



Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 02:15 PM JST

PDB ID : 9LRR / pdb_00009lrr
EMDB ID : EMD-63340
Title : Cryo-EM structure of Na⁺-translocating NADH-ubiquinone oxidoreductase NqrB-G141A mutant from *Vibrio cholerae* with bound korormicin A
Authors : Ishikawa-Fukuda, M.; Kishikawa, J.; Kato, T.; Murai, M.
Deposited on : 2025-02-01
Resolution : 2.68 Å(reported)
Based on initial model : 7XK7

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:

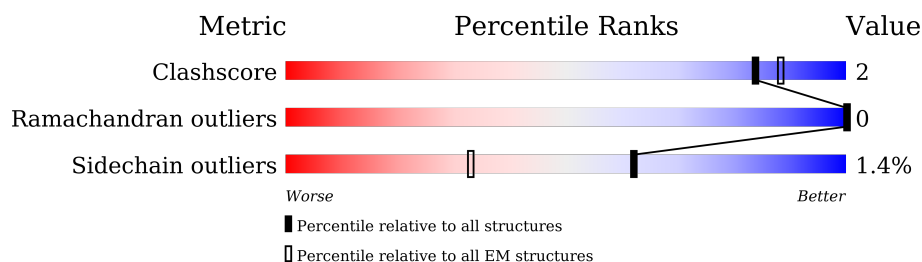
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 2.68 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 98%
2	B	415	 94% 5%
3	C	257	 91% 7%
4	D	210	 89% 9%
5	E	198	 90% 9%
6	F	414	 65% 92% 6%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15134 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	0	0
			3416	2165	584	650	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
			3178	2103	517	536	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	GLY	engineered mutation	UNP A5F5X0

- 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		

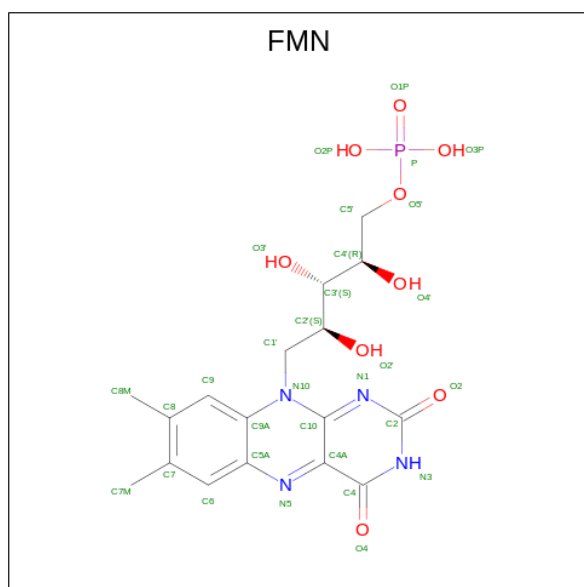
- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

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:

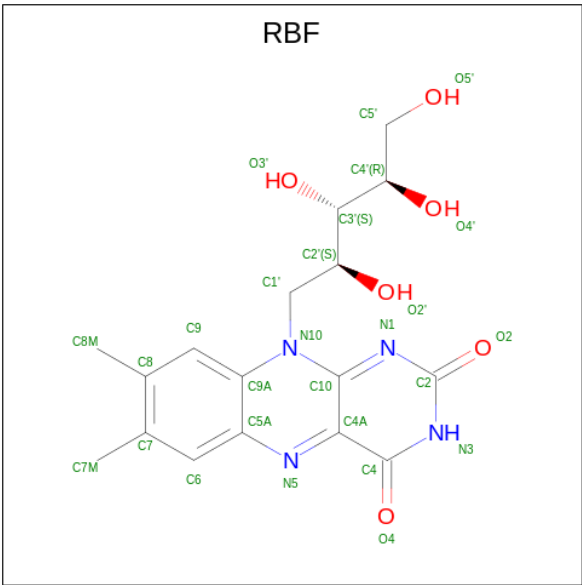
Chain	Residue	Modelled	Actual	Comment	Reference
F	409	HIS	-	expression tag	UNP A5F5Y4
F	410	HIS	-	expression tag	UNP A5F5Y4
F	411	HIS	-	expression tag	UNP A5F5Y4
F	412	HIS	-	expression tag	UNP A5F5Y4
F	413	HIS	-	expression tag	UNP A5F5Y4
F	414	HIS	-	expression tag	UNP A5F5Y4

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



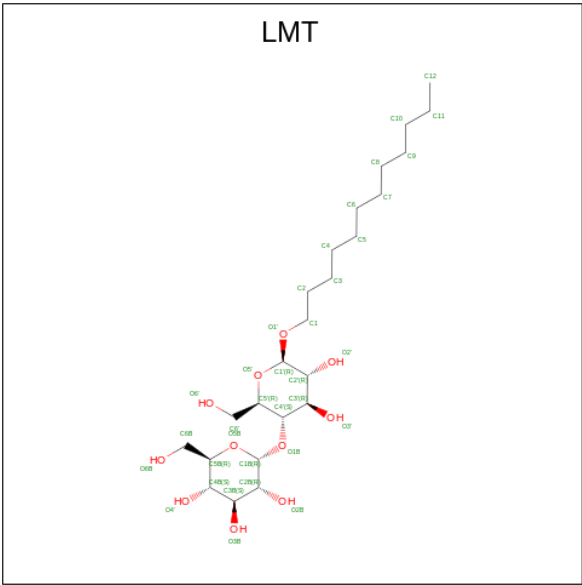
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
7	C	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



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

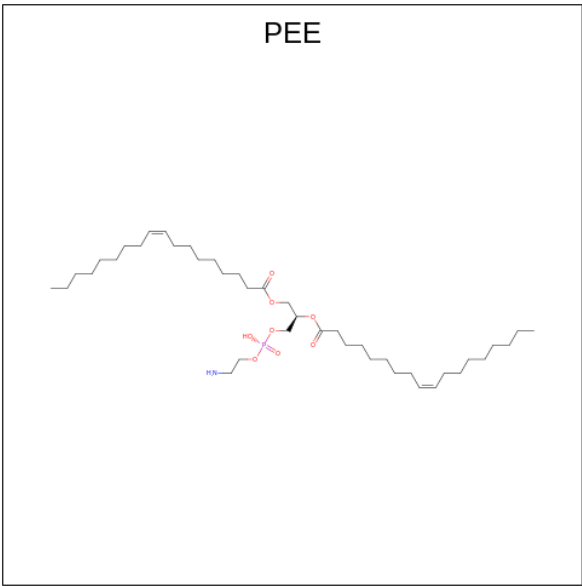
- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

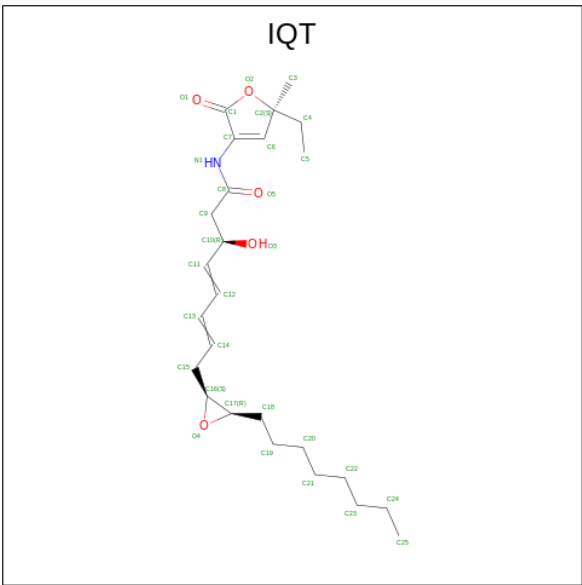
- Molecule 10 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

C₄₁H₇₈NO₈P).



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

- Molecule 11 is Korormicin (CCD ID: IQT) (formula: C₂₅H₃₉NO₅) (labeled as "Ligand of Interest" by depositor).

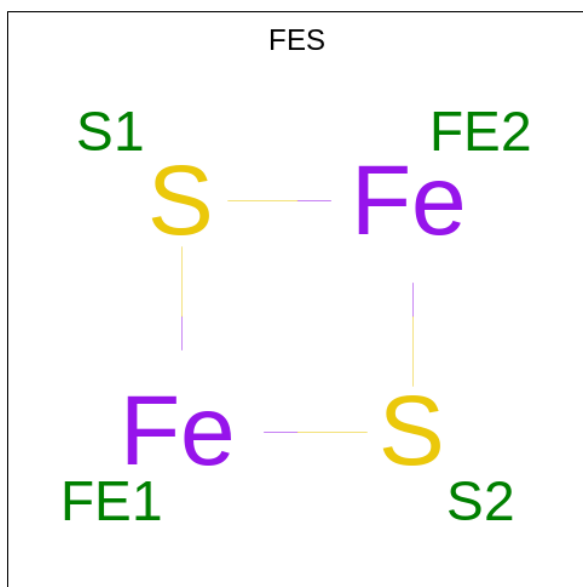


Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	N	O	0
			31	25	1	5	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

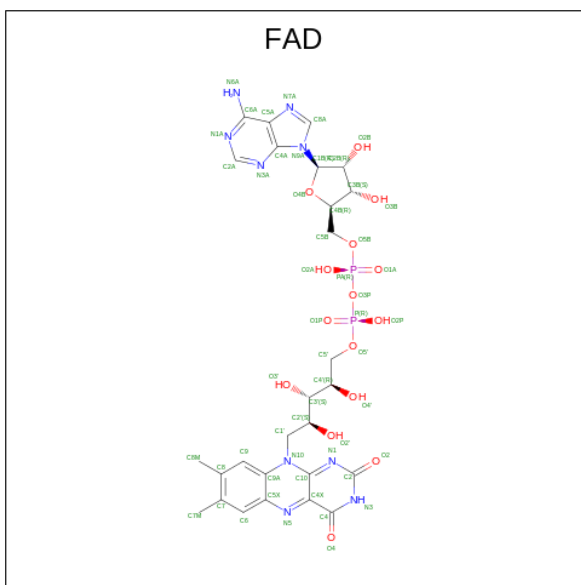
Mol	Chain	Residues	Atoms		AltConf
12	C	1	Total	Ca	0
			1	1	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 14 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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	18	Total 18	O 18	0
15	B	13	Total 13	O 13	0
15	C	1	Total 1	O 1	0
15	E	4	Total 4	O 4	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

Chain A:  98% .




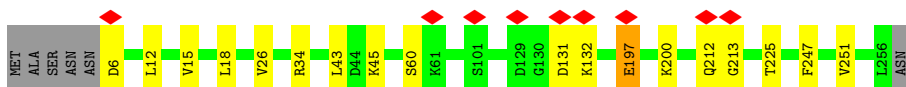
- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

Chain B:  94% 5% .




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

Chain C:  91% 7% .




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

Chain D:  89% 9% .



