1.8.5 (274361), 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

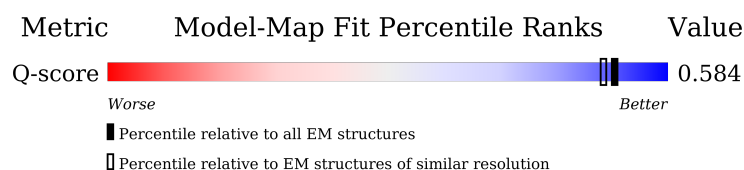
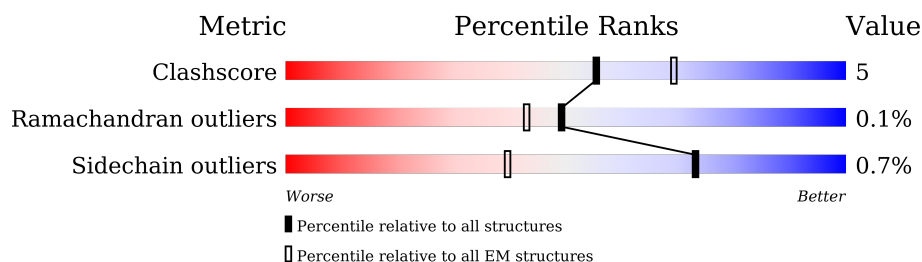
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



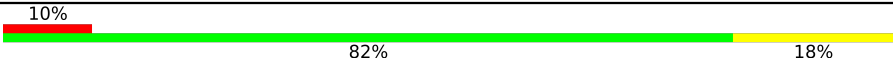
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	415	
3	C	257	
4	D	210	

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Mol	Chain	Length	Quality of chain
5	E	198	
6	F	414	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FES	F	501	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15186 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Na(+)-translocating NADH-quinone reductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	1	0
			3421	2168	585	651	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	412	Total	C	N	O	S	0	0
			3177	2102	517	536	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	N	O	S	0	0
			1902	1204	327	367	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1580	1048	250	272	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	198	Total	C	N	O	S	0	0
			1511	1013	230	257	11		

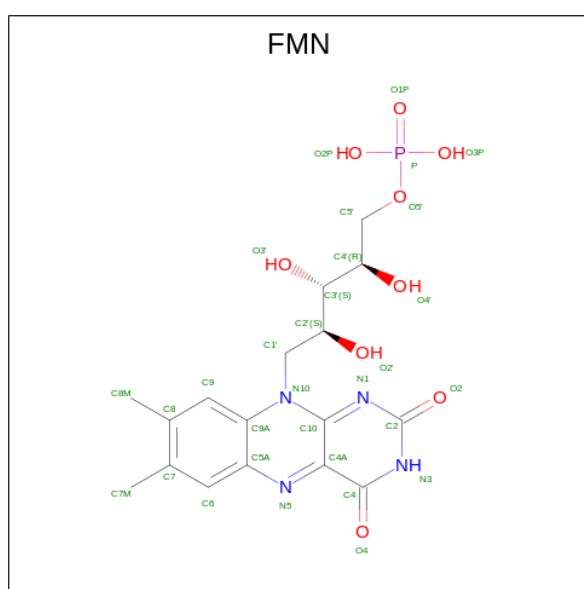
- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	408	Total	C	N	O	S	0	0
			3157	2021	517	595	24		

There are 6 discrepancies between the modelled and reference sequences:

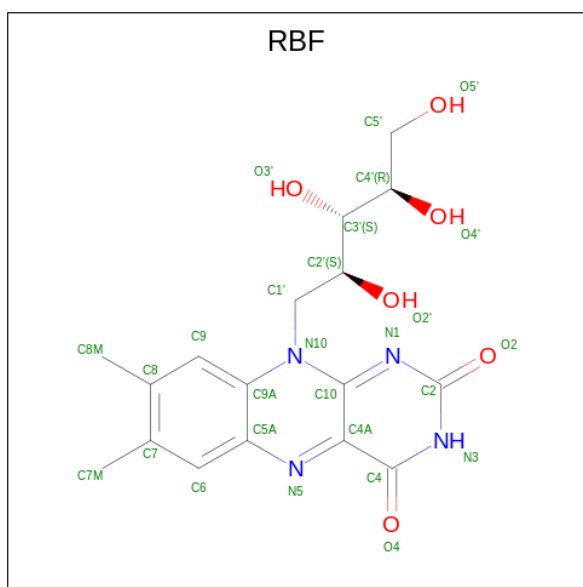
Chain	Residue	Modelled	Actual	Comment	Reference
F	409	HIS	-	expression tag	UNP A5F5Y4
F	410	HIS	-	expression tag	UNP A5F5Y4
F	411	HIS	-	expression tag	UNP A5F5Y4
F	412	HIS	-	expression tag	UNP A5F5Y4
F	413	HIS	-	expression tag	UNP A5F5Y4
F	414	HIS	-	expression tag	UNP A5F5Y4

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



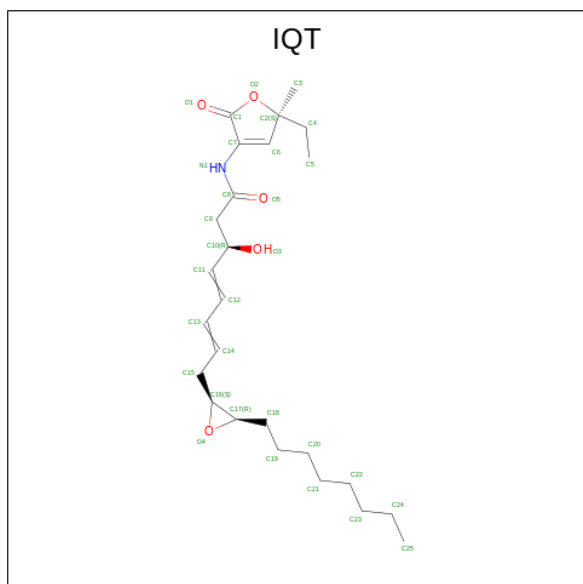
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			30	17	4	8	1	
7	C	1	Total	C	N	O	P	0
			30	17	4	8	1	

- Molecule 8 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



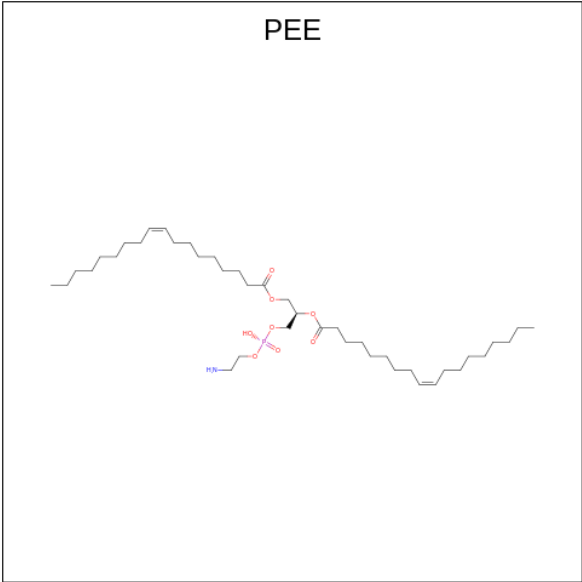
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			27	17	4	6	

- Molecule 9 is Korormicin (CCD ID: IQT) (formula: $C_{25}H_{39}NO_5$) (labeled as "Ligand of Interest" by depositor).



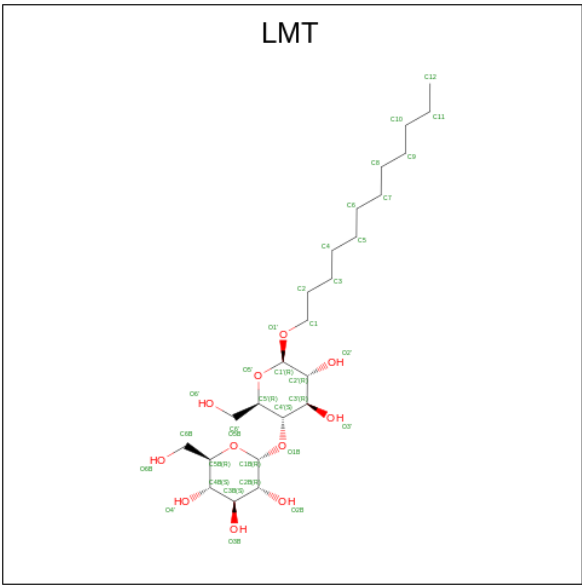
Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			31	25	1	5	

- Molecule 10 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
10	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
10	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			35	24	11	

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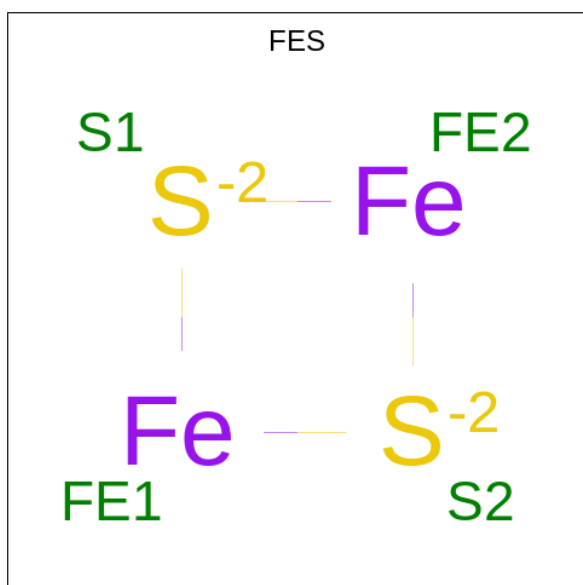
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Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			35	24	11	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

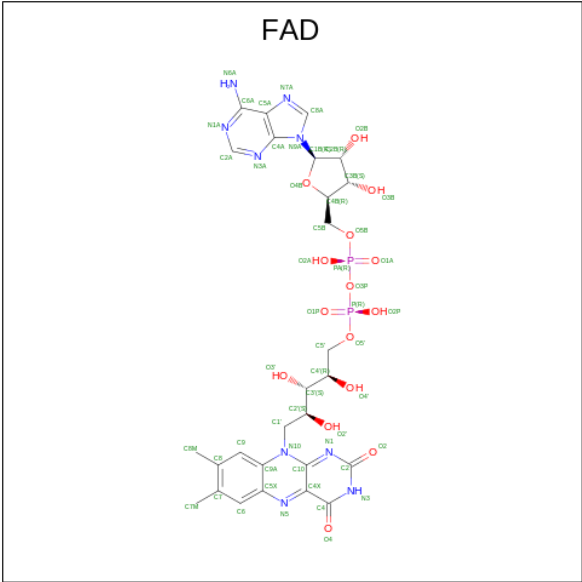
Mol	Chain	Residues	Atoms		AltConf
12	C	1	Total	Ca	0
			1	1	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	D	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: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	N	O	P	0
			53	27	9	15	2	

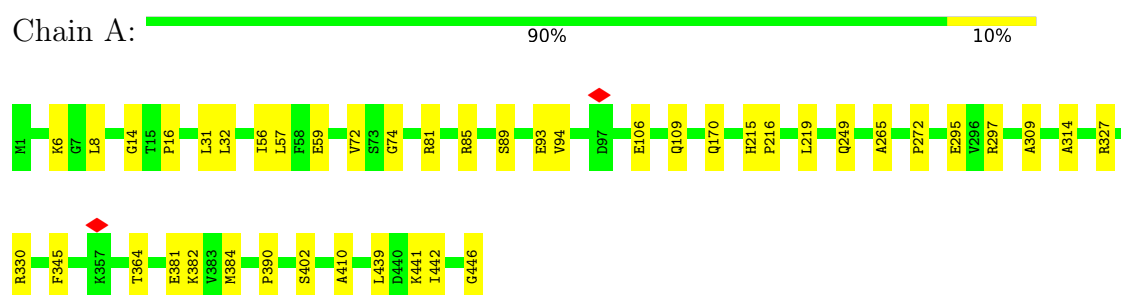
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	A	17	Total O 17 17	0
15	B	15	Total O 15 15	0
15	C	1	Total O 1 1	0
15	E	2	Total O 2 2	0

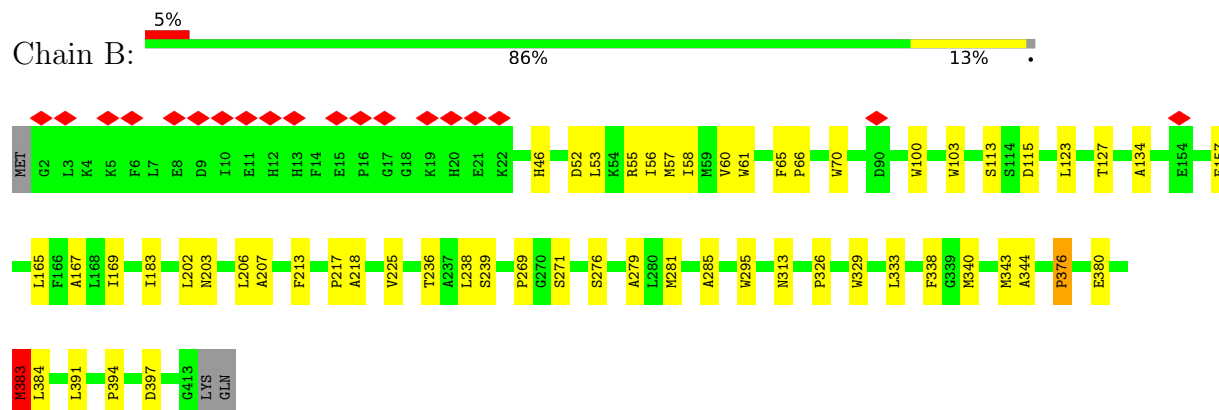
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

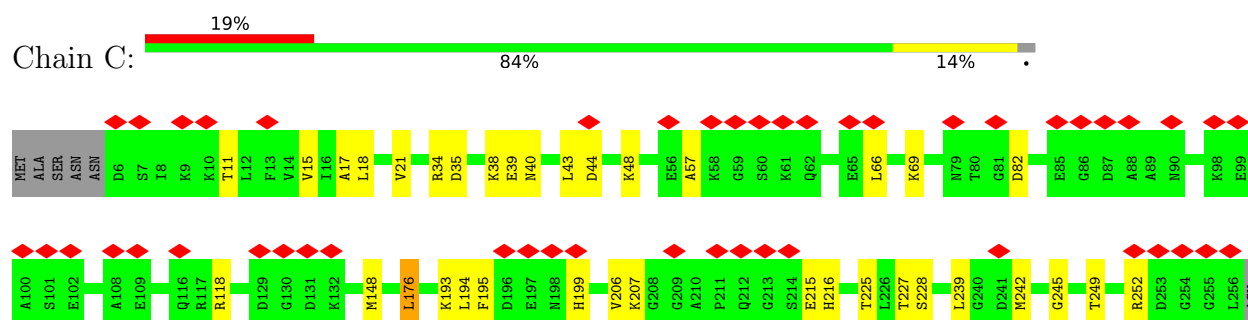
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



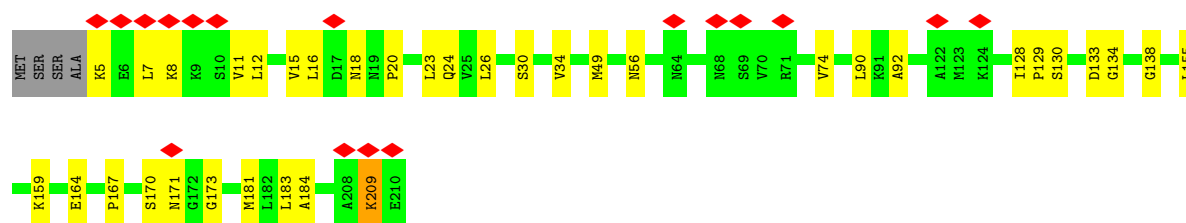
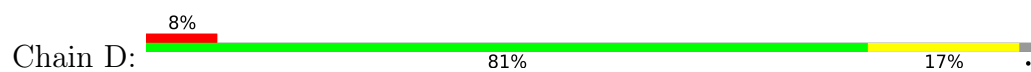
- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B



