



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:07 AM UTC

PDB ID : 7XK6 / pdb_00007xk6
EMDB ID : EMD-33245
Title : Cryo-EM structure of Na⁺-pumping NADH-ubiquinone oxidoreductase from *Vibrio cholerae*, with aurachin D-42
Authors : Kishikawa, J.; Ishikawa, M.; Masuya, T.; Murai, M.; Barquera, B.; Miyoshi, H.
Deposited on : 2022-04-19
Resolution : 3.00 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:

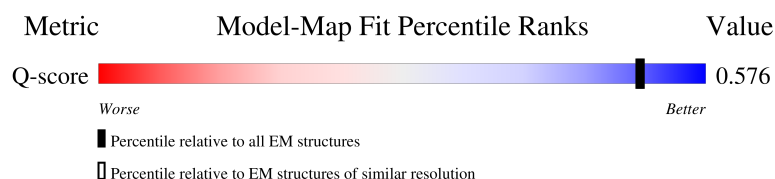
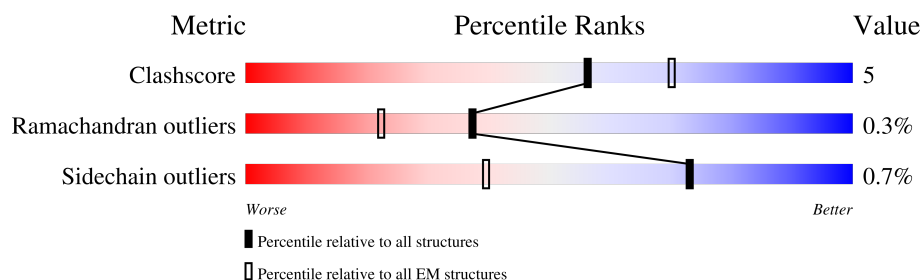
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.00 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	14081 (2.50 - 3.50)

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	 92% 8%
2	B	415	 88% 10%
3	C	257	 11% 85% 11%

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Mol	Chain	Length	Quality of chain
4	D	210	81% 15%
5	E	198	7% 85% 15%
6	F	414	17% 80% 18%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15123 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
			3173	2101	517	533	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	204	Total	C	N	O	S	0	0
			1558	1034	246	268	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
			1507	1011	230	255	11		

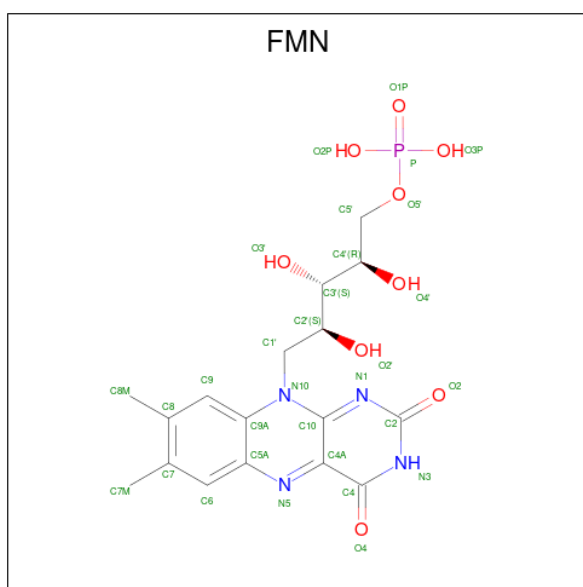
- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	408	Total	C	N	O	S	0	0
			3165	2027	519	595	24		

There are 6 discrepancies between the modelled and reference sequences:

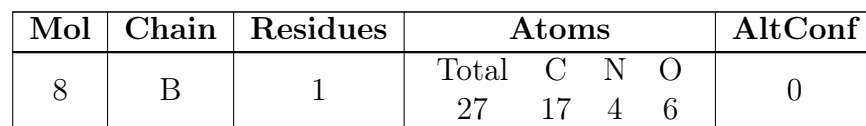
Chain	Residue	Modelled	Actual	Comment	Reference
F	409	HIS	-	expression tag	UNP A5F5Y4
F	410	HIS	-	expression tag	UNP A5F5Y4
F	411	HIS	-	expression tag	UNP A5F5Y4
F	412	HIS	-	expression tag	UNP A5F5Y4
F	413	HIS	-	expression tag	UNP A5F5Y4
F	414	HIS	-	expression tag	UNP A5F5Y4

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

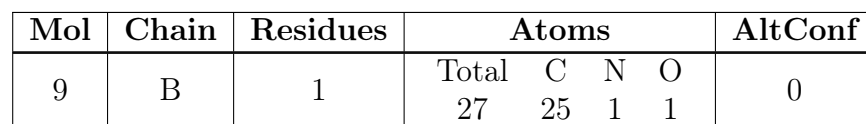


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			30	17	4	8	1	
7	C	1	Total	C	N	O	P	0
			30	17	4	8	1	

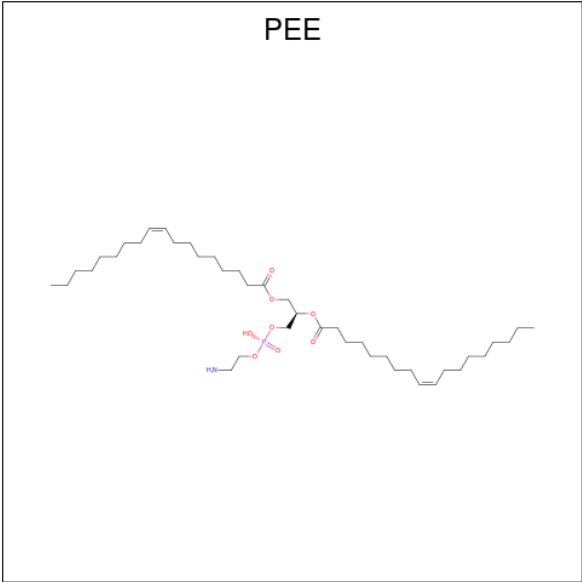
- Molecule 8 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



- Molecule 9 is Aurachin D (CCD ID: 0NI) (formula: $C_{25}H_{33}NO$) (labeled as "Ligand of Interest" by depositor).

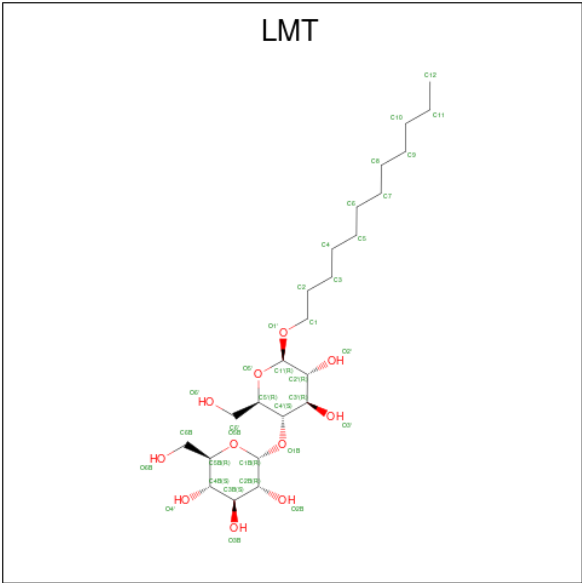


- Molecule 10 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$).



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	

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

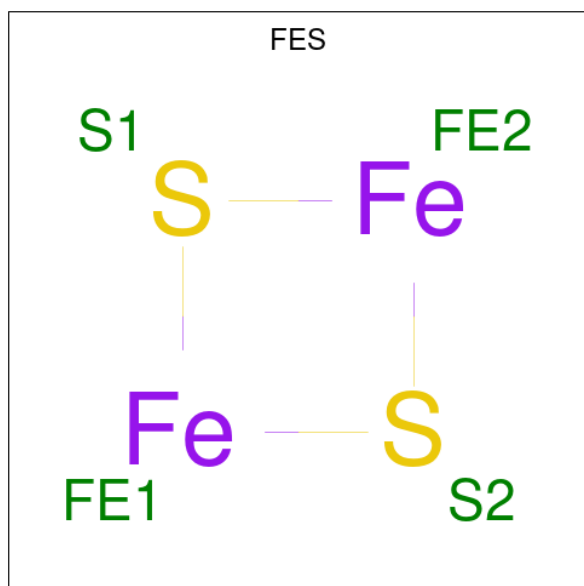


Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			35	24	11	
11	D	1	Total	C	O	0
			35	24	11	

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

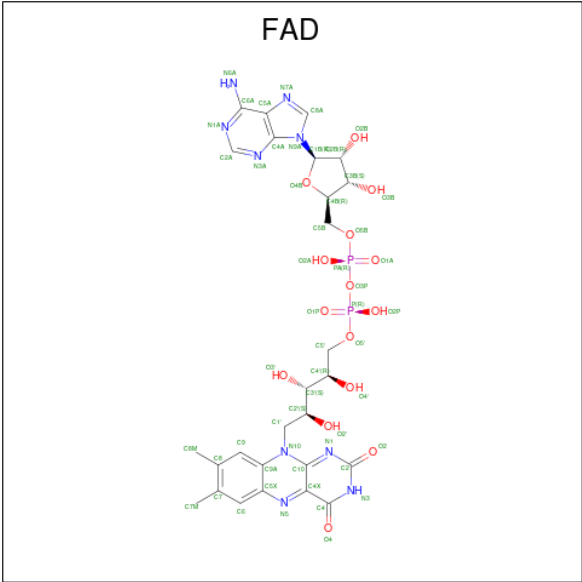
Mol	Chain	Residues	Atoms		AltConf
12	C	1	Total	Ca	0
			1	1	

- 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	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) (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	

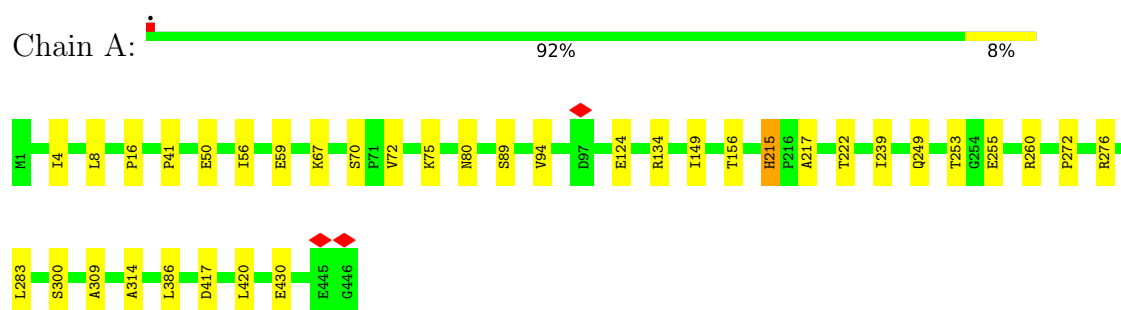
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	22	Total	O	0
			22	22	
15	B	20	Total	O	0
			20	20	
15	C	2	Total	O	0
			2	2	
15	D	2	Total	O	0
			2	2	
15	E	3	Total	O	0
			3	3	

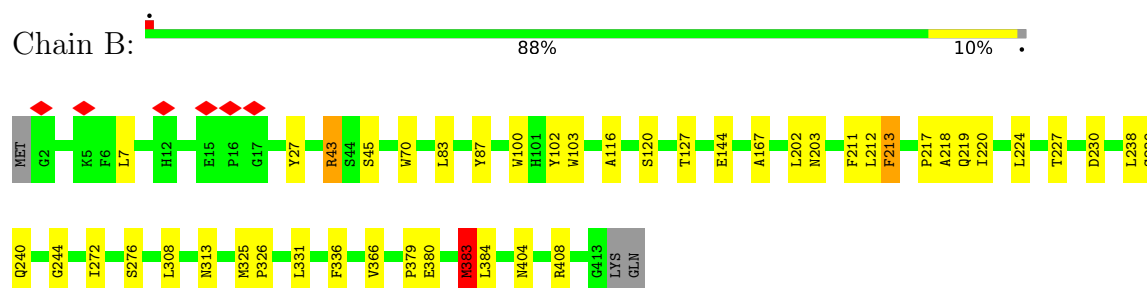
3 Residue-property plots

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.

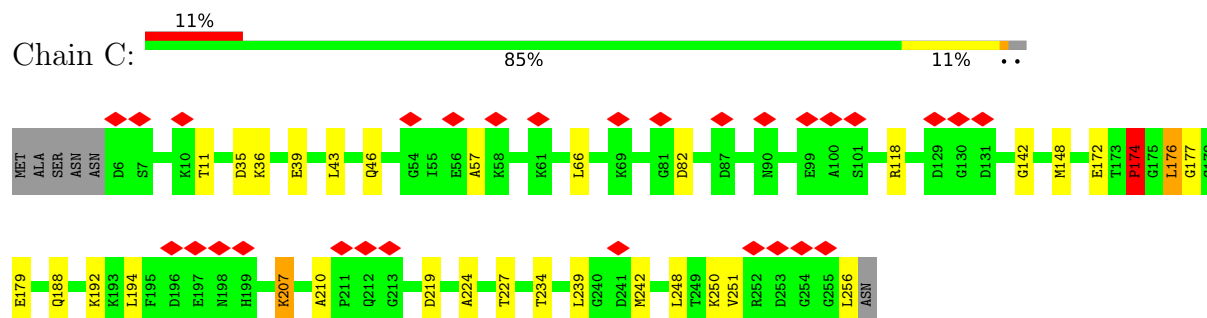
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



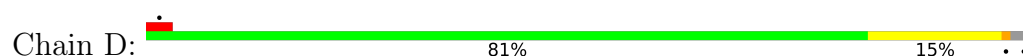
- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

