



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 06:39 PM UTC

PDB ID : 9HZL / pdb_00009hzl
EMDB ID : EMD-52525
Title : High resolution cryo-EM structure of human complex III in mitochondria
Authors : Nguyen, M.D.; Khawaja, A.; Rorbach, J.
Deposited on : 2025-01-14
Resolution : 2.52 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>.

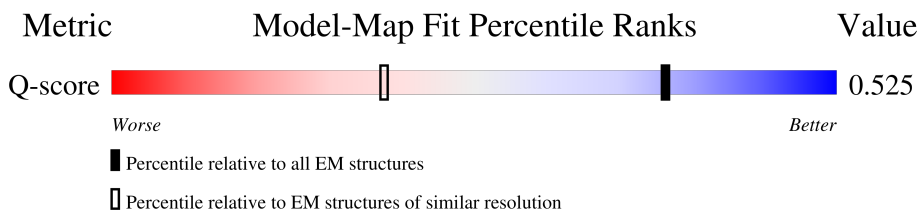
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
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

i

ELECTRON MICROSCOPY

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	7226 (2.02 - 3.02)

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
18	U10	J	406	-	X	-	-
18	U10	V	403	-	X	-	-
18	U10	V	404	-	X	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 68729 atoms, of which 34115 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 Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	81	Total	C	H	N	O	S	0	0
			1377	450	683	126	117	1		
1	N	81	Total	C	H	N	O	S	0	0
			1377	450	683	126	117	1		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	48	Total	C	H	N	O	S	0	0
			714	218	370	63	62	1		
2	C	187	Total	C	H	N	O	S	0	0
			2898	922	1441	255	274	6		
2	O	57	Total	C	H	N	O	S	0	0
			841	259	432	74	75	1		
2	P	196	Total	C	H	N	O	S	0	0
			3026	960	1505	264	290	7		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	62	Total	C	H	N	O	S	0	0
			1020	332	511	87	89	1		
3	Q	62	Total	C	H	N	O	S	0	0
			1020	332	511	87	89	1		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	73	Total	C	H	N	O	S	0	0
			1132	357	544	107	119	5		
4	R	74	Total	C	H	N	O	S	0	0
			1106	351	526	108	116	5		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	106	Total	C	H	N	O	S	0	0
			1831	589	910	162	168	2		
5	S	106	Total	C	H	N	O	S	0	0
			1831	589	910	162	168	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	52	Total	C	H	N	O		0	0
			869	293	435	74	67			
6	T	51	Total	C	H	N	O		0	0
			847	287	422	72	66			

- Molecule 7 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	241	Total	C	H	N	O	S	0	0
			3798	1231	1874	329	349	15		
7	U	241	Total	C	H	N	O	S	0	0
			3798	1231	1874	329	349	15		

- Molecule 8 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	379	Total	C	H	N	O	S	0	0
			6093	2022	3077	468	509	17		
8	V	379	Total	C	H	N	O	S	0	0
			6093	2022	3077	468	509	17		

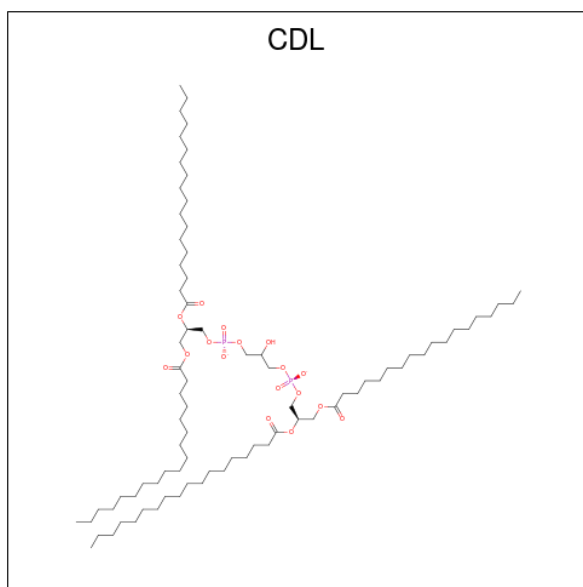
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	422	Total	C	H	N	O	S	0	0
			6315	1995	3141	556	613	10		
9	W	419	Total	C	H	N	O	S	0	0
			6301	1989	3139	553	610	10		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

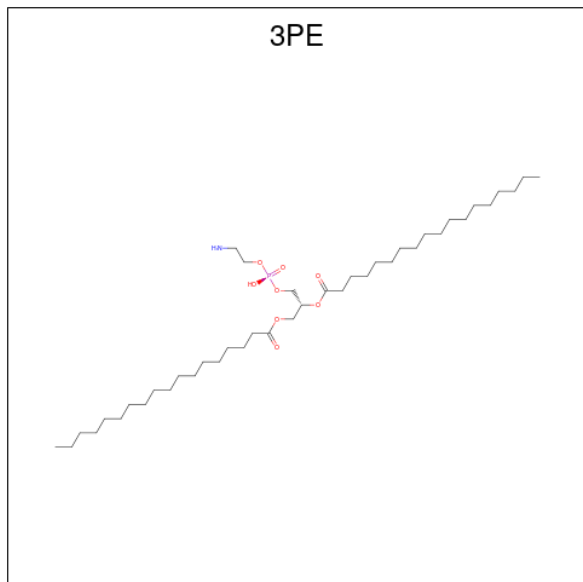
Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	446	Total	C	H	N	O	S	0	0
			6823	2169	3370	603	661	20		
10	Y	446	Total	C	H	N	O	S	0	0
			6823	2169	3370	603	661	20		

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



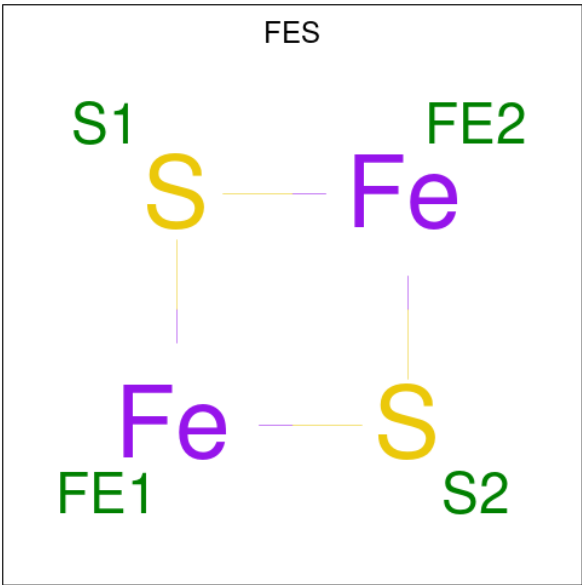
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	G	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	H	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	J	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	J	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	T	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	U	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	V	1	Total	C	H	O	P	0
			112	45	48	17	2	
11	Y	1	Total	C	H	O	P	0
			112	45	48	17	2	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



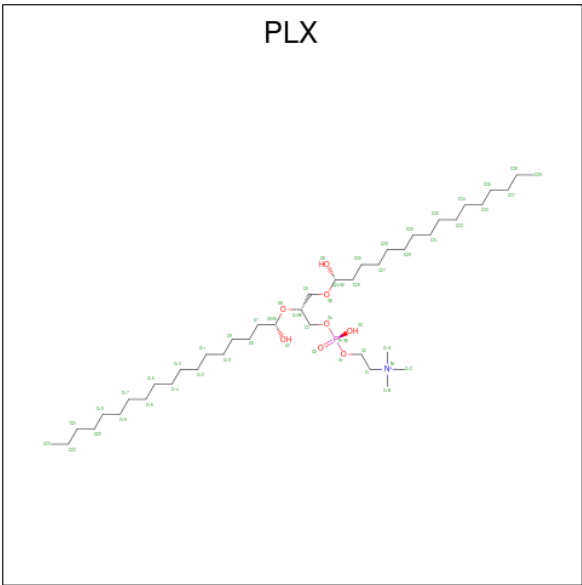
Mol	Chain	Residues	Atoms						AltConf
12	C	1	Total	C	H	N	O	P	0
			51	19	22	1	8	1	
12	C	1	Total	C	H	N	O	P	0
			53	23	20	1	8	1	
12	L	1	Total	C	H	N	O	P	0
			43	17	16	1	8	1	
12	U	1	Total	C	H	N	O	P	0
			103	37	56	1	8	1	
12	V	1	Total	C	H	N	O	P	0
			49	23	16	1	8	1	
12	Y	1	Total	C	H	N	O	P	0
			37	15	12	1	8	1	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



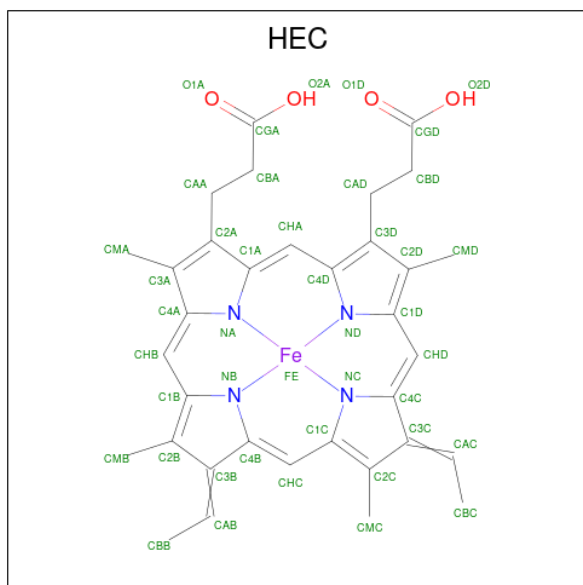
Mol	Chain	Residues	Atoms						AltConf
14	D	1	Total	C	H	N	O	P	0
			122	42	70	1	8	1	

