



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 02:55 pm BST

PDB ID : 9TAJ / pdb_00009taj
EMDB ID : EMD-55748
Title : E. coli Complex I WT purified in LMNG
Authors : Kovalova, T.; Beghiah, A.; Kaila, V.R.I.
Deposited on : 2025-11-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

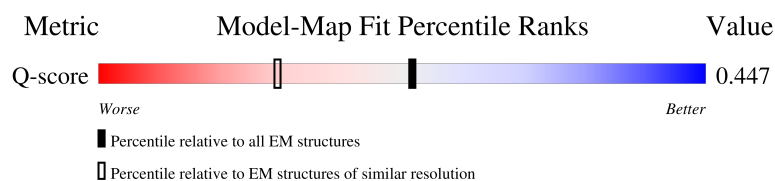
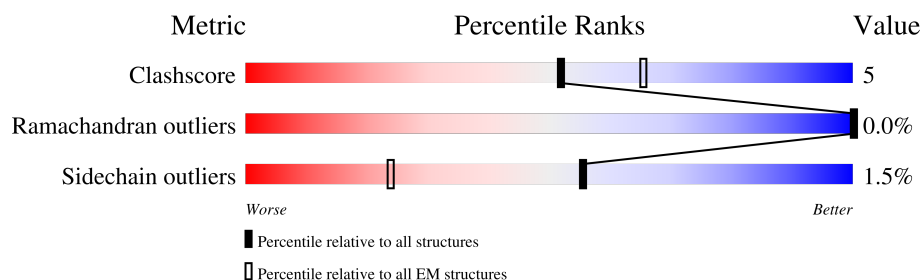
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



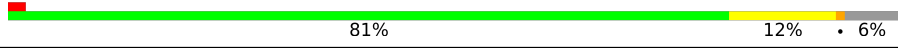
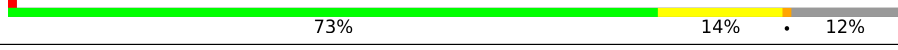
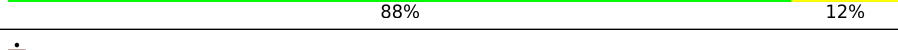
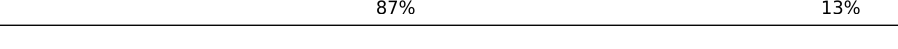
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	E	166	
2	F	461	
3	G	910	
4	I	180	

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Mol	Chain	Length	Quality of chain
5	B	220	
6	C	600	
7	H	325	
8	J	184	
9	K	100	
10	M	509	
11	A	147	
12	L	613	
13	N	485	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	B	301	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 38186 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 E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	156	Total	C	N	O	S	0	0
			1220	768	215	229	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	439	Total	C	N	O	S	0	0
			3407	2162	596	629	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 3 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	905	Total	C	N	O	S	0	0
			7027	4392	1269	1329	37		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P33602
G	2	LEU	-	expression tag	UNP P33602

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	145	Total	C	N	O	S	0	0
			1149	728	192	217	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	195	Total	C	N	O	S	0	0
			1551	985	269	281	16		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	589	Total	C	N	O	S	0	0
			4760	3049	828	859	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P33599
C	2	VAL	-	expression tag	UNP P33599
C	3	ASN	-	expression tag	UNP P33599
C	4	ASN	-	expression tag	UNP P33599

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	307	Total	C	N	O	S	0	0
			2404	1614	373	399	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	504	Total	C	N	O	S	1	0
			3964	2671	618	646	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	98	Total	C	N	O	S	0	0
			788	543	120	121	4		

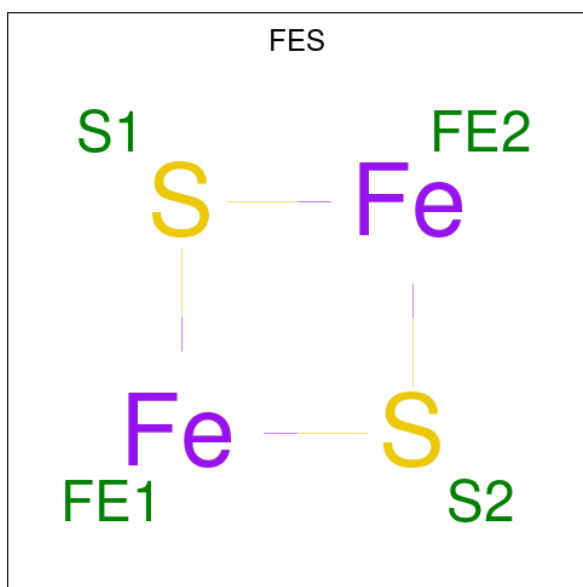
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit L.

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

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

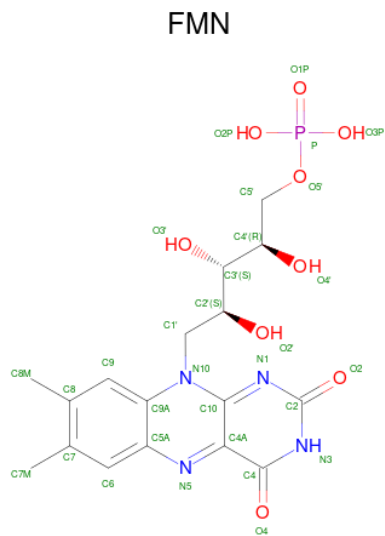


Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	Fe	S	0
			4	2	2	
14	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

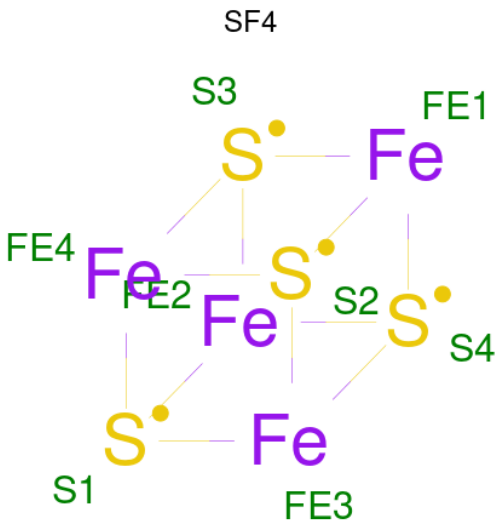
Mol	Chain	Residues	Atoms		AltConf
15	E	1	Total	Ca	0
			1	1	
15	G	3	Total	Ca	0
			3	3	
15	I	1	Total	Ca	0
			1	1	

- Molecule 16 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



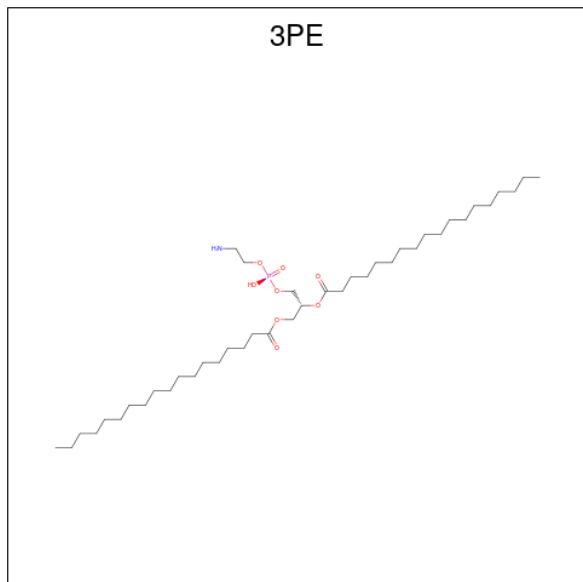
Mol	Chain	Residues	Atoms			AltConf
17	F	1	Total 8	Fe 4	S 4	0
17	G	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	I	1	Total	Fe	S	0
			8	4	4	
17	I	1	Total	Fe	S	0
			8	4	4	
17	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



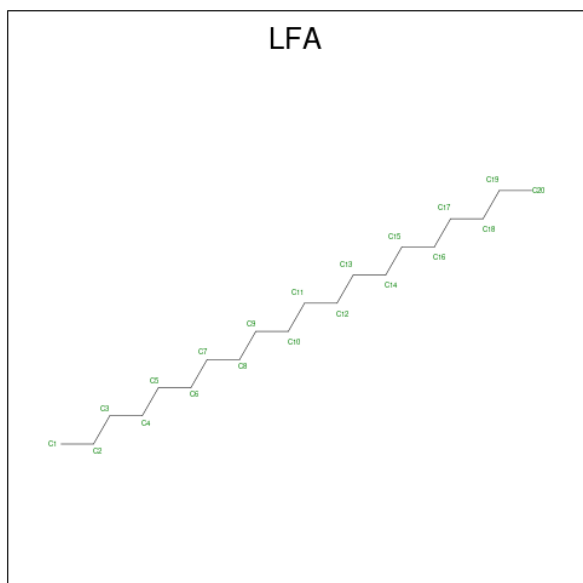
Mol	Chain	Residues	Atoms					AltConf
18	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	M	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	M	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
18	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 19 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



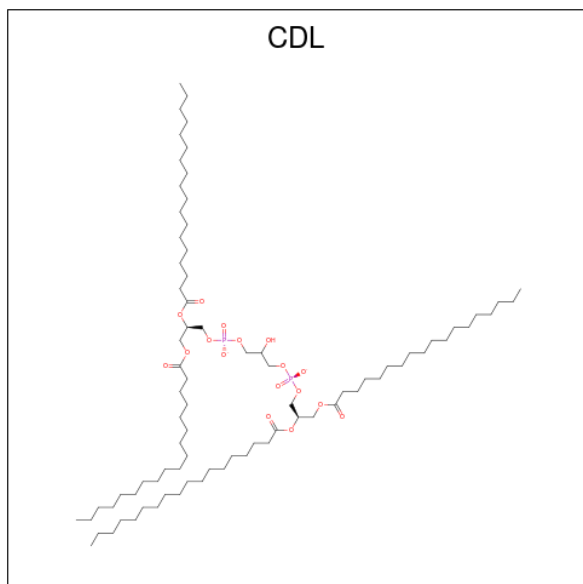
Mol	Chain	Residues	Atoms		AltConf
19	H	1	Total	C	0
			20	20	

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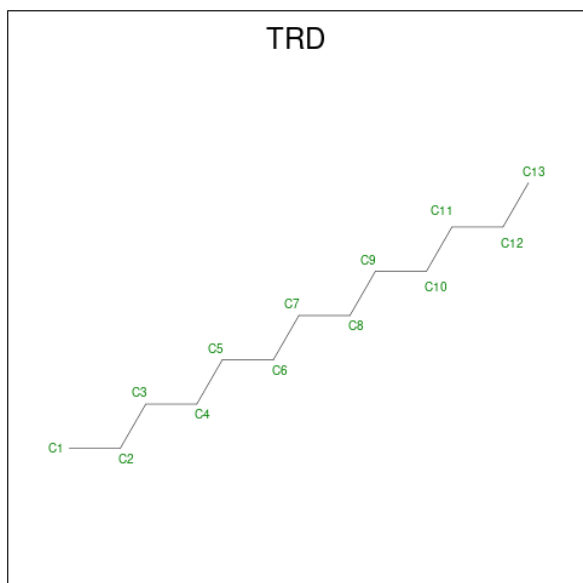
Mol	Chain	Residues	Atoms		AltConf
19	N	1	Total	C	0
			20	20	

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



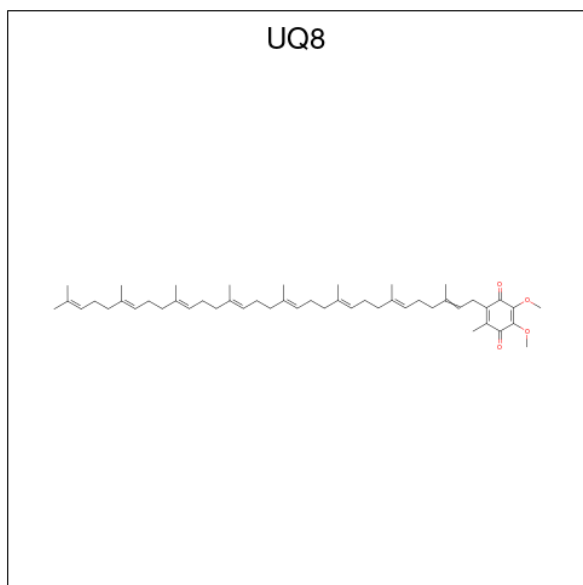
Mol	Chain	Residues	Atoms				AltConf
20	L	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 21 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



Mol	Chain	Residues	Atoms	AltConf
21	L	1	Total C 13 13	0
21	L	1	Total C 13 13	0
21	N	1	Total C 13 13	0

- Molecule 22 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	N	1	Total C O 53 49 4	0
22	N	1	Total C O 53 49 4	0

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	AltConf
23	E	5	Total O 5 5	0
23	F	42	Total O 42 42	0
23	G	138	Total O 138 138	0
23	I	18	Total O 18 18	0

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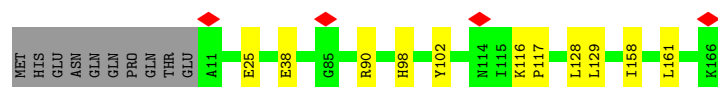
Mol	Chain	Residues	Atoms		AltConf
23	B	6	Total 6	O 6	0
23	C	53	Total 53	O 53	0
23	H	22	Total 22	O 22	0
23	J	8	Total 8	O 8	0
23	K	10	Total 10	O 10	0
23	M	40	Total 40	O 40	0
23	A	6	Total 6	O 6	0
23	L	44	Total 44	O 44	0
23	N	36	Total 36	O 36	0

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.

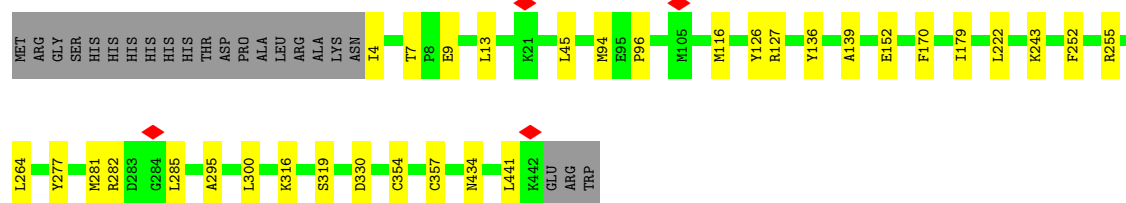
- Molecule 1: NADH-quinone oxidoreductase subunit E

Chain E: 



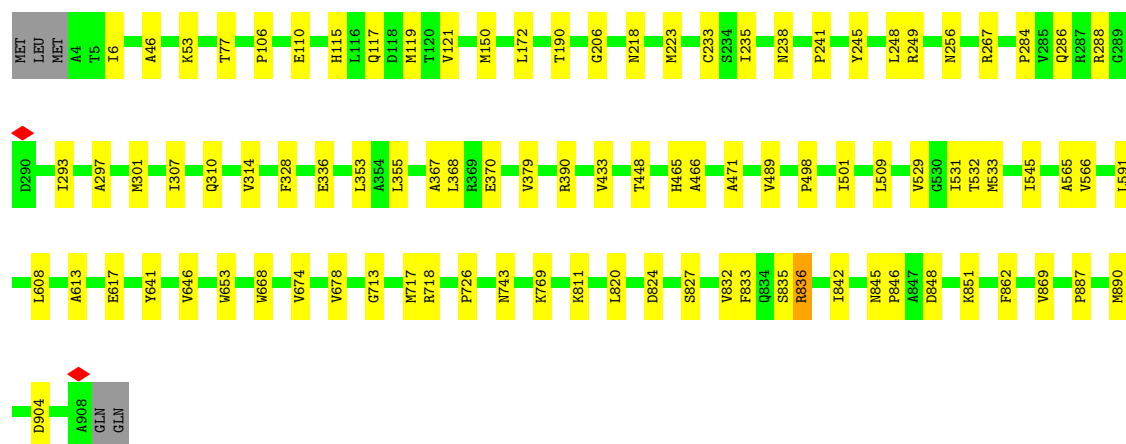
- Molecule 2: NADH-quinone oxidoreductase subunit F

Chain F: 



- Molecule 3: NADH-quinone oxidoreductase subunit G

Chain G: 



- Molecule 4: NADH-quinone oxidoreductase subunit I

Response	Percentage
Used a mobile app to book a flight	72%
Have not used a mobile app to book a flight	8%
Unsure	19%



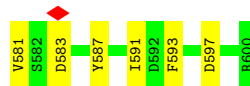
- Molecule 5: NADH-quinone oxidoreductase subunit B

62% 24% 11%



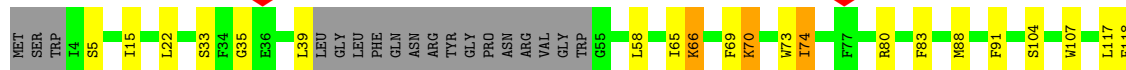
- Molecule 6: NADH-quinone oxidoreductase subunit C/D

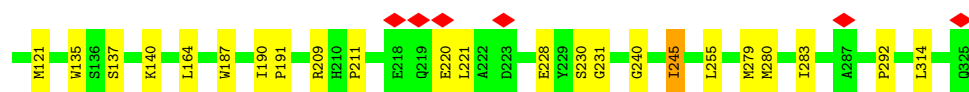
84% 14%



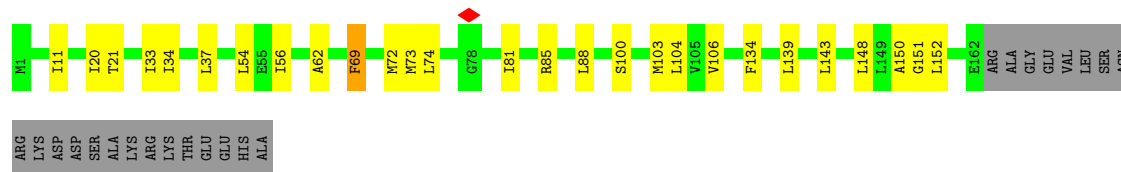
- Molecule 7: NADH-quinone oxidoreductase subunit H

81% 12% 6%

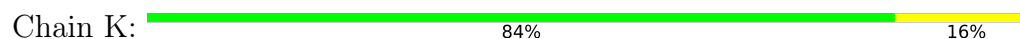




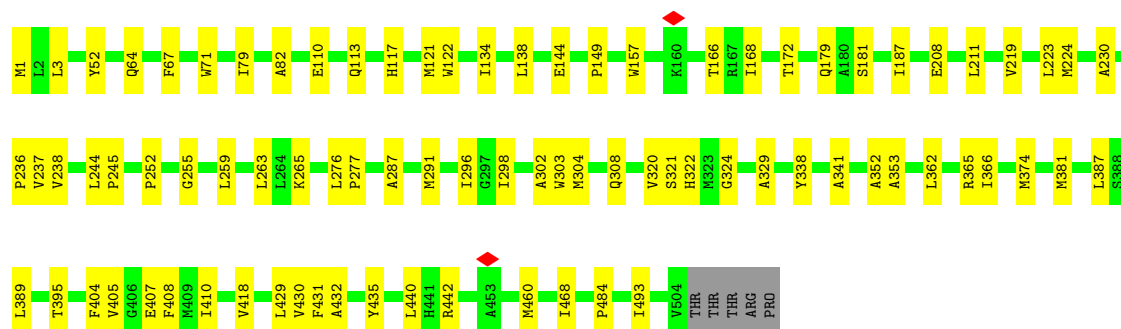
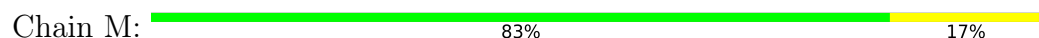
• Molecule 8: NADH-quinone oxidoreductase subunit J



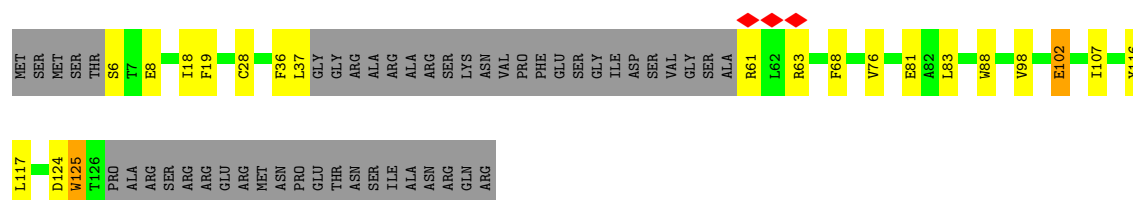
• Molecule 9: NADH-quinone oxidoreductase subunit K



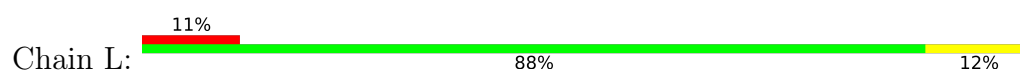
• Molecule 10: NADH-quinone oxidoreductase subunit M

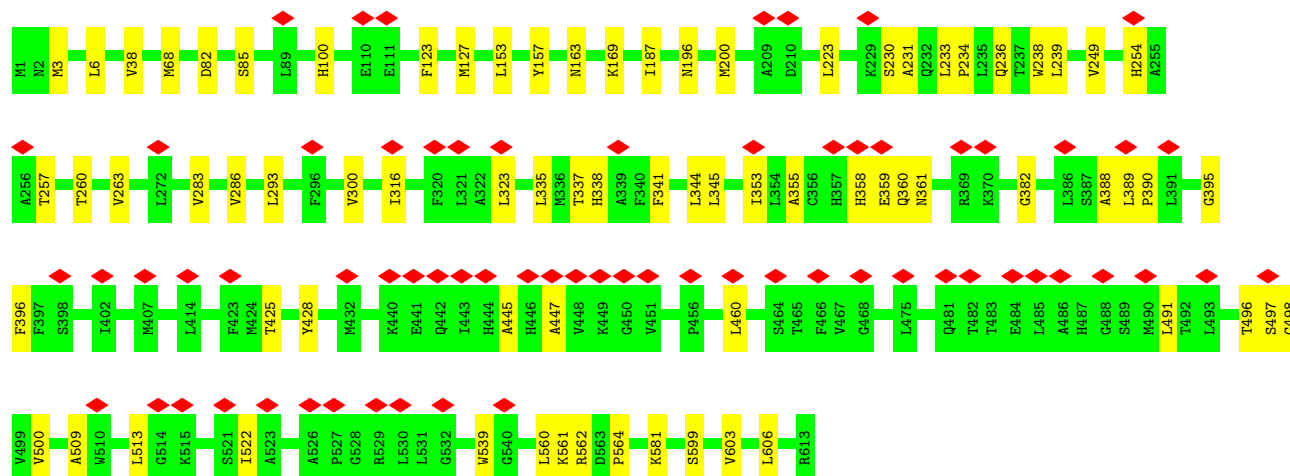


• Molecule 11: NADH-quinone oxidoreductase subunit A



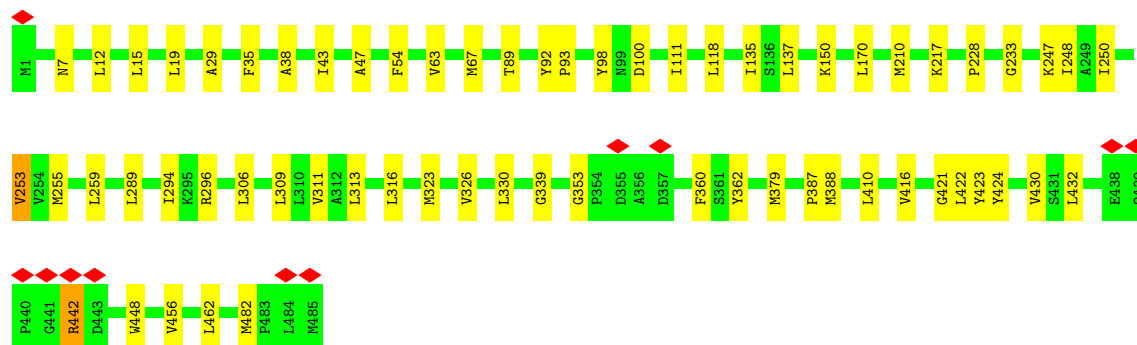
• Molecule 12: NADH-quinone oxidoreductase subunit L





- Molecule 13: NADH-quinone oxidoreductase subunit N

Chain N: 87% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.840	Depositor
Minimum map value	-0.721	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.234	Depositor
Map size (Å)	585.75, 585.75, 585.75	wwPDB
Map dimensions	710, 710, 710	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: CDL, TRD, SF4, FES, FMN, LFA, CA, UQ8, 3PE

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	E	0.13	0/1248	0.25	0/1691
2	F	0.14	0/3486	0.24	0/4713
3	G	0.14	0/7178	0.25	0/9733
4	I	0.14	0/1176	0.27	0/1590
5	B	0.21	0/1582	0.36	0/2140
6	C	0.14	0/4891	0.29	0/6637
7	H	0.21	0/2472	0.36	0/3361
8	J	0.10	0/1252	0.24	0/1708
9	K	0.11	0/769	0.23	0/1040
10	M	0.11	0/4090	0.24	0/5569
11	A	0.17	0/812	0.35	0/1105
12	L	0.11	0/4806	0.29	0/6549
13	N	0.11	0/3764	0.26	0/5138
All	All	0.14	0/37526	0.28	0/50974

