



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 9Q8I / pdb_00009q8i
EMDB ID : EMD-52895
Title : Cryo-EM structure of E. coli complex I variant V96P/N142M (NuoE)
Authors : Seifermann, T.; Wohlwend, D.; Friedrich, T.
Deposited on : 2025-02-24
Resolution : 2.35 Å(reported)

This is a wwPDB EM Validation Summary 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:

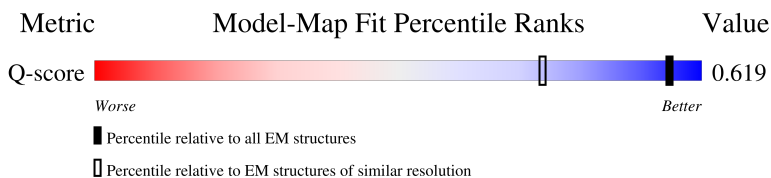
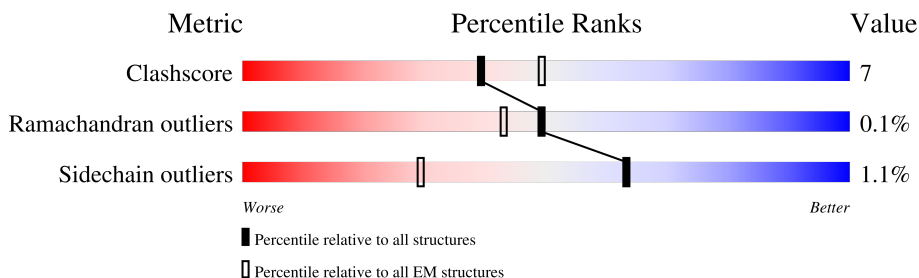
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.35 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	4607 (1.85 - 2.85)

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	147	
2	B	220	
3	C	596	
4	E	166	

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Mol	Chain	Length	Quality of chain
5	F	461	 80% 16% .
6	G	908	 86% 13% .
7	H	325	 77% 21% ..
8	I	180	 69% 12% .. 17%
9	J	184	 74% 22% .
10	K	100	 88% 12%
11	L	613	 83% 17%
12	M	509	 79% 19% ..
13	N	485	 80% 19%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 37648 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 NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			840	573	134	129	4		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	200	Total	C	N	O	S	0	0
			1601	1015	275	294	17		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	587	Total	C	N	O	S	0	0
			4746	3038	827	858	23		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	156	Total	C	N	O	S	0	0
			1220	769	214	228	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	96	PRO	VAL	engineered mutation	UNP P0AFD1
E	142	MET	ASN	engineered mutation	UNP P0AFD1

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	442	Total	C	N	O	S	0	0
			3429	2175	601	633	20		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	MET	-	initiating methionine	UNP P31979
F	-14	ARG	-	expression tag	UNP P31979
F	-13	GLY	-	expression tag	UNP P31979
F	-12	SER	-	expression tag	UNP P31979
F	-11	HIS	-	expression tag	UNP P31979
F	-10	HIS	-	expression tag	UNP P31979
F	-9	HIS	-	expression tag	UNP P31979
F	-8	HIS	-	expression tag	UNP P31979
F	-7	HIS	-	expression tag	UNP P31979
F	-6	HIS	-	expression tag	UNP P31979
F	-5	THR	-	expression tag	UNP P31979
F	-4	ASP	-	expression tag	UNP P31979
F	-3	PRO	-	expression tag	UNP P31979
F	-2	ALA	-	expression tag	UNP P31979
F	-1	LEU	-	expression tag	UNP P31979
F	0	ARG	-	expression tag	UNP P31979
F	1	ALA	-	expression tag	UNP P31979

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	907	Total	C	N	O	S	0	0
			7044	4402	1272	1332	38		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	320	Total	C	N	O	S	0	0
			2517	1690	395	413	19		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	149	Total	C	N	O	S	0	0
			1186	752	196	225	13		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	176	Total	C	N	O	S	0	0
			1331	884	210	230	7		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	100	Total	C	N	O	S	0	0
			761	494	132	130	5		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	613	Total	C	N	O	S	0	0
			4685	3113	753	787	32		

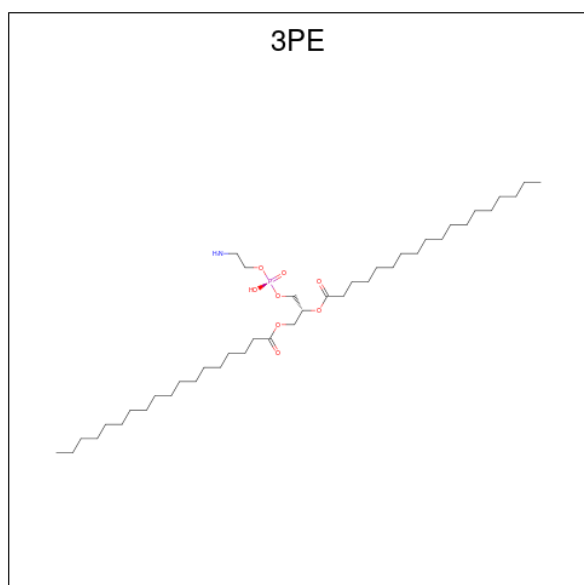
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	505	Total	C	N	O	S	0	0
			3960	2665	618	648	29		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit N.

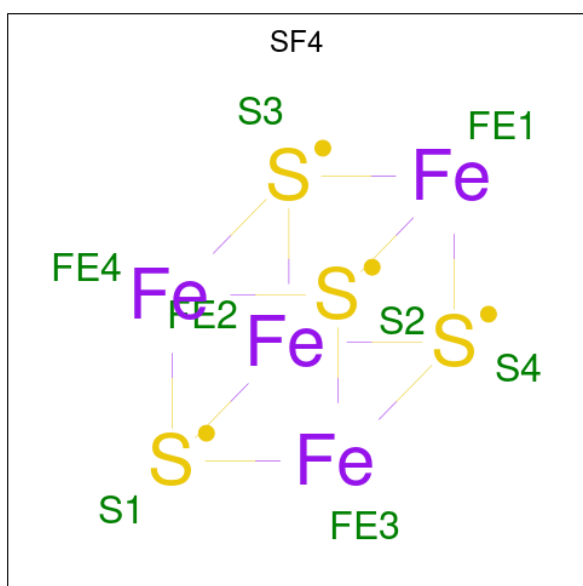
Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	485	Total	C	N	O	S	0	0
			3673	2448	582	623	20		

- Molecule 14 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
14	J	1	Total	C	N	O	P	0
			42	32	1	8	1	
14	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
14	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
14	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
14	N	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



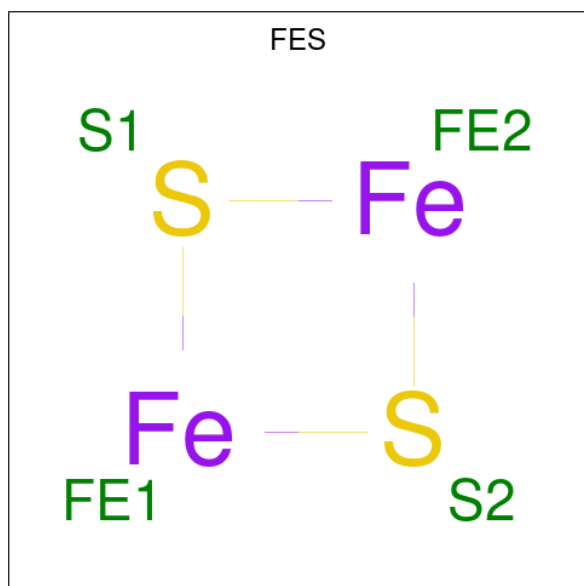
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	Fe	S	0
			8	4	4	

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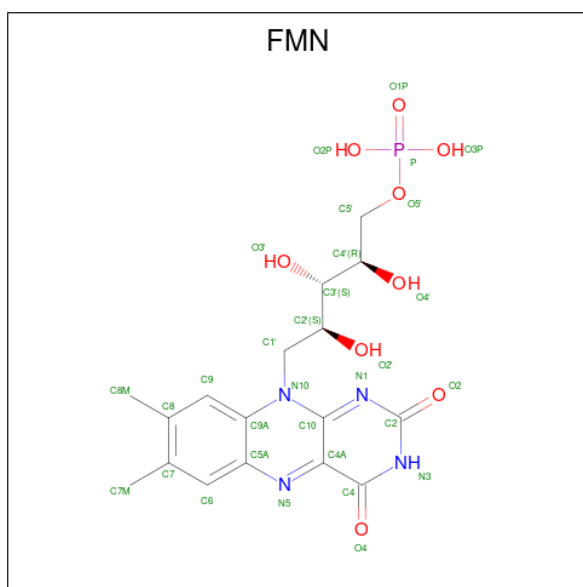
Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	Fe	S	0
			8	4	4	
15	G	1	Total	Fe	S	0
			8	4	4	
15	G	1	Total	Fe	S	0
			8	4	4	
15	G	1	Total	Fe	S	0
			8	4	4	
15	I	1	Total	Fe	S	0
			8	4	4	
15	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	E	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	Ca	0
			1	1	

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
19	G	1	Total	Cl	0
			1	1	
19	N	1	Total	Cl	0
			1	1	

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	O	0
			2	2	
20	B	8	Total	O	0
			8	8	
20	C	34	Total	O	0
			34	34	

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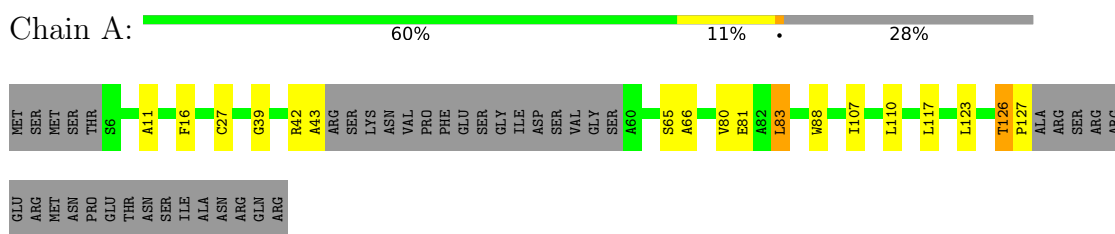
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Mol	Chain	Residues	Atoms		AltConf
20	E	1	Total 1	O 1	0
20	F	7	Total 7	O 7	0
20	G	33	Total 33	O 33	0
20	H	2	Total 2	O 2	0
20	I	10	Total 10	O 10	0
20	J	2	Total 2	O 2	0
20	K	1	Total 1	O 1	0
20	L	2	Total 2	O 2	0
20	M	10	Total 10	O 10	0
20	N	4	Total 4	O 4	0

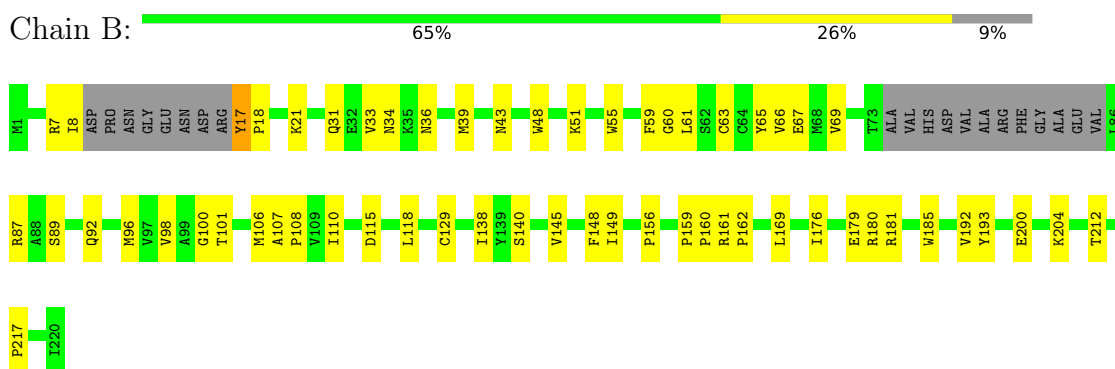
3 Residue-property plots

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.

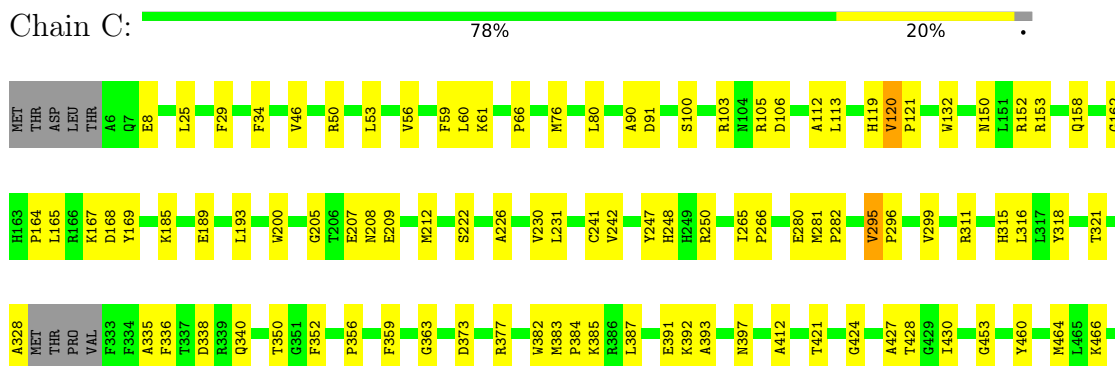
- Molecule 1: NADH-quinone oxidoreductase subunit A



- Molecule 2: NADH-quinone oxidoreductase subunit B



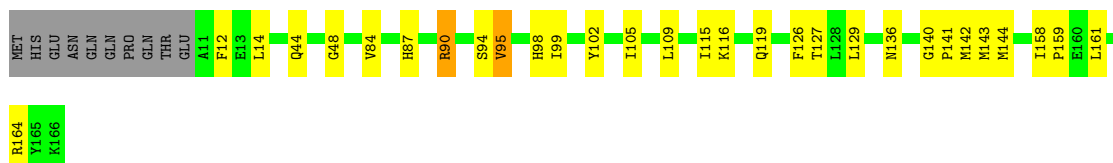
- Molecule 3: NADH-quinone oxidoreductase subunit C/D