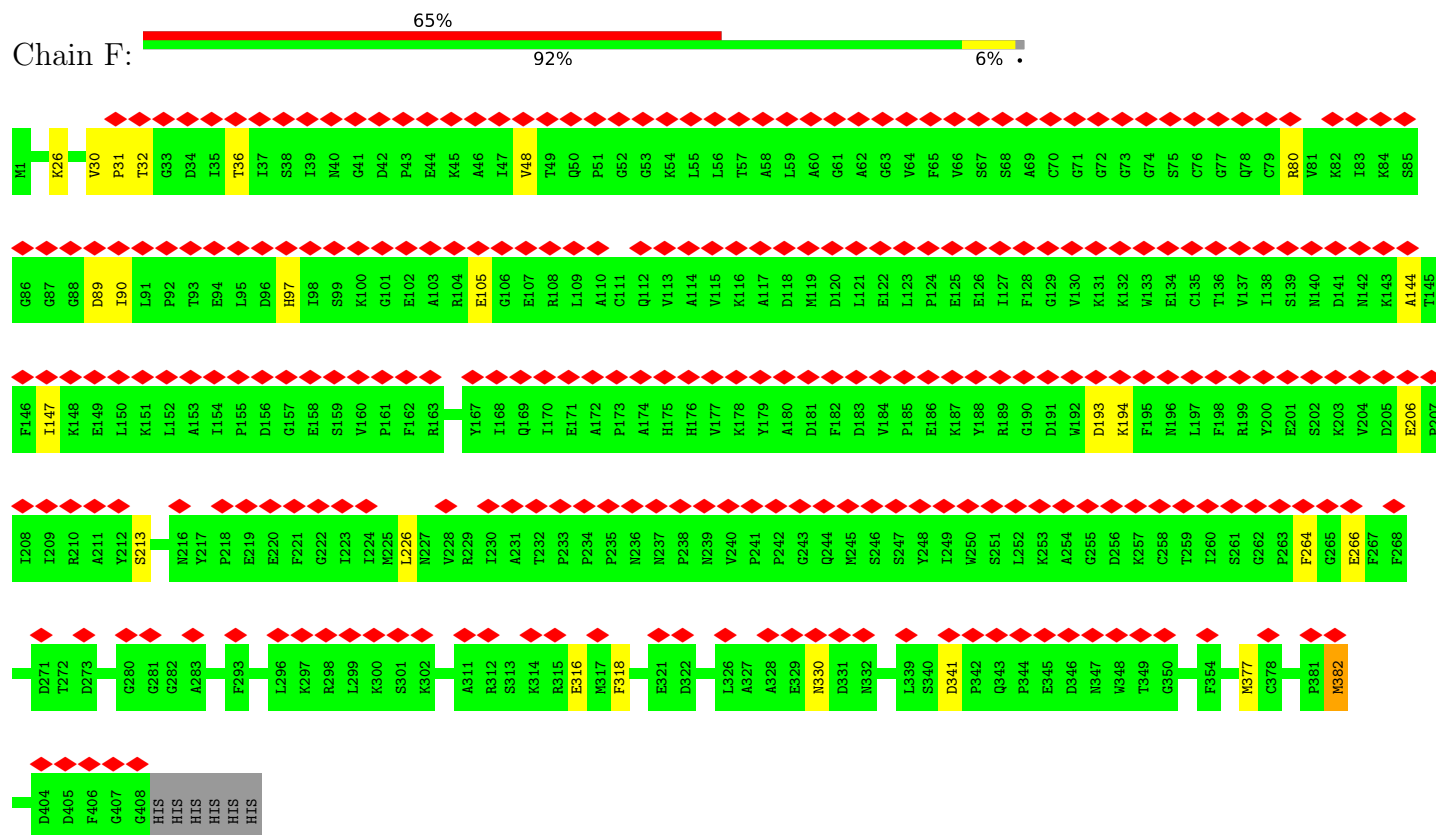
- Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E

Chain E:  90% 9% .



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

Chain F:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1035957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.995	Depositor
Minimum map value	-5.547	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.679	Depositor
Map size (\AA)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: FES, FAD, FMN, LMT, IQT, PEE, CA, 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	0/3480	0.47	0/4715
2	B	0.25	0/3276	0.44	0/4459
3	C	0.25	0/1934	0.45	0/2610
4	D	0.26	0/1612	0.44	0/2187
5	E	0.26	0/1544	0.45	1/2094 (0.0%)
6	F	0.25	0/3235	0.47	0/4381
All	All	0.25	0/15081	0.46	1/20446 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	133	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3463	5	0
2	B	3178	0	3157	12	0
3	C	1902	0	1911	11	0
4	D	1580	0	1667	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1511	0	1586	13	0
6	F	3157	0	3080	18	0
7	B	31	0	19	1	0
7	C	31	0	19	2	0
8	B	27	0	20	0	0
9	B	35	0	46	0	0
9	D	35	0	46	1	0
10	B	51	0	82	2	0
10	F	51	0	82	0	0
11	B	31	0	0	0	0
12	C	1	0	0	0	0
13	E	4	0	0	0	0
13	F	4	0	0	0	0
14	F	53	0	31	0	0
15	A	18	0	0	1	0
15	B	13	0	0	0	0
15	C	1	0	0	0	0
15	E	4	0	0	0	0
All	All	15134	0	15209	66	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 2.

All (66) 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)
6:F:206:GLU:N	6:F:206:GLU:OE1	2.05	0.89
2:B:154:GLU:N	2:B:154:GLU:OE1	2.13	0.81
3:C:225:THR:OG1	7:C:301:FMN:O3P	1.99	0.80
6:F:266:GLU:N	6:F:266:GLU:OE2	2.16	0.78
3:C:212:GLN:OE1	3:C:213:GLY:N	2.15	0.78
6:F:105:GLU:N	6:F:105:GLU:OE2	2.17	0.77
6:F:31:PRO:O	6:F:32:THR:OG1	2.02	0.72
5:E:48:VAL:HG21	5:E:116:ILE:HD11	1.72	0.72
5:E:197:GLN:N	5:E:197:GLN:OE1	2.23	0.69
6:F:89:ASP:OD1	6:F:90:ILE:N	2.27	0.67
4:D:133:ASP:OD1	4:D:137:ASN:ND2	2.31	0.64
1:A:35:GLU:OE2	15:A:501:HOH:O	2.17	0.58
6:F:316:GLU:N	6:F:316:GLU:OE2	2.35	0.58
5:E:31:VAL:HG12	5:E:31:VAL:O	2.05	0.56
3:C:43:LEU:HD21	3:C:60:SER:HB3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ARG:HA	2:B:58:ILE:HG22	1.89	0.54
3:C:6:ASP:N	3:C:6:ASP:OD1	2.41	0.54
6:F:382:MET:HE3	6:F:382:MET:H	1.74	0.53
5:E:133:ASP:O	5:E:133:ASP:OD1	2.26	0.52
2:B:397:ASP:O	2:B:401:VAL:HG23	2.09	0.51
3:C:131:ASP:OD1	3:C:132:LYS:N	2.44	0.51
5:E:48:VAL:O	5:E:52:SER:OG	2.23	0.51
1:A:133:THR:O	1:A:137:SER:N	2.45	0.49
3:C:34:ARG:NH1	5:E:74:ASP:OD1	2.43	0.49
2:B:49:ASP:OD1	2:B:50:SER:N	2.47	0.48
5:E:91:VAL:HG11	5:E:117:THR:HA	1.96	0.47
4:D:25:VAL:O	4:D:26:LEU:HD23	2.14	0.47
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.97	0.47
4:D:128:ILE:HB	4:D:129:PRO:HD3	1.96	0.47
6:F:382:MET:H	6:F:382:MET:CE	2.28	0.46
9:D:301:LMT:H1B	9:D:301:LMT:H5'	1.61	0.46
5:E:103:PRO:N	5:E:104:PRO:HD2	2.30	0.46
6:F:193:ASP:OD1	6:F:194:LYS:N	2.49	0.46
6:F:80:ARG:NH2	6:F:97:HIS:O	2.47	0.45
2:B:213:PHE:CZ	7:C:301:FMN:HM82	2.51	0.45
6:F:30:VAL:HG23	6:F:32:THR:HG23	1.99	0.45
5:E:28:PHE:O	5:E:32:SER:OG	2.31	0.45
3:C:197:GLU:C	3:C:197:GLU:OE1	2.55	0.44
5:E:96:MET:CE	6:F:26:LYS:HA	2.47	0.44
4:D:8:LYS:HA	4:D:11:VAL:HG22	2.00	0.44
10:B:504:PEE:H25	10:B:504:PEE:H19	1.89	0.44
2:B:100:TRP:HA	2:B:103:TRP:NE1	2.33	0.43
2:B:68:MET:HE2	2:B:164:ILE:HD11	1.99	0.43
4:D:38:LEU:HD23	4:D:161:PHE:CE2	2.53	0.43
2:B:370:LEU:O	2:B:374:VAL:HG22	2.19	0.43
1:A:392:LEU:HD13	2:B:401:VAL:HG21	1.99	0.43
6:F:89:ASP:OD1	6:F:89:ASP:C	2.56	0.43
5:E:53:VAL:HB	5:E:54:PRO:HD3	2.01	0.42
4:D:26:LEU:HD22	4:D:112:CYS:HB3	2.01	0.42
2:B:372:ARG:NH2	2:B:380:GLU:OE2	2.49	0.41
6:F:330:ASN:N	6:F:330:ASN:OD1	2.53	0.41
2:B:29:ALA:HB2	2:B:155:VAL:CG2	2.50	0.41
3:C:247:PHE:O	3:C:251:VAL:HG23	2.20	0.41
6:F:144:ALA:HB3	6:F:147:ILE:CG1	2.51	0.41
3:C:26:VAL:HG13	4:D:84:ILE:HG21	2.01	0.41
6:F:213:SER:O	6:F:226:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:504:PEE:H20	10:B:504:PEE:H14	1.45	0.41
1:A:333:GLU:OE1	1:A:333:GLU:HA	2.21	0.41
3:C:12:LEU:HA	3:C:15:VAL:HG22	2.02	0.41
6:F:318:PHE:CD1	6:F:318:PHE:N	2.88	0.41
4:D:184:ALA:HB2	5:E:22:PHE:CZ	2.56	0.40
6:F:36:THR:HG22	6:F:48:VAL:HG12	2.01	0.40
4:D:30:SER:O	4:D:34:VAL:HG22	2.21	0.40
2:B:238:LEU:HB2	7:B:501:FMN:O3P	2.21	0.40
3:C:18:LEU:CD2	4:D:74:VAL:HG13	2.52	0.40
5:E:48:VAL:CG2	5:E:116:ILE:HD11	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	437 (98%)	7 (2%)	0	100	100
2	B	410/415 (99%)	401 (98%)	9 (2%)	0	100	100
3	C	249/257 (97%)	243 (98%)	6 (2%)	0	100	100
4	D	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
5	E	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
6	F	406/414 (98%)	394 (97%)	12 (3%)	0	100	100
All	All	1909/1940 (98%)	1861 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	372 (99%)	4 (1%)	70	86
2	B	317/320 (99%)	314 (99%)	3 (1%)	75	89
3	C	200/205 (98%)	197 (98%)	3 (2%)	60	82
4	D	173/176 (98%)	168 (97%)	5 (3%)	37	64
5	E	165/165 (100%)	162 (98%)	3 (2%)	54	78
6	F	335/343 (98%)	331 (99%)	4 (1%)	67	85
All	All	1566/1585 (99%)	1544 (99%)	22 (1%)	62	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	260	ARG
1	A	357	LYS
1	A	374	MET
2	B	122	MET
2	B	261	MET
2	B	380	GLU
3	C	45	LYS
3	C	197	GLU
3	C	200	LYS
4	D	8	LYS
4	D	9	LYS
4	D	96	ASP
4	D	99	LYS
4	D	119	GLU
5	E	2	GLU
5	E	22	PHE
5	E	67	ASP
6	F	264	PHE
6	F	341	ASP
6	F	377	MET
6	F	382	MET

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
8	RBF	B	502	-	29,29,29	0.95	1 (3%)	41,43,43	0.91	0
14	FAD	F	503	-	53,58,58	0.90	2 (3%)	68,89,89	0.83	1 (1%)
13	FES	E	301	5,4	0,4,4	-	-	-		
7	FMN	B	501	-	33,33,33	0.58	0	48,50,50	0.72	1 (2%)
9	LMT	B	503	-	36,36,36	0.54	0	47,47,47	0.65	0
9	LMT	D	301	-	36,36,36	0.54	0	47,47,47	0.71	0
7	FMN	C	301	-	33,33,33	0.59	0	48,50,50	0.72	1 (2%)
11	IQT	B	505	-	31,32,32	1.99	5 (16%)	30,42,42	0.73	0
13	FES	F	502	6	0,4,4	-	-	-		
10	PEE	F	501	-	50,50,50	0.88	2 (4%)	53,55,55	0.59	0
10	PEE	B	504	-	50,50,50	0.88	2 (4%)	53,55,55	0.61	0

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
8	RBF	B	502	-	-	3/14/14/14	0/3/3/3
14	FAD	F	503	-	-	12/30/50/50	0/6/6/6
13	FES	E	301	5,4	-	-	0/1/1/1
7	FMN	B	501	-	-	6/18/18/18	0/3/3/3
9	LMT	B	503	-	-	9/21/61/61	0/2/2/2
9	LMT	D	301	-	-	7/21/61/61	0/2/2/2
7	FMN	C	301	-	-	5/18/18/18	0/3/3/3
11	IQT	B	505	-	-	9/27/46/46	0/2/2/2
13	FES	F	502	6	-	-	0/1/1/1
10	PEE	F	501	-	-	20/54/54/54	-
10	PEE	B	504	-	-	17/54/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	IQT	C6-C7	6.34	1.40	1.33
11	B	505	IQT	C13-C12	-5.54	1.28	1.44
11	B	505	IQT	C7-C1	-4.66	1.38	1.50
10	B	504	PEE	C39-C38	3.62	1.52	1.31
10	F	501	PEE	C18-C19	3.62	1.52	1.31
10	B	504	PEE	C18-C19	3.60	1.52	1.31
10	F	501	PEE	C39-C38	3.60	1.52	1.31
11	B	505	IQT	C7-N1	-3.47	1.32	1.41
14	F	503	FAD	C8A-N7A	-2.45	1.30	1.34
8	B	502	RBF	C5A-N5	-2.29	1.35	1.39
11	B	505	IQT	C8-N1	-2.24	1.32	1.37
14	F	503	FAD	C5X-N5	-2.18	1.35	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	503	FAD	O2P-P-O1P	2.09	122.56	112.24
7	C	301	FMN	C4-N3-C2	-2.07	121.81	125.64
7	B	501	FMN	C4-N3-C2	-2.07	121.82	125.64

There are no chirality outliers.