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	E	1220	0	1187	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3407	0	3374	21	0
3	G	7027	0	6829	51	0
4	I	1149	0	1113	9	0
5	B	1551	0	1549	47	0
6	C	4760	0	4677	59	0
7	H	2404	0	2459	40	0
8	J	1226	0	1297	25	0
9	K	760	0	817	16	0
10	M	3964	0	4063	52	0
11	A	788	0	803	19	0
12	L	4685	0	4831	48	0
13	N	3673	0	3836	49	0
14	E	4	0	0	0	0
14	G	4	0	0	0	0
15	E	1	0	0	0	0
15	G	3	0	0	0	0
15	I	1	0	0	0	0
16	F	31	0	19	1	0
17	B	8	0	0	2	0
17	F	8	0	0	1	0
17	G	24	0	0	0	0
17	I	16	0	0	0	0
18	A	89	0	129	4	0
18	H	102	0	164	1	0
18	J	102	0	164	6	0
18	L	233	0	351	5	0
18	M	140	0	211	5	0
18	N	93	0	140	4	0
19	H	20	0	42	0	0
19	N	20	0	42	2	0
20	L	100	0	156	4	0
21	L	26	0	56	0	0
21	N	13	0	28	0	0
22	N	106	0	148	24	0
23	A	6	0	0	0	0
23	B	6	0	0	0	0
23	C	53	0	0	0	0
23	E	5	0	0	0	0
23	F	42	0	0	0	0
23	G	138	0	0	0	0
23	H	22	0	0	0	0
23	I	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J	8	0	0	0	0
23	K	10	0	0	0	0
23	L	44	0	0	0	0
23	M	40	0	0	0	0
23	N	36	0	0	0	0
All	All	38186	0	38485	410	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 (410) 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:C:581:VAL:HG11	7:H:220:GLU:HG3	1.52	0.91
6:C:563:THR:HG21	6:C:597:ASP:O	1.73	0.88
5:B:101:THR:HG21	6:C:254:ARG:HD3	1.60	0.83
12:L:522:ILE:HD11	18:L:704:3PE:H221	1.60	0.83
5:B:91:ARG:HG3	7:H:230:SER:HB3	1.66	0.77
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.68	0.75
7:H:70:LYS:HG2	7:H:231:GLY:HA2	1.67	0.75
6:C:218:LEU:HD22	7:H:221:LEU:HG	1.69	0.74
12:L:223:LEU:HD13	12:L:283:VAL:HG22	1.71	0.73
3:G:307:ILE:O	3:G:310:GLN:HG2	1.90	0.72
6:C:218:LEU:HD22	7:H:221:LEU:CG	2.21	0.71
12:L:355:ALA:HB3	12:L:359:GLU:HA	1.74	0.68
6:C:236:GLN:HG2	6:C:243:VAL:HB	1.77	0.67
7:H:209:ARG:HG3	7:H:245:ILE:HD11	1.76	0.67
13:N:217:LYS:HB3	13:N:250:ILE:HD13	1.77	0.66
13:N:12:LEU:HD11	22:N:503:UQ8:H32A	1.77	0.66
6:C:408:SER:HB2	6:C:463:CYS:HB2	1.79	0.64
8:J:100:SER:HB3	9:K:16:VAL:HG13	1.79	0.64
10:M:1:MET:HG2	10:M:67:PHE:HB2	1.79	0.64
6:C:218:LEU:HD22	7:H:221:LEU:CD2	2.28	0.64
3:G:218:ASN:HD22	3:G:249:ARG:HD2	1.63	0.64
10:M:430:VAL:HG11	18:M:603:3PE:H381	1.80	0.63
13:N:47:ALA:HA	22:N:503:UQ8:H21	1.81	0.63
3:G:106:PRO:HD3	6:C:515:LEU:HD21	1.81	0.63
5:B:72:PHE:HD1	5:B:73:THR:H	1.47	0.63
12:L:231:ALA:HB1	12:L:236:GLN:HA	1.79	0.63
8:J:143:LEU:HD13	13:N:118:LEU:HD22	1.80	0.62
11:A:61:ARG:O	11:A:61:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:248:ILE:HG12	13:N:330:LEU:HD22	1.82	0.61
3:G:848:ASP:HA	3:G:851:LYS:HE3	1.81	0.61
6:C:200:LYS:HE3	6:C:200:LYS:HA	1.81	0.61
6:C:378:ARG:O	6:C:382:GLU:HG3	2.01	0.61
12:L:497:SER:HA	12:L:500:VAL:HB	1.83	0.61
10:M:219:VAL:HG22	18:N:506:3PE:H222	1.83	0.60
12:L:3:MET:HB3	12:L:6:LEU:HD12	1.83	0.60
3:G:355:LEU:HD21	3:G:545:ILE:HG13	1.83	0.60
6:C:218:LEU:HD22	7:H:221:LEU:HD21	1.84	0.59
8:J:148:LEU:HD13	11:A:81:GLU:HG2	1.82	0.59
7:H:280:MET:O	7:H:283:ILE:HG22	2.02	0.59
6:C:581:VAL:CG1	7:H:220:GLU:HG3	2.28	0.59
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.84	0.59
12:L:522:ILE:CD1	18:L:704:3PE:H221	2.30	0.59
13:N:54:PHE:CD1	22:N:503:UQ8:H33	2.37	0.59
10:M:181:SER:HB2	10:M:230:ALA:HA	1.84	0.58
13:N:38:ALA:HB1	22:N:503:UQ8:H3MA	1.84	0.58
10:M:179:GLN:HG2	13:N:422:LEU:HD11	1.84	0.58
8:J:104:LEU:HB2	9:K:16:VAL:HG21	1.86	0.58
10:M:172:THR:HG21	13:N:423:TYR:HD1	1.69	0.58
5:B:170:MET:O	5:B:174:GLU:HG2	2.04	0.58
6:C:76:ASP:HB3	6:C:562:ARG:HG3	1.87	0.57
18:J:202:3PE:H372	9:K:20:THR:HG21	1.87	0.57
6:C:468:MET:HE3	6:C:468:MET:HA	1.87	0.57
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.40	0.57
10:M:418:VAL:HG13	10:M:418:VAL:O	2.04	0.57
13:N:255:MET:HE2	13:N:313:LEU:HD12	1.86	0.57
6:C:391:LEU:HD22	6:C:478:LEU:HD12	1.87	0.56
13:N:247:LYS:HD3	13:N:306:LEU:HD11	1.86	0.56
3:G:301:MET:HE3	3:G:653:TRP:CE3	2.40	0.56
3:G:718:ARG:HD3	3:G:726:PRO:HG3	1.86	0.56
10:M:298:ILE:HG13	10:M:324:GLY:HA3	1.87	0.56
13:N:255:MET:HE3	13:N:326:VAL:HG21	1.86	0.56
8:J:150:ALA:HB2	13:N:111:ILE:HG21	1.87	0.56
5:B:185:TRP:HZ3	11:A:36:PHE:HA	1.71	0.55
5:B:96:MET:HE1	5:B:114:TYR:HB2	1.88	0.55
7:H:73:TRP:C	7:H:74:ILE:HG12	2.31	0.55
10:M:236:PRO:HB2	10:M:320:VAL:HG22	1.89	0.55
13:N:311:VAL:HG22	13:N:410:LEU:HD13	1.89	0.55
4:I:47:ARG:CZ	5:B:208:ARG:HD2	2.36	0.55
6:C:218:LEU:CD2	7:H:221:LEU:HG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:138:ILE:HG23	5:B:140:SER:H	1.71	0.55
2:F:357:CYS:HB3	17:F:502:SF4:S4	2.47	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.89	0.54
5:B:98:VAL:HG11	5:B:145:VAL:HG21	1.89	0.54
13:N:289:LEU:HD22	13:N:423:TYR:HD2	1.72	0.54
8:J:103:MET:HB2	12:L:603:VAL:HG12	1.89	0.54
5:B:87:ARG:H	5:B:87:ARG:HE	1.54	0.54
7:H:164:LEU:HD22	7:H:255:LEU:HD13	1.89	0.54
12:L:425:THR:HA	12:L:428:TYR:CE2	2.42	0.54
2:F:434:ASN:HB3	4:I:146:PRO:HD2	1.90	0.54
8:J:100:SER:HB3	9:K:16:VAL:CG1	2.37	0.54
13:N:294:ILE:HG21	13:N:360:PHE:HD2	1.73	0.53
3:G:307:ILE:HG21	3:G:591:LEU:HD13	1.91	0.53
5:B:48:TRP:HZ2	7:H:58:LEU:HD13	1.72	0.53
6:C:144:LEU:HB3	6:C:169:LEU:HB2	1.89	0.53
5:B:62:SER:HB3	17:B:301:SF4:S1	2.49	0.53
5:B:63:CYS:HB2	17:B:301:SF4:S2	2.49	0.53
5:B:91:ARG:HG3	7:H:230:SER:CB	2.36	0.53
13:N:43:ILE:HG12	22:N:503:UQ8:H12A	1.91	0.53
7:H:314:LEU:HD13	11:A:107:ILE:HD12	1.91	0.53
7:H:80:ARG:NH1	7:H:80:ARG:HB3	2.24	0.53
12:L:358:HIS:CD2	12:L:445:ALA:HA	2.43	0.53
12:L:355:ALA:HB3	12:L:359:GLU:CA	2.39	0.52
9:K:16:VAL:O	9:K:20:THR:HG22	2.09	0.52
13:N:150:LYS:HB2	13:N:150:LYS:NZ	2.24	0.52
2:F:441:LEU:HD21	6:C:496:ASP:HB2	1.91	0.52
6:C:175:ALA:HB2	6:C:258:LYS:HE3	1.91	0.52
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.90	0.52
10:M:362:LEU:HD13	10:M:381:MET:HE1	1.92	0.52
12:L:300:VAL:HG12	18:L:704:3PE:H31	1.91	0.52
6:C:133:ASN:ND2	6:C:422:TRP:HA	2.25	0.52
8:J:54:LEU:HD13	11:A:83:LEU:HD11	1.92	0.52
5:B:91:ARG:HH11	5:B:118:LEU:HD21	1.75	0.51
13:N:421:GLY:HA2	13:N:424:TYR:CE2	2.45	0.51
5:B:86:LEU:HD13	5:B:87:ARG:NE	2.25	0.51
18:J:201:3PE:H261	18:J:201:3PE:H392	1.92	0.51
10:M:387:LEU:HD13	10:M:468:ILE:HG21	1.91	0.51
12:L:263:VAL:HG13	12:L:323:LEU:HD11	1.91	0.51
12:L:82:ASP:H	12:L:85:SER:HB2	1.75	0.51
10:M:366:ILE:HD11	10:M:374:MET:HE2	1.92	0.51
12:L:355:ALA:HA	12:L:447:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.92	0.51
18:M:601:3PE:H232	12:L:187:ILE:HD11	1.92	0.51
10:M:341:ALA:HA	10:M:410:ILE:HD11	1.93	0.51
12:L:344:LEU:HB2	12:L:460:LEU:HB3	1.92	0.50
12:L:123:PHE:CE1	12:L:257:THR:HG21	2.47	0.50
1:E:98:HIS:HA	1:E:102:TYR:HD1	1.77	0.50
2:F:300:LEU:HD21	2:F:319:SER:HB2	1.93	0.50
6:C:501:THR:HG23	6:C:521:GLN:HB3	1.92	0.50
12:L:260:THR:HB	12:L:335:LEU:HD11	1.93	0.50
2:F:4:ILE:O	2:F:4:ILE:HG13	2.12	0.50
5:B:73:THR:HA	5:B:76:HIS:NE2	2.27	0.50
12:L:293:LEU:HG	12:L:539:TRP:CD1	2.46	0.50
12:L:388:ALA:HB1	12:L:396:PHE:HA	1.92	0.50
5:B:103:PHE:HE1	6:C:254:ARG:HG3	1.77	0.49
9:K:43:ALA:HB1	9:K:62:TYR:HD1	1.77	0.49
12:L:509:ALA:O	12:L:513:LEU:HB2	2.12	0.49
13:N:7:ASN:HB3	13:N:63:VAL:HG13	1.94	0.49
3:G:115:HIS:CE1	3:G:119:MET:HE3	2.46	0.49
7:H:190:ILE:HB	7:H:191:PRO:HD3	1.94	0.49
10:M:71:TRP:HB2	10:M:79:ILE:HG13	1.94	0.49
13:N:339:GLY:HA3	13:N:379:MET:HE3	1.92	0.49
3:G:117:GLN:HG2	6:C:516:ILE:HG23	1.94	0.49
3:G:218:ASN:ND2	3:G:249:ARG:HD2	2.26	0.49
10:M:208:GLU:HA	10:M:211:LEU:HD12	1.94	0.49
12:L:38:VAL:HG21	12:L:100:HIS:CE1	2.47	0.49
13:N:170:LEU:HD12	13:N:210:MET:HG2	1.94	0.49
7:H:280:MET:HA	7:H:283:ILE:HG22	1.94	0.49
5:B:91:ARG:NH1	5:B:118:LEU:HD21	2.27	0.49
6:C:397:ALA:O	6:C:401:ASN:HB2	2.12	0.49
6:C:576:ILE:HD11	6:C:583:ASP:HB3	1.95	0.49
8:J:34:ILE:HG23	18:J:201:3PE:H2F1	1.93	0.49
5:B:185:TRP:CZ3	11:A:36:PHE:HA	2.47	0.49
13:N:323:MET:HE3	13:N:482:MET:SD	2.53	0.49
6:C:403:ILE:HB	6:C:407:ARG:NH2	2.28	0.49
18:J:201:3PE:H2B1	18:J:201:3PE:H3D1	1.94	0.49
10:M:263:LEU:HD21	10:M:352:ALA:HB3	1.95	0.49
6:C:21:LEU:HD22	6:C:30:ARG:HH22	1.77	0.49
8:J:81:ILE:HG23	9:K:26:ARG:HH21	1.77	0.49
9:K:75:ILE:HD12	13:N:137:LEU:HD22	1.95	0.49
13:N:89:THR:HG21	13:N:456:VAL:HG21	1.95	0.49
5:B:64:CYS:HB3	5:B:99:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:367:ALA:HB3	3:G:370:GLU:HG3	1.94	0.48
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.95	0.48
6:C:24:PRO:O	6:C:28:GLU:HG3	2.14	0.48
6:C:200:LYS:HB2	6:C:203:GLU:HG2	1.96	0.48
8:J:62:ALA:HB1	11:A:76:VAL:HG22	1.95	0.48
6:C:387:MET:N	6:C:388:PRO:HD2	2.29	0.48
13:N:35:PHE:HE1	13:N:448:TRP:HZ2	1.61	0.48
8:J:134:PHE:CE1	11:A:88:TRP:HB2	2.49	0.48
6:C:201:PRO:HG2	6:C:208:ARG:HD3	1.96	0.47
10:M:287:ALA:O	10:M:291:MET:HG3	2.14	0.47
10:M:329:ALA:HB2	10:M:410:ILE:HG23	1.94	0.47
4:I:48:ILE:HG12	4:I:116:LEU:HG	1.97	0.47
6:C:133:ASN:HD21	6:C:422:TRP:HA	1.79	0.47
3:G:284:PRO:HD3	3:G:646:VAL:HB	1.97	0.47
2:F:282:ARG:HB2	2:F:285:LEU:HD12	1.95	0.47
8:J:85:ARG:HB3	8:J:88:LEU:HD12	1.95	0.47
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.95	0.47
12:L:239:LEU:HG	12:L:254:HIS:CE1	2.50	0.47
13:N:362:TYR:O	13:N:432:LEU:HD23	2.15	0.47
3:G:115:HIS:HE1	3:G:119:MET:HE3	1.78	0.47
3:G:288:ARG:HD2	3:G:293:ILE:HD13	1.97	0.47
5:B:46:VAL:O	5:B:50:ARG:HG3	2.14	0.47
7:H:135:TRP:CD1	8:J:72:MET:HG2	2.49	0.47
10:M:302:ALA:HB1	10:M:431:PHE:HB3	1.97	0.47
10:M:365:ARG:HH21	10:M:460:MET:HA	1.78	0.47
18:A:502:3PE:H3D1	13:N:19:LEU:HD13	1.96	0.47
12:L:230:SER:HB3	12:L:316:ILE:HG21	1.96	0.47
12:L:337:THR:HG21	12:L:395:GLY:HA2	1.96	0.47
22:N:503:UQ8:H20	22:N:503:UQ8:H17A	1.68	0.47
5:B:91:ARG:HD3	5:B:91:ARG:HA	1.49	0.47
8:J:139:LEU:HD13	13:N:67:MET:SD	2.54	0.47
8:J:151:GLY:HA2	9:K:75:ILE:HD11	1.96	0.47
10:M:82:ALA:HB3	10:M:134:ILE:HG21	1.97	0.47
3:G:531:ILE:HD11	3:G:533:MET:HE2	1.97	0.46
6:C:77:LEU:HB3	6:C:137:TYR:HB3	1.97	0.46
8:J:152:LEU:HD11	11:A:117:LEU:HD11	1.97	0.46
12:L:561:LYS:HG3	12:L:562:ARG:HG2	1.97	0.46
22:N:502:UQ8:H32	22:N:502:UQ8:H35	1.74	0.46
10:M:110:GLU:H	10:M:113:GLN:HG2	1.78	0.46
2:F:45:LEU:HD12	2:F:45:LEU:HA	1.83	0.46
6:C:73:MET:HE2	6:C:423:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:98:VAL:O	11:A:102:GLU:HG2	2.15	0.46
12:L:353:ILE:HA	12:L:359:GLU:HB2	1.97	0.46
13:N:98:TYR:CE2	13:N:100:ASP:HB3	2.50	0.46
22:N:503:UQ8:H32	22:N:503:UQ8:H35	1.63	0.46
10:M:157:TRP:O	10:M:252:PRO:HB3	2.15	0.46
22:N:503:UQ8:H10A	22:N:503:UQ8:H12	1.84	0.46
7:H:280:MET:C	7:H:283:ILE:HG22	2.41	0.46
10:M:263:LEU:HA	10:M:263:LEU:HD23	1.73	0.46
13:N:416:VAL:HG21	19:N:505:LFA:H172	1.96	0.46
22:N:503:UQ8:H12A	22:N:503:UQ8:H16	1.57	0.46
3:G:353:LEU:HD22	3:G:509:LEU:HG	1.98	0.46
22:N:503:UQ8:H42A	22:N:503:UQ8:H46	1.63	0.46
18:A:502:3PE:H391	13:N:15:LEU:HD22	1.97	0.46
20:L:703:CDL:H351	20:L:703:CDL:H382	1.66	0.46
18:N:504:3PE:H341	18:N:504:3PE:H251	1.98	0.46
1:E:116:LYS:HE3	1:E:116:LYS:HA	1.98	0.46
6:C:211:GLU:HG3	6:C:214:ASP:HB2	1.97	0.46
9:K:96:SER:HB2	9:K:99:ARG:HH12	1.81	0.46
10:M:304:MET:O	10:M:308:GLN:HG2	2.16	0.46
10:M:407:GLU:OE2	10:M:429:LEU:HD21	2.16	0.46
11:A:102:GLU:HG2	11:A:102:GLU:H	1.56	0.46
12:L:345:LEU:HG	12:L:382:GLY:HA3	1.98	0.46
6:C:133:ASN:HD21	6:C:422:TRP:CA	2.29	0.46
7:H:121:MET:HE3	8:J:56:ILE:HB	1.98	0.46
10:M:405:VAL:HG22	12:L:68:MET:HE2	1.98	0.46
8:J:69:PHE:O	8:J:73:MET:HB3	2.16	0.45
22:N:502:UQ8:H25B	22:N:502:UQ8:H27	1.78	0.45
5:B:101:THR:HA	5:B:129:CYS:HB3	1.98	0.45
6:C:328:GLN:HA	6:C:333:MET:HA	1.98	0.45
6:C:565:SER:HB3	6:C:593:PHE:HB2	1.98	0.45
10:M:122[A]:TRP:CE3	10:M:149:PRO:HG3	2.52	0.45
10:M:144:GLU:HB2	13:N:387:PRO:HG2	1.97	0.45
5:B:25:VAL:HG11	5:B:193:TYR:CE1	2.51	0.45
7:H:117:LEU:O	7:H:121:MET:HG3	2.16	0.45
9:K:98:MET:HE1	13:N:233:GLY:HA3	1.98	0.45
22:N:502:UQ8:H17A	22:N:502:UQ8:H13	1.66	0.45
2:F:136:TYR:HB3	2:F:139:ALA:HB3	1.99	0.45
3:G:328:PHE:CG	3:G:678:VAL:HG22	2.52	0.45
22:N:503:UQ8:H40	22:N:503:UQ8:H37A	1.63	0.45
3:G:190:THR:HG21	3:G:836:ARG:HD3	1.98	0.45
10:M:224:MET:HE3	10:M:224:MET:HB3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:216:MET:HE1	11:A:63:ARG:HD2	1.97	0.45
6:C:405:LYS:HB2	6:C:405:LYS:HE3	1.79	0.45
7:H:35:GLY:O	7:H:39:LEU:HD23	2.16	0.45
9:K:28:LEU:HD13	9:K:92:ILE:HD13	1.99	0.45
12:L:496:THR:C	12:L:498:GLY:H	2.25	0.45
3:G:887:PRO:HB2	3:G:890:MET:HG3	1.99	0.45
6:C:200:LYS:HB3	6:C:202:GLU:OE1	2.17	0.45
7:H:135:TRP:HB2	8:J:72:MET:SD	2.57	0.45
10:M:276:LEU:HB2	10:M:277:PRO:HD3	1.99	0.45
18:M:603:3PE:H242	12:L:169:LYS:HA	1.99	0.45
22:N:502:UQ8:H30	22:N:502:UQ8:H27A	1.70	0.45
22:N:502:UQ8:H40	22:N:502:UQ8:H37A	1.71	0.45
5:B:72:PHE:CZ	5:B:166:MET:HB2	2.51	0.45
6:C:212:ASN:HA	6:C:215:PHE:CE2	2.52	0.45
7:H:137:SER:HB2	7:H:228:GLU:HG3	1.98	0.45
7:H:211:PRO:HB2	7:H:292:PRO:HD2	1.98	0.45
10:M:442:ARG:HE	18:M:603:3PE:H112	1.82	0.45
2:F:94:MET:HE3	2:F:94:MET:HB2	1.87	0.44
7:H:88:MET:HE1	11:A:28:CYS:SG	2.58	0.44
10:M:244:LEU:HB3	10:M:245:PRO:HD3	1.99	0.44
12:L:127:MET:HB2	12:L:257:THR:HG23	2.00	0.44
12:L:233:LEU:HB2	12:L:286:VAL:HG13	1.98	0.44
9:K:43:ALA:HB1	9:K:62:TYR:CD1	2.52	0.44
3:G:713:GLY:O	3:G:717:MET:HG3	2.18	0.44
5:B:60:GLY:HA3	5:B:65:TYR:HB2	2.00	0.44
5:B:86:LEU:HD13	5:B:87:ARG:HE	1.82	0.44
6:C:74:LEU:HD23	6:C:133:ASN:HB2	1.99	0.44
9:K:12:ALA:O	9:K:16:VAL:HG23	2.18	0.44
7:H:70:LYS:CG	7:H:231:GLY:HA2	2.44	0.44
6:C:65:LYS:HE2	6:C:65:LYS:HB3	1.71	0.44
8:J:20:ILE:HG13	8:J:21:THR:HG23	2.00	0.44
22:N:502:UQ8:H12	22:N:502:UQ8:H15	1.62	0.44
3:G:301:MET:HE3	3:G:653:TRP:HE3	1.81	0.44
3:G:379:VAL:HB	3:G:433:VAL:HG12	1.99	0.44
4:I:42:PRO:HB3	5:B:215:ARG:HB2	1.99	0.44
2:F:127:ARG:HG2	2:F:170:PHE:HE2	1.83	0.44
5:B:50:ARG:HA	7:H:66:LYS:HG3	2.00	0.44
3:G:314:VAL:HG22	3:G:565:ALA:HB3	1.98	0.43
5:B:148:PHE:HD2	5:B:149:ILE:HG23	1.83	0.43
6:C:65:LYS:HD3	6:C:130:LEU:HD22	1.99	0.43
12:L:359:GLU:CD	12:L:360:GLN:HG3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:259:LEU:HB2	13:N:316:LEU:HD21	2.00	0.43
2:F:116:MET:HG2	2:F:222:LEU:HD13	2.00	0.43
10:M:255:GLY:O	10:M:259:LEU:HG	2.18	0.43
12:L:196:ASN:O	12:L:200:MET:HG3	2.17	0.43
2:F:7:THR:HG23	2:F:9:GLU:H	1.82	0.43
6:C:165:LYS:HD3	6:C:165:LYS:HA	1.67	0.43
6:C:168:PRO:HA	6:C:173:TYR:CD1	2.53	0.43
13:N:12:LEU:HD23	13:N:12:LEU:HA	1.83	0.43
5:B:38:PHE:O	5:B:42:LEU:HD22	2.18	0.43
10:M:265:LYS:HA	10:M:265:LYS:HD3	1.72	0.43
13:N:388:MET:HE2	13:N:388:MET:HB3	1.79	0.43
2:F:96:PRO:HB2	2:F:295:ALA:HB2	2.00	0.43
3:G:6:ILE:HG22	3:G:77:THR:HB	2.01	0.43
3:G:845:ASN:OD1	3:G:846:PRO:HD2	2.18	0.43
6:C:405:LYS:O	6:C:409:GLN:HB2	2.17	0.43
10:M:187:ILE:HG22	18:N:506:3PE:H282	2.01	0.43
12:L:491:LEU:HD12	12:L:491:LEU:HA	1.86	0.43
3:G:238:ASN:ND2	3:G:256:ASN:HD22	2.17	0.43
10:M:117:HIS:O	10:M:121:MET:HG2	2.18	0.43
1:E:161:LEU:HD12	1:E:161:LEU:HA	1.86	0.43
2:F:354:CYS:HA	3:G:46:ALA:O	2.19	0.43
16:F:501:FMN:HM81	16:F:501:FMN:HM73	1.84	0.43
3:G:110:GLU:HG3	3:G:206:GLY:HA2	2.01	0.43
3:G:233:CYS:SG	3:G:235:ILE:HG12	2.59	0.43
3:G:827:SER:HB3	3:G:833:PHE:CE2	2.54	0.43
4:I:100:ILE:HG21	5:B:135:MET:HB3	2.01	0.43
13:N:309:LEU:H	13:N:309:LEU:HD23	1.84	0.43
13:N:442:ARG:HD3	13:N:442:ARG:HA	1.83	0.43
10:M:322:HIS:CE1	10:M:395:THR:HG23	2.54	0.43
12:L:581:LYS:HD2	12:L:581:LYS:HA	1.81	0.43
10:M:238:VAL:HG21	10:M:296:ILE:HG22	1.99	0.43
3:G:150:MET:HE3	3:G:150:MET:O	2.19	0.42
10:M:365:ARG:NH2	10:M:460:MET:HA	2.34	0.42
3:G:501:ILE:HG12	3:G:532:THR:HB	2.01	0.42
3:G:848:ASP:O	3:G:851:LYS:HG2	2.19	0.42
5:B:92:GLN:H	5:B:92:GLN:HG2	1.48	0.42
7:H:15:ILE:HG23	11:A:18:ILE:HG21	2.01	0.42
6:C:233:ILE:HD13	6:C:247:PRO:HA	1.99	0.42
5:B:148:PHE:CD2	5:B:149:ILE:HG23	2.55	0.42
3:G:824:ASP:HB3	3:G:827:SER:HB2	2.02	0.42
12:L:231:ALA:HB2	12:L:238:TRP:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:560:LEU:HD23	12:L:564:PRO:HG2	2.00	0.42
1:E:25:GLU:CD	1:E:38:GLU:HG2	2.44	0.42
6:C:144:LEU:HA	6:C:168:PRO:HD2	2.02	0.42
6:C:169:LEU:HD23	6:C:169:LEU:HA	1.84	0.42
1:E:90:ARG:HA	1:E:129:LEU:O	2.20	0.42
18:M:602:3PE:H32	18:M:602:3PE:H321	1.55	0.42
18:N:506:3PE:H332	18:N:506:3PE:H361	1.79	0.42
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.02	0.42
7:H:187:TRP:CD2	18:H:401:3PE:H232	2.55	0.42
12:L:599:SER:O	12:L:603:VAL:HG13	2.18	0.42
13:N:462:LEU:CD1	22:N:502:UQ8:H22	2.50	0.42
2:F:126:TYR:CZ	2:F:127:ARG:HD2	2.54	0.42
3:G:53:LYS:HE3	3:G:53:LYS:HB2	1.88	0.42
6:C:402:THR:HA	6:C:405:LYS:HB3	2.02	0.42
10:M:259:LEU:HD22	10:M:353:ALA:HA	2.01	0.42
1:E:158:ILE:HD13	1:E:158:ILE:HA	1.88	0.42
2:F:255:ARG:HD3	2:F:330:ASP:OD2	2.20	0.42
3:G:121:VAL:HG21	6:C:520:LEU:HD12	2.01	0.42
3:G:498:PRO:HG2	3:G:529:VAL:HG23	2.01	0.42
5:B:46:VAL:HG22	7:H:69:PHE:CE1	2.55	0.42
7:H:74:ILE:HG23	7:H:83:PHE:CD2	2.55	0.42
9:K:100:GLY:HA2	13:N:296:ARG:NH1	2.33	0.42
11:A:116:TYR:HA	13:N:29:ALA:HB2	2.02	0.42
12:L:231:ALA:HB2	12:L:238:TRP:NE1	2.34	0.42
3:G:433:VAL:HG23	3:G:448:THR:HG23	2.01	0.41
10:M:3:LEU:HD23	10:M:3:LEU:HA	1.89	0.41
5:B:73:THR:HA	5:B:76:HIS:CD2	2.54	0.41
5:B:204:LYS:O	5:B:208:ARG:HG3	2.20	0.41
10:M:389:LEU:HA	10:M:440:LEU:HD21	2.02	0.41
3:G:267:ARG:HB2	3:G:820:LEU:HG	2.02	0.41
2:F:179:ILE:HD12	2:F:179:ILE:HA	1.86	0.41
8:J:33:ILE:O	8:J:37:LEU:HG	2.19	0.41
12:L:153:LEU:HD13	12:L:249:VAL:HG22	2.02	0.41
13:N:250:ILE:O	13:N:253:VAL:HG12	2.20	0.41
3:G:245:TYR:HA	3:G:641:TYR:CZ	2.55	0.41
4:I:36:GLU:HA	4:I:37:PRO:HD3	1.91	0.41
11:A:6:SER:C	11:A:8:GLU:H	2.29	0.41
5:B:48:TRP:HA	5:B:51:LYS:HG2	2.01	0.41
5:B:140:SER:HB3	6:C:160:MET:HE1	2.03	0.41
5:B:46:VAL:HA	7:H:65:ILE:HG21	2.02	0.41
6:C:569:LEU:HD13	6:C:572:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:74:LEU:HD22	9:K:84:HIS:ND1	2.36	0.41
18:J:201:3PE:H221	18:A:501:3PE:H322	2.01	0.41
18:L:701:3PE:H292	20:L:703:CDL:H872	2.02	0.41
13:N:38:ALA:HB3	22:N:503:UQ8:H4M	2.02	0.41
1:E:117:PRO:HA	1:E:128:LEU:HB3	2.03	0.41
3:G:297:ALA:HB1	3:G:668:TRP:CH2	2.56	0.41
5:B:180:ARG:HB2	5:B:193:TYR:HB2	2.02	0.41
7:H:118:PHE:HE1	18:A:501:3PE:H262	1.86	0.41
7:H:140:LYS:HE2	7:H:140:LYS:HB3	1.81	0.41
10:M:219:VAL:O	10:M:223:LEU:HG	2.21	0.41
11:A:37:LEU:HD23	11:A:37:LEU:HA	1.84	0.41
12:L:157:TYR:HB2	12:L:163:ASN:HD22	1.85	0.41
22:N:503:UQ8:H7A	22:N:503:UQ8:H10	1.58	0.41
2:F:152:GLU:OE1	2:F:152:GLU:HA	2.21	0.41
2:F:281:MET:HE3	2:F:281:MET:HB3	1.87	0.41
3:G:674:VAL:O	3:G:678:VAL:HG23	2.21	0.41
5:B:117:MET:HE2	5:B:117:MET:HB3	1.90	0.41
6:C:597:ASP:OD1	6:C:597:ASP:C	2.63	0.41
7:H:22:LEU:HB2	11:A:19:PHE:CE1	2.55	0.41
8:J:11:ILE:HD11	18:J:201:3PE:H3H2	2.03	0.41
10:M:52:TYR:CE2	10:M:64:GLN:HG3	2.55	0.41
10:M:166:THR:C	10:M:168:ILE:H	2.28	0.41
10:M:298:ILE:HA	10:M:321:SER:HA	2.02	0.41
10:M:404:PHE:O	10:M:408:PHE:HB2	2.21	0.41
2:F:264:LEU:HD21	2:F:277:TYR:CZ	2.55	0.41
4:I:106:GLU:HG3	4:I:115:GLN:HA	2.03	0.41
5:B:68:MET:HE3	5:B:126:MET:SD	2.61	0.41
6:C:587:TYR:O	6:C:591:ILE:HG23	2.20	0.41
3:G:241:PRO:HB3	3:G:248:LEU:HD11	2.03	0.40
3:G:862:PHE:HA	3:G:904:ASP:O	2.21	0.40
4:I:141:GLY:HA3	5:B:212:THR:HA	2.02	0.40
13:N:92:TYR:HB3	13:N:93:PRO:HD3	2.04	0.40
13:N:228:PRO:HB2	13:N:296:ARG:NH1	2.37	0.40
22:N:503:UQ8:H22A	22:N:503:UQ8:H25	1.67	0.40
3:G:811:LYS:HB3	3:G:811:LYS:HE2	1.84	0.40
6:C:217:PHE:HE1	6:C:236:GLN:HB2	1.85	0.40
13:N:289:LEU:HD23	13:N:289:LEU:HA	1.92	0.40
13:N:462:LEU:HD11	22:N:502:UQ8:H22	2.04	0.40
3:G:286:GLN:HB2	3:G:608:LEU:HD13	2.03	0.40
4:I:127:ARG:NH1	5:B:132:SER:HB3	2.35	0.40
7:H:91:PHE:HA	7:H:240:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:703:CDL:H572	20:L:703:CDL:H601	1.98	0.40
13:N:137:LEU:HD23	13:N:137:LEU:HA	1.90	0.40
22:N:502:UQ8:H12	22:N:502:UQ8:H10A	1.85	0.40
22:N:502:UQ8:H3M	22:N:503:UQ8:H8	2.02	0.40
5:B:182:PRO:HG3	5:B:191:GLY:H	1.86	0.40
11:A:68:PHE:CE1	11:A:125:TRP:HH2	2.39	0.40
12:L:338:HIS:HA	12:L:341:PHE:CE2	2.56	0.40
12:L:389:LEU:HA	12:L:390:PRO:HD3	1.96	0.40
18:L:705:3PE:H2B1	18:L:705:3PE:H2E2	1.87	0.40
2:F:243:LYS:HE3	2:F:243:LYS:HB3	1.85	0.40
8:J:106:VAL:HG11	12:L:606:LEU:HB3	2.04	0.40
10:M:484:PRO:HG3	20:L:703:CDL:HA62	2.04	0.40
19:N:505:LFA:H142	19:N:505:LFA:H171	1.85	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	E	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
2	F	437/461 (95%)	427 (98%)	10 (2%)	0	100	100
3	G	903/910 (99%)	874 (97%)	29 (3%)	0	100	100
4	I	143/180 (79%)	140 (98%)	3 (2%)	0	100	100
5	B	187/220 (85%)	177 (95%)	10 (5%)	0	100	100
6	C	587/600 (98%)	557 (95%)	30 (5%)	0	100	100
7	H	303/325 (93%)	289 (95%)	14 (5%)	0	100	100
8	J	160/184 (87%)	157 (98%)	3 (2%)	0	100	100
9	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
10	M	503/509 (99%)	486 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A	94/147 (64%)	89 (95%)	5 (5%)	0	100	100
12	L	611/613 (100%)	574 (94%)	36 (6%)	1 (0%)	43	76
13	N	483/485 (100%)	467 (97%)	15 (3%)	1 (0%)	43	76
All	All	4663/4900 (95%)	4482 (96%)	179 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	N	353	GLY
12	L	361	ASN