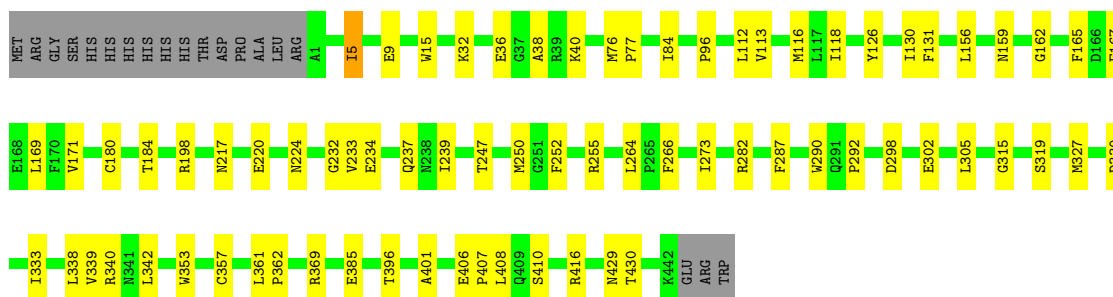
• Molecule 4: NADH-quinone oxidoreductase subunit E

Chain E: 76% 17% 6%



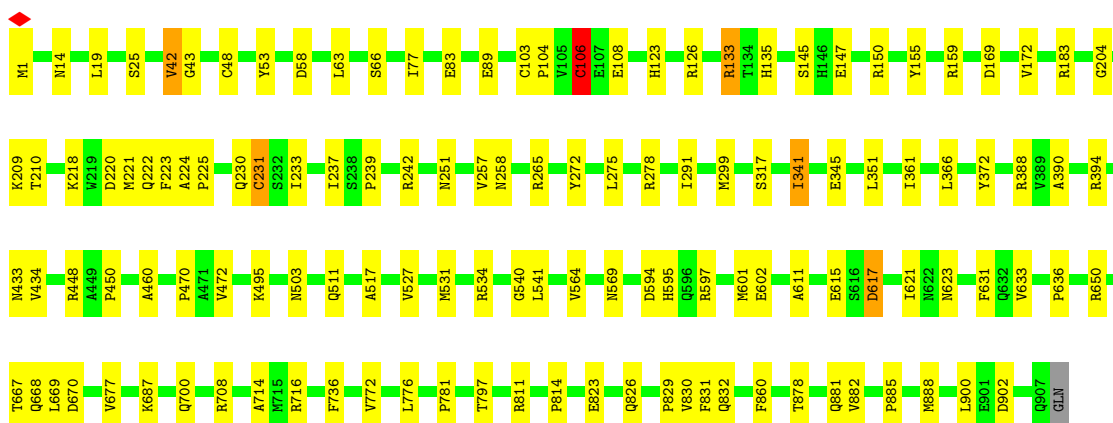
• Molecule 5: NADH-quinone oxidoreductase subunit F

Chain F: 80% 16% 4%



• Molecule 6: NADH-quinone oxidoreductase subunit G

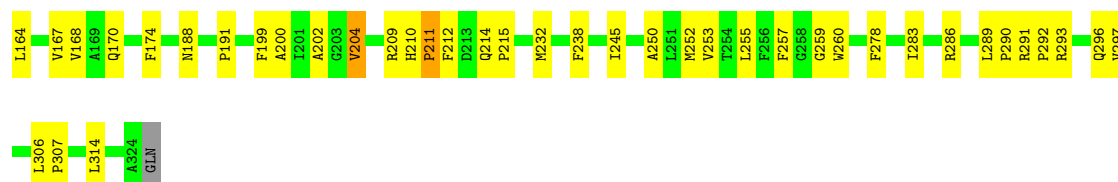
Chain G: 86% 13% 1%



• Molecule 7: NADH-quinone oxidoreductase subunit H

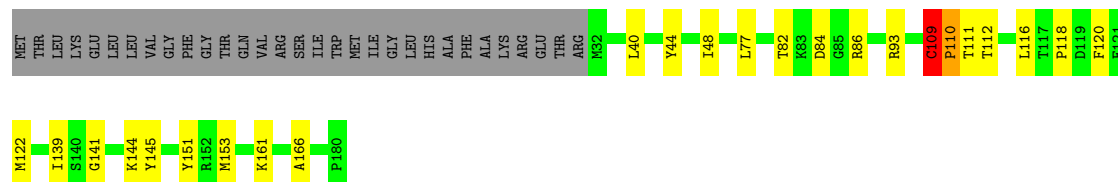
Chain H: 77% 21% 2%





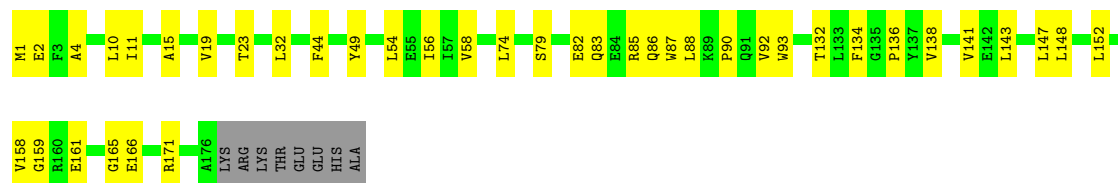
• Molecule 8: NADH-quinone oxidoreductase subunit I

Chain I: 69% 12% 17%



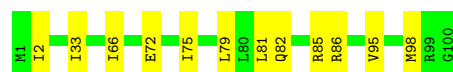
• Molecule 9: NADH-quinone oxidoreductase subunit J

Chain J: 74% 22% 4%



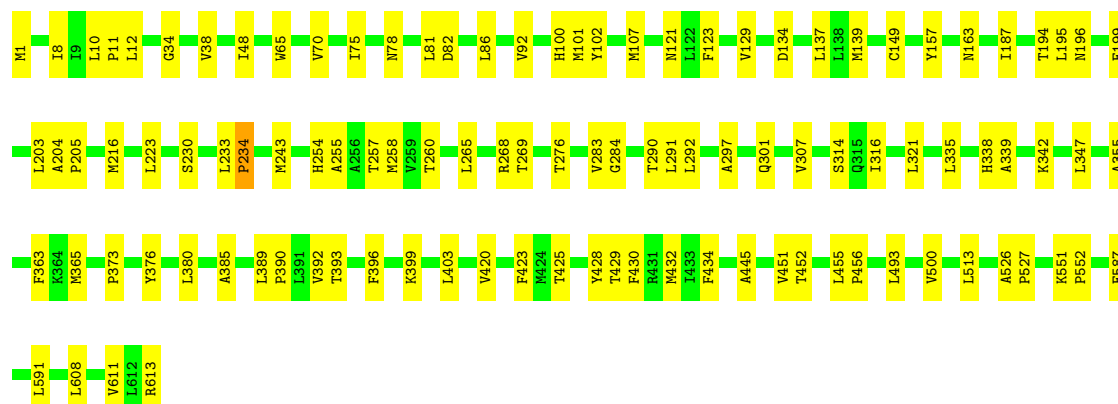
• Molecule 10: NADH-quinone oxidoreductase subunit K

Chain K: 88% 12% 0%



• Molecule 11: NADH-quinone oxidoreductase subunit L

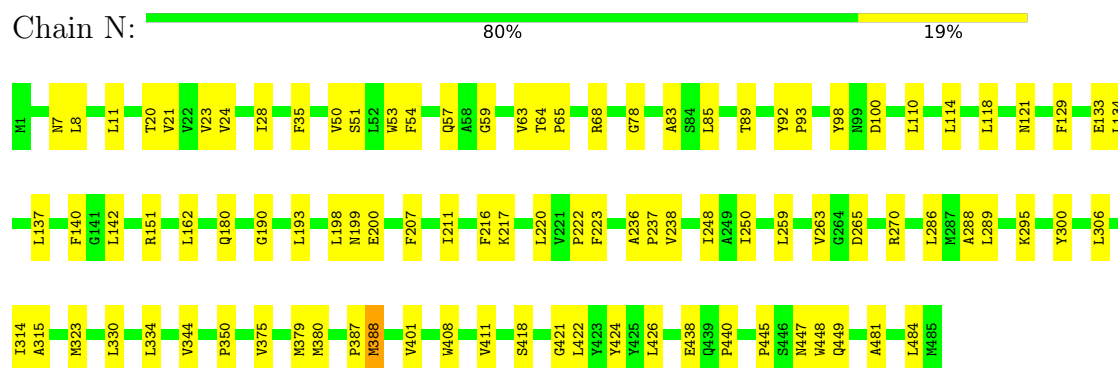
Chain L: 83% 17% 0%



• Molecule 12: NADH-quinone oxidoreductase subunit M



• Molecule 13: NADH-quinone oxidoreductase subunit N



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	95103, 95103, 95103, 95103	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.317	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	457.60004, 457.60004, 457.60004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.144, 1.144, 1.144	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CA, FES, 3PE, CL, SF4

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	0.93	0/865	1.17	0/1176
2	B	0.95	0/1634	1.14	0/2209
3	C	0.94	0/4875	1.13	3/6611 (0.0%)
4	E	0.97	0/1249	1.13	0/1692
5	F	0.96	0/3508	1.15	1/4742 (0.0%)
6	G	0.97	0/7195	1.14	1/9755 (0.0%)
7	H	0.96	0/2590	1.15	0/3522
8	I	0.95	0/1215	1.21	3/1642 (0.2%)
9	J	0.98	0/1357	1.18	0/1848
10	K	0.96	0/770	1.15	0/1040
11	L	0.95	0/4806	1.17	1/6549 (0.0%)
12	M	0.93	0/4081	1.14	2/5556 (0.0%)
13	N	0.96	0/3764	1.17	2/5138 (0.0%)
All	All	0.96	0/37909	1.15	13/51480 (0.0%)

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
4	E	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	109	CYS	CB-CA-C	-12.97	89.06	109.42
8	I	110	PRO	N-CA-C	-6.69	106.12	114.68
12	M	134	ILE	N-CA-C	-6.15	107.13	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	145	TYR	CB-CA-C	5.99	116.97	110.08
13	N	59	GLY	CA-C-O	-5.77	118.30	122.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	90	ARG	Sidechain

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	840	0	857	16	0
2	B	1601	0	1596	41	0
3	C	4746	0	4657	81	0
4	E	1220	0	1188	21	0
5	F	3429	0	3401	49	0
6	G	7044	0	6849	77	0
7	H	2517	0	2574	43	0
8	I	1186	0	1145	16	0
9	J	1331	0	1399	33	0
10	K	761	0	817	11	0
11	L	4685	0	4831	65	0
12	M	3960	0	4060	61	0
13	N	3673	0	3836	67	0
14	A	36	0	46	4	0
14	J	42	0	58	2	0
14	L	189	0	289	12	0
14	M	76	0	100	4	0
14	N	98	0	153	8	0
15	B	8	0	0	0	0
15	F	8	0	0	0	0
15	G	24	0	0	0	0
15	I	16	0	0	0	0
16	E	4	0	0	1	0
16	G	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	31	0	19	2	0
18	G	1	0	0	0	0
19	G	1	0	0	0	0
19	N	1	0	0	0	0
20	A	2	0	0	0	0
20	B	8	0	0	0	0
20	C	34	0	0	0	0
20	E	1	0	0	0	0
20	F	7	0	0	0	0
20	G	33	0	0	0	0
20	H	2	0	0	0	0
20	I	10	0	0	0	0
20	J	2	0	0	0	0
20	K	1	0	0	0	0
20	L	2	0	0	0	0
20	M	10	0	0	0	0
20	N	4	0	0	0	0
All	All	37648	0	37875	539	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 7.

The worst 5 of 539 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)
3:C:387:LEU:HD21	3:C:471:ARG:HG2	1.59	0.82
2:B:217:PRO:HD3	8:I:144:LYS:HB3	1.62	0.81
6:G:885:PRO:HB2	6:G:888:MET:HG3	1.66	0.77
11:L:157:TYR:HB2	11:L:163:ASN:HD22	1.54	0.73
13:N:78:GLY:HA3	14:N:502:3PE:H2B1	1.69	0.73

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	102/147 (69%)	101 (99%)	1 (1%)	0	100	100
2	B	194/220 (88%)	178 (92%)	16 (8%)	0	100	100
3	C	583/596 (98%)	563 (97%)	20 (3%)	0	100	100
4	E	154/166 (93%)	148 (96%)	6 (4%)	0	100	100
5	F	440/461 (95%)	424 (96%)	16 (4%)	0	100	100
6	G	905/908 (100%)	866 (96%)	38 (4%)	1 (0%)	48	59
7	H	316/325 (97%)	302 (96%)	14 (4%)	0	100	100
8	I	147/180 (82%)	141 (96%)	5 (3%)	1 (1%)	18	20
9	J	174/184 (95%)	172 (99%)	2 (1%)	0	100	100
10	K	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
11	L	611/613 (100%)	579 (95%)	31 (5%)	1 (0%)	43	52
12	M	503/509 (99%)	488 (97%)	15 (3%)	0	100	100
13	N	483/485 (100%)	474 (98%)	8 (2%)	1 (0%)	43	52
All	All	4710/4894 (96%)	4531 (96%)	175 (4%)	4 (0%)	49	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	N	388	MET
11	L	373	PRO
6	G	257	VAL
8	I	139	ILE

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	82/119 (69%)	80 (98%)	2 (2%)	43	57
2	B	177/192 (92%)	175 (99%)	2 (1%)	65	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	506/515 (98%)	497 (98%)	9 (2%)	51	66
4	E	129/139 (93%)	127 (98%)	2 (2%)	55	70
5	F	355/372 (95%)	353 (99%)	2 (1%)	78	87
6	G	735/736 (100%)	724 (98%)	11 (2%)	57	72
7	H	265/269 (98%)	263 (99%)	2 (1%)	73	84
8	I	128/154 (83%)	126 (98%)	2 (2%)	55	70
9	J	139/146 (95%)	139 (100%)	0	100	100
10	K	79/79 (100%)	78 (99%)	1 (1%)	61	76
11	L	485/485 (100%)	484 (100%)	1 (0%)	87	94
12	M	414/418 (99%)	408 (99%)	6 (1%)	59	73
13	N	385/385 (100%)	384 (100%)	1 (0%)	86	92
All	All	3879/4009 (97%)	3838 (99%)	41 (1%)	63	79

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	204	VAL
12	M	262	ILE
7	H	211	PRO
10	K	95	VAL
12	M	303	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
12	M	281	ASN
12	M	322	HIS
6	G	5	HIS
5	F	291	GLN
12	M	455	GLN