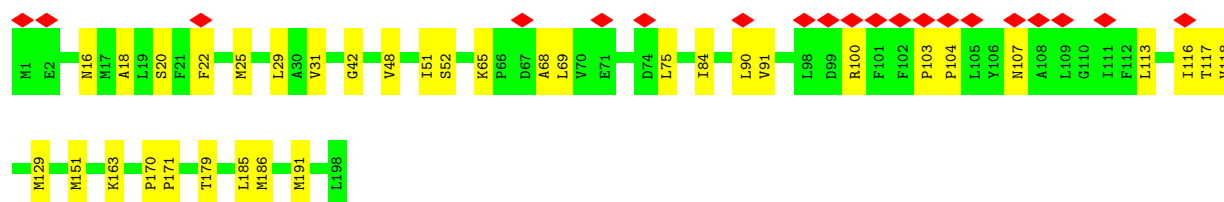
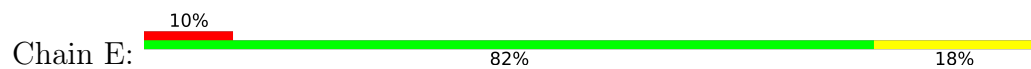
- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C



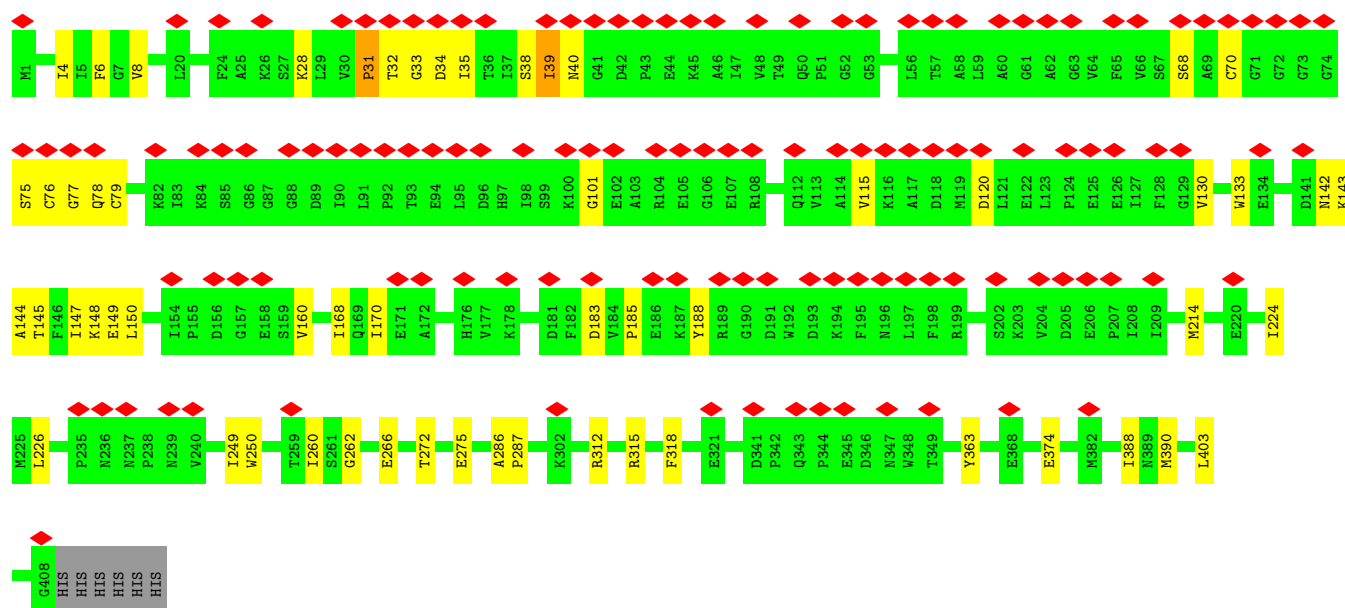
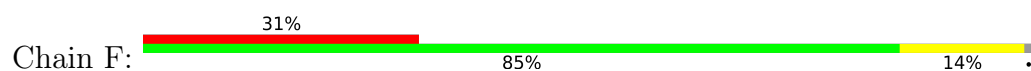
- Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50444	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.870	Depositor
Minimum map value	-2.517	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CA, FAD, IQT, RBF, LMT, FES, PEE

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	0.16	0/3485	0.39	0/4722
2	B	0.70	9/3275 (0.3%)	0.75	11/4457 (0.2%)
3	C	0.47	2/1934 (0.1%)	0.63	3/2610 (0.1%)
4	D	0.24	0/1612	0.53	1/2187 (0.0%)
5	E	0.15	0/1544	0.37	0/2094
6	F	0.18	0/3235	0.44	0/4381
All	All	0.39	11/15085 (0.1%)	0.54	15/20451 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	239	SER	CA-CB	-8.99	1.40	1.53
3	C	228	SER	CA-CB	-6.92	1.42	1.53
2	B	217	PRO	C-O	-6.83	1.15	1.24
3	C	225	THR	C-O	-6.16	1.15	1.23
2	B	236	THR	C-O	-6.03	1.16	1.24
2	B	269	PRO	C-O	-5.99	1.16	1.23
2	B	218	ALA	CA-CB	-5.44	1.46	1.54
2	B	383	MET	C-O	-5.22	1.17	1.24
2	B	271	SER	CA-CB	-5.19	1.44	1.53
2	B	338	PHE	C-O	-5.17	1.18	1.24
2	B	376	PRO	C-O	-5.12	1.17	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	THR	CB-CA-C	7.39	125.12	110.42
2	B	238	LEU	N-CA-C	-7.39	104.00	113.16
3	C	227	THR	N-CA-C	-7.01	104.35	113.12
2	B	225	VAL	N-CA-CB	-6.54	105.02	112.21
2	B	169	ILE	N-CA-C	-6.33	106.61	112.43
2	B	239	SER	N-CA-C	-6.16	106.30	113.88
2	B	167	ALA	O-C-N	-5.85	114.38	122.46
4	D	171	ASN	N-CA-C	-5.83	103.73	112.54
3	C	225	THR	N-CA-C	-5.55	106.18	113.17
2	B	213	PHE	CA-CB-CG	5.52	119.32	113.80
2	B	344	ALA	N-CA-C	-5.39	106.55	113.23
3	C	225	THR	CB-CA-C	-5.31	101.23	110.09
2	B	218	ALA	N-CA-CB	-5.16	103.50	110.67
2	B	217	PRO	N-CA-CB	-5.15	97.27	102.88
2	B	207	ALA	N-CA-C	-5.02	106.58	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	39	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3421	0	3467	26	0
2	B	3177	0	3154	29	0
3	C	1902	0	1910	21	0
4	D	1580	0	1669	22	0
5	E	1511	0	1588	24	0
6	F	3157	0	3083	37	0
7	B	30	0	19	0	0
7	C	30	0	19	1	0
8	B	27	0	20	1	0
9	B	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	102	0	164	8	0
10	C	51	0	82	3	0
11	B	70	0	90	0	0
12	C	1	0	0	0	0
13	D	4	0	0	0	0
13	F	4	0	0	2	0
14	F	53	0	31	0	0
15	A	17	0	0	3	0
15	B	15	0	0	1	0
15	C	1	0	0	0	0
15	E	2	0	0	0	0
All	All	15186	0	15296	153	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 5.

All (153) 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:397:ASP:OD2	15:B:601:HOH:O	1.98	0.81
1:A:215:HIS:HE1	15:A:515:HOH:O	1.65	0.78
6:F:39:ILE:HG22	6:F:40:ASN:H	1.55	0.72
6:F:160:VAL:HG21	6:F:224:ILE:HD11	1.71	0.72
3:C:40:ASN:ND2	4:D:92:ALA:O	2.24	0.71
2:B:165:LEU:HB3	2:B:343:MET:HE3	1.74	0.69
5:E:113:LEU:HA	5:E:116:ILE:HG22	1.75	0.68
4:D:5:LYS:HG3	4:D:7:LEU:H	1.57	0.67
6:F:70:CYS:HB2	6:F:76:CYS:HB3	1.74	0.67
1:A:446:GLY:HA3	6:F:101:GLY:HA3	1.78	0.66
5:E:100:ARG:NH2	6:F:28:LYS:O	2.29	0.65
6:F:143:LYS:NZ	6:F:149:GLU:OE1	2.25	0.64
10:B:506:PEE:H15	10:B:506:PEE:H49	1.78	0.64
4:D:56:ASN:HB3	4:D:130:SER:HB3	1.79	0.64
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.78	0.64
1:A:297:ARG:HH11	2:B:46:HIS:HD2	1.45	0.63
2:B:313:ASN:HD21	2:B:326:PRO:HA	1.63	0.62
2:B:113:SER:OG	2:B:115:ASP:OD1	2.17	0.62
1:A:384:MET:HE3	1:A:390:PRO:HG3	1.79	0.62
1:A:31:LEU:HD12	1:A:57:LEU:HD12	1.81	0.61
4:D:24:GLN:O	4:D:26:LEU:N	2.34	0.60
2:B:206:LEU:HD22	2:B:383:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLU:O	3:C:43:LEU:HG	2.01	0.60
6:F:78:GLN:NE2	6:F:266:GLU:OE1	2.33	0.60
1:A:309:ALA:HB1	1:A:314:ALA:HA	1.84	0.60
6:F:38:SER:HB2	6:F:120:ASP:HA	1.83	0.60
6:F:76:CYS:SG	6:F:77:GLY:N	2.75	0.59
3:C:118:ARG:NH1	3:C:242:MET:O	2.35	0.58
1:A:16:PRO:HA	1:A:272:PRO:HB2	1.84	0.58
6:F:275:GLU:OE2	6:F:363:TYR:OH	2.21	0.58
2:B:202:LEU:HD11	5:E:185:LEU:HB3	1.86	0.57
4:D:184:ALA:HB1	5:E:22:PHE:HZ	1.70	0.57
4:D:159:LYS:HG2	4:D:164:GLU:HA	1.88	0.56
2:B:203:ASN:OD1	8:B:502:RBF:N3	2.39	0.55
5:E:29:LEU:HD22	5:E:179:THR:HG22	1.89	0.55
6:F:35:ILE:HD11	6:F:115:VAL:HG12	1.89	0.54
1:A:216:PRO:HB3	1:A:219:LEU:HD12	1.89	0.54
4:D:167:PRO:HB2	4:D:173:GLY:HA3	1.91	0.54
5:E:48:VAL:O	5:E:52:SER:OG	2.22	0.54
6:F:75:SER:N	13:F:501:FES:S1	2.77	0.53
6:F:142:ASN:HD22	6:F:185:PRO:HD2	1.74	0.53
6:F:143:LYS:HD2	6:F:318:PHE:HB2	1.89	0.53
6:F:150:LEU:HD22	6:F:249:ILE:HG23	1.91	0.53
6:F:214:MET:HG2	6:F:224:ILE:HG23	1.91	0.53
6:F:31:PRO:C	6:F:33:GLY:H	2.18	0.52
6:F:130:VAL:HG13	6:F:262:GLY:HA3	1.91	0.52
6:F:4:ILE:O	6:F:8:VAL:HG23	2.10	0.52
6:F:272:THR:OG1	6:F:374:GLU:OE2	2.27	0.52
5:E:103:PRO:O	5:E:107:ASN:ND2	2.43	0.51
5:E:69:LEU:HD22	6:F:6:PHE:HZ	1.76	0.51
6:F:76:CYS:N	13:F:501:FES:S1	2.79	0.50
6:F:145:THR:HA	6:F:188:TYR:HB3	1.93	0.50
3:C:66:LEU:HA	3:C:69:LYS:HG2	1.94	0.50
2:B:134:ALA:HB2	10:B:506:PEE:H67	1.93	0.50
6:F:286:ALA:HB3	6:F:287:PRO:HD3	1.94	0.50
2:B:157:GLU:CD	2:B:157:GLU:H	2.20	0.49
4:D:133:ASP:OD1	4:D:134:GLY:N	2.45	0.49
6:F:183:ASP:OD1	6:F:183:ASP:N	2.44	0.49
4:D:18:ASN:HD22	4:D:23:LEU:HD23	1.76	0.49
4:D:15:VAL:HG12	4:D:16:LEU:HD12	1.94	0.49
1:A:215:HIS:CE1	15:A:515:HOH:O	2.50	0.49
6:F:170:ILE:HG12	6:F:260:ILE:HG22	1.95	0.49
4:D:183:LEU:HB3	5:E:191:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:GLY:O	3:C:249:THR:HG23	2.14	0.48
1:A:295:GLU:OE2	1:A:330:ARG:NH1	2.46	0.48
3:C:195:PHE:HB3	3:C:199:HIS:HA	1.96	0.48
2:B:55:ARG:HA	2:B:58:ILE:HG22	1.94	0.47
4:D:49:MET:HG2	4:D:138:GLY:HA3	1.97	0.47
5:E:84:ILE:HD11	5:E:118:VAL:HG13	1.95	0.47
1:A:32:LEU:HD23	1:A:89:SER:HB3	1.96	0.47
6:F:168:ILE:HG23	6:F:214:MET:HE2	1.97	0.46
3:C:34:ARG:O	3:C:38:LYS:HG2	2.15	0.46
5:E:129:MET:HE3	5:E:129:MET:HB3	1.91	0.46
1:A:170:GLN:OE1	1:A:249:GLN:NE2	2.47	0.46
3:C:82:ASP:N	3:C:82:ASP:OD1	2.49	0.46
2:B:326:PRO:HG2	2:B:329:TRP:HD1	1.81	0.46
3:C:249:THR:HG22	3:C:252:ARG:HH12	1.81	0.46
7:C:301:FMN:H1'2	7:C:301:FMN:H4'	1.60	0.46
10:C:303:PEE:H81	10:C:303:PEE:H74	1.80	0.45
2:B:61:TRP:CH2	2:B:65:PHE:HZ	2.35	0.45
2:B:394:PRO:HG3	5:E:163:LYS:HD2	1.98	0.45
5:E:51:ILE:HG22	5:E:90:LEU:HD11	1.97	0.45
1:A:382:LYS:NZ	15:A:502:HOH:O	2.41	0.45
1:A:56:ILE:HD11	1:A:59:GLU:HG3	1.99	0.45
4:D:128:ILE:CG2	4:D:129:PRO:HD3	2.47	0.45
1:A:410:ALA:O	1:A:439:LEU:HD21	2.17	0.45
6:F:133:TRP:HB2	6:F:260:ILE:HG12	1.98	0.45
2:B:100:TRP:HA	2:B:103:TRP:CD1	2.52	0.45
5:E:91:VAL:HG11	5:E:117:THR:HA	1.99	0.45
2:B:66:PRO:HB2	2:B:279:ALA:HB1	1.99	0.44
4:D:8:LYS:HA	4:D:11:VAL:HG22	2.00	0.44
1:A:74:GLY:HA3	1:A:93:GLU:O	2.17	0.44
1:A:106:GLU:HB2	1:A:109:GLN:HG3	2.00	0.44
3:C:44:ASP:O	3:C:48:LYS:HG2	2.18	0.44
3:C:215:GLU:HG3	3:C:216:HIS:CD2	2.52	0.44
1:A:81:ARG:NH1	1:A:85:ARG:O	2.49	0.43
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.52	0.43
4:D:184:ALA:HB1	5:E:22:PHE:CZ	2.51	0.43
4:D:30:SER:O	4:D:34:VAL:HG22	2.19	0.43
4:D:155:LEU:HD12	4:D:181:MET:HE3	1.99	0.43
6:F:68:SER:HA	6:F:79:CYS:SG	2.58	0.43
4:D:128:ILE:HG23	4:D:129:PRO:HD3	2.00	0.43
5:E:65:LYS:HG2	5:E:68:ALA:HB2	1.99	0.43
5:E:103:PRO:N	5:E:104:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASP:OD1	2:B:52:ASP:N	2.50	0.43
2:B:53:LEU:HD11	2:B:57:MET:HE2	2.01	0.43
2:B:281:MET:HE1	10:B:504:PEE:H13	2.01	0.43
3:C:176:LEU:HD12	3:C:176:LEU:HA	1.78	0.43
1:A:8:LEU:HD11	1:A:345:PHE:HZ	1.84	0.43
4:D:209:LYS:HA	4:D:209:LYS:HD2	1.68	0.43
5:E:75:LEU:HD11	6:F:6:PHE:CE2	2.54	0.42
3:C:18:LEU:HD13	4:D:74:VAL:HG13	2.01	0.42
2:B:56:ILE:O	2:B:60:VAL:HG23	2.19	0.42
10:B:504:PEE:H7	10:B:504:PEE:H49	1.82	0.42
2:B:340:MET:HE3	2:B:340:MET:HB3	1.72	0.42
6:F:144:ALA:HB3	6:F:147:ILE:HB	2.01	0.42
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.93	0.42
3:C:69:LYS:HE2	3:C:69:LYS:HB2	1.88	0.42
5:E:16:ASN:O	5:E:20:SER:HB3	2.19	0.42
5:E:42:GLY:HA3	5:E:151:MET:HG3	2.01	0.42
6:F:388:ILE:HD11	6:F:403:LEU:HD22	2.02	0.42
2:B:100:TRP:CZ3	10:B:506:PEE:H14	2.55	0.42
6:F:148:LYS:HE2	6:F:250:TRP:CZ3	2.54	0.42
2:B:183:ILE:HD12	2:B:183:ILE:HA	1.95	0.42
2:B:295:TRP:CZ3	10:B:504:PEE:H43	2.54	0.42
2:B:383:MET:HE2	2:B:384:LEU:HG	2.02	0.42
3:C:194:LEU:HD22	3:C:239:LEU:HD11	2.02	0.42
1:A:402:SER:HB3	1:A:442:ILE:HD11	2.01	0.42
5:E:170:PRO:HA	5:E:171:PRO:HD3	1.97	0.42
2:B:285:ALA:HB2	10:B:504:PEE:H67	2.01	0.42
3:C:35:ASP:O	3:C:39:GLU:HG3	2.20	0.41
4:D:11:VAL:HG23	4:D:12:LEU:HG	2.01	0.41
6:F:39:ILE:HG22	6:F:40:ASN:N	2.28	0.41
1:A:327:ARG:HB3	1:A:364:THR:HG22	2.02	0.41
1:A:441:LYS:HE2	1:A:441:LYS:HB3	1.80	0.41
5:E:18:ALA:O	5:E:25:MET:HE1	2.20	0.41
1:A:14:GLY:O	1:A:265:ALA:HB1	2.21	0.41
3:C:17:ALA:O	3:C:21:VAL:HG23	2.21	0.41
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.94	0.41
1:A:6:LYS:HD2	1:A:381:GLU:O	2.20	0.41
10:C:303:PEE:H49	10:C:303:PEE:H55	1.90	0.41
2:B:123:LEU:O	2:B:127:THR:HG23	2.20	0.41
10:B:506:PEE:H58	10:B:506:PEE:H53	1.96	0.41
3:C:193:LYS:HB2	3:C:216:HIS:CE1	2.56	0.41
6:F:214:MET:HA	6:F:226:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:VAL:HG12	5:E:31:VAL:O	2.20	0.40
6:F:312:ARG:HH22	6:F:315:ARG:HH21	1.70	0.40
3:C:148:MET:HE2	3:C:148:MET:HB2	1.97	0.40
2:B:391:LEU:HD22	5:E:186:MET:HG2	2.02	0.40
3:C:57:ALA:HB2	3:C:66:LEU:HD12	2.02	0.40
6:F:390:MET:HE3	6:F:390:MET:HB3	1.88	0.40
3:C:11:THR:O	3:C:15:VAL:HG13	2.22	0.40
10:C:303:PEE:H64	10:C:303:PEE:H58	1.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	445/446 (100%)	438 (98%)	7 (2%)	0	100	100
2	B	410/415 (99%)	403 (98%)	7 (2%)	0	100	100
3	C	249/257 (97%)	243 (98%)	6 (2%)	0	100	100
4	D	204/210 (97%)	195 (96%)	8 (4%)	1 (0%)	24	54
5	E	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
6	F	406/414 (98%)	391 (96%)	14 (3%)	1 (0%)	43	72
All	All	1910/1940 (98%)	1860 (97%)	48 (2%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	31	PRO
4	D	20	PRO