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	E	129/139 (93%)	129 (100%)	0	100	100
2	F	353/372 (95%)	350 (99%)	3 (1%)	73	86
3	G	733/738 (99%)	722 (98%)	11 (2%)	57	80
4	I	124/154 (80%)	121 (98%)	3 (2%)	43	73
5	B	171/192 (89%)	156 (91%)	15 (9%)	9	35
6	C	509/519 (98%)	501 (98%)	8 (2%)	55	79
7	H	254/269 (94%)	247 (97%)	7 (3%)	38	70
8	J	128/146 (88%)	127 (99%)	1 (1%)	73	86
9	K	79/79 (100%)	77 (98%)	2 (2%)	42	72
10	M	414/418 (99%)	412 (100%)	2 (0%)	81	89
11	A	79/119 (66%)	76 (96%)	3 (4%)	29	63
12	L	485/485 (100%)	485 (100%)	0	100	100
13	N	385/385 (100%)	381 (99%)	4 (1%)	68	84
All	All	3843/4015 (96%)	3784 (98%)	59 (2%)	55	80

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	13	LEU
2	F	252	PHE
2	F	316	LYS
3	G	172	LEU
3	G	223	MET
3	G	336	GLU
3	G	566	VAL
3	G	743	ASN
3	G	769	LYS
3	G	832	VAL
3	G	835	SER
3	G	836	ARG
3	G	842	ILE
3	G	869	VAL
4	I	64	ASN
4	I	77	LEU
4	I	147	GLU
5	B	8	ILE
5	B	19	LEU
5	B	20	GLN
5	B	50	ARG
5	B	63	CYS
5	B	69	VAL
5	B	85	VAL
5	B	86	LEU
5	B	89	SER
5	B	91	ARG
5	B	92	GLN
5	B	101	THR
5	B	183	LEU
5	B	207	GLU
5	B	219	GLU
6	C	36	ASP
6	C	124	VAL
6	C	210	THR
6	C	243	VAL
6	C	275	ILE
6	C	327	ILE
6	C	342	ASP
6	C	356	PHE
7	H	5	SER
7	H	33	SER

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Mol	Chain	Res	Type
7	H	66	LYS
7	H	70	LYS
7	H	74	ILE
7	H	245	ILE
7	H	279	MET
8	J	69	PHE
9	K	39	ILE
9	K	46	PHE
10	M	237	VAL
10	M	303	TRP
11	A	102	GLU
11	A	124	ASP
11	A	125	TRP
13	N	135	ILE
13	N	253	VAL
13	N	430	VAL
13	N	442	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	286	GLN
3	G	598	GLN
3	G	607	HIS
5	B	20	GLN
6	C	236	GLN
12	L	254	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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
18	3PE	M	601	-	46,46,50	0.53	0	49,51,55	0.57	1 (2%)
17	SF4	B	301	5	0,12,12	-	-	-		
18	3PE	L	702	-	46,46,50	0.53	0	49,51,55	0.55	1 (2%)
22	UQ8	N	502	-	53,53,53	1.15	2 (3%)	64,67,67	1.74	17 (26%)
18	3PE	L	701	-	41,41,50	0.56	0	44,46,55	0.58	1 (2%)
20	CDL	L	703	-	99,99,99	0.91	7 (7%)	105,111,111	1.09	4 (3%)
18	3PE	L	706	-	50,50,50	0.51	0	53,55,55	0.51	1 (1%)
18	3PE	J	202	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
18	3PE	L	704	-	41,41,50	0.56	0	44,46,55	0.55	1 (2%)
17	SF4	F	502	2	0,12,12	-	-	-		
18	3PE	N	504	-	41,41,50	0.56	0	44,46,55	0.56	1 (2%)
18	3PE	A	502	-	46,46,50	0.53	0	49,51,55	0.53	1 (2%)
17	SF4	I	202	4	0,12,12	-	-	-		
14	FES	E	201	1	0,4,4	-	-	-		
17	SF4	G	1001	3	0,12,12	-	-	-		
18	3PE	J	201	-	50,50,50	0.52	0	53,55,55	0.53	1 (1%)
18	3PE	L	705	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
18	3PE	M	603	-	41,41,50	0.57	0	44,46,55	0.56	1 (2%)
21	TRD	L	707	-	12,12,12	0.29	0	11,11,11	0.83	0
18	3PE	H	403	-	50,50,50	0.51	0	53,55,55	0.49	1 (1%)
18	3PE	M	602	-	50,50,50	0.52	0	53,55,55	0.55	1 (1%)
16	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.19	6 (12%)
17	SF4	I	203	4	0,12,12	-	-	-		
22	UQ8	N	503	-	53,53,53	1.14	2 (3%)	64,67,67	1.77	17 (26%)
18	3PE	N	506	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
18	3PE	A	501	-	41,41,50	0.56	0	44,46,55	0.57	1 (2%)
19	LFA	H	402	-	19,19,19	0.24	0	18,18,18	0.23	0
19	LFA	N	505	-	19,19,19	0.23	0	18,18,18	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	3PE	H	401	-	50,50,50	0.52	0	53,55,55	0.52	1 (1%)
17	SF4	G	1002	3	0,12,12	-	-	-		
17	SF4	G	1007	3	0,12,12	-	-	-		
21	TRD	N	501	-	12,12,12	0.29	0	11,11,11	0.83	0
21	TRD	L	708	-	12,12,12	0.29	0	11,11,11	0.85	0
14	FES	G	1003	3	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
18	3PE	M	601	-	-	18/50/50/54	-
18	3PE	L	702	-	-	18/50/50/54	-
22	UQ8	N	502	-	-	21/51/75/75	0/1/1/1
17	SF4	B	301	5	-	-	0/6/5/5
18	3PE	L	701	-	-	7/45/45/54	-
20	CDL	L	703	-	-	60/110/110/110	-
18	3PE	L	706	-	-	22/54/54/54	-
18	3PE	J	202	-	-	19/54/54/54	-
18	3PE	L	704	-	-	12/45/45/54	-
17	SF4	F	502	2	-	-	0/6/5/5
18	3PE	N	504	-	-	16/45/45/54	-
18	3PE	A	502	-	-	11/50/50/54	-
17	SF4	I	202	4	-	-	0/6/5/5
14	FES	E	201	1	-	-	0/1/1/1
17	SF4	G	1001	3	-	-	0/6/5/5
18	3PE	J	201	-	-	22/54/54/54	-
18	3PE	L	705	-	-	33/54/54/54	-
18	3PE	M	603	-	-	13/45/45/54	-
21	TRD	L	707	-	-	2/10/10/10	-
18	3PE	H	403	-	-	18/54/54/54	-
18	3PE	M	602	-	-	25/54/54/54	-
16	FMN	F	501	-	-	5/18/18/18	0/3/3/3
17	SF4	I	203	4	-	-	0/6/5/5
22	UQ8	N	503	-	-	15/51/75/75	0/1/1/1
18	3PE	N	506	-	-	30/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	A	501	-	-	16/45/45/54	-
19	LFA	H	402	-	-	1/17/17/17	-
19	LFA	N	505	-	-	7/17/17/17	-
18	3PE	H	401	-	-	14/54/54/54	-
17	SF4	G	1002	3	-	-	0/6/5/5
17	SF4	G	1007	3	-	-	0/6/5/5
21	TRD	N	501	-	-	1/10/10/10	-
21	TRD	L	708	-	-	3/10/10/10	-
14	FES	G	1003	3	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	502	UQ8	C6-C1	7.32	1.48	1.35
22	N	503	UQ8	C6-C1	7.21	1.48	1.35
16	F	501	FMN	C4A-N5	3.71	1.38	1.30
22	N	502	UQ8	C4-C3	2.97	1.48	1.36
22	N	503	UQ8	C4-C3	2.95	1.48	1.36
20	L	703	CDL	OB8-CB7	2.68	1.41	1.33
20	L	703	CDL	OA6-CA4	-2.61	1.40	1.46
20	L	703	CDL	OB6-CB4	-2.46	1.40	1.46
20	L	703	CDL	OA8-CA7	2.43	1.40	1.33
20	L	703	CDL	OB6-CB5	2.42	1.41	1.34
16	F	501	FMN	C10-N1	2.41	1.38	1.33
20	L	703	CDL	OA8-CA6	-2.11	1.40	1.45
20	L	703	CDL	OA6-CA5	2.08	1.40	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	502	UQ8	C7-C8-C9	-5.10	118.30	126.79
22	N	503	UQ8	C7-C8-C9	-4.48	119.34	126.79
20	L	703	CDL	OA6-CA5-C11	3.89	119.89	111.50
20	L	703	CDL	OB6-CB5-C51	3.89	119.89	111.50
22	N	503	UQ8	C15-C14-C16	3.67	121.45	115.27
22	N	503	UQ8	C32-C33-C34	-3.41	119.44	127.66
22	N	503	UQ8	C12-C13-C14	-3.39	119.49	127.66
22	N	503	UQ8	C22-C23-C24	-3.38	119.52	127.66
22	N	503	UQ8	C25-C24-C26	3.27	120.77	115.27
22	N	502	UQ8	C37-C38-C39	-3.24	119.85	127.66
22	N	502	UQ8	C30-C29-C31	3.12	120.52	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	502	UQ8	C15-C14-C16	3.10	120.48	115.27
16	F	501	FMN	C4-N3-C2	-3.07	119.97	125.64
22	N	503	UQ8	C20-C19-C21	3.01	120.33	115.27
22	N	503	UQ8	C35-C34-C36	3.00	120.32	115.27
22	N	502	UQ8	C20-C19-C21	3.00	120.31	115.27
22	N	503	UQ8	C37-C38-C39	-2.99	120.45	127.66
22	N	502	UQ8	C17-C18-C19	-2.99	120.47	127.66
22	N	502	UQ8	C32-C33-C34	-2.99	120.47	127.66
22	N	502	UQ8	C22-C23-C24	-2.93	120.60	127.66
22	N	502	UQ8	C27-C28-C29	-2.93	120.60	127.66
22	N	502	UQ8	C12-C13-C14	-2.90	120.67	127.66
22	N	502	UQ8	C35-C34-C36	2.75	119.89	115.27
20	L	703	CDL	OB8-CB7-C71	2.73	120.47	111.91
22	N	503	UQ8	C40-C39-C41	2.71	119.82	115.27
22	N	503	UQ8	C27-C28-C29	-2.67	121.24	127.66
16	F	501	FMN	C4A-C4-N3	2.65	119.92	113.19
16	F	501	FMN	C4A-C10-N10	2.63	120.33	116.48
22	N	503	UQ8	C10-C9-C11	2.62	119.68	115.27
22	N	502	UQ8	C10-C9-C11	2.60	119.65	115.27
20	L	703	CDL	OA8-CA7-C31	2.60	120.06	111.91
22	N	502	UQ8	C40-C39-C41	2.60	119.64	115.27
16	F	501	FMN	O4-C4-C4A	-2.55	119.84	126.60
22	N	502	UQ8	C25-C24-C26	2.50	119.48	115.27
22	N	502	UQ8	C46-C44-C45	2.49	120.09	114.60
22	N	503	UQ8	C1M-C1-C6	-2.48	120.35	124.40
22	N	503	UQ8	C46-C44-C45	2.41	119.92	114.60
22	N	502	UQ8	C42-C43-C44	-2.40	119.55	127.75
22	N	503	UQ8	C17-C18-C19	-2.39	121.91	127.66
22	N	503	UQ8	C30-C29-C31	2.39	119.28	115.27
18	L	701	3PE	O12-P-O14	2.38	124.00	112.24
18	L	705	3PE	O12-P-O14	2.35	123.85	112.24
18	A	501	3PE	O12-P-O14	2.35	123.84	112.24
18	M	601	3PE	O12-P-O14	2.34	123.81	112.24
18	A	502	3PE	O12-P-O14	2.33	123.78	112.24
18	M	602	3PE	O12-P-O14	2.33	123.76	112.24
18	J	201	3PE	O12-P-O14	2.33	123.75	112.24
18	N	506	3PE	O12-P-O14	2.32	123.72	112.24
18	H	401	3PE	O12-P-O14	2.32	123.71	112.24
18	N	504	3PE	O12-P-O14	2.31	123.67	112.24
18	L	702	3PE	O12-P-O14	2.31	123.66	112.24
18	L	704	3PE	O12-P-O14	2.30	123.61	112.24
18	J	202	3PE	O12-P-O14	2.27	123.48	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	706	3PE	O12-P-O14	2.27	123.46	112.24
16	F	501	FMN	C10-C4A-N5	-2.26	120.05	124.86
18	H	403	3PE	O12-P-O14	2.26	123.41	112.24
18	M	603	3PE	O12-P-O14	2.22	123.24	112.24
22	N	502	UQ8	C1M-C1-C6	-2.11	120.96	124.40
16	F	501	FMN	C4A-C10-N1	-2.06	119.94	124.73
22	N	503	UQ8	C42-C43-C44	-2.06	120.69	127.75

There are no chirality outliers.

All (409) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	F	501	FMN	C1'-C2'-C3'-O3'
16	F	501	FMN	C1'-C2'-C3'-C4'
18	H	401	3PE	C1-O11-P-O12
18	H	401	3PE	C2-C1-O11-P
18	H	401	3PE	C22-C21-O21-C2
18	H	403	3PE	C1-O11-P-O14
18	H	403	3PE	C11-O13-P-O11
18	H	403	3PE	C11-O13-P-O12
18	H	403	3PE	C11-O13-P-O14
18	H	403	3PE	C2-C1-O11-P
18	H	403	3PE	O13-C11-C12-N
18	J	201	3PE	C1-O11-P-O14
18	J	201	3PE	O13-C11-C12-N
18	J	201	3PE	O32-C31-O31-C3
18	J	201	3PE	C32-C31-O31-C3
18	J	202	3PE	C1-O11-P-O12
18	J	202	3PE	O13-C11-C12-N
18	J	202	3PE	O22-C21-O21-C2
18	M	601	3PE	C11-O13-P-O11
18	M	601	3PE	C11-O13-P-O12
18	M	601	3PE	O13-C11-C12-N
18	M	601	3PE	O11-C1-C2-O21
18	M	601	3PE	O22-C21-O21-C2
18	M	601	3PE	C22-C21-O21-C2
18	M	602	3PE	C1-O11-P-O12
18	M	602	3PE	C1-O11-P-O13
18	M	602	3PE	C1-O11-P-O14
18	M	602	3PE	C11-O13-P-O14
18	M	602	3PE	O13-C11-C12-N
18	M	602	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
18	M	602	3PE	C32-C31-O31-C3
18	M	603	3PE	C11-O13-P-O12
18	M	603	3PE	O13-C11-C12-N
18	M	603	3PE	C22-C21-O21-C2
18	A	501	3PE	C1-O11-P-O14
18	A	501	3PE	C11-O13-P-O12
18	A	501	3PE	O13-C11-C12-N
18	A	502	3PE	C1-O11-P-O14
18	L	702	3PE	O13-C11-C12-N
18	L	704	3PE	O13-C11-C12-N
18	L	705	3PE	C1-O11-P-O13
18	L	705	3PE	C1-O11-P-O14
18	L	705	3PE	C11-O13-P-O14
18	L	705	3PE	O13-C11-C12-N
18	L	705	3PE	O22-C21-O21-C2
18	L	706	3PE	C11-O13-P-O14
18	L	706	3PE	O22-C21-O21-C2
18	N	504	3PE	C1-O11-P-O12
18	N	504	3PE	C11-O13-P-O14
18	N	506	3PE	C11-O13-P-O14
18	N	506	3PE	O13-C11-C12-N
18	N	506	3PE	O22-C21-O21-C2
20	L	703	CDL	CB2-C1-CA2-OA2
20	L	703	CDL	CA2-OA2-PA1-OA3
20	L	703	CDL	CA2-OA2-PA1-OA4
20	L	703	CDL	CB2-OB2-PB2-OB3
20	L	703	CDL	CB2-OB2-PB2-OB4
22	N	502	UQ8	C35-C34-C36-C37
22	N	502	UQ8	C29-C31-C32-C33
22	N	502	UQ8	C30-C29-C31-C32
22	N	502	UQ8	C25-C24-C26-C27
22	N	502	UQ8	C23-C24-C26-C27
22	N	502	UQ8	C20-C19-C21-C22
22	N	503	UQ8	C20-C19-C21-C22
22	N	503	UQ8	C18-C19-C21-C22
22	N	503	UQ8	C9-C11-C12-C13
18	L	705	3PE	C32-C31-O31-C3
18	H	401	3PE	O32-C31-O31-C3
18	J	202	3PE	O32-C31-O31-C3
18	A	501	3PE	O32-C31-O31-C3
18	L	705	3PE	O32-C31-O31-C3
18	H	401	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
18	M	603	3PE	O22-C21-O21-C2
18	A	501	3PE	C32-C31-O31-C3
18	J	202	3PE	C22-C21-O21-C2
18	L	705	3PE	C22-C21-O21-C2
18	L	706	3PE	C22-C21-O21-C2
18	N	506	3PE	C22-C21-O21-C2
22	N	503	UQ8	C35-C34-C36-C37
22	N	503	UQ8	C30-C29-C31-C32
22	N	502	UQ8	C33-C34-C36-C37
22	N	502	UQ8	C28-C29-C31-C32
22	N	502	UQ8	C18-C19-C21-C22
22	N	503	UQ8	C33-C34-C36-C37
18	H	401	3PE	C32-C31-O31-C3
18	J	202	3PE	C32-C31-O31-C3
20	L	703	CDL	OB9-CB7-OB8-CB6
20	L	703	CDL	C71-CB7-OB8-CB6
22	N	502	UQ8	C40-C39-C41-C42
22	N	503	UQ8	C40-C39-C41-C42
22	N	502	UQ8	C38-C39-C41-C42
22	N	503	UQ8	C38-C39-C41-C42
22	N	502	UQ8	C24-C26-C27-C28
22	N	502	UQ8	C9-C11-C12-C13
22	N	503	UQ8	C34-C36-C37-C38
22	N	503	UQ8	C19-C21-C22-C23
20	L	703	CDL	CA2-C1-CB2-OB2
20	L	703	CDL	O1-C1-CA2-OA2
20	L	703	CDL	C51-CB5-OB6-CB4
18	L	704	3PE	C31-C32-C33-C34
18	L	705	3PE	C21-C22-C23-C24
20	L	703	CDL	CB5-C51-C52-C53
22	N	502	UQ8	C19-C21-C22-C23
20	L	703	CDL	O1-C1-CB2-OB2
18	H	401	3PE	C1-O11-P-O13
18	H	403	3PE	C1-O11-P-O13
18	J	202	3PE	C1-O11-P-O13
18	M	601	3PE	C1-O11-P-O13
18	M	602	3PE	C11-O13-P-O11
18	M	603	3PE	C11-O13-P-O11
18	A	501	3PE	C11-O13-P-O11
18	L	705	3PE	C11-O13-P-O11
18	N	504	3PE	C1-O11-P-O13
18	N	506	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
18	N	506	3PE	C11-O13-P-O11
20	L	703	CDL	CA2-OA2-PA1-OA5
20	L	703	CDL	CA3-OA5-PA1-OA2
20	L	703	CDL	CB2-OB2-PB2-OB5
20	L	703	CDL	CB3-OB5-PB2-OB2
20	L	703	CDL	OB7-CB5-OB6-CB4
22	N	503	UQ8	C28-C29-C31-C32
16	F	501	FMN	O2'-C2'-C3'-O3'
18	N	506	3PE	C31-C32-C33-C34
20	L	703	CDL	C11-CA5-OA6-CA4
18	J	201	3PE	C25-C26-C27-C28
18	J	201	3PE	C2A-C2B-C2C-C2D
18	M	602	3PE	C2A-C2B-C2C-C2D
18	A	502	3PE	C39-C3A-C3B-C3C
18	L	705	3PE	C27-C28-C29-C2A
18	L	706	3PE	C26-C27-C28-C29
18	L	706	3PE	C29-C2A-C2B-C2C
18	N	504	3PE	C32-C33-C34-C35
20	L	703	CDL	C77-C78-C79-C80
18	H	403	3PE	C3A-C3B-C3C-C3D
18	M	603	3PE	C29-C2A-C2B-C2C
20	L	703	CDL	C31-C32-C33-C34
20	L	703	CDL	OA7-CA5-OA6-CA4
18	N	504	3PE	C31-C32-C33-C34
16	F	501	FMN	O2'-C2'-C3'-C4'
18	A	501	3PE	C39-C3A-C3B-C3C
21	N	501	TRD	C11-C10-C9-C8
18	A	502	3PE	C38-C39-C3A-C3B
18	L	706	3PE	C2A-C2B-C2C-C2D
18	J	201	3PE	C21-C22-C23-C24
18	J	201	3PE	C28-C29-C2A-C2B
18	A	501	3PE	C32-C33-C34-C35
18	J	201	3PE	C34-C35-C36-C37
18	N	506	3PE	C22-C23-C24-C25
19	N	505	LFA	C13-C14-C15-C16
18	L	705	3PE	C23-C24-C25-C26
18	N	506	3PE	C36-C37-C38-C39
18	L	702	3PE	O22-C21-O21-C2
18	M	602	3PE	C22-C21-O21-C2
18	L	702	3PE	C22-C21-O21-C2
18	H	401	3PE	C27-C28-C29-C2A
18	L	702	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
18	L	706	3PE	C2B-C2C-C2D-C2E
18	H	403	3PE	C32-C33-C34-C35
18	L	705	3PE	C38-C39-C3A-C3B
18	L	706	3PE	C38-C39-C3A-C3B
18	N	506	3PE	C23-C24-C25-C26
20	L	703	CDL	C53-C54-C55-C56
20	L	703	CDL	C62-C63-C64-C65
20	L	703	CDL	C58-C59-C60-C61
18	J	201	3PE	C38-C39-C3A-C3B
21	L	707	TRD	C4-C5-C6-C7
18	M	602	3PE	O22-C21-O21-C2
18	M	601	3PE	C23-C24-C25-C26
18	A	502	3PE	C29-C2A-C2B-C2C
22	N	502	UQ8	C15-C14-C16-C17
22	N	502	UQ8	C13-C14-C16-C17
18	L	704	3PE	C22-C21-O21-C2
18	L	702	3PE	C25-C26-C27-C28
18	H	403	3PE	C36-C37-C38-C39
18	N	506	3PE	C2D-C2E-C2F-C2G
18	L	706	3PE	C3E-C3F-C3G-C3H
18	L	704	3PE	O22-C21-O21-C2
18	M	602	3PE	C34-C35-C36-C37
18	M	602	3PE	C28-C29-C2A-C2B
20	L	703	CDL	C75-C76-C77-C78
18	L	701	3PE	C21-C22-C23-C24
18	J	201	3PE	C29-C2A-C2B-C2C
18	A	501	3PE	C28-C29-C2A-C2B
20	L	703	CDL	C73-C74-C75-C76
18	J	201	3PE	O22-C21-O21-C2
18	L	705	3PE	C37-C38-C39-C3A
18	N	506	3PE	C2C-C2D-C2E-C2F
18	J	201	3PE	C22-C21-O21-C2
18	J	201	3PE	C2B-C2C-C2D-C2E
20	L	703	CDL	C80-C81-C82-C83
18	H	401	3PE	C24-C25-C26-C27
21	L	708	TRD	C4-C5-C6-C7
18	L	702	3PE	C3A-C3B-C3C-C3D
18	H	403	3PE	C3C-C3D-C3E-C3F
18	L	706	3PE	C3A-C3B-C3C-C3D
18	M	603	3PE	C32-C33-C34-C35
18	L	702	3PE	C27-C28-C29-C2A
18	H	403	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
18	J	202	3PE	C22-C23-C24-C25
20	L	703	CDL	C63-C64-C65-C66
18	J	201	3PE	C1-O11-P-O13
18	J	202	3PE	C11-O13-P-O11
18	L	706	3PE	C11-O13-P-O11
18	N	504	3PE	C26-C27-C28-C29
18	H	403	3PE	C33-C34-C35-C36
20	L	703	CDL	C72-C73-C74-C75
20	L	703	CDL	CB3-CB4-CB6-OB8
18	M	602	3PE	C3C-C3D-C3E-C3F
18	L	705	3PE	C35-C36-C37-C38
18	H	401	3PE	C2F-C2G-C2H-C2I
20	L	703	CDL	CB7-C71-C72-C73
18	N	506	3PE	C38-C39-C3A-C3B
18	J	201	3PE	C23-C24-C25-C26
20	L	703	CDL	C14-C15-C16-C17
18	L	706	3PE	C35-C36-C37-C38
18	L	705	3PE	C2C-C2D-C2E-C2F
20	L	703	CDL	C15-C16-C17-C18
18	J	202	3PE	C2C-C2D-C2E-C2F
18	N	506	3PE	C32-C33-C34-C35
18	L	705	3PE	O11-C1-C2-O21
20	L	703	CDL	C39-C40-C41-C42
18	H	401	3PE	C38-C39-C3A-C3B
18	M	602	3PE	C25-C26-C27-C28
18	N	506	3PE	C3B-C3C-C3D-C3E
20	L	703	CDL	C43-C44-C45-C46
18	J	202	3PE	C21-C22-C23-C24
21	L	708	TRD	C6-C7-C8-C9
19	N	505	LFA	C9-C10-C11-C12
18	L	706	3PE	C34-C35-C36-C37
18	N	504	3PE	O11-C1-C2-C3
22	N	503	UQ8	C24-C26-C27-C28
20	L	703	CDL	CA7-C31-C32-C33
18	J	202	3PE	C28-C29-C2A-C2B
18	L	706	3PE	C36-C37-C38-C39
18	J	201	3PE	C3D-C3E-C3F-C3G
18	J	202	3PE	C2-C1-O11-P
18	M	602	3PE	C2-C1-O11-P
18	L	705	3PE	C2-C1-O11-P
18	L	704	3PE	C23-C24-C25-C26
18	L	706	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
18	L	705	3PE	C28-C29-C2A-C2B
18	L	704	3PE	C11-O13-P-O11
18	L	706	3PE	C1-O11-P-O13
18	L	701	3PE	C38-C39-C3A-C3B
18	L	705	3PE	C25-C26-C27-C28
18	N	504	3PE	O11-C1-C2-O21
18	M	602	3PE	C22-C23-C24-C25
18	N	506	3PE	C27-C28-C29-C2A
18	M	602	3PE	O21-C2-C3-O31
18	L	705	3PE	O21-C2-C3-O31
18	L	706	3PE	O21-C2-C3-O31
18	J	202	3PE	C32-C33-C34-C35
18	M	601	3PE	C34-C35-C36-C37
18	A	502	3PE	C3D-C3E-C3F-C3G
20	L	703	CDL	C17-C18-C19-C20
18	M	603	3PE	C2-C1-O11-P
18	A	502	3PE	C2-C1-O11-P
18	N	504	3PE	C2-C1-O11-P
20	L	703	CDL	CA4-CA3-OA5-PA1
18	A	502	3PE	C3E-C3F-C3G-C3H
18	N	506	3PE	C2F-C2G-C2H-C2I
18	M	601	3PE	C3D-C3E-C3F-C3G
18	L	702	3PE	C32-C33-C34-C35
18	M	603	3PE	C37-C38-C39-C3A
20	L	703	CDL	C12-C13-C14-C15
18	M	601	3PE	C39-C3A-C3B-C3C
20	L	703	CDL	C78-C79-C80-C81
21	L	708	TRD	C5-C6-C7-C8
18	A	501	3PE	C27-C28-C29-C2A
18	M	601	3PE	O11-C1-C2-C3
18	H	403	3PE	C22-C21-O21-C2
18	L	706	3PE	C37-C38-C39-C3A
20	L	703	CDL	C31-CA7-OA8-CA6
18	A	501	3PE	C37-C38-C39-C3A
19	N	505	LFA	C15-C16-C17-C18
20	L	703	CDL	OB6-CB4-CB6-OB8
20	L	703	CDL	C54-C55-C56-C57
20	L	703	CDL	C55-C56-C57-C58
18	H	403	3PE	O22-C21-O21-C2
18	A	501	3PE	C29-C2A-C2B-C2C
20	L	703	CDL	C36-C37-C38-C39
20	L	703	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
18	L	702	3PE	C31-C32-C33-C34
18	N	504	3PE	C11-O13-P-O11
18	N	506	3PE	C2-C1-O11-P
20	L	703	CDL	CB4-CB3-OB5-PB2
18	H	403	3PE	C1-O11-P-O12
18	J	202	3PE	C11-O13-P-O12
18	M	601	3PE	C1-O11-P-O14
18	M	602	3PE	C11-O13-P-O12
18	A	501	3PE	C1-O11-P-O12
18	L	704	3PE	C11-O13-P-O12
18	L	705	3PE	C11-O13-P-O12
18	N	504	3PE	C1-O11-P-O14
18	N	506	3PE	C1-O11-P-O14
18	N	506	3PE	C11-O13-P-O12
20	L	703	CDL	CA3-OA5-PA1-OA4
20	L	703	CDL	CB3-OB5-PB2-OB4
18	H	401	3PE	O11-C1-C2-C3
18	L	706	3PE	O11-C1-C2-C3
20	L	703	CDL	OA9-CA7-OA8-CA6
18	H	403	3PE	C37-C38-C39-C3A
18	H	403	3PE	C12-C11-O13-P
18	J	202	3PE	C12-C11-O13-P
18	M	602	3PE	C12-C11-O13-P
18	N	506	3PE	C12-C11-O13-P
18	H	401	3PE	O11-C1-C2-O21
18	J	201	3PE	O11-C1-C2-O21
18	L	706	3PE	O11-C1-C2-O21
18	M	602	3PE	C2E-C2F-C2G-C2H
18	M	602	3PE	C1-C2-C3-O31
18	L	705	3PE	C1-C2-C3-O31
18	J	201	3PE	C2C-C2D-C2E-C2F
18	N	506	3PE	C3C-C3D-C3E-C3F
22	N	503	UQ8	C14-C16-C17-C18
20	L	703	CDL	C57-C58-C59-C60
22	N	502	UQ8	C5-C4-O4-C4M
18	A	502	3PE	C28-C29-C2A-C2B
18	L	705	3PE	O11-C1-C2-C3
18	M	603	3PE	C31-C32-C33-C34
18	N	506	3PE	C39-C3A-C3B-C3C
18	L	705	3PE	C2D-C2E-C2F-C2G
19	N	505	LFA	C14-C15-C16-C17
18	J	202	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
18	L	705	3PE	C2A-C2B-C2C-C2D
18	N	506	3PE	C3A-C3B-C3C-C3D
18	M	602	3PE	C2F-C2G-C2H-C2I
18	A	501	3PE	C1-O11-P-O13
18	A	502	3PE	C1-O11-P-O13
18	N	506	3PE	C37-C38-C39-C3A
18	A	501	3PE	C36-C37-C38-C39
18	N	506	3PE	C32-C31-O31-C3
19	H	402	LFA	C16-C17-C18-C19
18	L	701	3PE	C28-C29-C2A-C2B
22	N	502	UQ8	C14-C16-C17-C18
18	M	603	3PE	C28-C29-C2A-C2B
18	J	202	3PE	C3D-C3E-C3F-C3G
18	A	502	3PE	C2A-C2B-C2C-C2D
18	L	702	3PE	C34-C35-C36-C37
18	N	506	3PE	O32-C31-O31-C3
18	M	601	3PE	C2-C1-O11-P
22	N	503	UQ8	C5-C4-O4-C4M
18	M	602	3PE	C39-C3A-C3B-C3C
19	N	505	LFA	C16-C17-C18-C19
18	N	506	3PE	C2-C3-O31-C31
20	L	703	CDL	C40-C41-C42-C43
18	J	202	3PE	C38-C39-C3A-C3B
20	L	703	CDL	CB6-CB4-OB6-CB5
18	L	702	3PE	C2B-C2C-C2D-C2E
20	L	703	CDL	C52-C53-C54-C55
18	L	704	3PE	O11-C1-C2-C3
18	L	704	3PE	O21-C2-C3-O31
18	M	602	3PE	C3B-C3C-C3D-C3E
18	L	704	3PE	C33-C34-C35-C36
18	J	201	3PE	C2D-C2E-C2F-C2G
18	M	601	3PE	C33-C34-C35-C36
18	L	702	3PE	O11-C1-C2-O21
18	H	401	3PE	O13-C11-C12-N
18	L	701	3PE	O13-C11-C12-N
18	L	705	3PE	O31-C31-C32-C33
20	L	703	CDL	C12-C11-CA5-OA6
22	N	502	UQ8	C12-C11-C9-C10
18	L	701	3PE	O21-C21-C22-C23
18	L	705	3PE	C1-C2-O21-C21
18	N	504	3PE	O21-C21-C22-C23
18	M	603	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	L	702	3PE	O31-C31-C32-C33
18	L	702	3PE	C28-C29-C2A-C2B
18	L	705	3PE	O21-C21-C22-C23
18	L	702	3PE	C29-C2A-C2B-C2C
18	J	201	3PE	O11-C1-C2-C3
20	L	703	CDL	C56-C57-C58-C59
20	L	703	CDL	OA6-CA4-CA6-OA8
18	L	701	3PE	C31-C32-C33-C34
18	J	201	3PE	C3E-C3F-C3G-C3H
19	N	505	LFA	C6-C7-C8-C9
18	L	705	3PE	C29-C2A-C2B-C2C
18	M	601	3PE	C3C-C3D-C3E-C3F
22	N	503	UQ8	C3-C4-O4-C4M
18	M	603	3PE	C27-C28-C29-C2A
18	L	701	3PE	O22-C21-C22-C23
18	L	702	3PE	O32-C31-C32-C33
18	L	705	3PE	O22-C21-C22-C23
18	N	504	3PE	O22-C21-C22-C23
18	L	702	3PE	C38-C39-C3A-C3B
22	N	502	UQ8	C21-C22-C23-C24
18	N	506	3PE	C33-C34-C35-C36
18	L	705	3PE	O32-C31-C32-C33
18	N	504	3PE	C27-C28-C29-C2A
18	N	504	3PE	C28-C29-C2A-C2B
19	N	505	LFA	C10-C11-C12-C13
18	L	705	3PE	C32-C33-C34-C35
20	L	703	CDL	C12-C11-CA5-OA7
18	A	502	3PE	C1-O11-P-O12
18	L	706	3PE	C1-O11-P-O14
20	L	703	CDL	CB3-OB5-PB2-OB3
18	M	601	3PE	C12-C11-O13-P
18	L	702	3PE	C12-C11-O13-P
18	L	706	3PE	C12-C11-O13-P
18	N	504	3PE	C12-C11-O13-P
20	L	703	CDL	CB3-CB4-OB6-CB5
18	M	601	3PE	C32-C33-C34-C35
18	L	704	3PE	C25-C26-C27-C28
18	N	506	3PE	C21-C22-C23-C24
18	A	501	3PE	C38-C39-C3A-C3B
18	L	704	3PE	C39-C3A-C3B-C3C
16	F	501	FMN	N10-C1'-C2'-O2'
22	N	502	UQ8	C3-C4-O4-C4M