5.3.3 RNA ⓘ

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 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\# Z > 2$
17	FMN	F	502	-	33,33,33	0.35	0	48,50,50	0.43	0
14	3PE	L	703	-	46,46,50	0.31	0	49,51,55	0.44	0
15	SF4	G	1003	6	0,12,12	-	-	-		
14	3PE	N	502	-	50,50,50	0.28	0	53,55,55	0.33	0
15	SF4	G	1001	6	0,12,12	-	-	-		
14	3PE	M	601	-	38,38,50	0.31	0	41,43,55	0.37	0
14	3PE	J	201	-	41,41,50	0.31	0	44,46,55	0.33	0
14	3PE	L	701	-	39,39,50	0.31	0	42,44,55	0.33	0
15	SF4	B	301	2	0,12,12	-	-	-		
14	3PE	M	602	-	36,36,50	0.32	0	39,41,55	0.37	0
15	SF4	G	1002	6	0,12,12	-	-	-		
15	SF4	F	501	5	0,12,12	-	-	-		
14	3PE	N	501	-	46,46,50	0.29	0	49,51,55	0.41	0
14	3PE	A	201	-	35,35,50	0.33	0	38,40,55	0.36	0
15	SF4	I	201	8	0,12,12	-	-	-		
14	3PE	L	704	-	50,50,50	0.30	0	53,55,55	0.32	0
15	SF4	I	202	8	0,12,12	-	-	-		
16	FES	G	1004	6	0,4,4	-	-	-		
14	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.32	0
16	FES	E	201	4	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
17	FMN	F	502	-	-	9/18/18/18	0/3/3/3
14	3PE	L	703	-	-	9/50/50/54	-
15	SF4	G	1003	6	-	-	0/6/5/5
14	3PE	N	502	-	-	7/54/54/54	-
15	SF4	G	1001	6	-	-	0/6/5/5
14	3PE	M	601	-	-	8/42/42/54	-
14	3PE	J	201	-	-	9/45/45/54	-
14	3PE	L	701	-	-	6/43/43/54	-
15	SF4	B	301	2	-	-	0/6/5/5
14	3PE	M	602	-	-	13/40/40/54	-
15	SF4	G	1002	6	-	-	0/6/5/5
15	SF4	F	501	5	-	-	0/6/5/5
14	3PE	N	501	-	-	15/50/50/54	-
14	3PE	A	201	-	-	9/39/39/54	-
15	SF4	I	201	8	-	-	0/6/5/5
14	3PE	L	704	-	-	32/54/54/54	-
15	SF4	I	202	8	-	-	0/6/5/5
16	FES	G	1004	6	-	-	0/1/1/1
14	3PE	L	702	-	-	15/54/54/54	-
16	FES	E	201	4	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

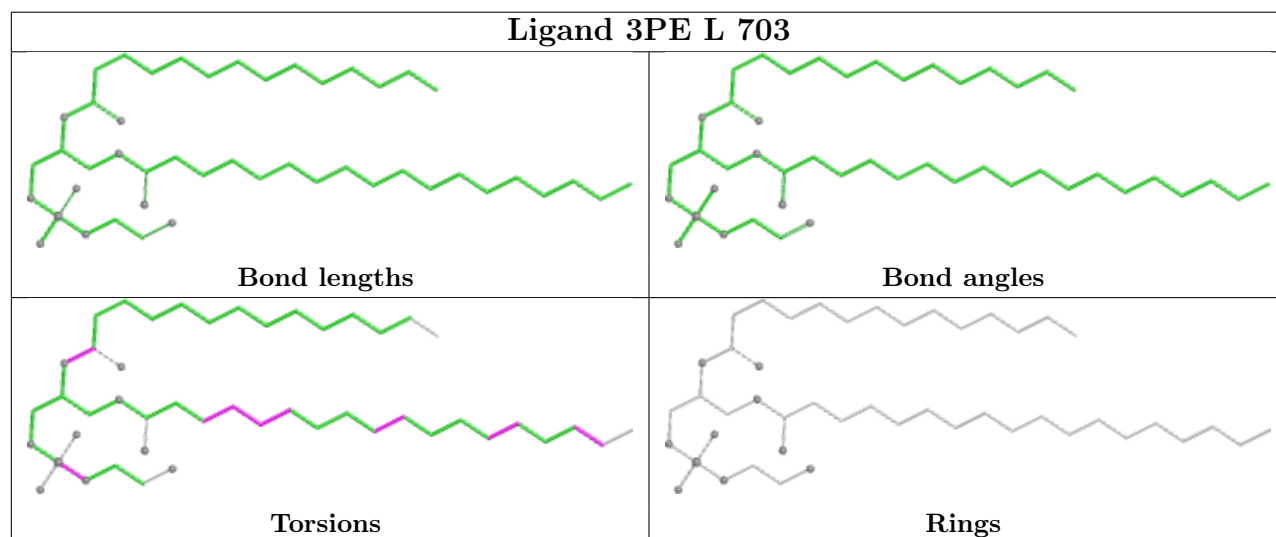
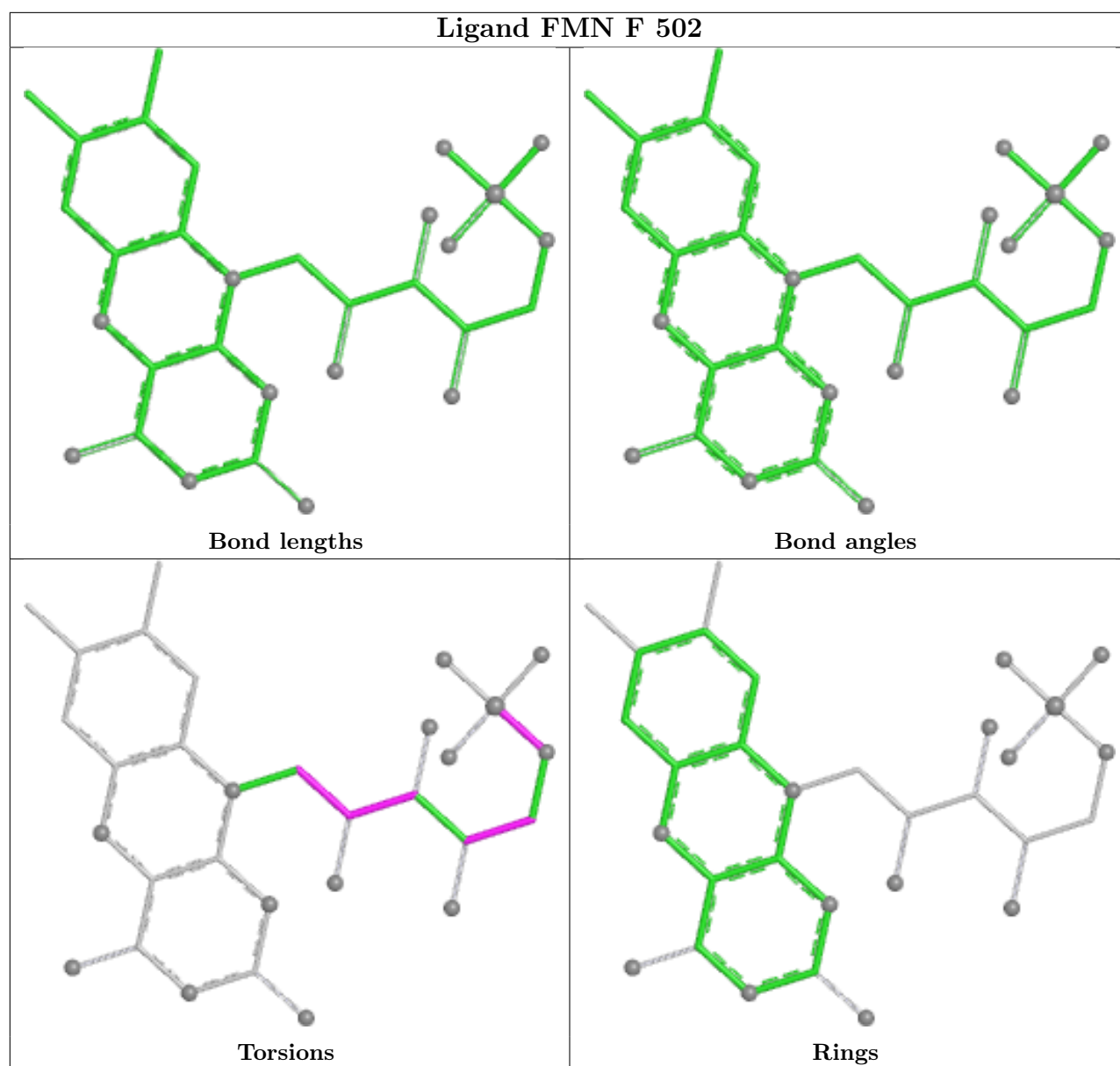
Mol	Chain	Res	Type	Atoms
14	L	701	3PE	C2-C1-O11-P
14	L	702	3PE	C1-O11-P-O14
14	L	702	3PE	C12-C11-O13-P
14	L	702	3PE	O32-C31-O31-C3
14	L	702	3PE	C32-C31-O31-C3

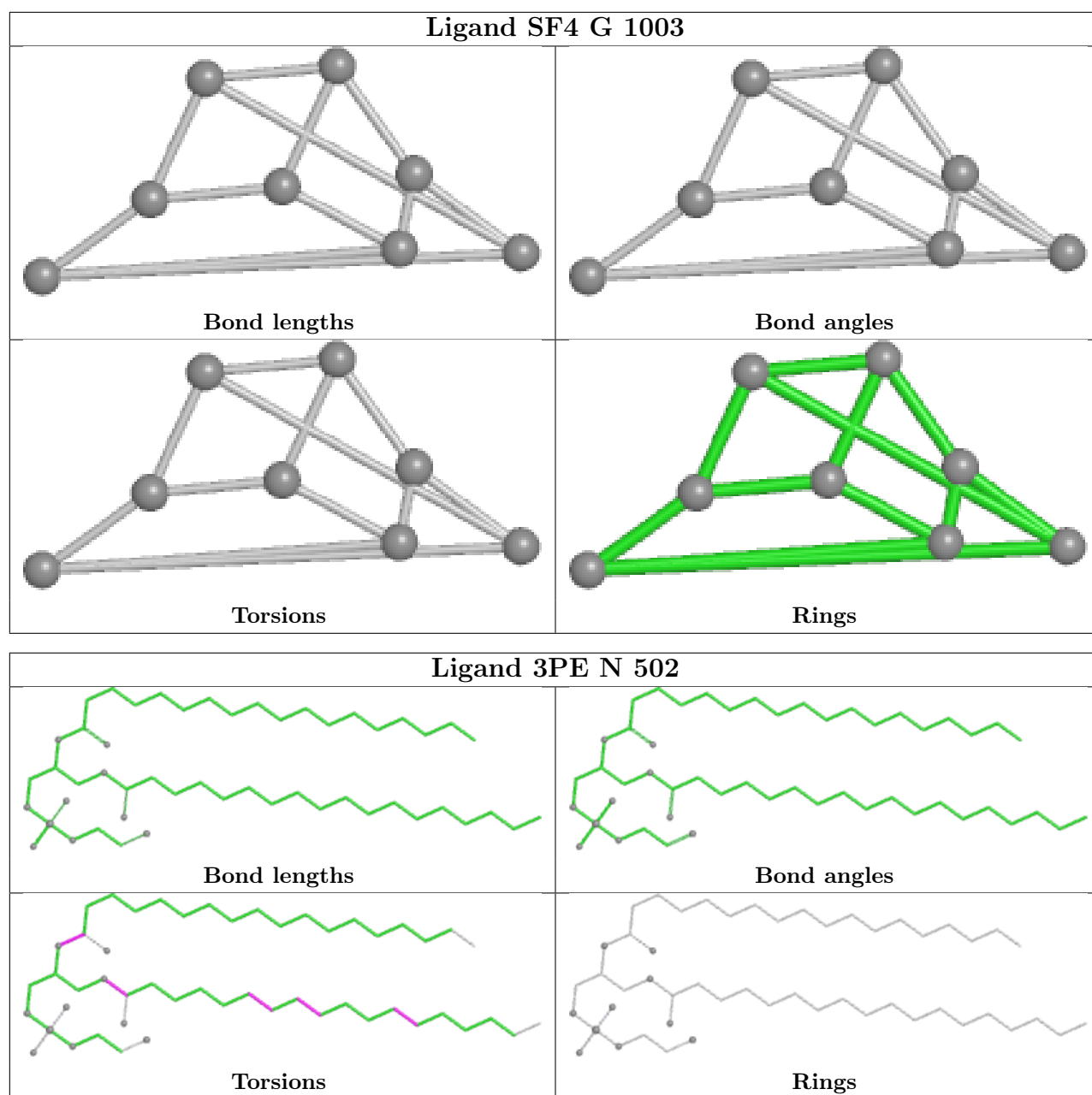
There are no ring outliers.