5.3.2 Protein sidechains ⓘ

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	376/376 (100%)	376 (100%)	0	100	100
2	B	317/320 (99%)	313 (99%)	4 (1%)	61	86
3	C	200/205 (98%)	197 (98%)	3 (2%)	57	84
4	D	173/176 (98%)	171 (99%)	2 (1%)	63	86
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	335/343 (98%)	333 (99%)	2 (1%)	78	93
All	All	1566/1585 (99%)	1555 (99%)	11 (1%)	73	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	333	LEU
2	B	376	PRO
2	B	380	GLU
2	B	383	MET
3	C	176	LEU
3	C	206	VAL
3	C	207	LYS
4	D	170	SER
4	D	209	LYS
6	F	32	THR
6	F	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
2	B	20	HIS
2	B	46	HIS
2	B	78	GLN
2	B	178	GLN
2	B	219	GLN

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Mol	Chain	Res	Type
2	B	240	GLN
2	B	243	GLN
2	B	313	ASN
2	B	354	ASN
3	C	37	GLN
3	C	40	ASN
3	C	46	GLN
3	C	216	HIS
4	D	18	ASN
4	D	56	ASN
4	D	75	GLN
4	D	88	GLN
4	D	176	GLN
4	D	205	GLN
5	E	57	ASN
5	E	119	ASN
6	F	97	HIS
6	F	142	ASN
6	F	239	ASN
6	F	295	GLN
6	F	356	HIS
6	F	362	ASN
6	F	384	ASN

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FES	D	301	-	0,4,4	-	-	-		
7	FMN	C	301	3	29,32,33	1.13	2 (6%)	40,47,50	0.92	2 (5%)
7	FMN	B	501	2	29,32,33	1.05	1 (3%)	40,47,50	0.80	1 (2%)
11	LMT	B	505	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
14	FAD	F	502	-	56,58,58	0.31	0	81,89,89	0.37	1 (1%)
13	FES	F	501	6	0,4,4	-	-	-		
11	LMT	B	507	-	36,36,36	1.18	5 (13%)	47,47,47	1.02	3 (6%)
10	PEE	B	506	-	50,50,50	1.14	6 (12%)	53,55,55	1.14	4 (7%)
9	IQT	B	503	-	31,32,32	1.74	4 (12%)	30,42,42	0.64	0
8	RBF	B	502	-	29,29,29	2.92	10 (34%)	41,43,43	1.87	9 (21%)
10	PEE	B	504	-	50,50,50	1.14	6 (12%)	53,55,55	1.10	3 (5%)
10	PEE	C	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.15	2 (3%)

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
13	FES	D	301	-	-	-	0/1/1/1
7	FMN	C	301	3	-	11/15/17/18	0/3/3/3
7	FMN	B	501	2	-	6/15/17/18	0/3/3/3
11	LMT	B	505	-	-	15/21/61/61	0/2/2/2
14	FAD	F	502	-	-	12/34/50/50	0/6/6/6
13	FES	F	501	6	-	-	0/1/1/1
11	LMT	B	507	-	-	11/21/61/61	0/2/2/2
10	PEE	B	506	-	-	26/54/54/54	-
9	IQT	B	503	-	-	11/27/46/46	0/2/2/2
8	RBF	B	502	-	-	6/14/14/14	0/3/3/3
10	PEE	B	504	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEE	C	303	-	-	29/54/54/54	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	RBF	C4A-N5	7.54	1.45	1.30
8	B	502	RBF	C10-N1	6.51	1.46	1.33
9	B	503	IQT	C6-C7	6.20	1.40	1.33
8	B	502	RBF	C5A-N5	5.22	1.49	1.39
8	B	502	RBF	C9A-N10	4.88	1.49	1.41
8	B	502	RBF	C2-N1	4.72	1.48	1.36
9	B	503	IQT	C7-C1	-4.57	1.38	1.50
9	B	503	IQT	C13-C12	-4.31	1.31	1.44
8	B	502	RBF	C2-N3	4.14	1.48	1.39
8	B	502	RBF	C4-N3	3.74	1.45	1.38
10	C	303	PEE	C39-C38	3.74	1.53	1.31
10	B	504	PEE	C18-C19	3.71	1.53	1.31
10	C	303	PEE	C18-C19	3.70	1.53	1.31
10	B	504	PEE	C39-C38	3.69	1.53	1.31
10	B	506	PEE	C39-C38	3.69	1.53	1.31
10	B	506	PEE	C18-C19	3.67	1.53	1.31
8	B	502	RBF	C10-N10	3.65	1.45	1.37
8	B	502	RBF	O2-C2	-3.14	1.18	1.24
7	C	301	FMN	C2-N3	-3.08	1.31	1.39
9	B	503	IQT	C7-N1	-2.78	1.34	1.41
11	B	507	LMT	O3'-C3'	-2.72	1.36	1.43
7	B	501	FMN	C2-N3	-2.69	1.32	1.39
8	B	502	RBF	O4-C4	-2.66	1.18	1.23
11	B	505	LMT	O3'-C3'	-2.63	1.36	1.43
10	B	506	PEE	O2-C2	-2.52	1.40	1.46
10	C	303	PEE	O2-C2	-2.49	1.40	1.46
10	B	504	PEE	O3-C30	2.47	1.40	1.33
11	B	507	LMT	O2B-C2B	-2.43	1.37	1.43
10	B	506	PEE	O3-C30	2.42	1.40	1.33
10	C	303	PEE	O3-C30	2.42	1.40	1.33
11	B	507	LMT	O2'-C2'	-2.40	1.37	1.43
11	B	505	LMT	O2'-C2'	-2.39	1.37	1.43
11	B	505	LMT	O2B-C2B	-2.35	1.37	1.43
11	B	505	LMT	O3B-C3B	-2.33	1.37	1.43
10	B	504	PEE	O2-C10	2.27	1.40	1.34
10	B	504	PEE	O2-C2	-2.22	1.41	1.46
7	C	301	FMN	O2-C2	-2.22	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	LMT	O4'-C4B	-2.18	1.37	1.43
10	C	303	PEE	O2-C10	2.13	1.40	1.34
10	C	303	PEE	O3-C3	-2.11	1.40	1.45
11	B	507	LMT	O3B-C3B	-2.10	1.38	1.43
11	B	507	LMT	O4'-C4B	-2.08	1.38	1.43
10	B	506	PEE	O2-C10	2.07	1.40	1.34
10	B	506	PEE	O3-C3	-2.07	1.40	1.45
10	B	504	PEE	O3-C3	-2.03	1.40	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	502	RBF	C7M-C7-C6	-6.29	107.87	119.49
8	B	502	RBF	C7M-C7-C8	5.68	132.38	120.74
10	C	303	PEE	O2-C10-C11	3.98	120.08	111.50
10	B	506	PEE	O2-C10-C11	3.86	119.81	111.50
10	B	504	PEE	O2-C10-C11	3.78	119.65	111.50
8	B	502	RBF	C4-N3-C2	-3.26	119.62	125.64
11	B	505	LMT	O5'-C5'-C4'	2.84	115.75	109.75
8	B	502	RBF	C4A-C4-N3	2.69	120.02	113.19
10	C	303	PEE	O3-C30-C31	2.67	120.27	111.91
11	B	507	LMT	C3'-C4'-C5'	-2.66	104.83	110.93
10	B	506	PEE	O3-C30-C31	2.63	120.17	111.91
14	F	502	FAD	P-O3P-PA	-2.62	123.85	132.83
8	B	502	RBF	C4A-C10-N10	2.56	120.23	116.48
10	B	504	PEE	O3-C30-C31	2.51	119.79	111.91
8	B	502	RBF	O4-C4-C4A	-2.40	120.23	126.60
8	B	502	RBF	C5A-C9A-N10	2.38	120.42	117.95
11	B	505	LMT	O5'-C5'-C6'	2.38	112.34	106.44
8	B	502	RBF	C10-C4A-N5	-2.24	120.10	124.86
7	C	301	FMN	N3-C2-N1	2.23	123.77	119.38
8	B	502	RBF	C9A-C5A-N5	-2.23	120.01	122.43
11	B	507	LMT	O5B-C5B-C6B	2.22	111.96	106.44
11	B	507	LMT	C1'-O5'-C5'	-2.11	109.55	113.69
7	C	301	FMN	C4-N3-C2	-2.11	121.75	125.64
7	B	501	FMN	C4A-C4-N3	2.09	118.51	113.19
10	B	506	PEE	C20-C19-C18	-2.02	109.22	124.73
10	B	504	PEE	C40-C39-C38	-2.01	109.33	124.73
10	B	506	PEE	C40-C39-C38	-2.00	109.35	124.73

There are no chirality outliers.

All (155) 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'
7	C	301	FMN	N10-C1'-C2'-O2'
7	C	301	FMN	C1'-C2'-C3'-C4'
7	C	301	FMN	C3'-C4'-C5'-O5'
7	C	301	FMN	O4'-C4'-C5'-O5'
8	B	502	RBF	N10-C1'-C2'-C3'
8	B	502	RBF	C2'-C3'-C4'-O4'
8	B	502	RBF	O3'-C3'-C4'-O4'
8	B	502	RBF	O3'-C3'-C4'-C5'
9	B	503	IQT	C10-C11-C12-C13
9	B	503	IQT	C12-C13-C14-C15
9	B	503	IQT	O4-C17-C18-C19
10	B	504	PEE	C1-O3P-P-O4P
10	B	506	PEE	O2-C2-C3-O3
10	B	506	PEE	C1-O3P-P-O2P
10	B	506	PEE	C1-O3P-P-O1P
10	B	506	PEE	C1-O3P-P-O4P
10	C	303	PEE	C1-O3P-P-O2P
10	C	303	PEE	C1-O3P-P-O1P
10	C	303	PEE	C1-O3P-P-O4P
11	B	505	LMT	C2'-C1'-O1'-C1
11	B	505	LMT	O5'-C1'-O1'-C1
11	B	505	LMT	C2-C1-O1'-C1'
11	B	507	LMT	O5'-C1'-O1'-C1
14	F	502	FAD	C1'-C2'-C3'-O3'
14	F	502	FAD	C1'-C2'-C3'-C4'
14	F	502	FAD	O2'-C2'-C3'-O3'
14	F	502	FAD	O2'-C2'-C3'-C4'
10	B	504	PEE	O5-C30-O3-C3
10	B	506	PEE	O5-C30-O3-C3
10	C	303	PEE	O5-C30-O3-C3
10	B	504	PEE	C31-C30-O3-C3
11	B	507	LMT	C3'-C4'-O1B-C1B
10	B	506	PEE	C31-C30-O3-C3
10	C	303	PEE	C31-C30-O3-C3
10	B	506	PEE	C17-C18-C19-C20
10	B	506	PEE	C37-C38-C39-C40
11	B	505	LMT	C4B-C5B-C6B-O6B
10	B	504	PEE	C11-C10-O2-C2
11	B	505	LMT	O5'-C5'-C6'-O6'
11	B	505	LMT	O5B-C5B-C6B-O6B
11	B	507	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
14	F	502	FAD	O3'-C3'-C4'-C5'
8	B	502	RBF	C2'-C3'-C4'-C5'
14	F	502	FAD	C2'-C3'-C4'-C5'
10	B	504	PEE	O4-C10-O2-C2
11	B	507	LMT	C4'-C5'-C6'-O6'
14	F	502	FAD	C2'-C3'-C4'-O4'
7	B	501	FMN	O3'-C3'-C4'-C5'
10	B	504	PEE	C4-O4P-P-O3P
10	C	303	PEE	C4-O4P-P-O3P
7	C	301	FMN	O2'-C2'-C3'-O3'
7	C	301	FMN	O3'-C3'-C4'-O4'
14	F	502	FAD	O3'-C3'-C4'-O4'
10	B	504	PEE	C35-C36-C37-C38
10	C	303	PEE	C12-C13-C14-C15
9	B	503	IQT	C21-C22-C23-C24
11	B	507	LMT	C2'-C1'-O1'-C1
10	B	504	PEE	C14-C15-C16-C17
10	B	504	PEE	C19-C20-C21-C22
11	B	505	LMT	C5-C6-C7-C8
10	B	504	PEE	C11-C12-C13-C14
10	C	303	PEE	C37-C38-C39-C40
10	B	506	PEE	C14-C15-C16-C17
11	B	505	LMT	C7-C8-C9-C10
10	B	506	PEE	C11-C10-O2-C2
10	B	504	PEE	C31-C32-C33-C34
10	B	504	PEE	C37-C38-C39-C40
10	B	506	PEE	C19-C20-C21-C22
10	B	506	PEE	O4-C10-O2-C2
10	C	303	PEE	C35-C36-C37-C38
11	B	507	LMT	C7-C8-C9-C10
11	B	507	LMT	C6-C7-C8-C9
7	C	301	FMN	O2'-C2'-C3'-C4'
11	B	507	LMT	C4B-C5B-C6B-O6B
11	B	505	LMT	C1-C2-C3-C4
9	B	503	IQT	C9-C10-C11-C12
10	B	506	PEE	C1-C2-C3-O3
10	B	506	PEE	C11-C12-C13-C14
11	B	505	LMT	O1'-C1-C2-C3
10	C	303	PEE	C34-C35-C36-C37
11	B	505	LMT	C3-C4-C5-C6
10	B	504	PEE	C34-C35-C36-C37
10	B	504	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	C	303	PEE	C36-C37-C38-C39
10	B	504	PEE	C12-C13-C14-C15
9	B	503	IQT	C20-C21-C22-C23
11	B	507	LMT	C2-C1-O1'-C1'
10	B	504	PEE	C41-C42-C43-C44
7	C	301	FMN	O3'-C3'-C4'-C5'
7	B	501	FMN	C2'-C3'-C4'-C5'
11	B	507	LMT	C11-C10-C9-C8
10	B	504	PEE	O3P-C1-C2-O2
7	C	301	FMN	C2'-C3'-C4'-O4'
11	B	505	LMT	C9-C10-C11-C12
11	B	507	LMT	C5'-C4'-O1B-C1B
9	B	503	IQT	C11-C10-C9-C8
10	B	504	PEE	C3-C2-O2-C10
10	B	504	PEE	C32-C33-C34-C35
10	C	303	PEE	C24-C25-C26-C27
11	B	505	LMT	C4-C5-C6-C7
14	F	502	FAD	C5B-O5B-PA-O3P
7	B	501	FMN	C2'-C3'-C4'-O4'
10	C	303	PEE	C2-C1-O3P-P
10	B	504	PEE	C1-O3P-P-O2P
10	B	504	PEE	C4-O4P-P-O1P
10	C	303	PEE	C4-O4P-P-O1P
14	F	502	FAD	C5B-O5B-PA-O2A
10	B	504	PEE	O3P-C1-C2-C3
9	B	503	IQT	O3-C10-C11-C12
7	C	301	FMN	C1'-C2'-C3'-O3'
10	C	303	PEE	C43-C44-C45-C46
10	C	303	PEE	C11-C12-C13-C14
8	B	502	RBF	N10-C1'-C2'-O2'
9	B	503	IQT	C6-C7-N1-C8
10	B	506	PEE	C41-C42-C43-C44
9	B	503	IQT	C19-C20-C21-C22
10	B	506	PEE	O3P-C1-C2-O2
10	C	303	PEE	C14-C15-C16-C17
10	B	504	PEE	C1-C2-C3-O3
10	C	303	PEE	C10-C11-C12-C13
10	C	303	PEE	C39-C40-C41-C42
7	C	301	FMN	C2'-C3'-C4'-C5'
10	B	504	PEE	C13-C14-C15-C16
10	B	506	PEE	C43-C44-C45-C46
10	C	303	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
10	B	506	PEE	C40-C41-C42-C43
10	C	303	PEE	C13-C14-C15-C16
9	B	503	IQT	C16-C17-C18-C19
10	C	303	PEE	C40-C41-C42-C43
11	B	505	LMT	O5B-C1B-O1B-C4'
7	B	501	FMN	O3'-C3'-C4'-O4'
10	C	303	PEE	C21-C22-C23-C24
10	C	303	PEE	C41-C42-C43-C44
10	C	303	PEE	O4-C10-O2-C2
14	F	502	FAD	O4'-C4'-C5'-O5'
10	B	504	PEE	C42-C43-C44-C45
10	B	506	PEE	O3P-C1-C2-C3
10	B	506	PEE	C18-C19-C20-C21
10	B	504	PEE	C36-C37-C38-C39
10	B	506	PEE	C36-C37-C38-C39
10	B	506	PEE	C38-C39-C40-C41
14	F	502	FAD	O4B-C4B-C5B-O5B
10	C	303	PEE	C11-C10-O2-C2
11	B	505	LMT	C2B-C1B-O1B-C4'
10	B	504	PEE	O2-C10-C11-C12
10	B	506	PEE	C12-C13-C14-C15
10	C	303	PEE	C18-C19-C20-C21
10	C	303	PEE	C4-O4P-P-O2P
10	C	303	PEE	O2-C10-C11-C12
10	B	506	PEE	C5-C4-O4P-P
10	B	506	PEE	C23-C24-C25-C26
10	B	506	PEE	C16-C17-C18-C19
10	B	504	PEE	O4-C10-C11-C12