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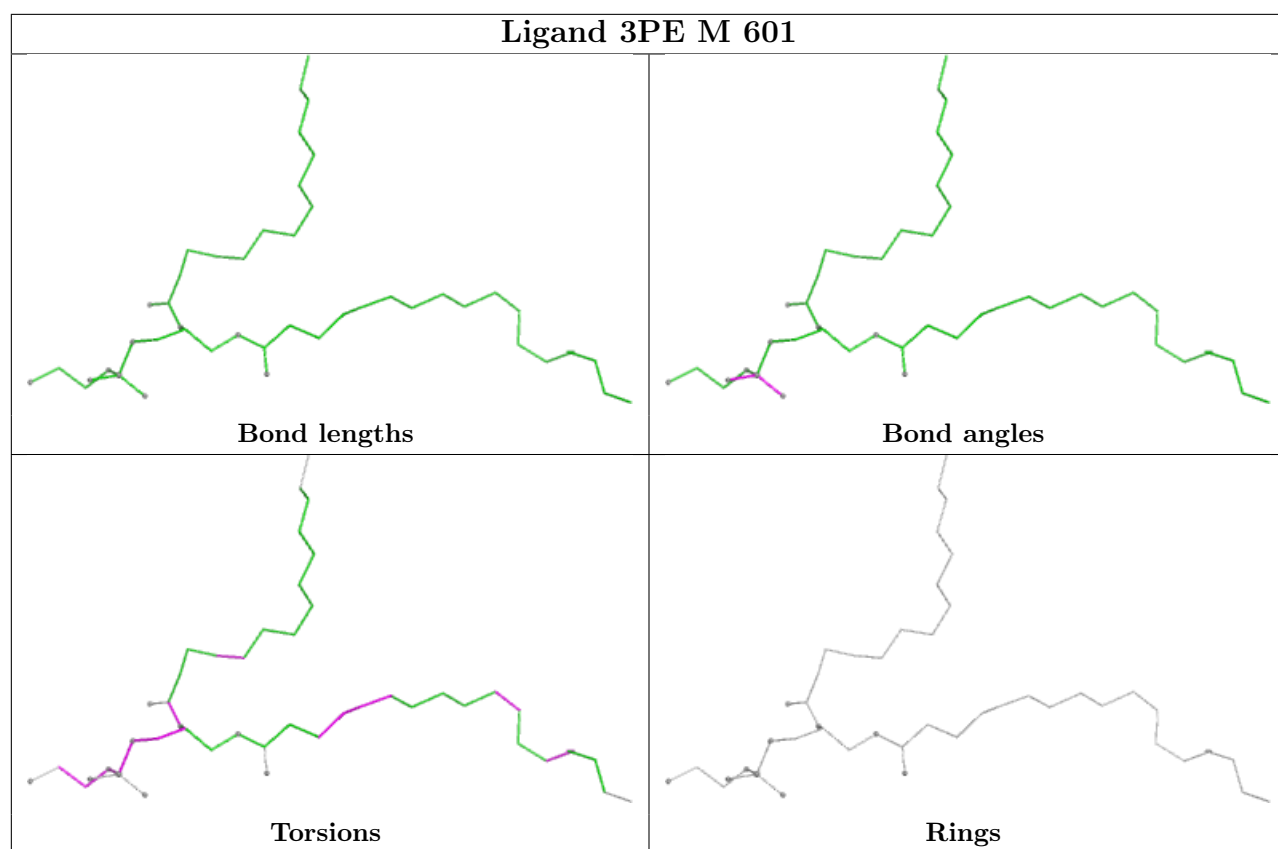
Mol	Chain	Res	Type	Atoms
21	L	707	TRD	C1-C2-C3-C4

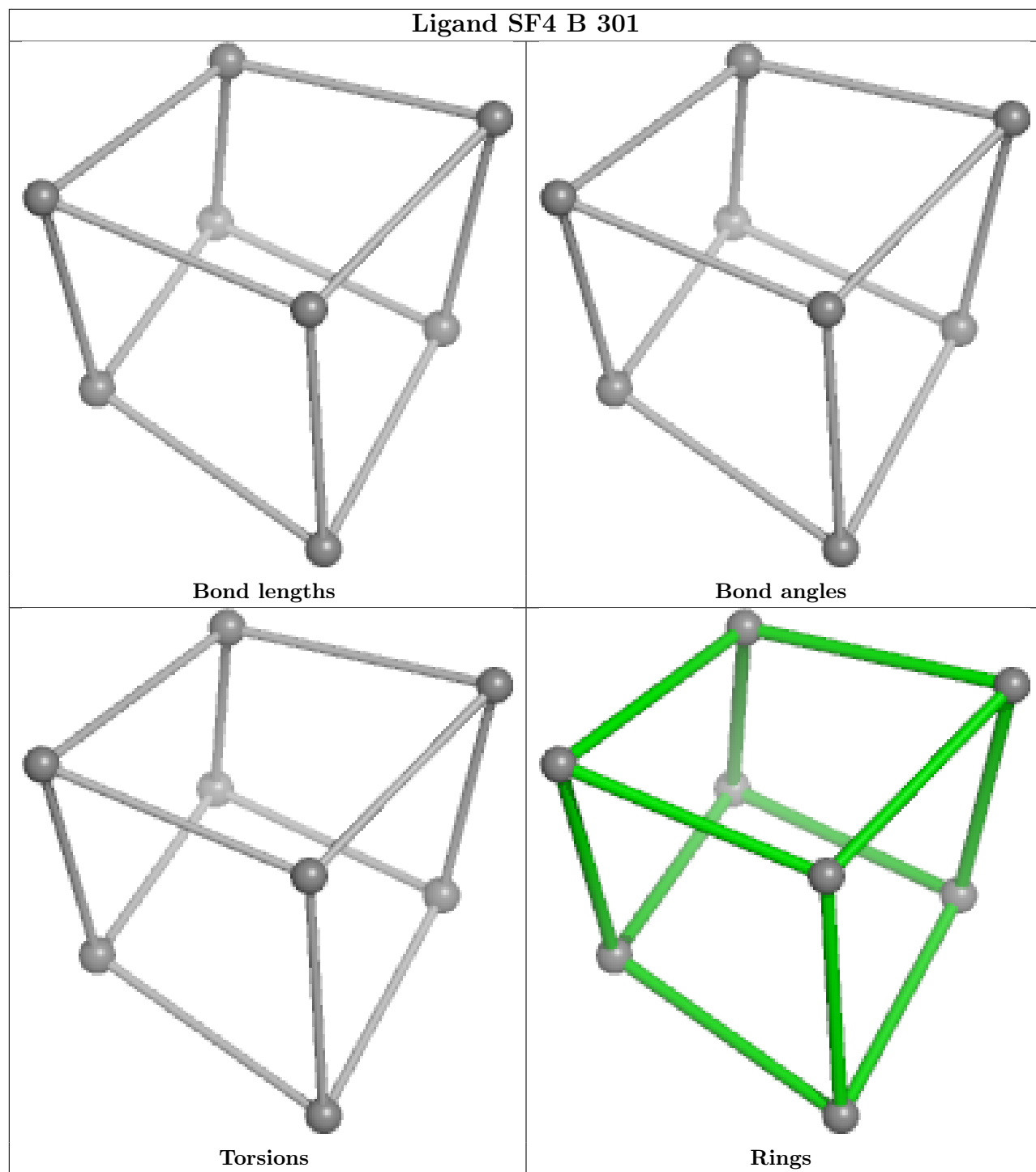
There are no ring outliers.

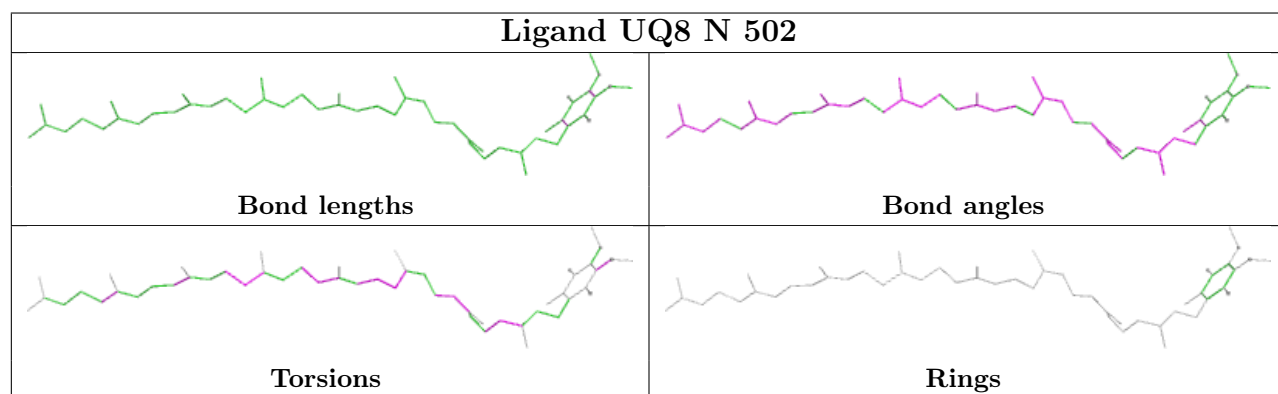
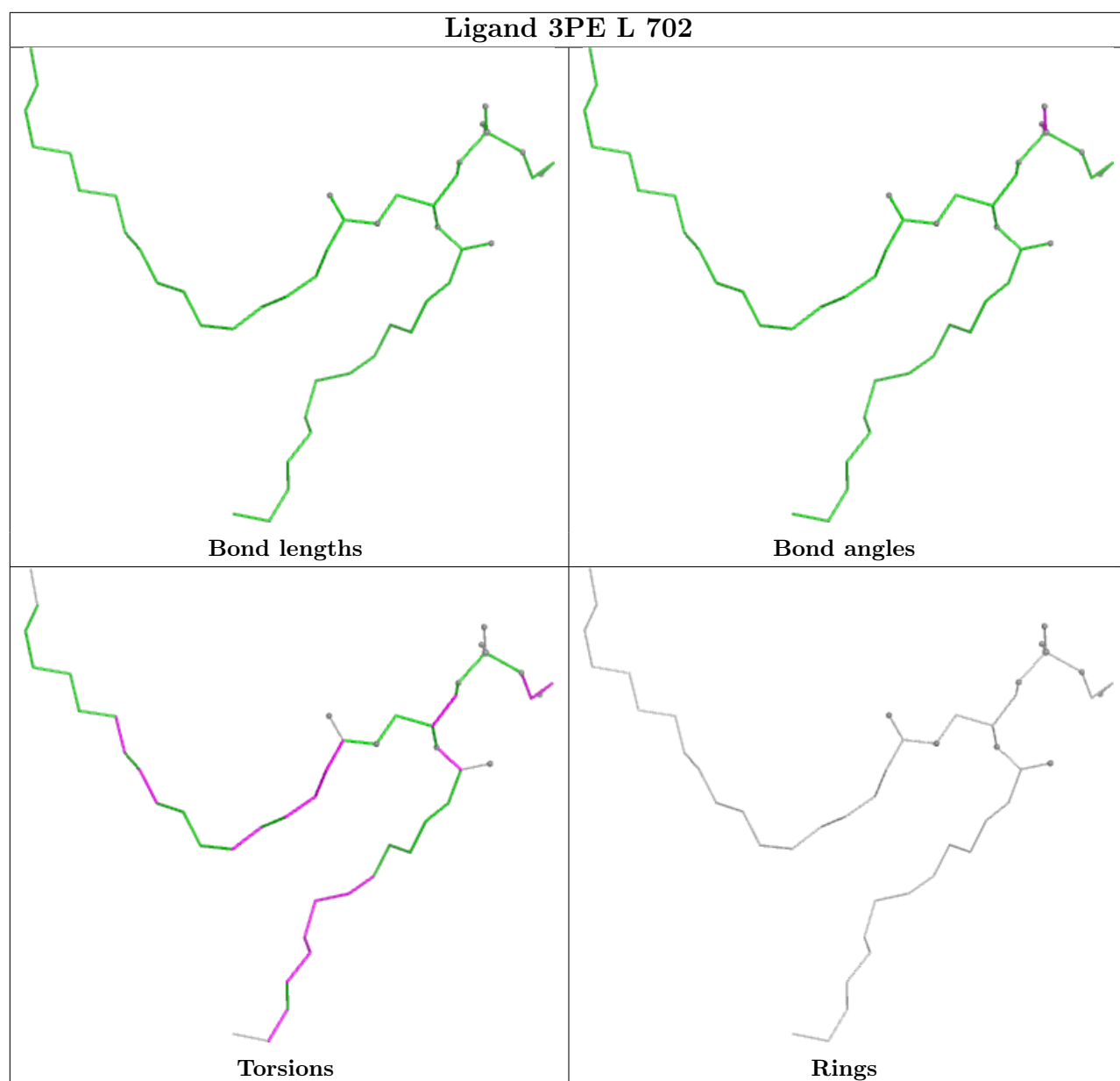
20 monomers are involved in 57 short contacts:

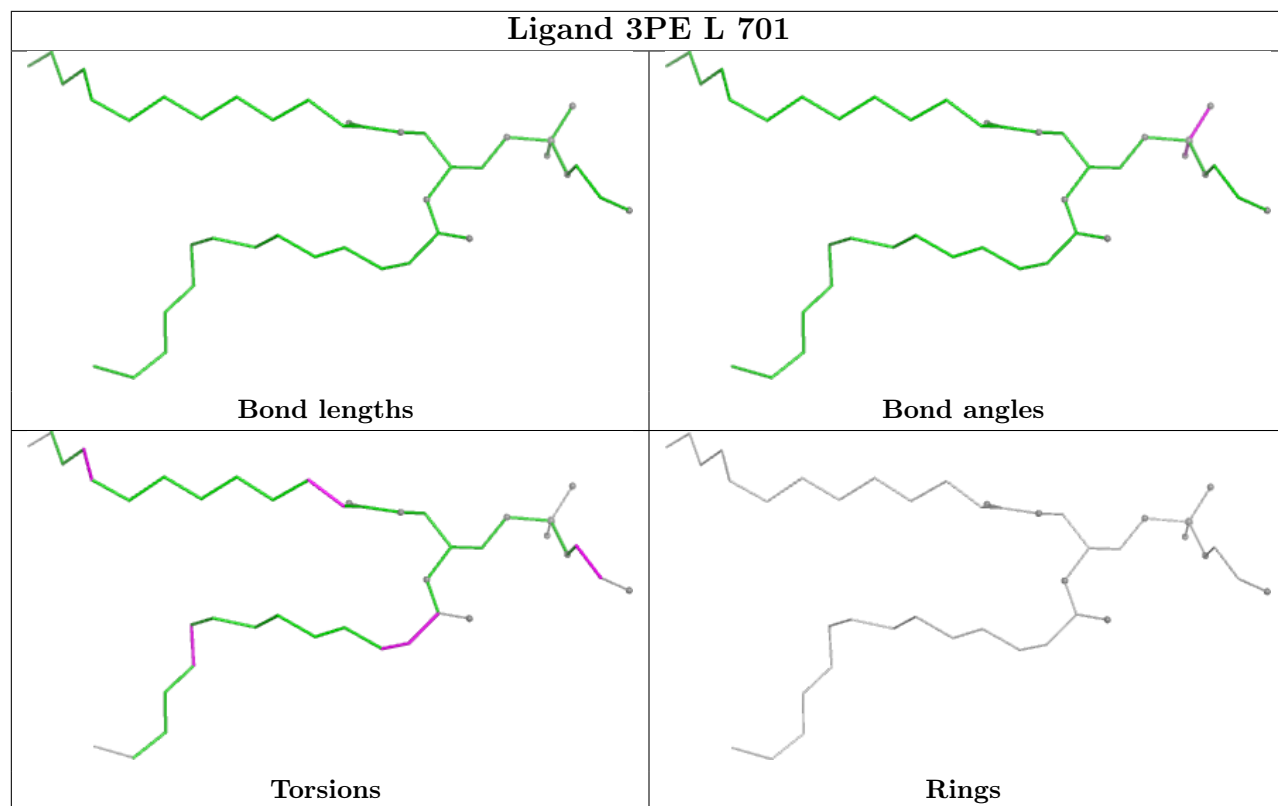
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	601	3PE	1	0
17	B	301	SF4	2	0
22	N	502	UQ8	10	0
18	L	701	3PE	1	0
20	L	703	CDL	4	0
18	J	202	3PE	1	0
18	L	704	3PE	3	0
17	F	502	SF4	1	0
18	N	504	3PE	1	0
18	A	502	3PE	2	0
18	J	201	3PE	5	0
18	L	705	3PE	1	0
18	M	603	3PE	3	0
18	M	602	3PE	1	0
16	F	501	FMN	1	0
22	N	503	UQ8	15	0
18	N	506	3PE	3	0
18	A	501	3PE	2	0
19	N	505	LFA	2	0
18	H	401	3PE	1	0

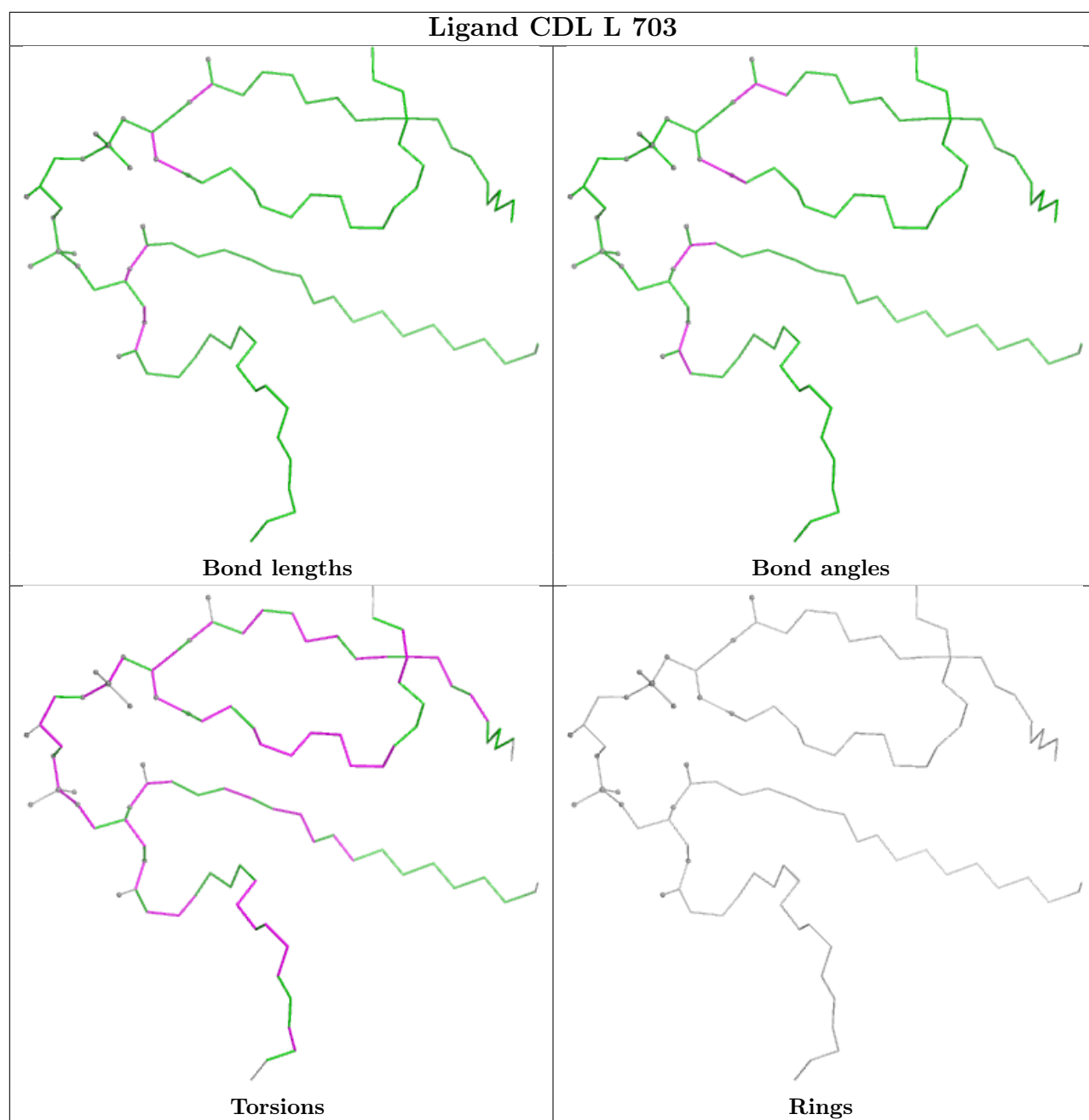
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

