



Full wwPDB EM Validation Report ⓘ

Nov 14, 2023 – 01:26 pm GMT

PDB ID : 8A1X
EMDB ID : EMD-15092
Title : Sodium pumping NADH-quinone oxidoreductase with inhibitor DQA
Authors : Hau, J.-L.; Kaltwasser, S.; Vonck, J.; Fritz, G.; Steuber, J.
Deposited on : 2022-06-02
Resolution : 3.20 Å (reported)
Based on initial model : 4P6V

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

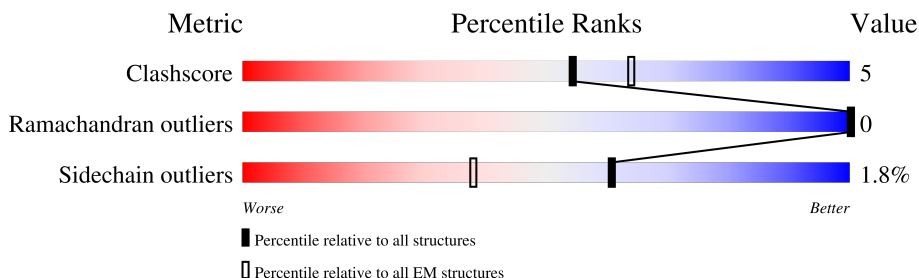
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	415	
3	C	257	
4	D	210	
5	E	198	
6	F	408	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29843 atoms, of which 14988 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	446	6879	2165	3463	584	650	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	396	6086	2018	3038	496	512	22	0	0

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

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

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

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

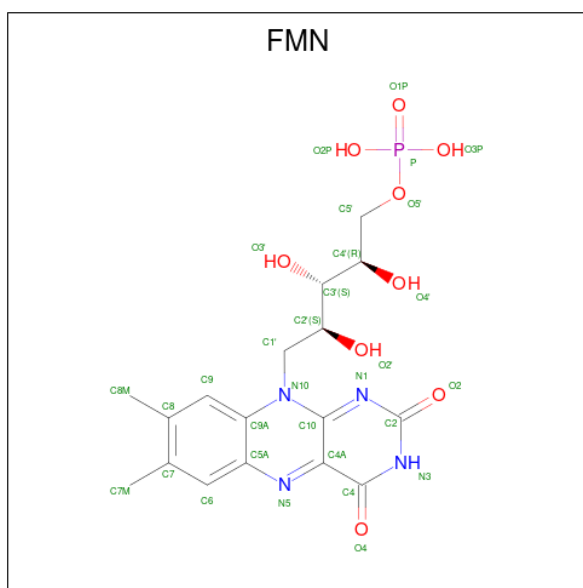
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

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

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

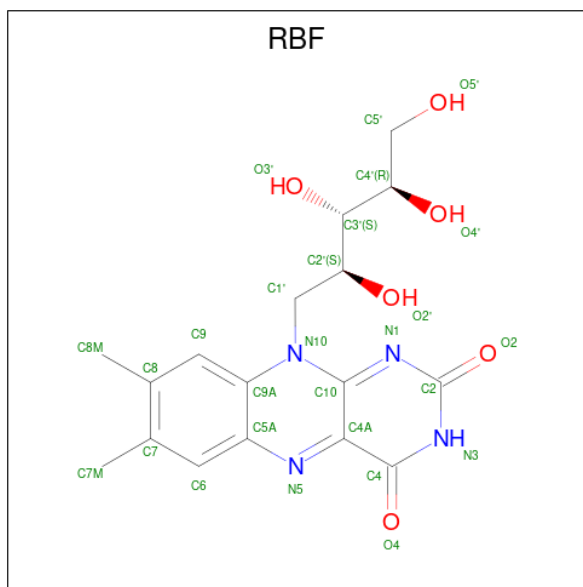
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	407	6246	2022	3089	518	594	23	0	0

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



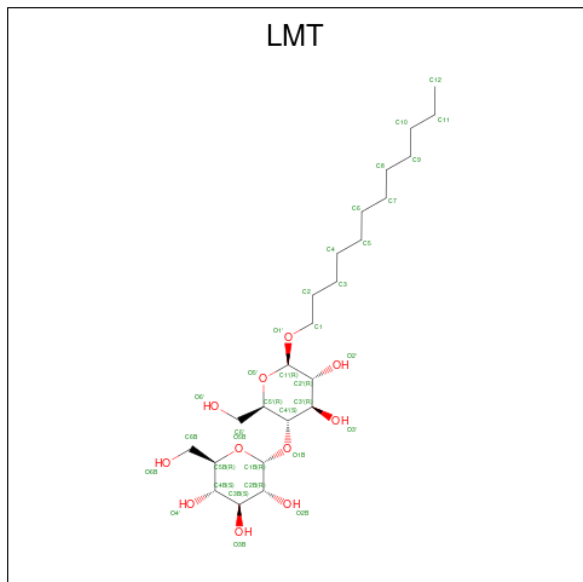
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
7	B	1	Total	C	H	N	O	P	0
			49	17	19	4	8	1	
7	C	1	Total	C	H	N	O	P	0
			49	17	19	4	8	1	

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



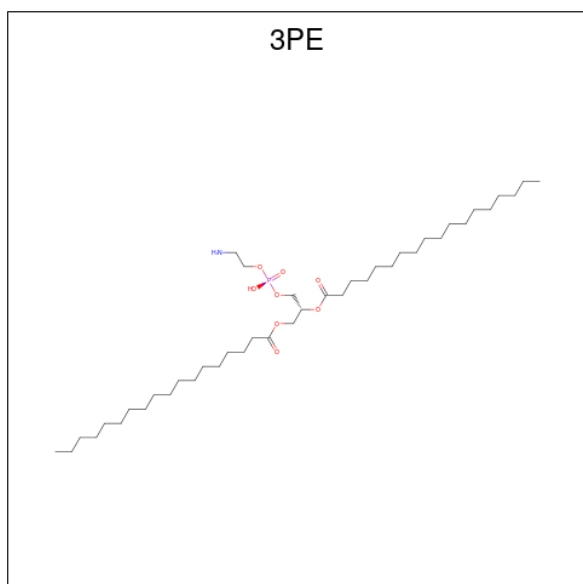
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
8	B	1	Total	C	H	N	O	0
			46	17	19	4	6	

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



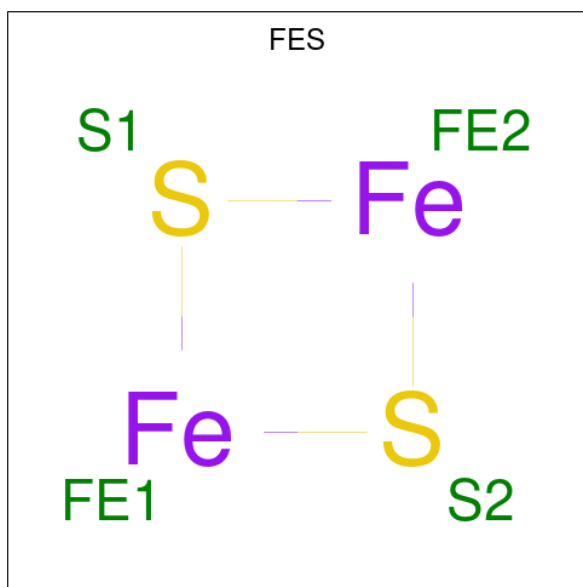
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	B	1	80	24	45	11	0
9	B	1	80	24	45	11	0
9	D	1	80	24	45	11	0

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



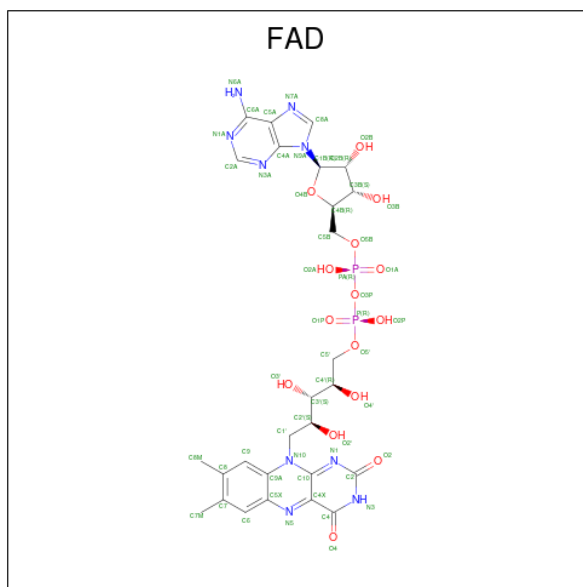
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
10	B	1	77	23	44	1	8	1	0
10	D	1	110	34	66	1	8	1	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

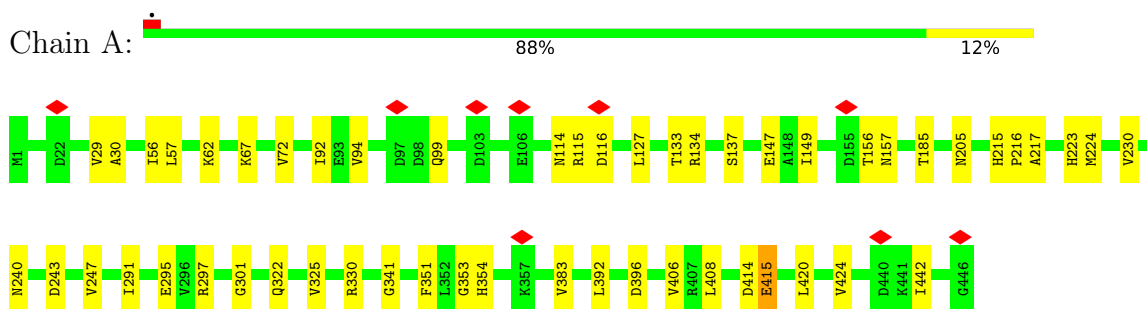


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
12	F	1	84	27	31	9	15	2	0

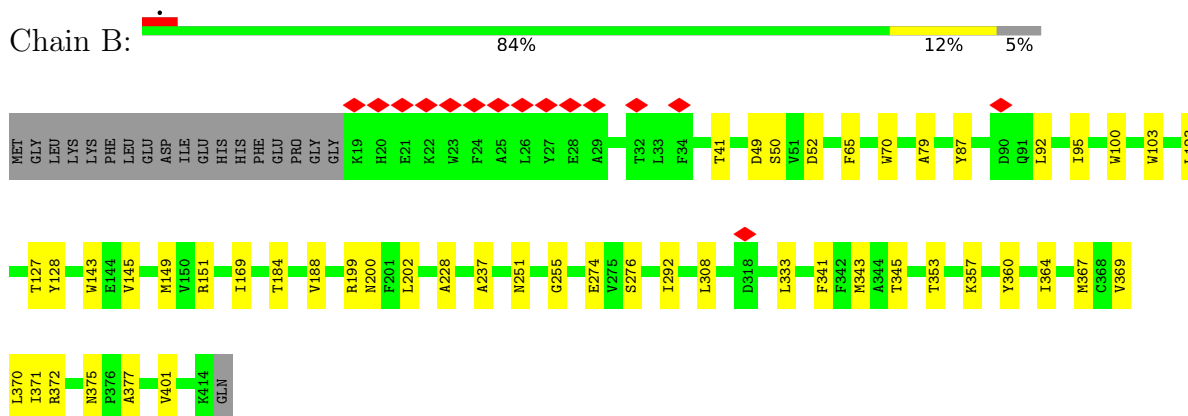
3 Residue-property plots

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.

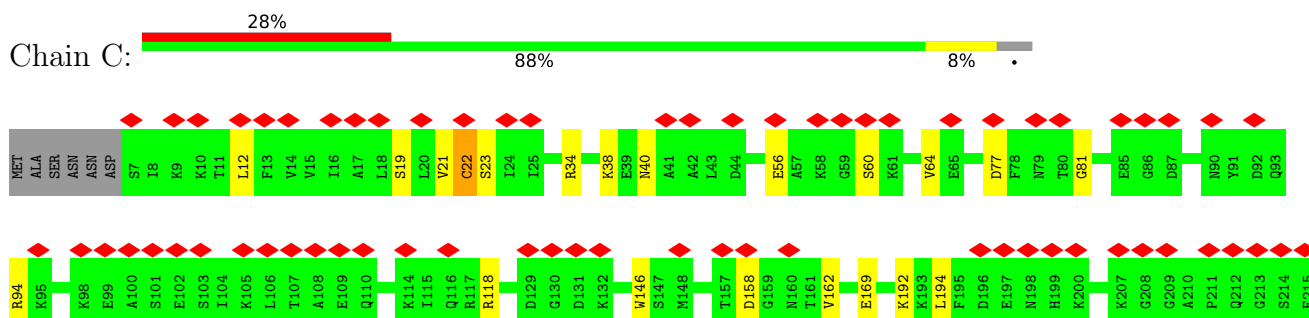
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A

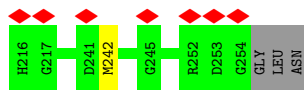


- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B



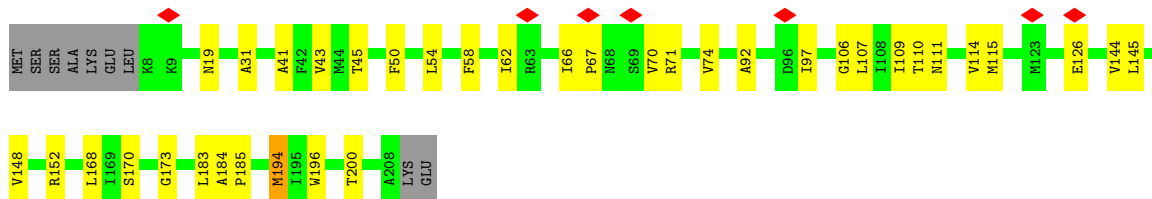
- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C