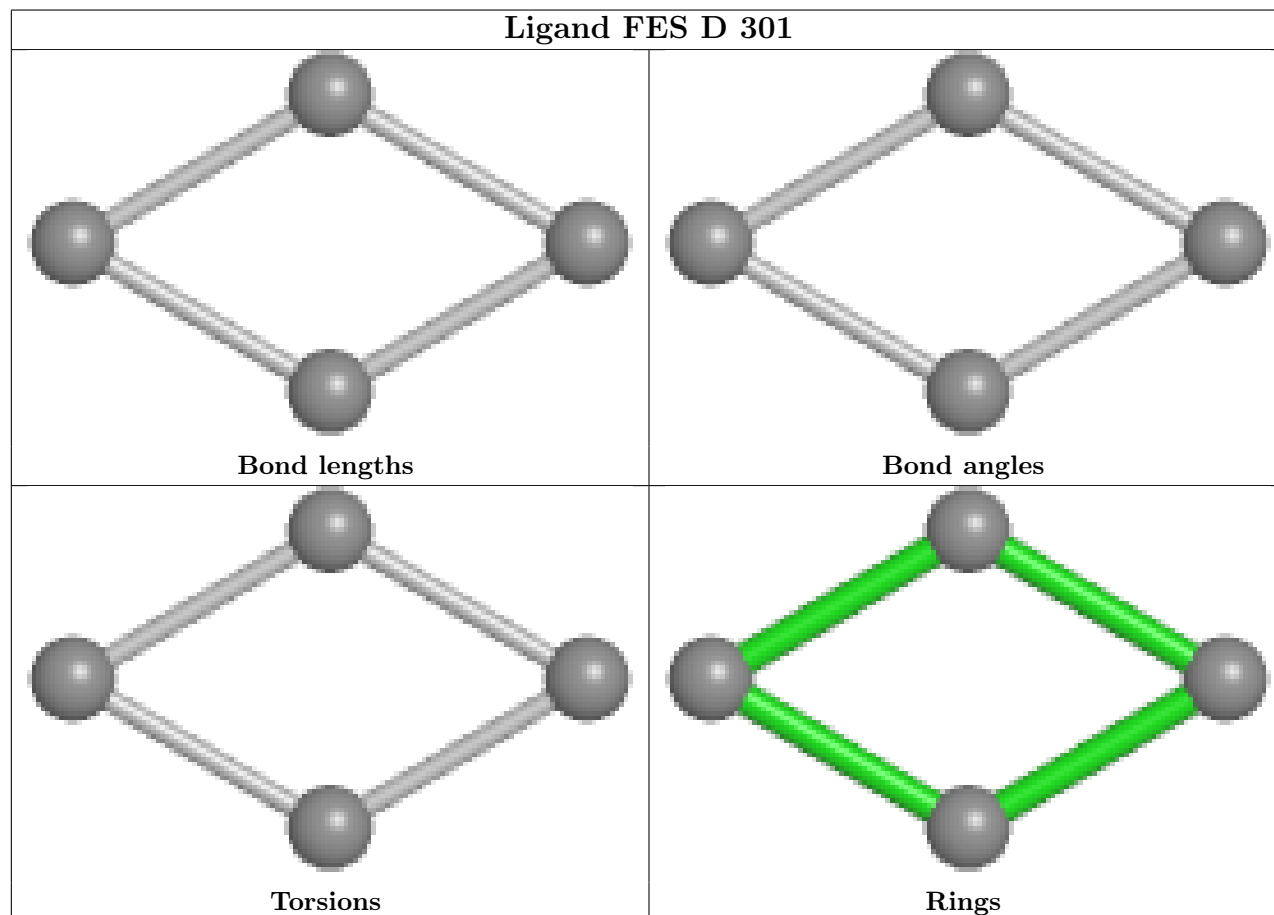
There are no ring outliers.

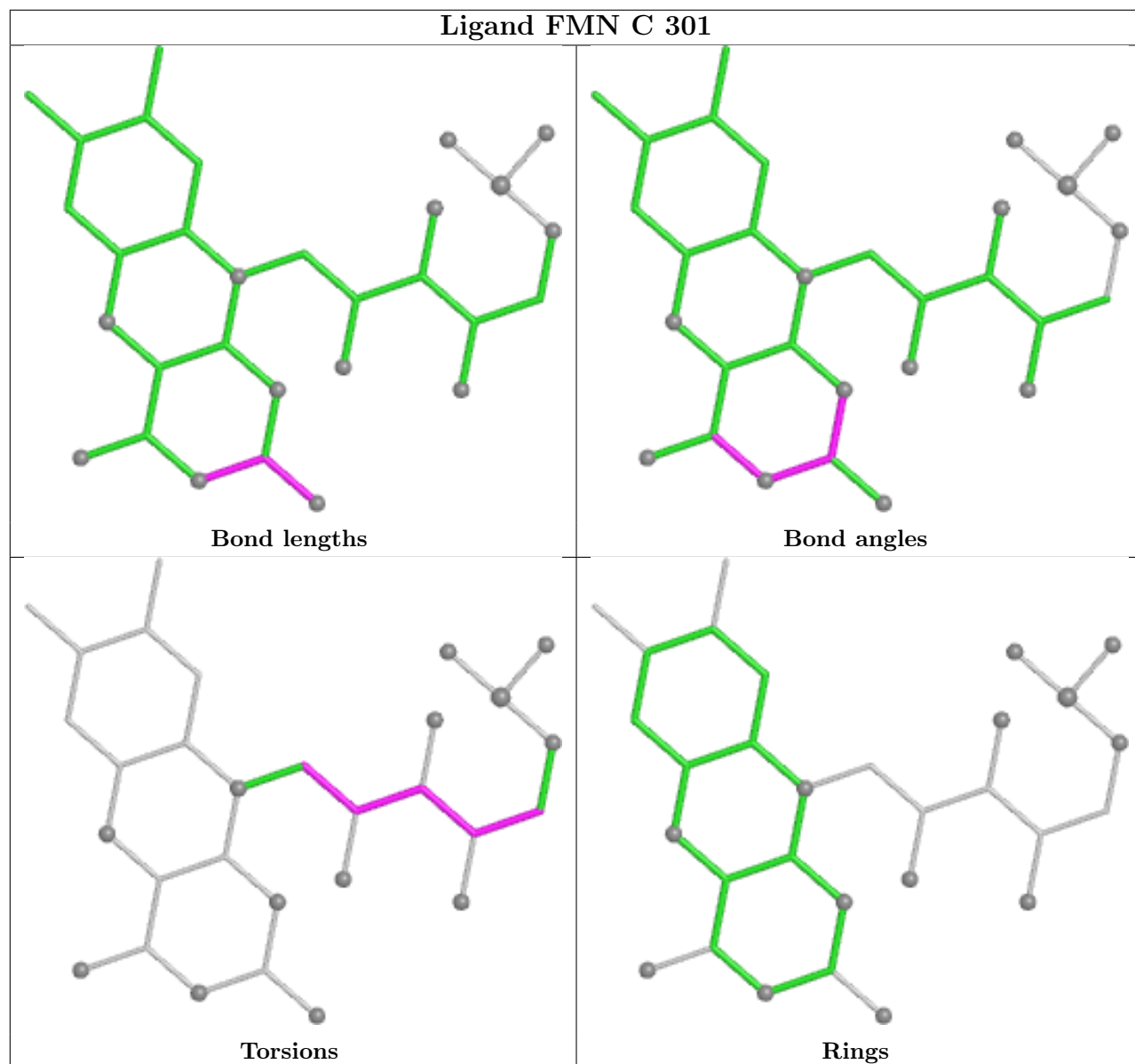
6 monomers are involved in 15 short contacts:

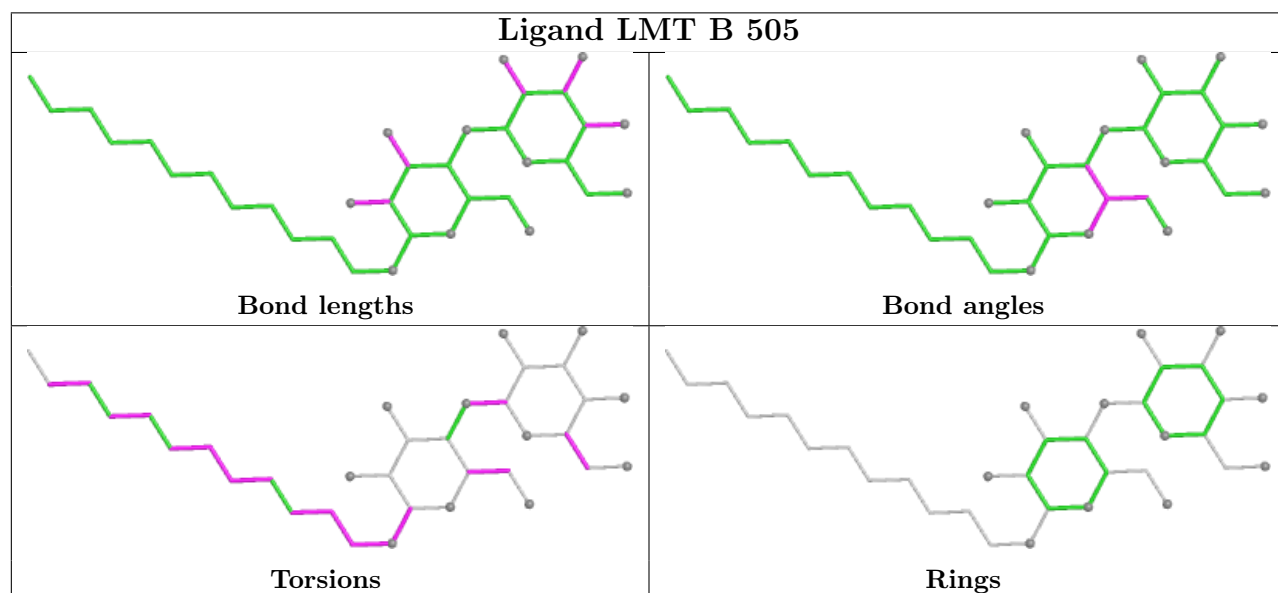
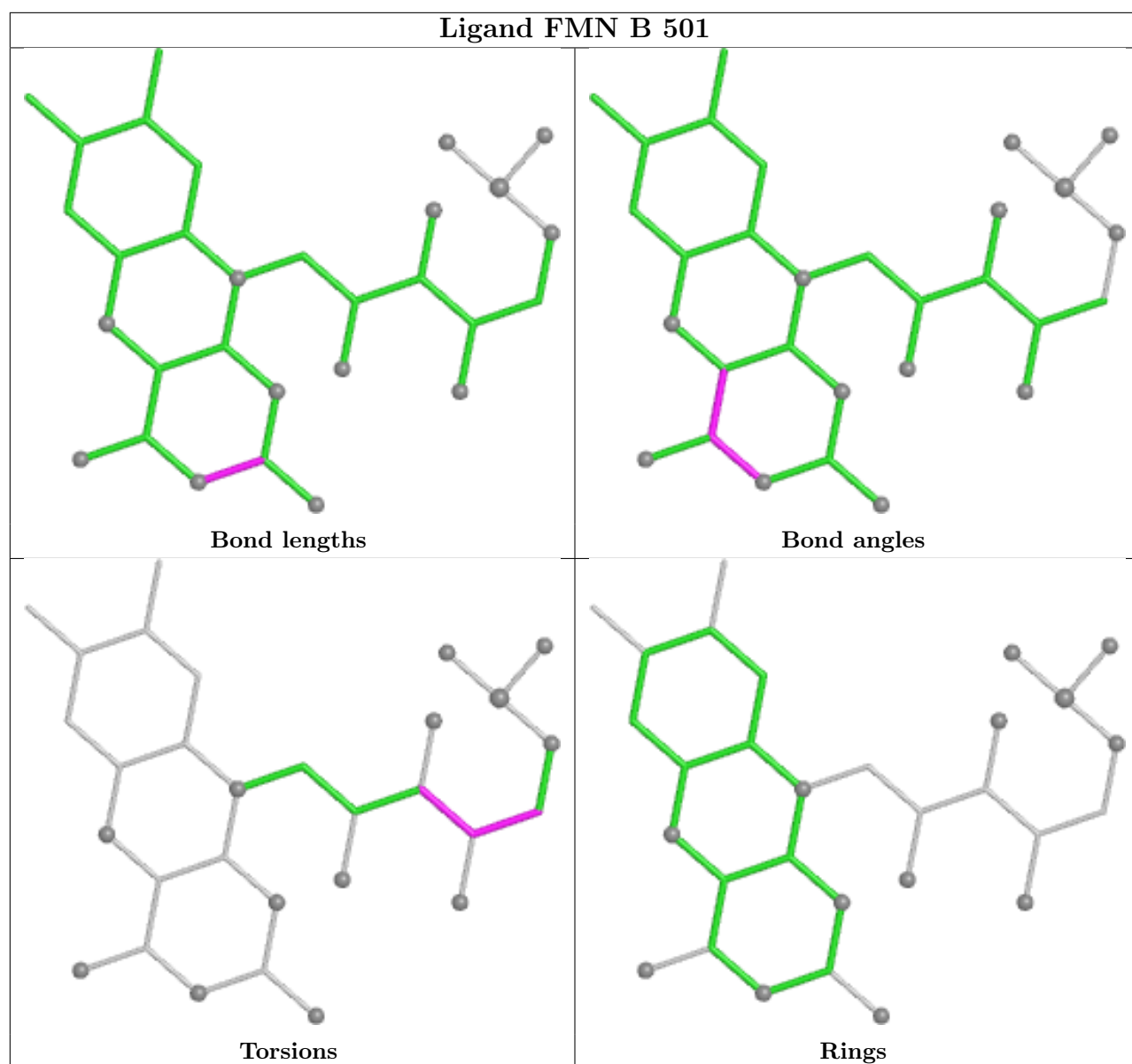
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	301	FMN	1	0
13	F	501	FES	2	0
10	B	506	PEE	4	0
8	B	502	RBF	1	0
10	B	504	PEE	4	0
10	C	303	PEE	3	0