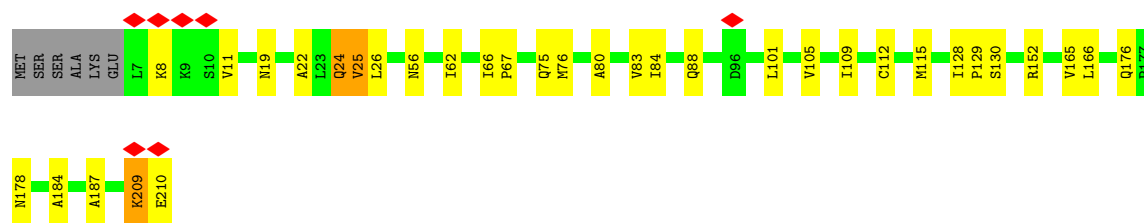


- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C

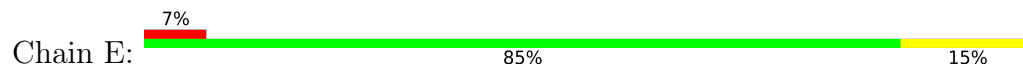


- Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

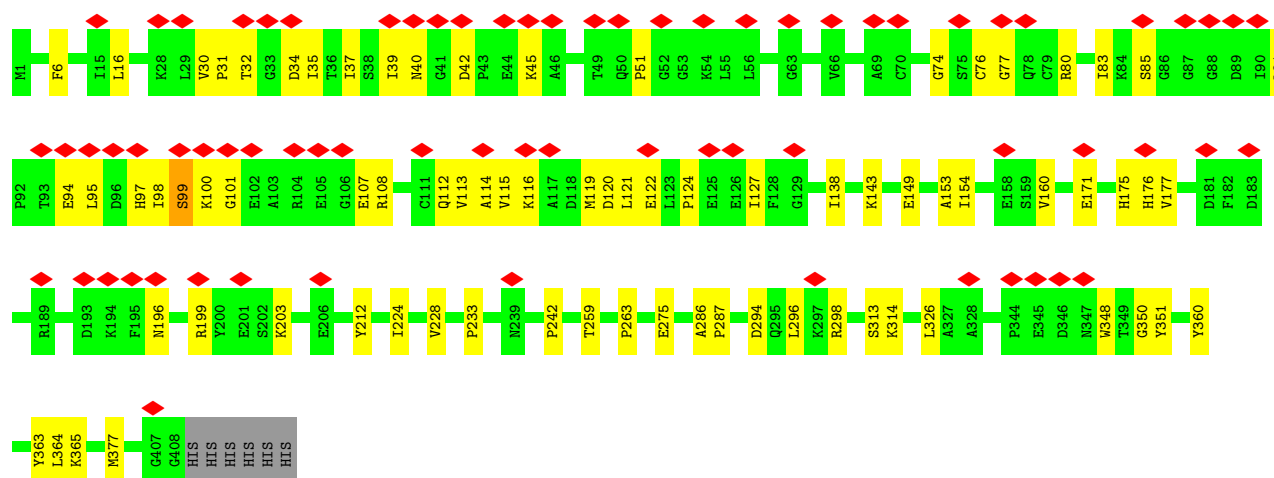
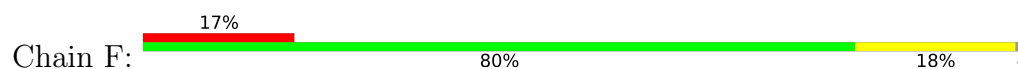




- Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



- 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	54284	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	3.716	Depositor
Minimum map value	-2.224	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.7	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FAD, RBF, CA, ONI, FMN, LMT, 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	0.19	0/3485	0.41	0/4722
2	B	0.67	5/3271 (0.2%)	0.80	7/4452 (0.2%)
3	C	0.44	1/1934 (0.1%)	0.65	5/2610 (0.2%)
4	D	0.24	0/1590	0.45	0/2160
5	E	0.17	0/1540	0.38	0/2089
6	F	0.20	0/3243	0.44	0/4389
All	All	0.39	6/15063 (0.0%)	0.56	12/20422 (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
1	A	0	1
2	B	0	1
4	D	0	1
6	F	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	239	SER	CA-CB	-6.88	1.44	1.53
2	B	217	PRO	C-O	-6.41	1.16	1.23
2	B	218	ALA	CA-CB	-5.83	1.46	1.54
3	C	224	ALA	CA-CB	-5.41	1.46	1.53
2	B	383	MET	C-O	-5.32	1.17	1.24
2	B	212	LEU	C-O	-5.30	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	PHE	CA-CB-CG	7.11	120.91	113.80
3	C	227	THR	N-CA-C	-6.79	105.15	113.50
2	B	336	PHE	N-CA-C	-6.36	105.18	113.12
3	C	174	PRO	N-CA-C	6.20	125.24	112.47
2	B	217	PRO	CB-CA-C	-6.03	103.25	110.00
3	C	172	GLU	CA-C-O	-6.02	115.02	121.94
2	B	211	PHE	O-C-N	-5.83	116.03	122.09
3	C	174	PRO	N-CA-CB	-5.65	97.32	103.25
3	C	207	LYS	CB-CA-C	-5.53	101.22	110.29
2	B	167	ALA	O-C-N	-5.34	114.63	122.43
2	B	227	THR	N-CA-CB	5.14	118.66	110.84
2	B	379	PRO	N-CA-C	5.11	120.25	113.86

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	HIS	Peptide
2	B	43	ARG	Peptide
4	D	24	GLN	Peptide
6	F	42	ASP	Peptide
6	F	99	SER	Peptide

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	3421	0	3467	24	0
2	B	3173	0	3149	21	0
3	C	1902	0	1910	17	0
4	D	1558	0	1639	24	0
5	E	1507	0	1584	22	0
6	F	3165	0	3105	46	0
7	B	30	0	19	0	0
7	C	30	0	19	1	0
8	B	27	0	20	2	0
9	B	27	0	0	1	0
10	B	102	0	164	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	35	0	44	0	0
11	D	35	0	44	1	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	22	0	0	4	0
15	B	20	0	0	0	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
All	All	15123	0	15195	148	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 (148) 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:39:ILE:HG22	6:F:121:LEU:HB2	1.65	0.77
6:F:80:ARG:NH1	6:F:107:GLU:OE1	2.21	0.73
6:F:171:GLU:HB3	6:F:259:THR:HG23	1.72	0.70
1:A:309:ALA:HB1	1:A:314:ALA:HA	1.73	0.70
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.76	0.67
1:A:222:THR:HG22	1:A:386:LEU:HD21	1.78	0.66
2:B:203:ASN:OD1	8:B:601:RBF:N3	2.29	0.65
6:F:275:GLU:OE2	6:F:363:TYR:OH	2.13	0.65
6:F:91:LEU:HD22	6:F:112:GLN:HB3	1.80	0.64
1:A:16:PRO:HA	1:A:272:PRO:HB2	1.81	0.62
6:F:74:GLY:O	6:F:97:HIS:NE2	2.32	0.62
5:E:65:LYS:HB3	5:E:68:ALA:HB2	1.81	0.62
4:D:76:MET:HE3	5:E:118:VAL:HG11	1.81	0.62
2:B:219:GLN:HE22	4:D:176:GLN:HE22	1.47	0.62
6:F:176:HIS:HD2	6:F:203:LYS:HE3	1.65	0.62
4:D:24:GLN:O	4:D:26:LEU:HG	2.00	0.62
1:A:260:ARG:NH2	15:A:502:HOH:O	2.31	0.62
4:D:26:LEU:HD22	4:D:112:CYS:HB3	1.82	0.61
6:F:296:LEU:HD12	6:F:326:LEU:HD13	1.82	0.61
2:B:313:ASN:HD21	2:B:326:PRO:HA	1.66	0.60
5:E:33:LYS:HG2	5:E:161:ARG:HH21	1.66	0.60
3:C:57:ALA:HB2	3:C:66:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ASN:HB3	4:D:22:ALA:HB3	1.86	0.57
1:A:149:ILE:CG2	15:A:521:HOH:O	2.53	0.57
6:F:45:LYS:HD2	6:F:45:LYS:H	1.69	0.56
3:C:194:LEU:HD22	3:C:239:LEU:HD11	1.86	0.56
6:F:160:VAL:HG21	6:F:224:ILE:HD11	1.87	0.56
6:F:114:ALA:HB1	6:F:116:LYS:HE2	1.87	0.56
1:A:249:GLN:O	1:A:253:THR:HG22	2.08	0.54
2:B:331:LEU:HD11	10:B:603:PEE:H24	1.89	0.54
2:B:213:PHE:HA	2:B:220:ILE:HG21	1.89	0.53
6:F:176:HIS:CD2	6:F:203:LYS:HE3	2.43	0.53
2:B:7:LEU:O	2:B:27:TYR:OH	2.26	0.52
3:C:43:LEU:HA	3:C:46:GLN:HE21	1.73	0.52
3:C:118:ARG:NH1	3:C:242:MET:O	2.36	0.52
6:F:212:TYR:HE2	6:F:228:VAL:HG13	1.75	0.52
5:E:75:LEU:HD21	6:F:6:PHE:HB3	1.91	0.52
3:C:251:VAL:HG23	3:C:256:LEU:HB2	1.92	0.52
4:D:56:ASN:HB3	4:D:130:SER:HB3	1.91	0.52
6:F:154:ILE:HD11	6:F:224:ILE:HG13	1.91	0.52
2:B:202:LEU:HD11	5:E:185:LEU:HB3	1.91	0.51
3:C:248:LEU:HA	3:C:251:VAL:HG12	1.91	0.51
4:D:25:VAL:HG21	5:E:176:LEU:HD21	1.92	0.51
3:C:82:ASP:HB3	3:C:250:LYS:NZ	2.26	0.51
4:D:184:ALA:HB1	5:E:22:PHE:HZ	1.76	0.51
3:C:35:ASP:OD1	3:C:36:LYS:N	2.45	0.50
6:F:40:ASN:H	6:F:122:GLU:HA	1.76	0.50
3:C:210:ALA:N	3:C:219:ASP:OD1	2.45	0.50
2:B:308:LEU:HD22	2:B:366:VAL:HG13	1.92	0.49
3:C:11:THR:HG23	4:D:67:PRO:HG3	1.94	0.49
6:F:175:HIS:HD2	6:F:177:VAL:HG13	1.77	0.49
1:A:430:GLU:OE2	2:B:43:ARG:NH1	2.45	0.49
6:F:76:CYS:SG	6:F:77:GLY:N	2.86	0.49
2:B:87:TYR:OH	2:B:230:ASP:O	2.21	0.49
8:B:601:RBF:HC3'	8:B:601:RBF:N1	2.28	0.49
3:C:35:ASP:O	3:C:39:GLU:HG3	2.14	0.48
5:E:64:LEU:HD13	5:E:79:ASN:HD22	1.77	0.48
2:B:100:TRP:HA	2:B:103:TRP:CD1	2.49	0.48
4:D:165:VAL:HG12	4:D:166:LEU:HD12	1.96	0.47
6:F:313:SER:OG	6:F:314:LYS:N	2.46	0.47
1:A:67:LYS:NZ	1:A:124:GLU:OE2	2.33	0.47
6:F:83:ILE:HD12	6:F:108:ARG:HD3	1.97	0.47
6:F:286:ALA:HB3	6:F:287:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:NH1	15:A:505:HOH:O	2.39	0.47
1:A:283:LEU:HD11	1:A:300:SER:HB3	1.97	0.47
5:E:161:ARG:NH1	5:E:179:THR:OG1	2.47	0.47
6:F:85:SER:HB3	6:F:120:ASP:HB2	1.96	0.47
3:C:176:LEU:HD12	3:C:176:LEU:HA	1.81	0.47
5:E:126:VAL:O	5:E:130:VAL:HG23	2.14	0.47
4:D:84:ILE:O	4:D:88:GLN:HG2	2.15	0.47
6:F:138:ILE:HD11	6:F:153:ALA:HB2	1.97	0.47
6:F:154:ILE:HD13	6:F:160:VAL:HG23	1.97	0.47
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.50	0.46
4:D:8:LYS:HA	4:D:11:VAL:HG12	1.97	0.46
5:E:29:LEU:HD22	5:E:179:THR:HG22	1.97	0.46
2:B:43:ARG:O	2:B:45:SER:N	2.46	0.45
5:E:84:ILE:HD11	5:E:118:VAL:HG13	1.97	0.45
2:B:383:MET:HE2	2:B:384:LEU:HG	1.98	0.45
2:B:127:THR:HG22	10:B:605:PEE:H57	1.98	0.45
6:F:233:PRO:HD3	6:F:242:PRO:HB3	1.99	0.45
6:F:100:LYS:HD3	6:F:100:LYS:H	1.81	0.45
1:A:134:ARG:NH2	1:A:417:ASP:OD2	2.49	0.45
6:F:360:TYR:HA	6:F:364:LEU:HB2	1.97	0.45
6:F:348:TRP:HE1	6:F:351:TYR:H	1.65	0.45
1:A:50:GLU:HA	1:A:75:LYS:HA	1.99	0.44
10:B:603:PEE:H64	10:B:603:PEE:H71	1.81	0.44
4:D:184:ALA:HB1	5:E:22:PHE:CZ	2.52	0.44
3:C:148:MET:HE2	3:C:148:MET:HB2	1.92	0.44
2:B:144:GLU:HG2	9:B:602:ONI:C13	2.48	0.44
4:D:83:VAL:HG21	4:D:109:ILE:CG1	2.47	0.44
1:A:8:LEU:HB3	1:A:420:LEU:HD21	2.00	0.44
3:C:142:GLY:HA3	3:C:234:THR:HB	1.99	0.44
3:C:82:ASP:HB3	3:C:250:LYS:HZ1	1.82	0.44
6:F:294:ASP:OD1	6:F:298:ARG:NH2	2.50	0.43
5:E:63:VAL:HG23	5:E:64:LEU:HG	2.01	0.43
7:C:301:FMN:H4'	7:C:301:FMN:H1'2	1.67	0.43
5:E:59:VAL:O	5:E:63:VAL:HG22	2.18	0.43
6:F:143:LYS:HD2	6:F:149:GLU:HB2	2.00	0.43
6:F:124:PRO:HD2	6:F:127:ILE:HD13	2.00	0.43
6:F:377:MET:HE2	6:F:377:MET:HB3	1.92	0.43
1:A:80:ASN:HD22	1:A:89:SER:HB2	1.84	0.43
4:D:128:ILE:HB	4:D:129:PRO:HD3	2.00	0.43
4:D:178:ASN:HD22	11:D:301:LMT:H82	1.83	0.43
6:F:196:ASN:O	6:F:199:ARG:NE	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:MET:HE2	4:D:115:MET:HE2	2.01	0.42
1:A:156:THR:HB	1:A:215:HIS:HB2	2.00	0.42
5:E:94:LEU:O	5:E:98:LEU:HD12	2.19	0.42
6:F:16:LEU:HD23	6:F:16:LEU:HA	1.88	0.42
6:F:115:VAL:HG12	6:F:115:VAL:O	2.19	0.42
1:A:70:SER:OG	1:A:72:VAL:O	2.37	0.42
1:A:215:HIS:ND1	1:A:215:HIS:O	2.53	0.42
6:F:37:ILE:HG12	6:F:119:MET:HB2	2.00	0.42
1:A:239:ILE:CG2	15:A:521:HOH:O	2.67	0.42
5:E:5:ILE:O	5:E:9:VAL:HG23	2.20	0.42
6:F:95:LEU:O	6:F:99:SER:OG	2.22	0.42
1:A:56:ILE:HD12	1:A:67:LYS:HG2	2.01	0.42
4:D:209:LYS:HE3	4:D:209:LYS:HB2	1.37	0.42
6:F:35:ILE:HG12	6:F:51:PRO:HG3	2.01	0.42
4:D:101:LEU:HB3	4:D:105:VAL:HG23	2.02	0.42
2:B:83:LEU:HD11	2:B:102:TYR:CZ	2.55	0.42
6:F:108:ARG:HH12	6:F:113:VAL:HG13	1.85	0.42
1:A:253:THR:HG23	1:A:255:GLU:H	1.84	0.41
6:F:365:LYS:HE2	6:F:365:LYS:HB3	1.77	0.41
1:A:4:ILE:HG13	1:A:217:ALA:HB2	2.02	0.41
4:D:80:ALA:HA	4:D:83:VAL:HG22	2.02	0.41
4:D:152:ARG:NH1	4:D:187:ALA:HB2	2.34	0.41
5:E:176:LEU:HD23	5:E:176:LEU:HA	1.89	0.41
2:B:238:LEU:HD23	2:B:325:MET:HE1	2.02	0.41
2:B:100:TRP:HA	2:B:103:TRP:NE1	2.36	0.41
6:F:348:TRP:CD1	6:F:350:GLY:H	2.38	0.41
5:E:17:MET:SD	5:E:146:SER:HB2	2.61	0.41
5:E:57:ASN:HB2	5:E:129:MET:SD	2.61	0.41
1:A:41:PRO:HA	1:A:59:GLU:O	2.21	0.41
1:A:215:HIS:O	1:A:215:HIS:CG	2.74	0.41
6:F:94:GLU:HA	6:F:98:ILE:HG22	2.02	0.41
2:B:116:ALA:HB1	2:B:120:SER:HB2	2.02	0.41
2:B:404:ASN:HD21	2:B:408:ARG:HH22	1.68	0.40
6:F:98:ILE:HD12	6:F:98:ILE:HA	1.97	0.40
6:F:100:LYS:O	6:F:101:GLY:C	2.63	0.40
4:D:75:GLN:NE2	4:D:115:MET:SD	2.94	0.40
4:D:76:MET:HE2	4:D:115:MET:CE	2.52	0.40
5:E:10:LYS:HA	5:E:14:ILE:HG12	2.02	0.40
6:F:160:VAL:CG1	6:F:263:PRO:HG3	2.51	0.40
3:C:177:GLY:C	3:C:179:GLU:H	2.29	0.40
3:C:188:GLN:O	3:C:192:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:GLY:O	5:E:46:ILE:HG13	2.21	0.40
4:D:62:ILE:O	4:D:66:ILE:HG13	2.20	0.40
6:F:108:ARG:NH1	6:F:113:VAL:HG22	2.36	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	445/446 (100%)	432 (97%)	13 (3%)	0	100	100
2	B	410/415 (99%)	398 (97%)	10 (2%)	2 (0%)	24	60
3	C	249/257 (97%)	241 (97%)	7 (3%)	1 (0%)	30	65
4	D	202/210 (96%)	195 (96%)	6 (3%)	1 (0%)	24	60
5	E	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
6	F	406/414 (98%)	383 (94%)	21 (5%)	2 (0%)	24	60
All	All	1908/1940 (98%)	1838 (96%)	64 (3%)	6 (0%)	37	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	174	PRO
6	F	31	PRO
2	B	244	GLY
2	B	272	ILE
6	F	32	THR
4	D	25	VAL