All (88) 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	O3'-C3'-C4'-C5'
9	B	503	LMT	C2-C1-O1'-C1'
9	D	301	LMT	O5'-C1'-O1'-C1
10	B	504	PEE	C1-O3P-P-O1P
10	F	501	PEE	C5-C4-O4P-P
10	F	501	PEE	O4P-C4-C5-N
11	B	505	IQT	C11-C12-C13-C14
11	B	505	IQT	C10-C11-C12-C13
11	B	505	IQT	C12-C13-C14-C15
14	F	503	FAD	C5B-O5B-PA-O1A
14	F	503	FAD	C5B-O5B-PA-O2A
14	F	503	FAD	C1'-C2'-C3'-O3'
14	F	503	FAD	C1'-C2'-C3'-C4'
14	F	503	FAD	C5'-O5'-P-O1P
10	F	501	PEE	O5-C30-O3-C3
10	F	501	PEE	C31-C30-O3-C3
7	C	301	FMN	O3'-C3'-C4'-O4'
7	C	301	FMN	C2'-C3'-C4'-O4'
9	D	301	LMT	C5'-C4'-O1B-C1B
10	B	504	PEE	C11-C12-C13-C14
10	F	501	PEE	C14-C15-C16-C17
14	F	503	FAD	O2'-C2'-C3'-C4'
7	C	301	FMN	C2'-C3'-C4'-C5'
14	F	503	FAD	O2'-C2'-C3'-O3'
10	B	504	PEE	C12-C13-C14-C15
9	D	301	LMT	C6-C7-C8-C9
11	B	505	IQT	C21-C22-C23-C24
8	B	502	RBF	C2'-C3'-C4'-O4'
9	D	301	LMT	C2'-C1'-O1'-C1
10	B	504	PEE	C11-C10-O2-C2
9	B	503	LMT	C1-C2-C3-C4
10	B	504	PEE	C43-C44-C45-C46
9	D	301	LMT	C2-C1-O1'-C1'
10	B	504	PEE	C19-C20-C21-C22
10	F	501	PEE	C39-C40-C41-C42
10	B	504	PEE	O4-C10-O2-C2
9	D	301	LMT	C3'-C4'-O1B-C1B
7	B	501	FMN	C4'-C5'-O5'-P
10	F	501	PEE	C2-C1-O3P-P
10	B	504	PEE	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	504	PEE	O3P-C1-C2-O2
8	B	502	RBF	C2'-C3'-C4'-C5'
11	B	505	IQT	C14-C15-C16-O4
10	F	501	PEE	C10-C11-C12-C13
8	B	502	RBF	O3'-C3'-C4'-O4'
11	B	505	IQT	C13-C14-C15-C16
9	B	503	LMT	C7-C8-C9-C10
9	B	503	LMT	C2-C3-C4-C5
9	B	503	LMT	O1'-C1-C2-C3
11	B	505	IQT	C1-C7-N1-C8
14	F	503	FAD	C5'-O5'-P-O3P
10	F	501	PEE	C40-C41-C42-C43
10	F	501	PEE	C1-O3P-P-O4P
14	F	503	FAD	C5'-O5'-P-O2P
11	B	505	IQT	C6-C7-N1-C8
7	B	501	FMN	C2'-C3'-C4'-O4'
10	B	504	PEE	C18-C19-C20-C21
9	B	503	LMT	C3-C4-C5-C6
9	B	503	LMT	C5'-C4'-O1B-C1B
10	B	504	PEE	O3P-C1-C2-C3
10	B	504	PEE	C36-C37-C38-C39
10	B	504	PEE	C4-O4P-P-O3P
10	F	501	PEE	C4-O4P-P-O3P
10	F	501	PEE	C12-C13-C14-C15
9	B	503	LMT	C3'-C4'-O1B-C1B
11	B	505	IQT	C20-C21-C22-C23
9	D	301	LMT	C7-C8-C9-C10
14	F	503	FAD	O4B-C4B-C5B-O5B
10	F	501	PEE	C38-C39-C40-C41
10	B	504	PEE	C16-C17-C18-C19
10	B	504	PEE	C14-C15-C16-C17
9	B	503	LMT	C4'-C5'-C6'-O6'
7	C	301	FMN	O4'-C4'-C5'-O5'
10	F	501	PEE	C34-C35-C36-C37
10	B	504	PEE	O2-C10-C11-C12
10	F	501	PEE	C16-C17-C18-C19
14	F	503	FAD	C5B-O5B-PA-O3P
14	F	503	FAD	P-O3P-PA-O1A
10	F	501	PEE	C18-C19-C20-C21
10	F	501	PEE	C35-C36-C37-C38
7	B	501	FMN	O3'-C3'-C4'-O4'
10	B	504	PEE	O4-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	F	501	PEE	C1-O3P-P-O2P
10	F	501	PEE	C4-O4P-P-O1P
10	F	501	PEE	C36-C37-C38-C39
7	B	501	FMN	O3'-C3'-C4'-C5'

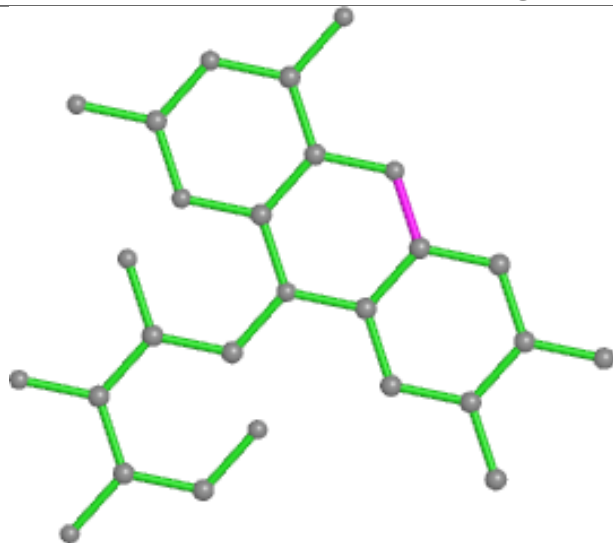
There are no ring outliers.

4 monomers are involved in 6 short contacts:

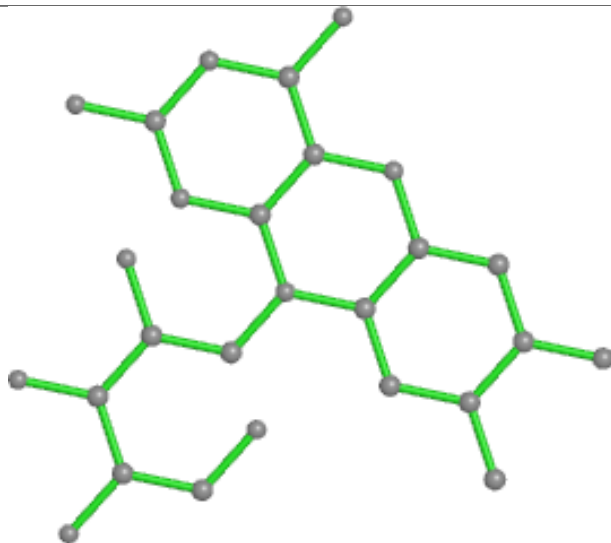
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	FMN	1	0
9	D	301	LMT	1	0
7	C	301	FMN	2	0
10	B	504	PEE	2	0