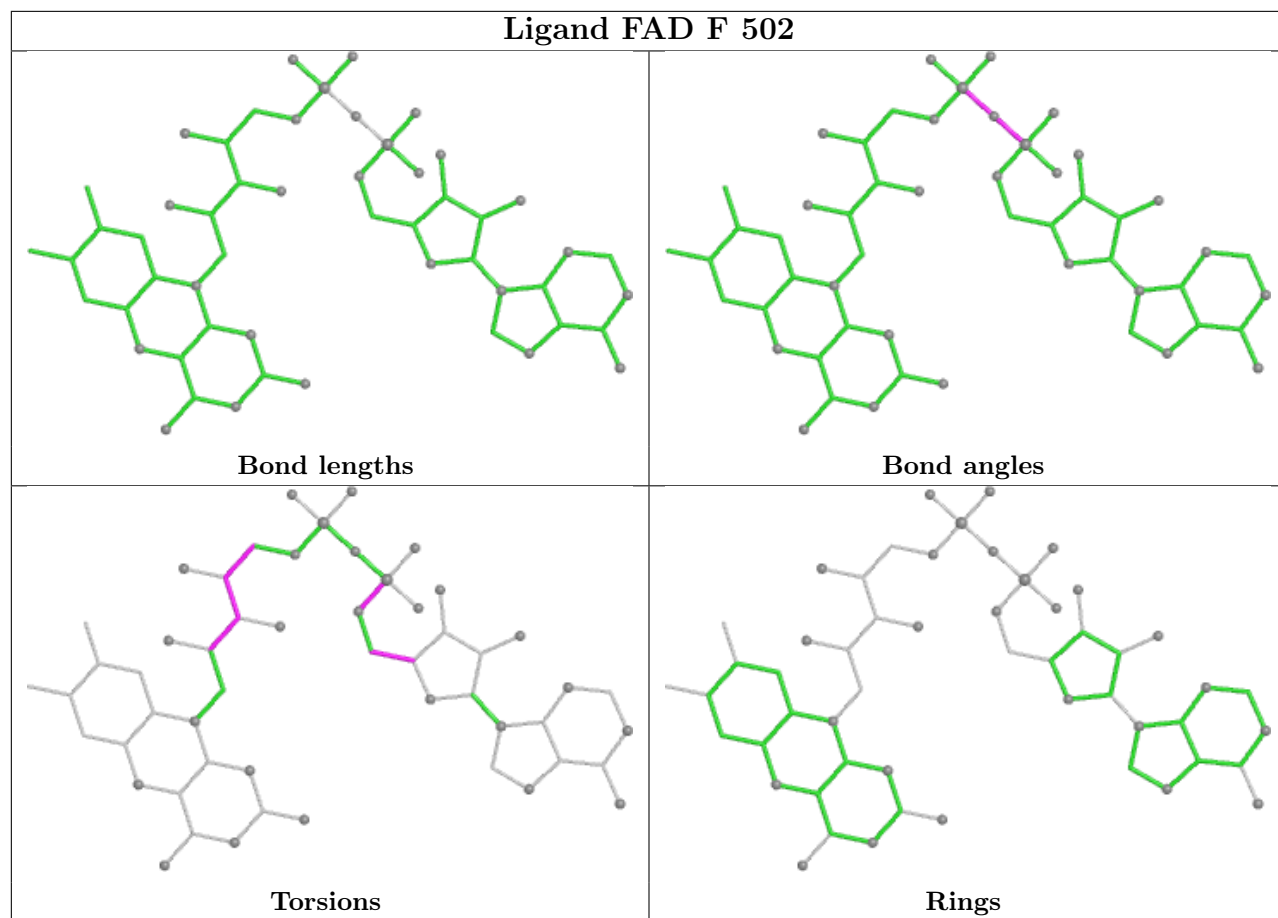
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

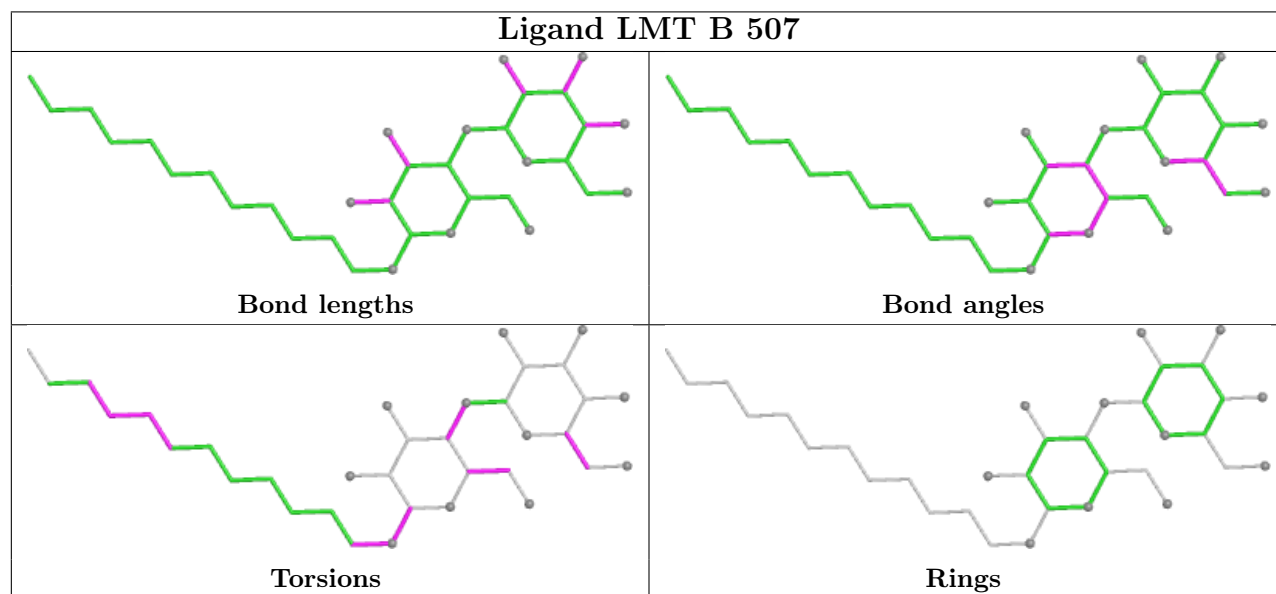
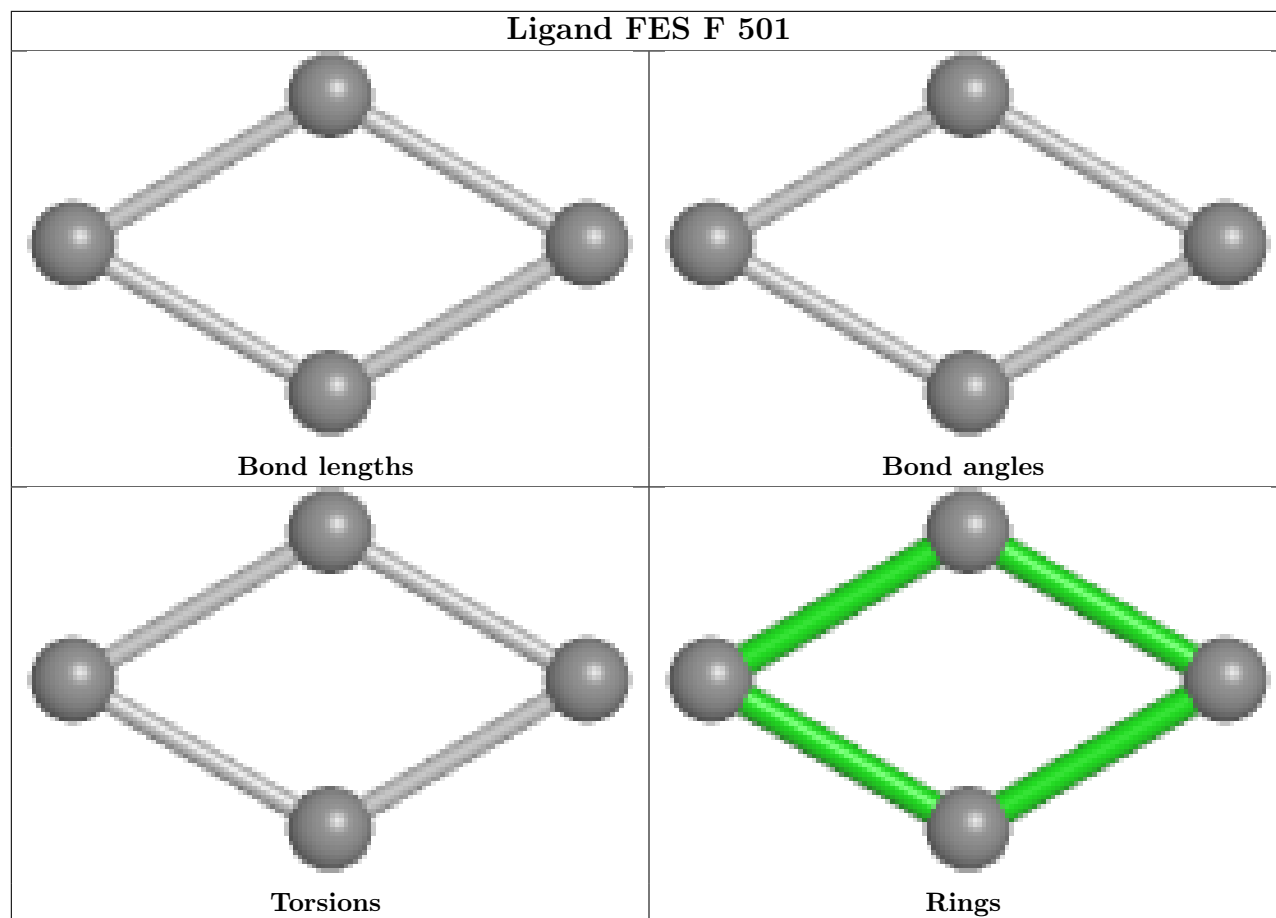
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

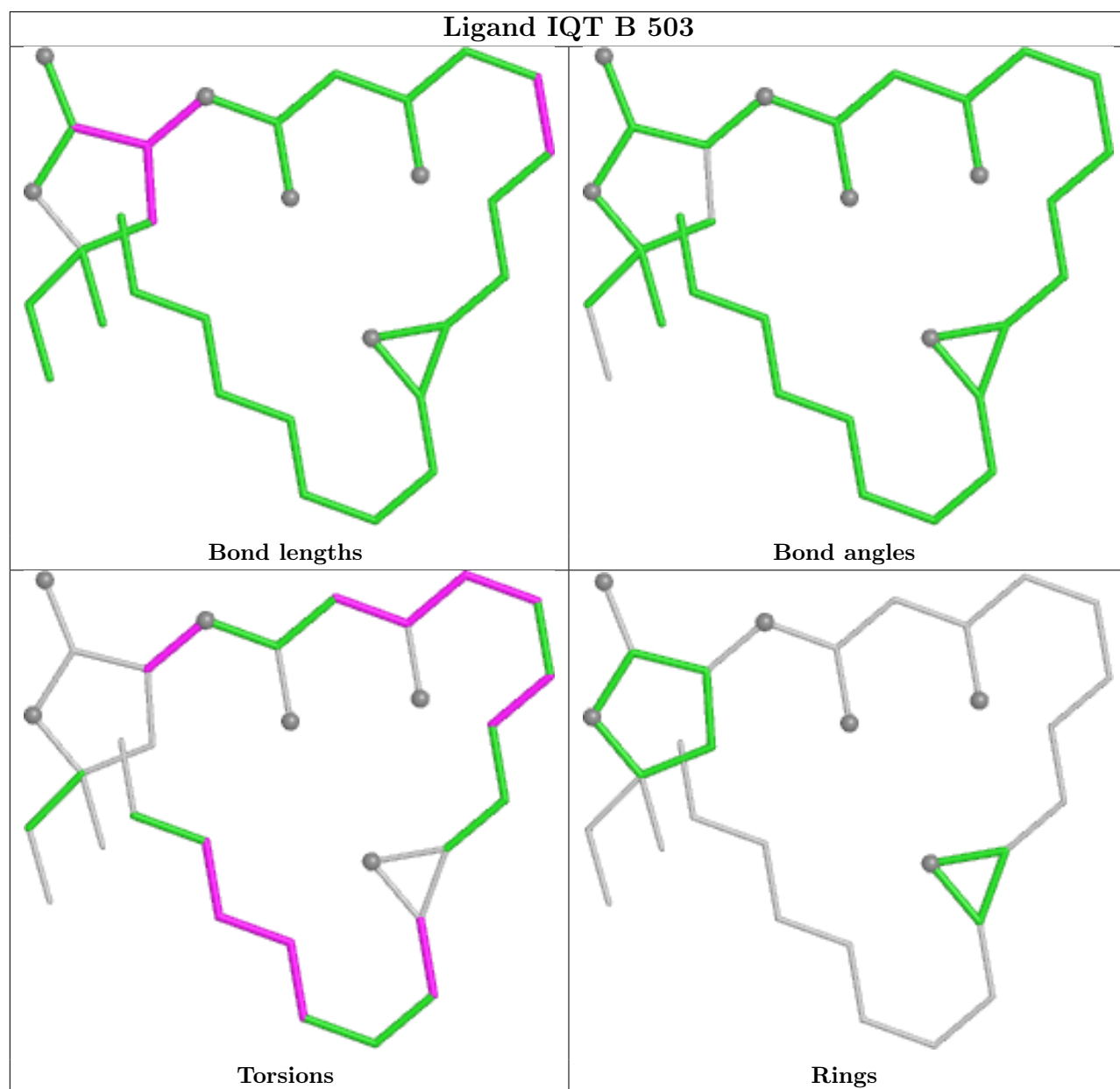
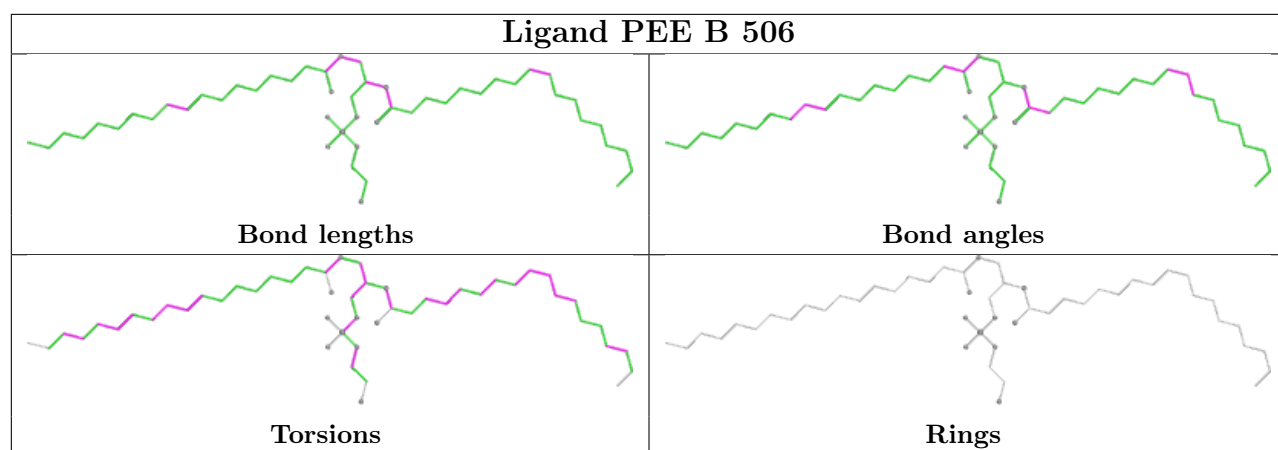