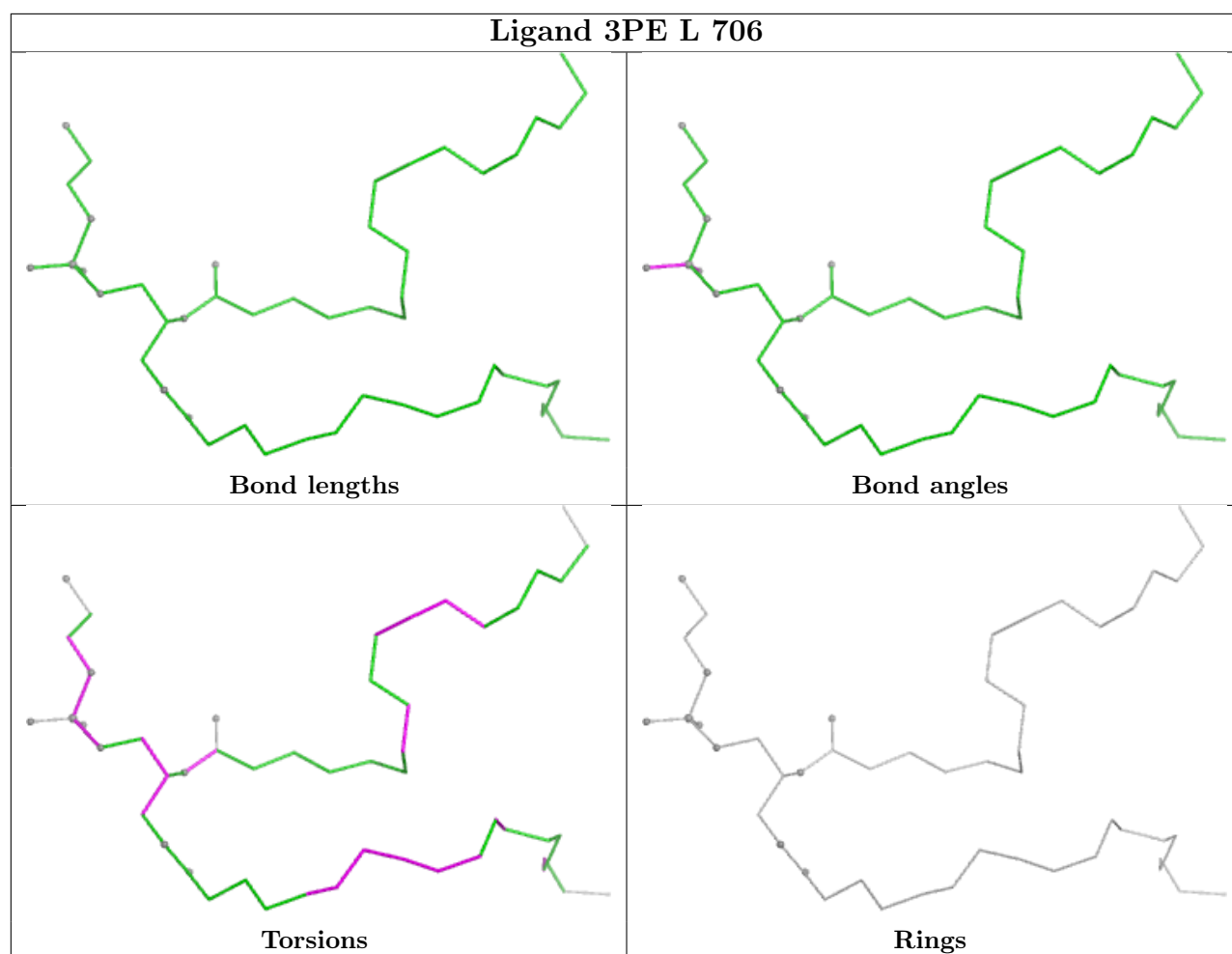


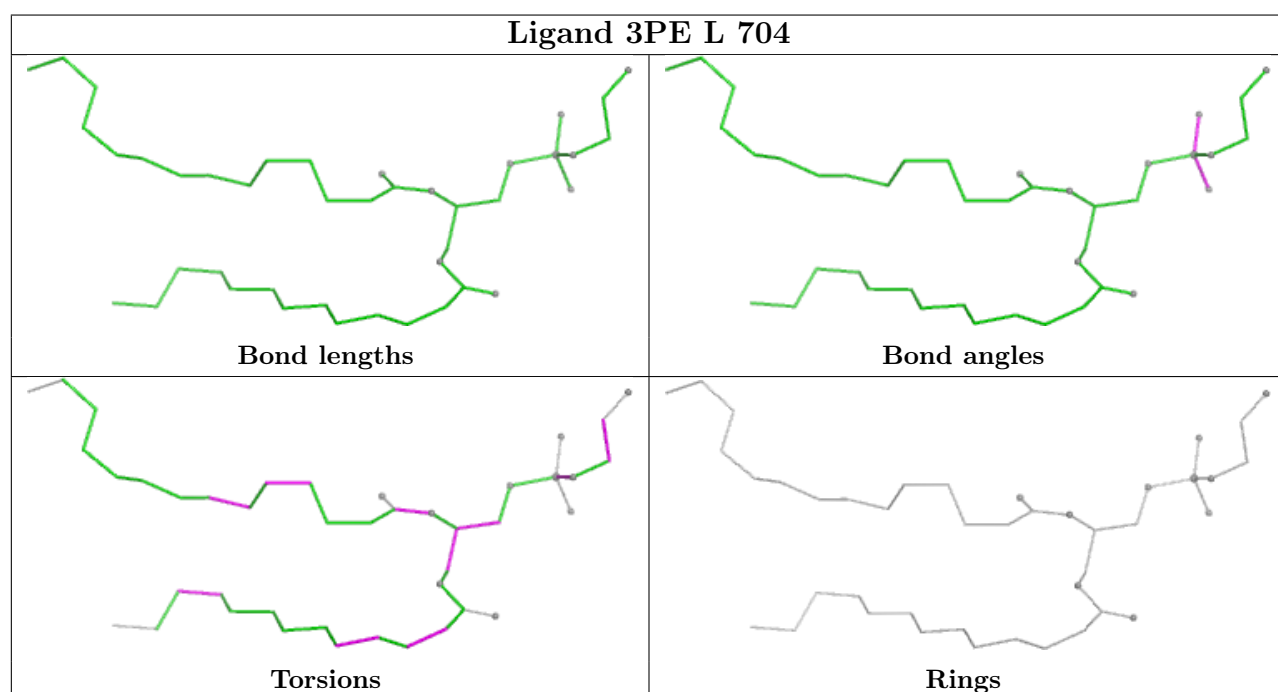


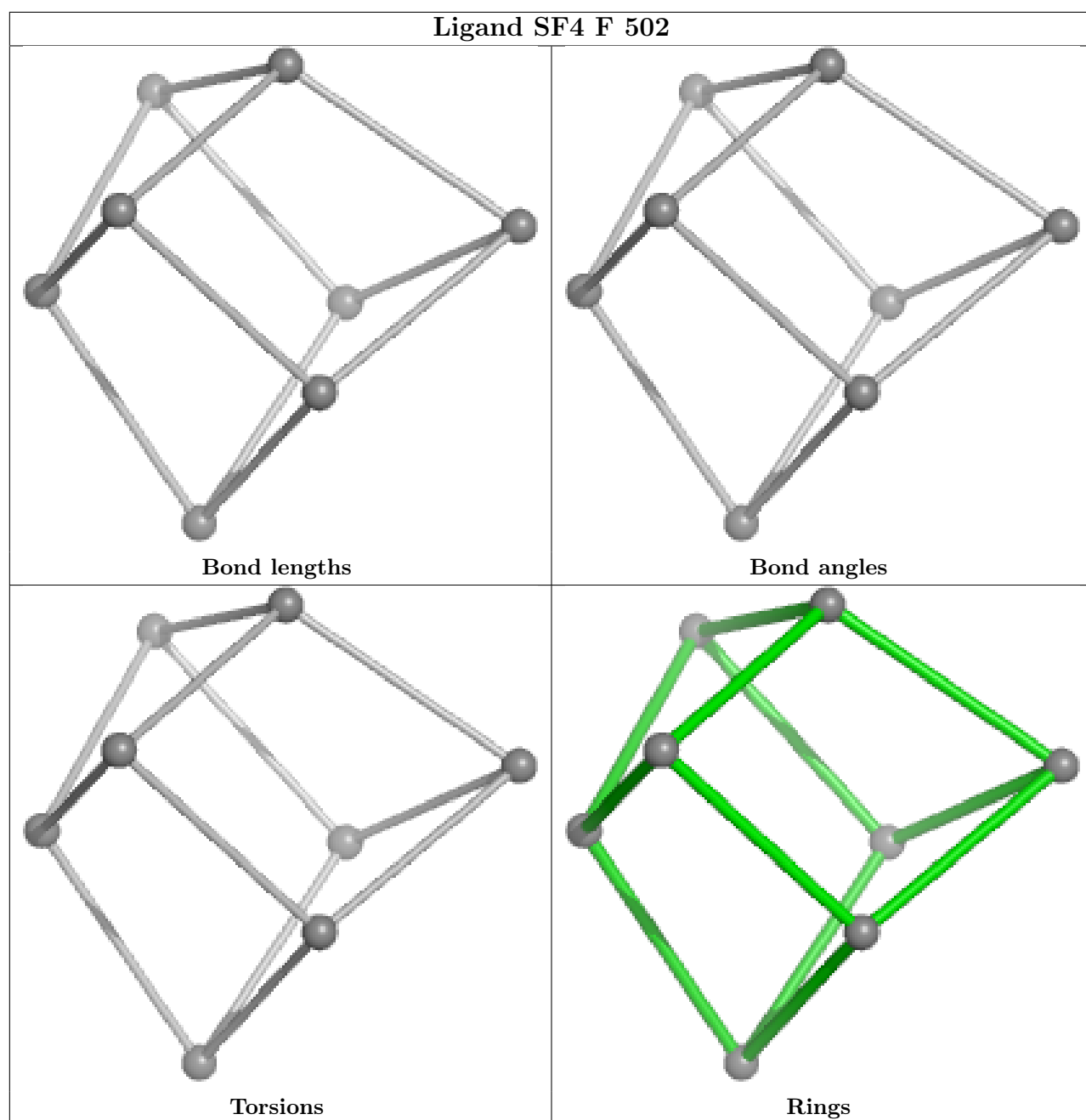


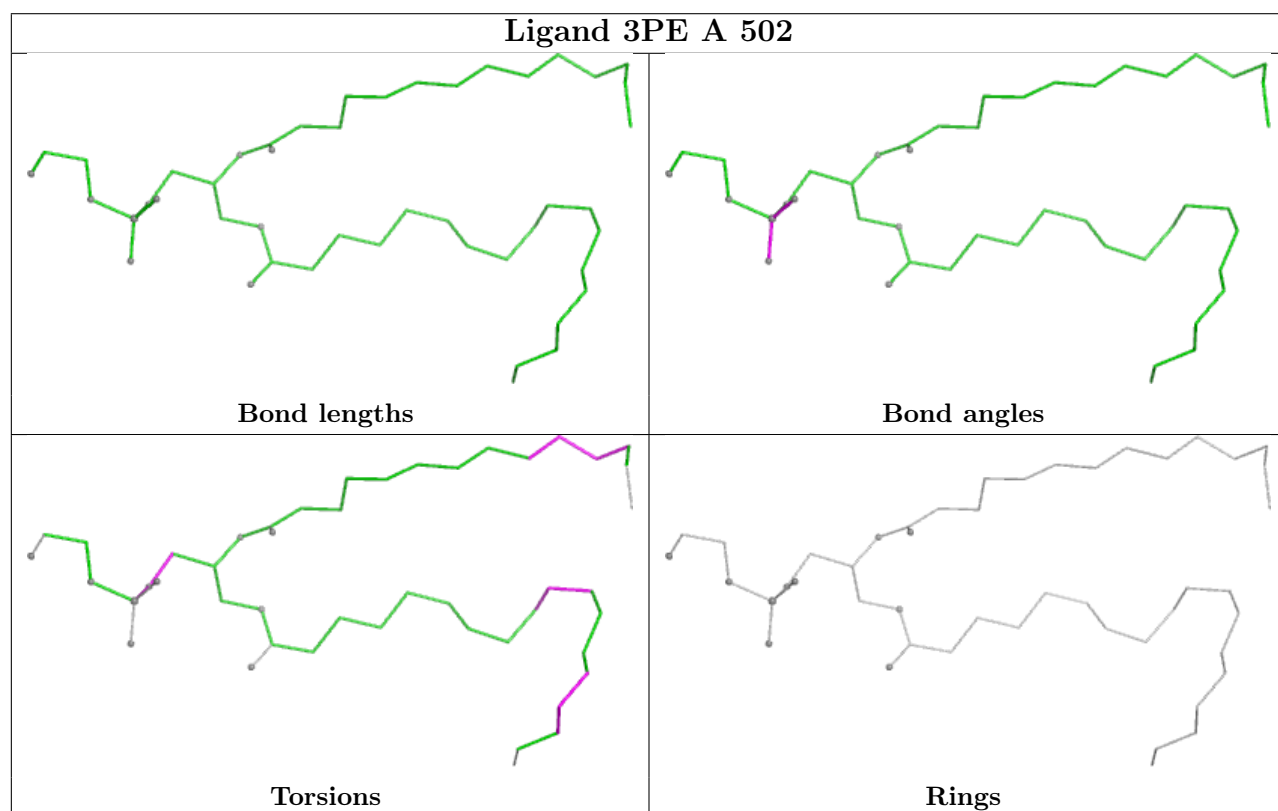
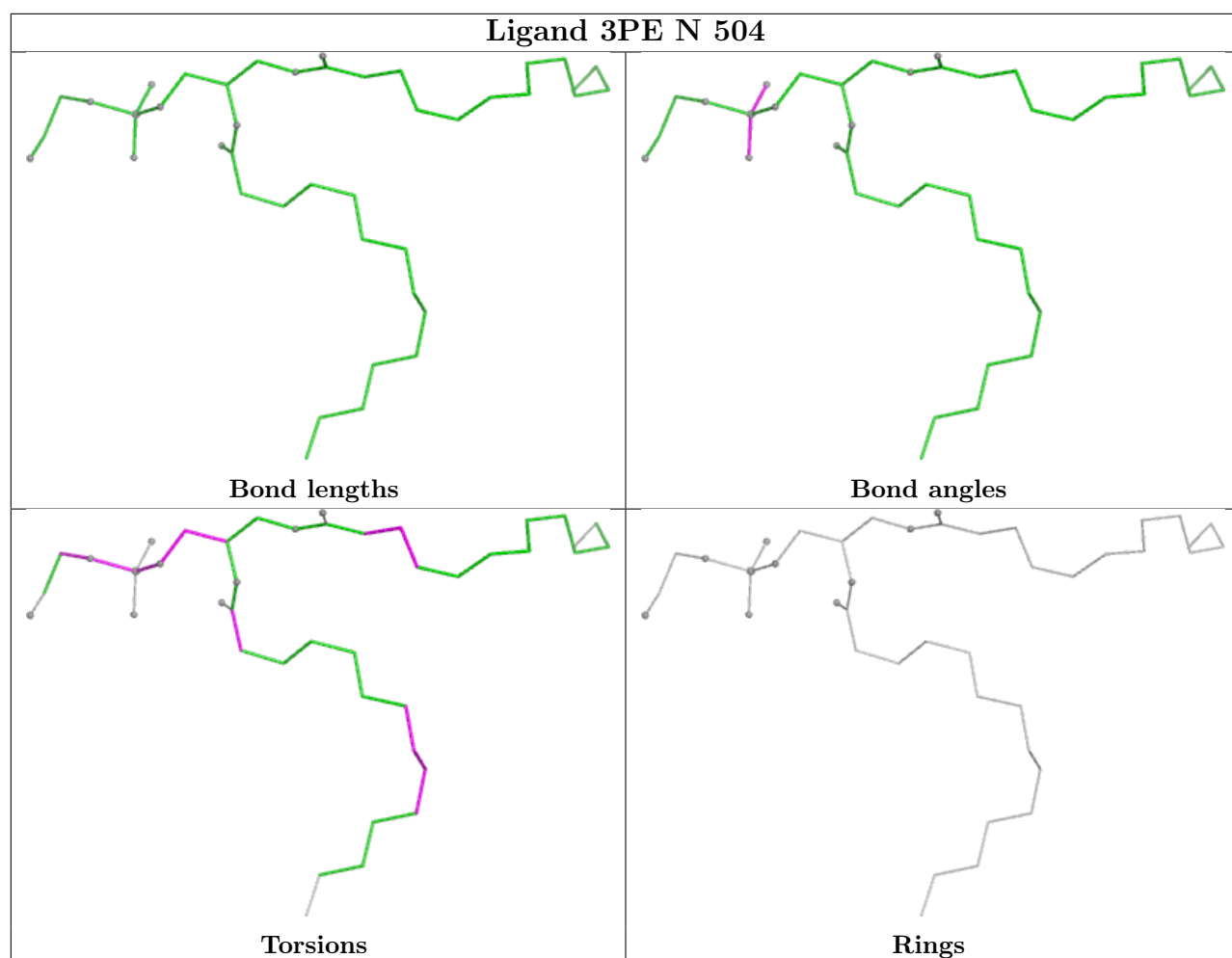