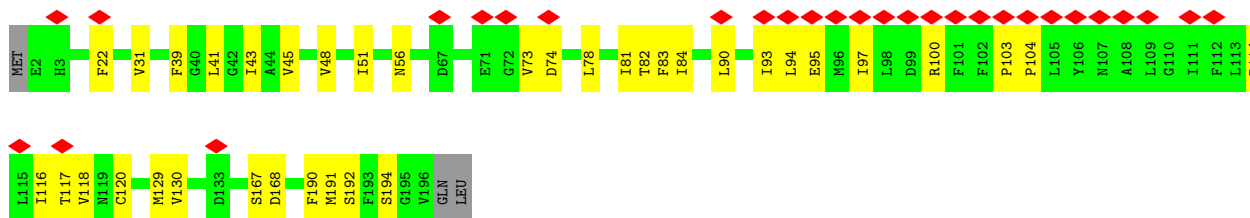
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

Chain D: 78% 17%



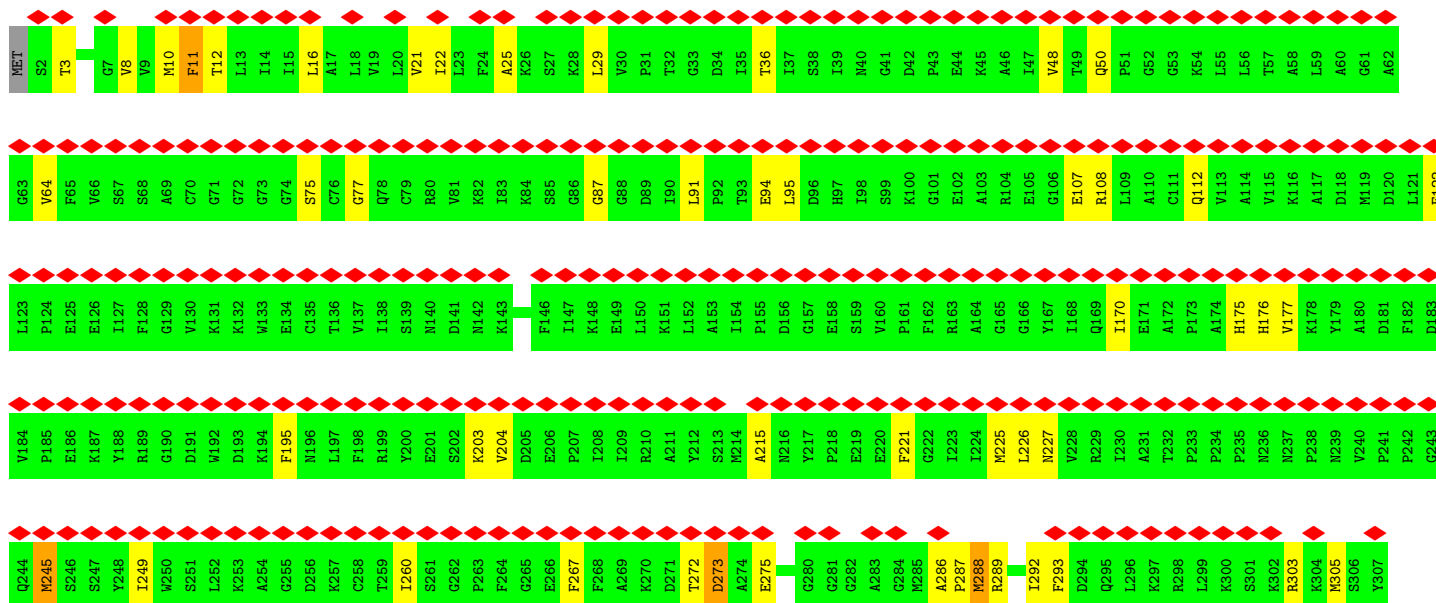
• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E

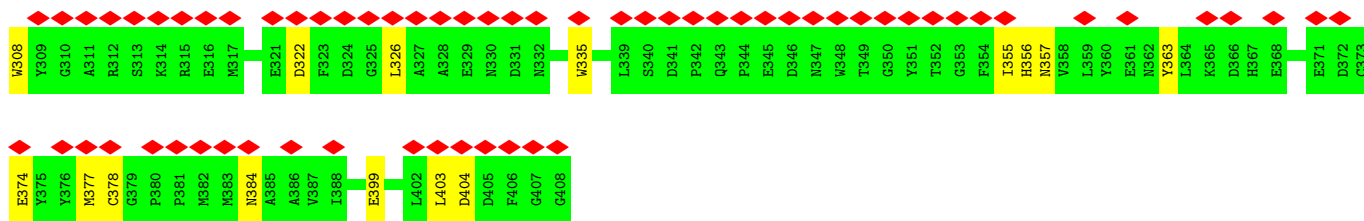
Chain E: 15% 80% 19%



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

Chain F: 84% 84% 15%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	273218	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	60168	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.128	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0325	Depositor
Map size (Å)	249.30402, 249.30402, 249.30402	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24652, 1.24652, 1.24652	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FAD, FMN, LMT, 3PE, 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	0/3141	0.43	0/4277
3	C	0.25	0/1914	0.45	0/2583
4	D	0.25	0/1568	0.45	0/2130
5	E	0.27	0/1519	0.45	0/2061
6	F	0.26	0/3235	0.47	0/4379
All	All	0.25	0/14857	0.45	0/20145