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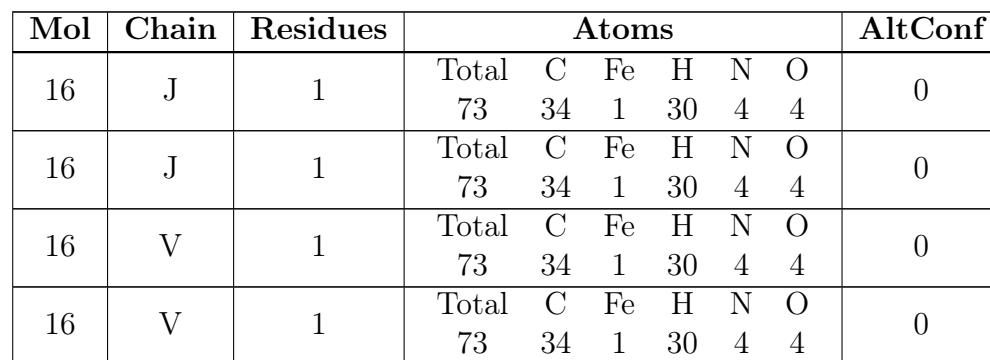
Mol	Chain	Residues	Atoms					AltConf	
14	T	1	Total	C	H	N	O	P	0
			122	42	70	1	8	1	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

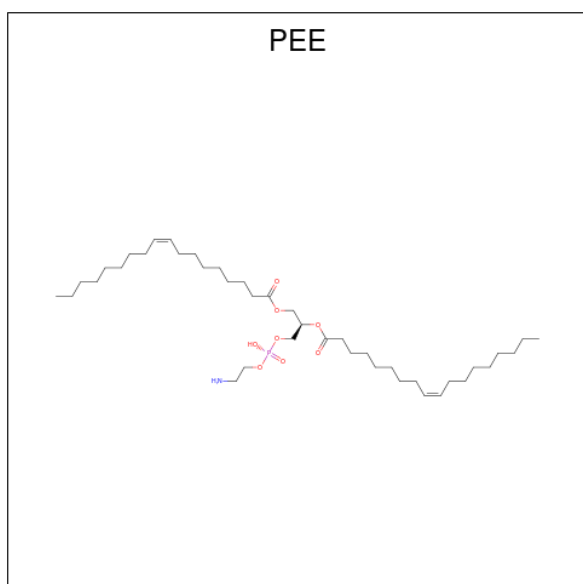


Mol	Chain	Residues	Atoms						AltConf
15	H	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	U	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

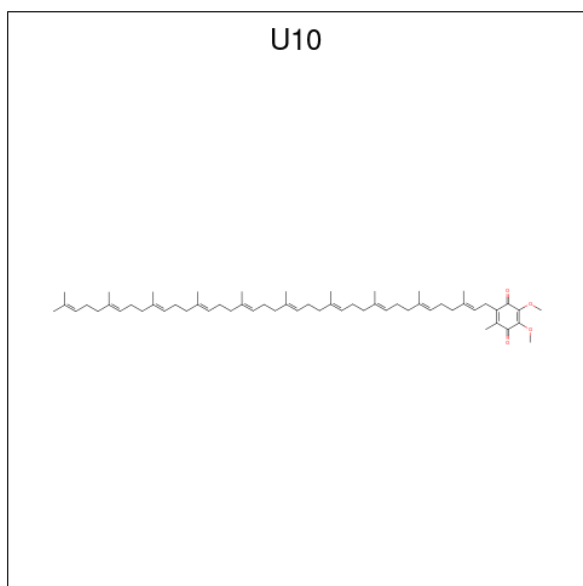


- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



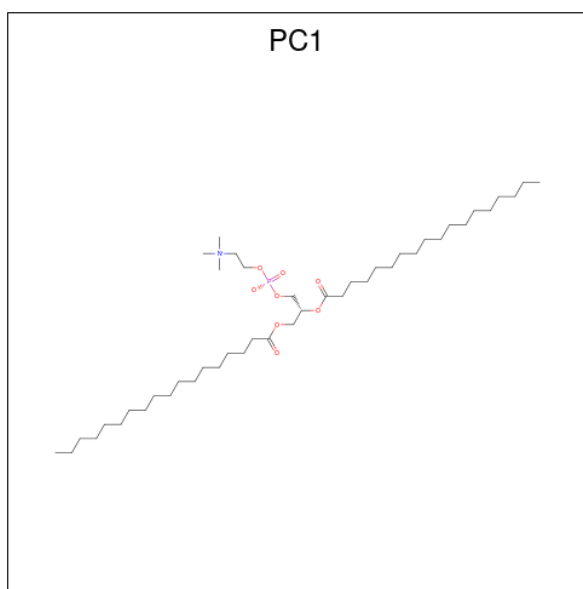
Mol	Chain	Residues	Atoms					AltConf
17	J	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 18 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	J	1	Total	C	H	O	0
			150	59	87	4	
18	J	1	Total	C	H	O	0
			150	59	87	4	
18	V	1	Total	C	H	O	0
			150	59	87	4	
18	V	1	Total	C	H	O	0
			150	59	87	4	

- Molecule 19 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
19	P	1	109	35	64	1	8	1	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213731	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.643	Depositor
Minimum map value	-14.750	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.54	Depositor
Map size (\AA)	420.0, 420.0, 420.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.875, 0.875, 0.875	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CDL	G	101	-	63,63,99	1.43	7 (11%)	69,75,111	1.05	4 (5%)
18	U10	J	406	-	63,63,63	2.90	35 (55%)	78,79,79	7.92	43 (55%)
14	PLX	D	101	-	51,51,51	1.03	4 (7%)	53,59,59	0.75	0
13	FES	C	302	2	0,4,4	-	-	-	-	-
18	U10	V	403	-	63,63,63	2.83	30 (47%)	78,79,79	7.50	44 (56%)
16	HEM	V	401	8	50,50,50	1.45	8 (16%)	67,82,82	1.09	2 (2%)
16	HEM	V	402	8	50,50,50	1.42	7 (14%)	67,82,82	1.23	6 (8%)
11	CDL	U	403	-	63,63,99	1.43	8 (12%)	69,75,111	1.17	4 (5%)
11	CDL	Y	501	-	63,63,99	1.43	7 (11%)	69,75,111	1.17	4 (5%)
18	U10	J	405	-	63,63,63	2.97	30 (47%)	78,79,79	8.16	38 (48%)
12	3PE	C	303	-	32,32,50	1.21	4 (12%)	35,37,55	1.10	2 (5%)
12	3PE	C	301	-	28,28,50	1.28	4 (14%)	31,33,55	1.13	2 (6%)
12	3PE	L	501	-	26,26,50	1.32	3 (11%)	29,31,55	1.14	2 (6%)
12	3PE	U	401	-	46,46,50	1.07	4 (8%)	49,51,55	0.99	2 (4%)
11	CDL	A	101	-	63,63,99	1.42	7 (11%)	69,75,111	1.09	4 (5%)
16	HEM	J	401	8	50,50,50	1.47	7 (14%)	67,82,82	1.04	2 (2%)
18	U10	V	404	-	63,63,63	2.92	35 (55%)	78,79,79	7.49	37 (47%)
11	CDL	J	404	-	63,63,99	1.42	8 (12%)	69,75,111	1.14	4 (5%)
15	HEC	H	401	-	46,50,50	1.83	6 (13%)	58,82,82	1.91	5 (8%)
13	FES	P	301	2	0,4,4	-	-	-	-	-
12	3PE	Y	502	-	24,24,50	1.34	3 (12%)	27,29,55	1.22	2 (7%)
11	CDL	V	406	-	63,63,99	1.44	8 (12%)	69,75,111	1.03	3 (4%)
12	3PE	V	405	-	32,32,50	1.21	3 (9%)	35,37,55	1.10	2 (5%)
19	PC1	P	302	-	44,44,53	1.41	7 (15%)	50,52,61	0.70	1 (2%)
11	CDL	H	402	-	63,63,99	1.42	8 (12%)	69,75,111	1.12	4 (5%)
17	PEE	J	403	-	48,48,50	1.19	3 (6%)	51,53,55	1.01	2 (3%)
14	PLX	T	102	-	51,51,51	1.05	5 (9%)	53,59,59	0.73	0
15	HEC	U	402	7	46,50,50	1.84	5 (10%)	58,82,82	1.96	6 (10%)
16	HEM	J	402	8	50,50,50	1.40	6 (12%)	67,82,82	1.18	5 (7%)
11	CDL	J	407	-	63,63,99	1.43	8 (12%)	69,75,111	1.05	4 (5%)
11	CDL	T	101	-	63,63,99	1.42	8 (12%)	69,75,111	1.13	5 (7%)