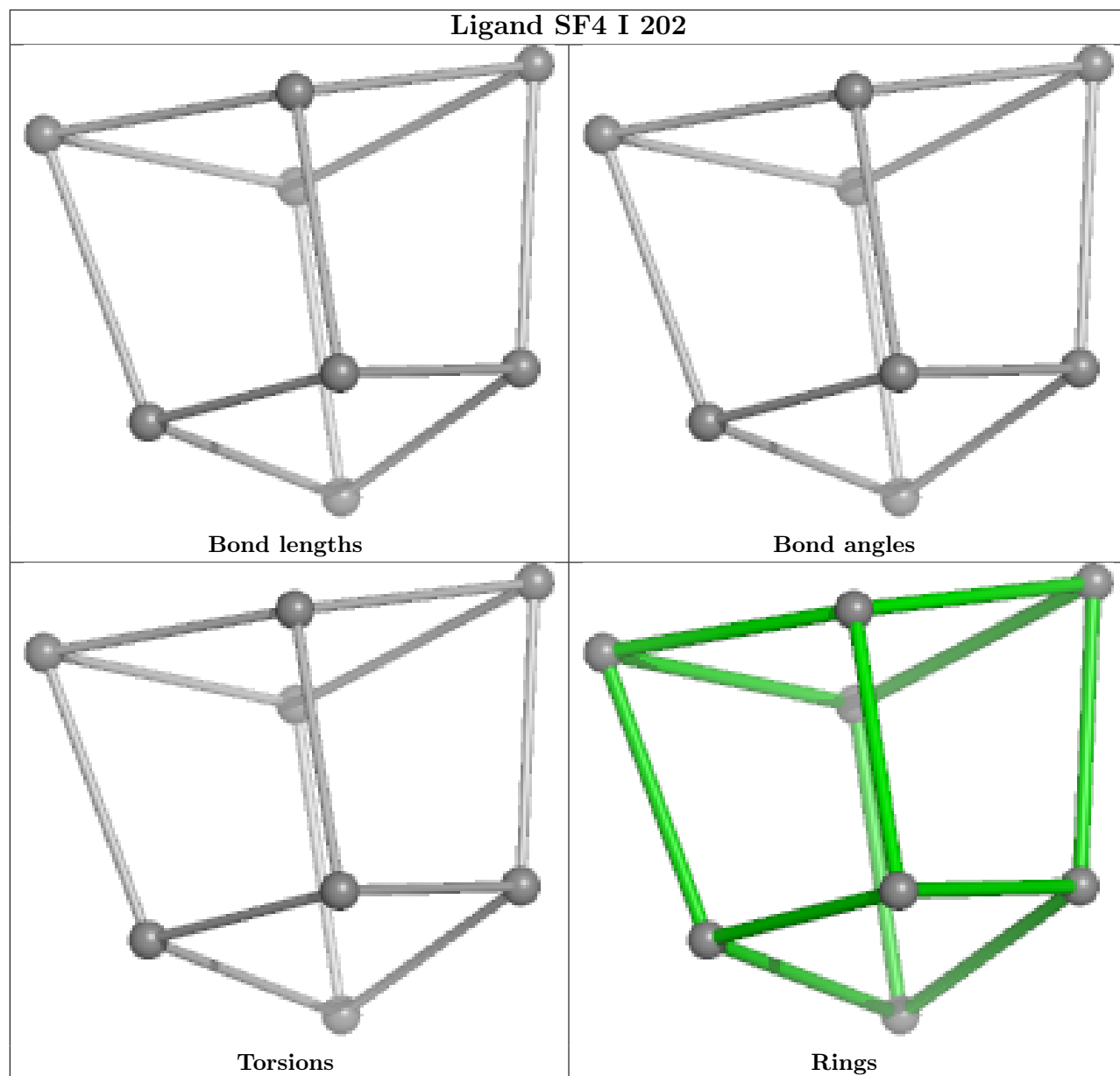


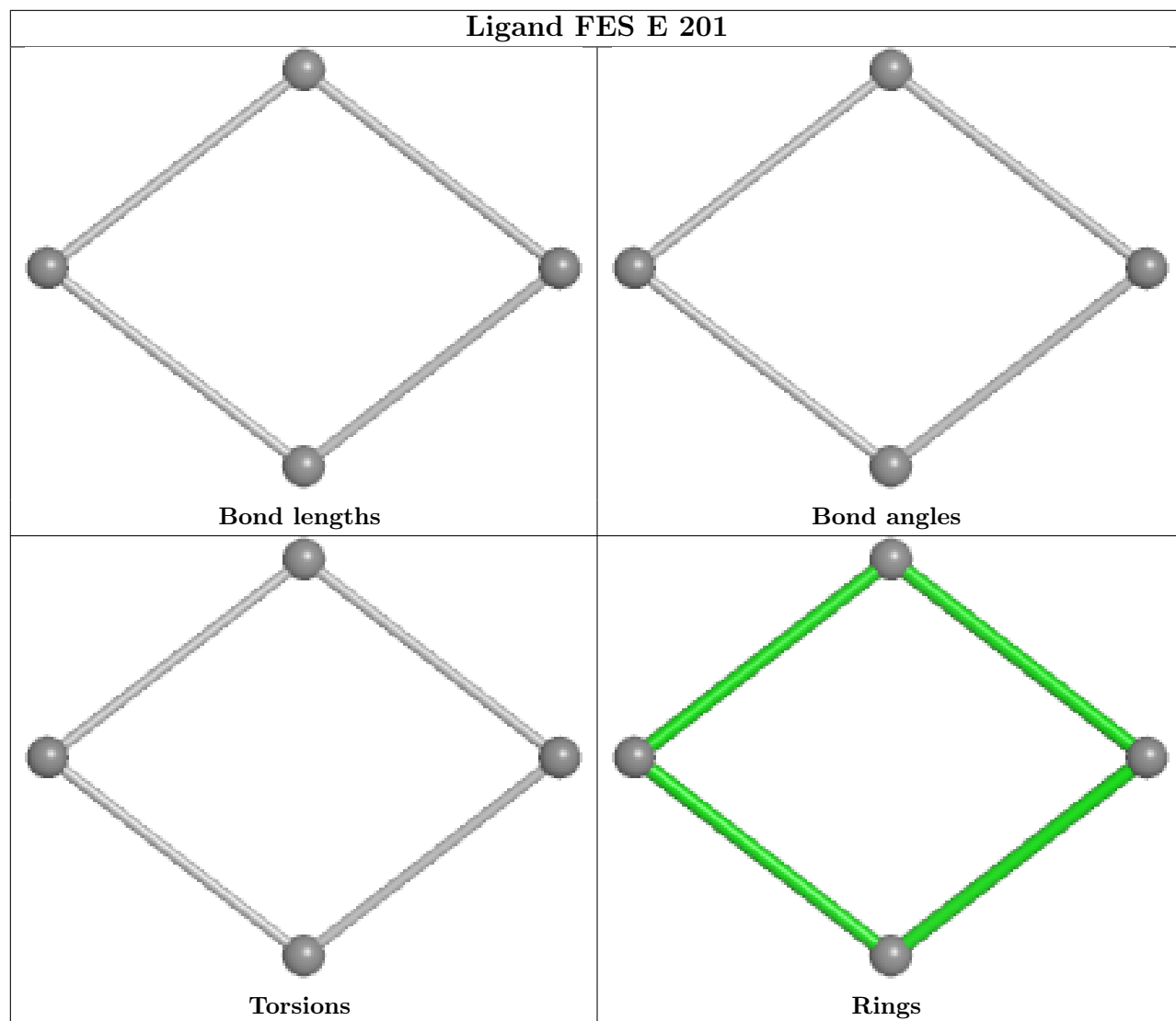


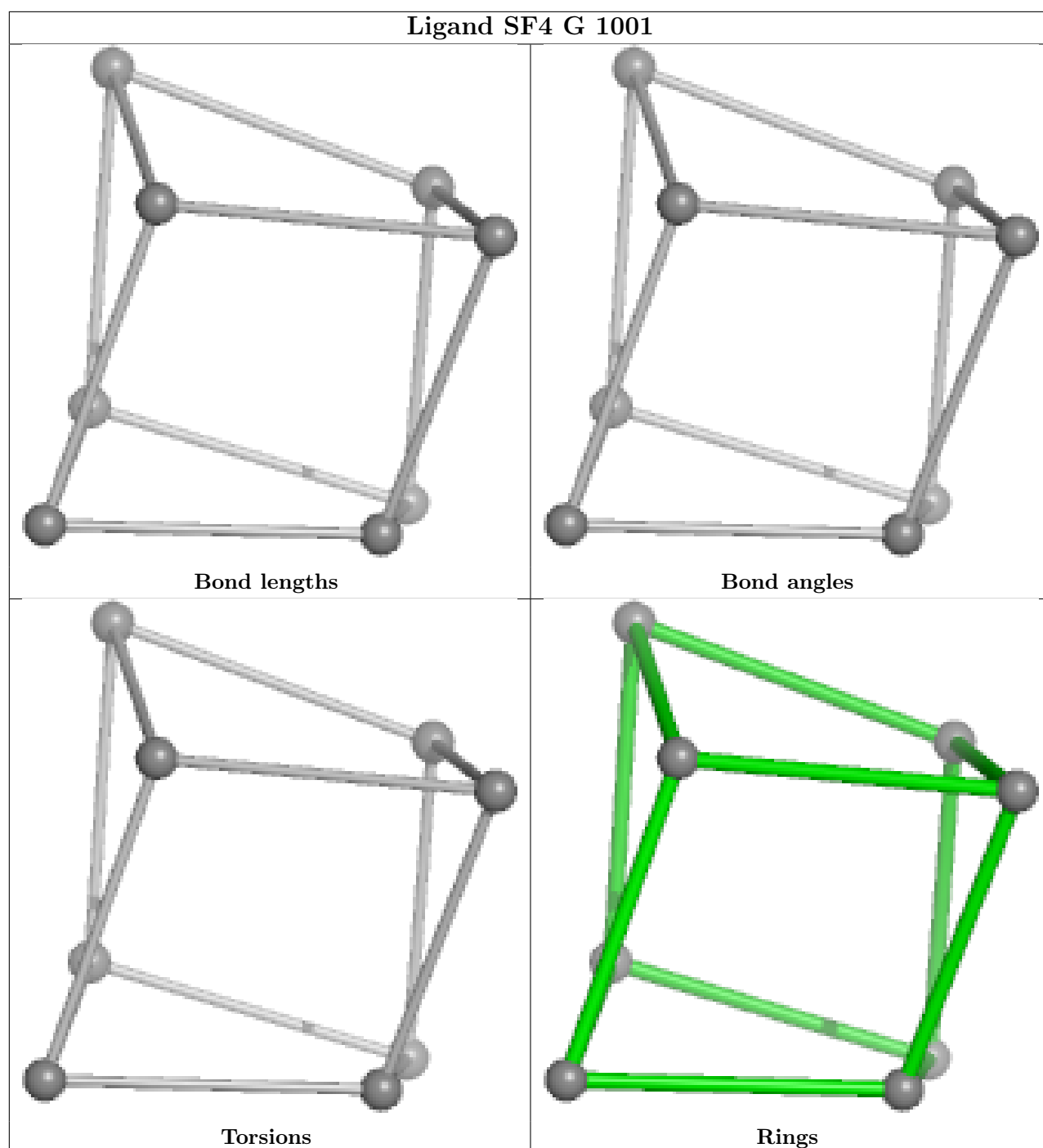


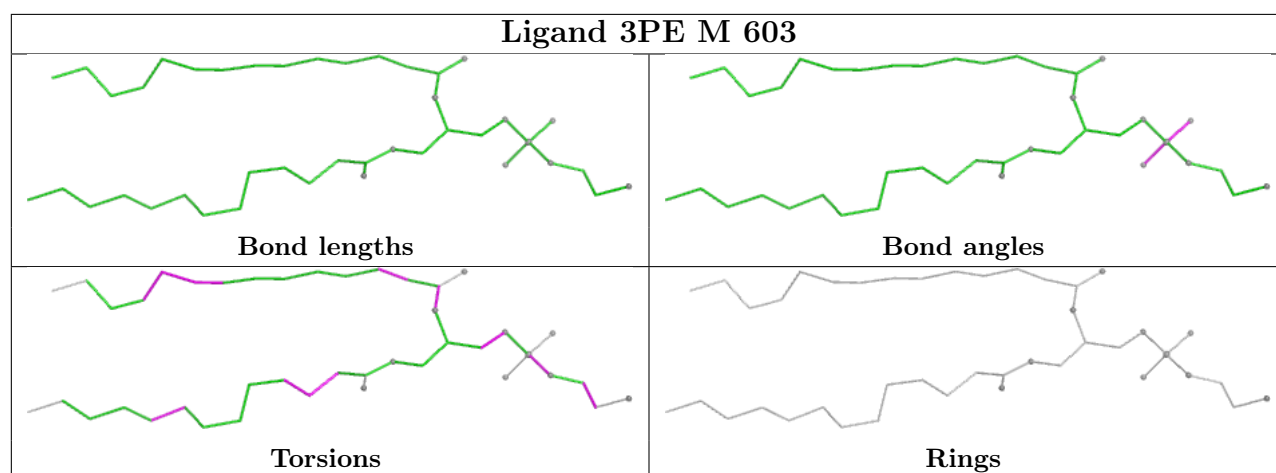
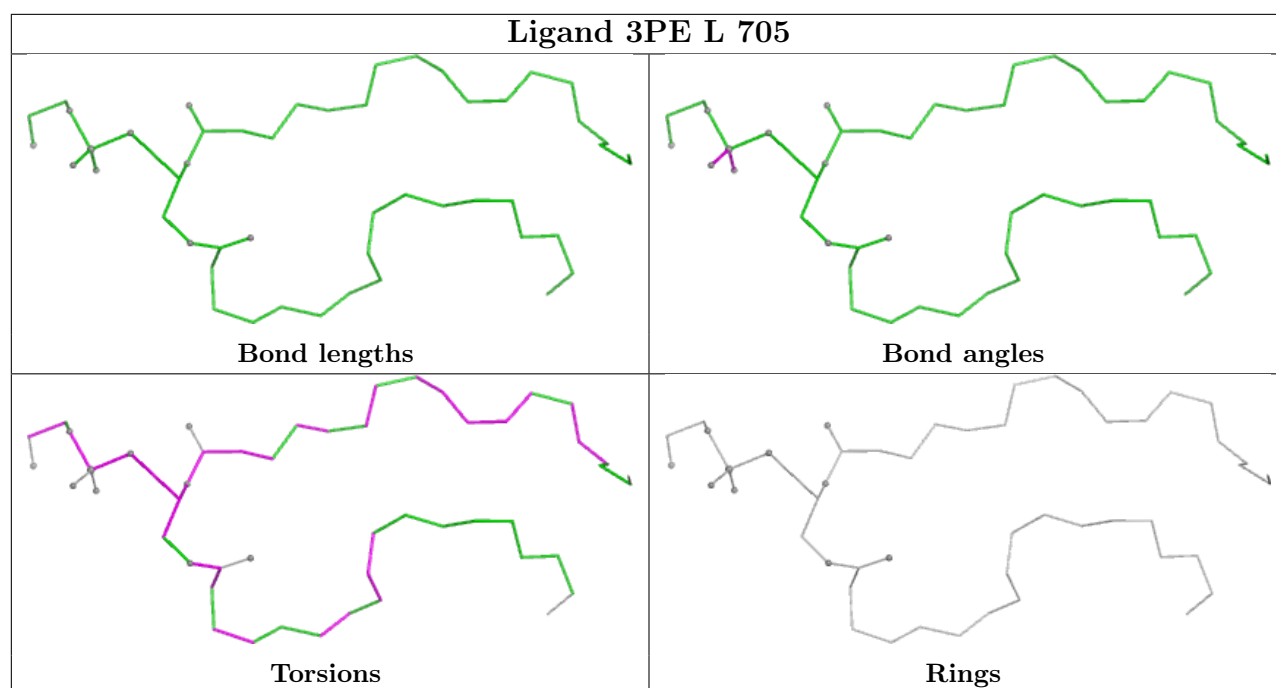
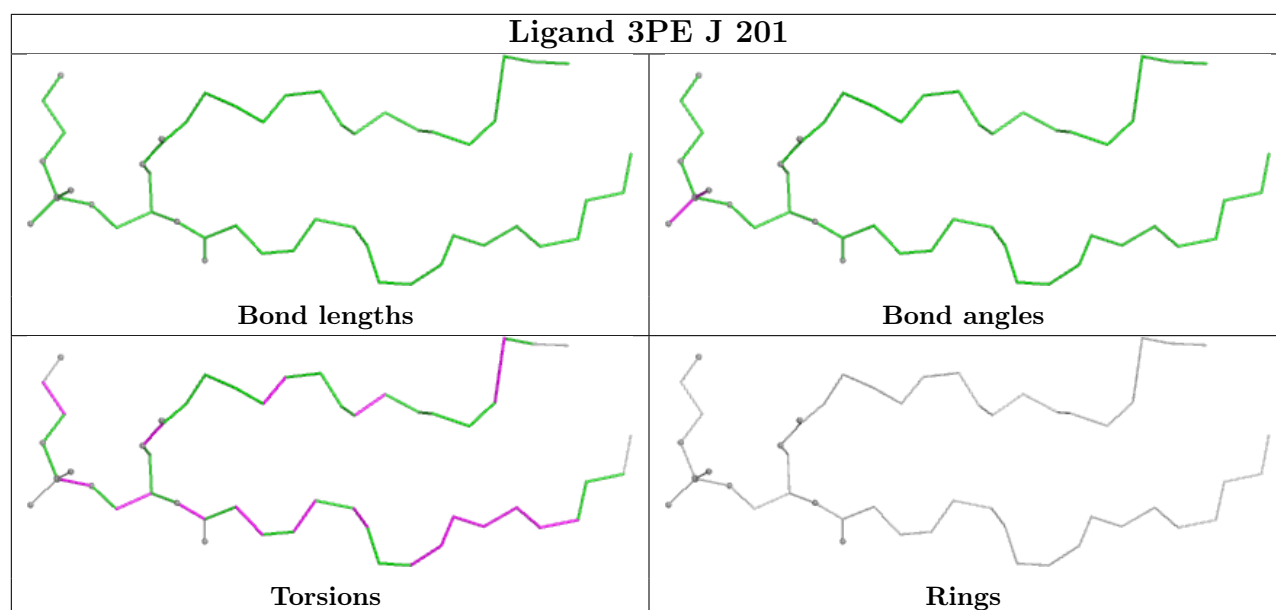


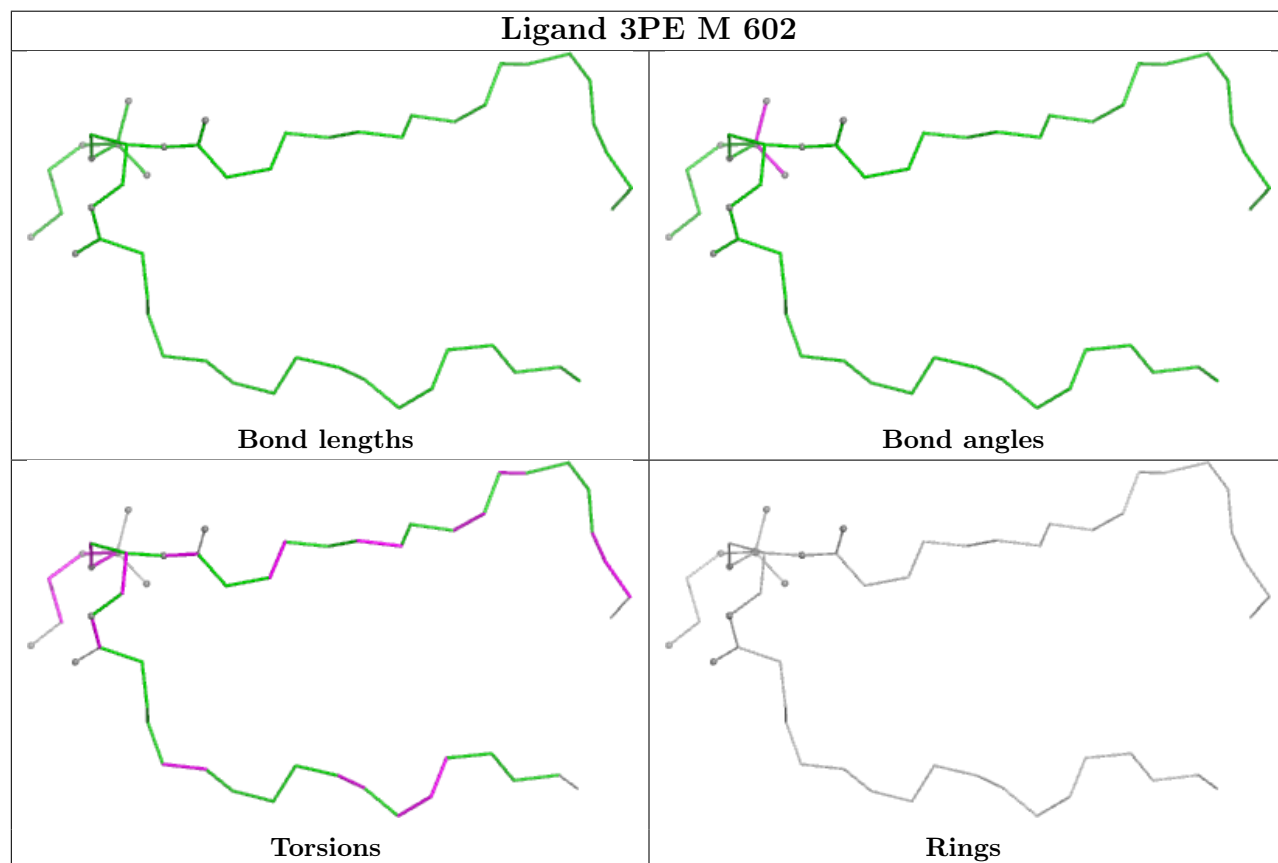
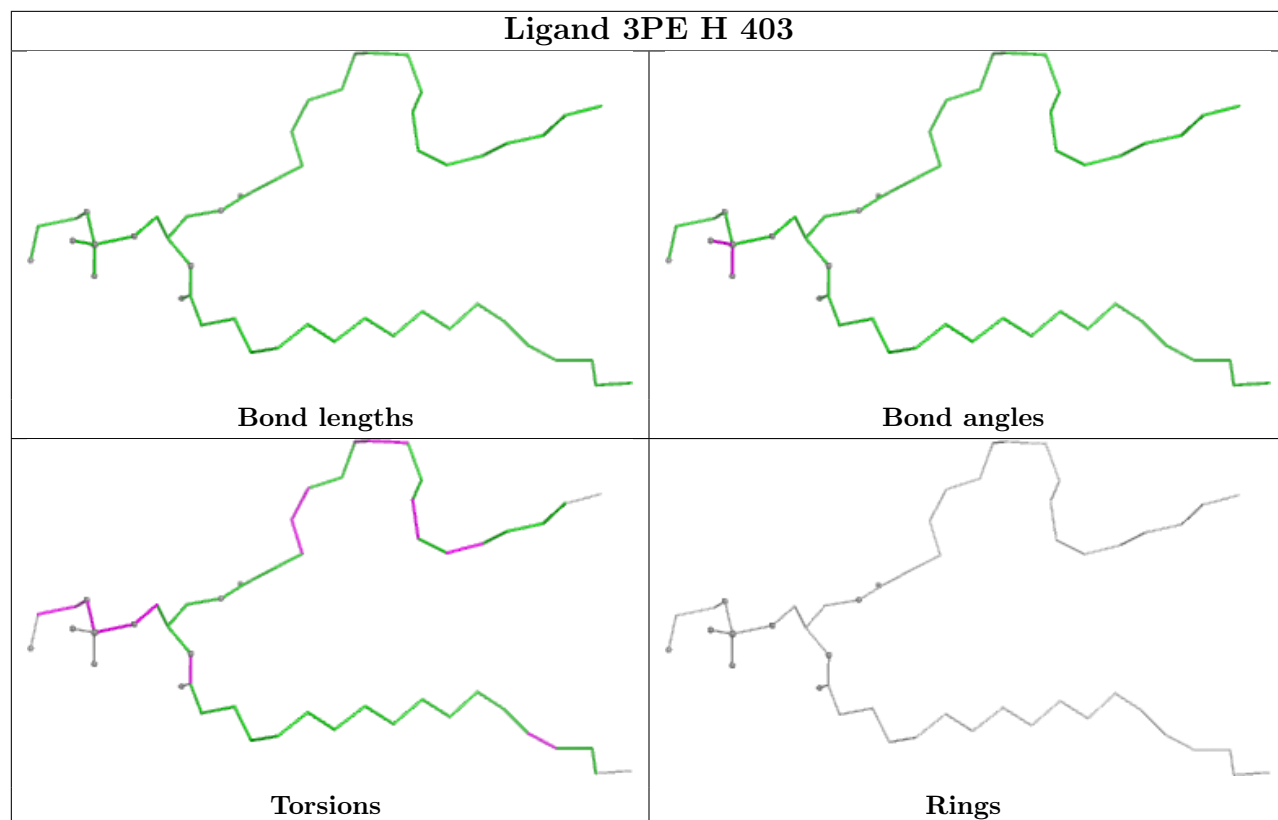


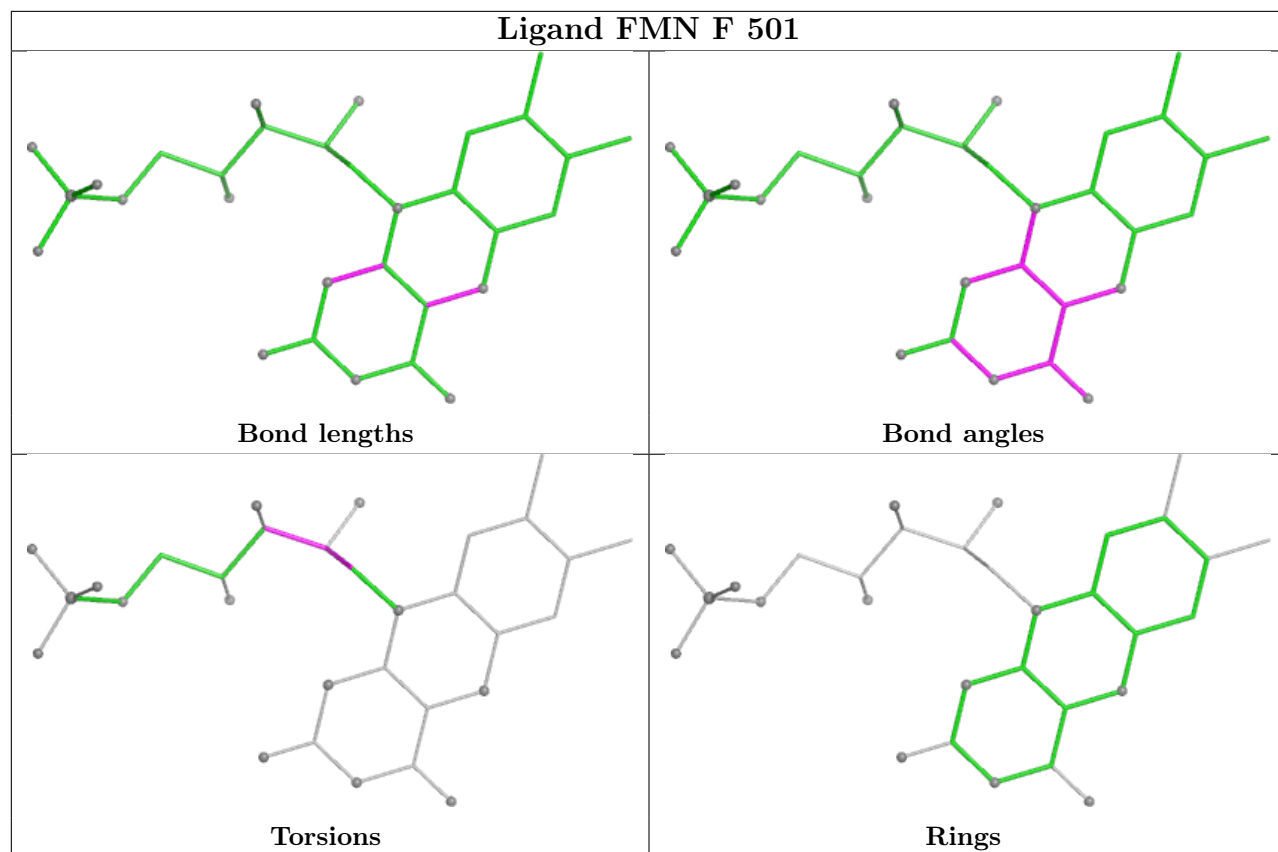




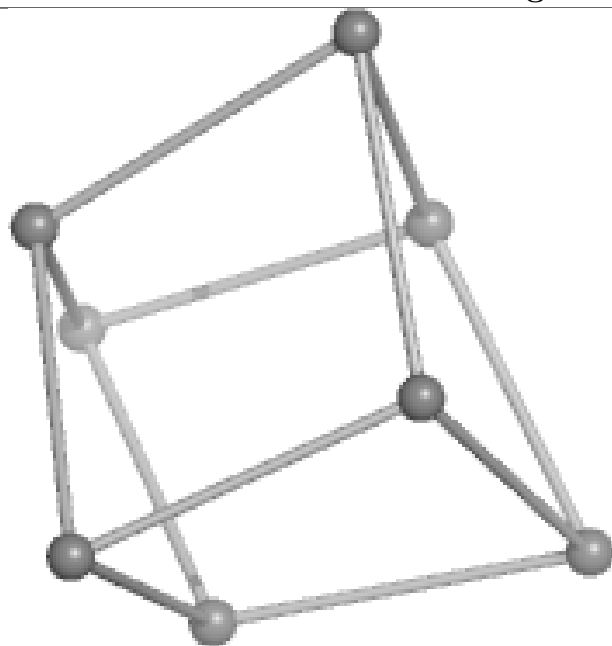




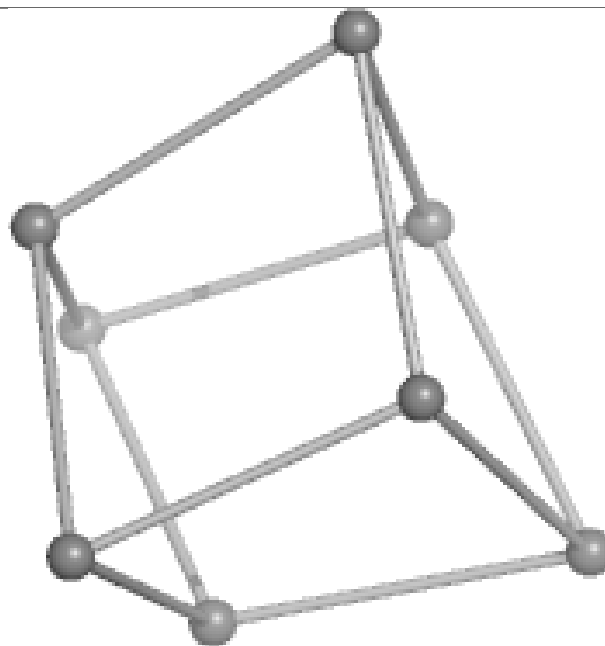




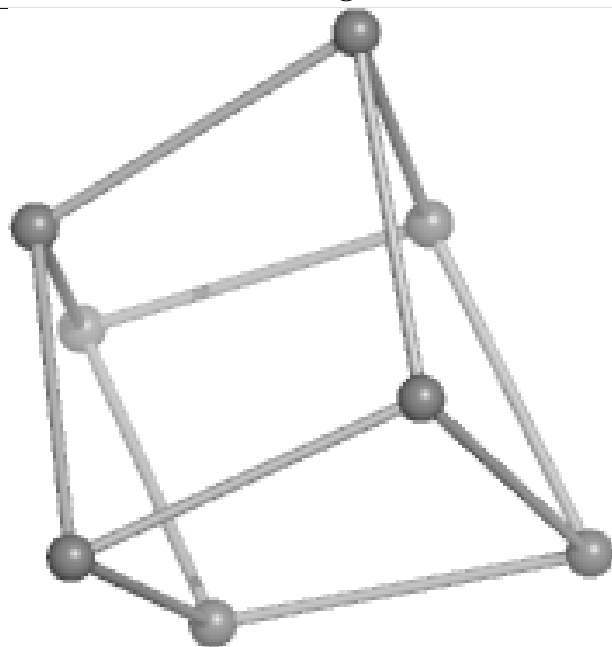
Ligand SF4 I 203



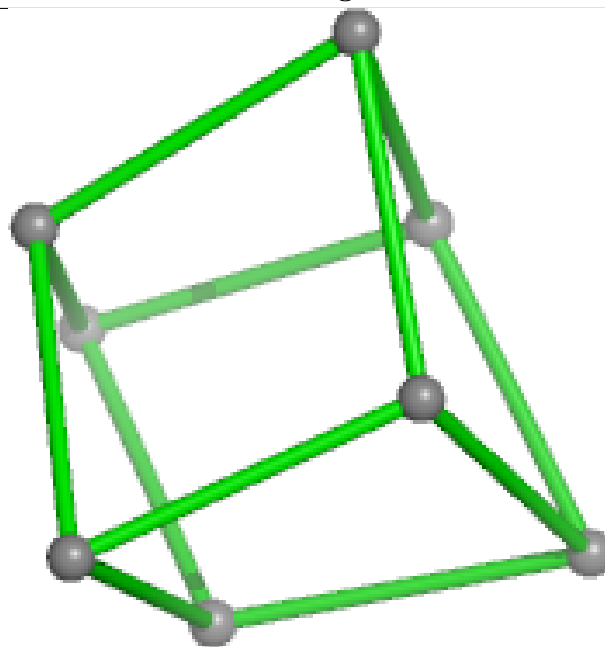
Bond lengths



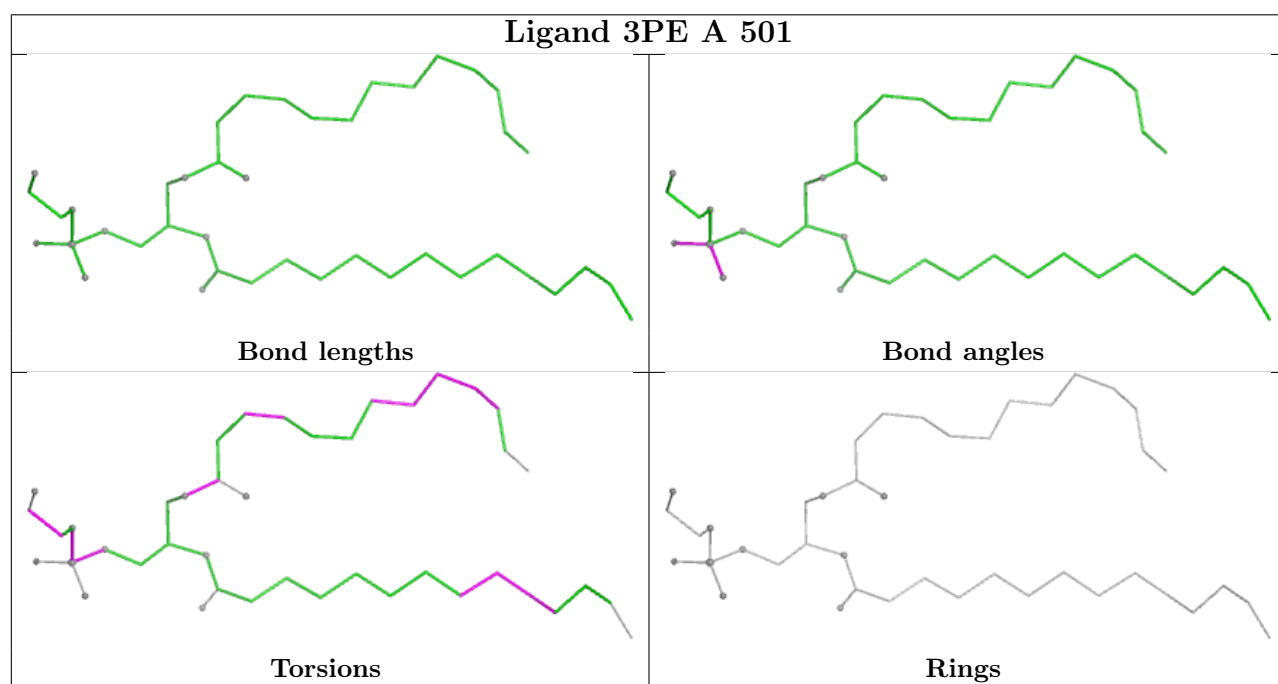
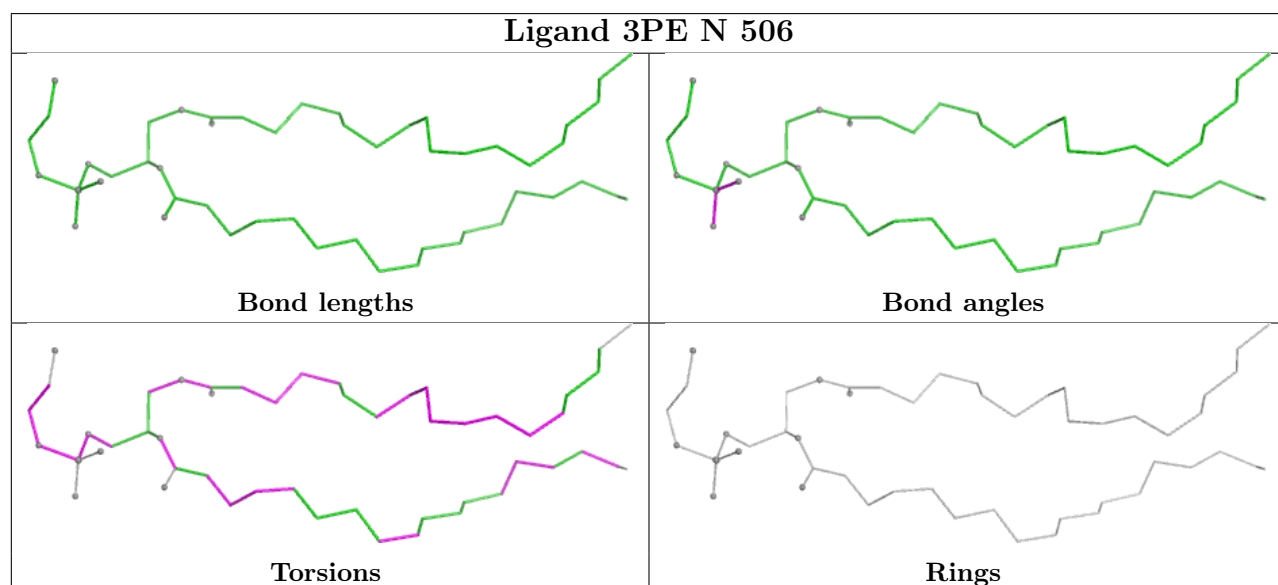
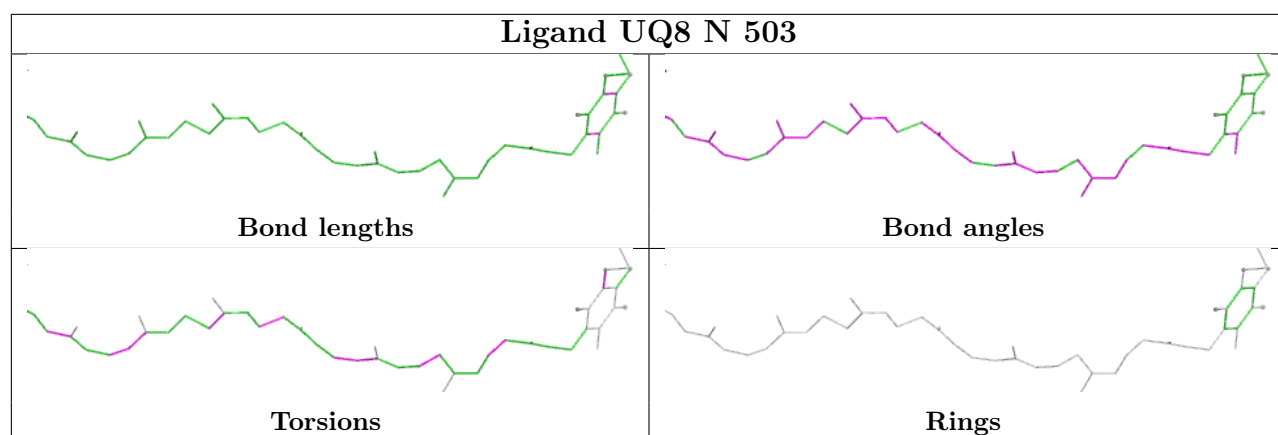
Bond angles