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3463	3463	31	0
2	B	3048	3038	3038	34	0
3	C	1882	1892	1892	15	0
4	D	1536	1618	1618	23	0
5	E	1486	1555	1555	30	0
6	F	3157	3089	3089	47	0
7	B	30	19	19	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	30	19	19	1	0
8	B	27	19	20	1	0
9	B	70	90	90	2	0
9	D	35	45	45	1	0
10	B	33	44	40	0	0
10	D	44	66	62	2	0
11	E	4	0	0	0	0
11	F	4	0	0	1	0
12	F	53	31	31	0	0
All	All	14855	14988	14981	161	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 (161) 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)
5:E:78:LEU:O	5:E:82:THR:OG1	1.89	0.89
3:C:40:ASN:ND2	4:D:92:ALA:O	2.09	0.84
6:F:275:GLU:OE2	6:F:363:TYR:OH	1.96	0.82
1:A:414:ASP:OD1	1:A:415:GLU:N	2.15	0.80
6:F:8:VAL:O	6:F:12:THR:HG23	1.83	0.79
2:B:274:GLU:OE2	7:B:501:FMN:O3'	2.01	0.78
4:D:41:ALA:O	4:D:45:THR:HG23	1.86	0.74
6:F:303:ARG:NH2	6:F:374:GLU:OE1	2.25	0.70
4:D:196:TRP:O	4:D:200:THR:HG23	1.90	0.70
3:C:34:ARG:NH2	5:E:74:ASP:OD1	2.24	0.69
3:C:60:SER:O	3:C:64:VAL:HG23	1.93	0.69
3:C:56:GLU:OE1	3:C:56:GLU:N	2.26	0.68
6:F:288:MET:O	6:F:292:ILE:HD12	1.93	0.68
2:B:341:PHE:O	2:B:345:THR:OG1	2.09	0.67
2:B:333:LEU:O	2:B:372:ARG:NH2	2.27	0.66
9:B:504:LMT:O3'	9:B:504:LMT:O5B	2.14	0.65
6:F:227:ASN:HB2	6:F:286:ALA:HB2	1.79	0.64
4:D:58:PHE:O	4:D:62:ILE:HG22	1.98	0.63
1:A:114:ASN:OD1	1:A:115:ARG:N	2.33	0.62
2:B:123:LEU:O	2:B:127:THR:HG23	2.00	0.62
2:B:360:TYR:CZ	2:B:364:ILE:HD11	2.35	0.62
5:E:100:ARG:NE	6:F:29:LEU:O	2.33	0.61
5:E:45:VAL:HG23	5:E:116:ILE:HD11	1.83	0.60
1:A:133:THR:O	1:A:137:SER:N	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ARG:NH2	5:E:168:ASP:OD2	2.36	0.58
1:A:217:ALA:O	1:A:223:HIS:NE2	2.35	0.58
2:B:49:ASP:OD1	2:B:50:SER:N	2.36	0.58
6:F:107:GLU:OE1	6:F:107:GLU:N	2.37	0.58
1:A:134:ARG:HG3	1:A:230:VAL:HG21	1.86	0.57
2:B:377:ALA:O	7:C:1000:FMN:O2'	2.23	0.57
4:D:200:THR:HG21	10:D:301:3PE:H341	1.85	0.56
5:E:48:VAL:HG21	5:E:116:ILE:HG21	1.87	0.56
5:E:74:ASP:OD1	5:E:74:ASP:O	2.24	0.56
2:B:308:LEU:HD23	2:B:369:VAL:HB	1.88	0.55
5:E:94:LEU:HD23	5:E:97:ILE:HD11	1.88	0.55
1:A:127:LEU:HD23	1:A:247:VAL:HG22	1.89	0.55
2:B:92:LEU:O	2:B:95:ILE:HG22	2.07	0.55
4:D:107:LEU:HD12	5:E:120:CYS:SG	2.47	0.55
1:A:392:LEU:HD13	2:B:401:VAL:HG11	1.90	0.54
3:C:162:VAL:HG12	3:C:192:LYS:O	2.08	0.54
5:E:97:ILE:HG22	6:F:29:LEU:HD11	1.88	0.54
1:A:57:LEU:HD11	1:A:92:ILE:HD11	1.91	0.53
6:F:356:HIS:NE2	6:F:357:ASN:OD1	2.42	0.53
3:C:146:TRP:HZ3	5:E:194:SER:HG	1.58	0.52
6:F:95:LEU:HD23	6:F:95:LEU:O	2.10	0.52
5:E:83:PHE:CZ	5:E:130:VAL:HG21	2.45	0.51
5:E:31:VAL:HG21	5:E:41:LEU:HD22	1.93	0.51
2:B:200:ASN:ND2	2:B:202:LEU:O	2.44	0.51
6:F:170:ILE:HG22	6:F:260:ILE:HG22	1.93	0.51
6:F:225:MET:O	6:F:226:LEU:HD23	2.10	0.51
2:B:251:ASN:O	2:B:255:GLY:N	2.43	0.50
6:F:25:ALA:O	6:F:29:LEU:HB2	2.11	0.50
2:B:145:VAL:O	2:B:149:MET:HG3	2.12	0.50
1:A:216:PRO:HG3	1:A:420:LEU:HD12	1.94	0.50
6:F:36:THR:HG22	6:F:48:VAL:HG22	1.94	0.50
3:C:77:ASP:O	3:C:81:GLY:N	2.43	0.50
2:B:87:TYR:HD1	2:B:95:ILE:HG21	1.77	0.49
5:E:95:GLU:OE1	5:E:114:PRO:HD3	2.12	0.49
6:F:91:LEU:HD12	6:F:112:GLN:NE2	2.27	0.49
1:A:351:PHE:O	1:A:354:HIS:ND1	2.41	0.49
2:B:199:ARG:O	5:E:167:SER:OG	2.29	0.49
4:D:62:ILE:HG12	4:D:62:ILE:O	2.12	0.49
2:B:169:ILE:HD13	2:B:343:MET:HE1	1.95	0.49
6:F:203:LYS:NZ	6:F:204:VAL:O	2.45	0.49
1:A:147:GLU:OE1	1:A:147:GLU:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:PHE:CZ	4:D:54:LEU:HD22	2.48	0.49
6:F:175:HIS:HD2	6:F:177:VAL:HG13	1.78	0.49
9:D:302:LMT:O1B	9:D:302:LMT:O6'	2.29	0.48
5:E:81:ILE:HA	5:E:84:ILE:HG22	1.95	0.48
5:E:51:ILE:HG22	5:E:90:LEU:HD13	1.95	0.48
1:A:240:ASN:ND2	1:A:243:ASP:OD2	2.46	0.48
6:F:94:GLU:OE2	6:F:108:ARG:NH2	2.46	0.48
4:D:152:ARG:NH2	4:D:183:LEU:O	2.47	0.48
4:D:168:LEU:O	4:D:173:GLY:N	2.45	0.48
6:F:170:ILE:HD12	6:F:249:ILE:HD11	1.95	0.48
4:D:31:ALA:HA	4:D:145:LEU:HD11	1.96	0.47
1:A:396:ASP:OD2	1:A:408:LEU:HD12	2.14	0.47
1:A:114:ASN:OD1	1:A:116:ASP:N	2.44	0.47
4:D:70:VAL:HG12	6:F:22:ILE:HG21	1.96	0.47
6:F:122:GLU:HA	6:F:122:GLU:OE1	2.14	0.47
3:C:94:ARG:NH2	3:C:169:GLU:OE1	2.43	0.47
4:D:19:ASN:HD21	4:D:144:VAL:HG23	1.79	0.47
4:D:184:ALA:HB1	5:E:22:PHE:HE1	1.80	0.47
5:E:83:PHE:CE2	5:E:130:VAL:HG21	2.50	0.47
2:B:52:ASP:OD1	2:B:52:ASP:N	2.47	0.47
3:C:12:LEU:HD11	6:F:16:LEU:HD11	1.96	0.47
6:F:292:ILE:HD12	6:F:292:ILE:H	1.80	0.46
3:C:23:SER:OG	6:F:8:VAL:HG22	2.15	0.46
4:D:110:THR:HG22	5:E:118:VAL:O	2.15	0.46
5:E:114:PRO:O	5:E:117:THR:OG1	2.29	0.46
2:B:169:ILE:HG22	7:B:501:FMN:HM83	1.97	0.46
6:F:286:ALA:HB3	6:F:287:PRO:CD	2.46	0.46
6:F:245:MET:O	6:F:249:ILE:HG12	2.17	0.45
2:B:375:ASN:ND2	5:E:192:SER:O	2.50	0.45
1:A:301:GLY:N	1:A:322:GLN:O	2.43	0.45
2:B:143:TRP:HE1	2:B:184:THR:HG1	1.62	0.45
1:A:406:VAL:HG21	1:A:442:ILE:CD1	2.47	0.45
4:D:148:VAL:HG23	4:D:194:MET:HE1	1.98	0.45
6:F:50:GLN:OE1	6:F:50:GLN:N	2.49	0.44
2:B:237:ALA:HB3	2:B:333:LEU:HD22	1.99	0.44
2:B:79:ALA:HB2	2:B:228:ALA:HB3	1.98	0.44
3:C:19:SER:O	3:C:23:SER:HB2	2.17	0.44
4:D:62:ILE:O	4:D:62:ILE:CG1	2.65	0.44
6:F:87:GLY:O	6:F:108:ARG:NH1	2.51	0.44
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.99	0.44
5:E:103:PRO:N	5:E:104:PRO:HD2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD12	1:A:67:LYS:HG2	1.99	0.44
1:A:157:ASN:OD1	1:A:215:HIS:NE2	2.51	0.44
5:E:43:ILE:N	5:E:43:ILE:HD13	2.33	0.43
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.53	0.43
2:B:308:LEU:HD21	2:B:370:LEU:HG	2.00	0.43
4:D:66:ILE:HG13	4:D:67:PRO:HD2	2.00	0.43
4:D:111:ASN:O	4:D:114:VAL:HG22	2.18	0.43
5:E:93:ILE:HD11	6:F:21:VAL:HG12	2.00	0.43
1:A:134:ARG:HB2	1:A:224:MET:SD	2.58	0.43
1:A:149:ILE:HD12	1:A:185:THR:HB	2.00	0.43
6:F:225:MET:C	6:F:226:LEU:HD23	2.38	0.43
6:F:308:TRP:HB3	6:F:355:ILE:HD11	2.01	0.43
1:A:156:THR:OG1	1:A:215:HIS:O	2.32	0.43
6:F:273:ASP:N	6:F:273:ASP:OD1	2.52	0.43
1:A:62:LYS:NZ	6:F:399:GLU:OE2	2.52	0.43
1:A:383:VAL:HG11	1:A:424:VAL:HG11	2.01	0.43
1:A:295:GLU:OE2	1:A:330:ARG:NH1	2.50	0.43
3:C:21:VAL:HG23	3:C:22:CYS:N	2.34	0.43
4:D:185:PRO:HD3	5:E:191:MET:HE2	2.00	0.43
6:F:272:THR:HG22	6:F:273:ASP:H	1.84	0.43
6:F:292:ILE:HG23	6:F:305:MET:HE2	2.01	0.43
1:A:341:GLY:O	1:A:353:GLY:N	2.52	0.42
4:D:106:GLY:O	4:D:109:ILE:HG12	2.19	0.42
2:B:100:TRP:HA	2:B:103:TRP:NE1	2.34	0.42
2:B:292:ILE:HG22	8:B:502:RBF:HC71	2.02	0.42
1:A:29:VAL:HG12	1:A:30:ALA:N	2.33	0.42
9:B:504:LMT:O2B	9:B:504:LMT:H4'	2.18	0.42
5:E:73:VAL:HG23	6:F:3:THR:HG22	2.02	0.42
1:A:406:VAL:HG21	1:A:442:ILE:HD12	2.02	0.42
2:B:353:THR:O	2:B:357:LYS:N	2.47	0.42
5:E:129:MET:C	5:E:129:MET:SD	2.98	0.42
6:F:288:MET:HG2	6:F:378:CYS:SG	2.59	0.42
3:C:118:ARG:NH1	3:C:242:MET:O	2.47	0.42
6:F:215:ALA:HA	6:F:286:ALA:O	2.19	0.42
6:F:293:PHE:CE1	6:F:326:LEU:HD11	2.55	0.42
2:B:367:MET:HE1	2:B:371:ILE:HD11	2.02	0.42
5:E:39:PHE:O	5:E:43:ILE:HG12	2.20	0.41
6:F:77:GLY:N	11:F:1502:FES:S1	2.85	0.41
4:D:43:VAL:HG21	4:D:97:ILE:HG21	2.01	0.41
2:B:128:TYR:CE2	2:B:228:ALA:HB1	2.55	0.41
6:F:377:MET:SD	6:F:384:ASN:OD1	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:OD1	1:A:114:ASN:C	2.58	0.41
6:F:377:MET:HE1	6:F:403:LEU:HD13	2.02	0.41
2:B:237:ALA:CB	2:B:333:LEU:HD22	2.51	0.41
2:B:128:TYR:CZ	2:B:228:ALA:HB1	2.55	0.41
6:F:215:ALA:N	6:F:225:MET:O	2.35	0.41
6:F:377:MET:SD	6:F:378:CYS:N	2.94	0.41
1:A:291:ILE:HD12	1:A:325:VAL:HG11	2.02	0.41
3:C:23:SER:OG	6:F:8:VAL:HA	2.20	0.41
4:D:67:PRO:CG	4:D:74:VAL:HG21	2.51	0.41
5:E:81:ILE:HD11	6:F:11:PHE:CE1	2.57	0.40
2:B:188:VAL:HG11	10:D:301:3PE:H2A2	2.03	0.40
6:F:64:VAL:O	6:F:64:VAL:HG23	2.20	0.40
3:C:162:VAL:HB	3:C:194:LEU:HD21	2.03	0.40
1:A:297:ARG:NH1	2:B:41:THR:O	2.53	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%)	435 (98%)	9 (2%)	0	100	100
2	B	394/415 (95%)	392 (100%)	2 (0%)	0	100	100
3	C	246/257 (96%)	243 (99%)	3 (1%)	0	100	100
4	D	199/210 (95%)	189 (95%)	10 (5%)	0	100	100
5	E	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
6	F	405/408 (99%)	399 (98%)	6 (2%)	0	100	100
All	All	1881/1934 (97%)	1844 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/376 (100%)	373 (99%)	3 (1%)	81	93
2	B	304/320 (95%)	303 (100%)	1 (0%)	92	96
3	C	198/205 (97%)	195 (98%)	3 (2%)	65	85
4	D	168/176 (96%)	163 (97%)	5 (3%)	41	73
5	E	162/165 (98%)	160 (99%)	2 (1%)	71	88
6	F	336/337 (100%)	322 (96%)	14 (4%)	30	65
All	All	1544/1579 (98%)	1516 (98%)	28 (2%)	61	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	205	ASN
1	A	415	GLU
2	B	65	PHE
3	C	22	CYS
3	C	38	LYS
3	C	158	ASP
4	D	71	ARG
4	D	115	MET
4	D	126	GLU
4	D	170	SER
4	D	194	MET
5	E	56	ASN
5	E	190	PHE
6	F	10	MET
6	F	11	PHE
6	F	75	SER
6	F	176	HIS
6	F	195	PHE
6	F	221	PHE
6	F	245	MET
6	F	267	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	273	ASP
6	F	288	MET
6	F	289	ARG
6	F	322	ASP
6	F	335	TRP
6	F	404	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
2	B	101	HIS
3	C	68	ASN
4	D	68	ASN
6	F	175	HIS
6	F	362	ASN
6	F	400	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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
7	FMN	C	1000	3	29,32,33	1.12	2 (6%)	40,47,50	1.31	6 (15%)
10	3PE	B	505	-	32,32,50	0.62	0	35,37,55	0.63	1 (2%)
9	LMT	B	503	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)
11	FES	E	1001	5,4	0,4,4	-	-	-	-	-
9	LMT	D	302	-	36,36,36	1.17	5 (13%)	47,47,47	0.96	2 (4%)
9	LMT	B	504	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	3 (6%)
8	RBF	B	502	-	29,29,29	0.58	0	41,43,43	0.68	1 (2%)
7	FMN	B	501	2	29,32,33	1.12	2 (6%)	40,47,50	1.32	8 (20%)
10	3PE	D	301	-	43,43,50	0.54	0	46,48,55	0.66	2 (4%)
12	FAD	F	1501	-	53,58,58	0.45	0	68,89,89	0.52	2 (2%)
11	FES	F	1502	6	0,4,4	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FMN	C	1000	3	-	2/15/17/18	0/3/3/3
10	3PE	B	505	-	-	13/36/36/54	-
9	LMT	B	503	-	-	9/21/61/61	0/2/2/2
11	FES	E	1001	5,4	-	-	0/1/1/1
9	LMT	D	302	-	-	7/21/61/61	0/2/2/2
9	LMT	B	504	-	-	9/21/61/61	0/2/2/2
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
10	3PE	D	301	-	-	13/47/47/54	-
12	FAD	F	1501	-	-	5/30/50/50	0/6/6/6
11	FES	F	1502	6	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1000	FMN	C4A-N5	3.73	1.38	1.30
7	B	501	FMN	C4A-N5	3.66	1.37	1.30
9	D	302	LMT	O3'-C3'	-2.77	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	LMT	O3'-C3'	-2.72	1.36	1.43
9	B	504	LMT	O3'-C3'	-2.70	1.36	1.43
7	B	501	FMN	C10-N1	2.62	1.38	1.33
7	C	1000	FMN	C10-N1	2.56	1.38	1.33
9	B	504	LMT	O2B-C2B	-2.41	1.37	1.43
9	B	503	LMT	O2'-C2'	-2.36	1.37	1.43
9	B	503	LMT	O3B-C3B	-2.36	1.37	1.43
9	B	504	LMT	O3B-C3B	-2.35	1.37	1.43
9	D	302	LMT	O2B-C2B	-2.35	1.37	1.43
9	B	503	LMT	O2B-C2B	-2.34	1.37	1.43
9	D	302	LMT	O3B-C3B	-2.34	1.37	1.43
9	D	302	LMT	O2'-C2'	-2.32	1.37	1.43
9	B	504	LMT	O2'-C2'	-2.31	1.37	1.43
9	B	503	LMT	O4'-C4B	-2.14	1.37	1.43
9	D	302	LMT	O4'-C4B	-2.11	1.38	1.43
9	B	504	LMT	O4'-C4B	-2.10	1.38	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	FMN	C4-N3-C2	-3.19	119.74	125.64
7	C	1000	FMN	C4-N3-C2	-3.15	119.83	125.64
10	D	301	3PE	C2-O21-C21	2.86	124.84	117.79
7	C	1000	FMN	C4A-C10-N10	2.79	120.56	116.48
7	B	501	FMN	C4A-C4-N3	2.70	120.05	113.19
7	C	1000	FMN	C4A-C4-N3	2.69	120.01	113.19
9	B	504	LMT	C3'-C4'-C5'	-2.66	104.83	110.93
7	B	501	FMN	C4A-C10-N10	2.57	120.23	116.48
9	B	503	LMT	C1'-O5'-C5'	-2.56	108.66	113.69
7	B	501	FMN	O4-C4-C4A	-2.49	120.00	126.60
7	C	1000	FMN	O4-C4-C4A	-2.47	120.05	126.60
7	B	501	FMN	C10-C4A-N5	-2.46	119.64	124.86
12	F	1501	FAD	P-O3P-PA	-2.45	124.40	132.83
9	B	504	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
9	D	302	LMT	C3'-C4'-C5'	-2.44	105.34	110.93
7	B	501	FMN	C4A-C10-N1	-2.39	119.19	124.73
10	B	505	3PE	O12-P-O14	2.36	123.93	112.24
10	D	301	3PE	O12-P-O14	2.34	123.81	112.24
7	C	1000	FMN	C10-C4A-N5	-2.34	119.90	124.86
7	C	1000	FMN	C4A-C10-N1	-2.33	119.32	124.73
9	B	503	LMT	C3'-C4'-C5'	-2.30	105.66	110.93
9	D	302	LMT	C1'-O5'-C5'	-2.28	109.20	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	1501	FAD	C5A-C6A-N6A	2.28	123.81	120.35
9	B	504	LMT	O5B-C5B-C4B	2.08	113.47	109.69
7	B	501	FMN	C9A-C5A-N5	-2.06	120.19	122.43
7	B	501	FMN	C4-C4A-C10	2.04	120.22	116.79
8	B	502	RBF	C4-N3-C2	-2.03	121.90	125.64

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1000	FMN	O4'-C4'-C5'-O5'
9	B	503	LMT	C2'-C1'-O1'-C1
9	B	503	LMT	O5'-C1'-O1'-C1
9	B	504	LMT	C2'-C1'-O1'-C1
9	B	504	LMT	O5'-C1'-O1'-C1
9	D	302	LMT	O5'-C1'-O1'-C1
10	B	505	3PE	C1-O11-P-O12
10	B	505	3PE	C1-O11-P-O13
10	B	505	3PE	C1-O11-P-O14
10	B	505	3PE	C11-O13-P-O14
10	B	505	3PE	O13-C11-C12-N
10	D	301	3PE	O22-C21-O21-C2
12	F	1501	FAD	C5'-O5'-P-O1P
12	F	1501	FAD	C5'-O5'-P-O2P
12	F	1501	FAD	C5'-O5'-P-O3P
9	B	504	LMT	C2B-C1B-O1B-C4'
10	D	301	3PE	C22-C21-O21-C2
9	D	302	LMT	C4'-C5'-C6'-O6'
9	D	302	LMT	O5'-C5'-C6'-O6'
9	B	504	LMT	O5B-C5B-C6B-O6B
9	D	302	LMT	C2'-C1'-O1'-C1
10	B	505	3PE	C11-O13-P-O11
9	B	504	LMT	C5'-C4'-O1B-C1B
9	B	503	LMT	O5B-C1B-O1B-C4'
9	B	503	LMT	C6-C7-C8-C9
10	D	301	3PE	C32-C33-C34-C35
9	D	302	LMT	C2-C1-O1'-C1'
9	B	503	LMT	C5'-C4'-O1B-C1B
9	B	504	LMT	C4B-C5B-C6B-O6B
10	D	301	3PE	C28-C29-C2A-C2B
10	D	301	3PE	C22-C23-C24-C25
7	C	1000	FMN	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	D	301	3PE	C1-C2-C3-O31
12	F	1501	FAD	O4B-C4B-C5B-O5B
12	F	1501	FAD	C3B-C4B-C5B-O5B
9	B	504	LMT	C3'-C4'-O1B-C1B
9	B	503	LMT	C3-C4-C5-C6
10	B	505	3PE	O11-C1-C2-C3
9	B	503	LMT	C3'-C4'-O1B-C1B
9	B	504	LMT	C11-C10-C9-C8
9	B	504	LMT	O5B-C1B-O1B-C4'
9	B	503	LMT	C11-C10-C9-C8
10	B	505	3PE	C11-O13-P-O12
10	B	505	3PE	C12-C11-O13-P
10	B	505	3PE	O11-C1-C2-O21
9	B	503	LMT	C7-C8-C9-C10
10	D	301	3PE	O21-C2-C3-O31
10	D	301	3PE	C3-C2-O21-C21
7	B	501	FMN	C4'-C5'-O5'-P
10	D	301	3PE	C1-O11-P-O13
10	D	301	3PE	C11-O13-P-O11
9	D	302	LMT	C6-C7-C8-C9
9	D	302	LMT	C5'-C4'-O1B-C1B
10	B	505	3PE	C1-C2-O21-C21
10	D	301	3PE	C39-C3A-C3B-C3C
10	D	301	3PE	C1-O11-P-O14
10	B	505	3PE	C24-C25-C26-C27
10	B	505	3PE	C3-C2-O21-C21
10	D	301	3PE	C29-C2A-C2B-C2C