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	315/320 (98%)	311 (99%)	4 (1%)	61	81
3	C	200/205 (98%)	197 (98%)	3 (2%)	57	80
4	D	170/176 (97%)	168 (99%)	2 (1%)	63	82
5	E	164/165 (99%)	164 (100%)	0	100	100
6	F	337/343 (98%)	335 (99%)	2 (1%)	78	88
All	All	1562/1585 (98%)	1551 (99%)	11 (1%)	73	86

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

Mol	Chain	Res	Type
2	B	224	LEU
2	B	240	GLN
2	B	380	GLU
2	B	383	MET
3	C	174	PRO
3	C	176	LEU
3	C	207	LYS
4	D	209	LYS
4	D	210	GLU
6	F	30	VAL
6	F	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	80	ASN
1	A	108	ASN
1	A	109	GLN
1	A	215	HIS
1	A	320	HIS

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Mol	Chain	Res	Type
2	B	74	ASN
2	B	78	GLN
2	B	156	ASN
2	B	178	GLN
2	B	219	GLN
2	B	240	GLN
2	B	243	GLN
2	B	251	ASN
2	B	313	ASN
2	B	354	ASN
2	B	404	ASN
3	C	37	GLN
3	C	46	GLN
3	C	160	ASN
4	D	24	GLN
4	D	75	GLN
4	D	88	GLN
4	D	205	GLN
5	E	79	ASN
6	F	78	GLN
6	F	112	GLN
6	F	176	HIS
6	F	356	HIS
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 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	$\# Z > 2$
10	PEE	B	603	-	50,50,50	1.15	6 (12%)	53,55,55	1.21	5 (9%)
7	FMN	B	600	2	29,32,33	1.12	2 (6%)	41,47,50	0.89	2 (4%)
14	FAD	F	502	-	58,58,58	0.36	0	85,89,89	0.31	0
10	PEE	B	605	-	50,50,50	1.17	6 (12%)	53,55,55	1.15	4 (7%)
7	FMN	C	301	3	29,32,33	1.15	2 (6%)	41,47,50	0.91	2 (4%)
13	FES	E	301	4	0,4,4	-	-	-	-	-
9	ONI	B	602	-	28,28,28	0.78	1 (3%)	35,37,37	0.61	1 (2%)
11	LMT	D	301	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	2 (4%)
13	FES	F	501	-	0,4,4	-	-	-	-	-
8	RBF	B	601	-	29,29,29	2.86	10 (34%)	42,43,43	1.91	10 (23%)
11	LMT	B	604	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEE	B	603	-	-	30/54/54/54	-
7	FMN	B	600	2	-	12/15/17/18	0/3/3/3
14	FAD	F	502	-	-	10/34/50/50	0/6/6/6
10	PEE	B	605	-	-	18/54/54/54	-
7	FMN	C	301	3	-	5/15/17/18	0/3/3/3
13	FES	E	301	4	-	-	0/1/1/1
9	ONI	B	602	-	-	8/17/17/17	0/2/2/2
11	LMT	D	301	-	-	11/21/61/61	0/2/2/2
13	FES	F	501	-	-	-	0/1/1/1
8	RBF	B	601	-	-	10/14/14/14	0/3/3/3
11	LMT	B	604	-	-	10/21/61/61	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	601	RBF	C4A-N5	6.69	1.45	1.30
8	B	601	RBF	C10-N1	6.53	1.46	1.33
8	B	601	RBF	C5A-N5	5.37	1.49	1.39
8	B	601	RBF	C2-N1	4.85	1.47	1.36
8	B	601	RBF	C9A-N10	4.77	1.49	1.41
8	B	601	RBF	C2-N3	4.32	1.48	1.39
10	B	605	PEE	C39-C38	3.81	1.53	1.31
10	B	603	PEE	C39-C38	3.79	1.53	1.31
10	B	605	PEE	C18-C19	3.77	1.53	1.31
10	B	603	PEE	C18-C19	3.74	1.52	1.31
8	B	601	RBF	C10-N10	3.66	1.45	1.37
8	B	601	RBF	C4-N3	3.59	1.45	1.38
8	B	601	RBF	O2-C2	-3.11	1.18	1.24
7	C	301	FMN	C2-N3	-2.95	1.32	1.39
8	B	601	RBF	O4-C4	-2.77	1.18	1.23
11	D	301	LMT	O3'-C3'	-2.68	1.36	1.43
10	B	605	PEE	O2-C2	-2.63	1.40	1.46
7	B	600	FMN	C2-N3	-2.60	1.33	1.39
11	B	604	LMT	O3'-C3'	-2.56	1.36	1.43
11	D	301	LMT	O2'-C2'	-2.50	1.36	1.43
11	B	604	LMT	O2B-C2B	-2.47	1.36	1.43
10	B	605	PEE	O3-C30	2.41	1.40	1.33
9	B	602	ONI	C1-C2	2.41	1.40	1.36
10	B	603	PEE	O3-C30	2.38	1.40	1.33
10	B	603	PEE	O2-C2	-2.33	1.41	1.46
11	B	604	LMT	O3B-C3B	-2.33	1.37	1.43
11	B	604	LMT	O2'-C2'	-2.28	1.37	1.43
11	D	301	LMT	O2B-C2B	-2.22	1.37	1.43
10	B	603	PEE	O2-C10	2.20	1.40	1.34
11	D	301	LMT	O3B-C3B	-2.19	1.37	1.43
10	B	605	PEE	O2-C10	2.19	1.40	1.34
7	B	600	FMN	O2'-C2'	-2.16	1.38	1.43
10	B	605	PEE	O3-C3	-2.15	1.40	1.45
11	B	604	LMT	O4'-C4B	-2.14	1.37	1.43
11	D	301	LMT	O1'-C1'	-2.14	1.36	1.40
10	B	603	PEE	O3-C3	-2.12	1.40	1.45
11	B	604	LMT	O1'-C1'	-2.06	1.36	1.40
7	C	301	FMN	O2-C2	-2.02	1.20	1.24
11	D	301	LMT	O4'-C4B	-2.01	1.38	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	601	RBF	C7M-C7-C6	-6.72	107.73	119.57
8	B	601	RBF	C7M-C7-C8	5.69	132.37	120.76
10	B	603	PEE	O2-C10-C11	4.18	120.53	111.48
10	B	605	PEE	O2-C10-C11	3.81	119.72	111.48
8	B	601	RBF	C4-N3-C2	-3.42	119.57	125.64
10	B	603	PEE	O3-C30-C31	2.92	120.75	111.83
11	B	604	LMT	C1'-O5'-C5'	-2.83	108.19	113.72
10	B	605	PEE	O3-C30-C31	2.72	120.11	111.83
11	B	604	LMT	C3'-C4'-C5'	-2.69	104.97	110.93
8	B	601	RBF	C4A-C4-N3	2.69	120.09	113.25
8	B	601	RBF	C4A-C10-N10	2.66	120.29	116.48
8	B	601	RBF	C5A-C9A-N10	2.63	120.34	117.97
11	D	301	LMT	C1'-O5'-C5'	-2.61	108.62	113.72
8	B	601	RBF	O4-C4-C4A	-2.41	120.16	126.53
9	B	602	ONI	C-C1-C2	-2.33	121.89	126.19
7	B	600	FMN	C4'-C3'-C2'	-2.33	109.69	113.57
8	B	601	RBF	C10-C4A-N5	-2.27	120.18	124.81
8	B	601	RBF	C9A-C5A-N5	-2.22	120.10	122.45
7	C	301	FMN	C4-N3-C2	-2.21	121.72	125.64
11	D	301	LMT	C3'-C4'-C5'	-2.16	106.15	110.93
7	B	600	FMN	C4-N3-C2	-2.13	121.86	125.64
10	B	603	PEE	C20-C19-C18	-2.11	109.04	124.83
8	B	601	RBF	C4'-C3'-C2'	-2.08	110.10	113.57
11	B	604	LMT	C3B-C4B-C5B	-2.06	106.49	110.23
10	B	605	PEE	C17-C18-C19	-2.03	109.59	124.83
7	C	301	FMN	O4'-C4'-C5'	-2.02	105.52	109.99
10	B	603	PEE	C40-C39-C38	-2.02	109.67	124.83
10	B	605	PEE	C40-C39-C38	-2.02	109.69	124.83
10	B	603	PEE	C37-C38-C39	-2.02	109.70	124.83

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	600	FMN	C1'-C2'-C3'-O3'
7	B	600	FMN	C1'-C2'-C3'-C4'
7	B	600	FMN	C2'-C3'-C4'-C5'
7	B	600	FMN	O3'-C3'-C4'-O4'
7	B	600	FMN	O3'-C3'-C4'-C5'
7	B	600	FMN	C3'-C4'-C5'-O5'
7	B	600	FMN	O4'-C4'-C5'-O5'
7	C	301	FMN	C3'-C4'-C5'-O5'
7	C	301	FMN	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	B	601	RBF	N10-C1'-C2'-C3'
8	B	601	RBF	C2'-C3'-C4'-O4'
8	B	601	RBF	O3'-C3'-C4'-O4'
8	B	601	RBF	O3'-C3'-C4'-C5'
10	B	603	PEE	C11-C10-O2-C2
10	B	603	PEE	O4-C10-O2-C2
10	B	603	PEE	C1-O3P-P-O1P
10	B	603	PEE	C1-O3P-P-O4P
10	B	603	PEE	C4-O4P-P-O3P
10	B	603	PEE	C4-O4P-P-O2P
10	B	603	PEE	C4-O4P-P-O1P
10	B	603	PEE	O5-C30-O3-C3
10	B	603	PEE	C31-C30-O3-C3
10	B	605	PEE	O2-C2-C3-O3
11	B	604	LMT	C2-C1-O1'-C1'
14	F	502	FAD	O4B-C4B-C5B-O5B
14	F	502	FAD	N10-C1'-C2'-O2'
14	F	502	FAD	N10-C1'-C2'-C3'
14	F	502	FAD	C5'-O5'-P-O1P
14	F	502	FAD	C5'-O5'-P-O2P
14	F	502	FAD	C5'-O5'-P-O3P
10	B	605	PEE	O5-C30-O3-C3
11	D	301	LMT	C4B-C5B-C6B-O6B
10	B	605	PEE	C31-C30-O3-C3
9	B	602	0NI	C15-C16-C17-C18
9	B	602	0NI	C15-C16-C17-C19
11	B	604	LMT	C4'-C5'-C6'-O6'
11	D	301	LMT	O5B-C5B-C6B-O6B
7	B	600	FMN	C2'-C3'-C4'-O4'
11	B	604	LMT	O5'-C5'-C6'-O6'
14	F	502	FAD	C3B-C4B-C5B-O5B
9	B	602	0NI	C17-C19-C20-C21
8	B	601	RBF	C2'-C3'-C4'-C5'
10	B	605	PEE	C37-C38-C39-C40
7	B	600	FMN	O2'-C2'-C3'-C4'
8	B	601	RBF	O4'-C4'-C5'-O5'
10	B	603	PEE	C10-C11-C12-C13
10	B	605	PEE	C10-C11-C12-C13
7	B	600	FMN	O2'-C2'-C3'-O3'
8	B	601	RBF	C3'-C4'-C5'-O5'
10	B	603	PEE	C37-C38-C39-C40
11	D	301	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	B	604	LMT	C1-C2-C3-C4
11	B	604	LMT	C3-C4-C5-C6
10	B	605	PEE	C34-C35-C36-C37
11	D	301	LMT	C2-C3-C4-C5
11	D	301	LMT	C5-C6-C7-C8
11	B	604	LMT	O1'-C1-C2-C3
10	B	603	PEE	C43-C44-C45-C46
10	B	605	PEE	C12-C13-C14-C15
9	B	602	0NI	C13-C12-C14-C15
11	D	301	LMT	C1-C2-C3-C4
10	B	603	PEE	C14-C15-C16-C17
11	D	301	LMT	C3-C4-C5-C6
11	B	604	LMT	C11-C10-C9-C8
10	B	603	PEE	C11-C12-C13-C14
10	B	603	PEE	C12-C13-C14-C15
10	B	603	PEE	C3-C2-O2-C10
10	B	603	PEE	C34-C35-C36-C37
10	B	605	PEE	C21-C22-C23-C24
10	B	603	PEE	O2-C2-C3-O3
10	B	605	PEE	C14-C15-C16-C17
10	B	605	PEE	C13-C14-C15-C16
11	B	604	LMT	C4-C5-C6-C7
10	B	603	PEE	C44-C45-C46-C47
10	B	605	PEE	C40-C41-C42-C43
11	D	301	LMT	C7-C8-C9-C10
9	B	602	0NI	C18-C17-C19-C20
10	B	603	PEE	C13-C14-C15-C16
9	B	602	0NI	C16-C17-C19-C20
10	B	603	PEE	C20-C21-C22-C23
10	B	603	PEE	O3P-C1-C2-O2
14	F	502	FAD	C3'-C4'-C5'-O5'
10	B	605	PEE	C19-C20-C21-C22
11	D	301	LMT	O5'-C5'-C6'-O6'
10	B	603	PEE	O3P-C1-C2-C3
7	B	600	FMN	N10-C1'-C2'-O2'
7	C	301	FMN	N10-C1'-C2'-O2'
8	B	601	RBF	N10-C1'-C2'-O2'
10	B	605	PEE	C1-C2-C3-O3
10	B	603	PEE	C1-O3P-P-O2P
9	B	602	0NI	C11-C12-C14-C15
10	B	603	PEE	C21-C22-C23-C24
11	D	301	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	B	605	PEE	C16-C17-C18-C19
10	B	605	PEE	C36-C37-C38-C39
11	B	604	LMT	O5'-C1'-O1'-C1
9	B	602	0NI	C12-C14-C15-C16
10	B	603	PEE	C19-C20-C21-C22
11	D	301	LMT	C9-C10-C11-C12
8	B	601	RBF	O2'-C2'-C3'-C4'
14	F	502	FAD	P-O3P-PA-O1A
10	B	603	PEE	C2-C1-O3P-P
7	C	301	FMN	O2'-C2'-C3'-O3'
10	B	603	PEE	C31-C32-C33-C34
7	C	301	FMN	O2'-C2'-C3'-C4'
10	B	603	PEE	C1-C2-C3-O3
11	B	604	LMT	C5'-C4'-O1B-C1B
10	B	603	PEE	C22-C23-C24-C25
10	B	605	PEE	C18-C19-C20-C21
10	B	605	PEE	O2-C10-C11-C12
8	B	601	RBF	O2'-C2'-C3'-O3'
7	B	600	FMN	N10-C1'-C2'-C3'
10	B	605	PEE	O4-C10-C11-C12
14	F	502	FAD	P-O3P-PA-O2A