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

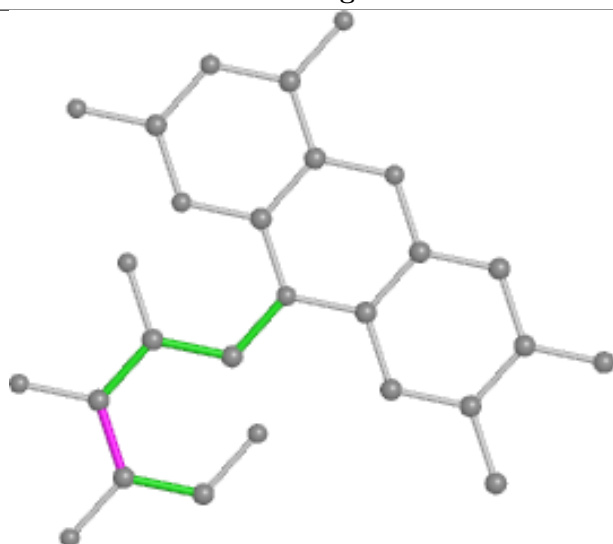
Ligand RBF B 502



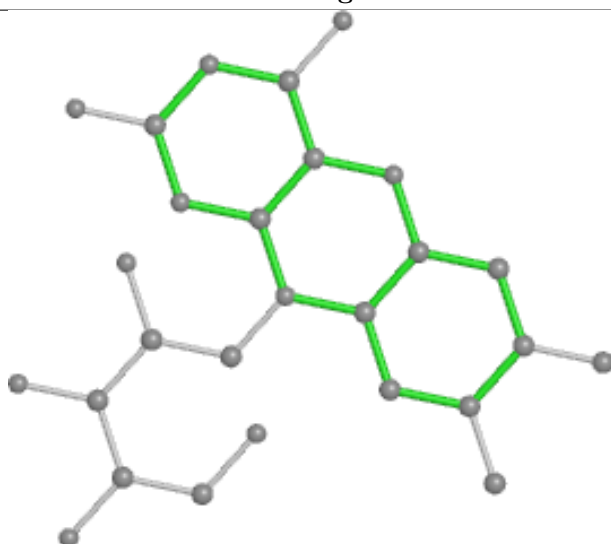
Bond lengths



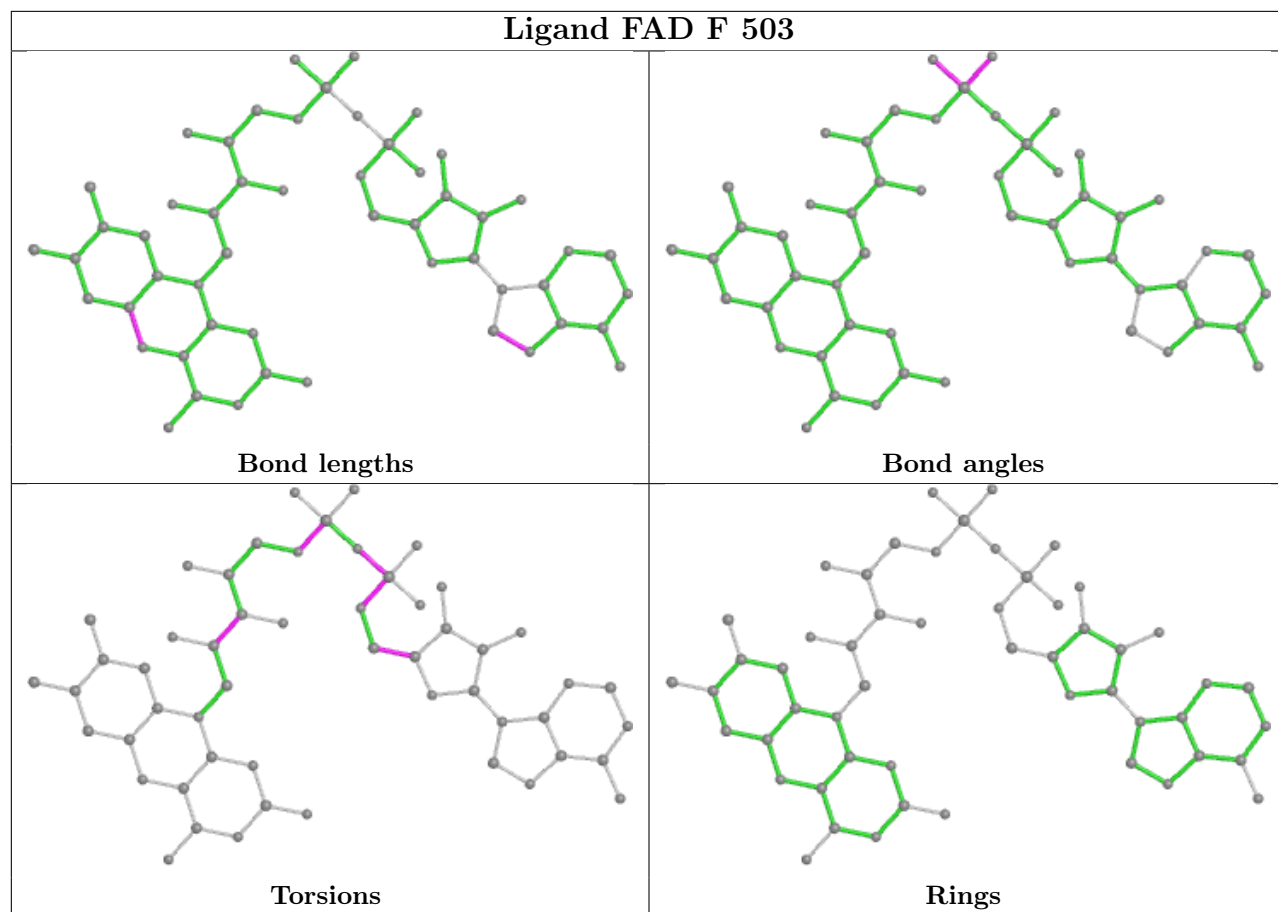
Bond angles

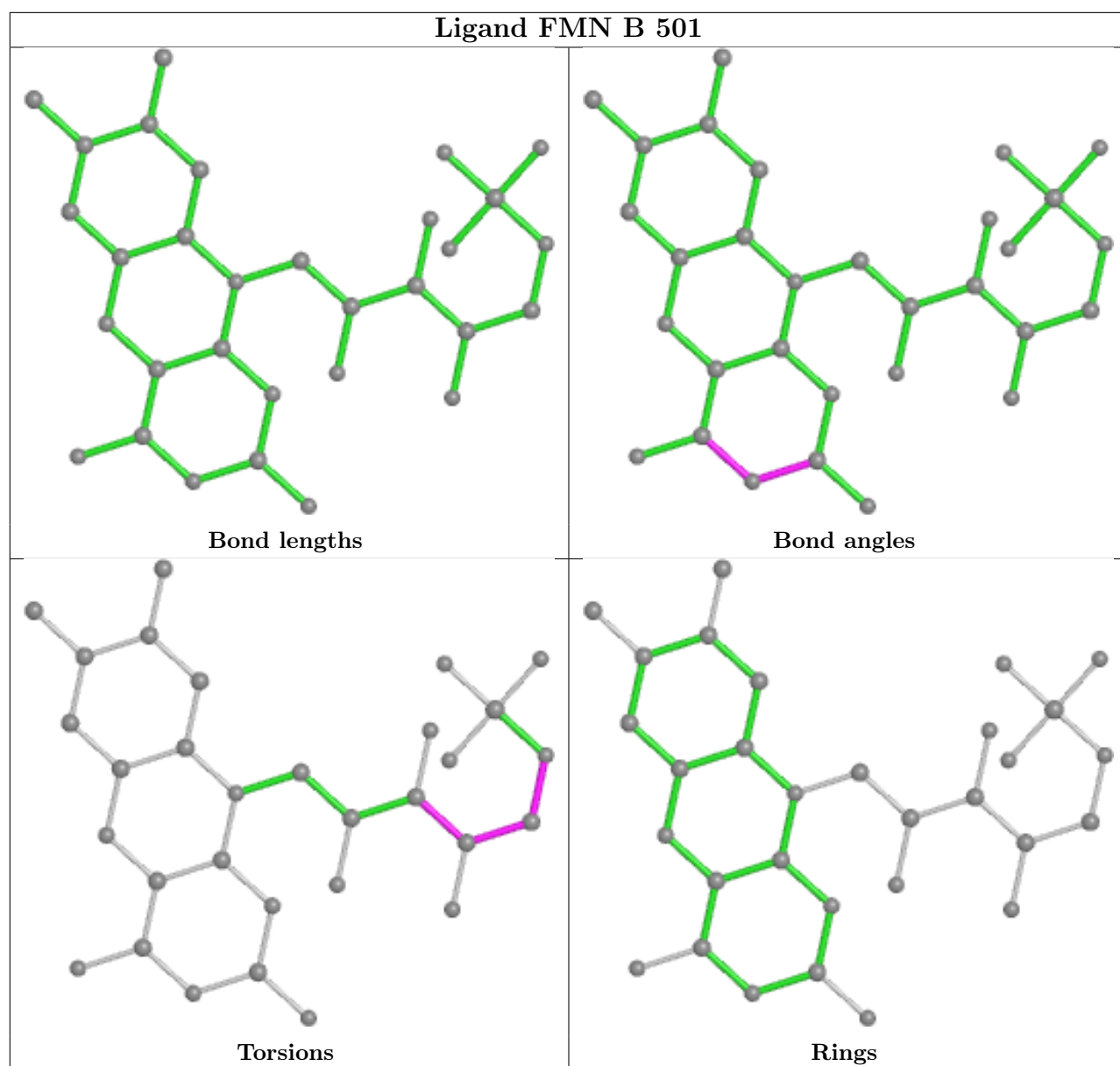


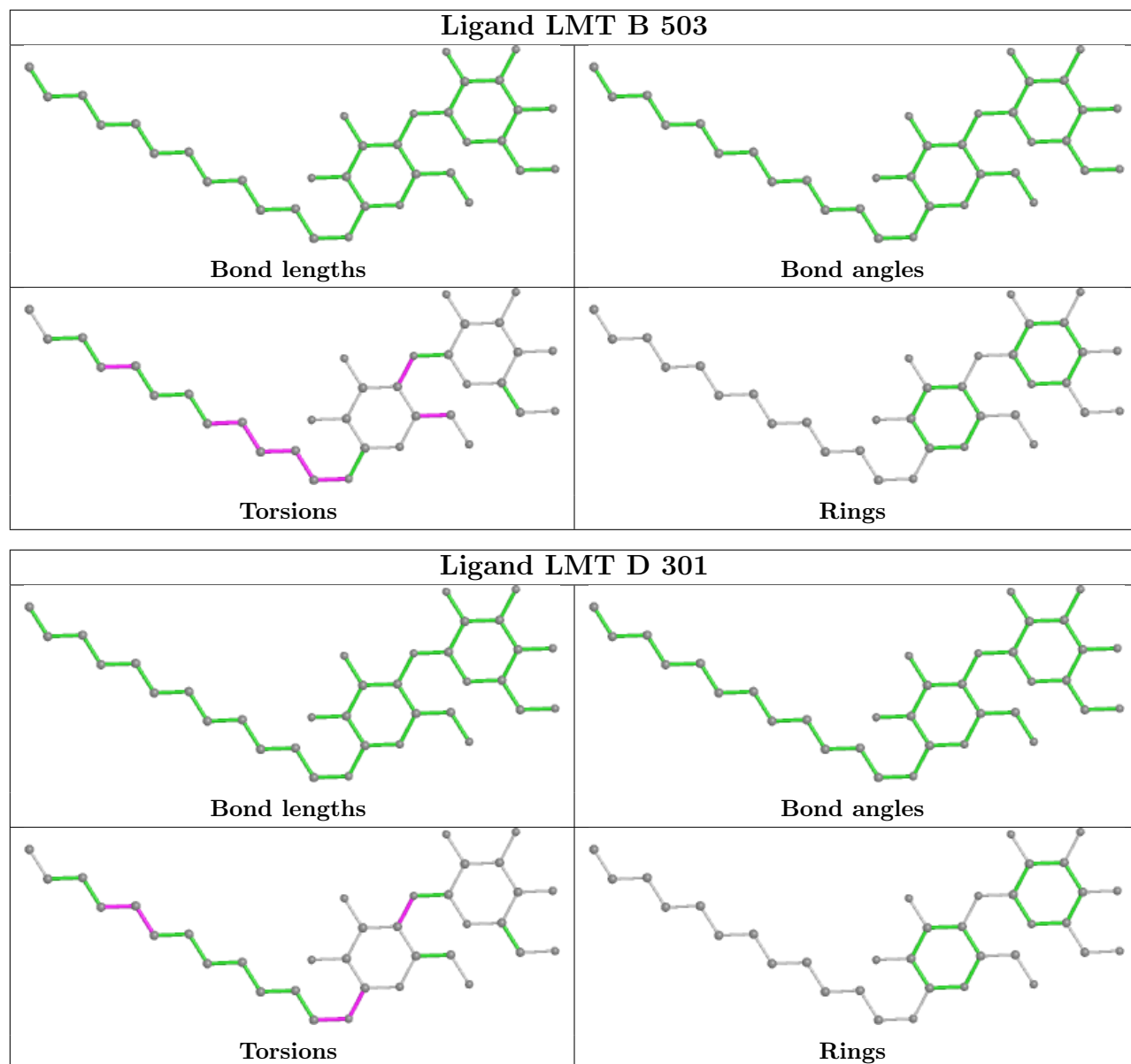
Torsions

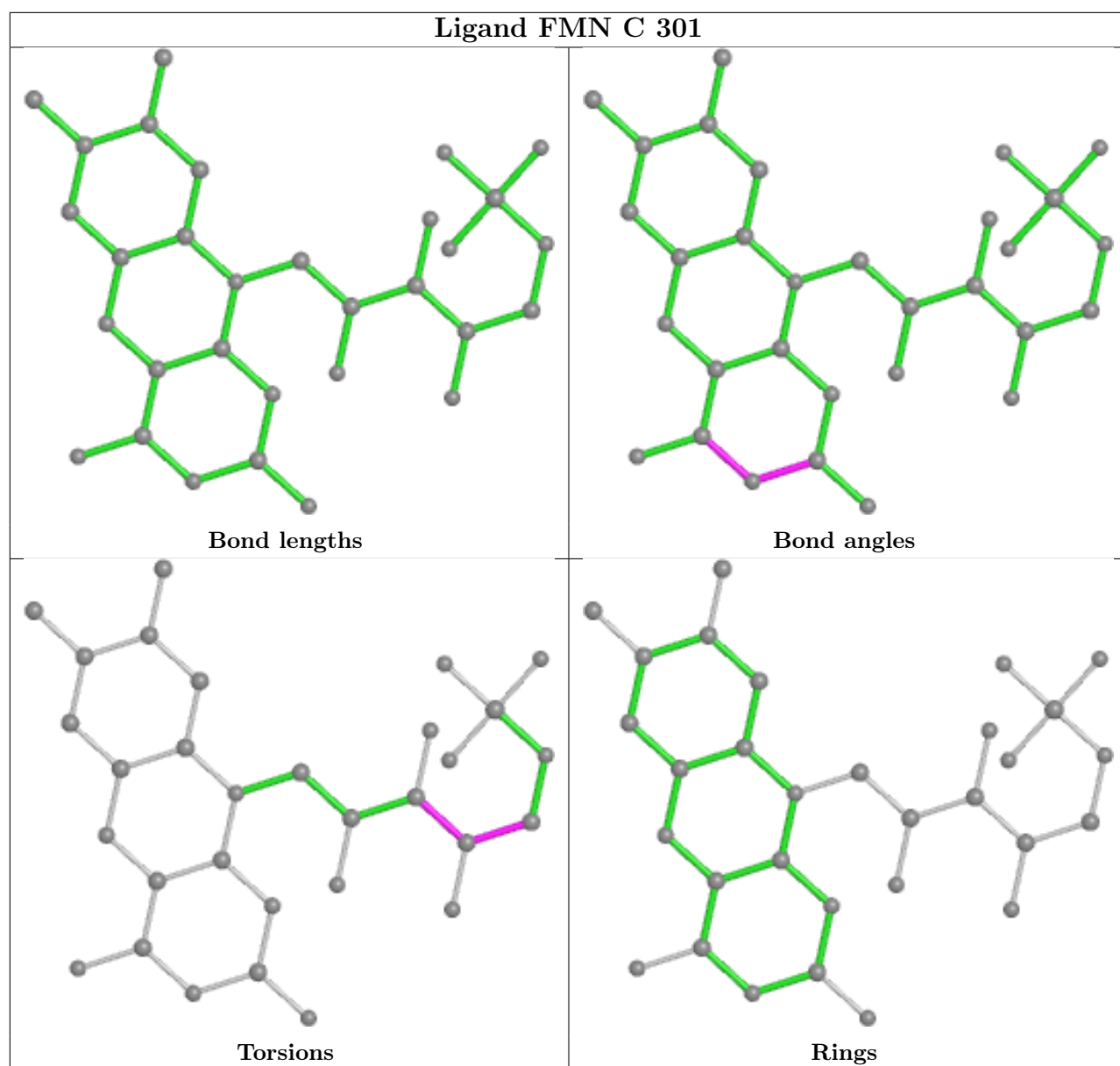


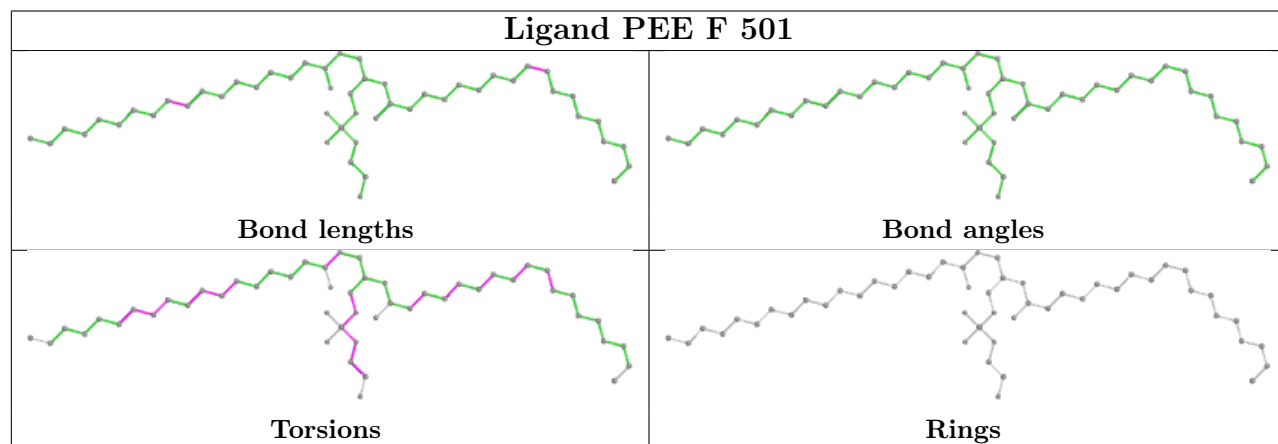
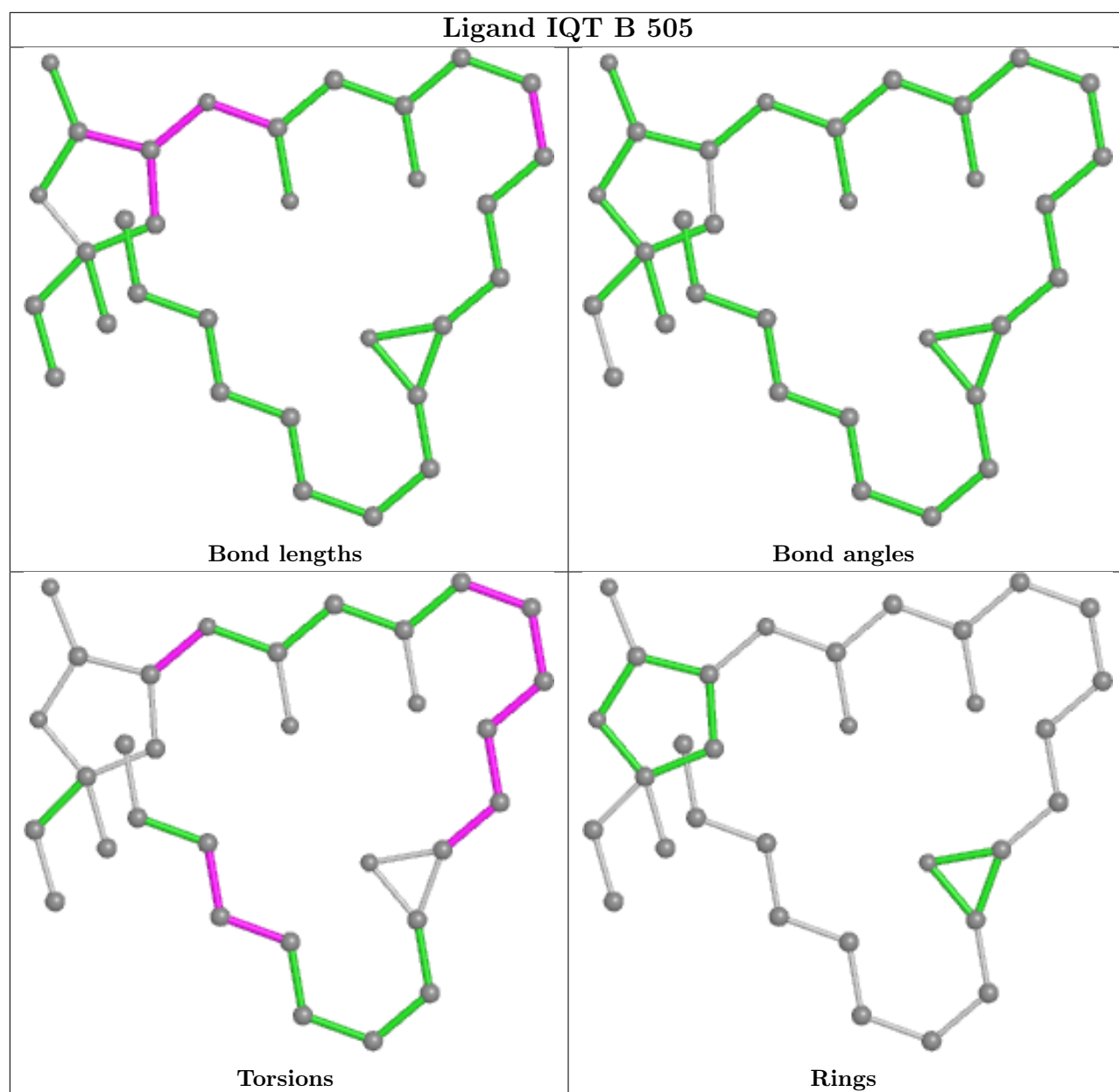
Rings

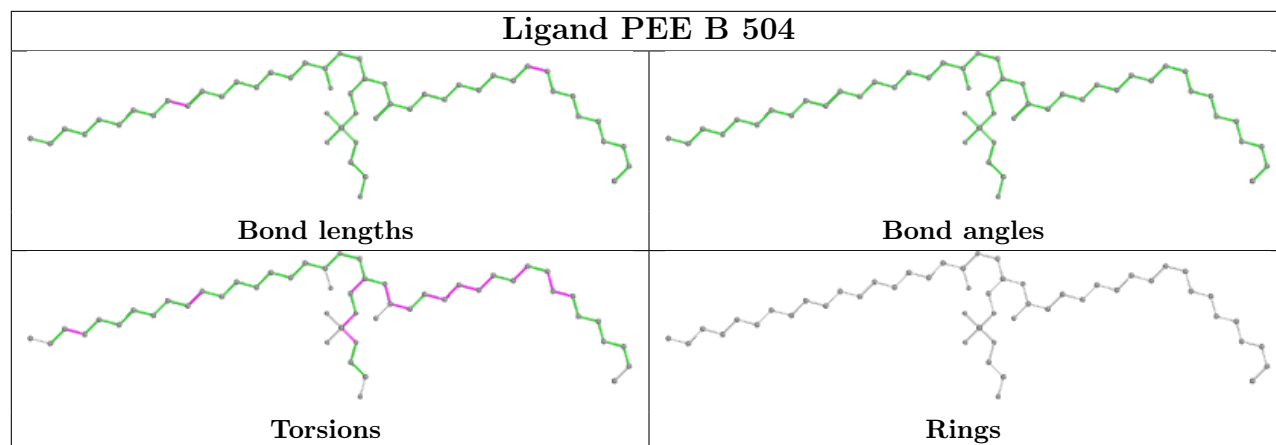












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

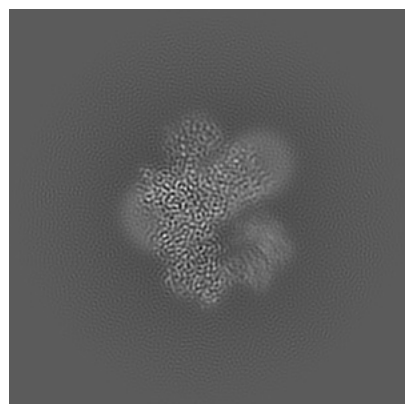