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
11	CDL	G	101	-	-	31/74/74/110	-
18	U10	J	406	-	-	18/63/87/87	0/1/1/1
14	PLX	D	101	-	-	8/55/55/55	-
13	FES	C	302	2	-	-	0/1/1/1
18	U10	V	403	-	-	25/63/87/87	0/1/1/1
16	HEM	V	401	8	-	5/14/54/54	-
16	HEM	V	402	8	-	5/14/54/54	-
11	CDL	U	403	-	-	12/74/74/110	-
11	CDL	Y	501	-	-	19/74/74/110	-
18	U10	J	405	-	-	19/63/87/87	0/1/1/1
12	3PE	C	303	-	-	6/36/36/54	-
12	3PE	C	301	-	-	11/32/32/54	-
12	3PE	L	501	-	-	9/30/30/54	-
12	3PE	U	401	-	-	12/50/50/54	-
11	CDL	A	101	-	-	21/74/74/110	-
16	HEM	J	401	8	-	2/14/54/54	-
18	U10	V	404	-	-	20/63/87/87	0/1/1/1
11	CDL	J	404	-	-	28/74/74/110	-
15	HEC	H	401	-	-	6/14/54/54	-
13	FES	P	301	2	-	-	0/1/1/1
12	3PE	Y	502	-	-	6/28/28/54	-
11	CDL	V	406	-	-	27/74/74/110	-
12	3PE	V	405	-	-	14/36/36/54	-
19	PC1	P	302	-	-	10/48/48/57	-
11	CDL	H	402	-	-	21/74/74/110	-
17	PEE	J	403	-	-	11/52/52/54	-
14	PLX	T	102	-	-	8/55/55/55	-
15	HEC	U	402	7	-	9/14/54/54	-
16	HEM	J	402	8	-	4/14/54/54	-
11	CDL	J	407	-	-	18/74/74/110	-
11	CDL	T	101	-	-	20/74/74/110	-