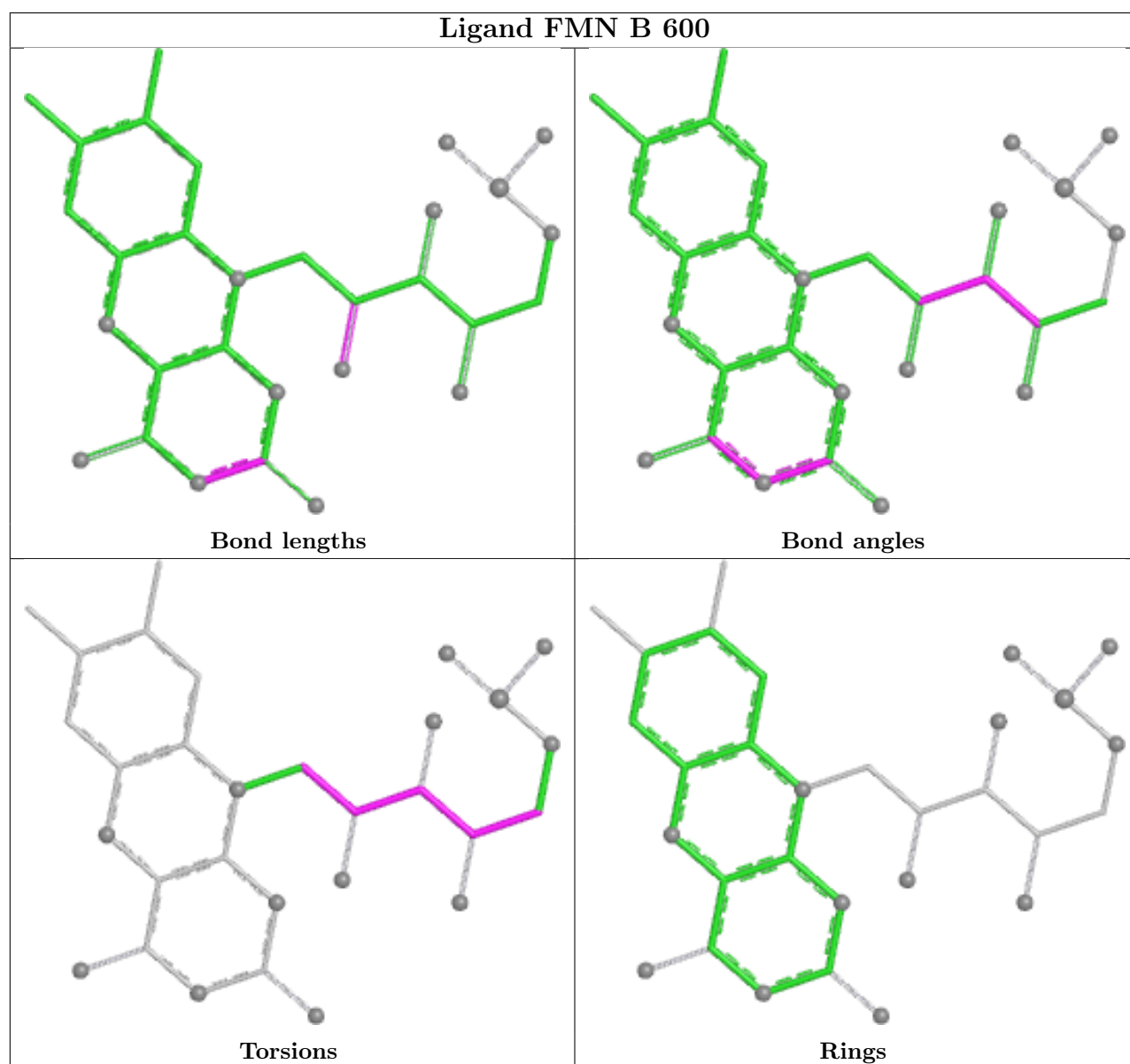
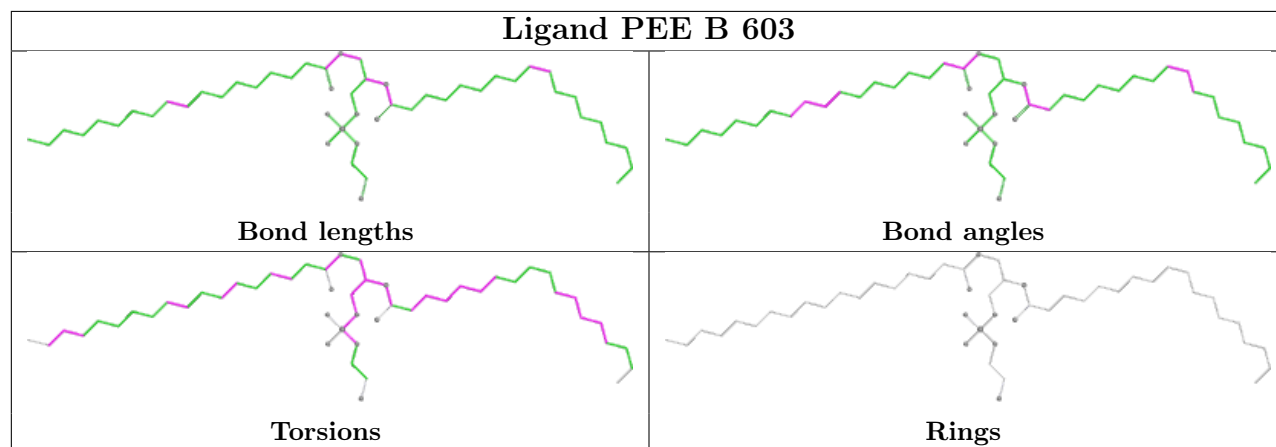
There are no ring outliers.

6 monomers are involved in 8 short contacts:

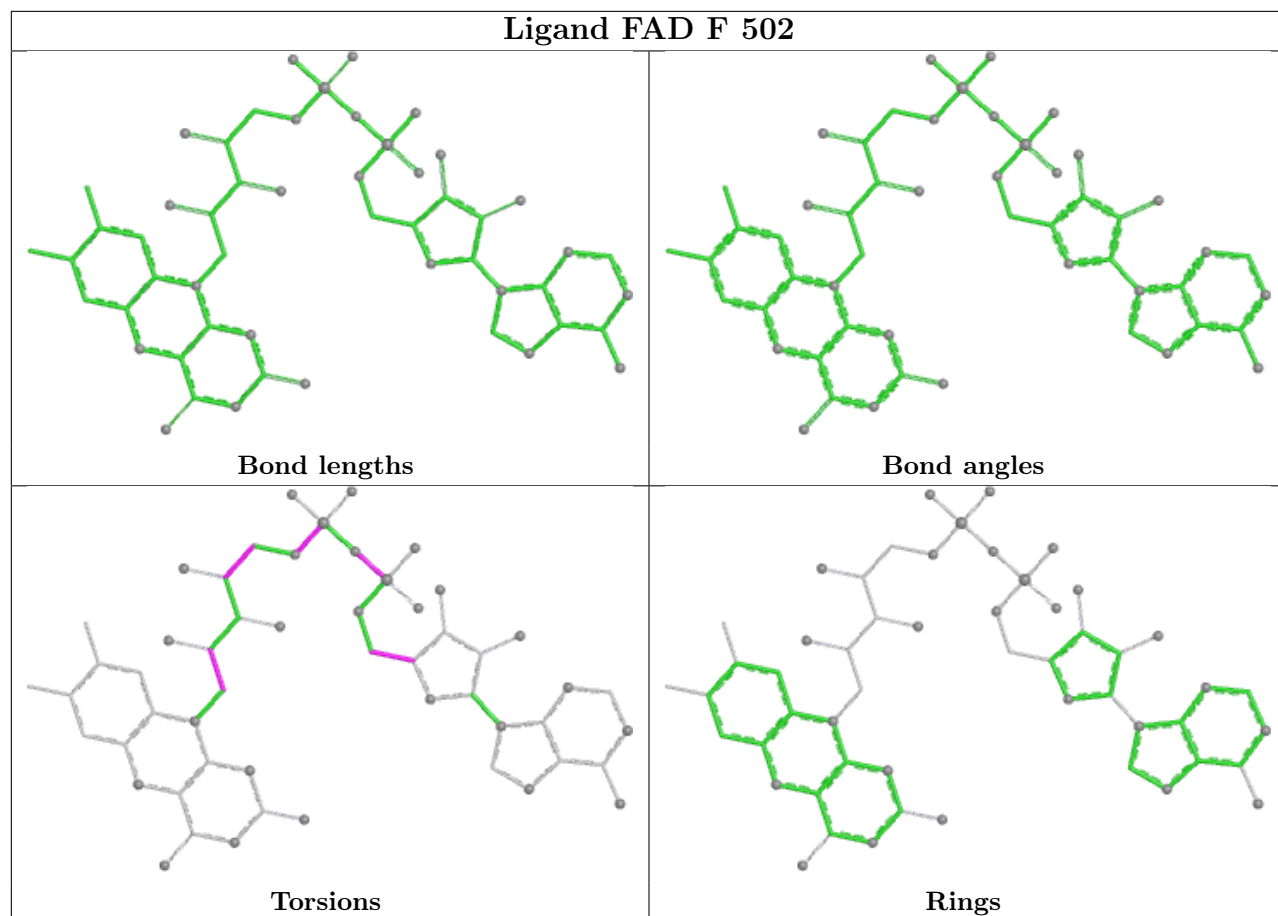
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	603	PEE	2	0
10	B	605	PEE	1	0
7	C	301	FMN	1	0
9	B	602	0NI	1	0
11	D	301	LMT	1	0
8	B	601	RBF	2	0

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

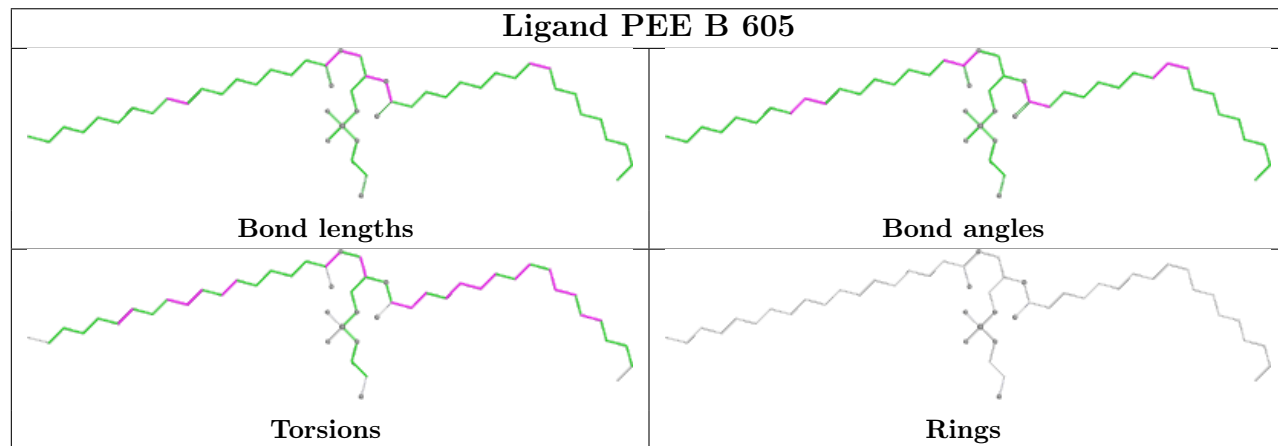
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