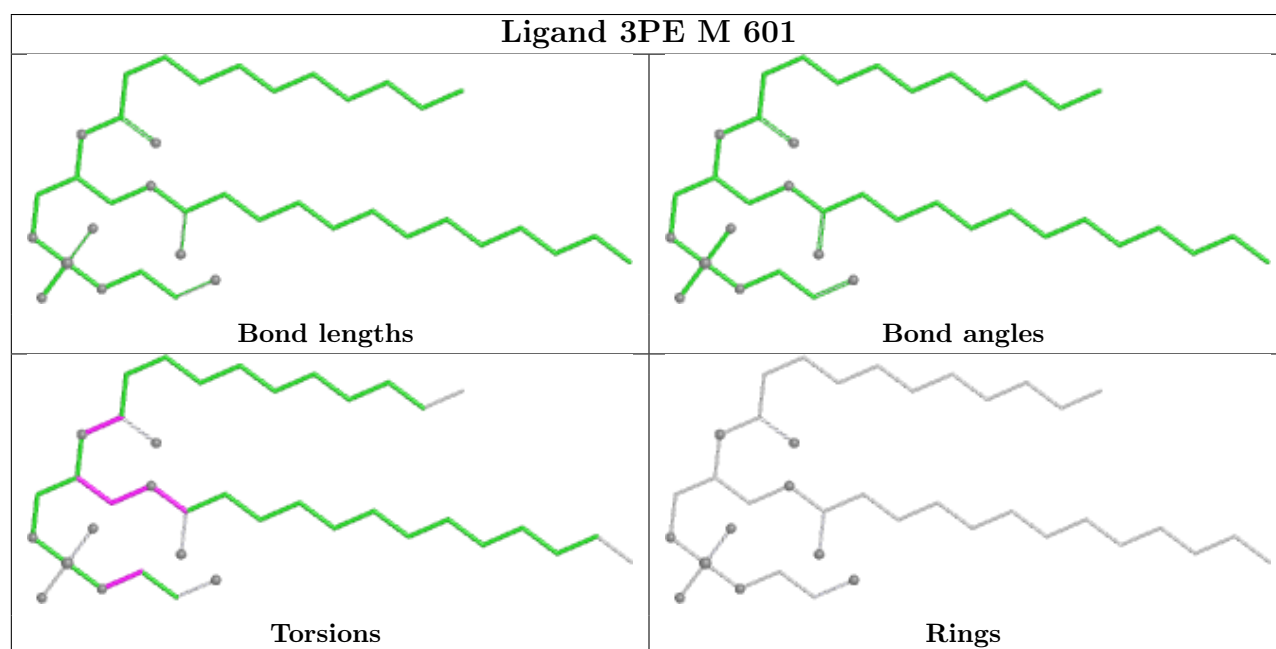
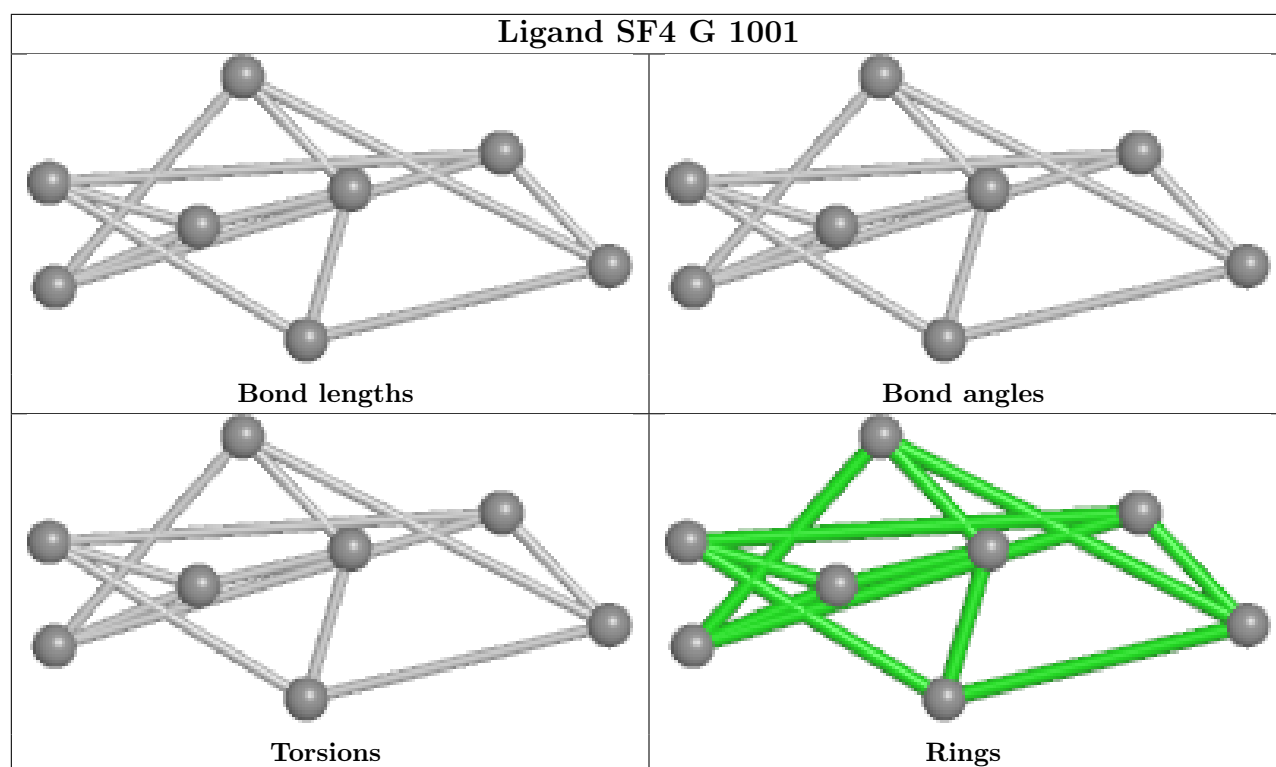
13 monomers are involved in 32 short contacts:

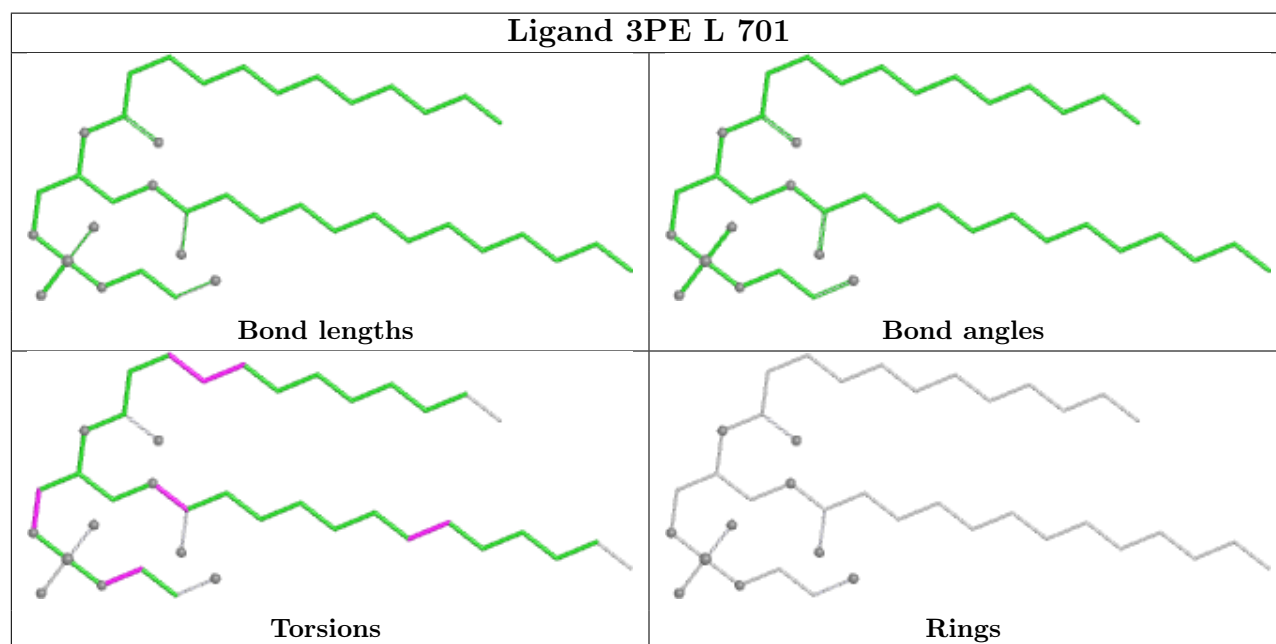
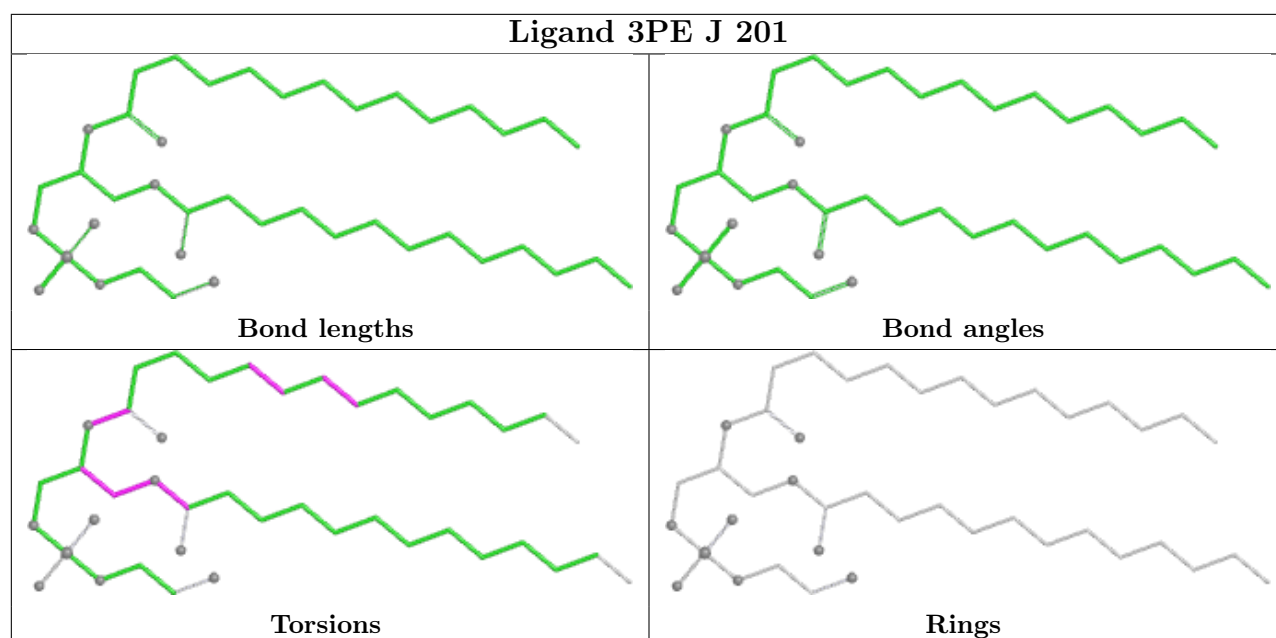
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	F	502	FMN	2	0
14	L	703	3PE	2	0
14	N	502	3PE	4	0
14	M	601	3PE	2	0
14	J	201	3PE	2	0
14	L	701	3PE	3	0
14	M	602	3PE	2	0
14	N	501	3PE	4	0
14	A	201	3PE	4	0
14	L	704	3PE	1	0
16	G	1004	FES	1	0
14	L	702	3PE	6	0
16	E	201	FES	1	0

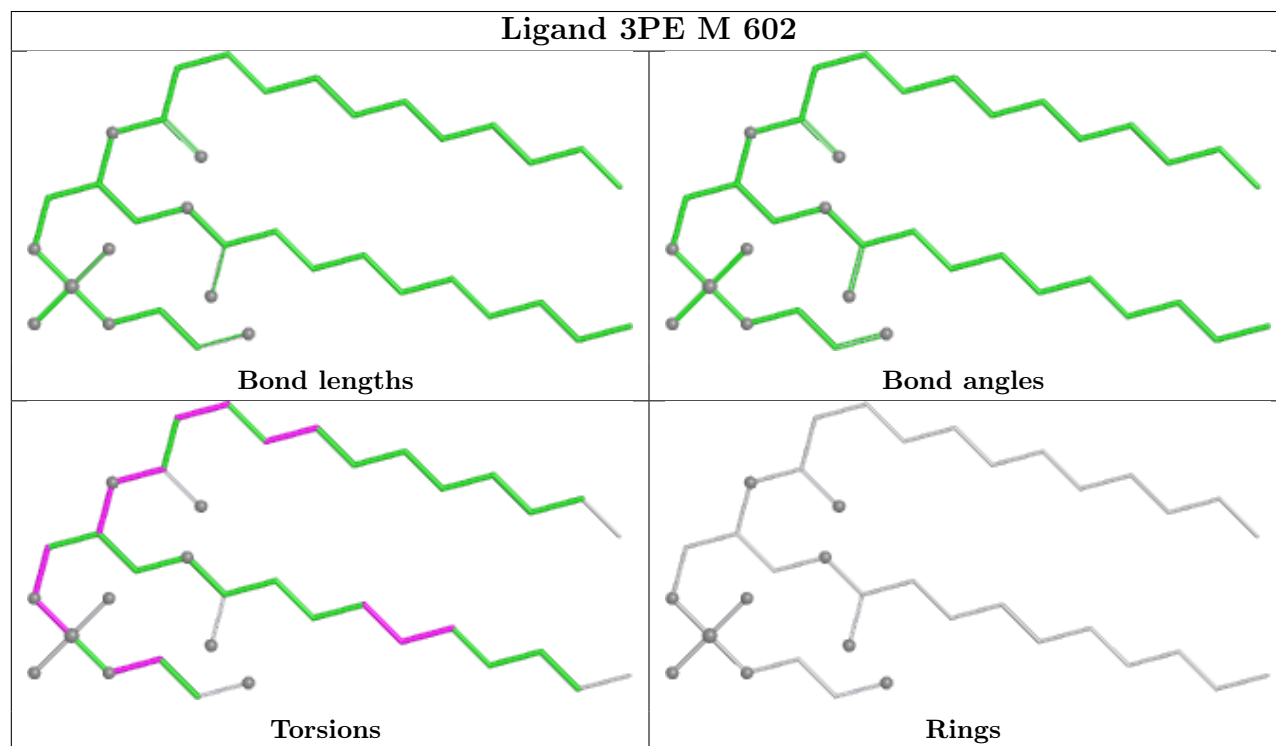
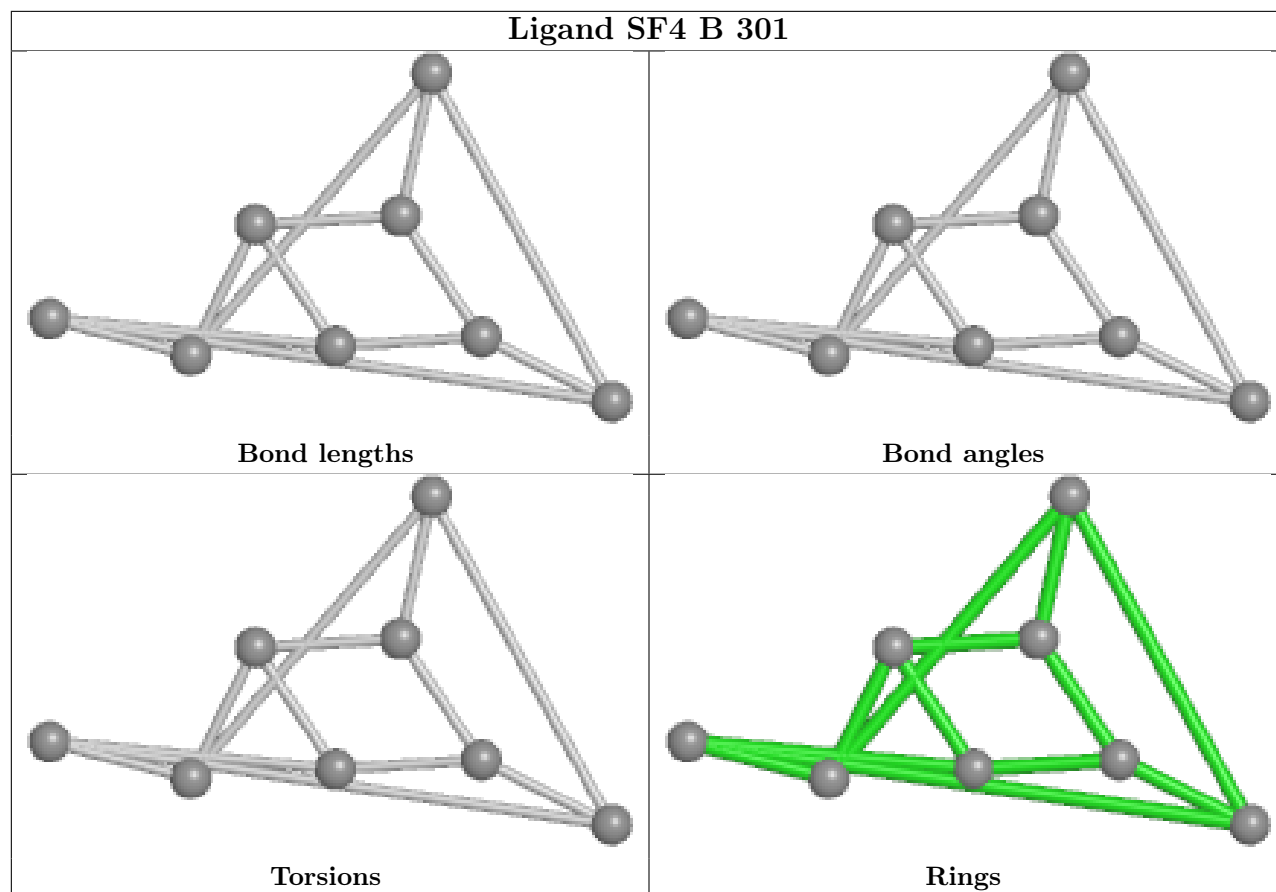
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