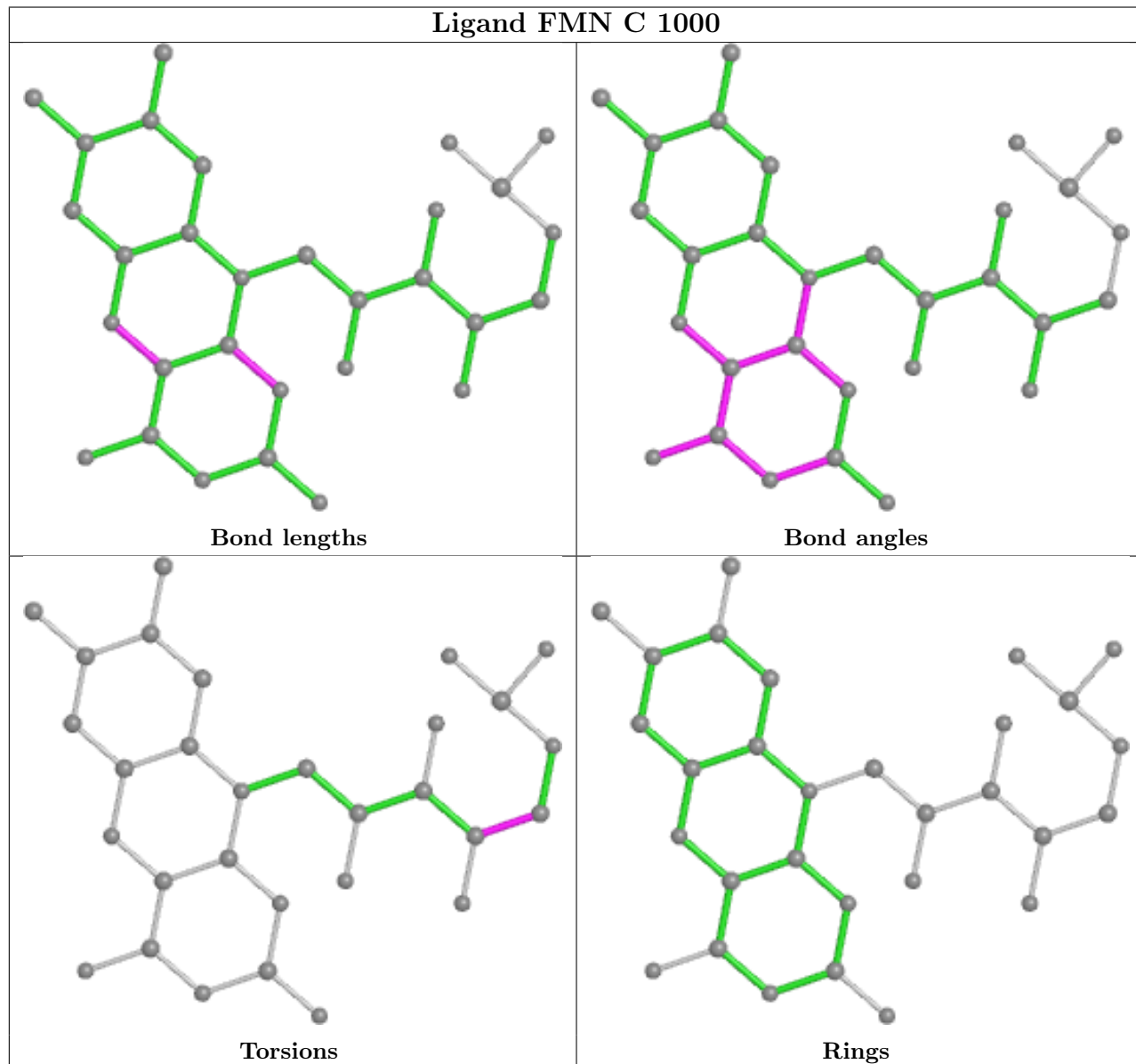
There are no ring outliers.

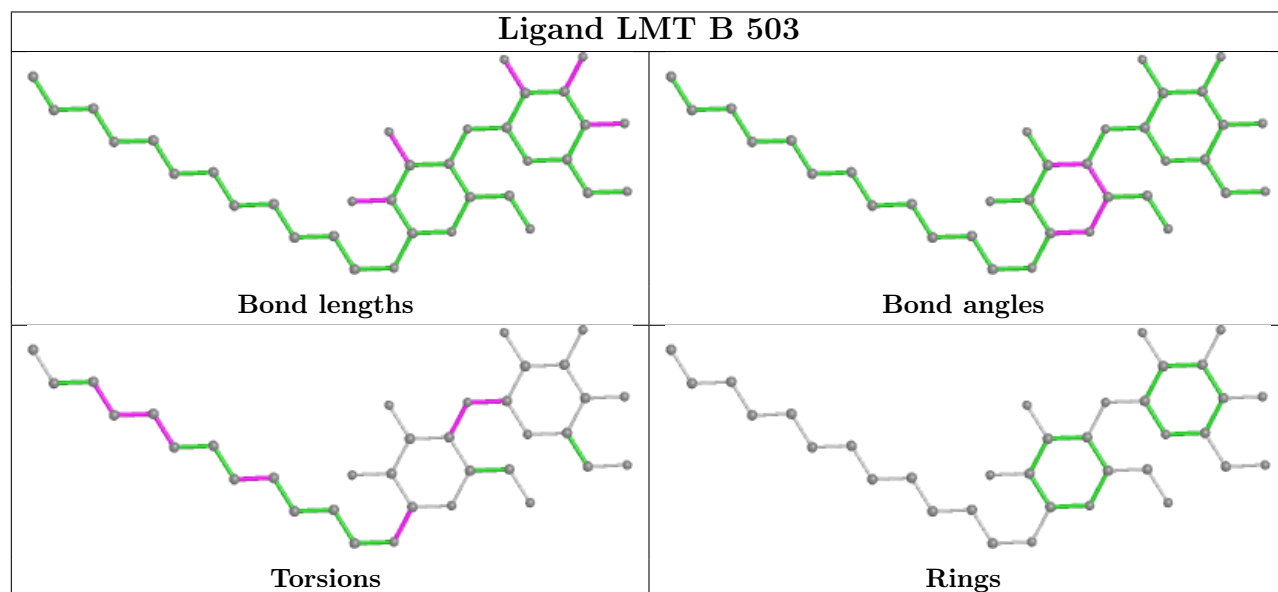
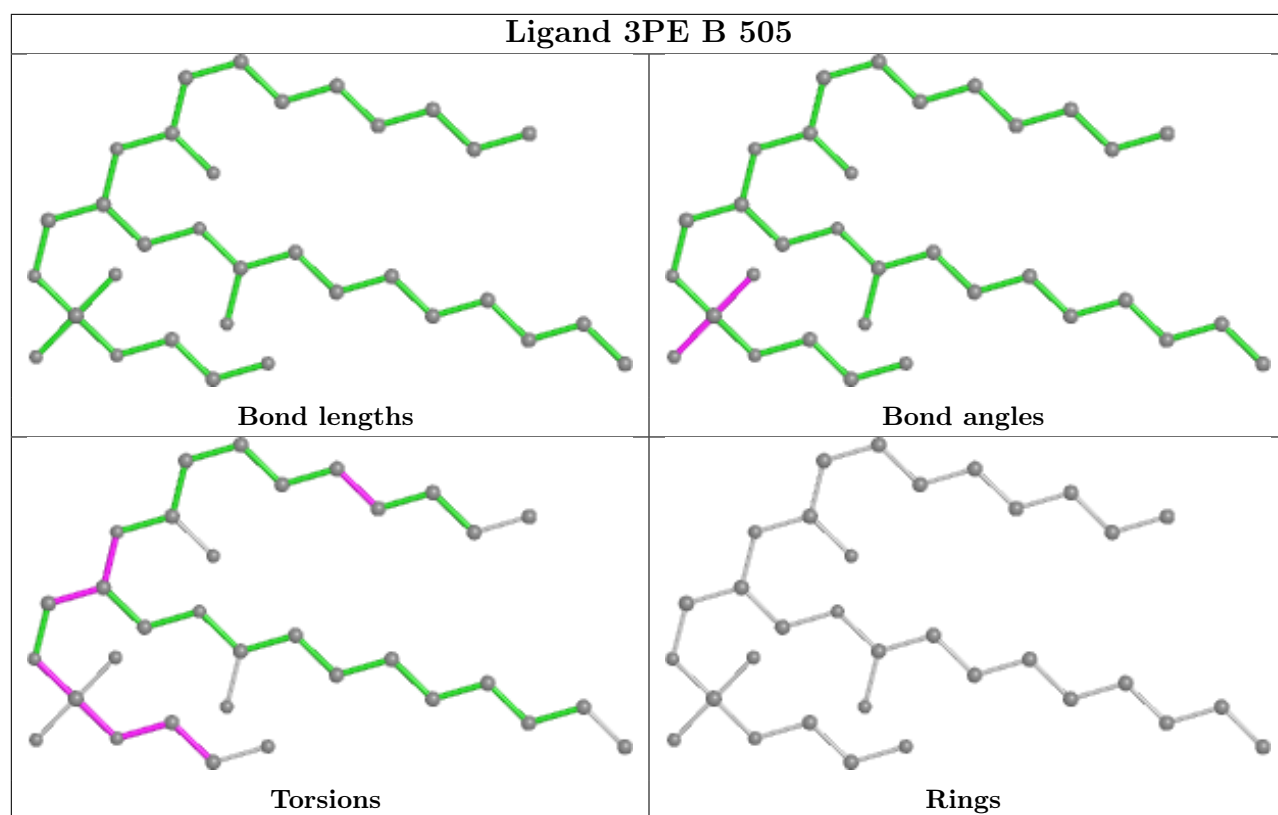
7 monomers are involved in 10 short contacts:

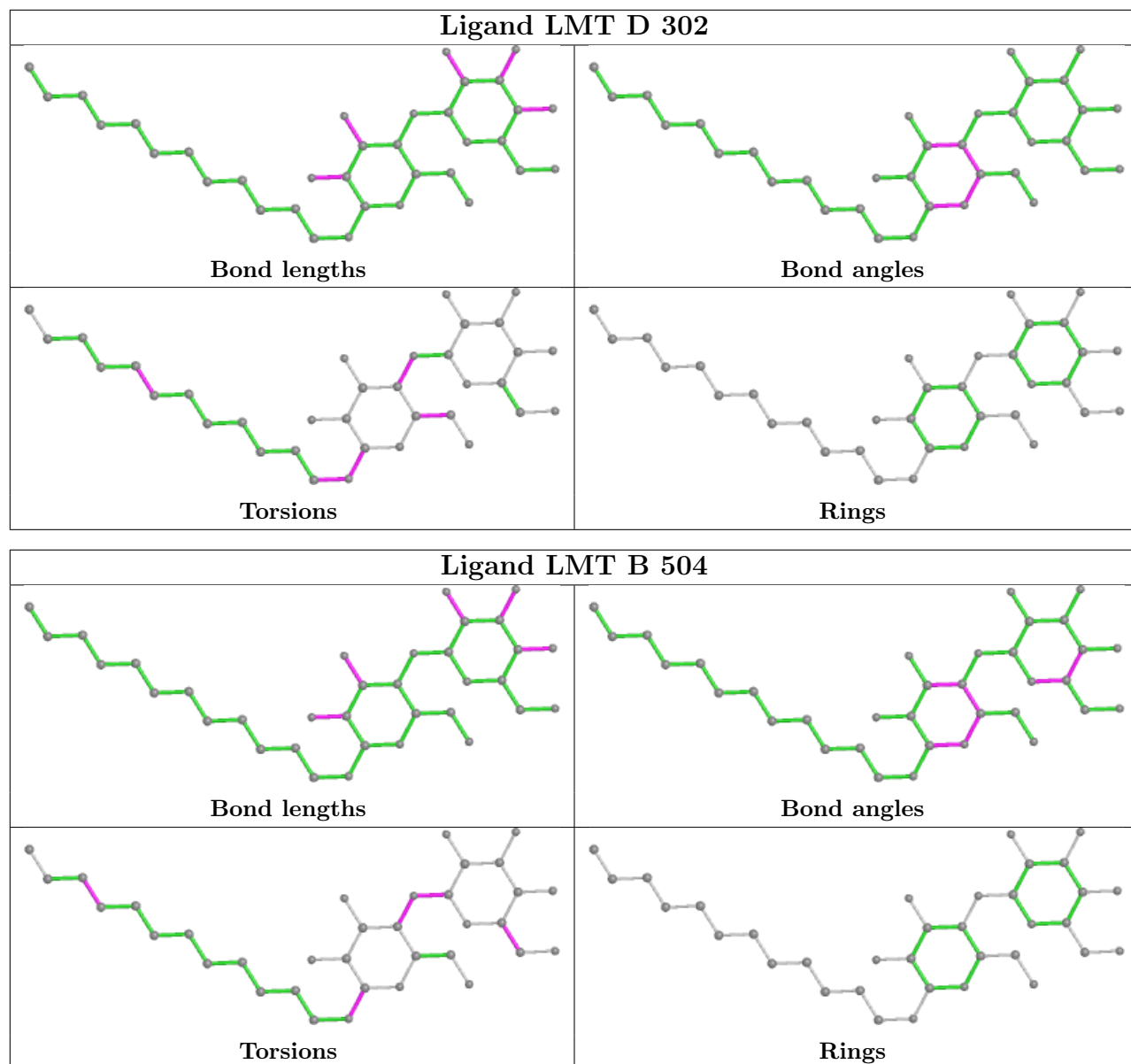
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1000	FMN	1	0
9	D	302	LMT	1	0
9	B	504	LMT	2	0
8	B	502	RBF	1	0
7	B	501	FMN	2	0
10	D	301	3PE	2	0
11	F	1502	FES	1	0