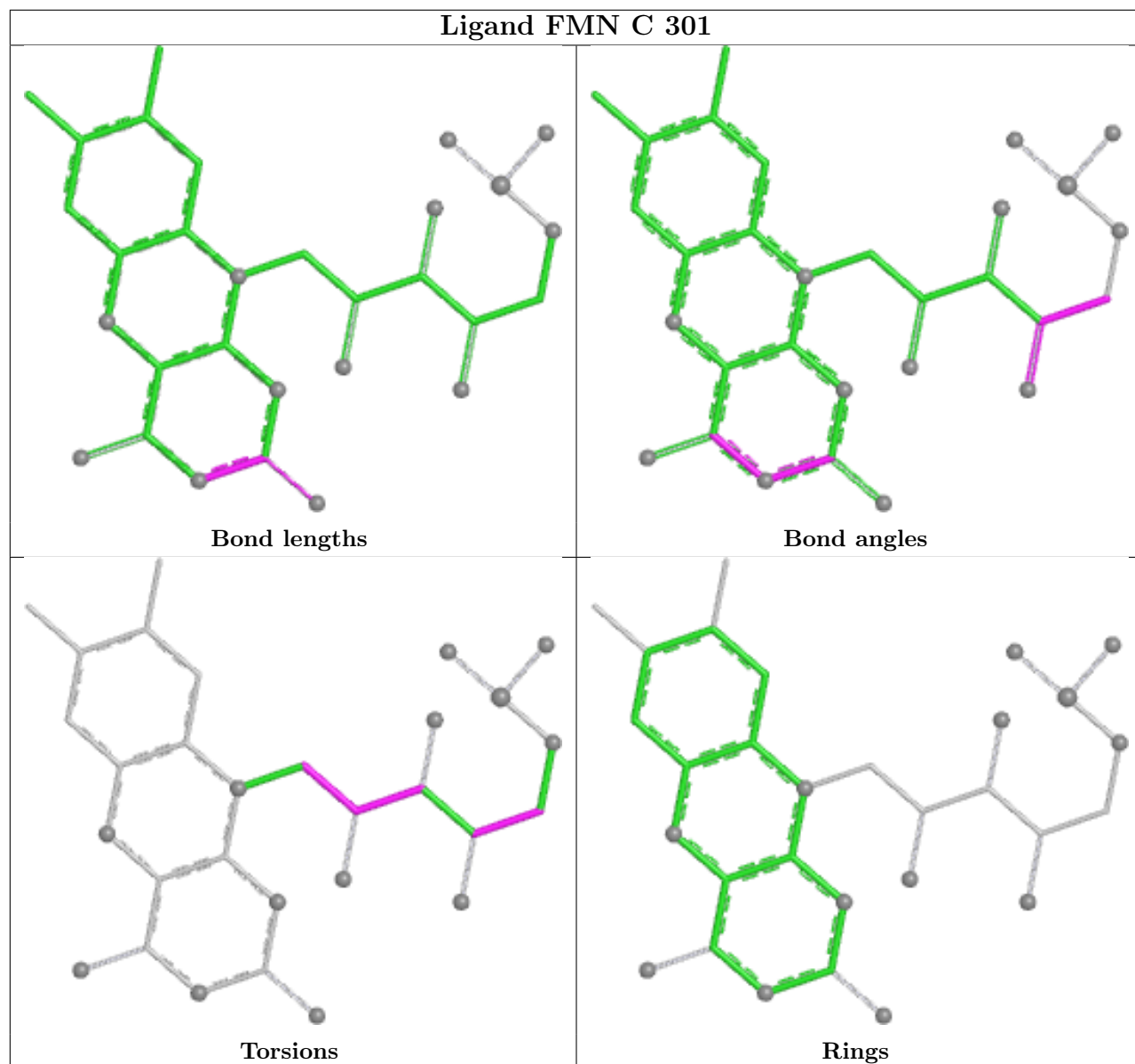


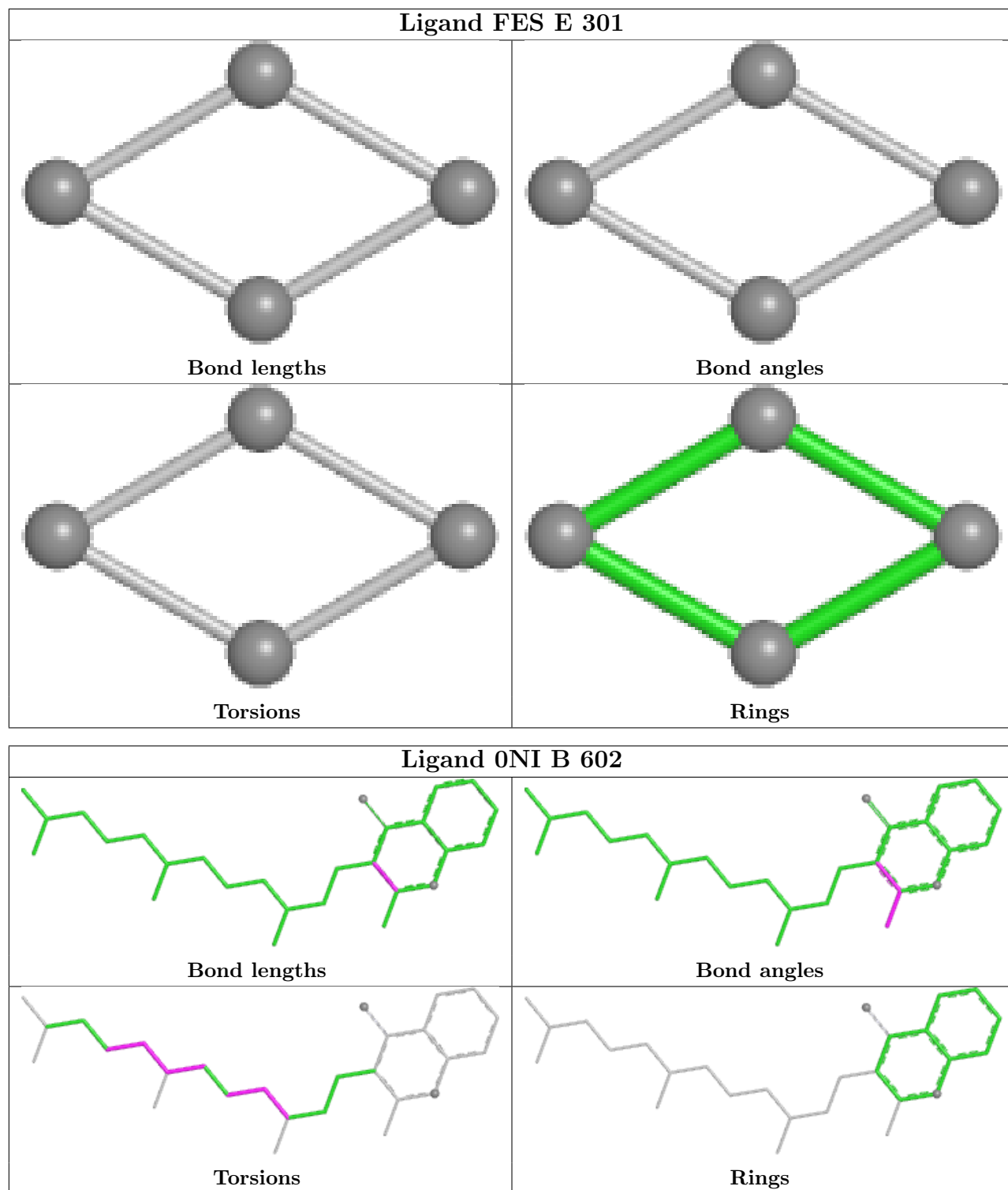
Ligand FAD F 502

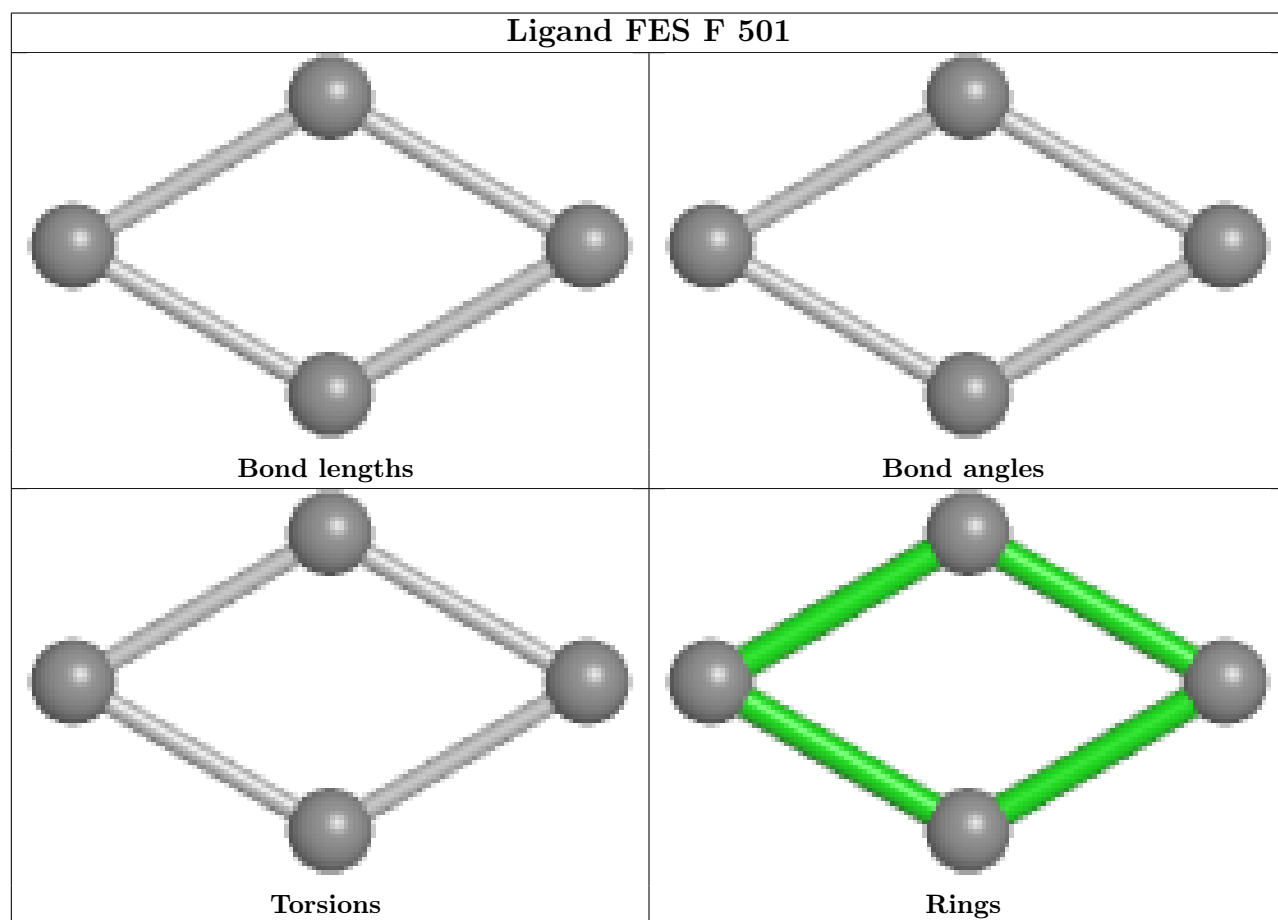
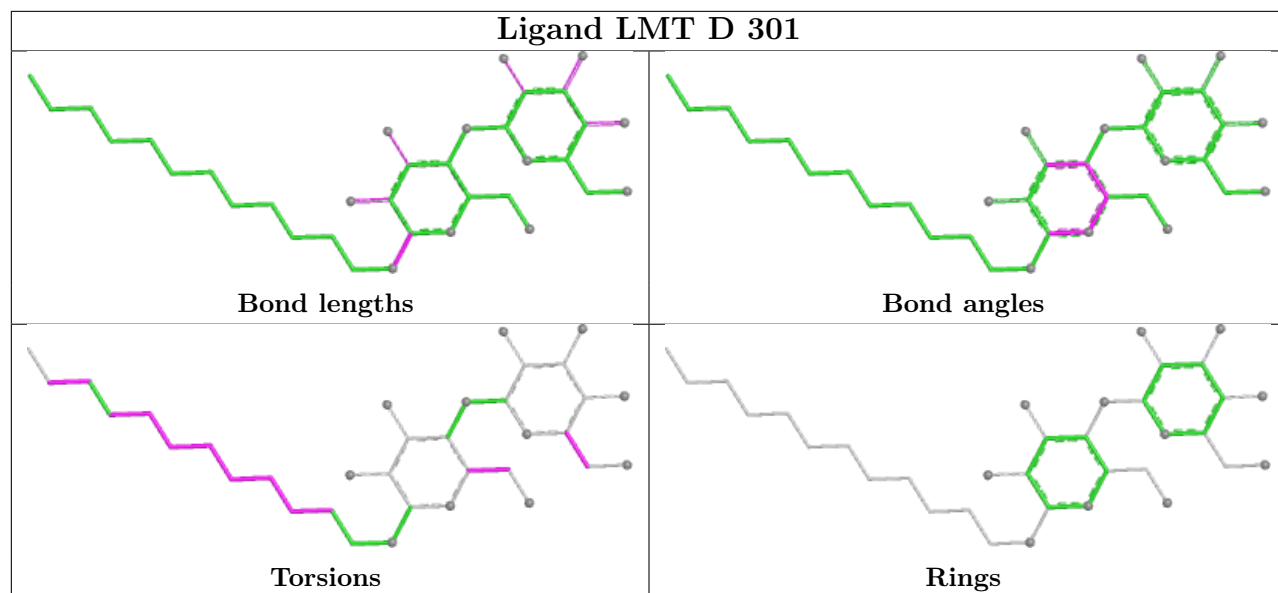