All (278) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	404	U10	C6-C1	11.16	1.55	1.35
18	J	405	U10	C6-C1	10.44	1.53	1.35
18	J	406	U10	C6-C1	10.42	1.53	1.35
18	V	403	U10	C6-C1	9.69	1.52	1.35
15	H	401	HEC	CAB-C3B	6.19	1.55	1.35
15	U	402	HEC	CAB-C3B	6.19	1.55	1.35
15	H	401	HEC	CAC-C3C	6.07	1.54	1.35
15	U	402	HEC	CAC-C3C	6.06	1.54	1.35
18	V	403	U10	C36-C34	5.76	1.63	1.51
15	U	402	HEC	C3D-C2D	5.68	1.53	1.38
15	H	401	HEC	C3D-C2D	5.67	1.53	1.38
18	J	406	U10	C46-C44	5.47	1.62	1.51
18	V	404	U10	C46-C44	5.23	1.62	1.51
18	J	406	U10	C16-C14	5.21	1.62	1.51
18	J	405	U10	C46-C44	5.20	1.62	1.51
18	V	404	U10	C36-C34	5.18	1.62	1.51
18	V	404	U10	C16-C14	5.15	1.61	1.51
18	J	405	U10	C11-C9	5.14	1.61	1.51
18	V	403	U10	C46-C44	5.11	1.61	1.51
18	J	405	U10	C26-C24	5.02	1.61	1.51
18	J	405	U10	C16-C14	5.01	1.61	1.51
18	J	405	U10	C31-C29	4.97	1.61	1.51
18	V	403	U10	C26-C24	4.95	1.61	1.51
18	J	405	U10	C36-C34	4.95	1.61	1.51
18	V	403	U10	C4-C3	4.89	1.53	1.36
18	J	405	U10	C21-C19	4.84	1.61	1.51
18	J	406	U10	C31-C29	4.82	1.61	1.51
18	J	405	U10	C4-C3	4.78	1.53	1.36
18	J	405	U10	C41-C39	4.78	1.61	1.51
18	J	406	U10	C4-C3	4.77	1.53	1.36
18	V	404	U10	C4-C3	4.68	1.53	1.36
18	V	404	U10	C21-C19	4.61	1.60	1.51
18	J	406	U10	C21-C19	4.56	1.60	1.51
18	V	403	U10	C41-C39	4.54	1.60	1.51
18	V	403	U10	C21-C19	4.40	1.60	1.51
18	J	406	U10	C41-C39	4.38	1.60	1.51
18	J	406	U10	C36-C34	4.38	1.60	1.51
18	V	404	U10	C26-C24	4.35	1.60	1.51
18	V	403	U10	C16-C14	4.33	1.60	1.51
18	V	404	U10	C51-C49	4.29	1.60	1.51
18	J	406	U10	C26-C24	4.25	1.60	1.51
18	J	406	U10	C51-C49	4.17	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	404	U10	C41-C39	4.14	1.59	1.51
18	J	406	U10	C11-C9	4.08	1.59	1.51
18	V	404	U10	C11-C9	4.08	1.59	1.51
18	V	403	U10	C11-C9	4.08	1.59	1.51
18	V	403	U10	C31-C29	3.99	1.59	1.51
18	J	405	U10	C51-C49	3.98	1.59	1.51
16	V	402	HEM	FE-ND	3.93	2.07	1.94
18	V	403	U10	C51-C49	3.88	1.59	1.51
16	J	401	HEM	FE-ND	3.86	2.06	1.94
18	V	404	U10	C31-C29	3.86	1.59	1.51
16	V	401	HEM	FE-ND	3.84	2.06	1.94
16	J	401	HEM	FE-NA	3.75	2.07	1.95
18	J	406	U10	C7-C8	3.73	1.56	1.50
11	U	403	CDL	OA8-CA7	3.58	1.43	1.33
17	J	403	PEE	O3-C30	3.55	1.43	1.33
11	Y	501	CDL	OA8-CA7	3.48	1.43	1.33
11	G	101	CDL	OA8-CA7	3.48	1.43	1.33
11	V	406	CDL	OB8-CB7	3.48	1.43	1.33
11	V	406	CDL	OA8-CA7	3.47	1.43	1.33
11	G	101	CDL	OB8-CB7	3.46	1.43	1.33
11	J	407	CDL	OB8-CB7	3.45	1.43	1.33
11	J	407	CDL	OA8-CA7	3.45	1.43	1.33
11	U	403	CDL	OB8-CB7	3.43	1.43	1.33
11	A	101	CDL	OA8-CA7	3.42	1.43	1.33
16	V	401	HEM	FE-NA	3.42	2.06	1.95
11	A	101	CDL	OB8-CB7	3.42	1.43	1.33
11	Y	501	CDL	OB8-CB7	3.42	1.43	1.33
11	H	402	CDL	OA8-CA7	3.41	1.43	1.33
11	T	101	CDL	OA8-CA7	3.41	1.43	1.33
11	T	101	CDL	OB8-CB7	3.41	1.43	1.33
11	J	404	CDL	OA8-CA7	3.40	1.43	1.33
11	J	404	CDL	OB8-CB7	3.40	1.43	1.33
11	V	406	CDL	OA6-CA5	3.38	1.43	1.34
11	H	402	CDL	OB8-CB7	3.38	1.43	1.33
18	J	405	U10	C7-C8	3.36	1.55	1.50
11	T	101	CDL	OA6-CA5	3.36	1.43	1.34
11	J	407	CDL	OA6-CA5	3.36	1.43	1.34
11	G	101	CDL	OA6-CA5	3.35	1.43	1.34
11	Y	501	CDL	OA6-CA5	3.33	1.43	1.34
11	A	101	CDL	OA6-CA5	3.28	1.43	1.34
11	U	403	CDL	OA6-CA5	3.27	1.43	1.34
11	J	404	CDL	OA6-CA5	3.27	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	402	CDL	OA6-CA5	3.26	1.43	1.34
16	V	402	HEM	FE-NA	3.21	2.05	1.95
16	J	401	HEM	FE-NB	3.20	2.04	1.94
16	J	402	HEM	FE-ND	3.20	2.04	1.94
19	P	302	PC1	O31-C31	3.09	1.42	1.33
18	V	403	U10	C7-C8	3.09	1.55	1.50
16	V	401	HEM	FE-NC	3.07	2.05	1.95
19	P	302	PC1	O21-C21	3.06	1.42	1.34
16	J	402	HEM	FE-NB	3.05	2.04	1.94
17	J	403	PEE	O2-C10	3.03	1.42	1.34
11	A	101	CDL	OB6-CB4	-3.03	1.39	1.46
11	H	402	CDL	OB6-CB4	-3.03	1.39	1.46
16	V	401	HEM	CAC-C3C	2.97	1.55	1.47
18	V	404	U10	C40-C39	2.96	1.57	1.50
16	J	402	HEM	FE-NC	2.95	2.04	1.95
16	V	402	HEM	CAC-C3C	2.95	1.55	1.47
16	J	401	HEM	CAC-C3C	2.93	1.55	1.47
16	J	401	HEM	CAB-C3B	2.93	1.55	1.47
16	J	402	HEM	CAC-C3C	2.93	1.55	1.47
16	V	402	HEM	CAB-C3B	2.92	1.55	1.47
18	V	404	U10	C7-C8	2.91	1.55	1.50
16	J	402	HEM	CAB-C3B	2.91	1.55	1.47
11	V	406	CDL	OB6-CB4	-2.91	1.39	1.46
16	V	401	HEM	CAB-C3B	2.90	1.55	1.47
11	U	403	CDL	OB6-CB5	2.90	1.42	1.34
16	J	402	HEM	FE-NA	2.90	2.04	1.95
11	A	101	CDL	OA6-CA4	-2.88	1.39	1.46
11	H	402	CDL	OA6-CA4	-2.88	1.39	1.46
11	J	404	CDL	OB6-CB4	-2.88	1.39	1.46
11	Y	501	CDL	OB6-CB4	-2.87	1.39	1.46
11	J	407	CDL	OB6-CB5	2.87	1.42	1.34
11	U	403	CDL	OA6-CA4	-2.84	1.39	1.46
11	Y	501	CDL	OB6-CB5	2.84	1.42	1.34
11	G	101	CDL	OB6-CB5	2.83	1.42	1.34
11	G	101	CDL	OB6-CB4	-2.83	1.39	1.46
11	V	406	CDL	OB6-CB5	2.83	1.42	1.34
11	T	101	CDL	OB6-CB4	-2.83	1.39	1.46
11	J	404	CDL	OB6-CB5	2.83	1.42	1.34
16	J	401	HEM	FE-NC	2.83	2.04	1.95
11	J	404	CDL	OA6-CA4	-2.82	1.40	1.46
18	V	404	U10	C7-C6	2.82	1.56	1.51
11	U	403	CDL	OB6-CB4	-2.80	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	401	HEM	FE-NB	2.77	2.03	1.94
11	V	406	CDL	OA6-CA4	-2.76	1.40	1.46
11	Y	501	CDL	OA6-CA4	-2.76	1.40	1.46
16	V	402	HEM	FE-NB	2.76	2.03	1.94
11	T	101	CDL	OA6-CA4	-2.75	1.40	1.46
11	T	101	CDL	OB6-CB5	2.74	1.42	1.34
19	P	302	PC1	P-O13	2.74	1.70	1.59
11	J	407	CDL	OA6-CA4	-2.74	1.40	1.46
18	J	406	U10	C7-C6	2.74	1.56	1.51
11	H	402	CDL	OB6-CB5	2.73	1.42	1.34
11	J	407	CDL	OB6-CB4	-2.73	1.40	1.46
12	L	501	3PE	O31-C31	2.72	1.41	1.33