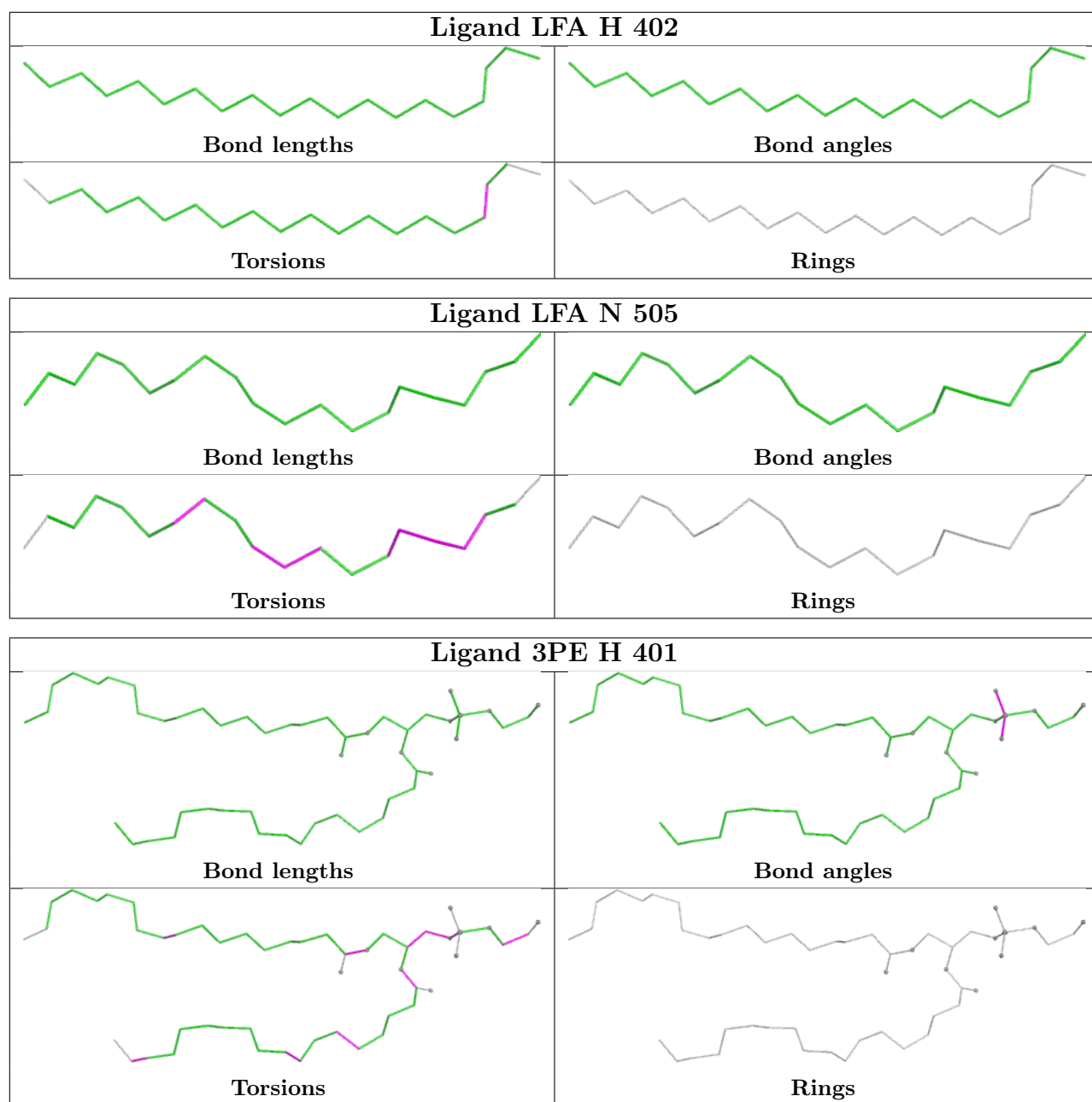


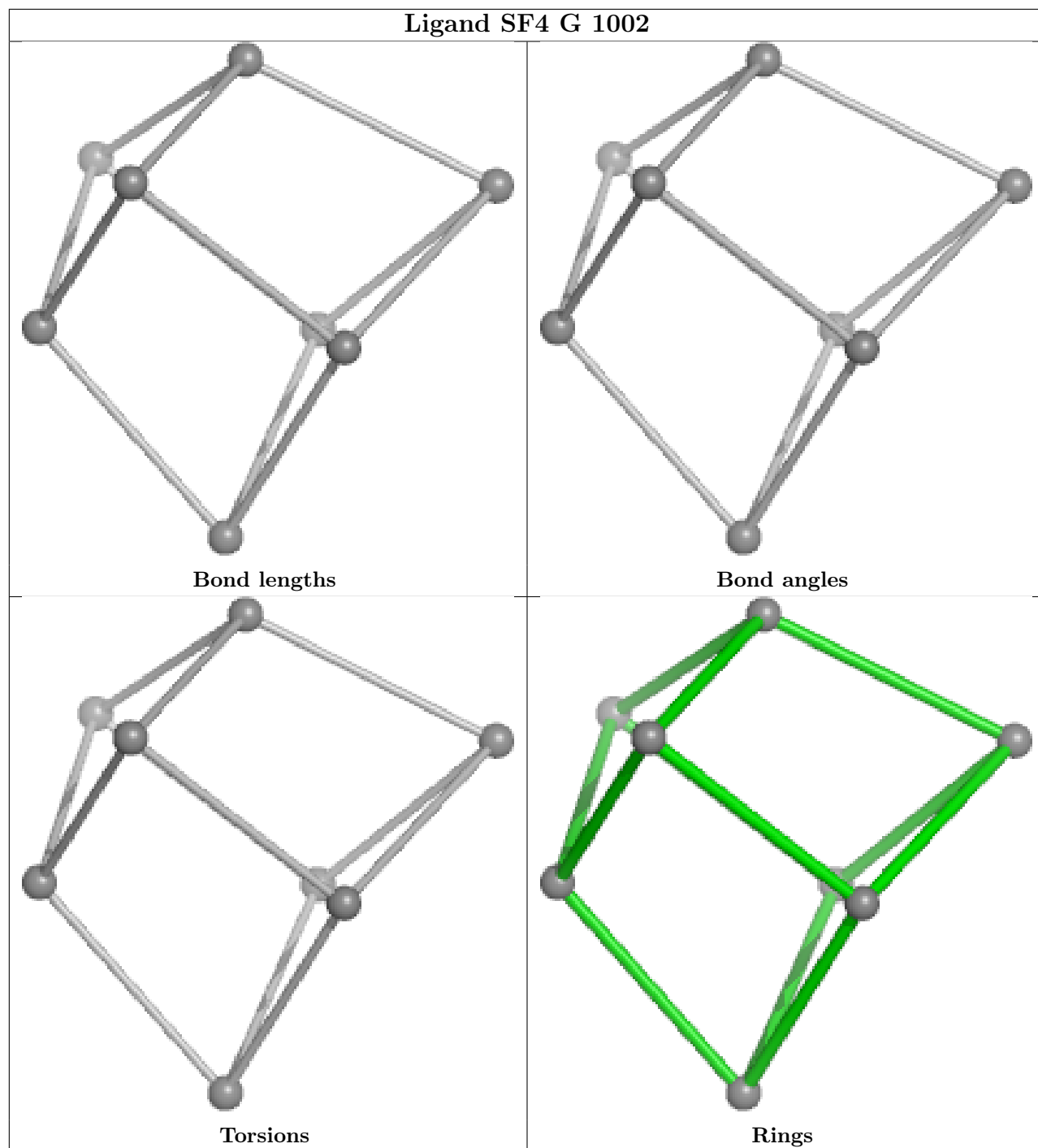
Torsions

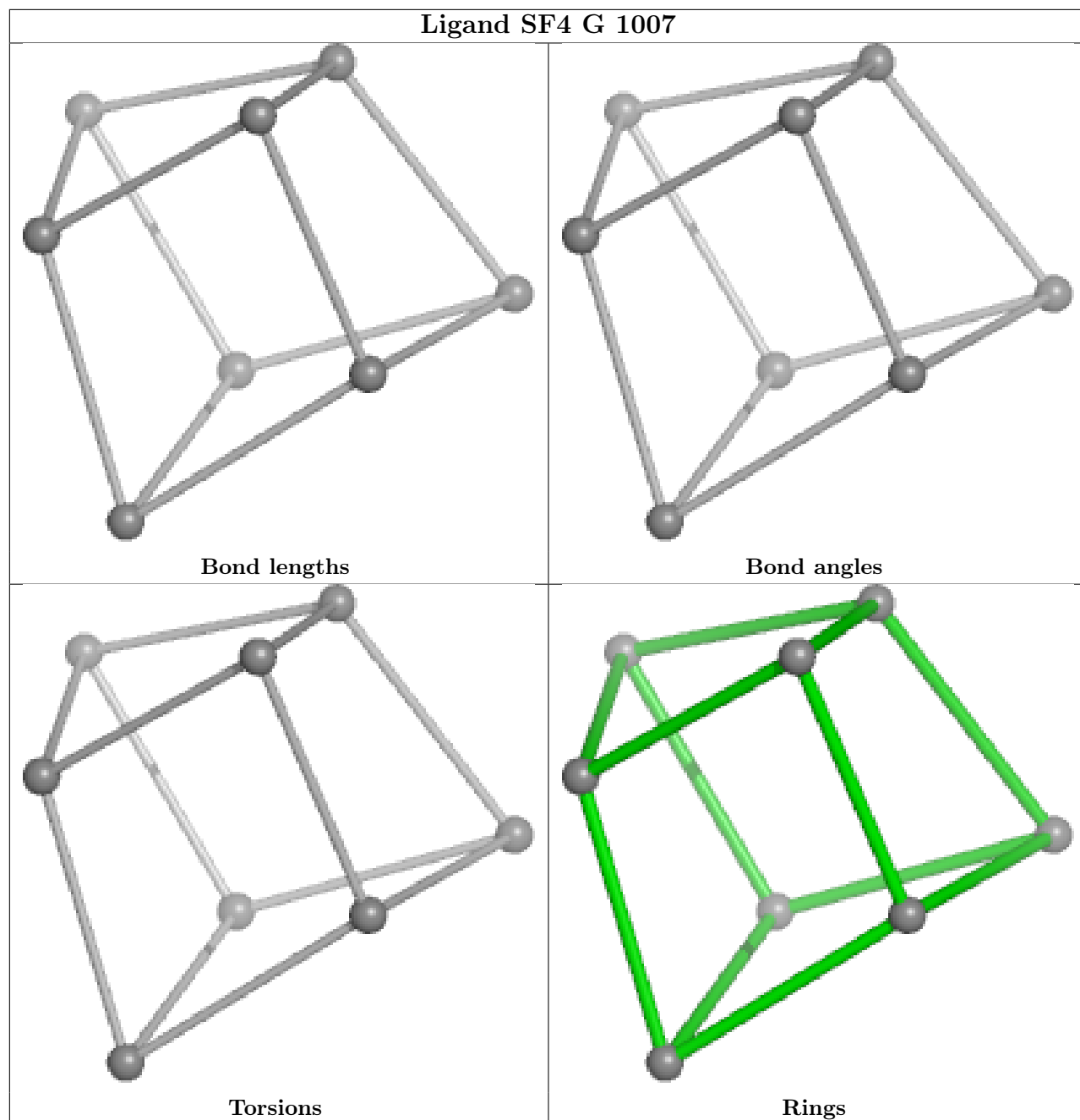


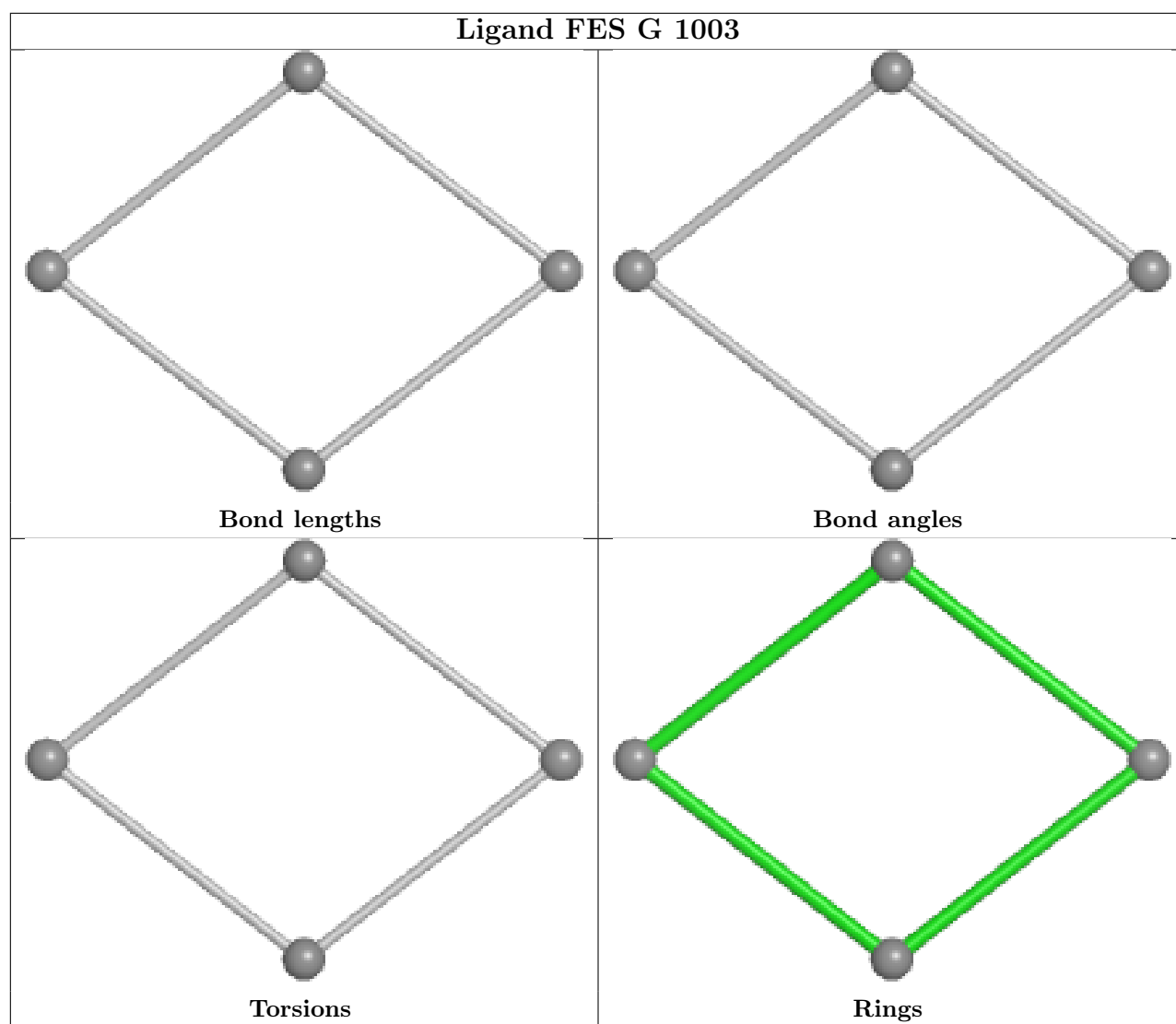
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

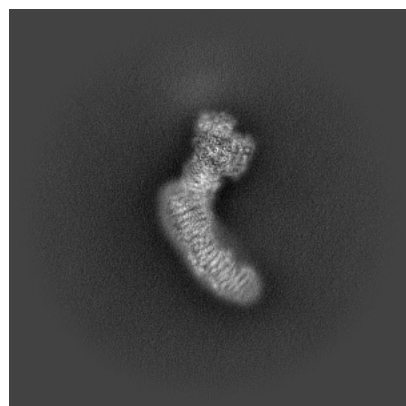
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55748. These allow visual inspection of the internal detail of the map and identification of artifacts.

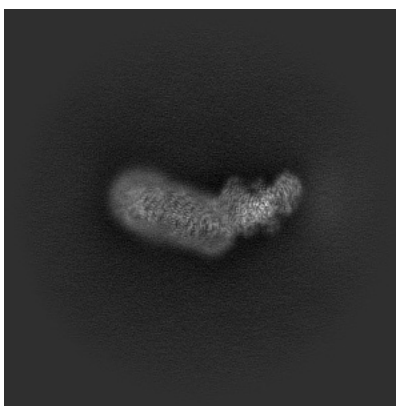
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

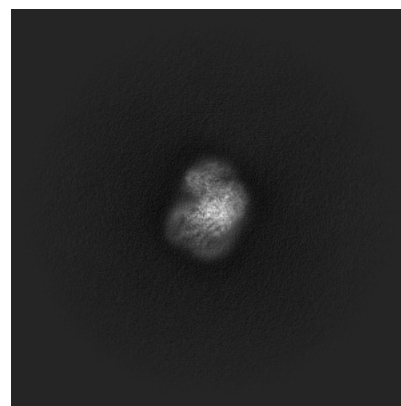
6.1.1 Primary map



X

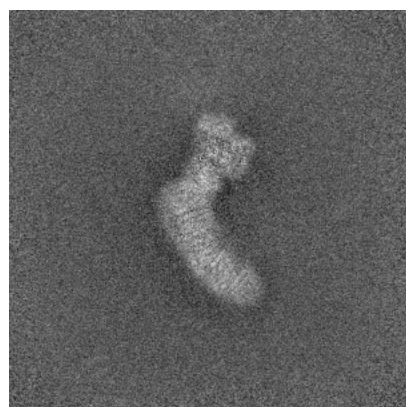


Y

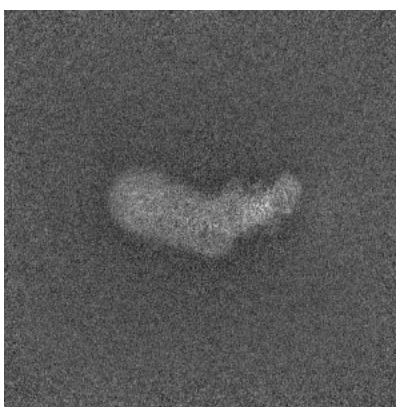


Z

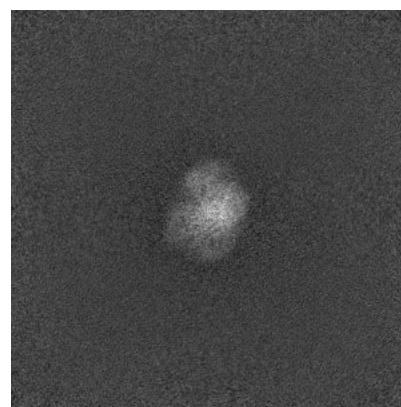
6.1.2 Raw map



X



Y

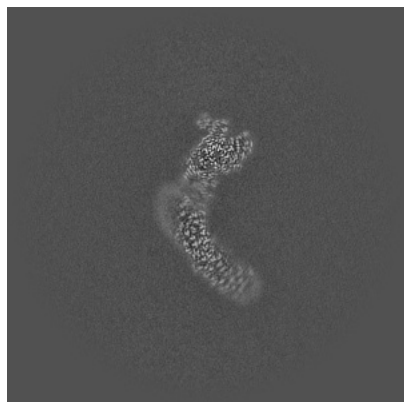


Z

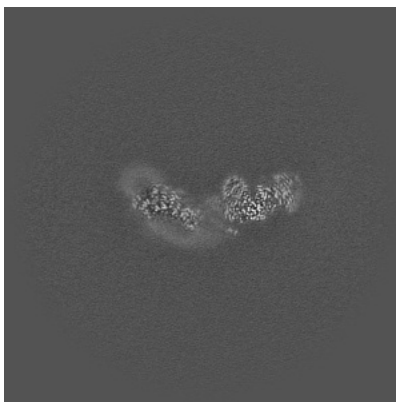
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

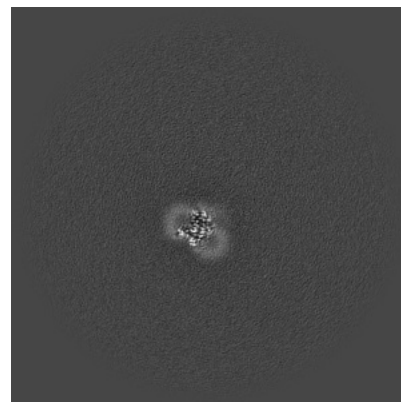
6.2.1 Primary map



X Index: 355

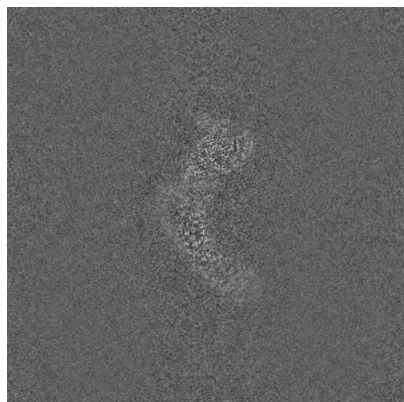


Y Index: 355

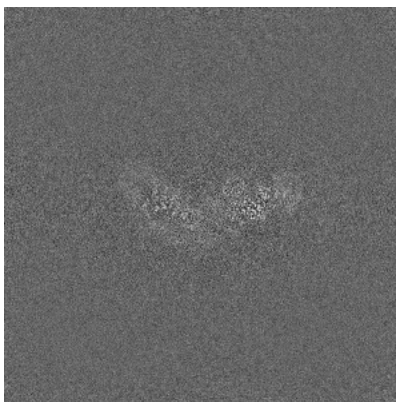


Z Index: 355

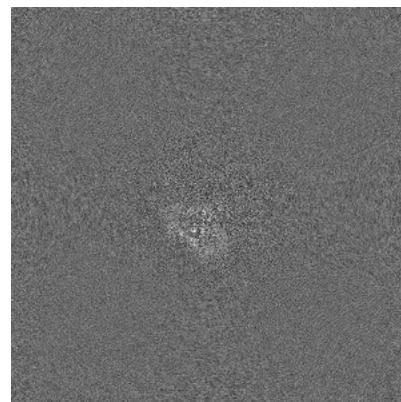
6.2.2 Raw map



X Index: 355



Y Index: 355



Z Index: 355

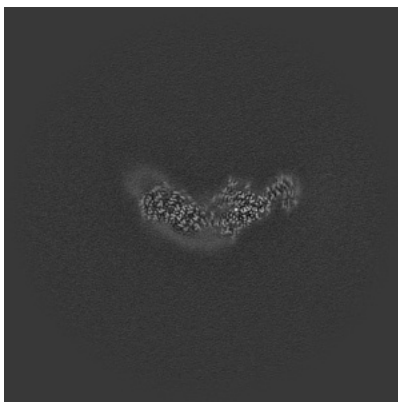
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

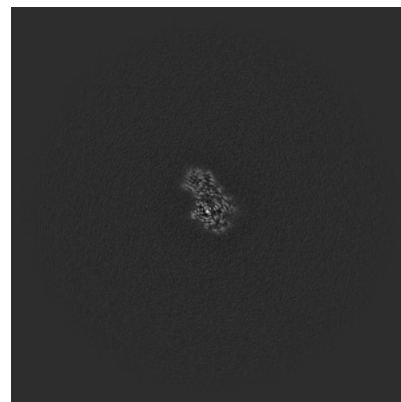
6.3.1 Primary map



X Index: 349

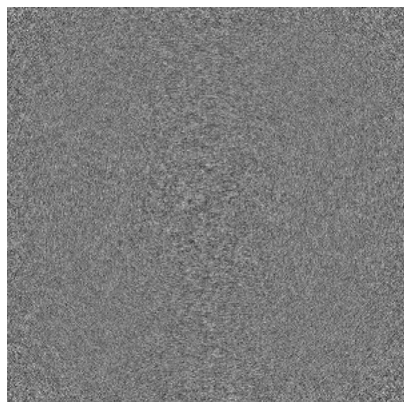


Y Index: 344

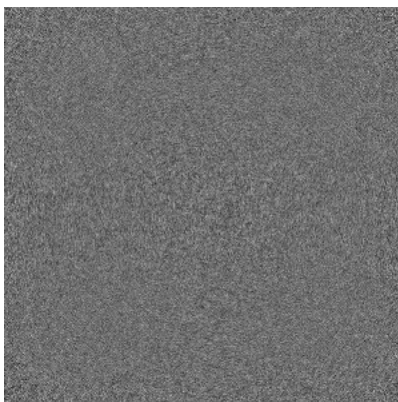


Z Index: 427

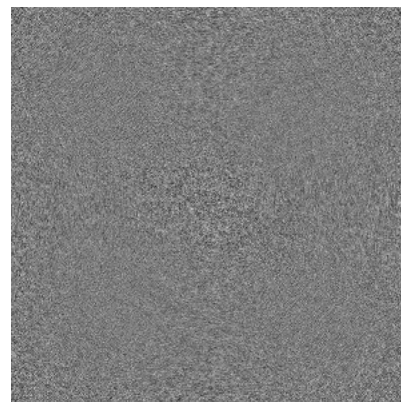
6.3.2 Raw map



X Index: 0



Y Index: 0

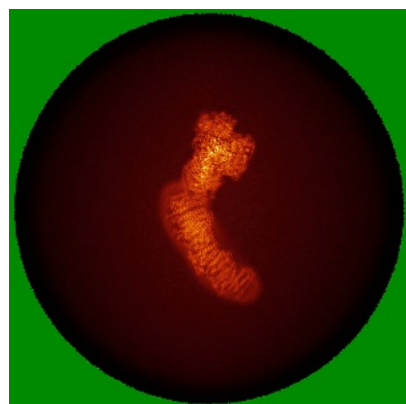


Z Index: 0

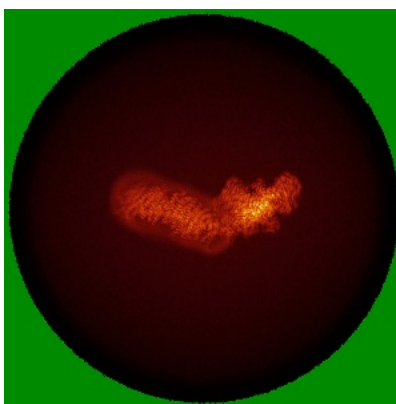
The images above show the largest variance slices of the map in three orthogonal directions.