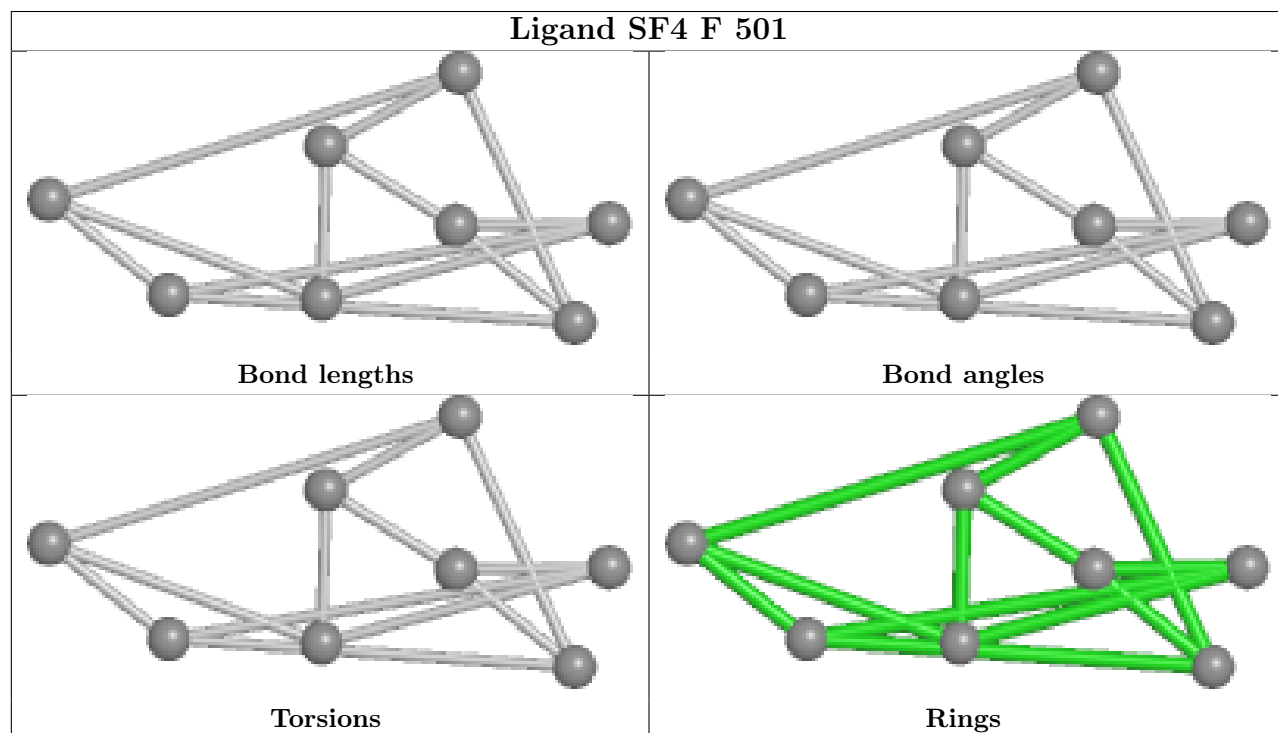
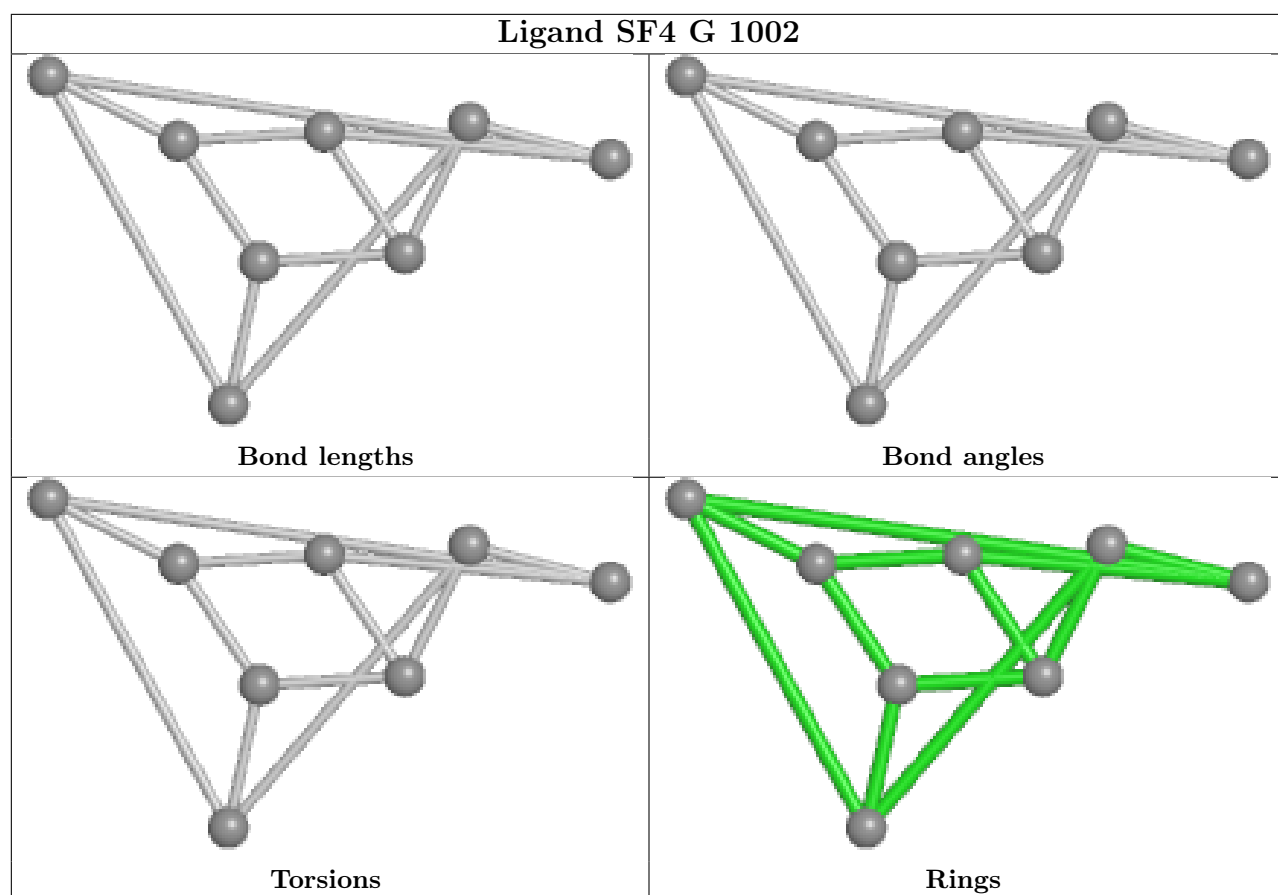


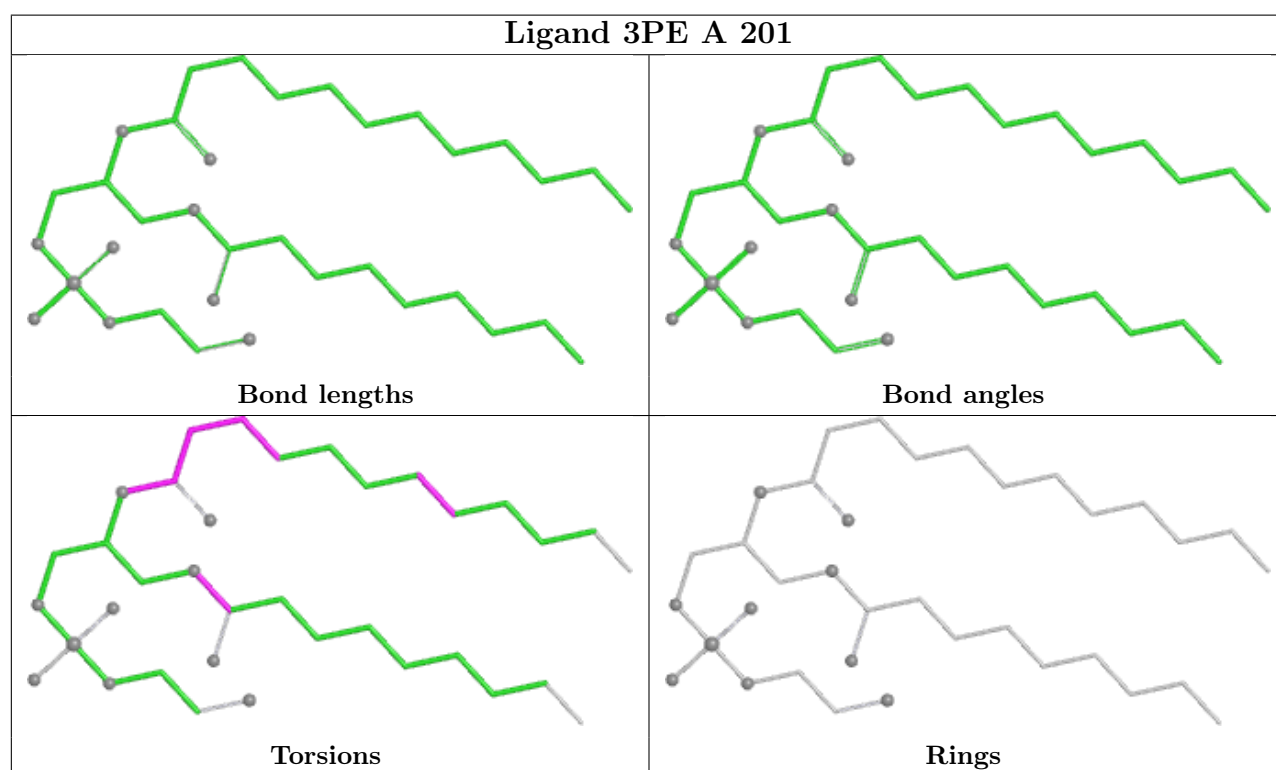
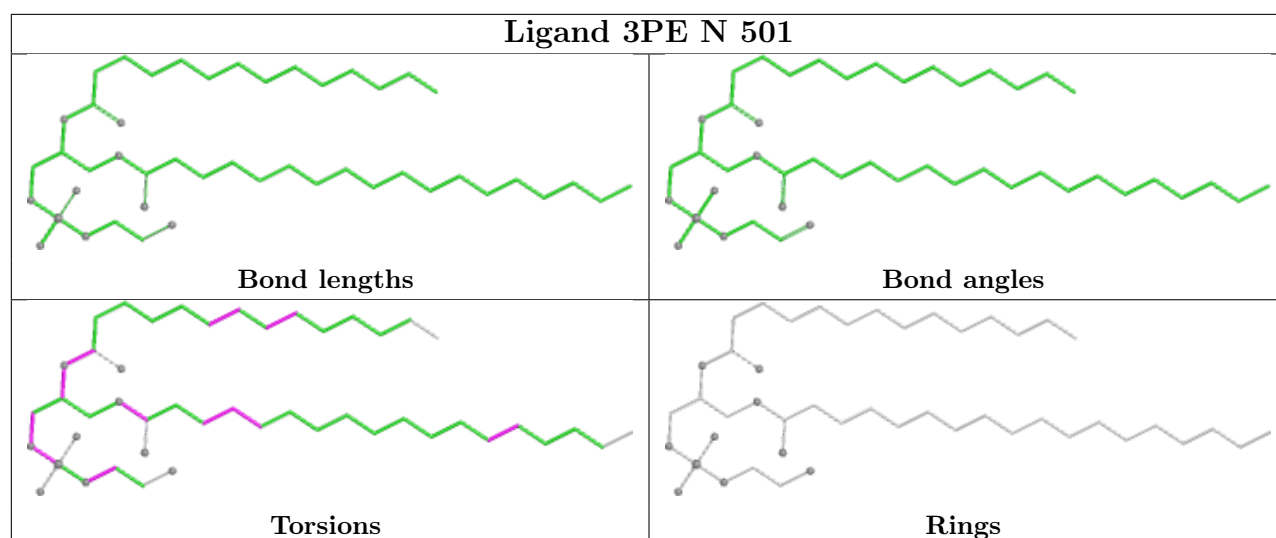