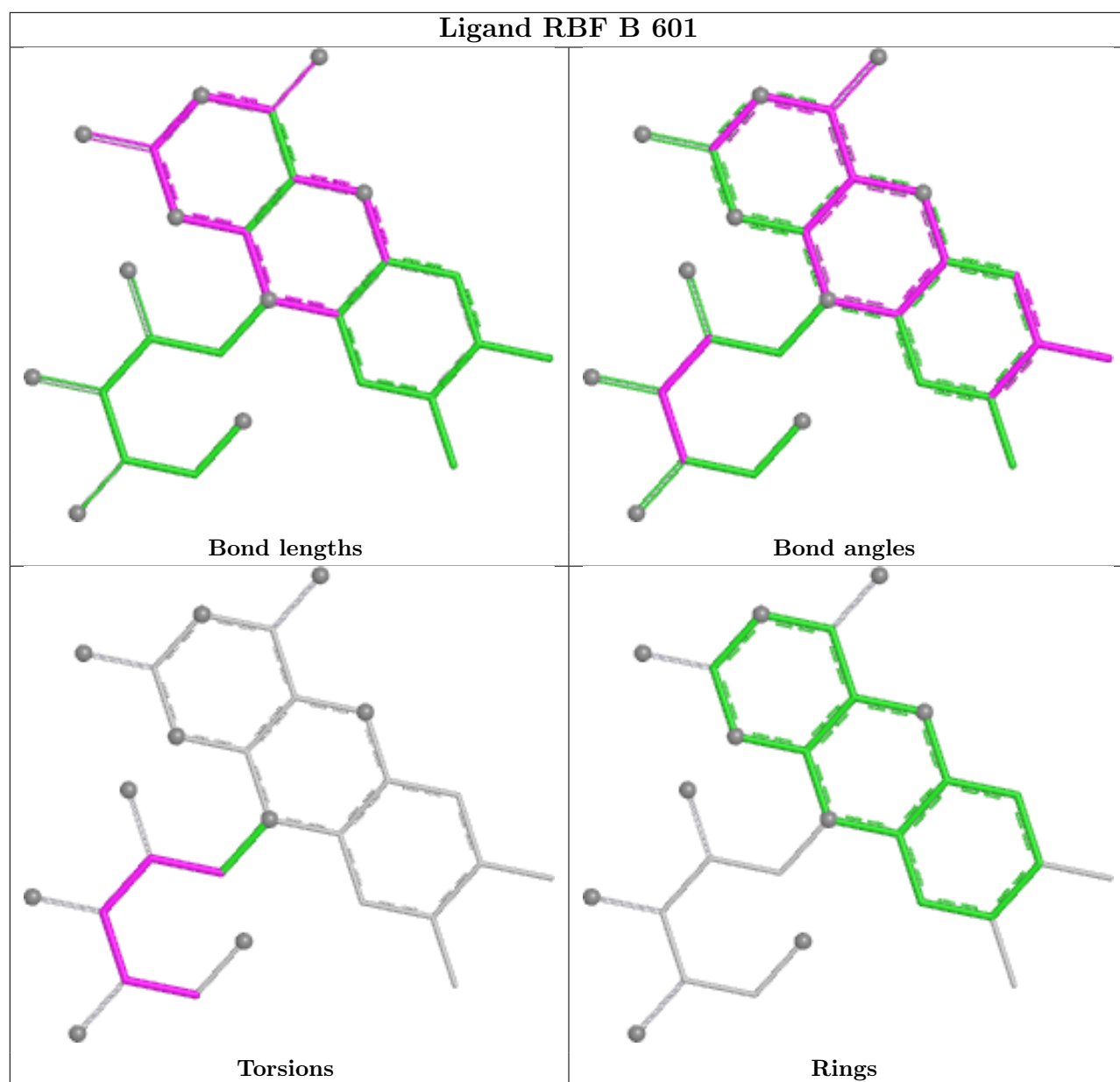
Ligand PEE B 605

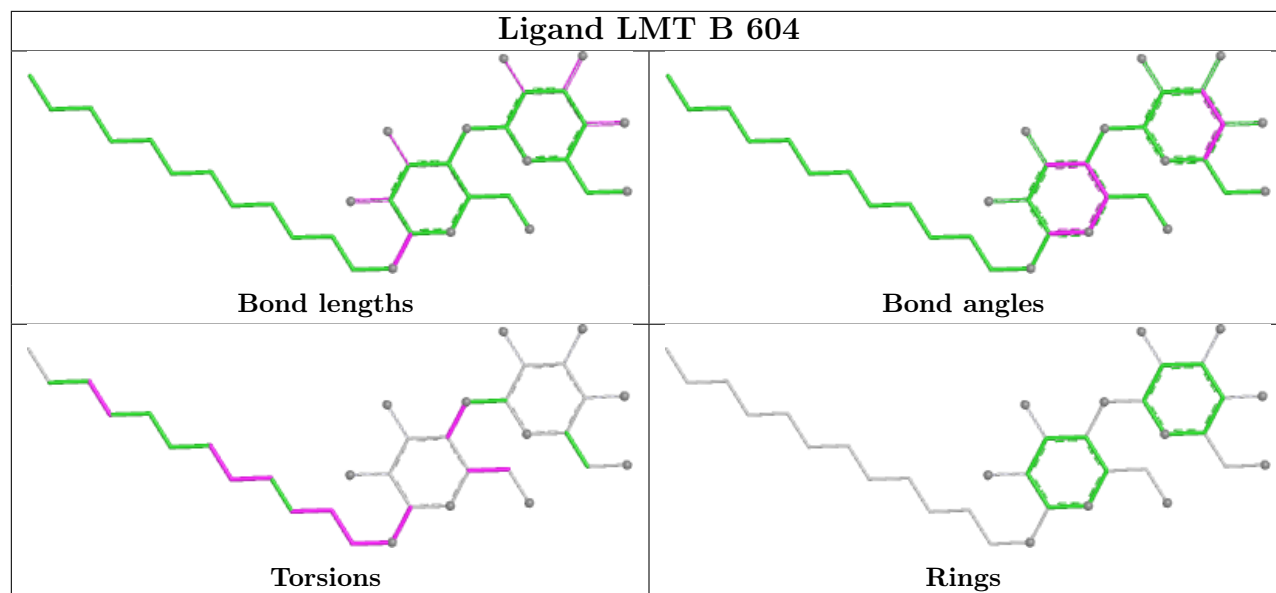












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

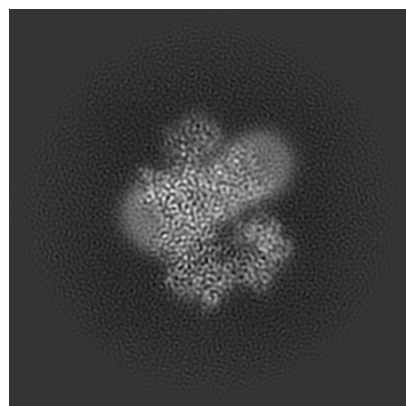
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33245. These allow visual inspection of the internal detail of the map and identification of artifacts.

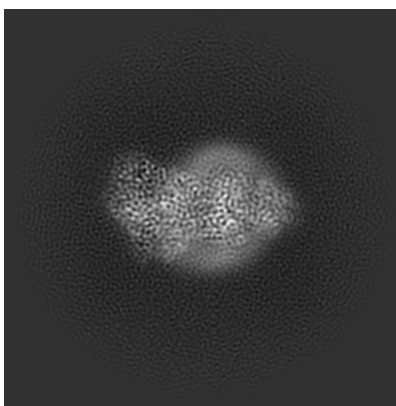
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

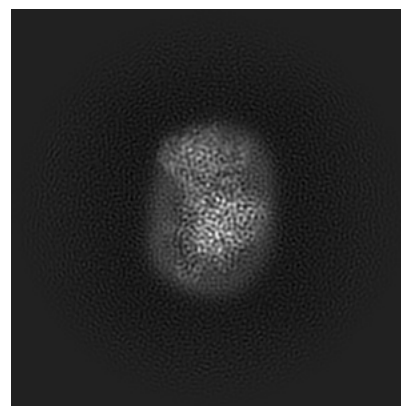
6.1.1 Primary map



X

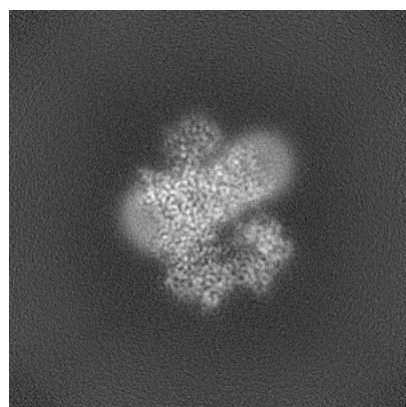


Y

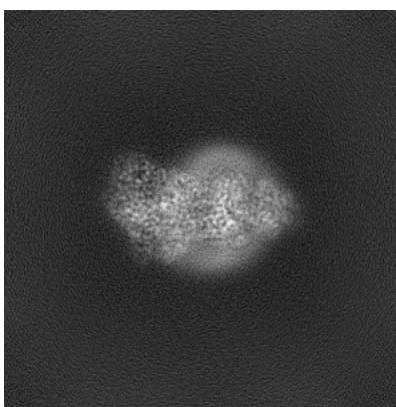


Z

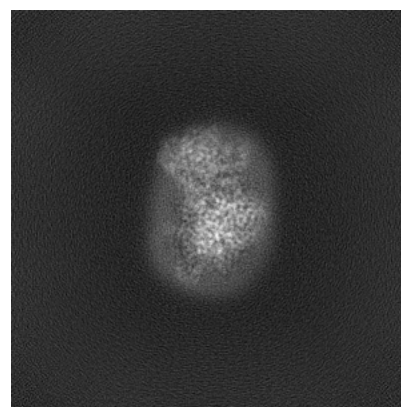
6.1.2 Raw map



X



Y

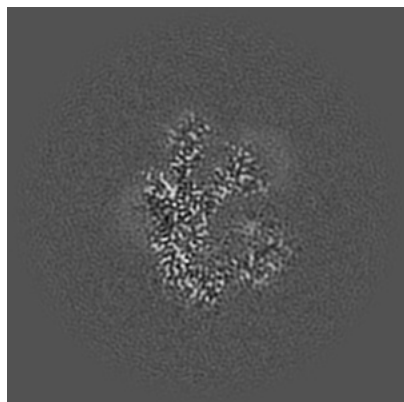


Z

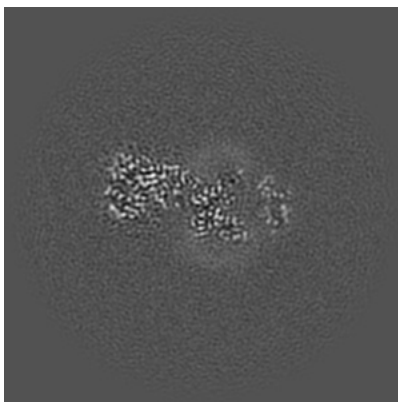
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

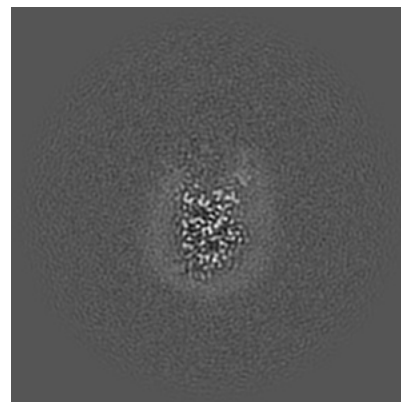
6.2.1 Primary map



X Index: 160

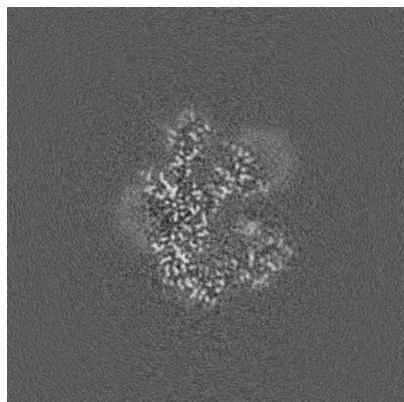


Y Index: 160

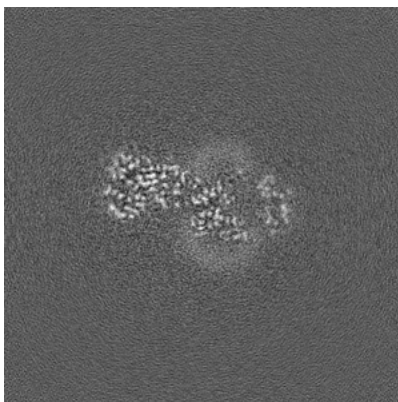


Z Index: 160

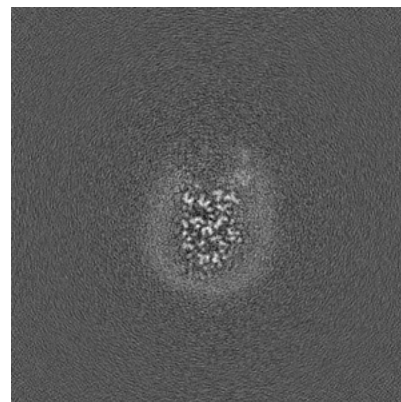
6.2.2 Raw map



X Index: 160



Y Index: 160

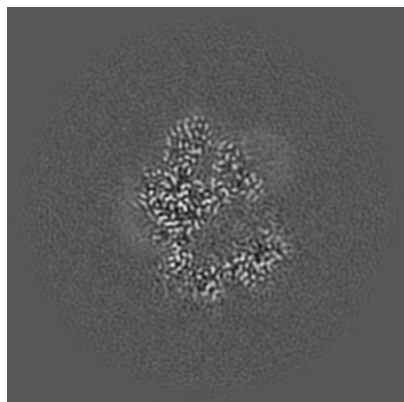


Z Index: 160

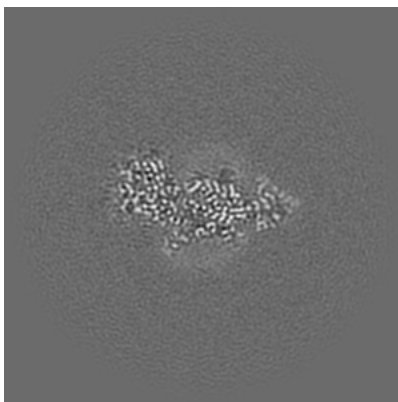
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

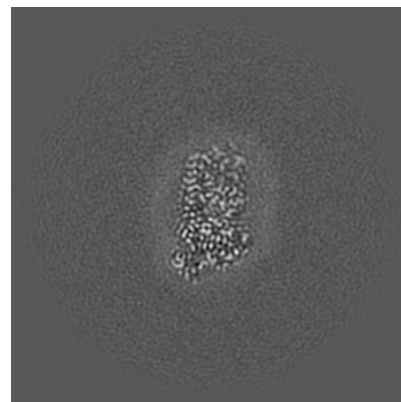
6.3.1 Primary map



X Index: 154

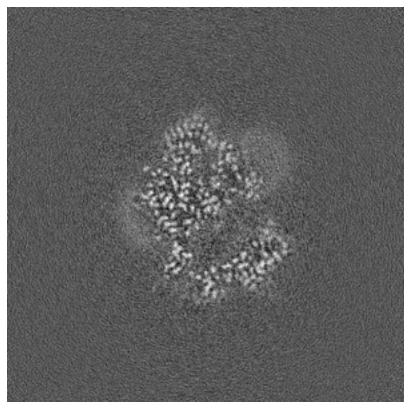


Y Index: 140

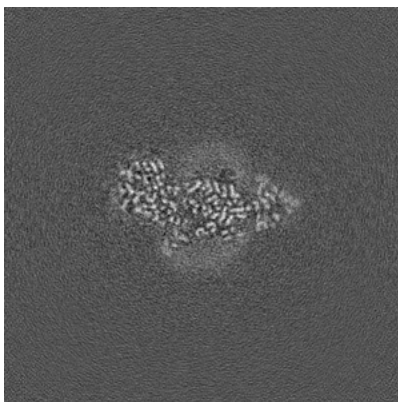


Z Index: 176

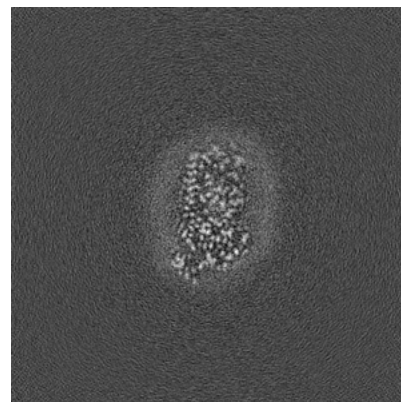
6.3.2 Raw map



X Index: 153



Y Index: 140

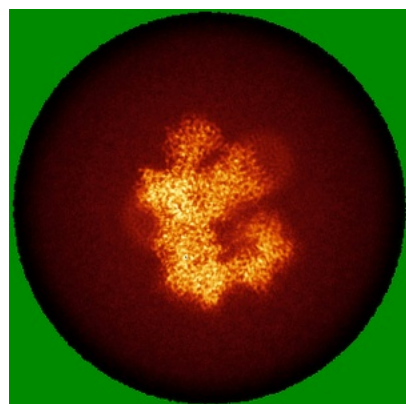


Z Index: 176

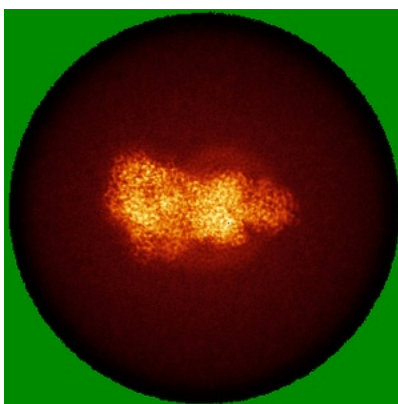
The images above show the largest variance slices of the map in three orthogonal directions.