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63340. These allow visual inspection of the internal detail of the map and identification of artifacts.

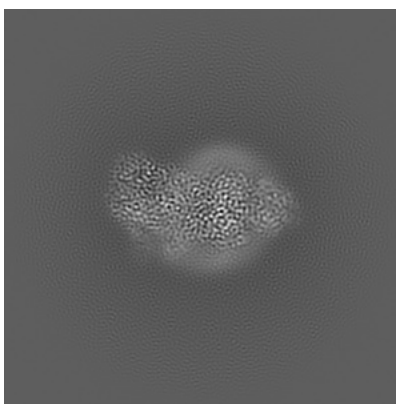
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

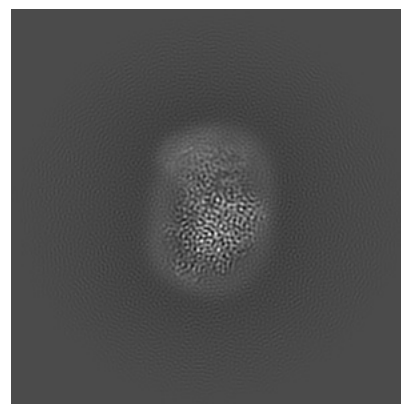
6.1.1 Primary map



X

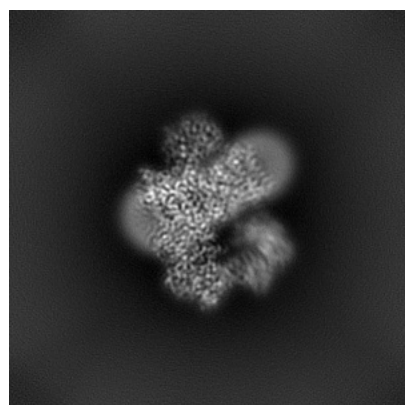


Y

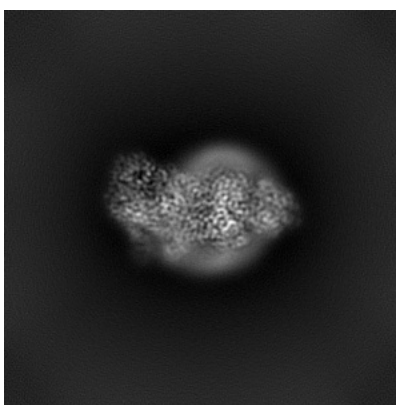


Z

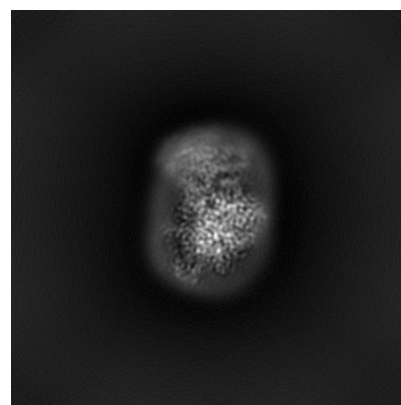
6.1.2 Raw map



X



Y

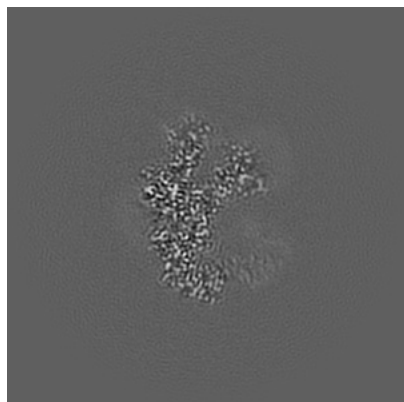


Z

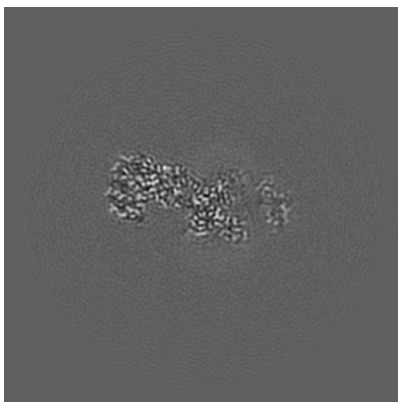
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