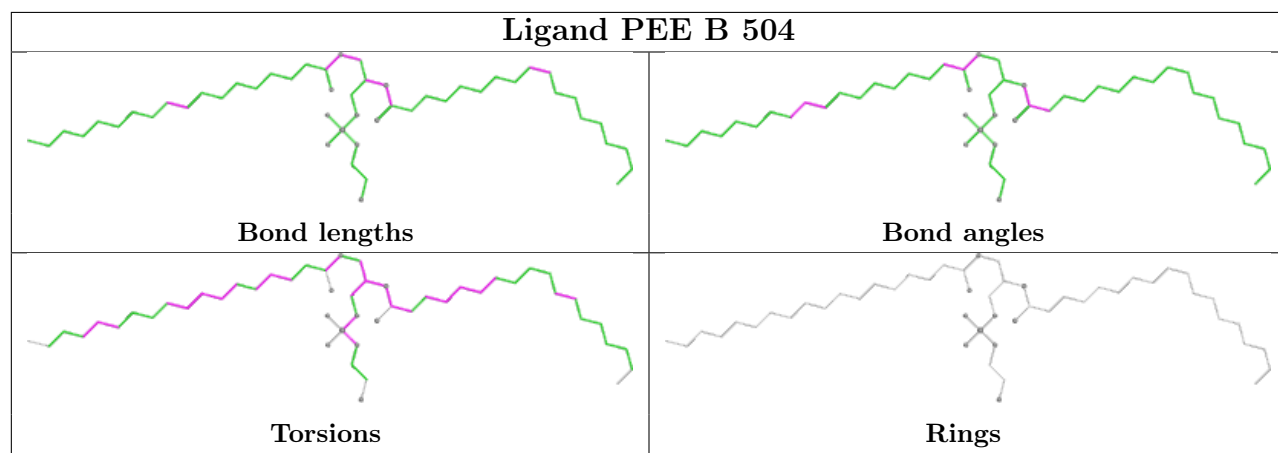
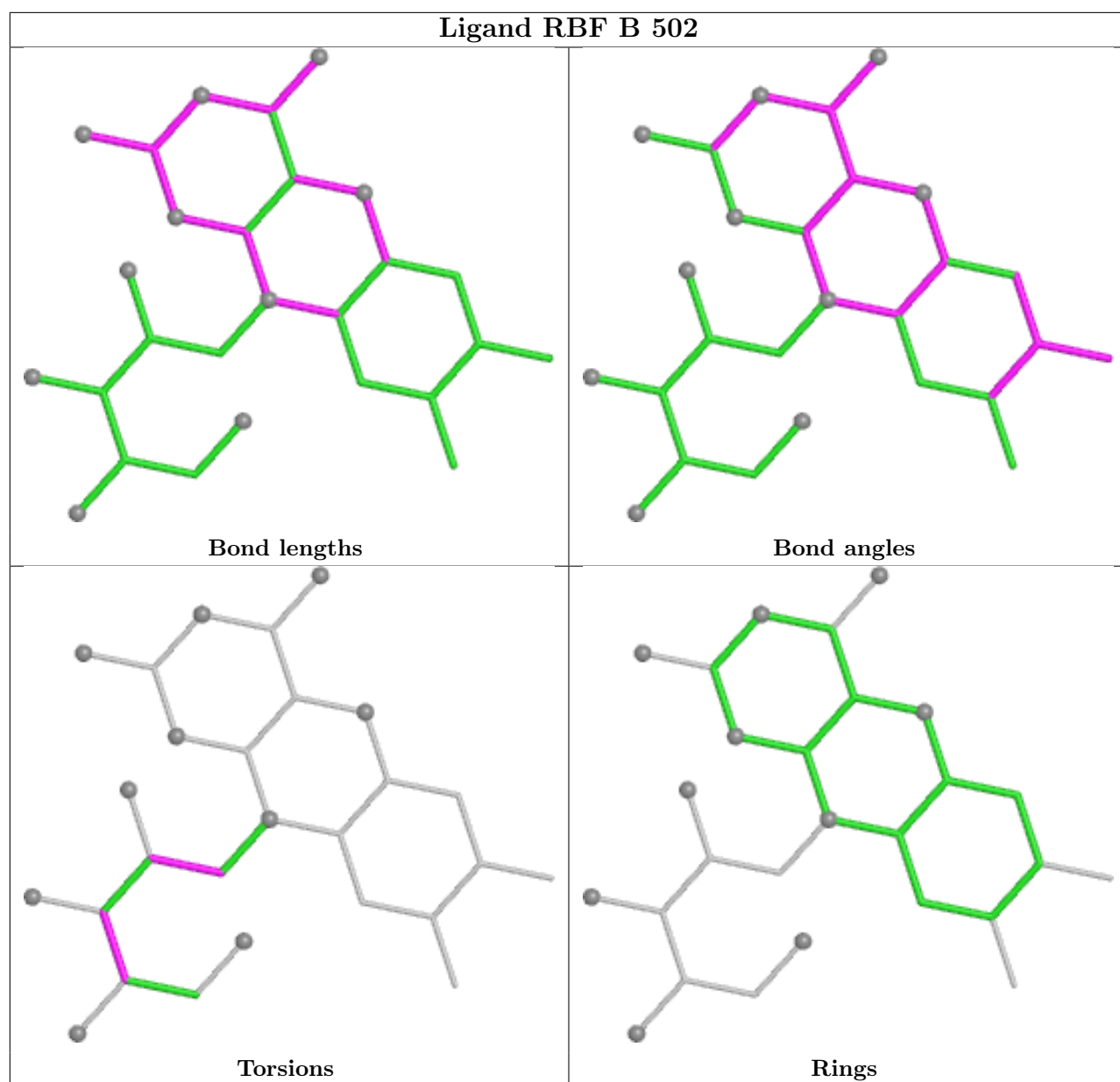


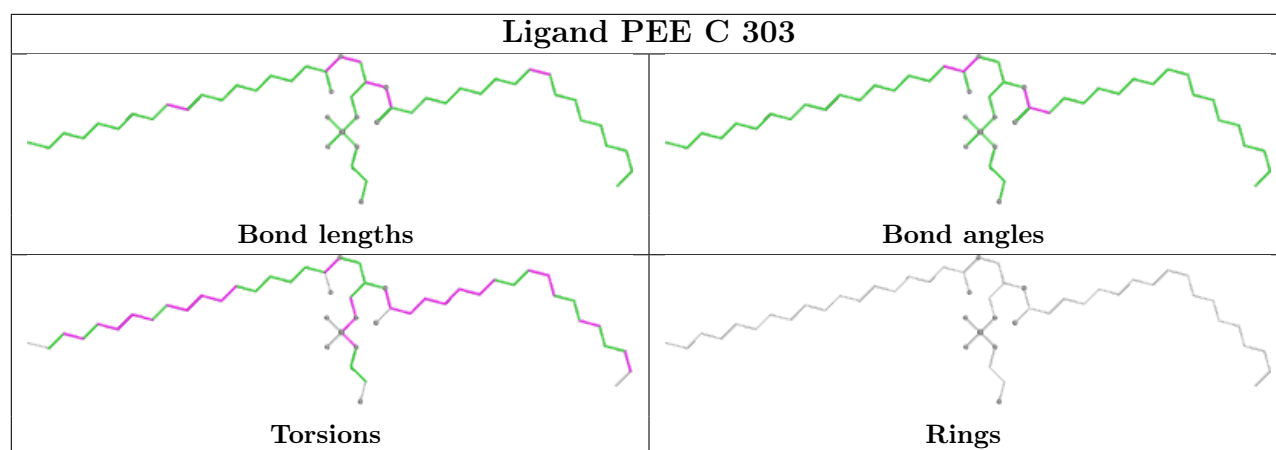












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

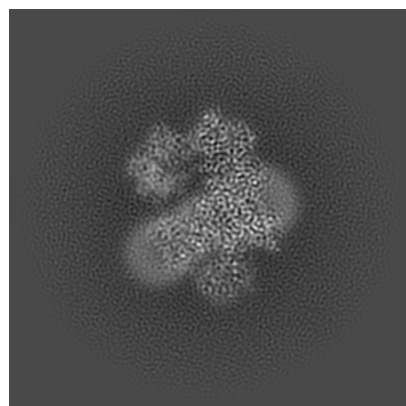
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33246. These allow visual inspection of the internal detail of the map and identification of artifacts.

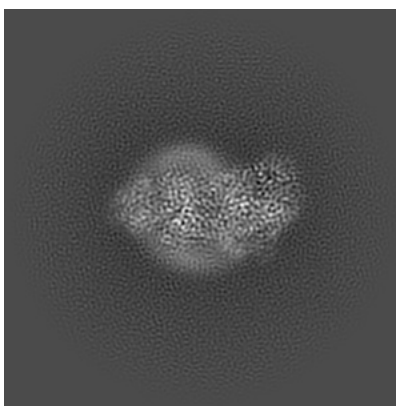
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

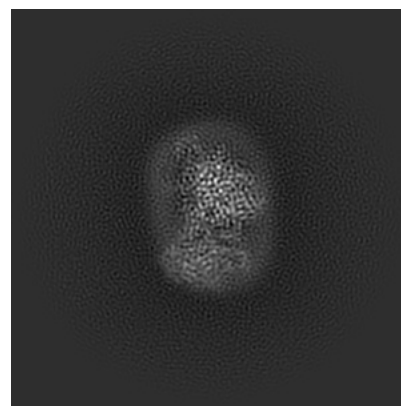
6.1.1 Primary map



X

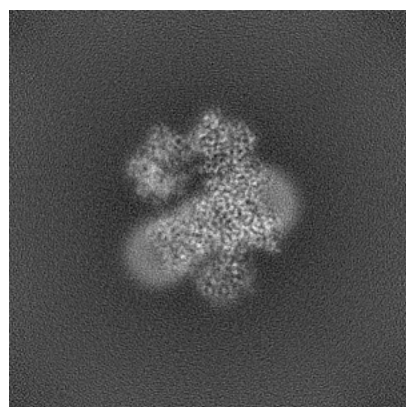


Y

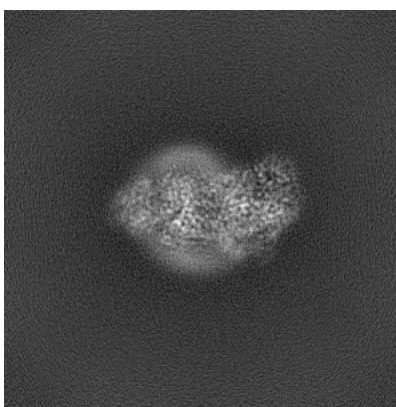


Z

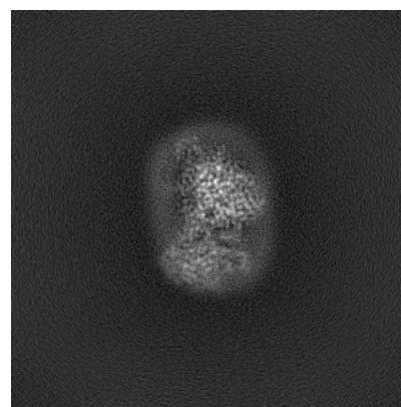
6.1.2 Raw map



X



Y

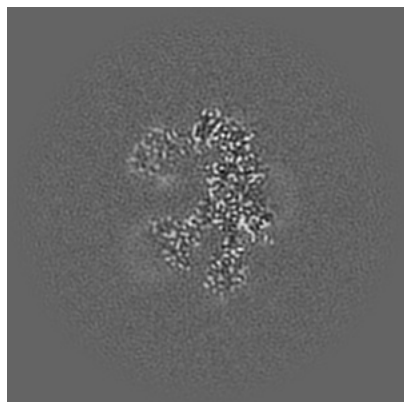


Z

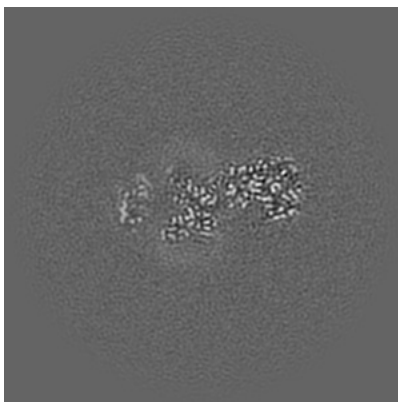
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

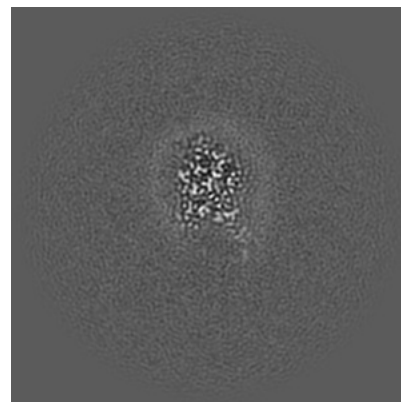
6.2.1 Primary map



X Index: 160

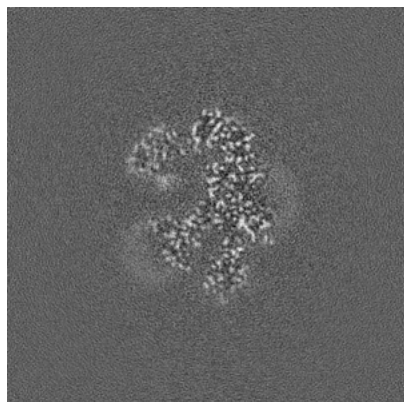


Y Index: 160

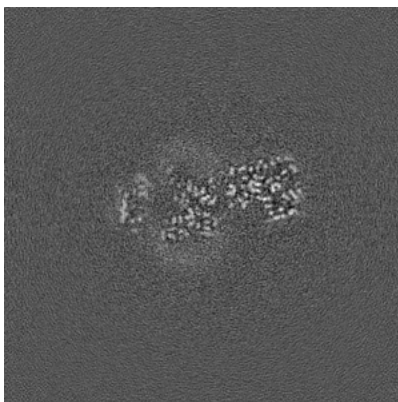


Z Index: 160

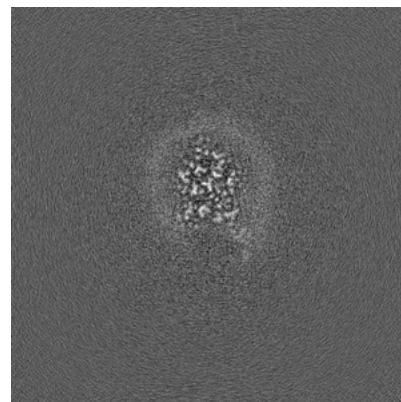
6.2.2 Raw map



X Index: 160



Y Index: 160

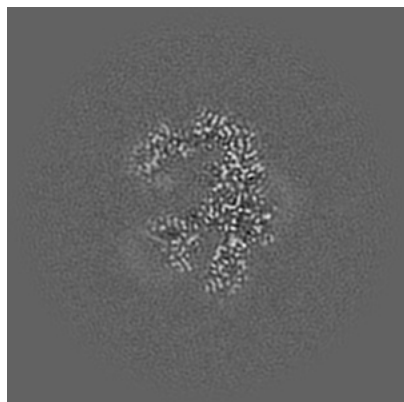


Z Index: 160

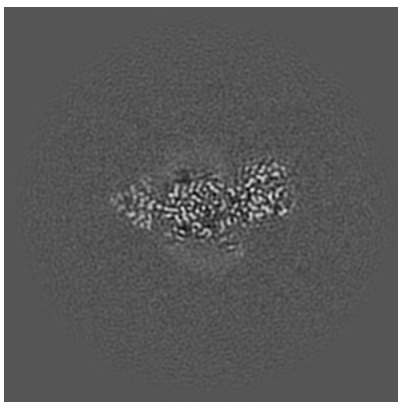
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

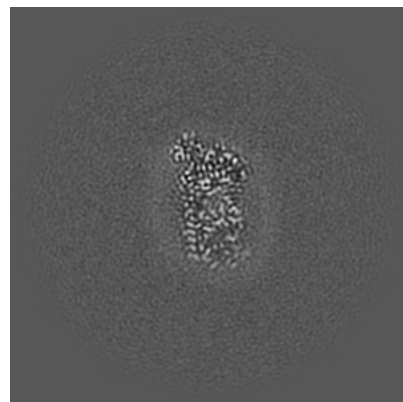
6.3.1 Primary map



X Index: 158

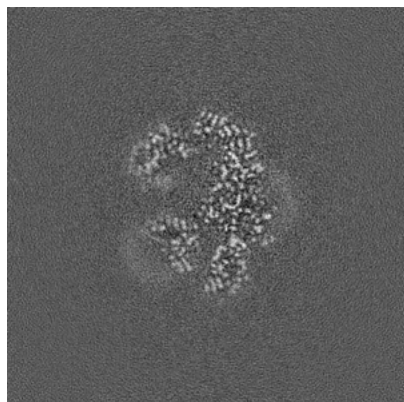


Y Index: 180

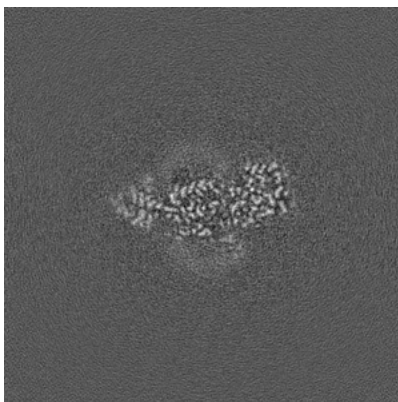


Z Index: 143

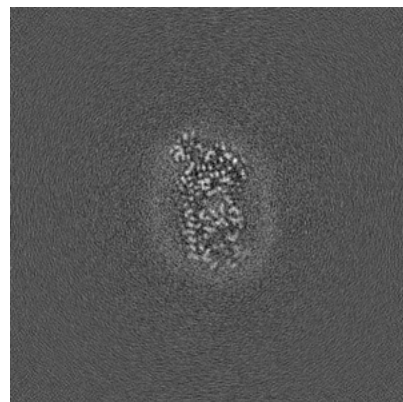
6.3.2 Raw map



X Index: 158



Y Index: 181

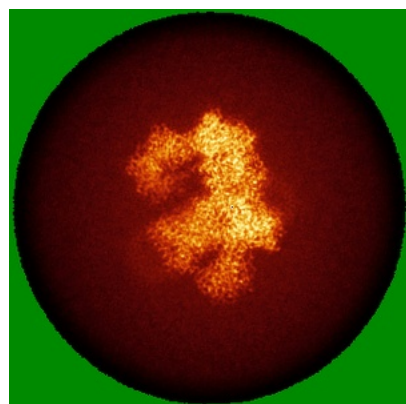


Z Index: 143

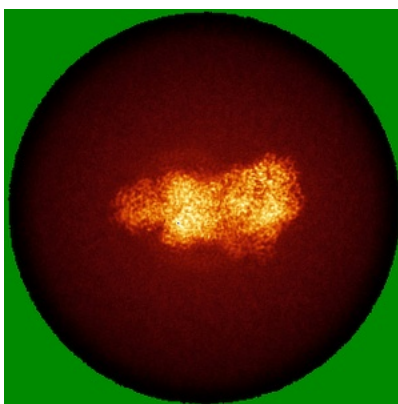
The images above show the largest variance slices of the map in three orthogonal directions.