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

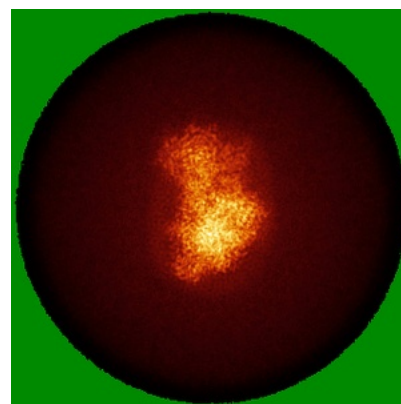
6.4.1 Primary map



X

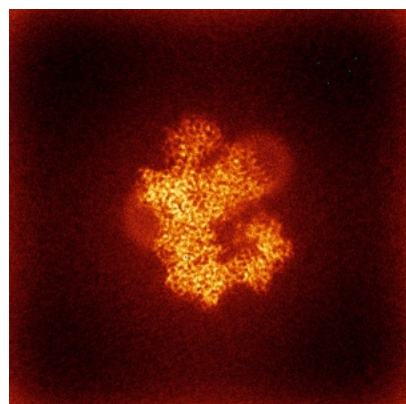


Y

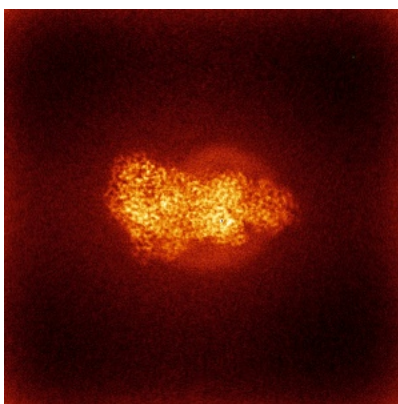


Z

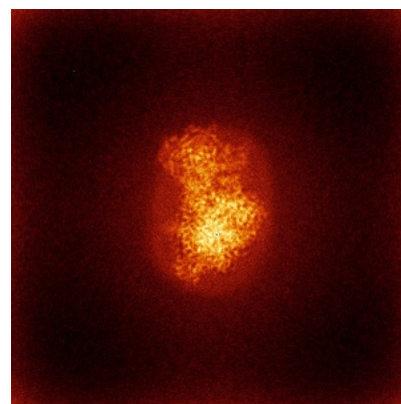
6.4.2 Raw map



X



Y



Z

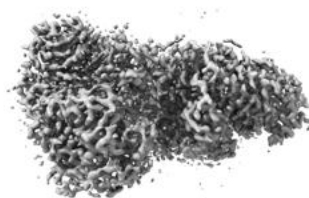
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

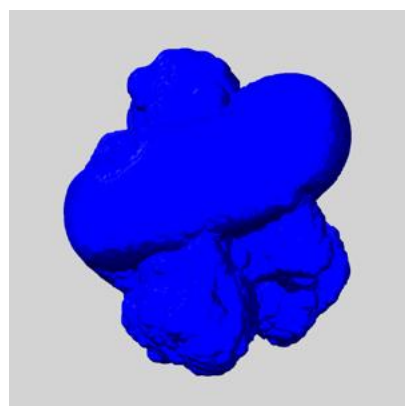
6.6 Mask visualisation [i](#)

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

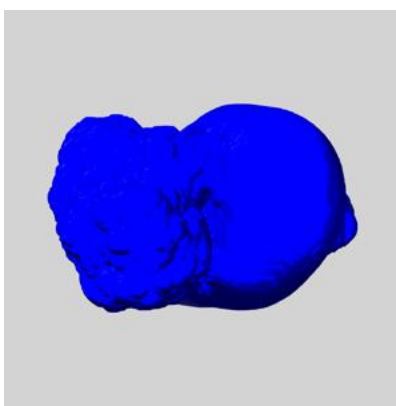
A mask typically either:

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

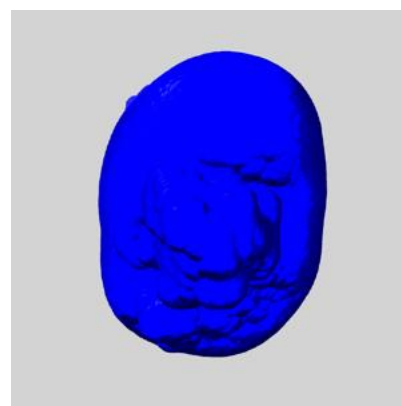
6.6.1 emd_33245_msk_1.map [i](#)



X



Y

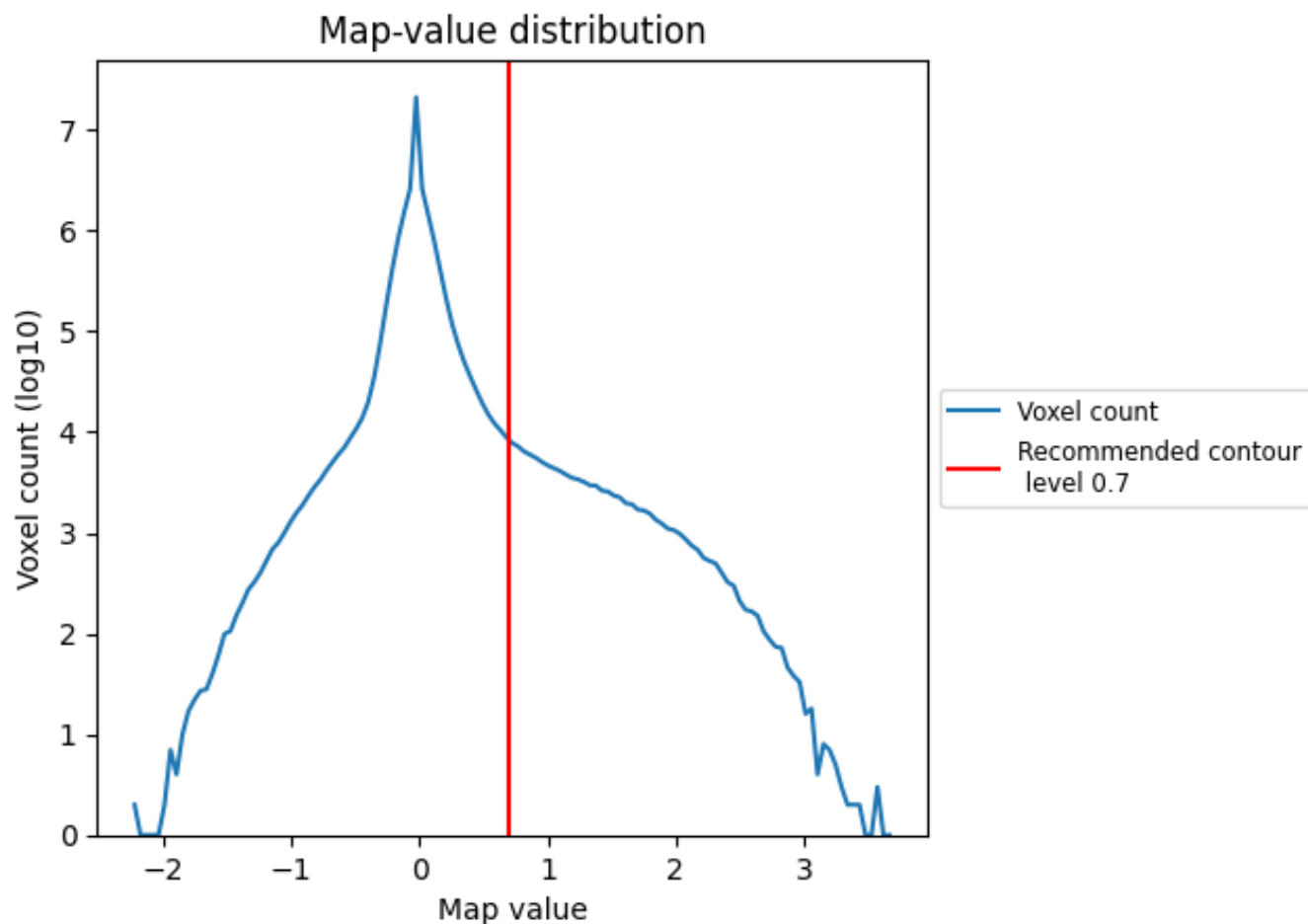


Z

7 Map analysis [i](#)

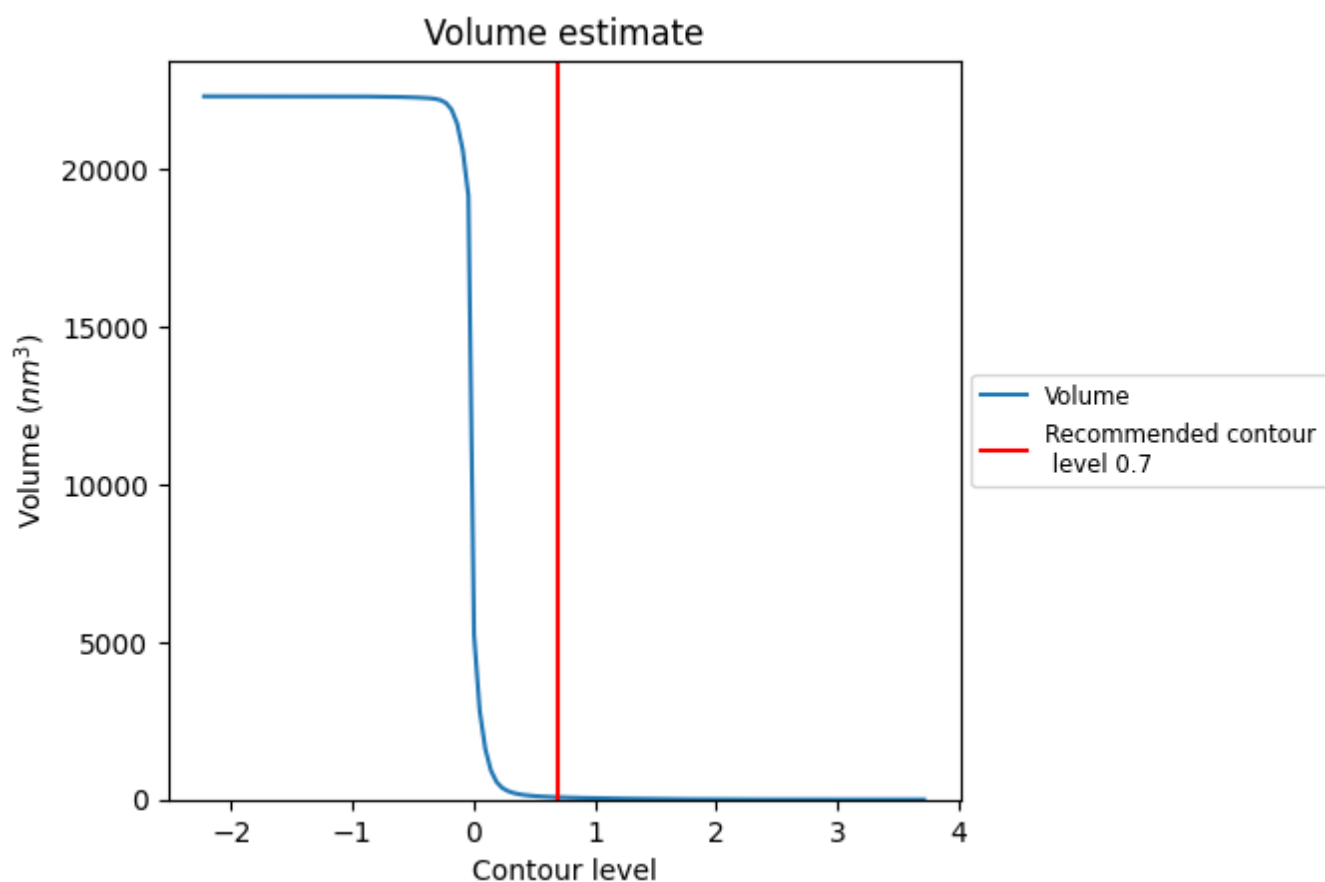
This section contains the results of statistical analysis of the map.

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.