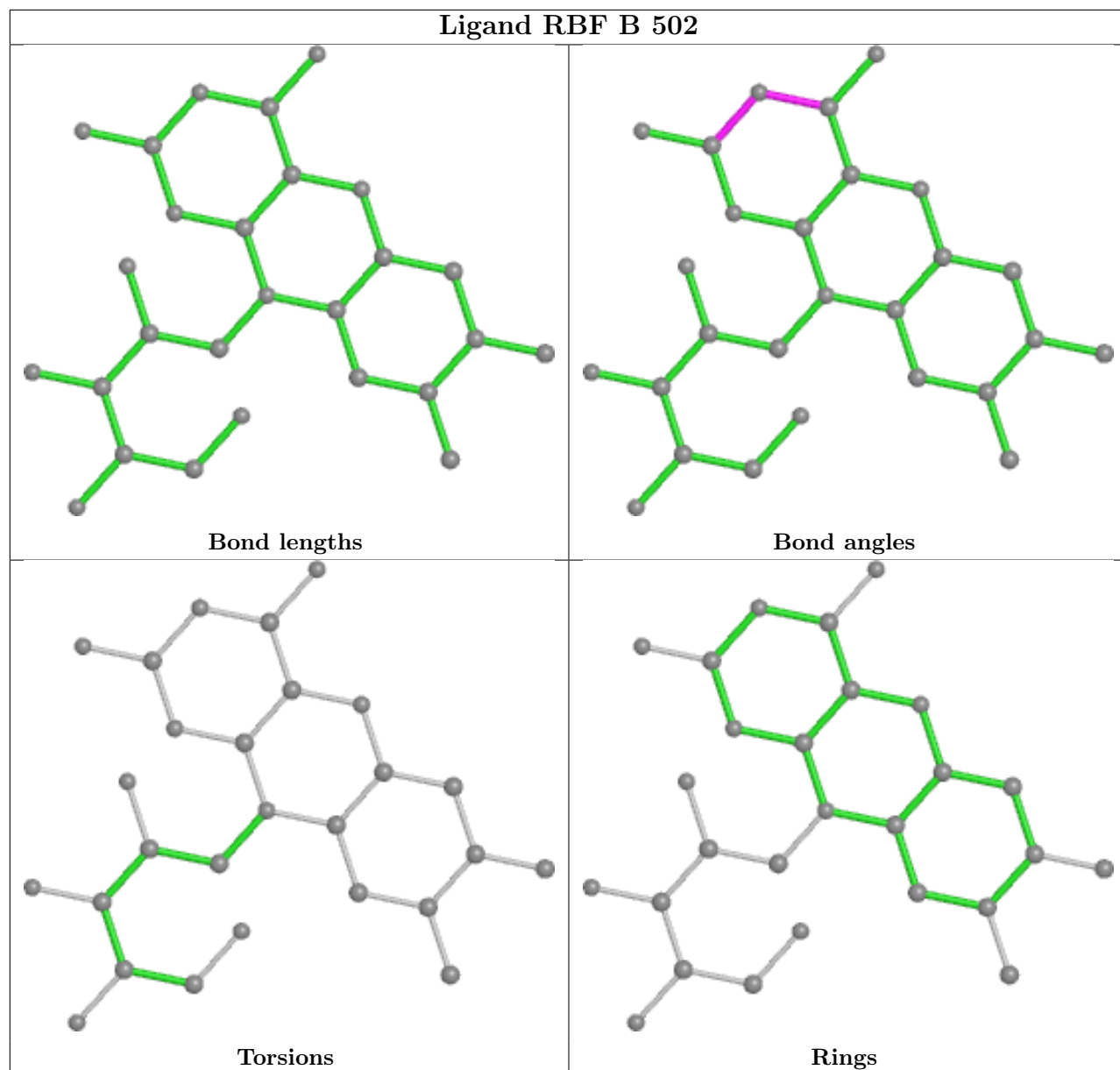
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

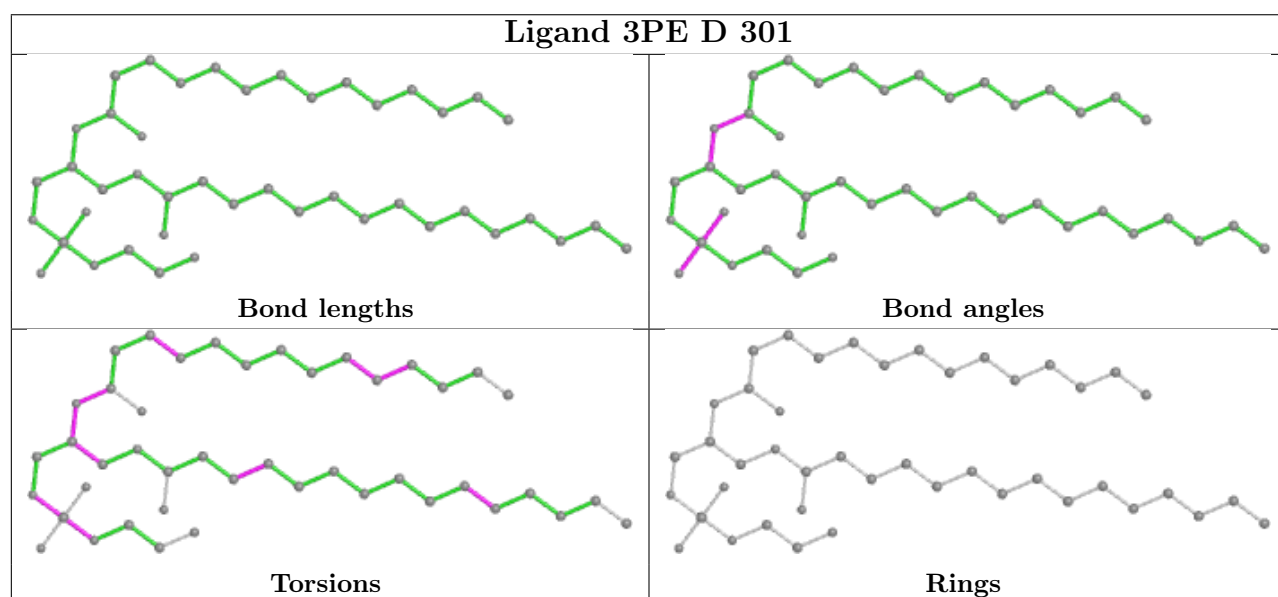
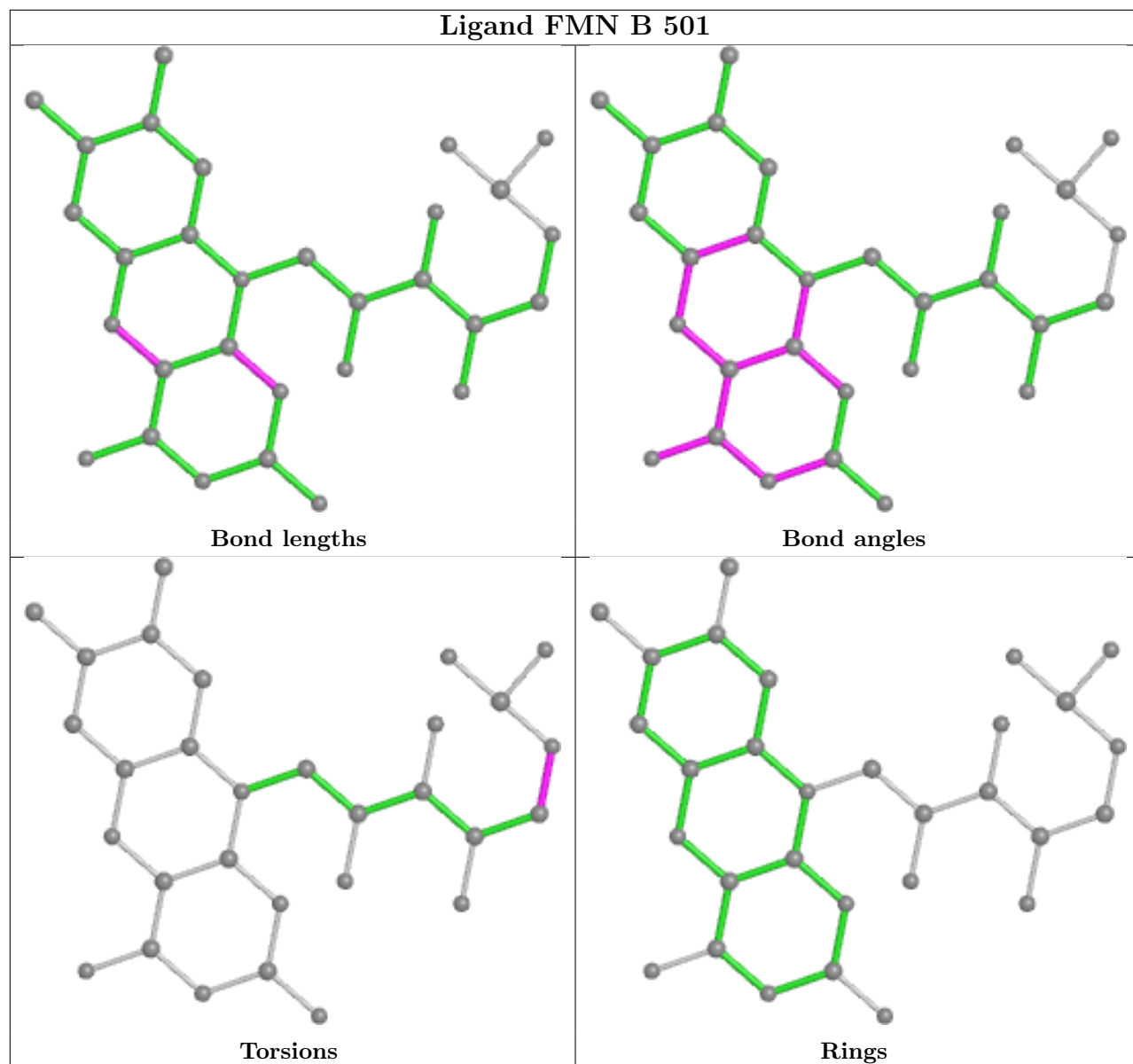
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

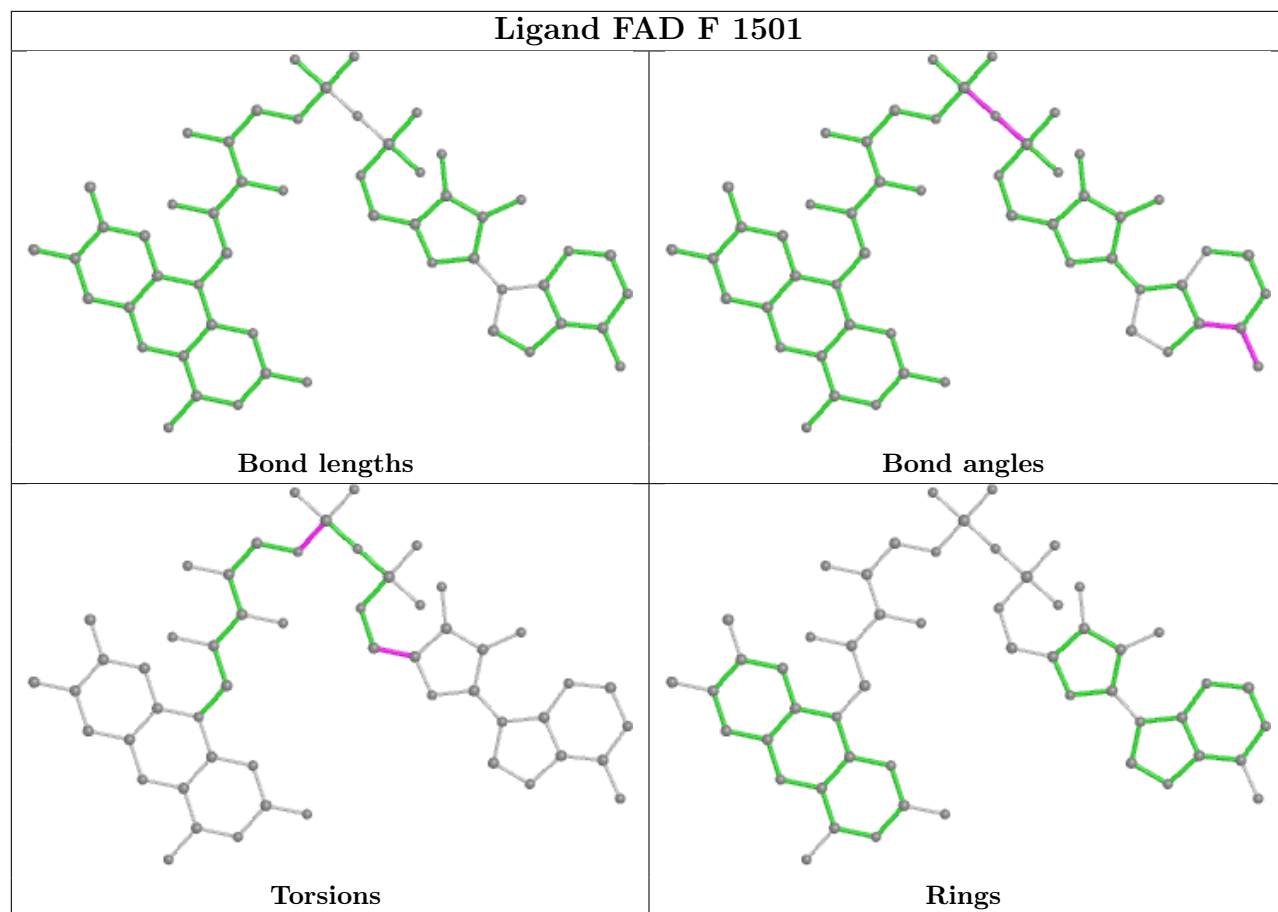












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

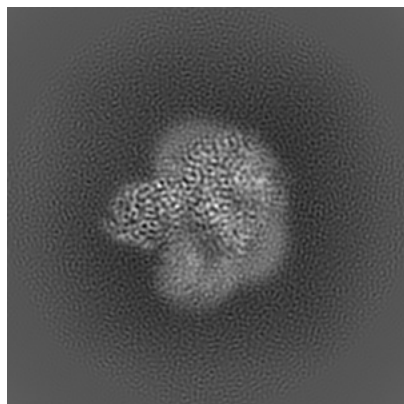
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15092. These allow visual inspection of the internal detail of the map and identification of artifacts.