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

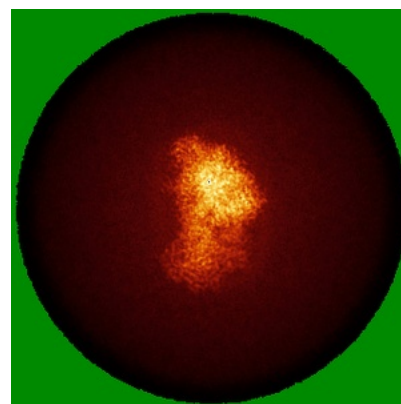
6.4.1 Primary map



X

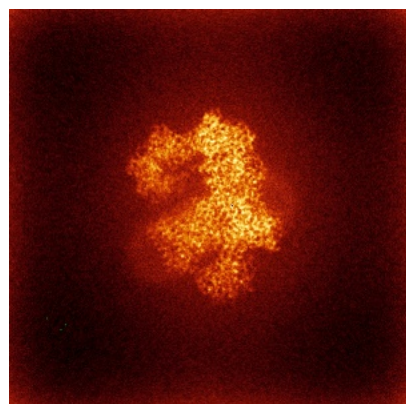


Y

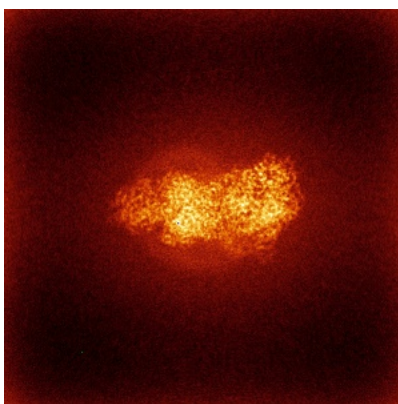


Z

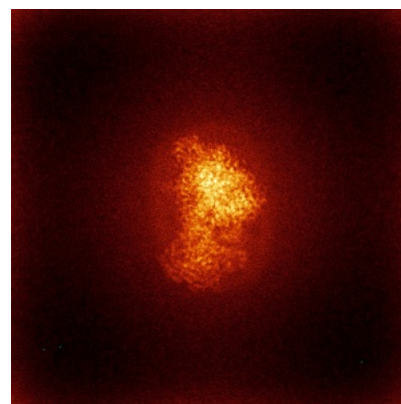
6.4.2 Raw map



X



Y

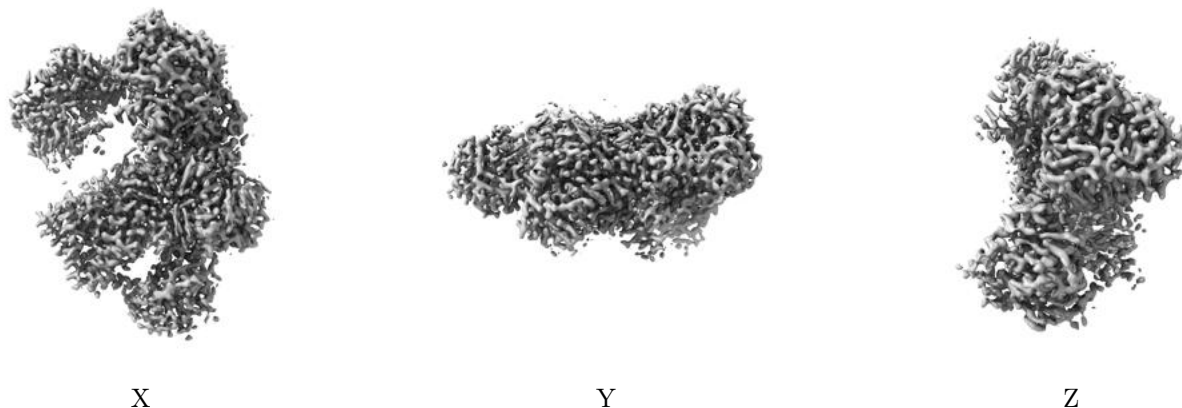


Z

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

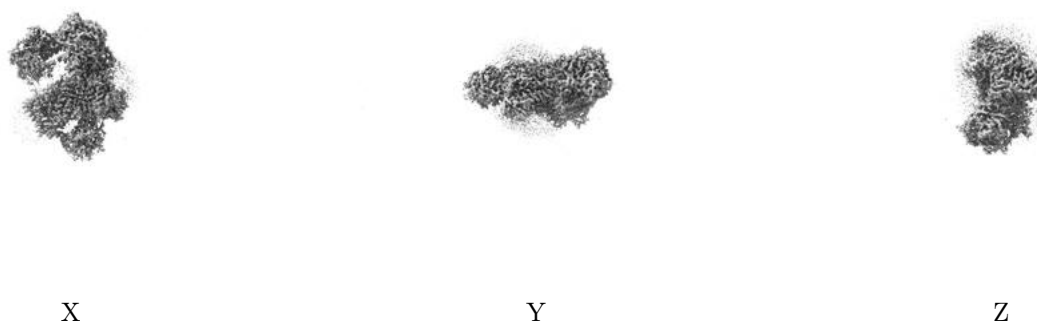
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

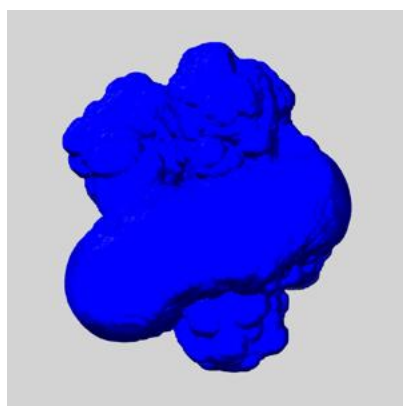
6.6 Mask visualisation [i](#)

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

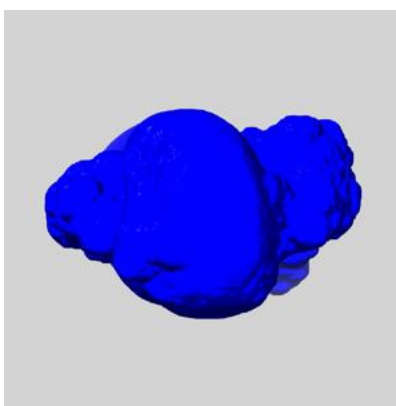
A mask typically either:

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

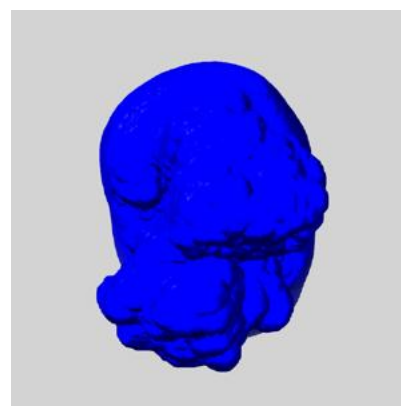
6.6.1 emd_33246_msk_1.map [i](#)



X



Y

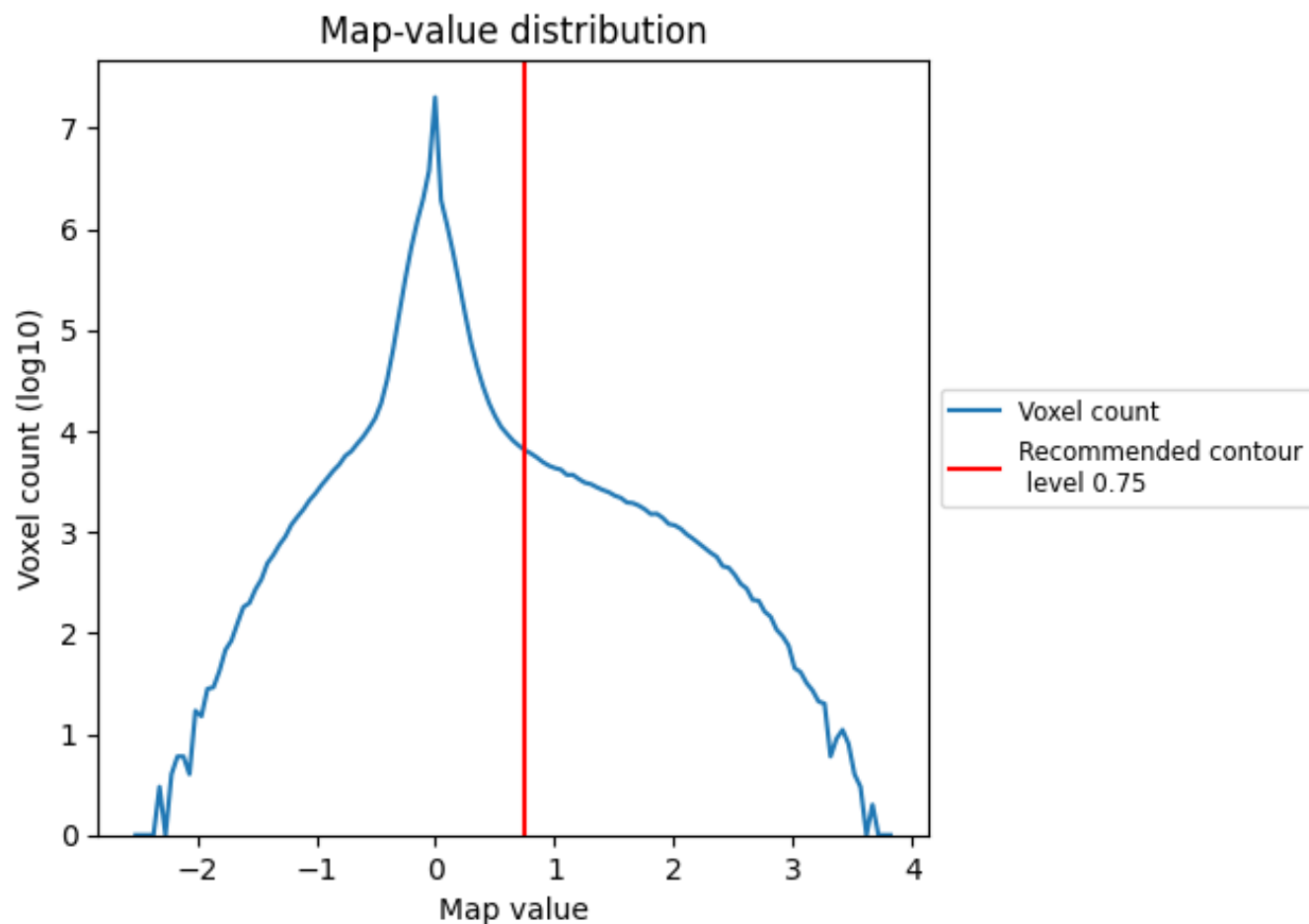


Z

7 Map analysis [i](#)

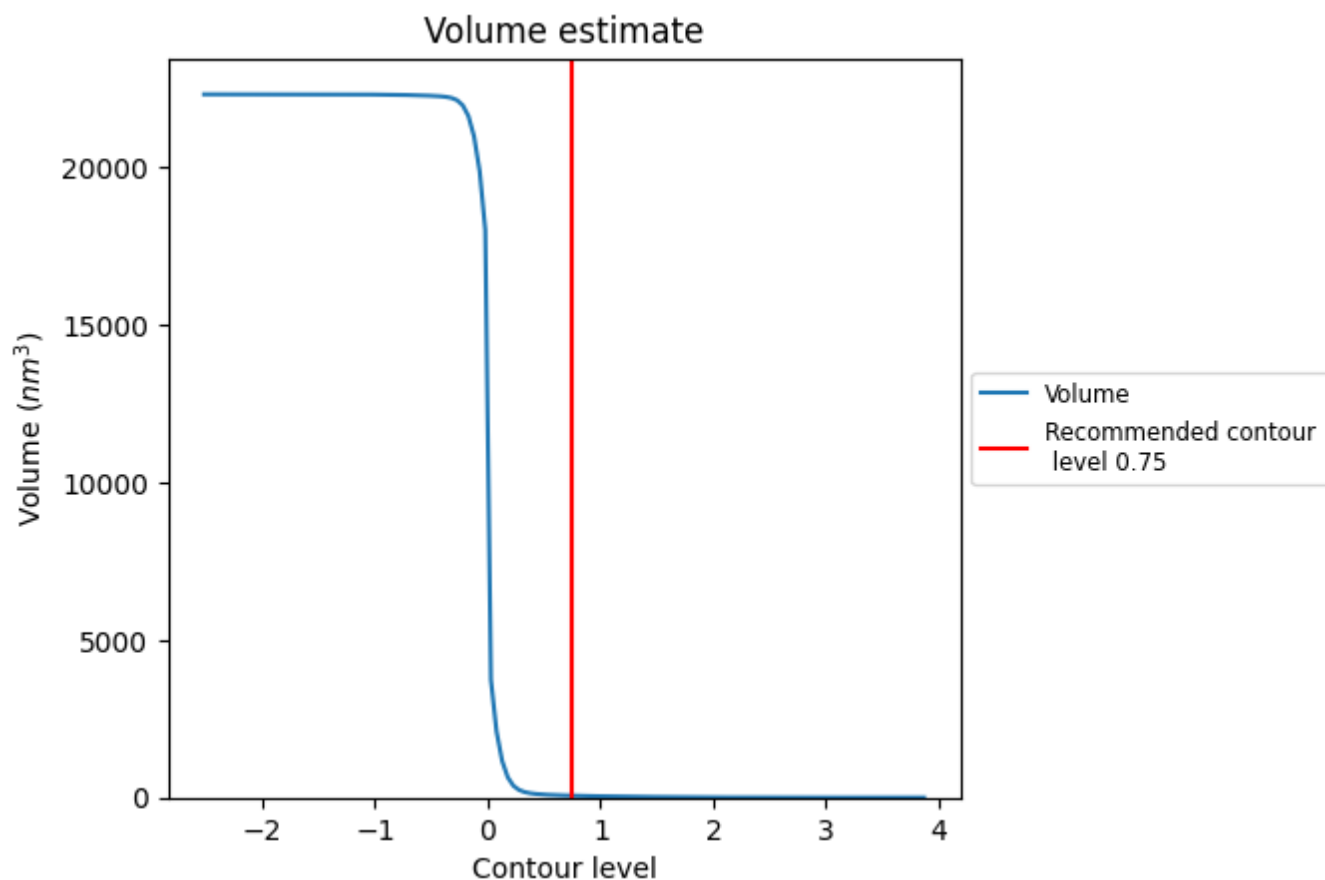
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