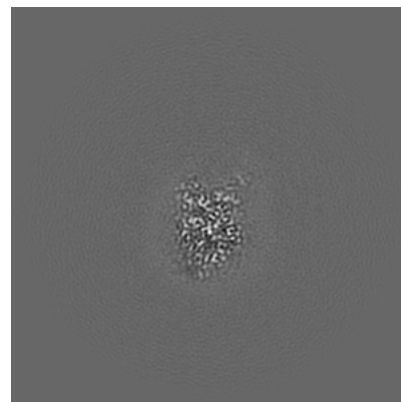
6.2.1 Primary map



X Index: 160

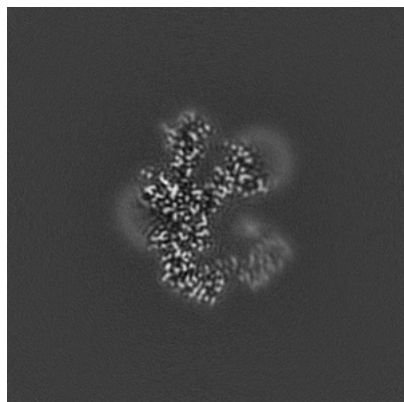


Y Index: 160

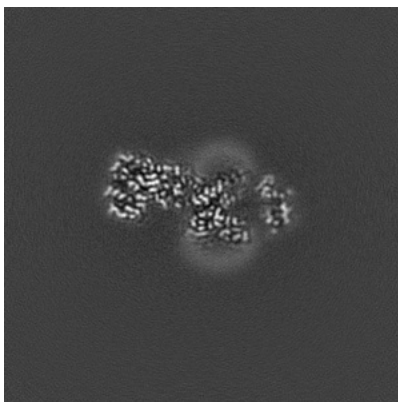


Z Index: 160

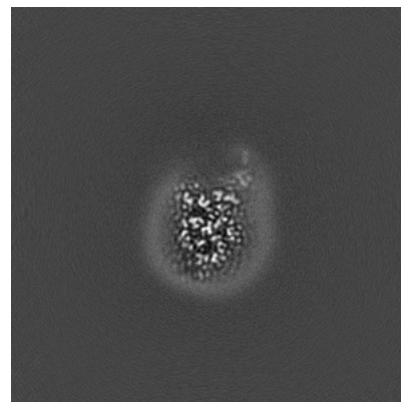
6.2.2 Raw map



X Index: 160



Y Index: 160

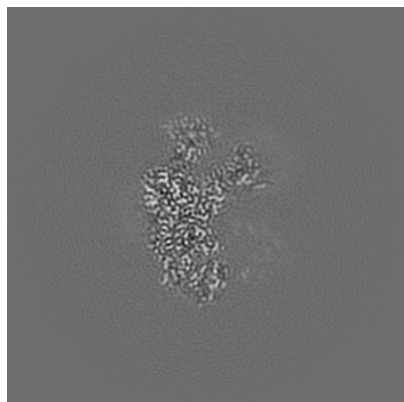


Z Index: 160

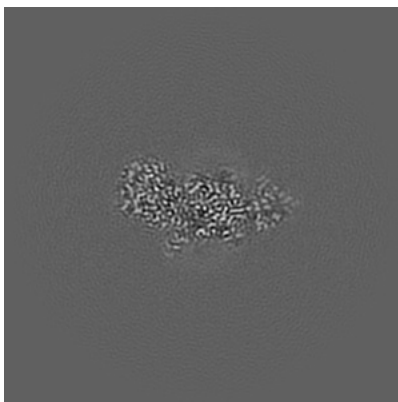
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

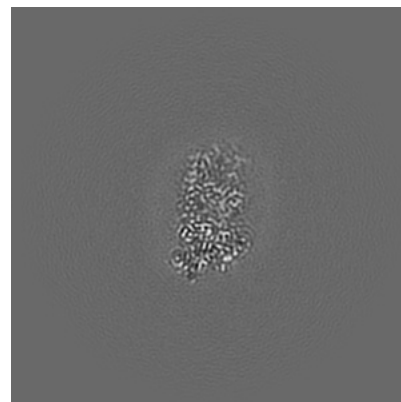
6.3.1 Primary map



X Index: 165

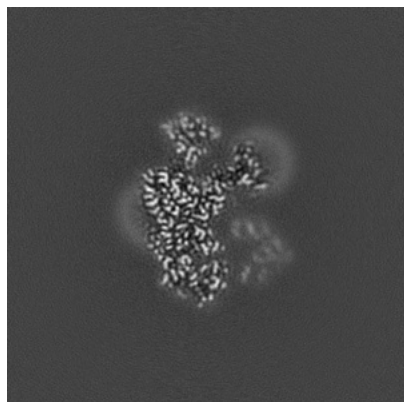


Y Index: 140

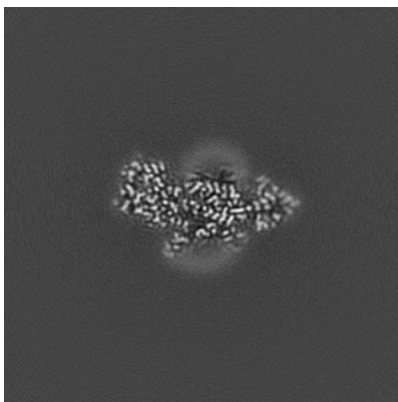


Z Index: 177

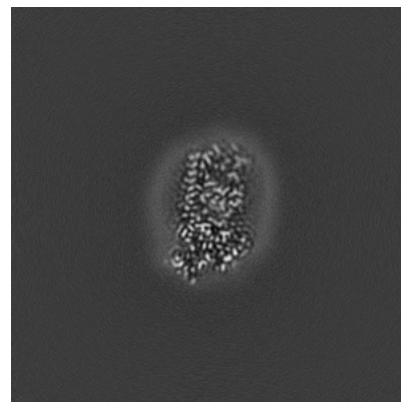
6.3.2 Raw map



X Index: 165



Y Index: 140

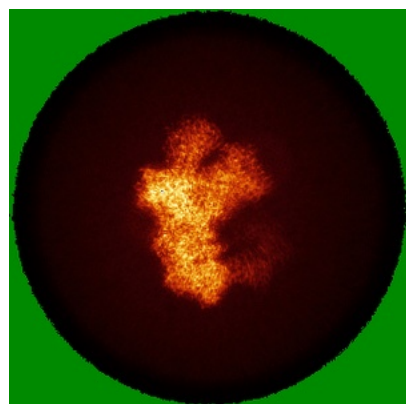


Z Index: 177

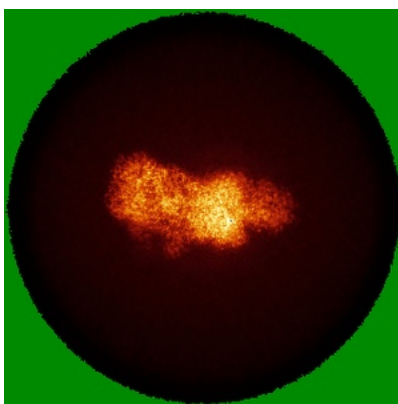
The images above show the largest variance slices of the map in three orthogonal directions.

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

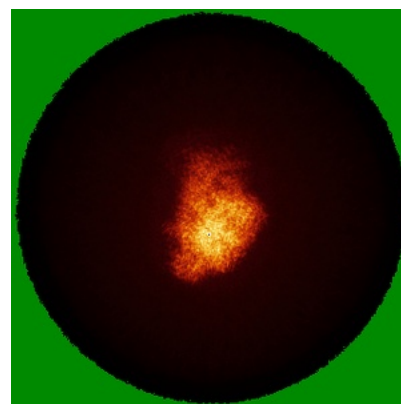
6.4.1 Primary map



X

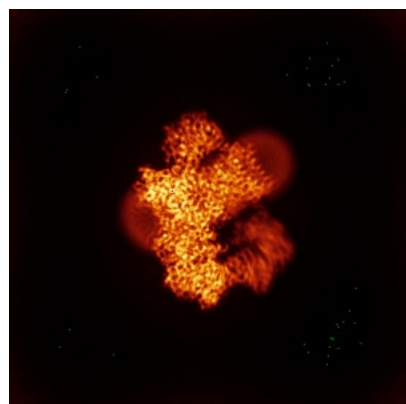


Y

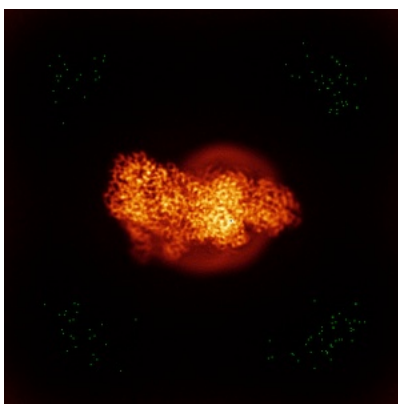


Z

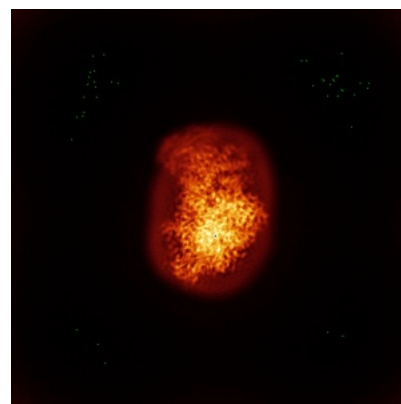
6.4.2 Raw map



X



Y



Z

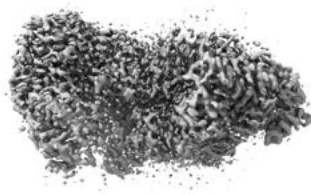
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



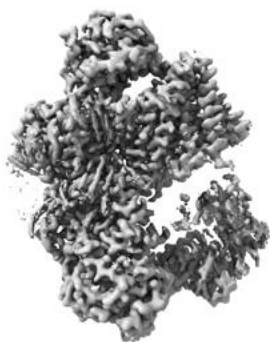
Y



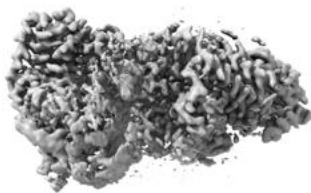
Z

The images above show the 3D surface view of the map at the recommended contour level 0.679. 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.