12	C	303	3PE	O31-C31	2.71	1.41	1.33
11	G	101	CDL	OA6-CA4	-2.71	1.40	1.46
18	J	406	U10	C22-C23	2.70	1.58	1.50
16	V	402	HEM	FE-NC	2.70	2.04	1.95
18	J	405	U10	C17-C18	2.69	1.58	1.50
11	A	101	CDL	OB6-CB5	2.69	1.41	1.34
12	U	401	3PE	O31-C31	2.69	1.41	1.33
12	Y	502	3PE	O31-C31	2.69	1.41	1.33
12	C	301	3PE	O31-C31	2.65	1.41	1.33
12	V	405	3PE	O31-C31	2.64	1.41	1.33
18	J	405	U10	C7-C6	2.63	1.56	1.51
18	J	405	U10	C42-C43	2.63	1.58	1.50
19	P	302	PC1	P-O11	2.60	1.69	1.59
18	J	406	U10	C17-C18	2.60	1.58	1.50
18	J	405	U10	C47-C48	2.59	1.58	1.50
12	C	301	3PE	O21-C21	2.58	1.41	1.34
18	V	403	U10	C40-C39	2.58	1.57	1.50
18	V	403	U10	C32-C33	2.56	1.58	1.50
12	U	401	3PE	O21-C21	2.55	1.41	1.34
18	J	406	U10	C20-C19	2.54	1.56	1.50
18	V	403	U10	C16-C17	2.54	1.62	1.53
14	D	101	PLX	O6-C4	-2.54	1.41	1.44
12	V	405	3PE	O21-C21	2.53	1.41	1.34
12	Y	502	3PE	O21-C21	2.52	1.41	1.34
12	L	501	3PE	O21-C21	2.52	1.41	1.34
18	J	405	U10	C37-C38	2.52	1.58	1.50
18	J	405	U10	C12-C13	2.52	1.58	1.50
18	J	406	U10	C6-C5	2.51	1.53	1.46
18	V	404	U10	C20-C19	2.51	1.56	1.50
12	C	303	3PE	O21-C21	2.51	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	102	PLX	C7-C6	2.50	1.56	1.50
17	J	403	PEE	O2-C2	-2.49	1.40	1.46
18	J	405	U10	C27-C28	2.48	1.58	1.50
18	J	405	U10	C22-C23	2.47	1.58	1.50
18	V	404	U10	C25-C24	2.46	1.56	1.50
18	J	406	U10	C40-C39	2.46	1.56	1.50
18	J	405	U10	C30-C29	2.46	1.56	1.50
18	J	406	U10	C27-C28	2.43	1.57	1.50
14	T	102	PLX	C25-C24	2.43	1.55	1.50
18	V	403	U10	C25-C24	2.43	1.56	1.50
18	V	403	U10	C50-C49	2.42	1.56	1.50
18	J	405	U10	C32-C33	2.42	1.57	1.50
18	V	404	U10	C37-C38	2.40	1.57	1.50
18	V	404	U10	C12-C13	2.40	1.57	1.50
18	V	403	U10	C22-C23	2.39	1.57	1.50
18	V	403	U10	C20-C19	2.35	1.56	1.50
14	D	101	PLX	C7-C6	2.35	1.55	1.50
18	V	404	U10	C30-C29	2.35	1.56	1.50
18	V	403	U10	C46-C47	2.34	1.61	1.53
18	J	406	U10	C35-C34	2.34	1.56	1.50
12	U	401	3PE	O21-C2	-2.34	1.41	1.46
12	V	405	3PE	O21-C2	-2.33	1.41	1.46
18	V	403	U10	C42-C43	2.33	1.57	1.50
18	V	404	U10	C32-C33	2.31	1.57	1.50
12	C	303	3PE	O21-C2	-2.31	1.41	1.46
18	J	405	U10	C25-C24	2.31	1.56	1.50
18	V	404	U10	C27-C28	2.31	1.57	1.50
12	L	501	3PE	O21-C2	-2.31	1.41	1.46
18	J	405	U10	C6-C5	2.30	1.53	1.46
12	Y	502	3PE	O21-C2	-2.30	1.41	1.46
12	C	301	3PE	O21-C2	-2.29	1.41	1.46
18	J	406	U10	C12-C13	2.28	1.57	1.50
18	V	403	U10	C6-C5	2.28	1.52	1.46
14	T	102	PLX	P1-O4	2.27	1.68	1.59
14	T	102	PLX	O6-C4	-2.27	1.41	1.44
14	D	101	PLX	C25-C24	2.27	1.55	1.50
18	V	403	U10	C36-C37	2.27	1.61	1.53
18	V	404	U10	C35-C34	2.27	1.56	1.50
18	V	404	U10	C22-C23	2.27	1.57	1.50
11	J	404	CDL	PB2-OB2	2.27	1.68	1.59
18	J	406	U10	C47-C48	2.27	1.57	1.50
18	V	404	U10	C42-C43	2.26	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	407	CDL	PB2-OB2	2.26	1.68	1.59
18	V	403	U10	C15-C14	2.25	1.56	1.50
11	T	101	CDL	PB2-OB2	2.25	1.68	1.59
11	G	101	CDL	PB2-OB2	2.25	1.68	1.59
18	V	404	U10	C6-C5	2.25	1.52	1.46
11	V	406	CDL	PB2-OB2	2.25	1.68	1.59
18	J	405	U10	C35-C34	2.24	1.56	1.50
11	U	403	CDL	PB2-OB2	2.24	1.68	1.59
18	J	406	U10	C10-C9	2.24	1.56	1.50
18	J	406	U10	C25-C24	2.23	1.56	1.50
18	V	404	U10	C17-C18	2.23	1.57	1.50
11	Y	501	CDL	PB2-OB2	2.22	1.68	1.59
15	H	401	HEC	C3C-C2C	-2.22	1.33	1.41
18	V	404	U10	C50-C49	2.22	1.56	1.50
19	P	302	PC1	O21-C2	-2.22	1.41	1.46
18	J	405	U10	C40-C39	2.21	1.56	1.50
11	A	101	CDL	PB2-OB2	2.21	1.68	1.59
18	V	404	U10	C15-C14	2.19	1.56	1.50
14	D	101	PLX	P1-O4	2.19	1.68	1.59
11	H	402	CDL	PB2-OB2	2.17	1.67	1.59
15	U	402	HEC	C3C-C2C	-2.17	1.33	1.41
15	H	401	HEC	C3B-C2B	-2.17	1.33	1.41
18	J	406	U10	C15-C14	2.17	1.56	1.50
18	J	406	U10	C42-C43	2.15	1.57	1.50
18	V	403	U10	O4-C4	2.14	1.41	1.36
18	V	403	U10	C47-C48	2.14	1.57	1.50
19	P	302	PC1	C22-C21	2.14	1.56	1.50
11	V	406	CDL	PB2-OB5	2.14	1.67	1.59
18	V	404	U10	C47-C48	2.13	1.56	1.50
18	V	403	U10	O3-C3	2.13	1.41	1.36
18	V	404	U10	C21-C22	2.13	1.60	1.53
18	V	403	U10	C17-C18	2.13	1.56	1.50
18	J	406	U10	C36-C37	2.12	1.60	1.53
15	U	402	HEC	C3B-C2B	-2.12	1.34	1.41
18	J	406	U10	C21-C22	2.12	1.60	1.53
18	J	405	U10	C50-C49	2.10	1.55	1.50
18	V	404	U10	C52-C53	2.10	1.56	1.50
18	J	406	U10	C11-C12	2.10	1.60	1.53
18	J	406	U10	C30-C29	2.09	1.55	1.50
18	V	404	U10	O4-C4M	-2.09	1.40	1.45
12	C	301	3PE	P-O11	2.09	1.67	1.59
18	J	405	U10	C26-C27	2.09	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	404	U10	C1-C2	2.08	1.54	1.47
18	V	404	U10	C36-C37	2.07	1.60	1.53
18	V	403	U10	C7-C6	2.07	1.55	1.51
18	J	406	U10	O3-C3	2.07	1.41	1.36
18	J	406	U10	C50-C49	2.06	1.55	1.50
11	H	402	CDL	PB2-OB5	2.06	1.67	1.59
18	J	406	U10	C37-C38	2.06	1.56	1.50
11	T	101	CDL	PB2-OB5	2.05	1.67	1.59
12	U	401	3PE	P-O11	2.05	1.67	1.59
18	J	406	U10	C32-C33	2.05	1.56	1.50
11	J	404	CDL	PB2-OB5	2.05	1.67	1.59
11	U	403	CDL	PB2-OB5	2.05	1.67	1.59
14	T	102	PLX	P1-O1	2.04	1.67	1.59
16	V	402	HEM	C2A-C3A	-2.04	1.33	1.38
18	V	404	U10	O3-C3	2.04	1.41	1.36
11	J	407	CDL	PB2-OB5	2.04	1.67	1.59
18	V	403	U10	O2-C2	-2.03	1.18	1.23
18	J	406	U10	O4-C4	2.02	1.41	1.36
16	V	401	HEM	CMD-C2D	2.02	1.54	1.50
19	P	302	PC1	C15-N	-2.02	1.44	1.50
16	J	401	HEM	CMD-C2D	2.02	1.54	1.50
15	H	401	HEC	CMC-C2C	2.01	1.54	1.50
18	J	405	U10	C15-C14	2.01	1.55	1.50
18	J	405	U10	C45-C44	2.01	1.55	1.50
16	V	401	HEM	C2A-C3A	-2.01	1.33	1.38
12	C	303	3PE	P-O11	2.00	1.67	1.59