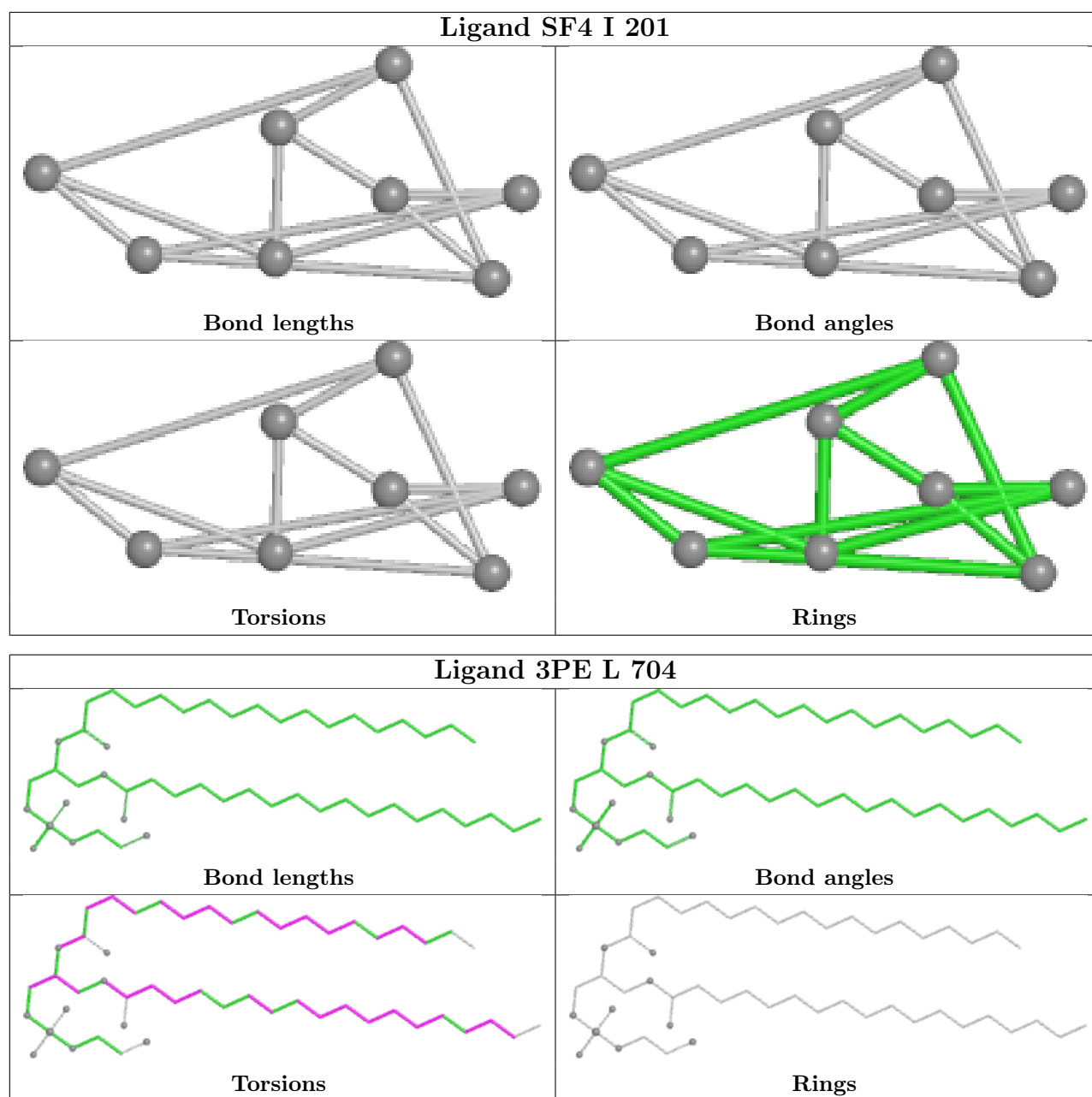


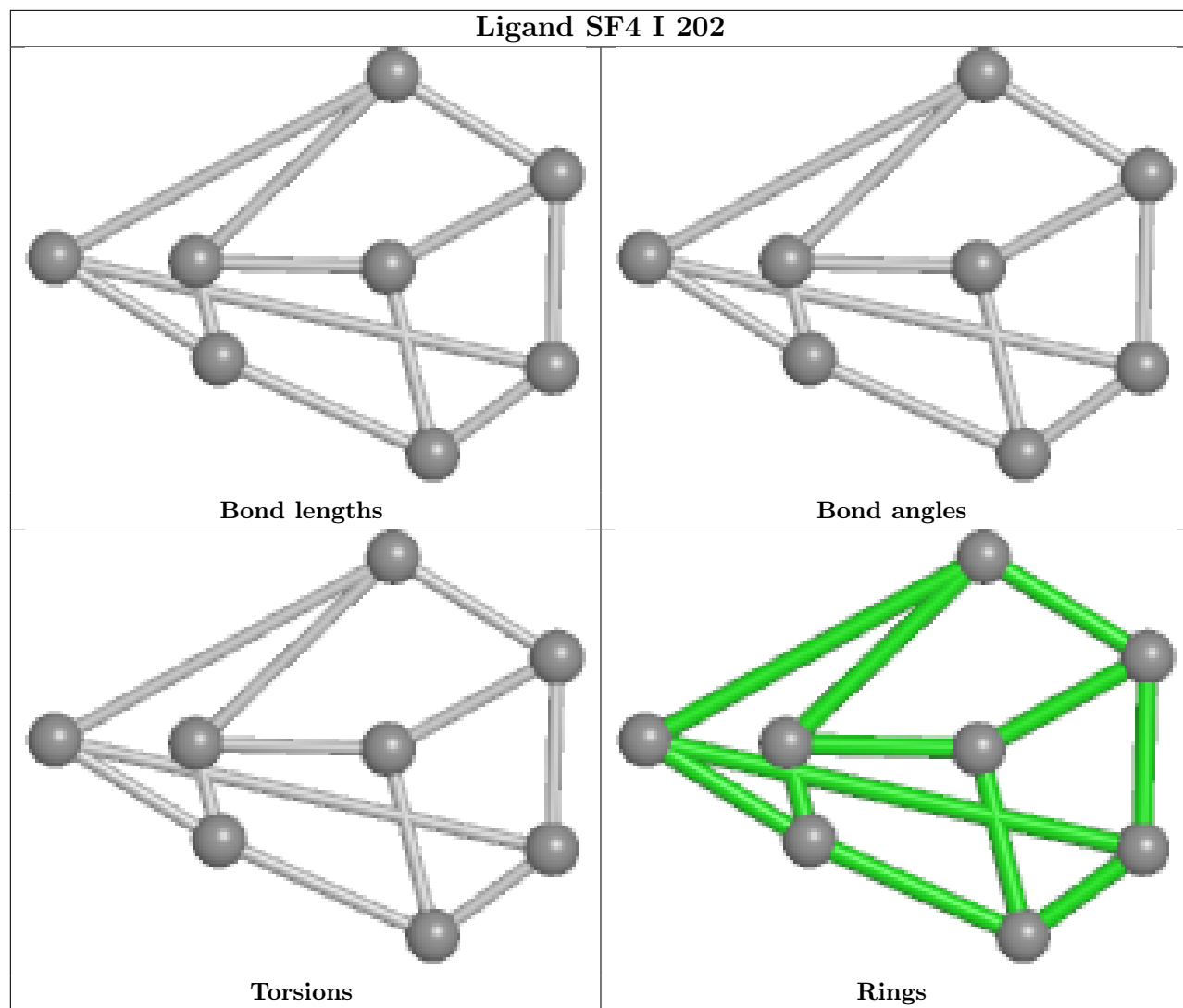


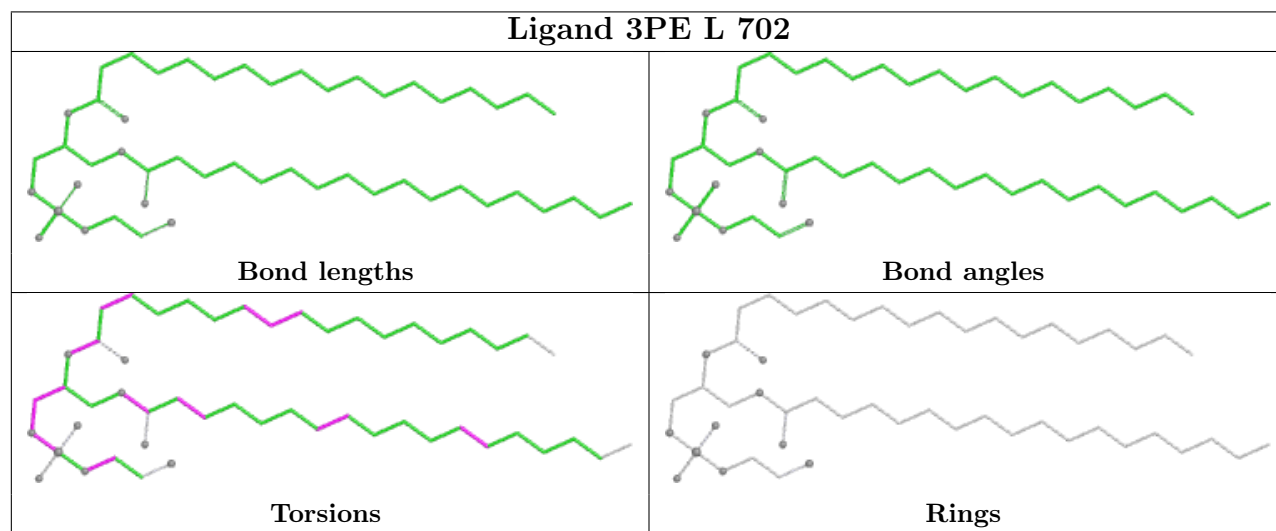
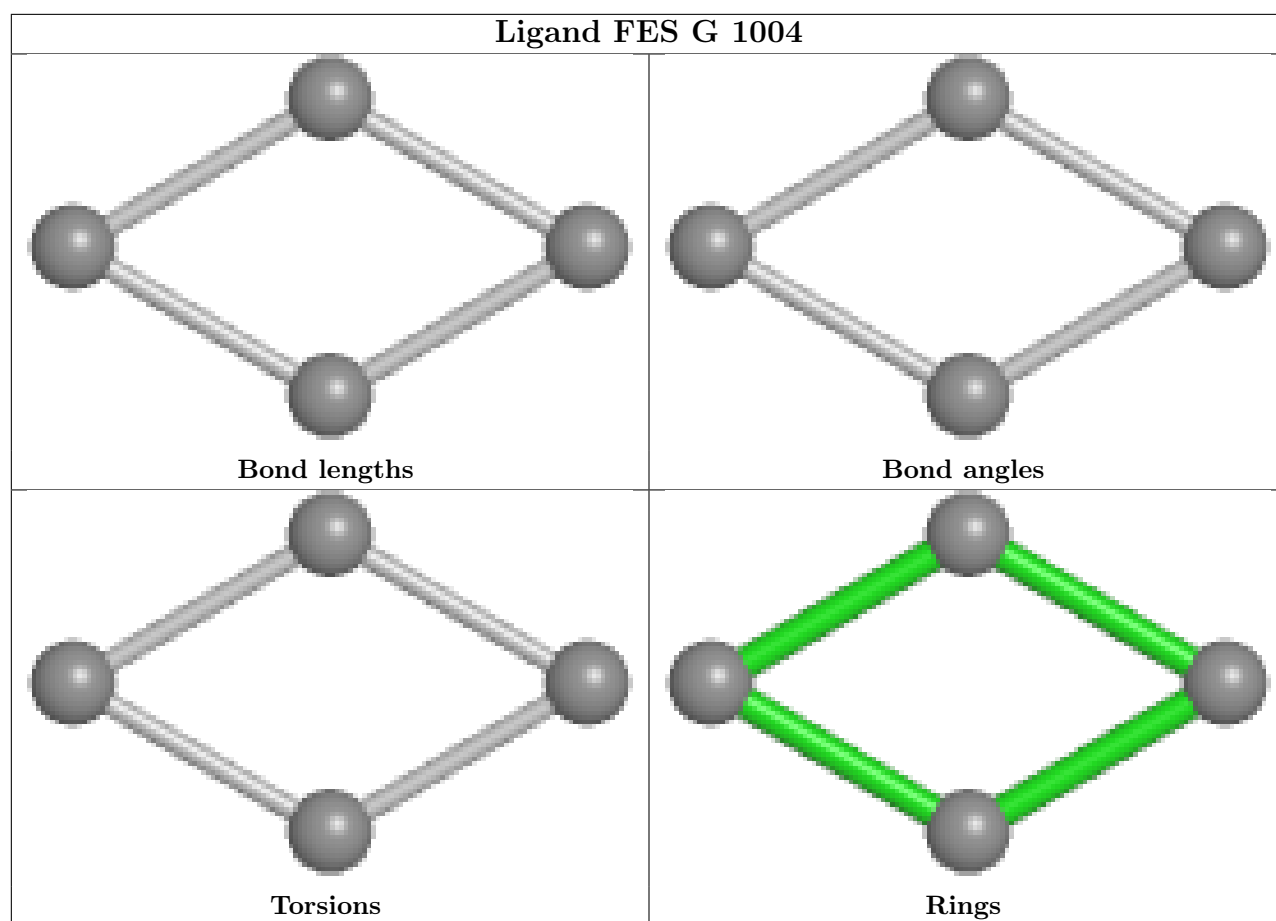