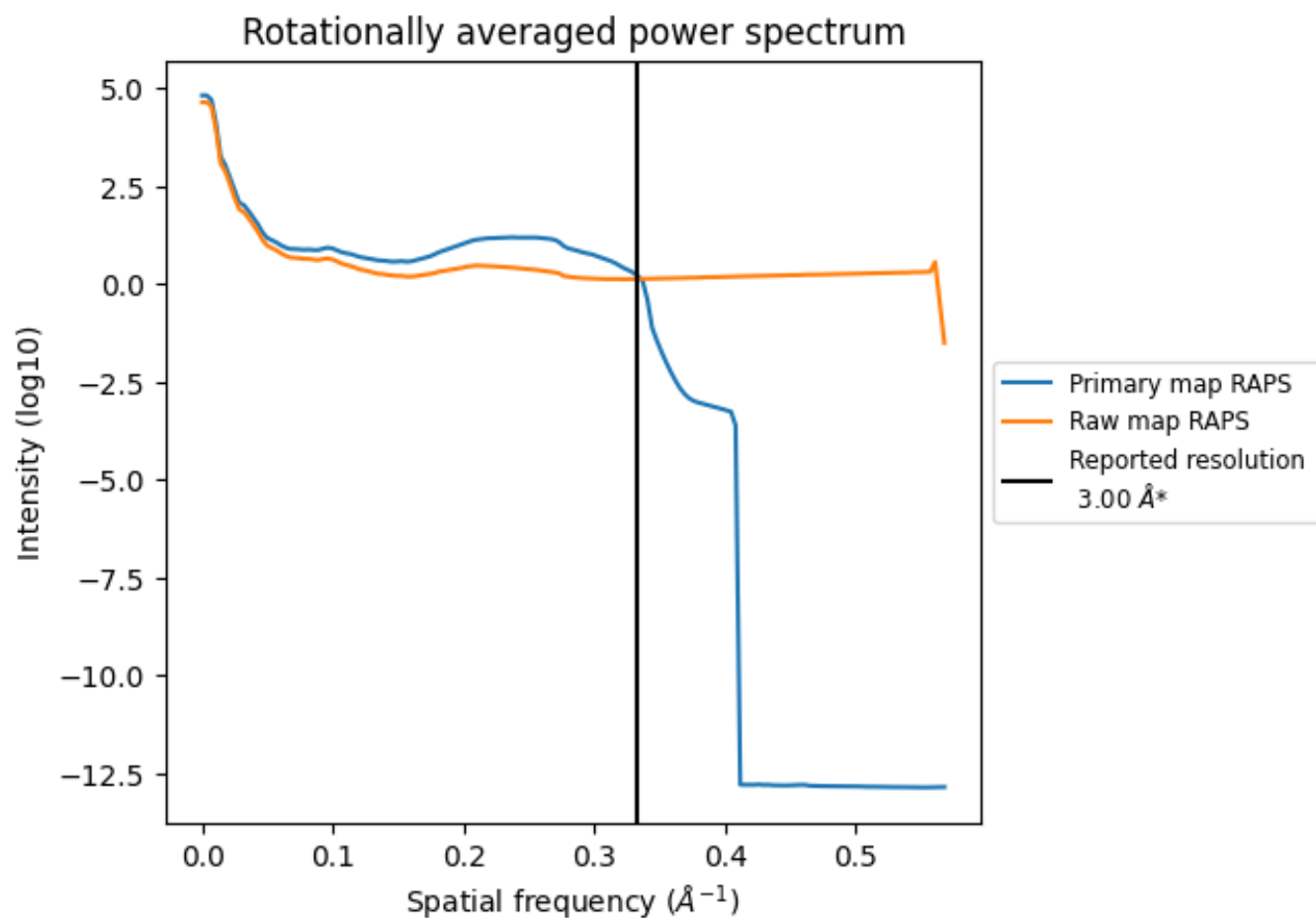
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm³; this corresponds to an approximate mass of 65 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 ⓘ

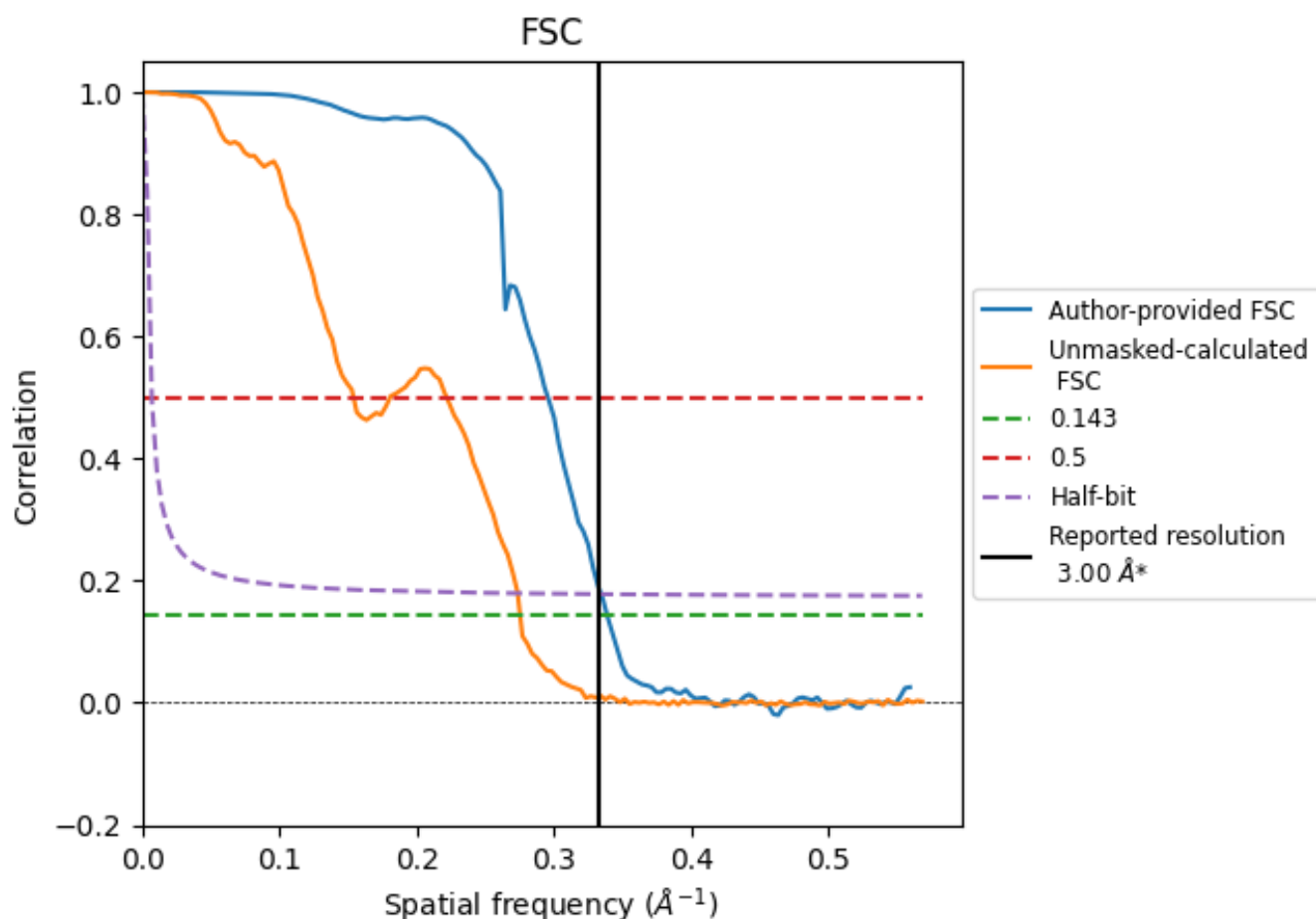


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

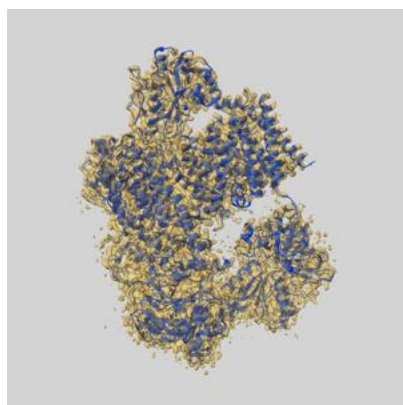
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.38	2.99
Unmasked-calculated*	3.63	6.50	3.65

*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 3.63 differs from the reported value 3.0 by more than 10 %

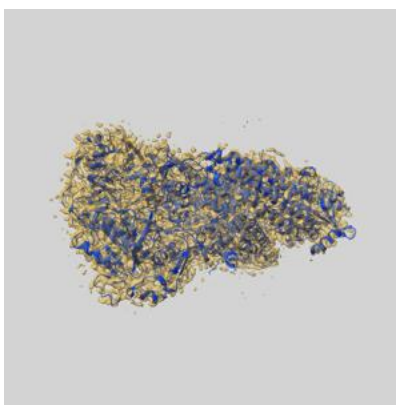
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33245 and PDB model 7XK6. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

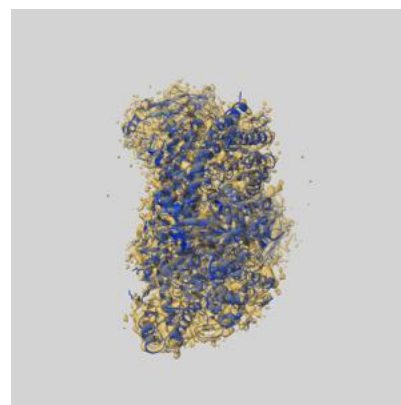
9.1 Map-model overlay [i](#)



X



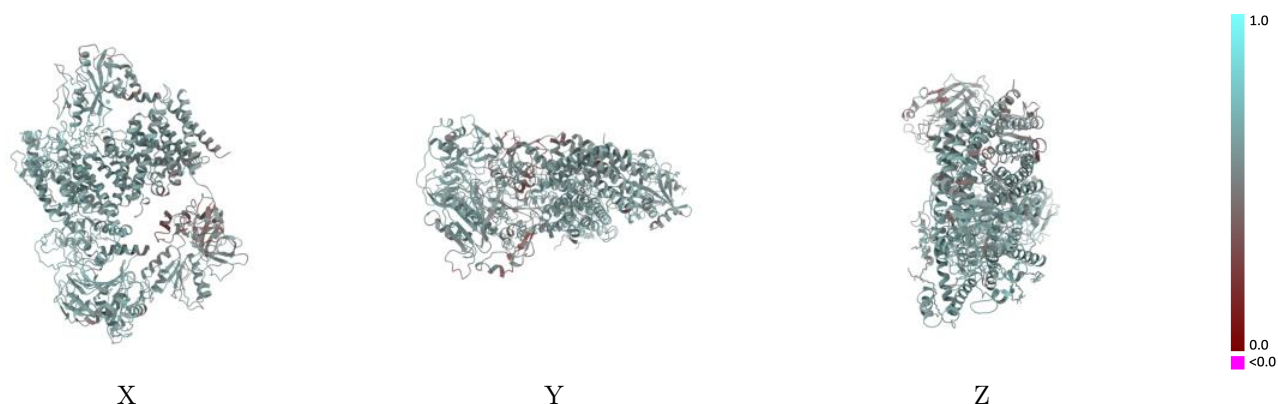
Y



Z

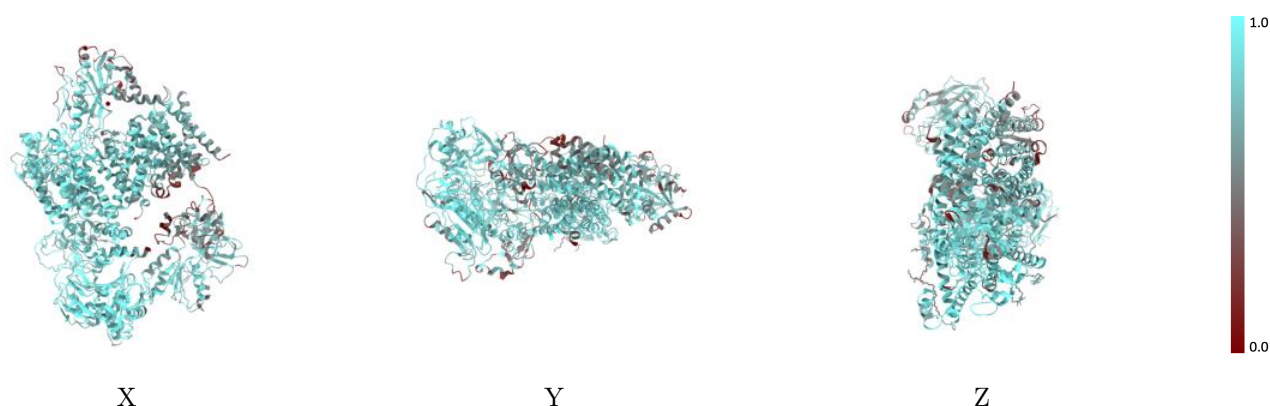
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



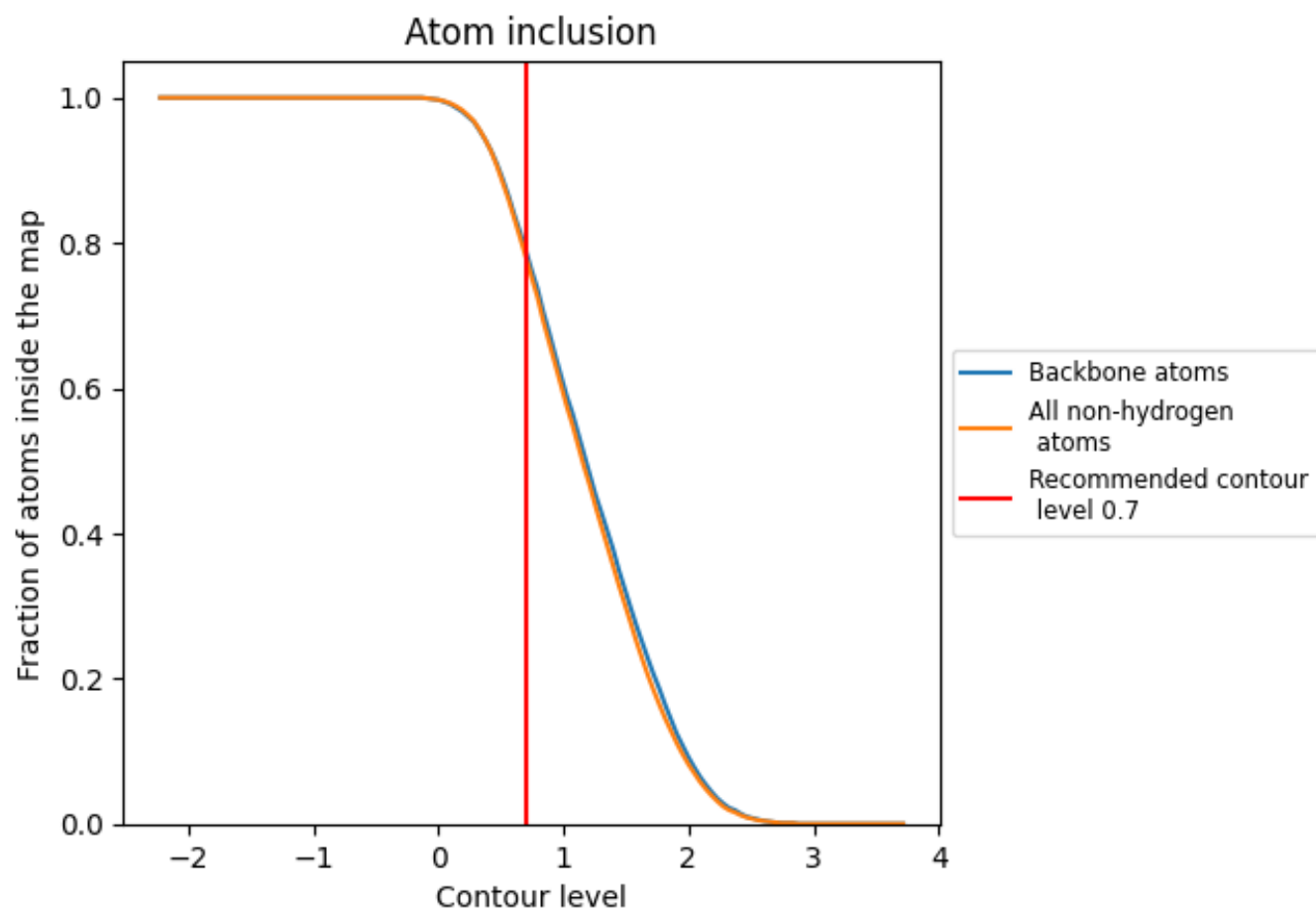
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.5760
A	0.8640	0.5990
B	0.8720	0.6110
C	0.6880	0.5690
D	0.7860	0.5850
E	0.7620	0.5800
F	0.6660	0.5100

1.0

0.0

<0.0