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C10-C9-C11	-20.60	79.48	115.23
18	J	406	U10	C40-C39-C41	-19.02	82.21	115.23
18	V	403	U10	C10-C9-C8	18.63	171.47	123.63
18	J	406	U10	C40-C39-C38	18.62	171.44	123.63
18	J	405	U10	C20-C19-C18	18.43	170.95	123.63
18	V	404	U10	C10-C9-C8	17.44	168.41	123.63
18	J	405	U10	C11-C9-C8	-17.37	82.17	121.17
18	J	406	U10	C25-C24-C23	17.33	168.13	123.63
18	J	406	U10	C10-C9-C8	17.16	167.69	123.63
18	J	406	U10	C15-C14-C16	-16.92	85.87	115.23
18	J	405	U10	C50-C49-C48	16.85	166.90	123.63
18	J	405	U10	C40-C39-C38	16.50	166.01	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C15-C14-C16	-16.39	86.77	115.23
18	J	405	U10	C20-C19-C21	-16.28	86.97	115.23
18	V	403	U10	C20-C19-C18	15.64	163.79	123.63
18	V	404	U10	C45-C44-C43	15.63	163.76	123.63
18	J	405	U10	C35-C34-C36	-15.55	88.24	115.23
18	J	406	U10	C50-C49-C48	15.32	162.97	123.63
18	V	404	U10	C40-C39-C38	15.32	162.97	123.63
18	V	404	U10	C50-C49-C51	-15.29	88.69	115.23
18	V	404	U10	C25-C24-C26	-15.26	88.74	115.23
18	J	405	U10	C25-C24-C23	15.20	162.67	123.63
18	V	403	U10	C50-C49-C48	15.09	162.38	123.63
18	J	406	U10	C25-C24-C26	-15.07	89.07	115.23
18	V	404	U10	C30-C29-C28	15.06	162.30	123.63
18	J	405	U10	C50-C49-C51	-15.01	89.18	115.23
18	V	404	U10	C25-C24-C23	14.96	162.06	123.63
18	V	403	U10	C15-C14-C13	14.91	161.91	123.63
18	J	405	U10	C10-C9-C8	14.80	161.64	123.63
18	J	406	U10	C20-C19-C18	14.71	161.40	123.63
18	J	405	U10	C45-C44-C43	14.55	161.00	123.63
18	V	403	U10	C40-C39-C41	-14.50	90.05	115.23
18	J	406	U10	C10-C9-C11	-14.42	90.19	115.23
18	V	404	U10	C30-C29-C31	-14.33	90.35	115.23
18	V	403	U10	C25-C24-C23	14.31	160.38	123.63
18	V	403	U10	C30-C29-C28	14.23	160.16	123.63
18	V	404	U10	C50-C49-C48	14.23	160.16	123.63
18	V	403	U10	C50-C49-C51	-14.20	90.58	115.23
18	J	406	U10	C35-C34-C36	-14.11	90.74	115.23
18	J	406	U10	C30-C29-C28	14.08	159.78	123.63
18	V	404	U10	C35-C34-C33	14.07	159.75	123.63
18	J	406	U10	C20-C19-C21	-14.06	90.82	115.23
18	V	404	U10	C35-C34-C36	-14.04	90.85	115.23
18	V	404	U10	C45-C44-C46	-13.97	90.99	115.23
18	J	406	U10	C45-C44-C43	13.90	159.33	123.63
18	V	404	U10	C20-C19-C18	13.82	159.13	123.63
18	J	405	U10	C40-C39-C41	-13.74	91.38	115.23
18	J	405	U10	C45-C44-C46	-13.68	91.48	115.23
18	V	403	U10	C45-C44-C43	13.61	158.59	123.63
18	V	404	U10	C15-C14-C13	13.59	158.52	123.63
18	V	403	U10	C40-C39-C38	13.58	158.51	123.63
18	J	405	U10	C30-C29-C28	13.50	158.31	123.63
18	J	406	U10	C50-C49-C51	-13.42	91.94	115.23
18	J	405	U10	C30-C29-C31	-13.33	92.09	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C25-C24-C26	-13.31	92.13	115.23
18	V	403	U10	C11-C9-C8	-13.15	91.66	121.17
18	V	403	U10	C35-C34-C33	13.07	157.18	123.63
18	V	403	U10	C45-C44-C46	-13.06	92.55	115.23
18	V	404	U10	C40-C39-C41	-12.97	92.72	115.23
18	J	405	U10	C35-C34-C33	12.96	156.91	123.63
18	J	406	U10	C30-C29-C31	-12.89	92.86	115.23
18	V	404	U10	C20-C19-C21	-12.76	93.09	115.23
18	J	405	U10	C15-C14-C13	12.75	156.36	123.63
18	V	403	U10	C30-C29-C31	-12.65	93.27	115.23
18	J	406	U10	C41-C39-C38	-12.50	93.10	121.17
18	V	403	U10	C35-C34-C36	-12.48	93.56	115.23
18	V	404	U10	C10-C9-C11	-12.20	94.05	115.23
18	V	403	U10	C20-C19-C21	-11.93	94.53	115.23
18	J	406	U10	C35-C34-C33	11.75	153.81	123.63
18	V	403	U10	C15-C14-C16	-11.59	95.12	115.23
18	V	404	U10	C15-C14-C16	-11.32	95.57	115.23
18	J	406	U10	C15-C14-C13	11.24	152.49	123.63
18	V	403	U10	C47-C48-C49	11.00	152.81	127.62
18	V	403	U10	C10-C9-C11	-10.82	96.44	115.23
18	V	403	U10	C8-C7-C6	10.68	138.40	112.08
18	V	404	U10	C11-C9-C8	-10.64	97.29	121.17
18	J	405	U10	C21-C19-C18	-10.40	97.83	121.17
18	J	406	U10	C7-C8-C9	-9.81	109.93	126.83
18	J	406	U10	C45-C44-C46	-9.79	98.24	115.23
18	V	403	U10	C25-C24-C26	-9.39	98.92	115.23
18	J	405	U10	C7-C8-C9	-9.17	111.03	126.83
18	V	403	U10	C26-C24-C23	-9.12	100.68	121.17
15	H	401	HEC	CBC-CAC-C3C	-9.01	109.42	127.43
18	J	406	U10	C11-C9-C8	-9.00	100.97	121.17
15	U	402	HEC	CBC-CAC-C3C	-8.94	109.57	127.43
18	V	404	U10	C7-C8-C9	-8.91	111.48	126.83
18	J	405	U10	C41-C39-C38	-8.84	101.33	121.17
18	V	403	U10	C21-C19-C18	-8.77	101.48	121.17
18	J	406	U10	C32-C33-C34	-8.39	108.41	127.62
18	J	406	U10	C46-C44-C43	-8.36	102.40	121.17
18	J	406	U10	C26-C24-C23	-8.28	102.58	121.17
15	H	401	HEC	CBB-CAB-C3B	-8.16	111.12	127.43
18	V	403	U10	C16-C14-C13	-8.15	102.87	121.17
15	U	402	HEC	CBB-CAB-C3B	-8.09	111.25	127.43
18	J	405	U10	C51-C49-C48	-7.82	103.61	121.17
18	V	404	U10	C41-C39-C38	-7.51	104.31	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C12-C13-C14	-7.49	110.48	127.62
18	V	404	U10	C46-C44-C43	-7.36	104.64	121.17
18	J	406	U10	C51-C49-C48	-7.33	104.72	121.17
18	J	405	U10	C26-C24-C23	-7.14	105.15	121.17
18	J	406	U10	C22-C23-C24	7.09	143.86	127.62
18	V	404	U10	C16-C14-C13	-6.81	105.89	121.17
18	J	405	U10	C32-C33-C34	-6.74	112.19	127.62
18	V	403	U10	C51-C49-C48	-6.71	106.11	121.17
18	V	403	U10	C31-C29-C28	-6.64	106.27	121.17
18	J	406	U10	C31-C29-C28	-6.49	106.61	121.17
18	V	404	U10	C31-C29-C28	-6.17	107.31	121.17
18	J	405	U10	C46-C44-C43	-6.11	107.46	121.17
18	J	406	U10	C12-C13-C14	6.10	141.59	127.62
18	J	406	U10	C21-C19-C18	-5.97	107.77	121.17
18	V	404	U10	C21-C19-C18	-5.96	107.79	121.17
18	V	404	U10	C7-C6-C5	-5.77	111.82	118.52
18	V	403	U10	C46-C44-C43	-5.52	108.78	121.17
18	V	404	U10	C26-C24-C23	-5.34	109.18	121.17
18	V	403	U10	C37-C38-C39	5.32	139.80	127.62
18	V	403	U10	C36-C34-C33	-5.31	109.25	121.17
18	J	405	U10	C31-C29-C28	-5.30	109.27	121.17
18	V	404	U10	C36-C34-C33	-5.25	109.38	121.17