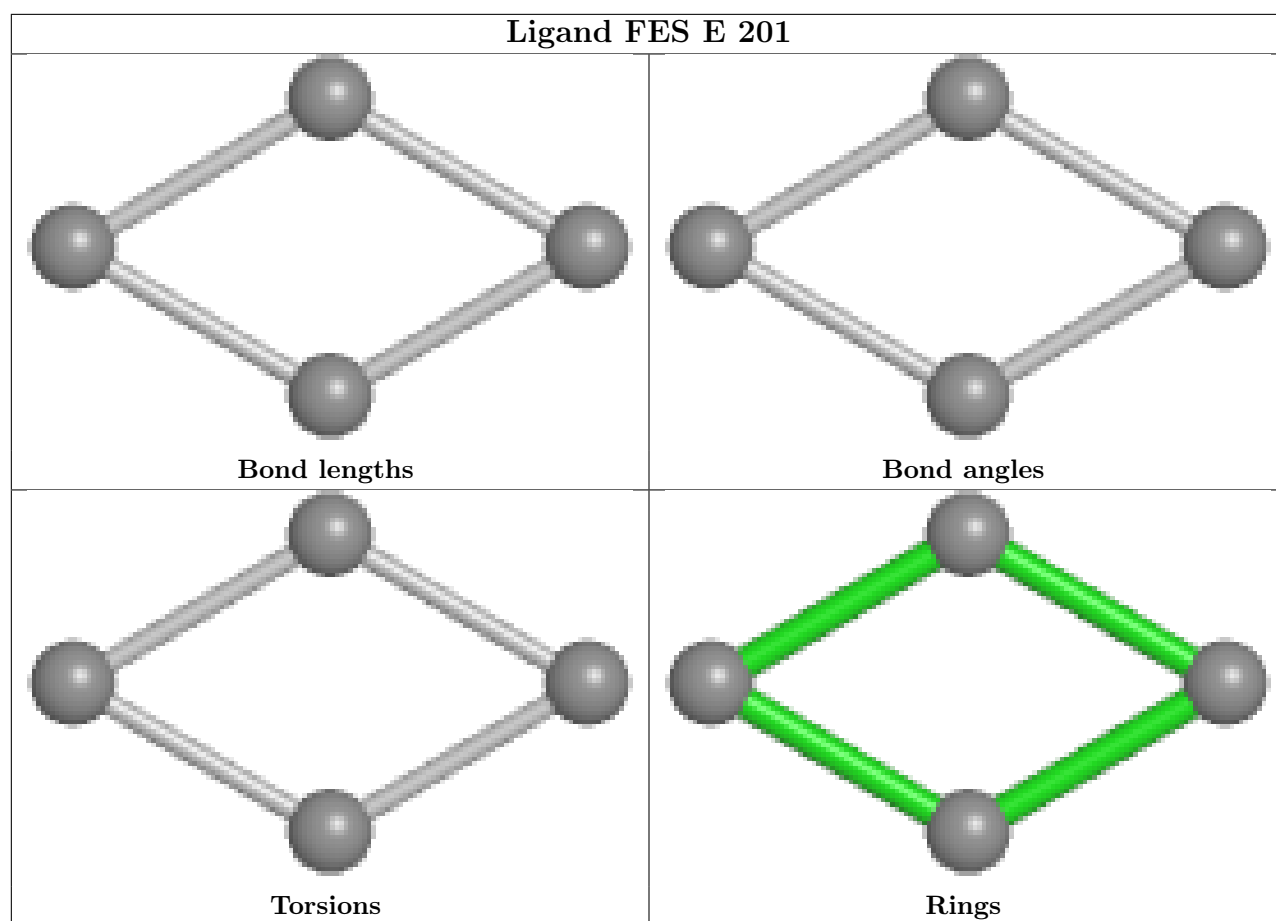












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

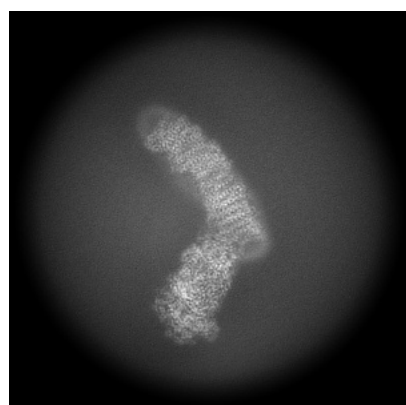
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52895. These allow visual inspection of the internal detail of the map and identification of artifacts.

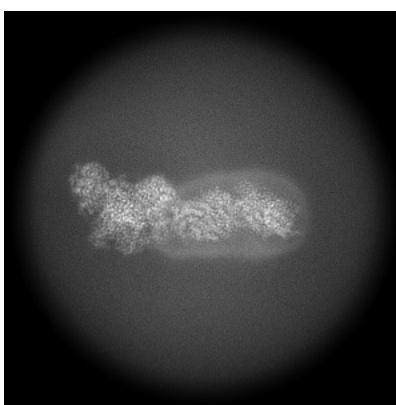
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

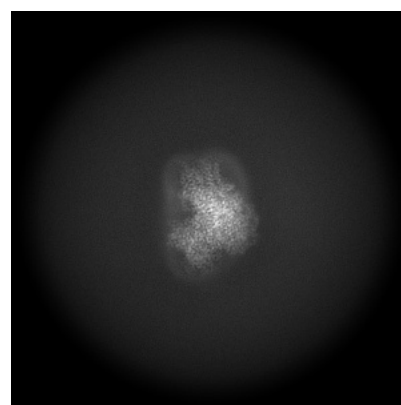
6.1.1 Primary map



X



Y

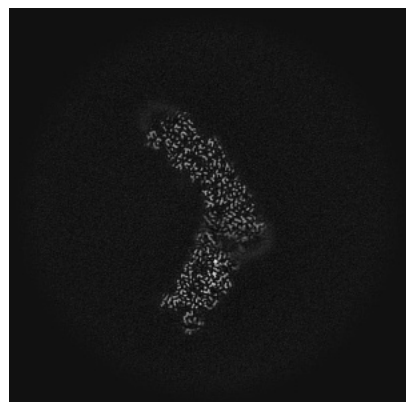


Z

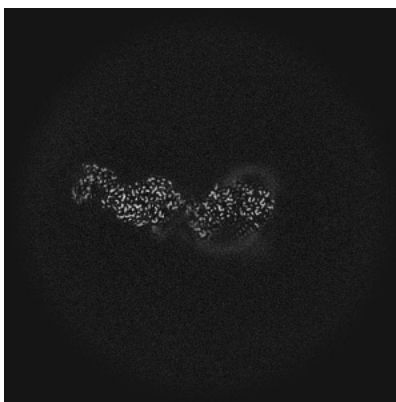
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

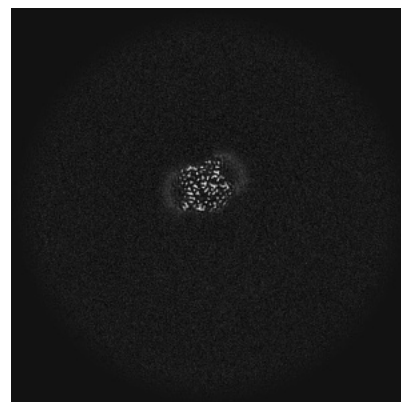
6.2.1 Primary map



X Index: 200



Y Index: 200

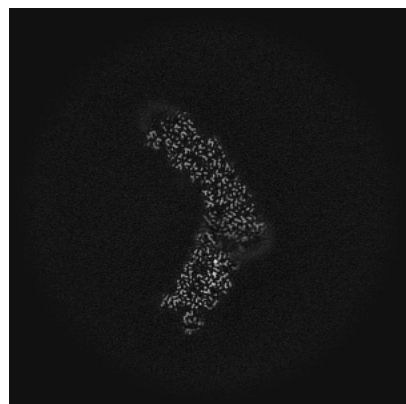


Z Index: 200

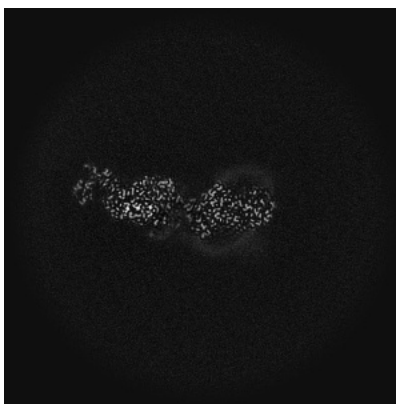
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

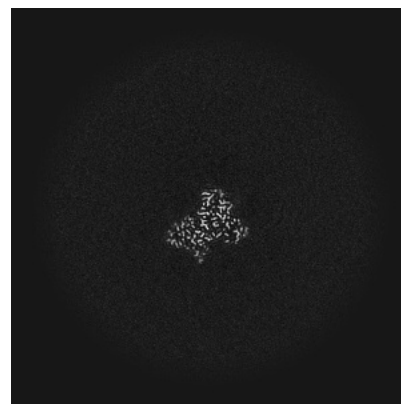
6.3.1 Primary map



X Index: 200



Y Index: 205



Z Index: 119

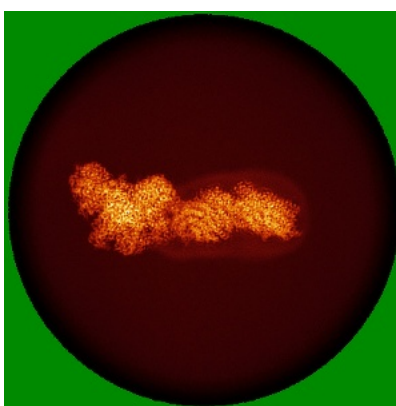
The images above show the largest variance slices of the map in three orthogonal directions.

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

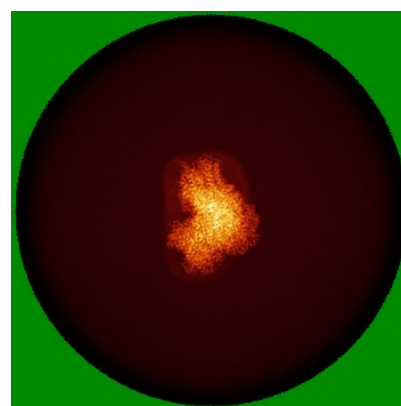
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