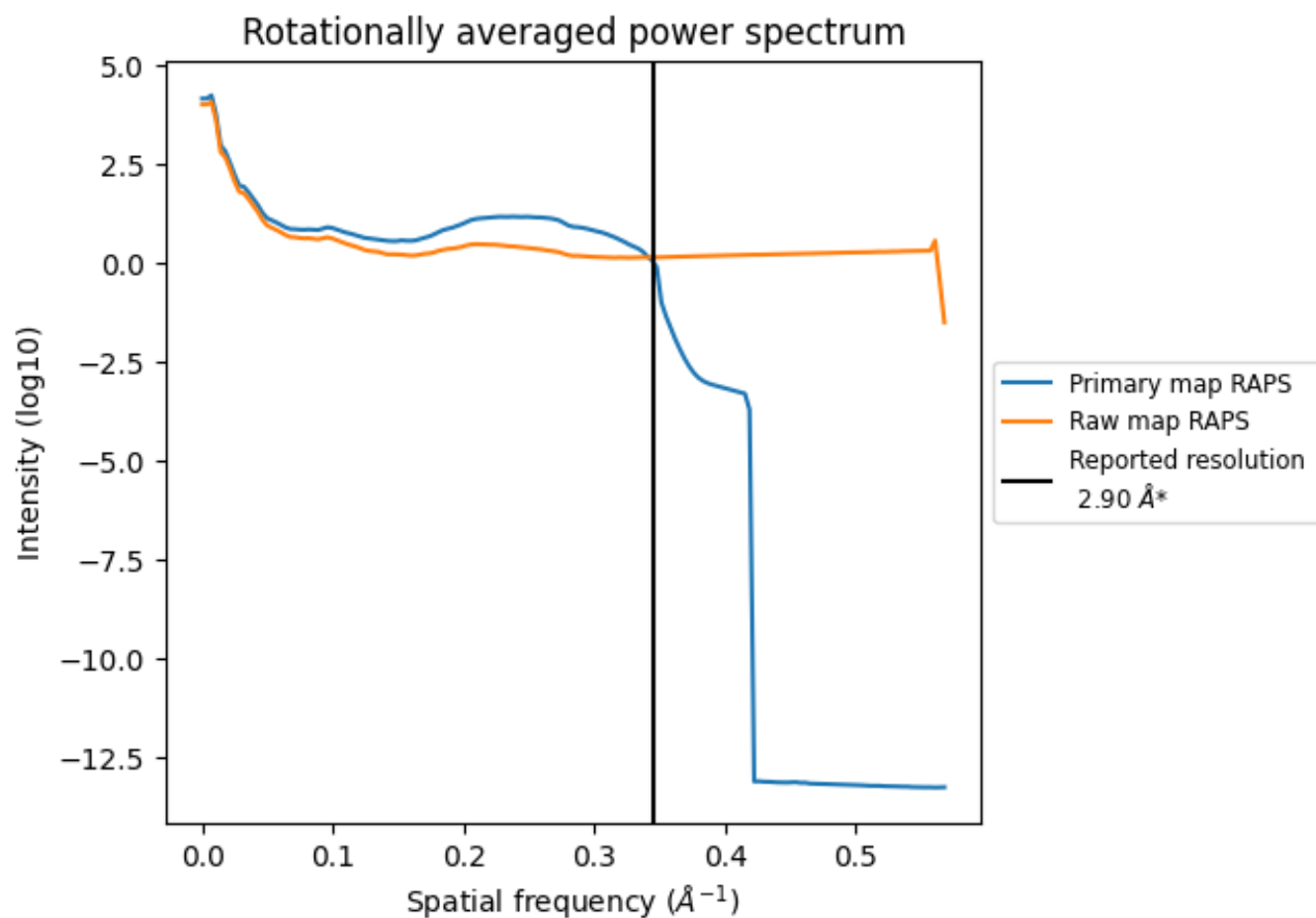
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 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 ⓘ

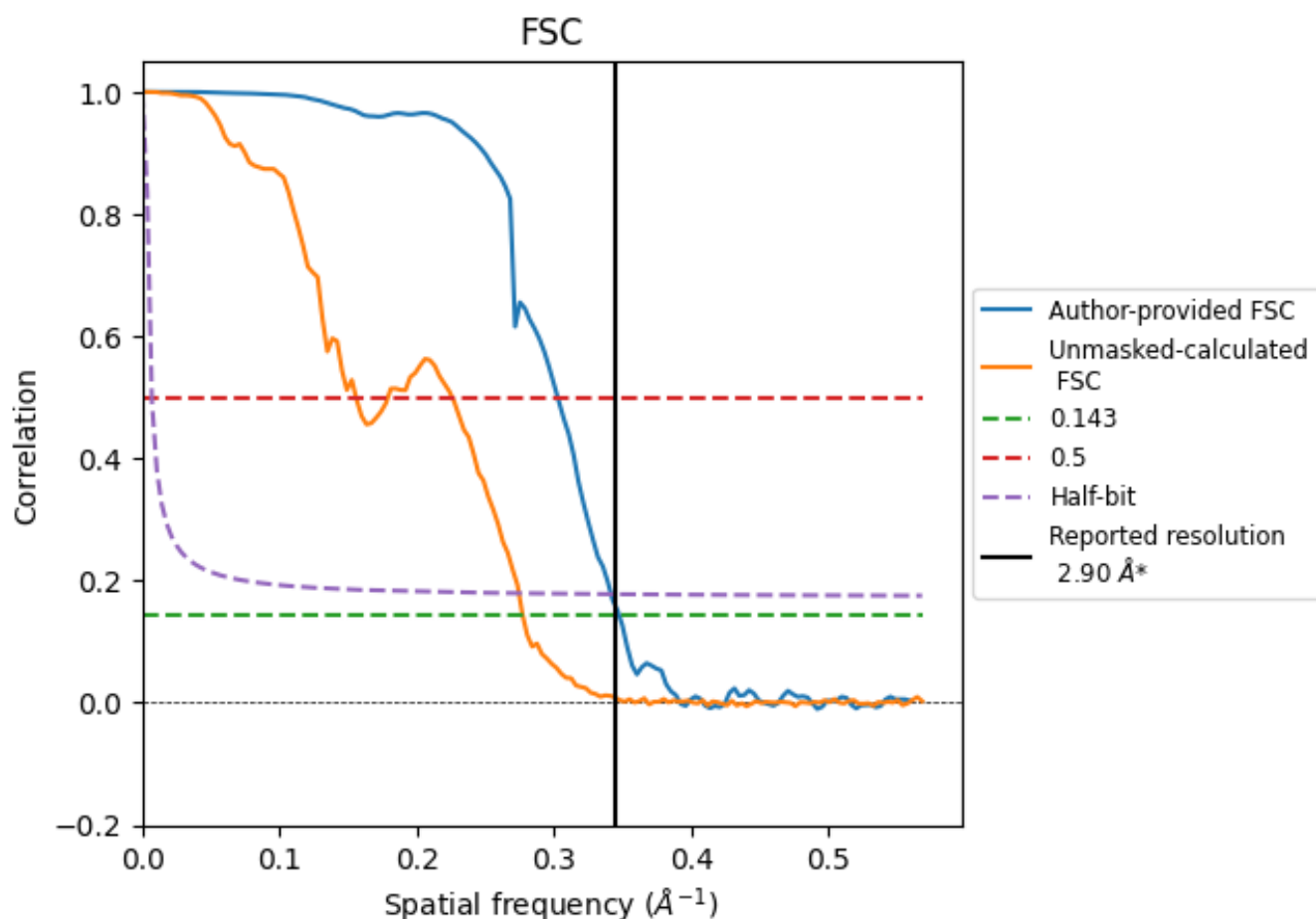


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

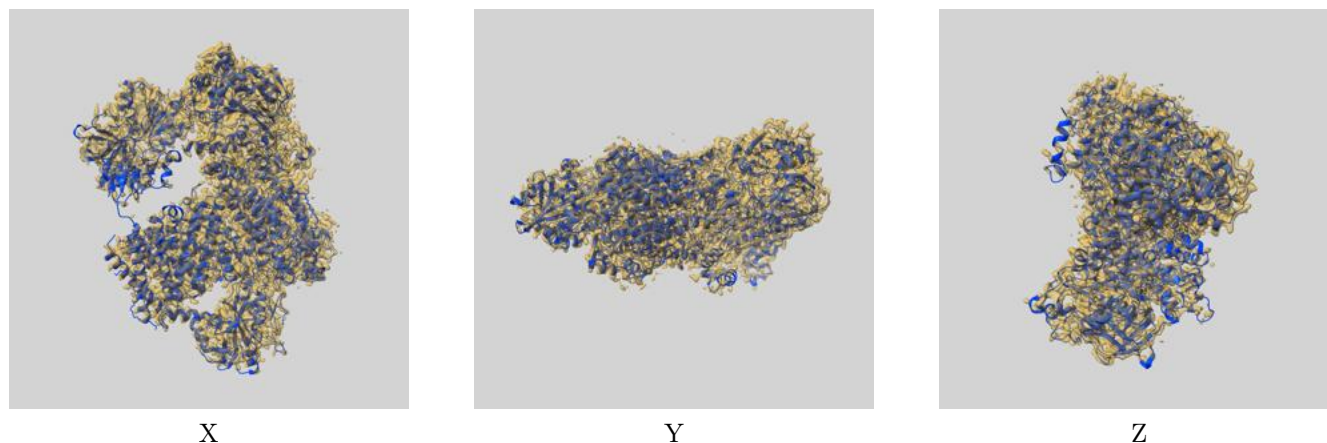
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.30	2.93
Unmasked-calculated*	3.61	6.42	3.64

*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 3.61 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

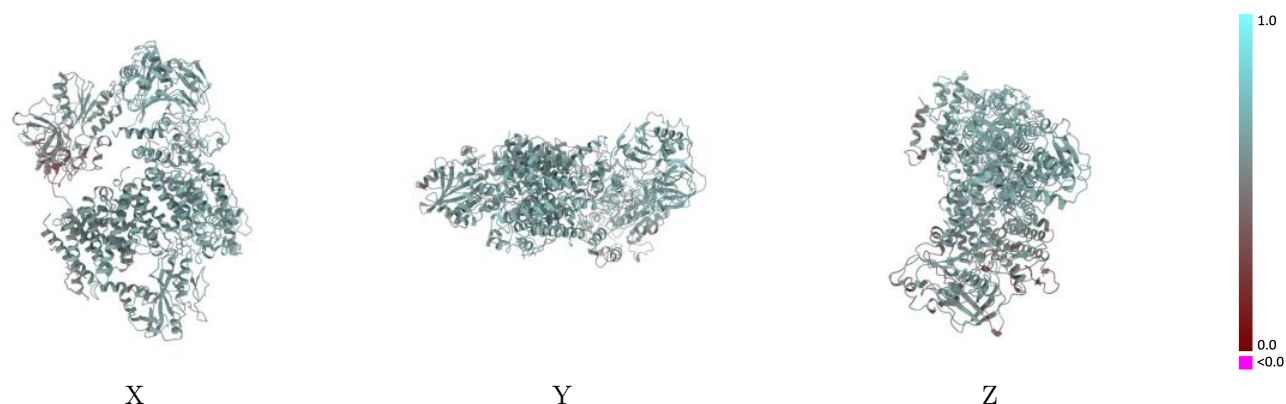
This section contains information regarding the fit between EMDB map EMD-33246 and PDB model 7XK7. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



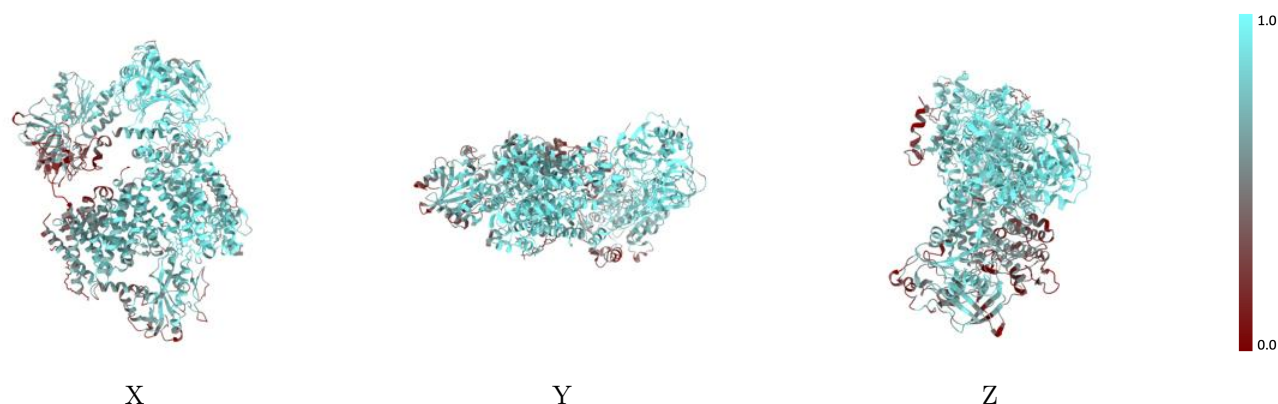
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



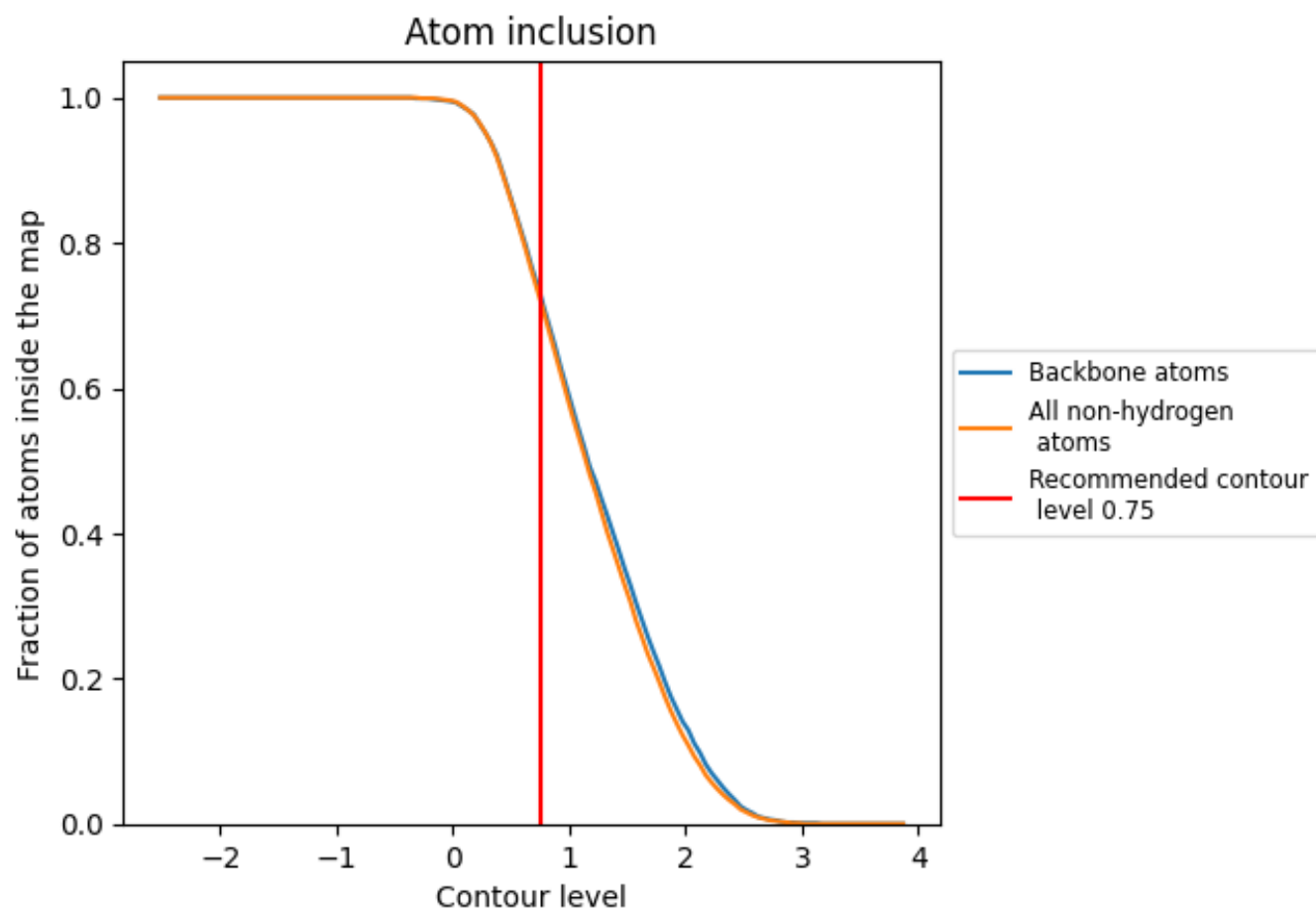
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.5840
A	0.8500	0.6150
B	0.8240	0.6160
C	0.6180	0.5720
D	0.7410	0.5910
E	0.7290	0.5910
F	0.5410	0.5190

1.0

0.0

<0.0