18	J	406	U10	C37-C38-C39	-5.15	115.83	127.62
18	V	403	U10	C27-C28-C29	-4.86	116.50	127.62
18	V	404	U10	C47-C48-C49	-4.83	116.57	127.62
18	V	404	U10	C17-C18-C19	-4.80	116.64	127.62
18	V	403	U10	C42-C43-C44	-4.79	116.67	127.62
18	V	403	U10	C41-C39-C38	-4.70	110.62	121.17
18	V	403	U10	C12-C13-C14	-4.48	117.36	127.62
18	V	404	U10	C51-C49-C48	-4.48	111.11	121.17
11	U	403	CDL	OB6-CB5-C51	4.38	120.96	111.48
18	V	404	U10	C22-C23-C24	-4.35	117.66	127.62
11	J	404	CDL	OB6-CB5-C51	4.17	120.49	111.48
11	T	101	CDL	OA6-CA5-C11	4.11	120.38	111.48
11	J	407	CDL	OB6-CB5-C51	4.10	120.36	111.48
11	Y	501	CDL	OB6-CB5-C51	4.10	120.35	111.48
12	Y	502	3PE	O21-C21-C22	4.09	120.32	111.48
11	H	402	CDL	OB6-CB5-C51	4.05	120.25	111.48
18	J	406	U10	C17-C18-C19	-4.04	118.38	127.62
18	V	404	U10	C12-C13-C14	4.04	136.87	127.62
12	L	501	3PE	O21-C21-C22	4.01	120.15	111.48
12	V	405	3PE	O21-C21-C22	3.97	120.06	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	404	U10	C27-C28-C29	-3.91	118.67	127.62
11	A	101	CDL	OB6-CB5-C51	3.89	119.90	111.48
18	J	406	U10	C42-C43-C44	-3.85	118.82	127.62
12	C	303	3PE	O21-C21-C22	3.83	119.76	111.48
12	C	301	3PE	O21-C21-C22	3.78	119.67	111.48
11	G	101	CDL	OA6-CA5-C11	3.74	119.56	111.48
12	U	401	3PE	O21-C21-C22	3.71	119.52	111.48
11	Y	501	CDL	OA6-CA5-C11	3.64	119.35	111.48
15	U	402	HEC	C4D-ND-C1D	3.63	111.74	105.82
18	J	405	U10	C17-C18-C19	3.61	135.89	127.62
18	V	403	U10	C32-C33-C34	3.61	135.88	127.62
11	J	404	CDL	OA6-CA5-C11	3.60	119.27	111.48
11	A	101	CDL	OA6-CA5-C11	3.60	119.27	111.48
11	V	406	CDL	OB6-CB5-C51	3.57	119.20	111.48
11	U	403	CDL	OA6-CA5-C11	3.56	119.19	111.48
18	V	403	U10	C17-C18-C19	-3.53	119.54	127.62
15	H	401	HEC	C4D-ND-C1D	3.46	111.46	105.82
18	V	403	U10	C7-C6-C1	-3.43	119.01	124.89
18	J	406	U10	C42-C41-C39	-3.42	101.85	113.19
11	T	101	CDL	OB6-CB5-C51	3.40	118.85	111.48
11	V	406	CDL	OA6-CA5-C11	3.40	118.83	111.48
18	V	404	U10	C32-C33-C34	-3.36	119.93	127.62
11	J	407	CDL	OA6-CA5-C11	3.33	118.68	111.48
11	G	101	CDL	OB6-CB5-C51	3.26	118.53	111.48
11	H	402	CDL	OA6-CA5-C11	3.23	118.47	111.48
18	V	403	U10	C22-C23-C24	-3.21	120.29	127.62
18	J	405	U10	C36-C34-C33	-3.19	114.02	121.17
18	V	403	U10	C1M-C1-C6	-3.08	119.39	124.45
11	U	403	CDL	OA8-CA7-C31	3.08	121.22	111.83
18	J	406	U10	C36-C34-C33	-3.07	114.28	121.17
18	J	405	U10	C27-C28-C29	3.06	134.64	127.62
11	Y	501	CDL	OA8-CA7-C31	3.04	121.12	111.83
18	J	405	U10	C7-C6-C1	-3.04	119.67	124.89
18	V	403	U10	C7-C8-C9	-3.03	121.62	126.83
18	J	406	U10	C47-C48-C49	-3.01	120.74	127.62
17	J	403	PEE	C40-C39-C38	2.97	147.12	124.83
11	V	406	CDL	OB8-CB7-C71	2.95	120.82	111.83
18	V	403	U10	C12-C11-C9	-2.86	103.70	113.19
18	J	405	U10	C1M-C1-C6	-2.84	119.77	124.45
17	J	403	PEE	O2-C10-C11	2.79	117.52	111.48
16	J	402	HEM	C3B-C2B-C1B	2.76	108.48	106.41
18	J	406	U10	C32-C31-C29	2.75	122.30	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	406	U10	C27-C28-C29	2.71	133.82	127.62
11	Y	501	CDL	OB8-CB7-C71	2.69	120.04	111.83
15	U	402	HEC	C2A-C1A-NA	-2.66	107.75	110.32
16	V	402	HEM	C3B-C2B-C1B	2.65	108.40	106.41
11	G	101	CDL	OB8-CB7-C71	2.62	119.83	111.83
18	J	405	U10	C37-C38-C39	2.59	133.56	127.62
18	J	406	U10	C7-C6-C1	-2.56	120.50	124.89
11	H	402	CDL	OB8-CB7-C71	2.55	119.61	111.83
16	V	402	HEM	C1B-NB-C4B	2.52	108.19	105.21
11	J	407	CDL	OB8-CB7-C71	2.50	119.47	111.83
18	V	404	U10	C37-C38-C39	-2.50	121.89	127.62
18	J	406	U10	C1M-C1-C6	-2.49	120.35	124.45
18	J	405	U10	C31-C32-C33	2.49	124.34	112.02
12	U	401	3PE	O31-C31-C32	2.49	119.43	111.83
11	H	402	CDL	OA8-CA7-C31	2.46	119.34	111.83
11	U	403	CDL	OB8-CB7-C71	2.45	119.30	111.83
11	A	101	CDL	OA8-CA7-C31	2.44	119.27	111.83
12	L	501	3PE	O31-C31-C32	2.44	119.27	111.83
11	J	404	CDL	OB8-CB7-C71	2.43	119.24	111.83
19	P	302	PC1	O21-C21-C22	2.41	116.70	111.48
16	V	402	HEM	C3B-C4B-NB	-2.41	107.74	109.47
12	Y	502	3PE	O31-C31-C32	2.39	119.13	111.83
11	J	404	CDL	OA8-CA7-C31	2.37	119.08	111.83
12	C	301	3PE	O31-C31-C32	2.37	119.06	111.83
18	J	406	U10	C31-C32-C33	2.36	123.71	112.02
18	J	405	U10	C42-C43-C44	2.36	133.02	127.62
16	V	402	HEM	C4D-ND-C1D	2.35	107.99	105.21
18	V	403	U10	C27-C26-C24	2.35	120.97	113.19
16	V	402	HEM	CHC-C1C-NC	2.35	127.01	124.45
18	J	406	U10	C52-C53-C54	-2.34	119.83	127.64
18	V	403	U10	C56-C54-C55	2.34	119.97	114.59
15	H	401	HEC	C2A-C1A-NA	-2.33	108.08	110.32
16	J	402	HEM	C1B-NB-C4B	2.32	107.96	105.21
12	C	303	3PE	O31-C31-C32	2.30	118.85	111.83
16	J	402	HEM	C4D-ND-C1D	2.28	107.91	105.21
15	U	402	HEC	CAA-C2A-C3A	-2.27	123.61	127.87
11	T	101	CDL	OB8-CB7-C71	2.26	118.73	111.83
11	G	101	CDL	OA8-CA7-C31	2.26	118.72	111.83
18	J	406	U10	C8-C7-C6	-2.25	106.53	112.08
16	V	402	HEM	CBA-CAA-C2A	-2.25	106.30	112.53
16	V	401	HEM	C1B-NB-C4B	2.25	107.87	105.21
11	T	101	CDL	CB4-OB6-CB5	-2.25	112.42	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C42-C41-C39	2.22	120.53	113.19
18	J	405	U10	C11-C12-C13	2.20	122.92	112.02
12	V	405	3PE	O31-C31-C32	2.20	118.55	111.83
15	U	402	HEC	CHA-C1A-C2A	2.19	128.31	124.86
16	J	402	HEM	C3B-C4B-NB	-2.18	107.90	109.47
11	A	101	CDL	OB8-CB7-C71	2.15	118.39	111.83
16	J	401	HEM	C1B-NB-C4B	2.15	107.75	105.21
16	J	402	HEM	CHC-C1C-NC	2.14	126.78	124.45
18	J	406	U10	C56-C54-C55	2.12	119.47	114.59
16	J	401	HEM	C3B-C2B-C1B	2.11	107.99	106.41
11	T	101	CDL	OA8-CA7-C31	2.10	118.25	111.83
18	V	404	U10	C7-C6-C1	2.10	128.49	124.89
16	V	401	HEM	C3B-C2B-C1B	2.08	107.98	106.41
18	V	403	U10	C52-C51-C49	-2.08	106.31	113.19
18	V	403	U10	C42-C41-C39	-2.06	106.35	113.19
11	J	407	CDL	OA8-CA7-C31	2.02	117.99	111.83
15	H	401	HEC	CAA-CBA-CGA	-2.01	108.33	113.67