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

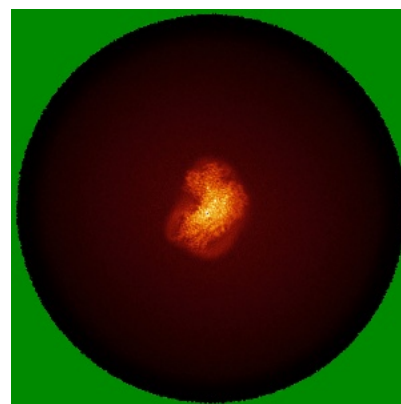
6.4.1 Primary map



X

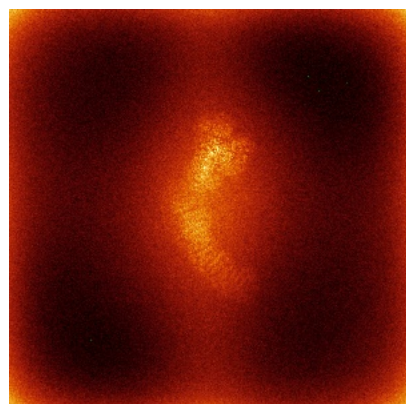


Y

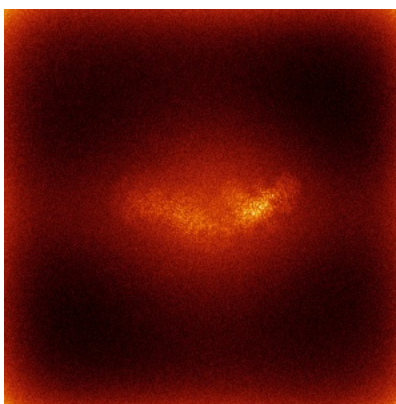


Z

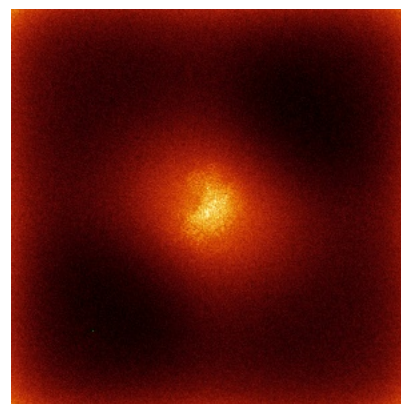
6.4.2 Raw map



X



Y

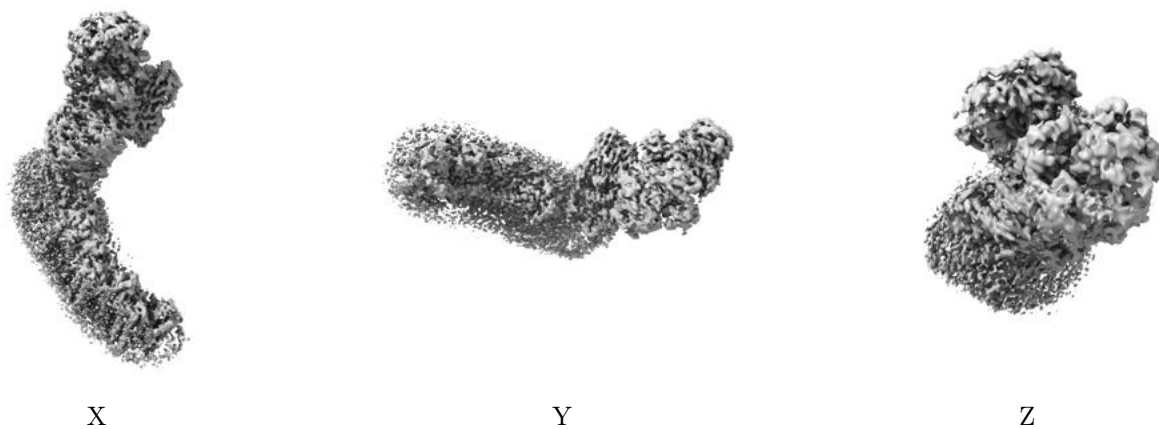


Z

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.

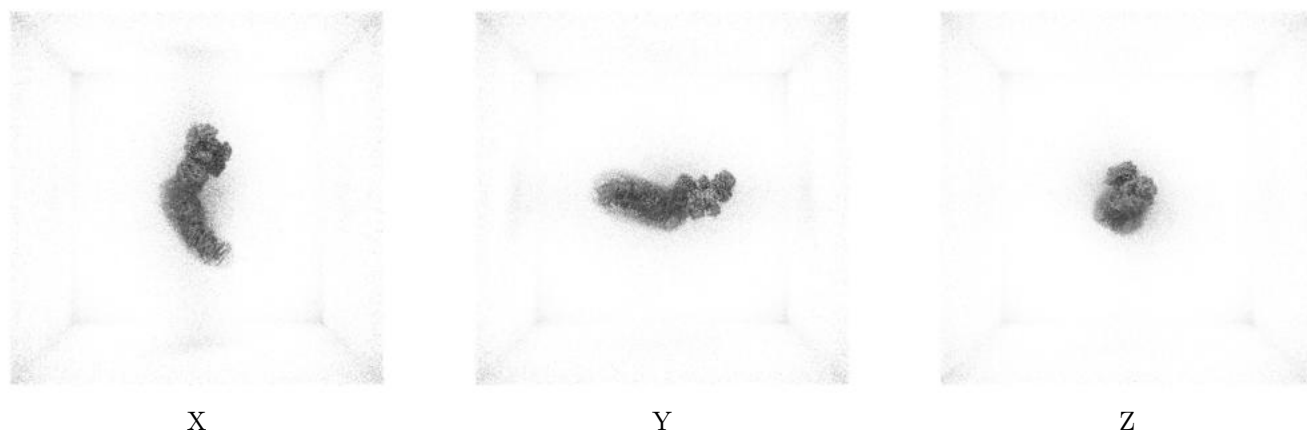
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.234. 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.

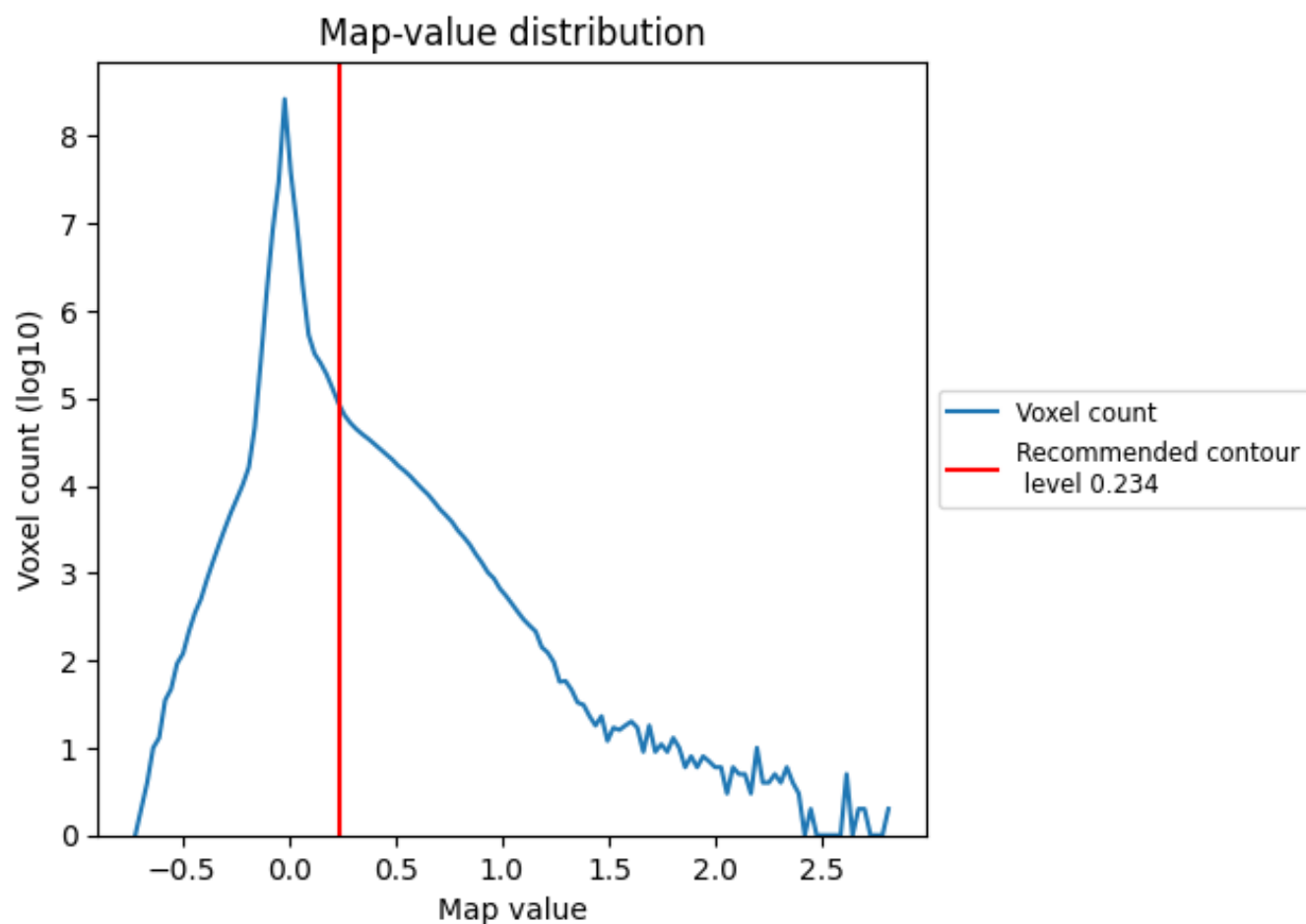
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

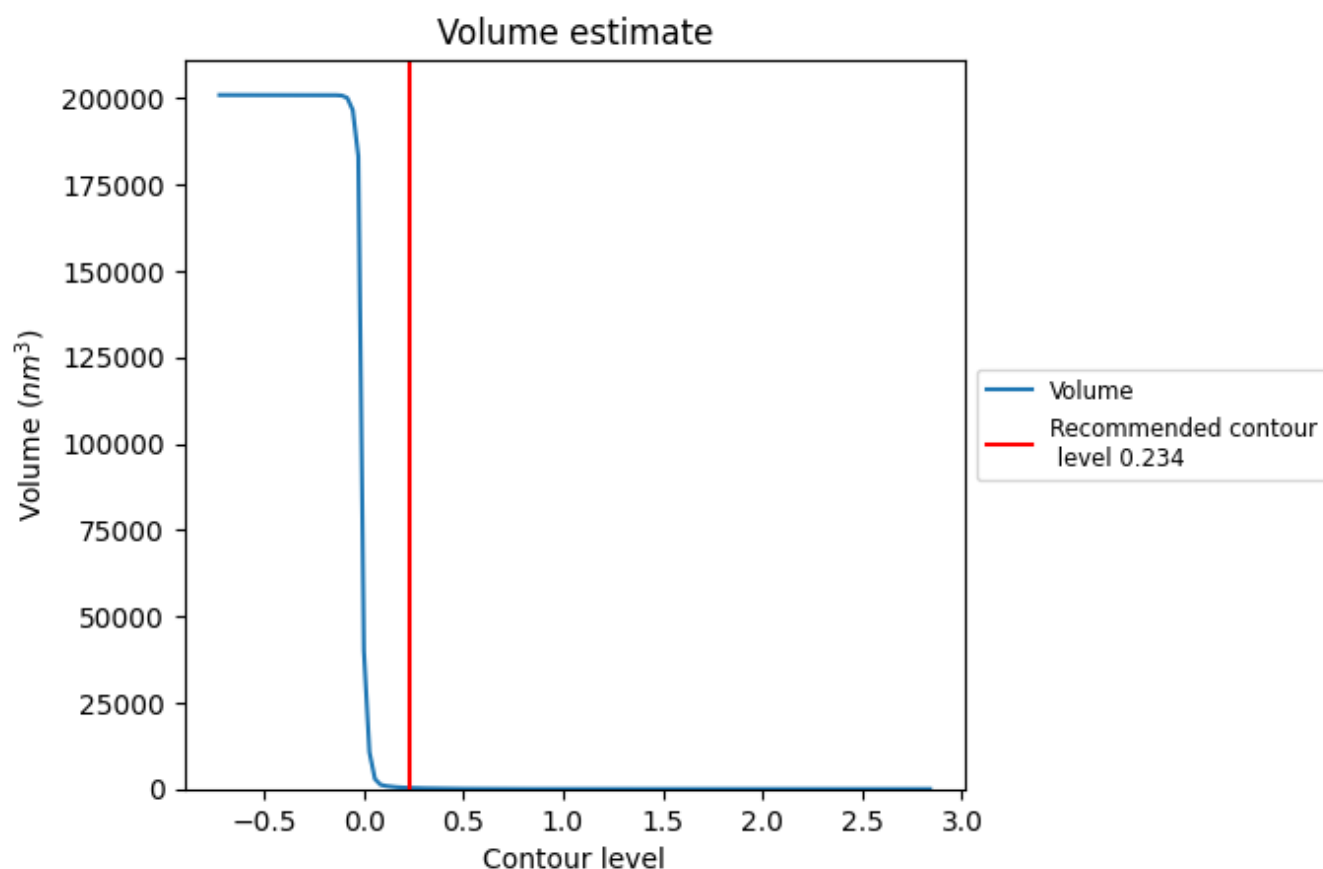
This section contains the results of statistical analysis of the map.

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.

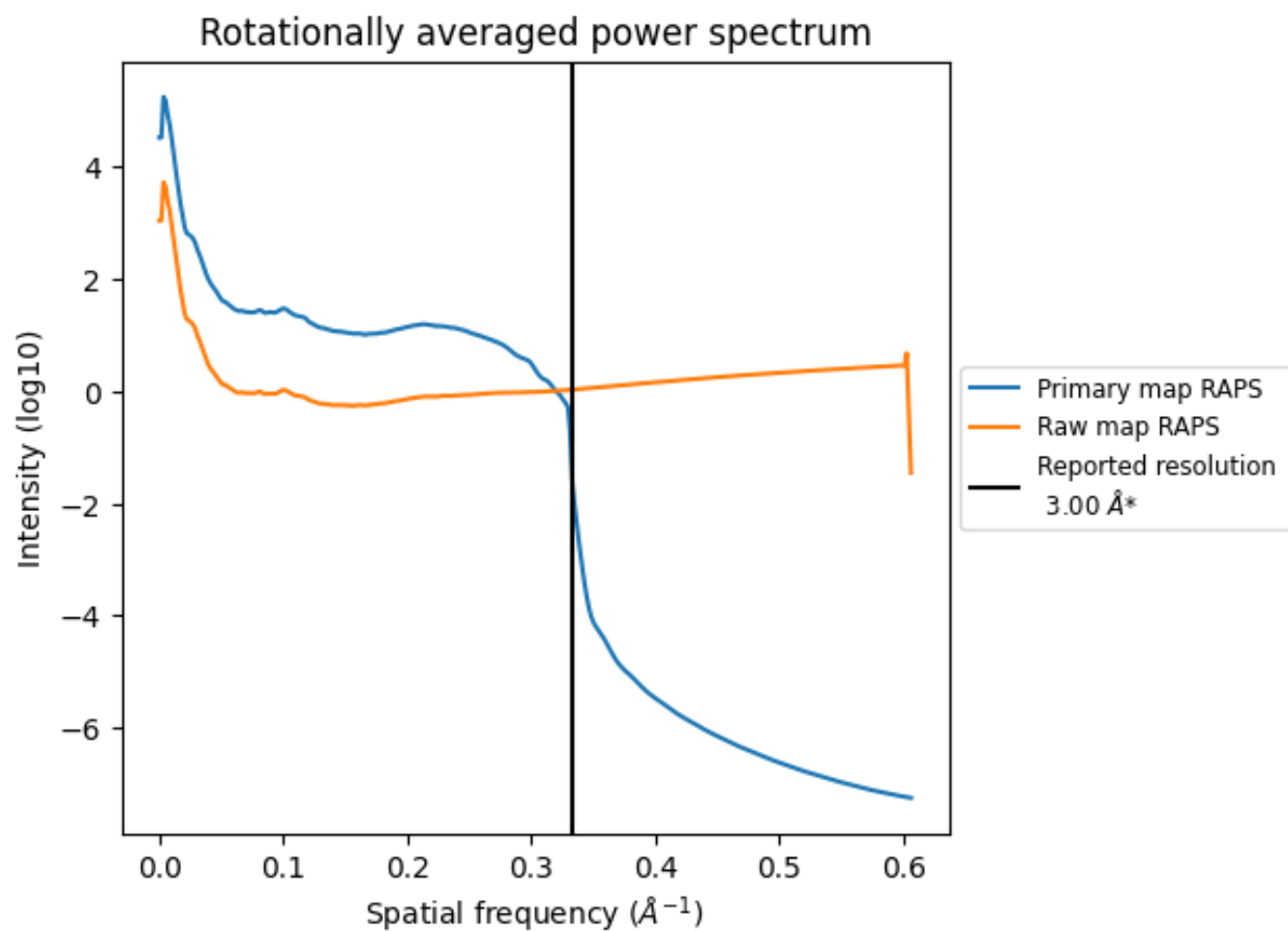
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm³; this corresponds to an approximate mass of 267 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 ⓘ

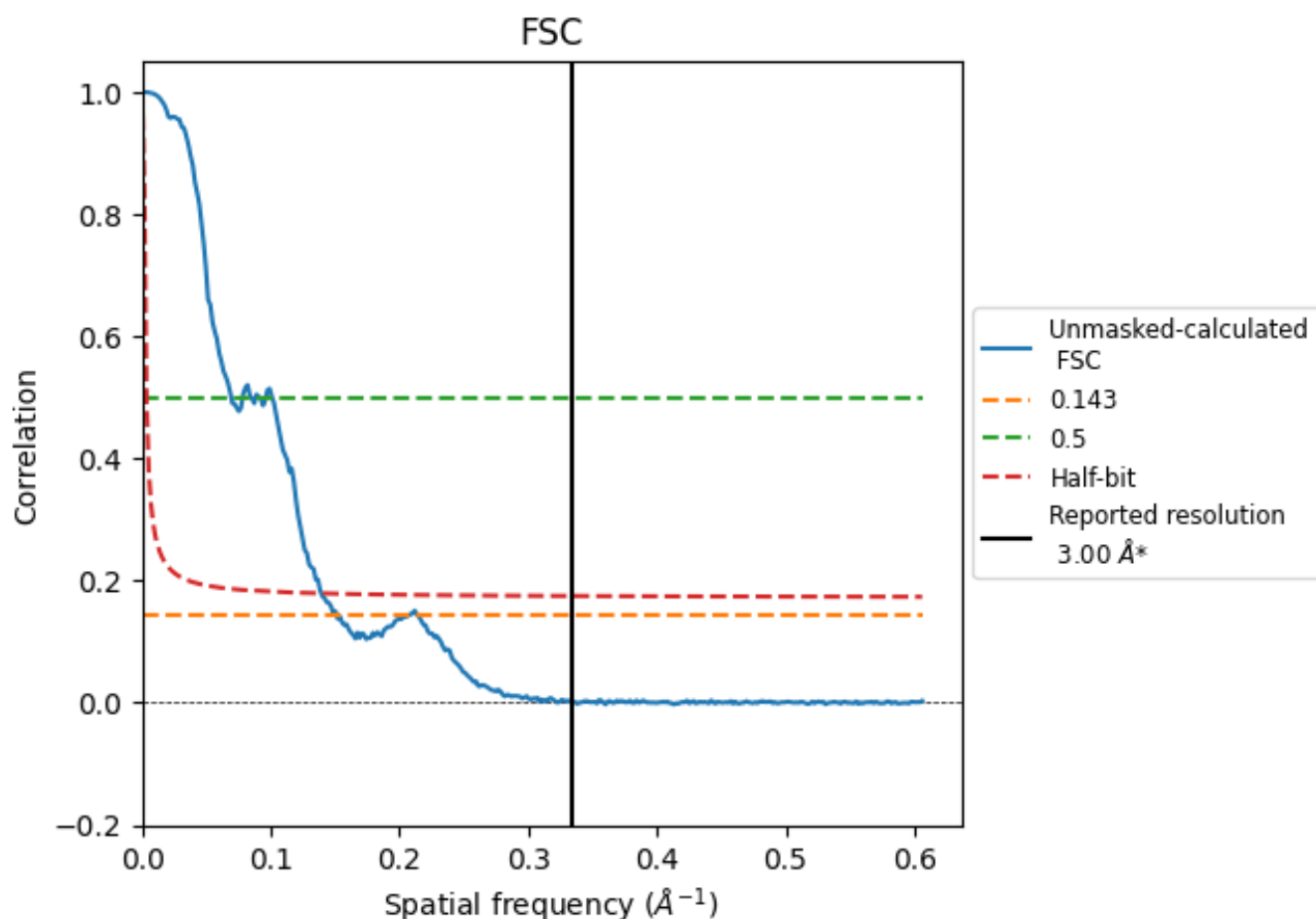


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

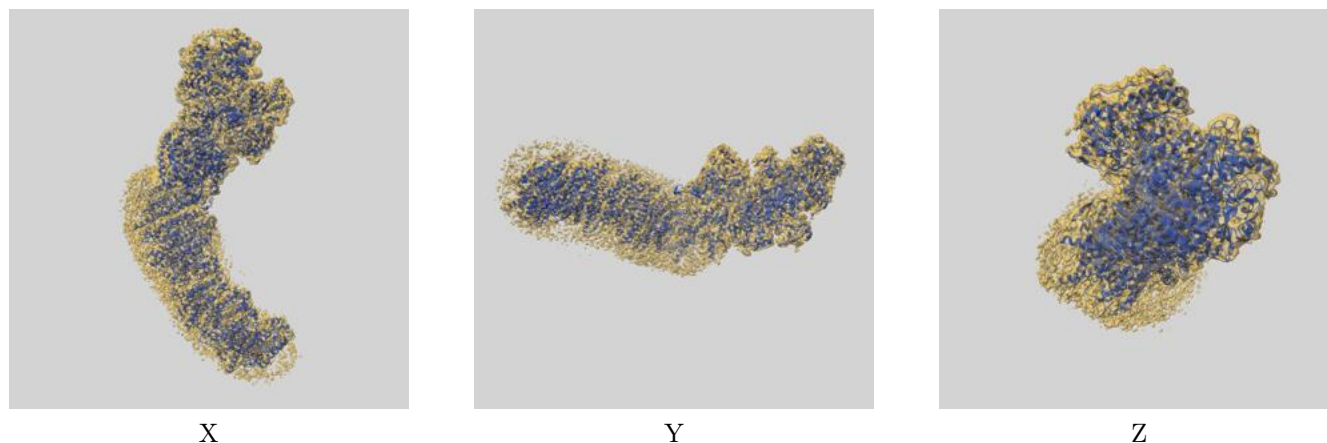
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.62	14.47	7.19

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

9 Map-model fit [i](#)

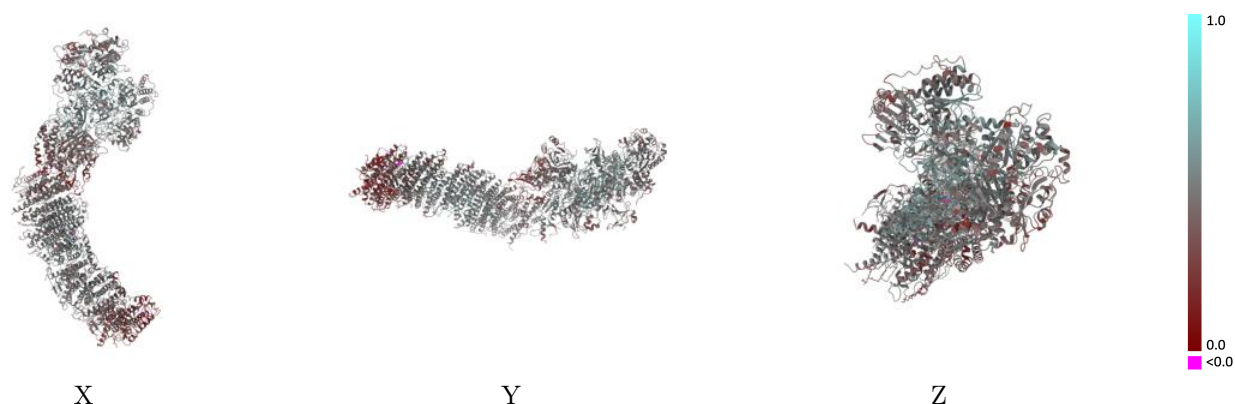
This section contains information regarding the fit between EMDB map EMD-55748 and PDB model 9TAJ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



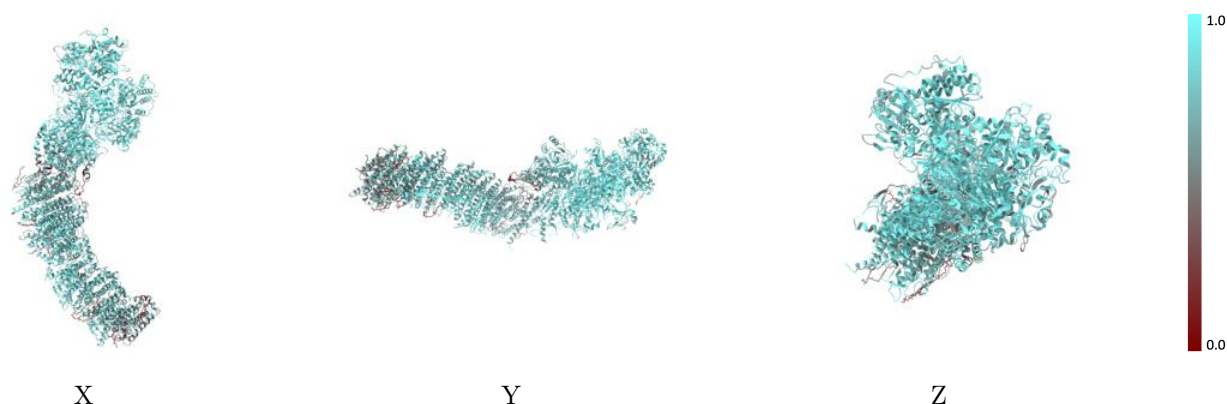
The images above show the 3D surface view of the map at the recommended contour level 0.234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



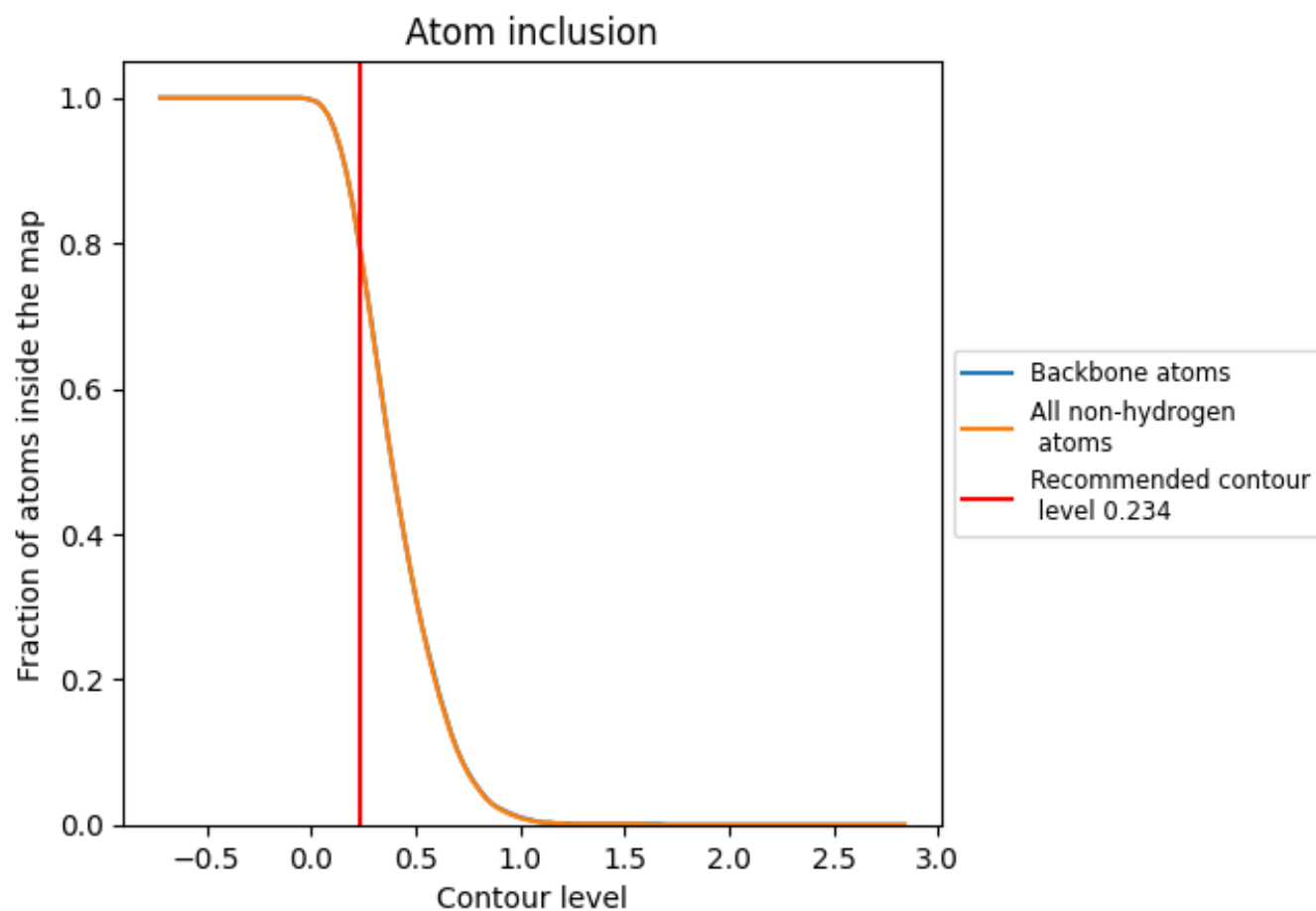
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.234).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.4470
A	0.7450	0.4380
B	0.8300	0.4730
C	0.7700	0.4010
E	0.8200	0.4330
F	0.8310	0.4550
G	0.8850	0.4990
H	0.7460	0.4060
I	0.9300	0.5450
J	0.7900	0.4710
K	0.8540	0.5000
L	0.6450	0.3470
M	0.8000	0.4670
N	0.8270	0.4850

1.0

0.0

<0.0