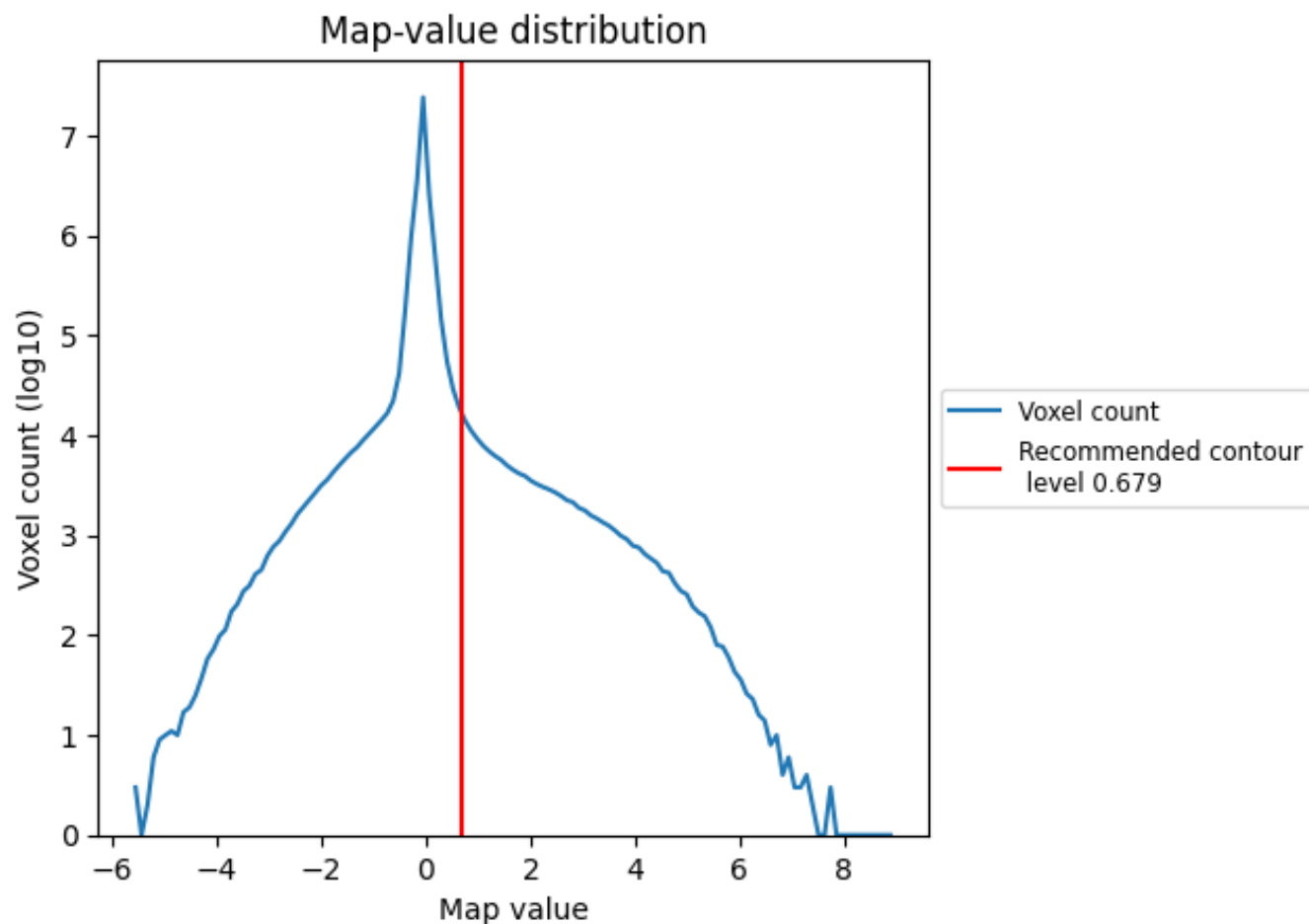
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

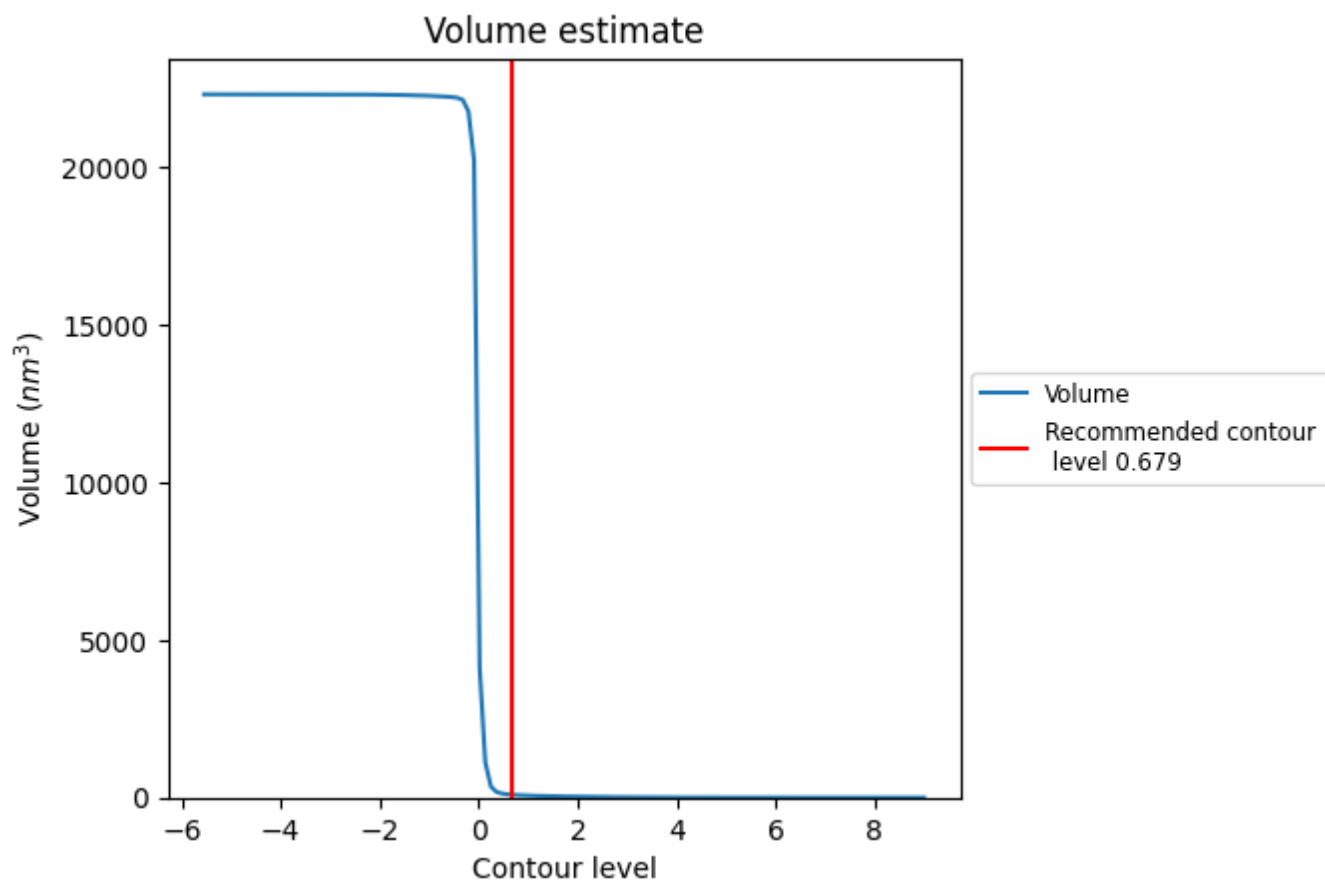
This section contains the results of statistical analysis of the map.

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.

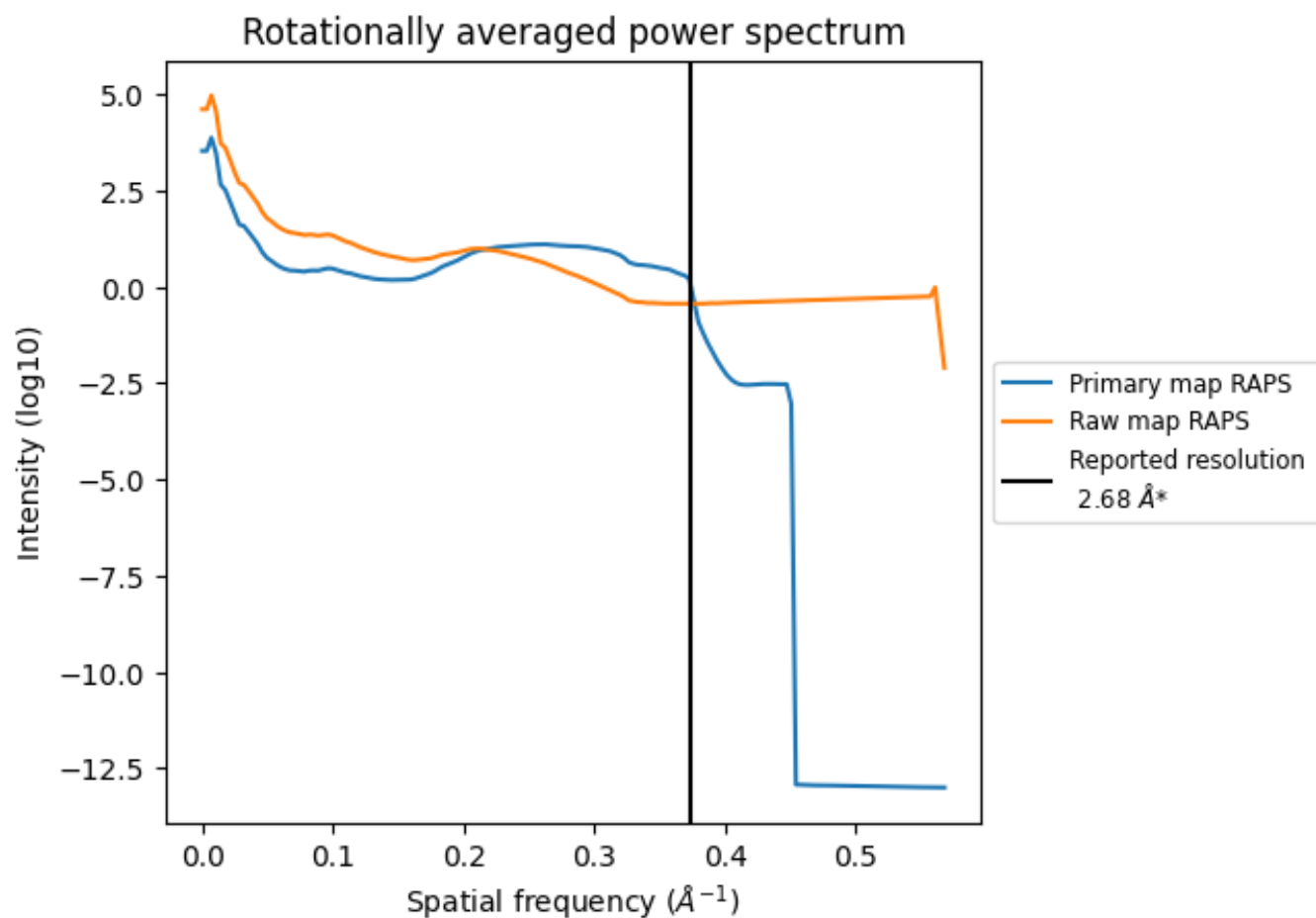
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