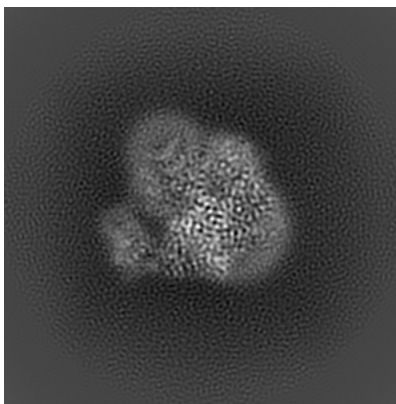
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

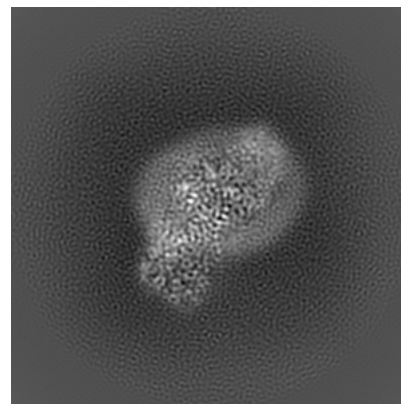
6.1.1 Primary map



X

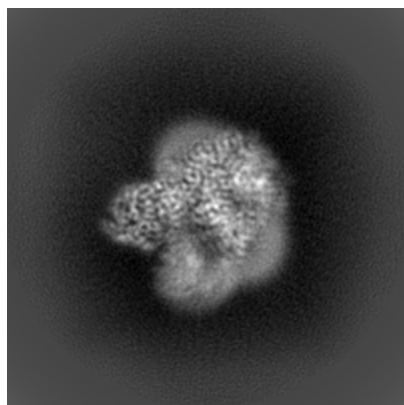


Y

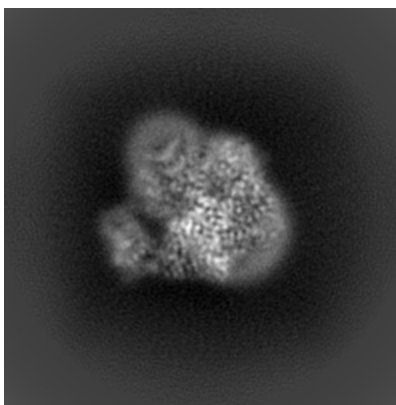


Z

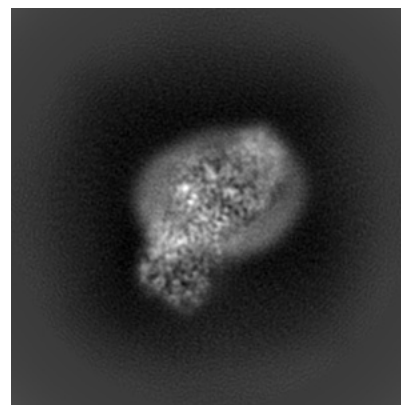
6.1.2 Raw map



X



Y

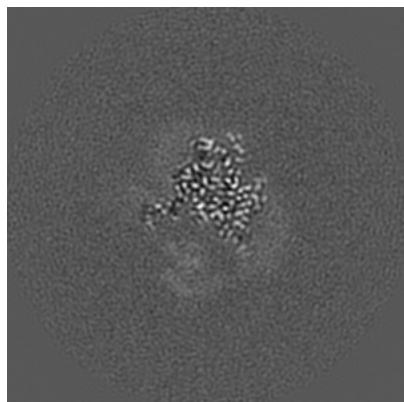


Z

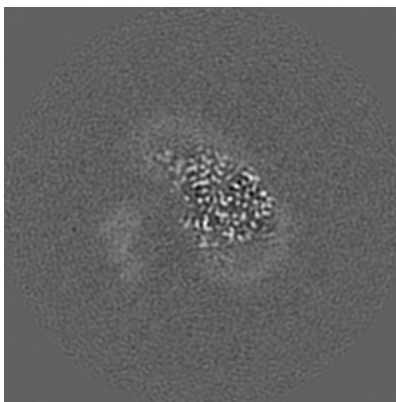
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

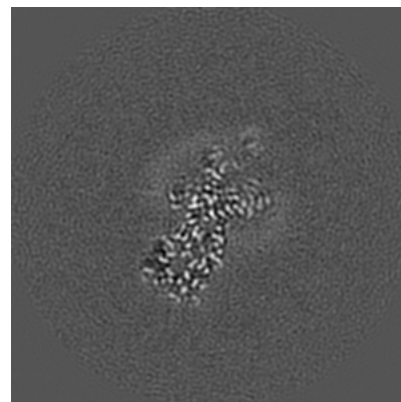
6.2.1 Primary map



X Index: 100

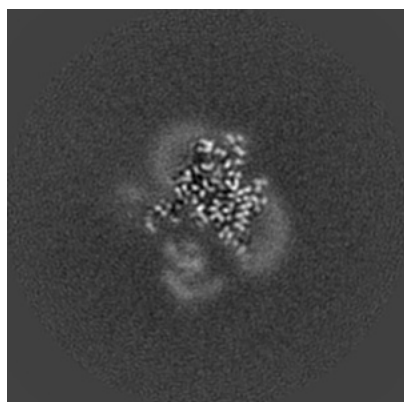


Y Index: 100

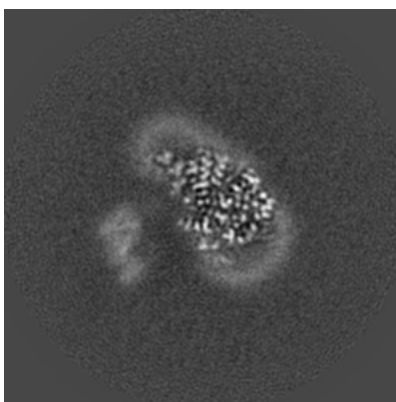


Z Index: 100

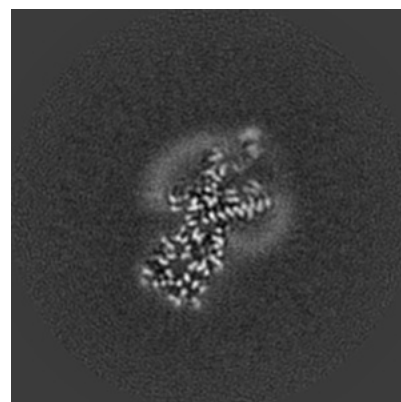
6.2.2 Raw map



X Index: 100



Y Index: 100

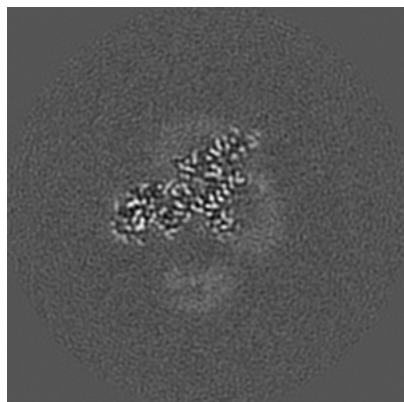


Z Index: 100

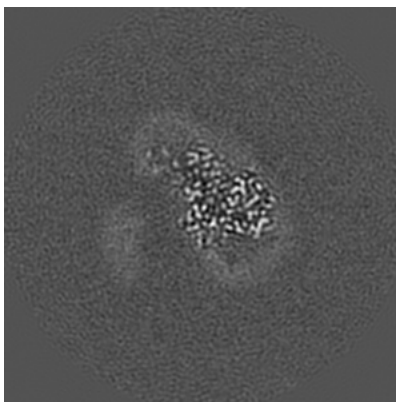
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

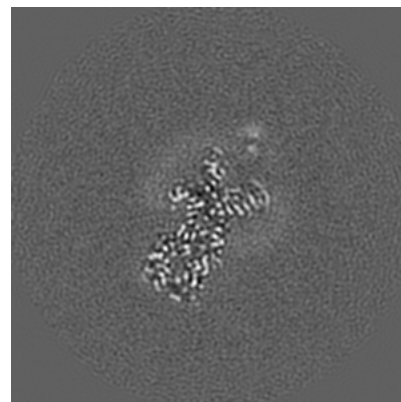
6.3.1 Primary map



X Index: 91

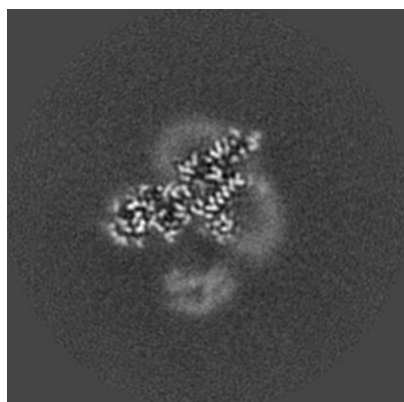


Y Index: 102

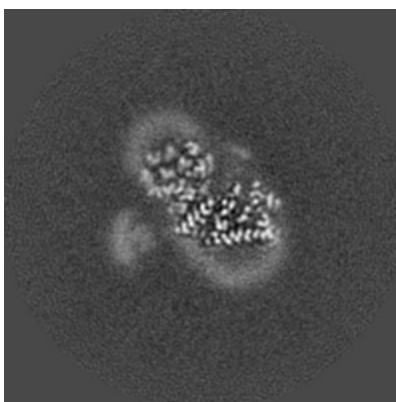


Z Index: 101

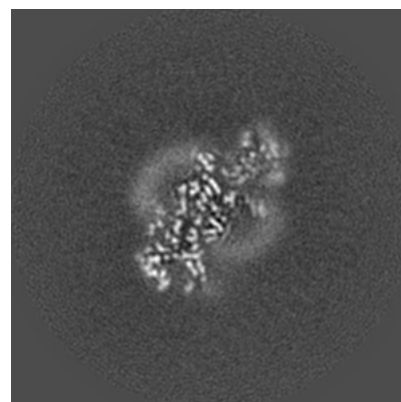
6.3.2 Raw map



X Index: 91



Y Index: 109

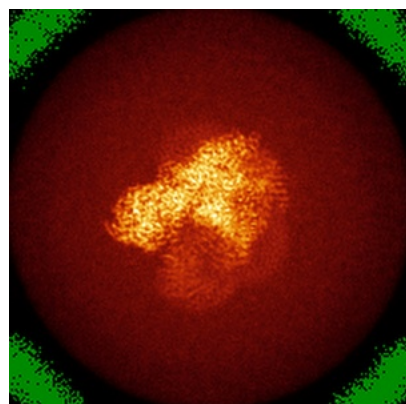


Z Index: 110

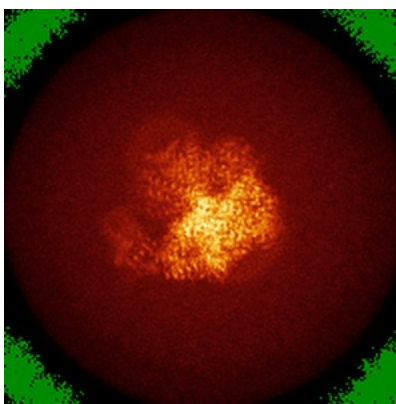
The images above show the largest variance slices of the map in three orthogonal directions.