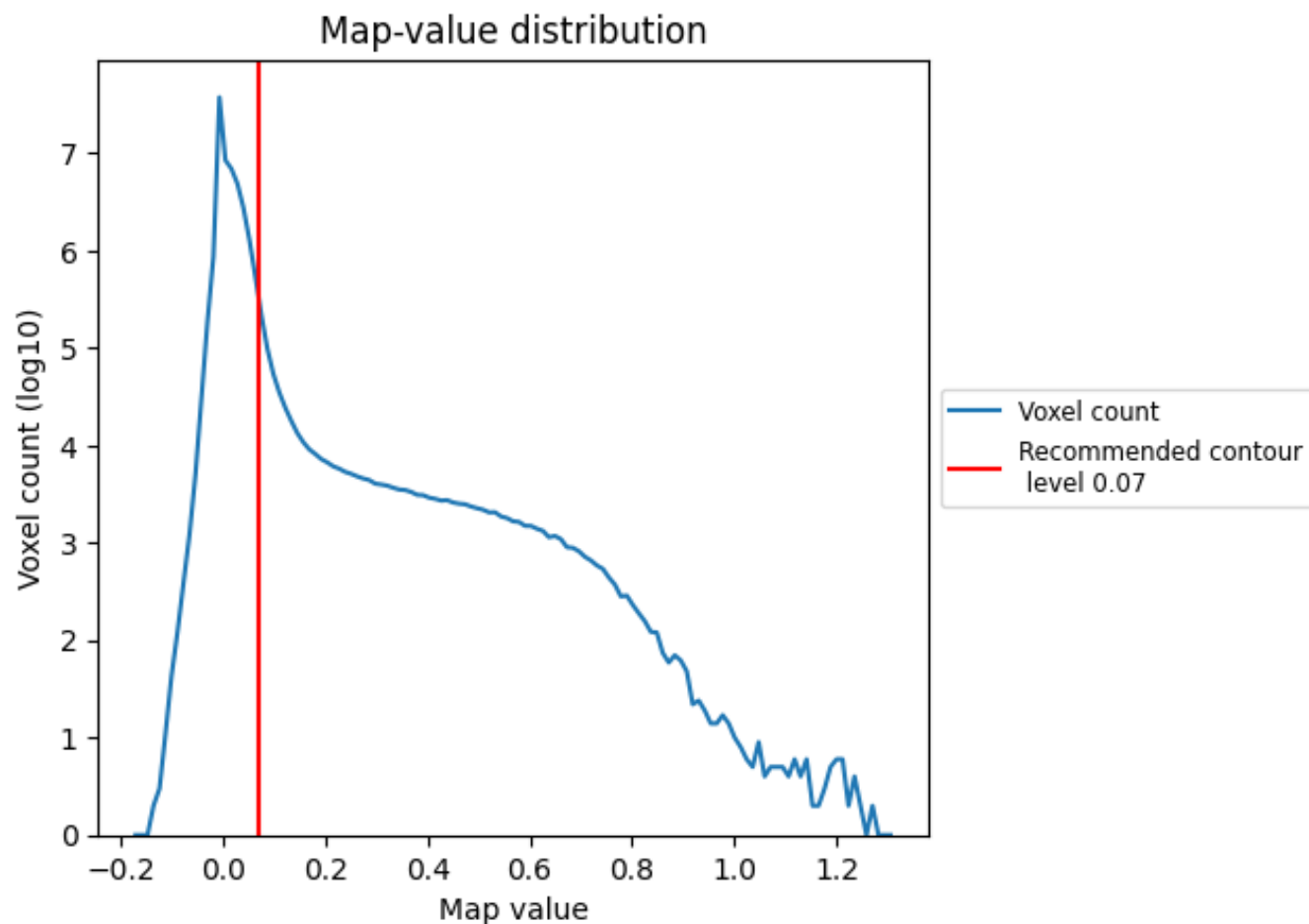
6.6 Mask visualisation

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

7 Map analysis [i](#)

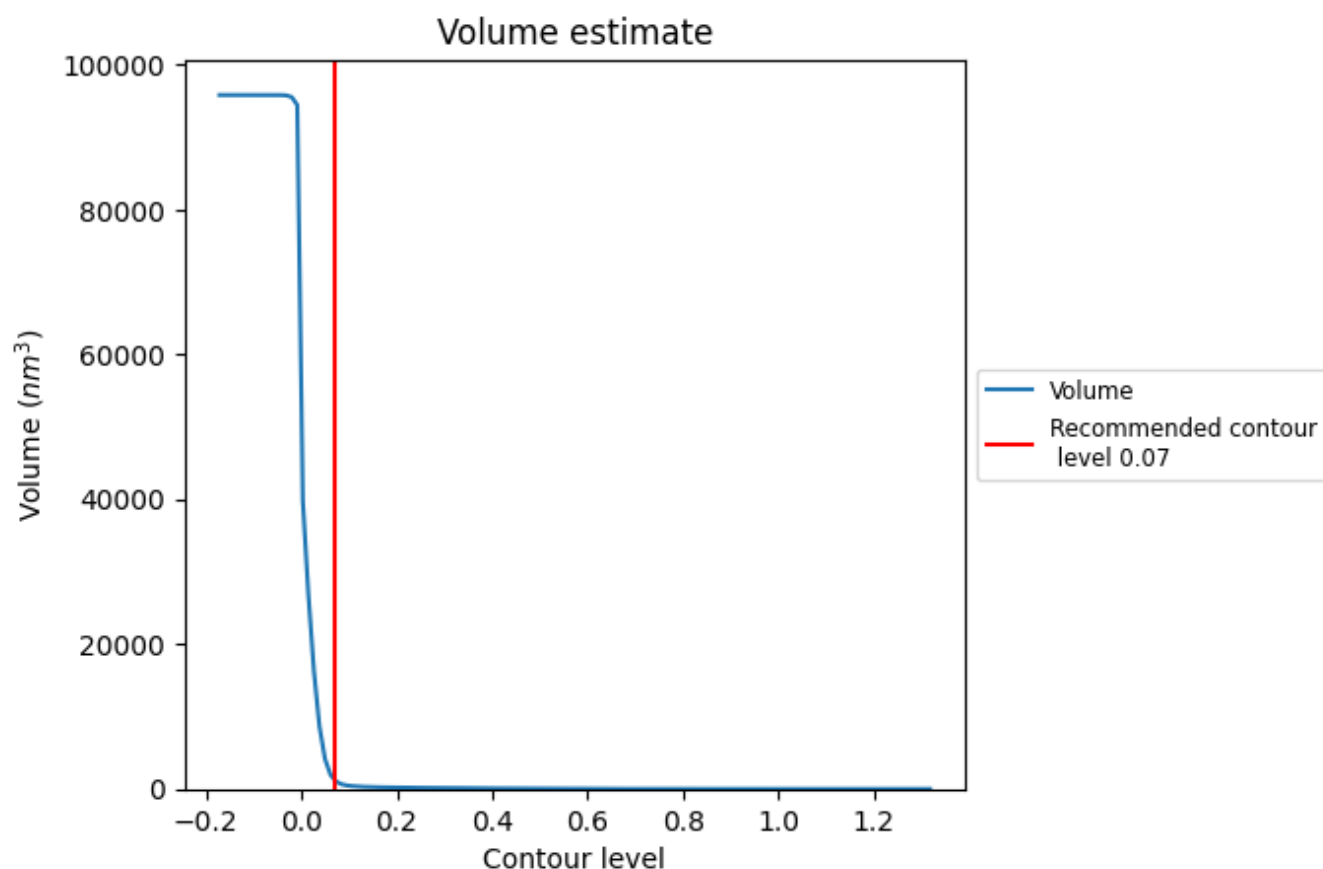
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

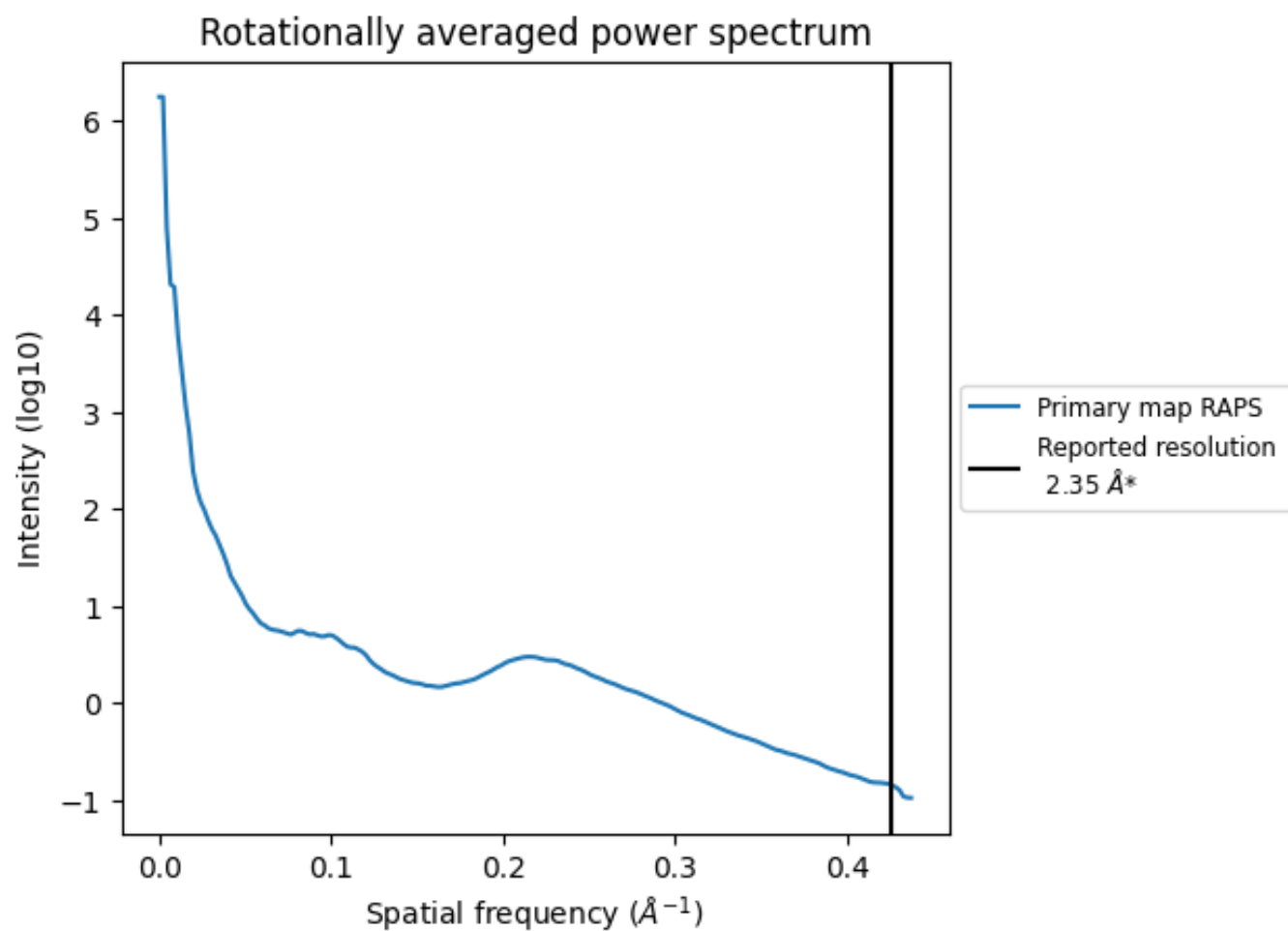
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1253 nm³; this corresponds to an approximate mass of 1132 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 0.426 Å⁻¹

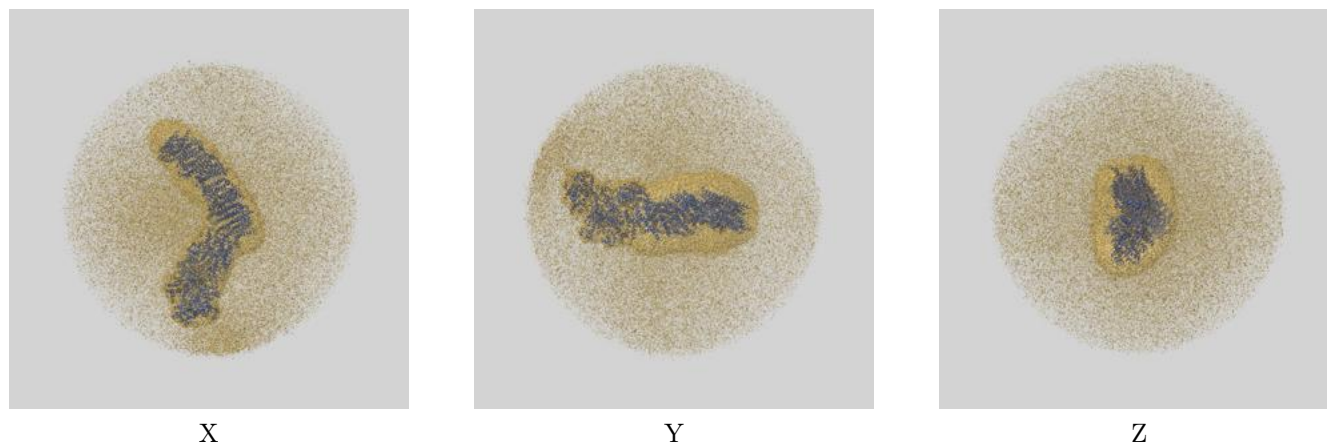
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

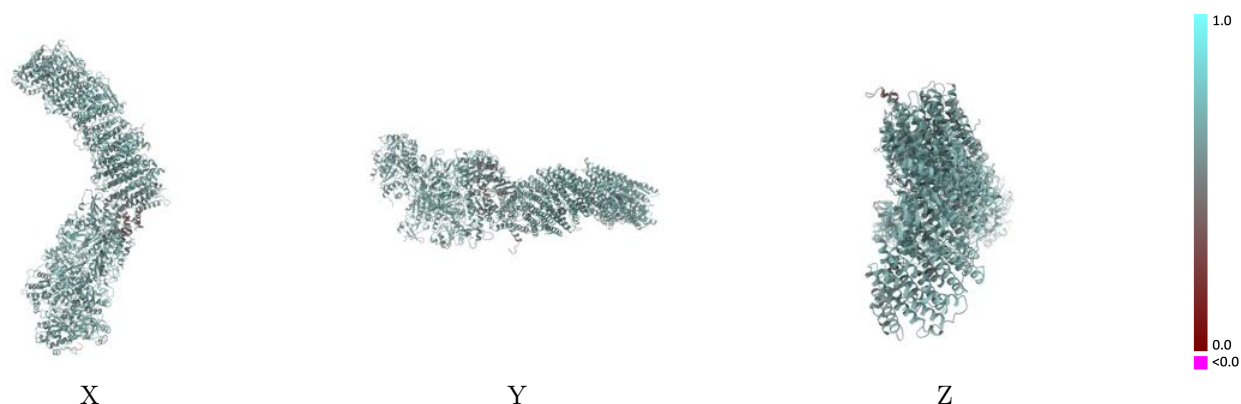
This section contains information regarding the fit between EMDB map EMD-52895 and PDB model 9Q8I. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.07 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](#)

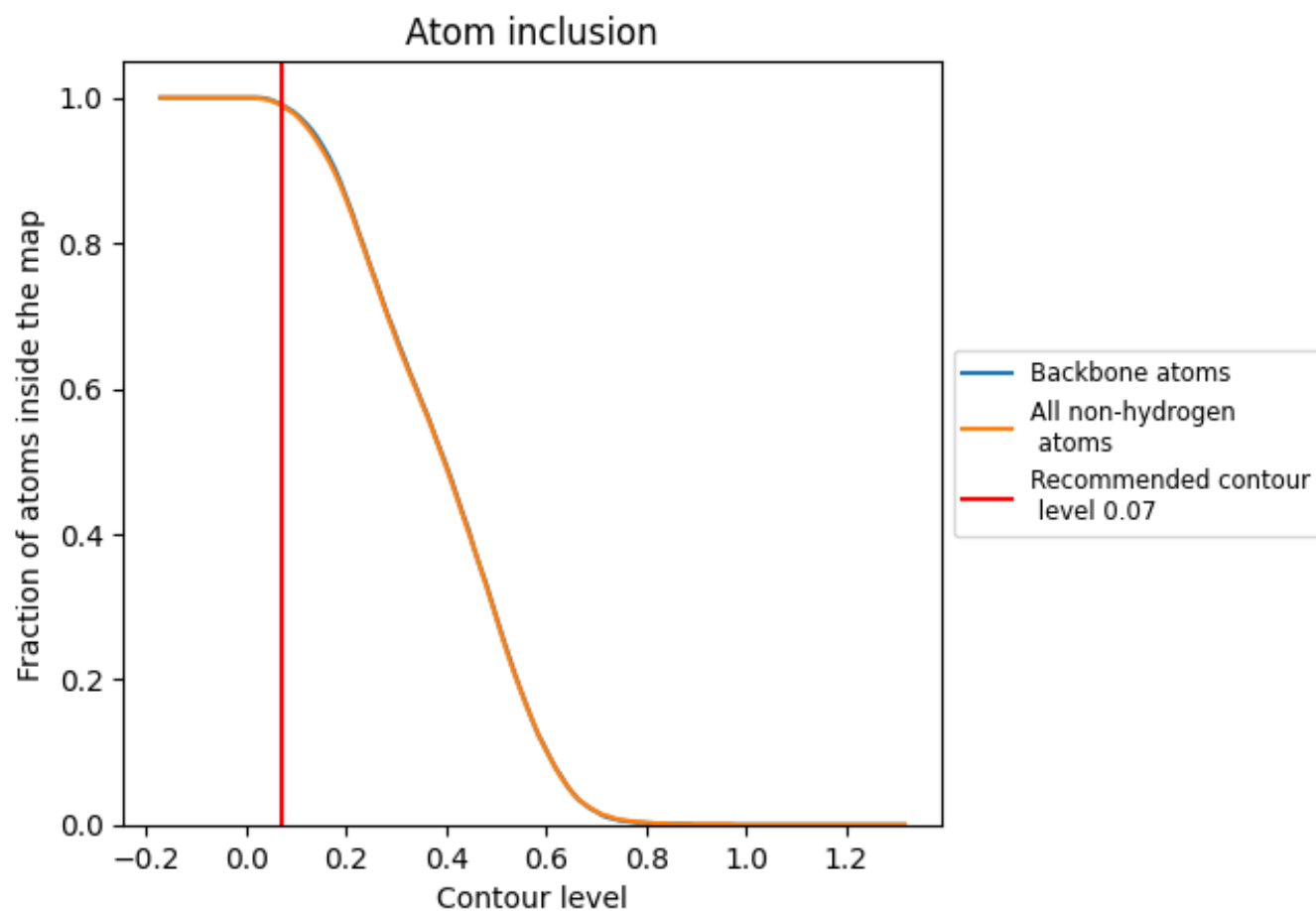


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9900	0.6190
A	0.9910	0.6010
B	0.9780	0.5890
C	0.9890	0.6130
E	0.9870	0.5950
F	0.9880	0.6100
G	0.9910	0.6340
H	0.9890	0.5760
I	0.9920	0.6410
J	0.9920	0.6170
K	0.9950	0.6460
L	0.9890	0.6160
M	0.9940	0.6360
N	0.9950	0.6310

1.0

0.0

<0.0