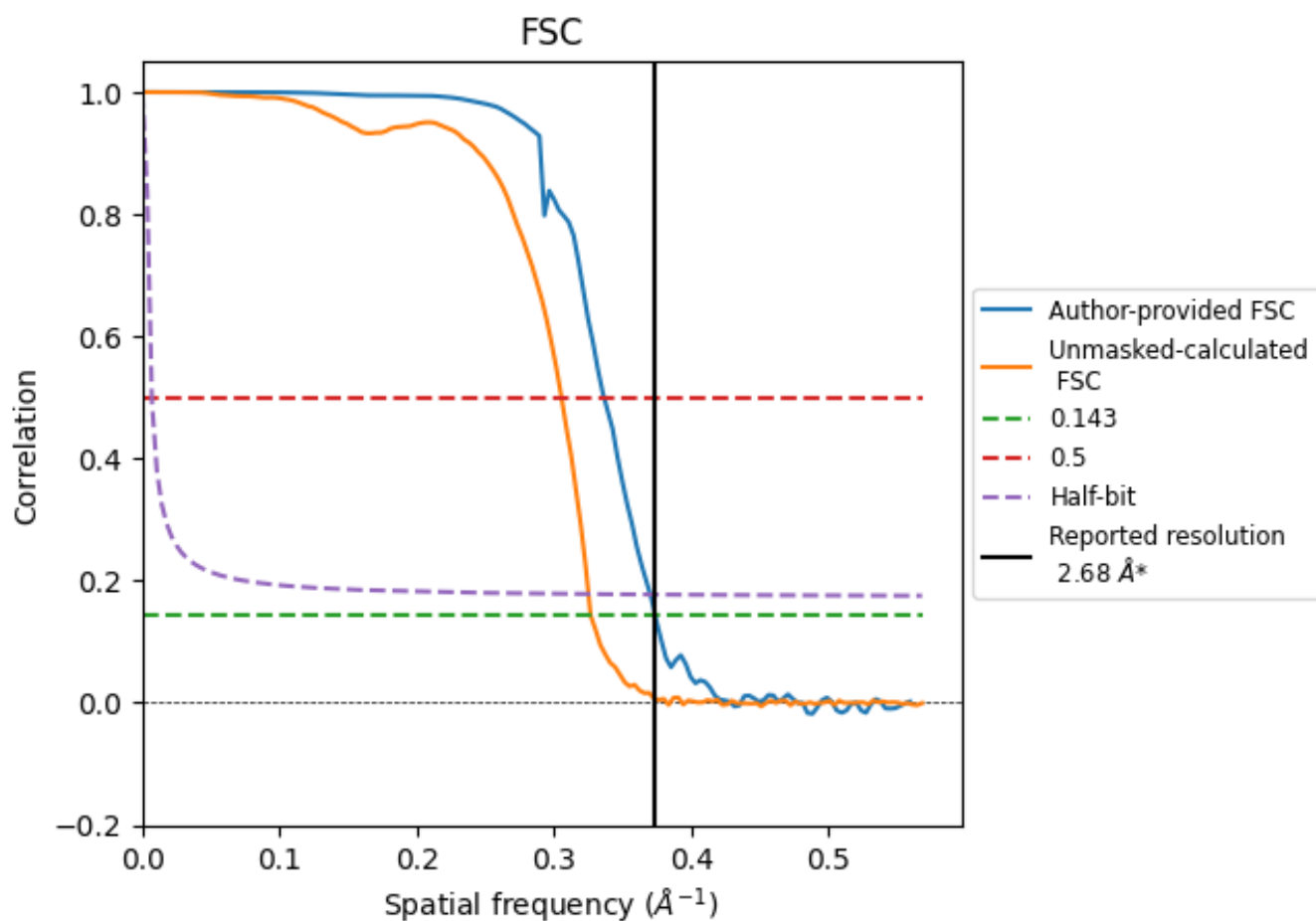


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 \AA^{-1}

8.2 Resolution estimates [i](#)

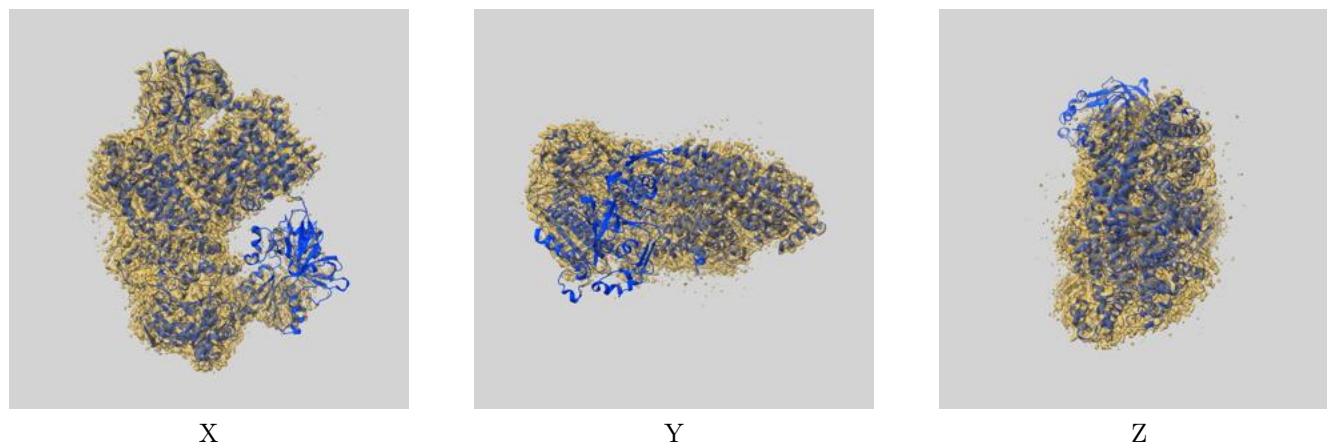
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	2.97	2.70
Unmasked-calculated*	3.06	3.27	3.08

*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 3.06 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

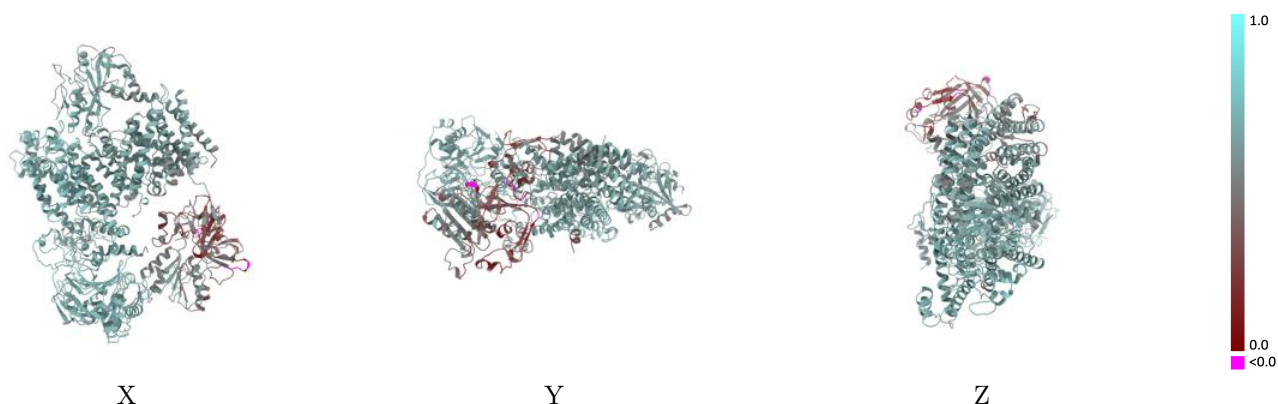
This section contains information regarding the fit between EMDB map EMD-63340 and PDB model 9LRR. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



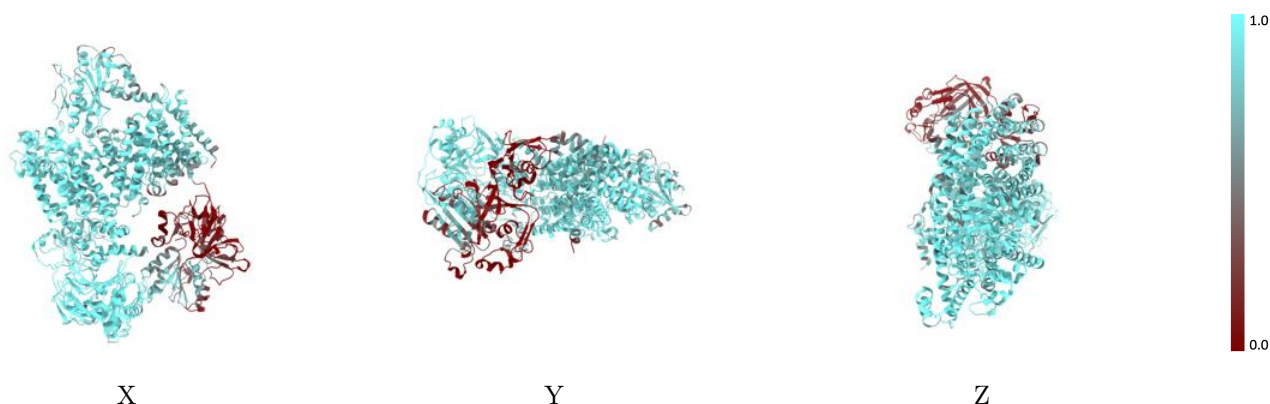
The images above show the 3D surface view of the map at the recommended contour level 0.679 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



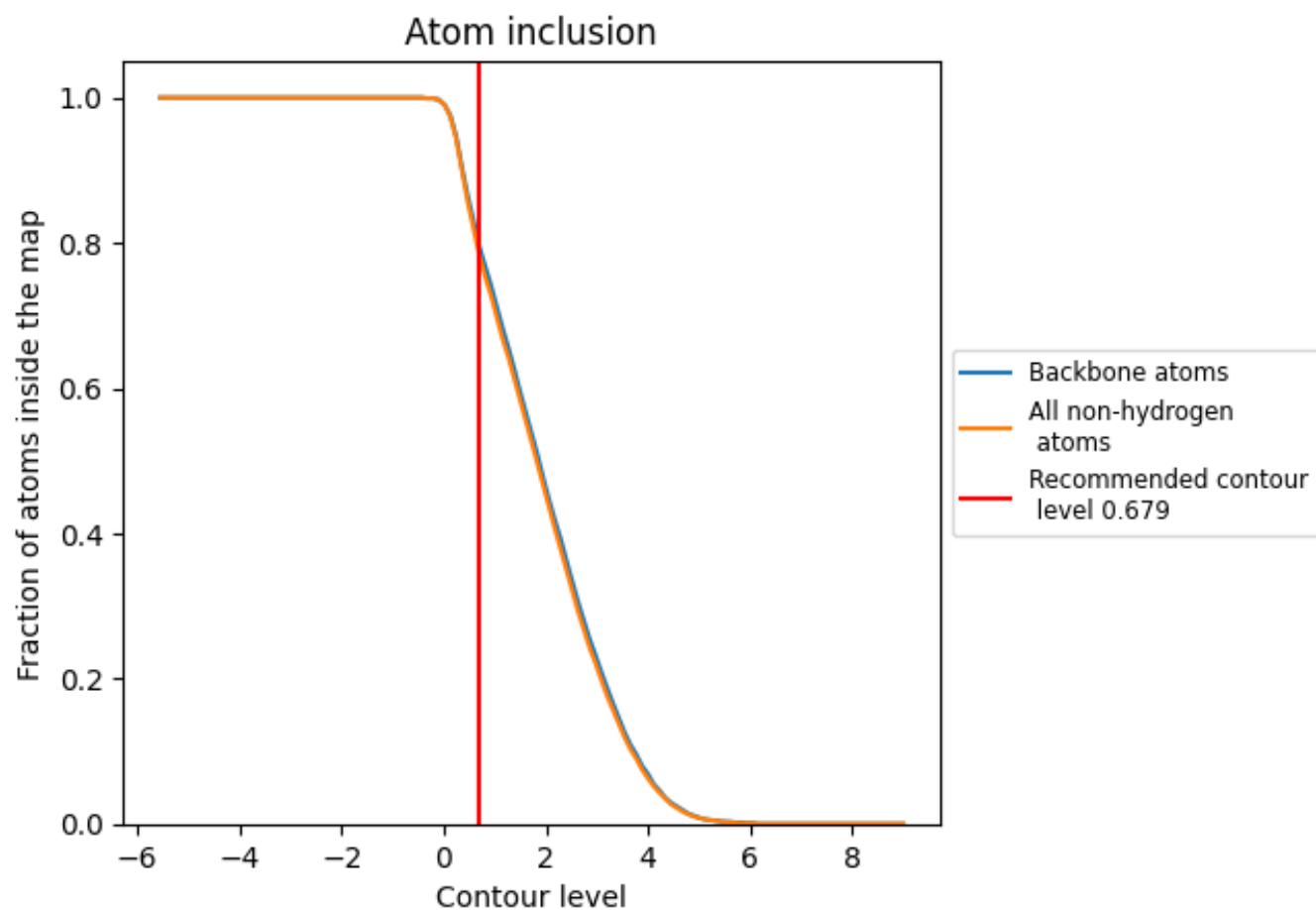
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.679).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.679) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7890	<div></div> 0.5760
A	<div></div> 0.9590	<div></div> 0.6460
B	<div></div> 0.9610	<div></div> 0.6460
C	<div></div> 0.8360	<div></div> 0.5920
D	<div></div> 0.9100	<div></div> 0.6140
E	<div></div> 0.8890	<div></div> 0.6110
F	<div></div> 0.3040	<div></div> 0.3880

1.0

0.0

<0.0