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

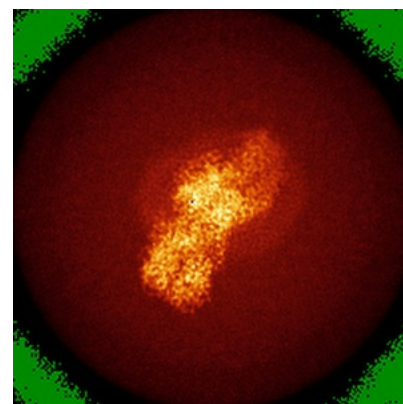
6.4.1 Primary map



X

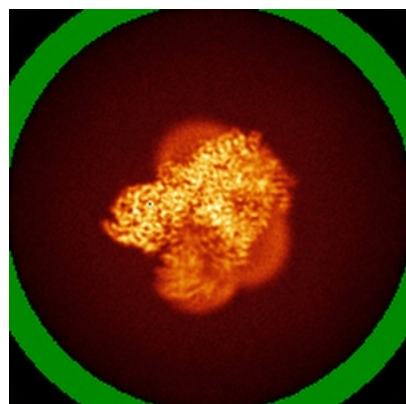


Y

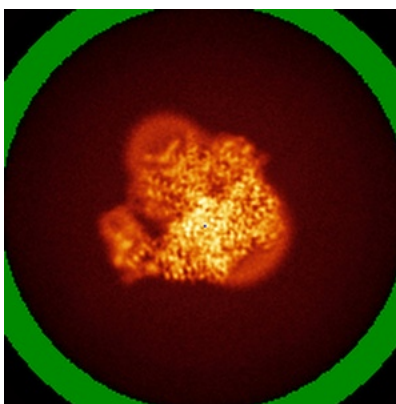


Z

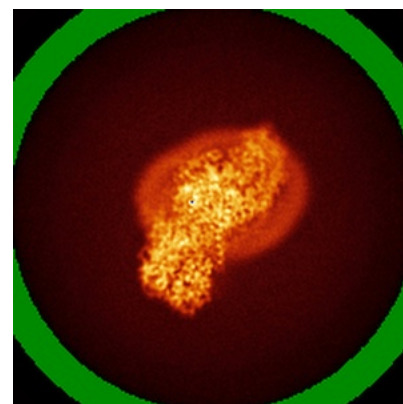
6.4.2 Raw map



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.

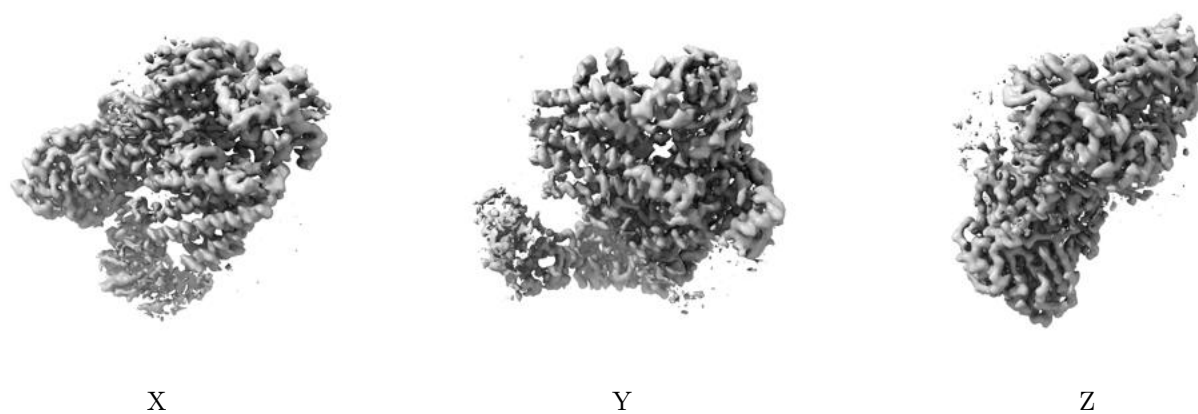
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0325. 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.

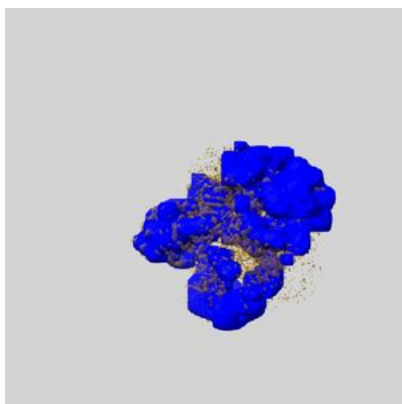
6.6 Mask visualisation [i](#)

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

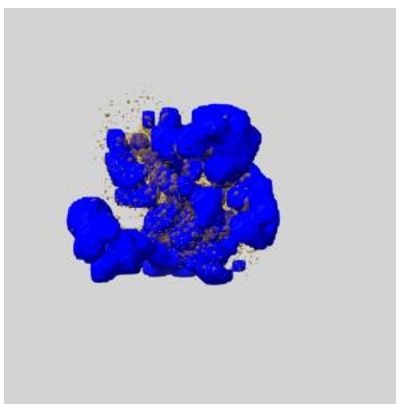
A mask typically either:

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

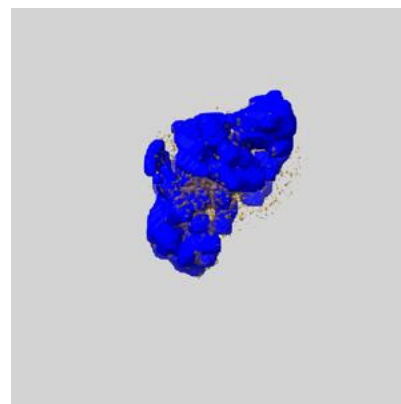
6.6.1 emd_15092_msk_1.map [i](#)



X



Y

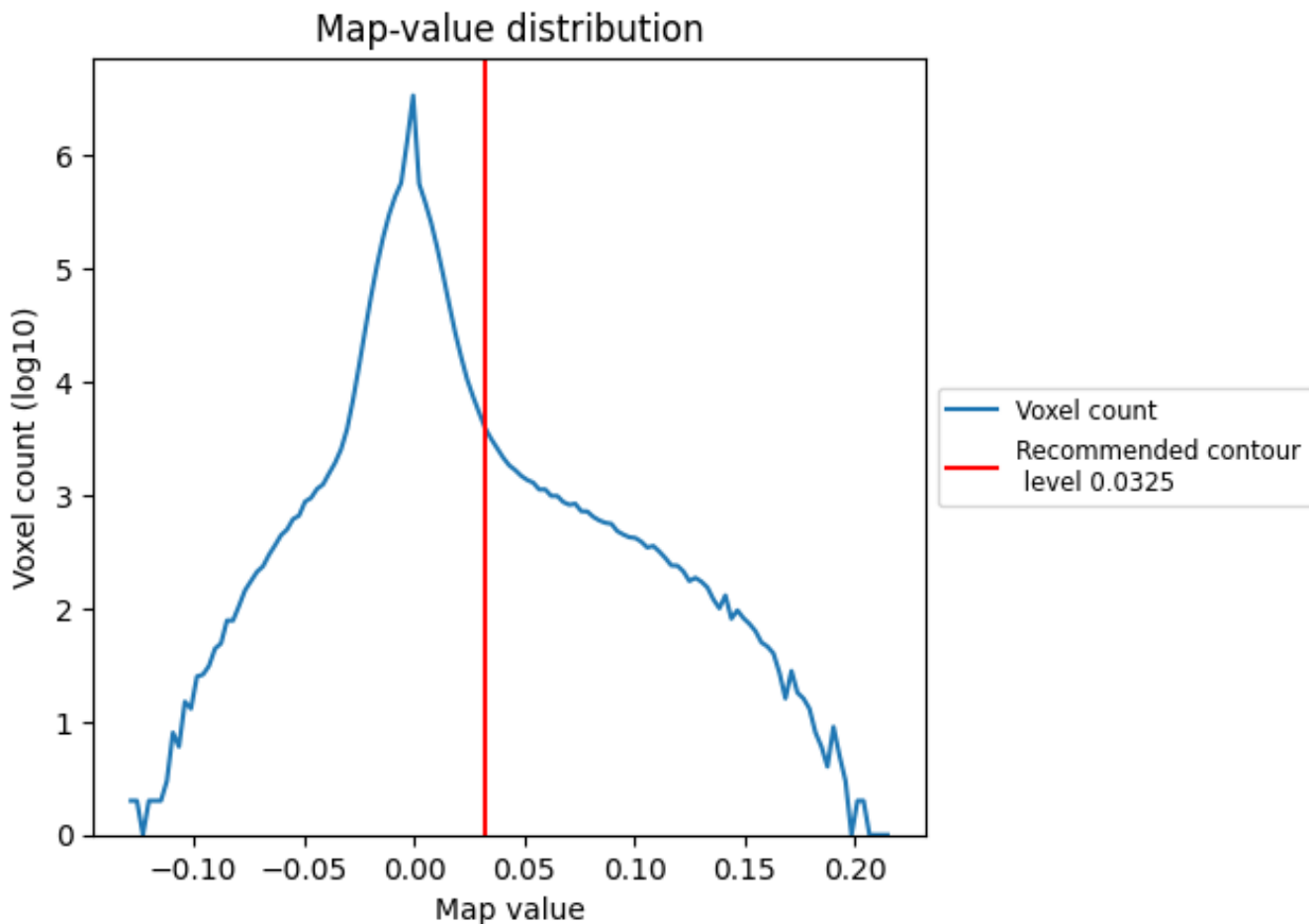


Z

7 Map analysis [i](#)

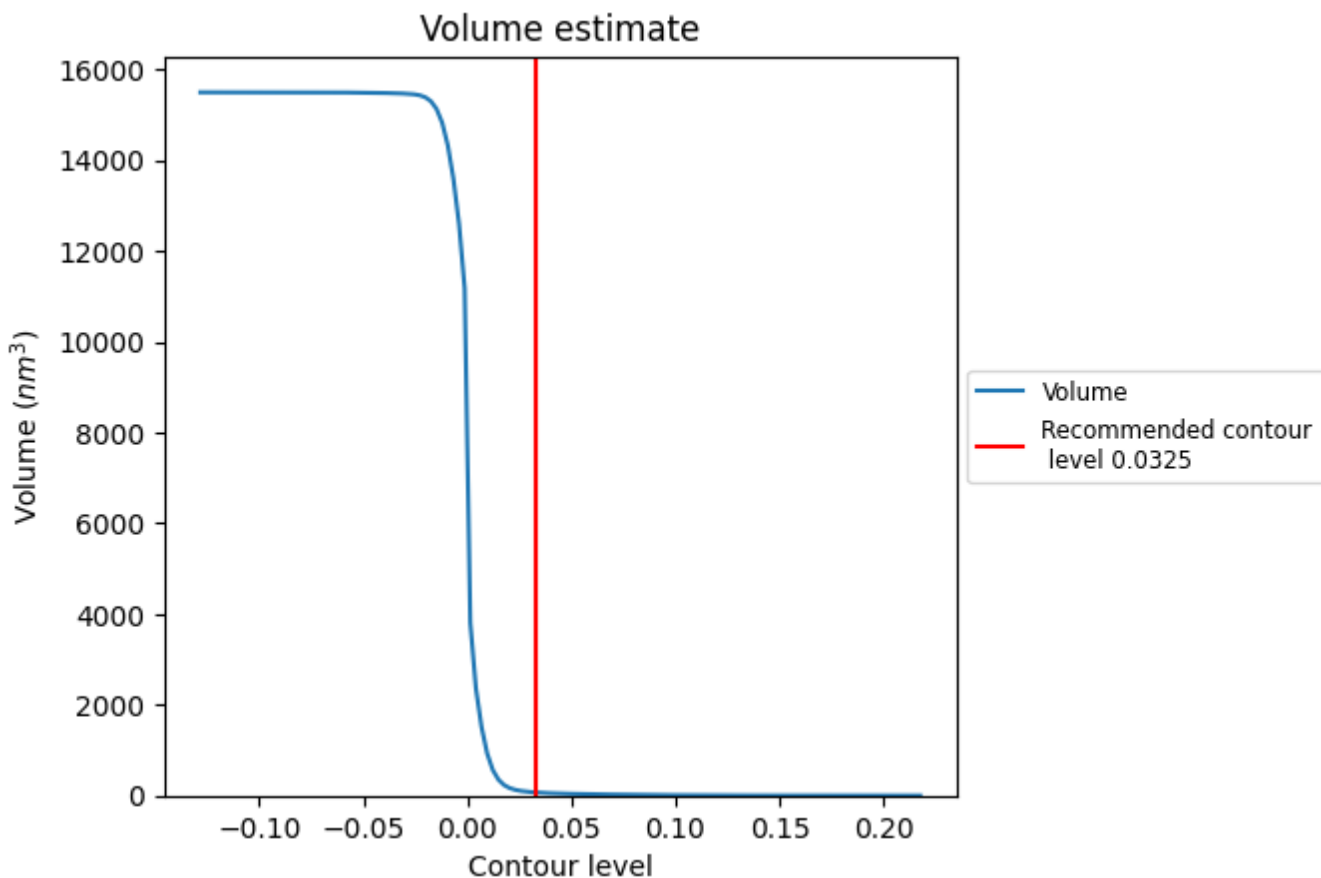
This section contains the results of statistical analysis of the map.

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.

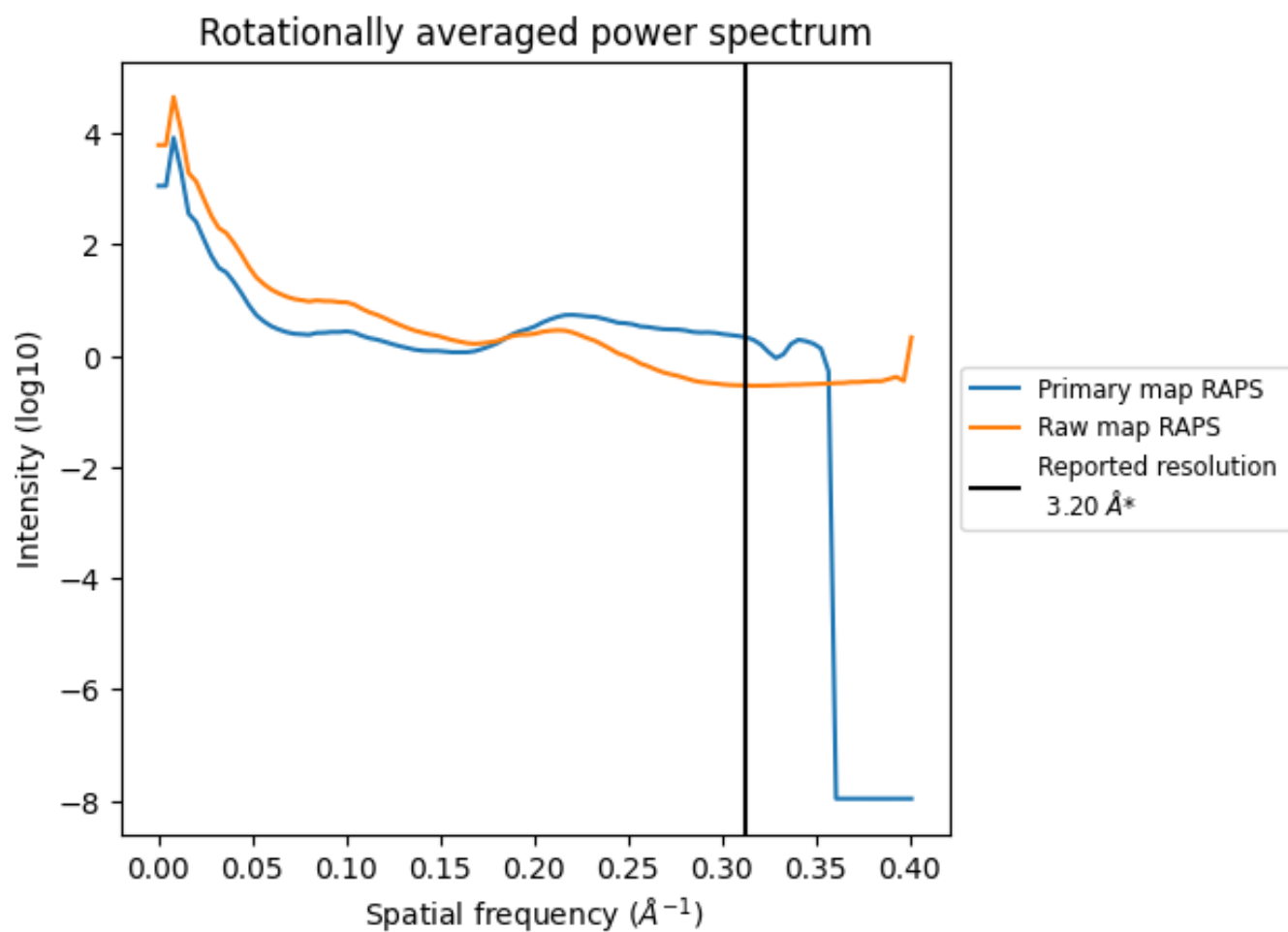
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 63 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

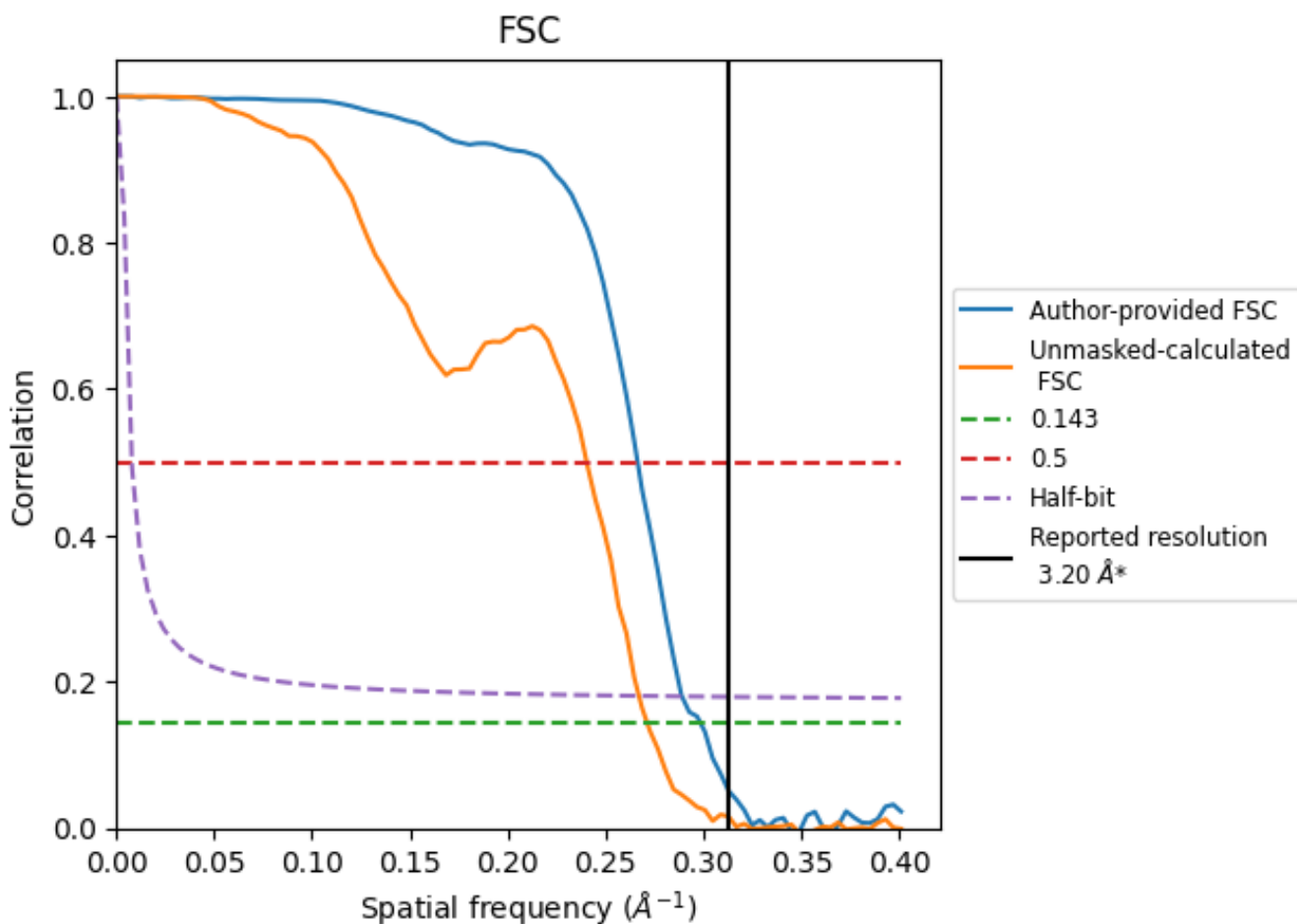


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

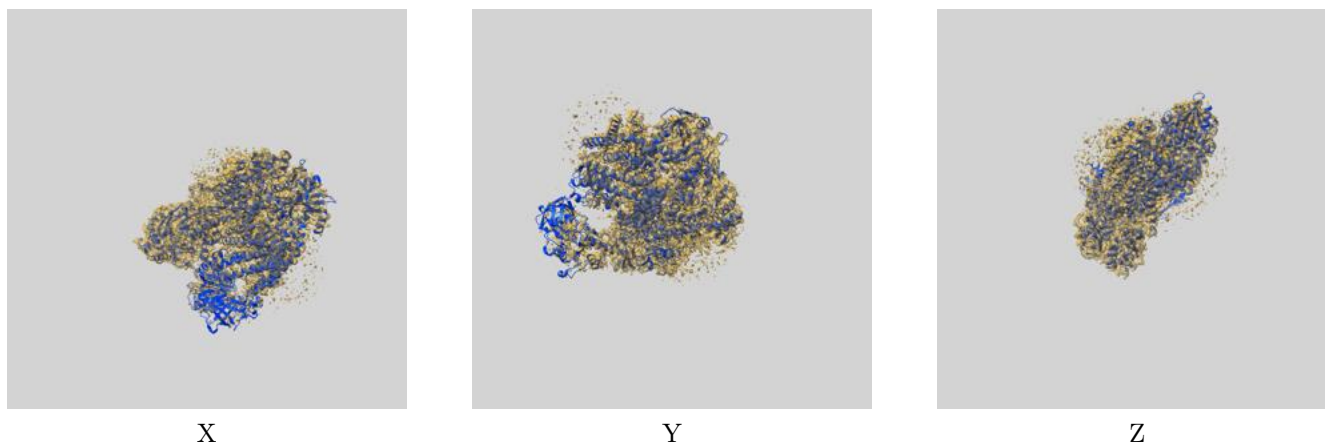
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.35	3.75	3.46
Unmasked-calculated*	3.68	4.16	3.74

*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 3.68 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

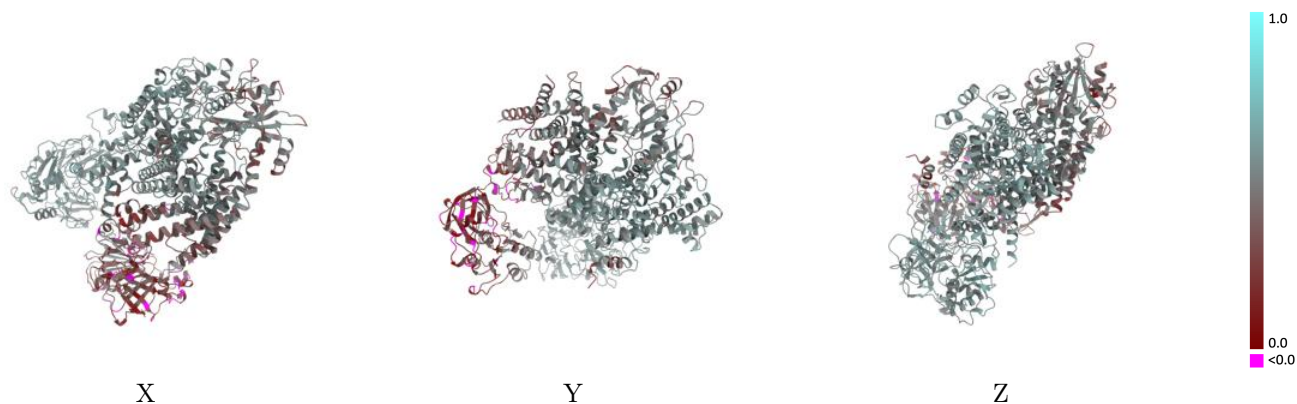
This section contains information regarding the fit between EMDB map EMD-15092 and PDB model 8A1X. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0325 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](#)



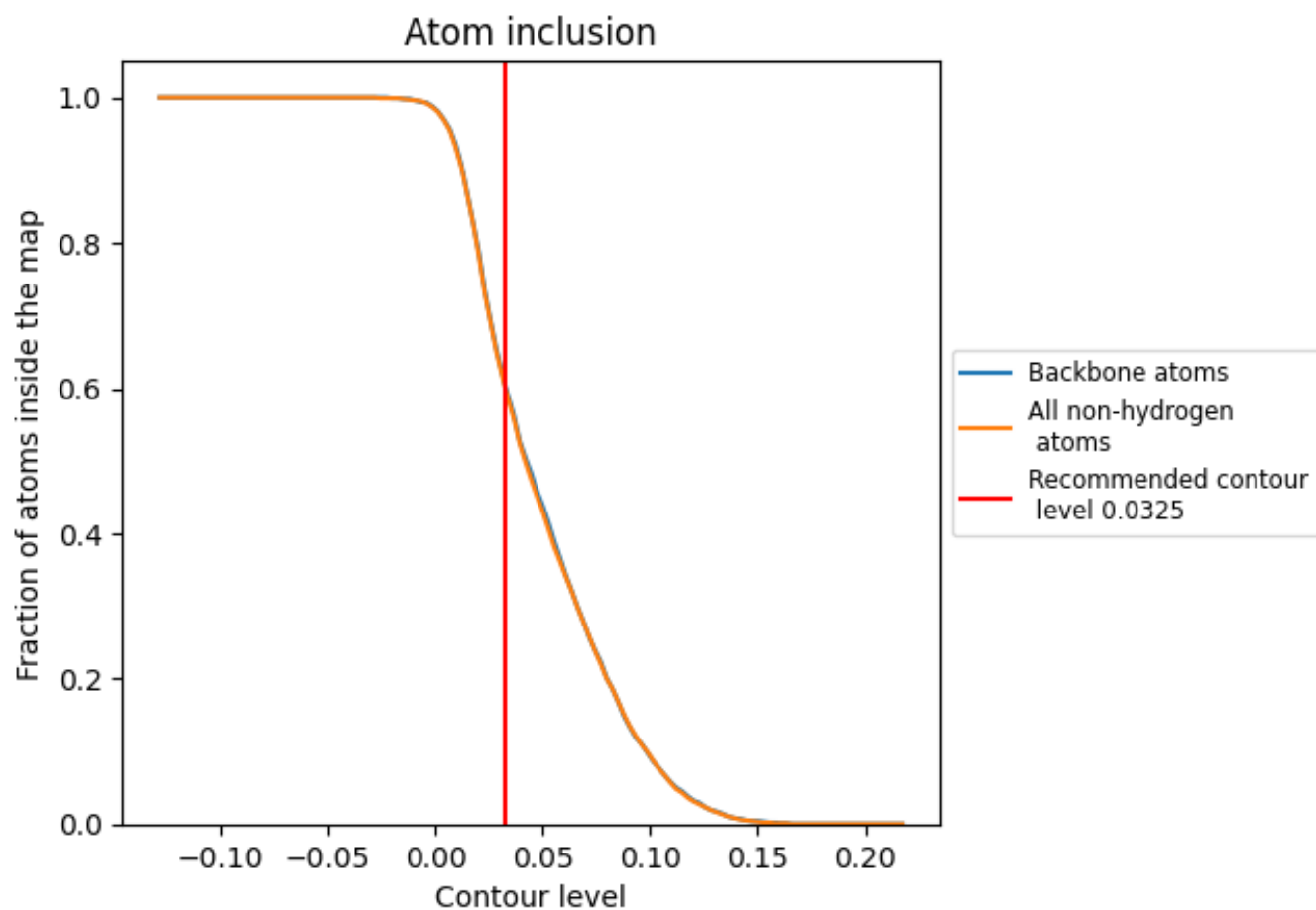
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0325).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6010	0.4670
A	0.7860	0.5540
B	0.7870	0.5430
C	0.5270	0.4570
D	0.6910	0.5060
E	0.6630	0.4810
F	0.1850	0.2810