There are no chirality outliers.

All (405) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	101	CDL	CA2-OA2-PA1-OA4
11	A	101	CDL	CA2-OA2-PA1-OA5
11	A	101	CDL	CA3-OA5-PA1-OA2
11	A	101	CDL	C1-CB2-OB2-PB2
11	A	101	CDL	CB2-OB2-PB2-OB4
11	A	101	CDL	CB2-OB2-PB2-OB5
11	A	101	CDL	CB3-OB5-PB2-OB3
11	G	101	CDL	CA2-C1-CB2-OB2
11	G	101	CDL	OA6-CA4-CA6-OA8
11	G	101	CDL	CB2-OB2-PB2-OB3
11	G	101	CDL	CB2-OB2-PB2-OB4
11	G	101	CDL	CB2-OB2-PB2-OB5
11	H	402	CDL	CA3-OA5-PA1-OA2
11	H	402	CDL	CA3-OA5-PA1-OA3
11	H	402	CDL	OA7-CA5-OA6-CA4
11	H	402	CDL	C11-CA5-OA6-CA4
11	H	402	CDL	C51-CB5-OB6-CB4
11	J	404	CDL	CA3-OA5-PA1-OA2
11	J	404	CDL	CA3-OA5-PA1-OA3
11	J	404	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
11	J	404	CDL	CB3-OB5-PB2-OB2
11	J	404	CDL	CB3-OB5-PB2-OB3
11	J	404	CDL	CB3-OB5-PB2-OB4
11	J	404	CDL	OB7-CB5-OB6-CB4
11	J	404	CDL	OB9-CB7-OB8-CB6
11	J	404	CDL	C71-CB7-OB8-CB6
11	J	407	CDL	CA2-OA2-PA1-OA3
11	J	407	CDL	CA3-OA5-PA1-OA2
11	J	407	CDL	CA3-OA5-PA1-OA3
11	J	407	CDL	OB7-CB5-OB6-CB4
11	J	407	CDL	C51-CB5-OB6-CB4
11	J	407	CDL	OB9-CB7-OB8-CB6
11	J	407	CDL	C71-CB7-OB8-CB6
11	T	101	CDL	C11-CA5-OA6-CA4
11	T	101	CDL	OB7-CB5-OB6-CB4
11	T	101	CDL	OB9-CB7-OB8-CB6
11	T	101	CDL	C71-CB7-OB8-CB6
11	U	403	CDL	OA9-CA7-OA8-CA6
11	U	403	CDL	C31-CA7-OA8-CA6
11	U	403	CDL	C1-CB2-OB2-PB2
11	U	403	CDL	CB3-OB5-PB2-OB2
11	U	403	CDL	CB3-OB5-PB2-OB3
11	U	403	CDL	OB7-CB5-OB6-CB4
11	V	406	CDL	OB6-CB4-CB6-OB8
11	Y	501	CDL	CA2-C1-CB2-OB2
11	Y	501	CDL	C51-CB5-OB6-CB4
12	C	301	3PE	C1-O11-P-O13
12	C	301	3PE	C11-O13-P-O11
12	C	301	3PE	C11-O13-P-O14
12	C	301	3PE	O22-C21-O21-C2
12	C	301	3PE	C22-C21-O21-C2
12	L	501	3PE	O22-C21-O21-C2
12	L	501	3PE	C22-C21-O21-C2
12	V	405	3PE	C11-O13-P-O12
12	V	405	3PE	C11-O13-P-O14
12	V	405	3PE	C12-C11-O13-P
12	V	405	3PE	O13-C11-C12-N
12	Y	502	3PE	C11-O13-P-O11
12	Y	502	3PE	C11-O13-P-O14
12	Y	502	3PE	O22-C21-O21-C2
12	Y	502	3PE	C22-C21-O21-C2
14	D	101	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
14	D	101	PLX	N1-C1-C2-O1
15	H	401	HEC	C2B-C3B-CAB-CBB
15	H	401	HEC	C4B-C3B-CAB-CBB
15	H	401	HEC	C2C-C3C-CAC-CBC
15	H	401	HEC	C4C-C3C-CAC-CBC
15	U	402	HEC	C1A-C2A-CAA-CBA
15	U	402	HEC	C3A-C2A-CAA-CBA
15	U	402	HEC	C2B-C3B-CAB-CBB
15	U	402	HEC	C4B-C3B-CAB-CBB
15	U	402	HEC	C2C-C3C-CAC-CBC
15	U	402	HEC	C4C-C3C-CAC-CBC
15	U	402	HEC	C3D-CAD-CBD-CGD
17	J	403	PEE	C1-O3P-P-O1P
17	J	403	PEE	C1-O3P-P-O4P
18	J	406	U10	C21-C22-C23-C24
18	J	406	U10	C37-C38-C39-C40
18	V	403	U10	C19-C21-C22-C23
18	V	403	U10	C47-C48-C49-C51
18	V	404	U10	C1-C6-C7-C8
18	V	404	U10	C5-C6-C7-C8
19	P	302	PC1	C1-O11-P-O12
19	P	302	PC1	C1-O11-P-O13
19	P	302	PC1	C2-C1-O11-P
11	G	101	CDL	OB9-CB7-OB8-CB6
11	Y	501	CDL	OA9-CA7-OA8-CA6
11	Y	501	CDL	OB9-CB7-OB8-CB6
11	G	101	CDL	C71-CB7-OB8-CB6
11	Y	501	CDL	C31-CA7-OA8-CA6
11	Y	501	CDL	C71-CB7-OB8-CB6
11	V	406	CDL	OB9-CB7-OB8-CB6
11	H	402	CDL	OB7-CB5-OB6-CB4
11	T	101	CDL	OA7-CA5-OA6-CA4
11	V	406	CDL	C71-CB7-OB8-CB6
11	J	404	CDL	C51-CB5-OB6-CB4
11	T	101	CDL	C51-CB5-OB6-CB4
11	U	403	CDL	C51-CB5-OB6-CB4
18	J	405	U10	C17-C18-C19-C20
11	Y	501	CDL	OB7-CB5-OB6-CB4
11	J	407	CDL	O1-C1-CA2-OA2
12	C	301	3PE	C32-C31-O31-C3
11	A	101	CDL	C51-CB5-OB6-CB4
18	J	406	U10	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
18	J	406	U10	C43-C44-C46-C47
18	V	403	U10	C23-C24-C26-C27
18	J	405	U10	C9-C11-C12-C13
18	J	405	U10	C14-C16-C17-C18
18	J	405	U10	C19-C21-C22-C23
18	J	405	U10	C24-C26-C27-C28
18	J	405	U10	C39-C41-C42-C43
18	J	405	U10	C44-C46-C47-C48
18	J	405	U10	C49-C51-C52-C53
18	J	406	U10	C24-C26-C27-C28
18	J	406	U10	C34-C36-C37-C38
18	V	403	U10	C29-C31-C32-C33
18	V	404	U10	C39-C41-C42-C43
11	T	101	CDL	CA4-CA3-OA5-PA1
18	V	403	U10	C37-C38-C39-C41
11	G	101	CDL	C11-CA5-OA6-CA4
12	U	401	3PE	C2-C3-O31-C31
12	C	301	3PE	O32-C31-O31-C3
11	V	406	CDL	CA2-C1-CB2-OB2
11	V	406	CDL	C72-C73-C74-C75
18	V	403	U10	C25-C24-C26-C27
11	G	101	CDL	O1-C1-CB2-OB2
11	Y	501	CDL	O1-C1-CB2-OB2
11	A	101	CDL	OB7-CB5-OB6-CB4
18	V	403	U10	C47-C48-C49-C50
18	J	405	U10	C34-C36-C37-C38
18	V	403	U10	C39-C41-C42-C43
11	V	406	CDL	CB7-C71-C72-C73
11	A	101	CDL	C1-CA2-OA2-PA1
11	G	101	CDL	CB7-C71-C72-C73
11	V	406	CDL	O1-C1-CB2-OB2
11	G	101	CDL	OA7-CA5-OA6-CA4
11	H	402	CDL	CB5-C51-C52-C53
18	V	404	U10	C46-C47-C48-C49
11	J	407	CDL	C31-CA7-OA8-CA6
11	Y	501	CDL	C11-CA5-OA6-CA4
11	Y	501	CDL	OA7-CA5-OA6-CA4
18	V	404	U10	C34-C36-C37-C38
11	G	101	CDL	CA4-CA3-OA5-PA1
11	U	403	CDL	C11-CA5-OA6-CA4
12	U	401	3PE	C32-C31-O31-C3
11	G	101	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
17	J	403	PEE	C40-C41-C42-C43
11	H	402	CDL	C31-CA7-OA8-CA6
19	P	302	PC1	C38-C39-C3A-C3B
11	G	101	CDL	C11-C12-C13-C14
14	D	101	PLX	C11-C10-C9-C8
11	G	101	CDL	C51-C52-C53-C54
11	G	101	CDL	CA5-C11-C12-C13
14	D	101	PLX	C25-C26-C27-C28
11	J	404	CDL	C11-CA5-OA6-CA4
11	Y	501	CDL	CB4-CB3-OB5-PB2
11	J	407	CDL	OA9-CA7-OA8-CA6
11	U	403	CDL	OA7-CA5-OA6-CA4
11	H	402	CDL	C71-CB7-OB8-CB6
11	J	404	CDL	C31-CA7-OA8-CA6
11	H	402	CDL	OA9-CA7-OA8-CA6
11	G	101	CDL	CB5-C51-C52-C53
16	V	401	HEM	C4D-C3D-CAD-CBD
14	T	102	PLX	C25-C26-C27-C28
18	V	404	U10	C41-C42-C43-C44
12	U	401	3PE	O32-C31-O31-C3
18	J	406	U10	C12-C13-C14-C16
11	J	404	CDL	OA7-CA5-OA6-CA4
11	G	101	CDL	OB5-CB3-CB4-OB6
12	U	401	3PE	C22-C23-C24-C25
19	P	302	PC1	C39-C3A-C3B-C3C
18	J	405	U10	C29-C31-C32-C33
11	V	406	CDL	C51-CB5-OB6-CB4
12	L	501	3PE	C32-C31-O31-C3
18	J	406	U10	C26-C27-C28-C29
11	J	407	CDL	CB2-C1-CA2-OA2
11	T	101	CDL	C71-C72-C73-C74
11	J	404	CDL	CA4-CA6-OA8-CA7
11	H	402	CDL	OB9-CB7-OB8-CB6
11	G	101	CDL	OA5-CA3-CA4-CA6
12	V	405	3PE	C22-C21-O21-C2
11	G	101	CDL	CA3-CA4-CA6-OA8
11	V	406	CDL	CB3-CB4-CB6-OB8
12	U	401	3PE	C1-C2-C3-O31
11	A	101	CDL	C31-CA7-OA8-CA6
11	H	402	CDL	CA7-C31-C32-C33
11	J	404	CDL	OA9-CA7-OA8-CA6
18	J	406	U10	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
11	V	406	CDL	CA4-CA3-OA5-PA1
12	U	401	3PE	C33-C34-C35-C36
11	T	101	CDL	C31-C32-C33-C34
12	L	501	3PE	O32-C31-O31-C3
12	V	405	3PE	C32-C31-O31-C3
11	V	406	CDL	C75-C76-C77-C78
18	J	406	U10	C7-C8-C9-C10
12	C	301	3PE	C2-C1-O11-P
16	V	401	HEM	C2D-C3D-CAD-CBD
11	G	101	CDL	OB5-CB3-CB4-CB6
17	J	403	PEE	O3P-C1-C2-C3
11	V	406	CDL	C52-C53-C54-C55
12	C	301	3PE	C21-C22-C23-C24
11	A	101	CDL	OA9-CA7-OA8-CA6
12	V	405	3PE	C26-C27-C28-C29
11	J	404	CDL	CA3-CA4-CA6-OA8
19	P	302	PC1	C3D-C3E-C3F-C3G
11	J	404	CDL	C11-C12-C13-C14
18	V	403	U10	C46-C47-C48-C49
11	Y	501	CDL	OA5-CA3-CA4-OA6
17	J	403	PEE	O3P-C1-C2-O2
11	U	403	CDL	C1-CA2-OA2-PA1
16	V	402	HEM	C2A-CAA-CBA-CGA
11	U	403	CDL	C31-C32-C33-C34
18	J	406	U10	C14-C16-C17-C18
17	J	403	PEE	C38-C39-C40-C41
11	T	101	CDL	OB5-CB3-CB4-CB6
18	J	405	U10	C36-C37-C38-C39
18	V	403	U10	C36-C37-C38-C39
11	G	101	CDL	C72-C73-C74-C75
12	V	405	3PE	O32-C31-O31-C3
11	V	406	CDL	OB7-CB5-OB6-CB4
12	V	405	3PE	O22-C21-O21-C2
11	Y	501	CDL	CA7-C31-C32-C33
11	Y	501	CDL	CB6-CB4-OB6-CB5
11	G	101	CDL	C74-C75-C76-C77
11	G	101	CDL	C55-C56-C57-C58
16	J	402	HEM	C4B-C3B-CAB-CBB
16	J	402	HEM	C4C-C3C-CAC-CBC
16	V	401	HEM	C4C-C3C-CAC-CBC
16	V	402	HEM	C4B-C3B-CAB-CBB
16	V	402	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
12	L	501	3PE	C12-C11-O13-P
12	Y	502	3PE	C12-C11-O13-P
11	J	404	CDL	OA6-CA4-CA6-OA8
12	U	401	3PE	O21-C2-C3-O31
14	T	102	PLX	N1-C1-C2-O1
11	G	101	CDL	C33-C34-C35-C36
14	D	101	PLX	C13-C14-C15-C16
11	H	402	CDL	C32-C33-C34-C35
11	J	404	CDL	OB5-CB3-CB4-CB6
11	A	101	CDL	C12-C13-C14-C15
11	G	101	CDL	C31-C32-C33-C34
17	J	403	PEE	C16-C17-C18-C19
11	H	402	CDL	C1-CB2-OB2-PB2
11	T	101	CDL	C1-CA2-OA2-PA1
11	J	404	CDL	OB5-CB3-CB4-OB6
11	T	101	CDL	OB5-CB3-CB4-OB6
11	V	406	CDL	C71-C72-C73-C74
11	V	406	CDL	C74-C75-C76-C77
12	C	303	3PE	C1-C2-C3-O31
11	J	404	CDL	C31-C32-C33-C34
11	T	101	CDL	C14-C15-C16-C17
11	V	406	CDL	C32-C33-C34-C35
11	A	101	CDL	CA2-OA2-PA1-OA3
11	A	101	CDL	CA3-OA5-PA1-OA4
11	A	101	CDL	CB2-OB2-PB2-OB3
11	H	402	CDL	CA3-OA5-PA1-OA4
11	H	402	CDL	CB3-OB5-PB2-OB3
11	J	404	CDL	CB2-OB2-PB2-OB5
11	J	407	CDL	CA2-OA2-PA1-OA5
11	J	407	CDL	CB2-OB2-PB2-OB4
11	T	101	CDL	CB2-OB2-PB2-OB3
11	T	101	CDL	CB2-OB2-PB2-OB5
11	V	406	CDL	CA3-OA5-PA1-OA3
11	V	406	CDL	CB3-OB5-PB2-OB3
12	C	301	3PE	C1-O11-P-O14
12	L	501	3PE	C11-O13-P-O11
12	L	501	3PE	C11-O13-P-O12
12	L	501	3PE	C11-O13-P-O14
12	V	405	3PE	C11-O13-P-O11
12	Y	502	3PE	C1-O11-P-O14
14	T	102	PLX	C3-O4-P1-O2
14	T	102	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
19	P	302	PC1	C1-O11-P-O14
18	J	405	U10	C37-C38-C39-C40
18	J	405	U10	C15-C14-C16-C17
11	A	101	CDL	CB4-CB3-OB5-PB2
11	J	404	CDL	CB4-CB3-OB5-PB2
11	T	101	CDL	C1-CB2-OB2-PB2
11	V	406	CDL	C1-CB2-OB2-PB2
12	V	405	3PE	C2-C1-O11-P
12	U	401	3PE	C31-C32-C33-C34
11	G	101	CDL	C34-C35-C36-C37
11	T	101	CDL	C73-C74-C75-C76
11	V	406	CDL	OB5-CB3-CB4-CB6
11	G	101	CDL	OA5-CA3-CA4-OA6
11	H	402	CDL	OA5-CA3-CA4-OA6
18	J	406	U10	C5-C4-O4-C4M
12	C	303	3PE	O21-C2-C3-O31
11	V	406	CDL	C11-C12-C13-C14
11	T	101	CDL	C51-C52-C53-C54
18	V	404	U10	C31-C32-C33-C34
12	C	303	3PE	C22-C21-O21-C2
11	G	101	CDL	C73-C74-C75-C76
11	J	407	CDL	CA4-CA3-OA5-PA1
18	V	404	U10	C5-C4-O4-C4M
12	U	401	3PE	C2C-C2D-C2E-C2F
18	J	405	U10	C12-C11-C9-C10
18	J	405	U10	C20-C19-C21-C22
18	V	403	U10	C35-C34-C36-C37
18	V	403	U10	C38-C39-C41-C42
18	V	403	U10	C48-C49-C51-C52
18	V	403	U10	C14-C16-C17-C18
12	C	303	3PE	C22-C23-C24-C25
18	V	403	U10	C50-C49-C51-C52
18	V	404	U10	C25-C24-C26-C27
14	T	102	PLX	C18-C19-C20-C21
18	V	403	U10	C40-C39-C41-C42
18	V	404	U10	C30-C29-C31-C32
16	J	401	HEM	C3D-CAD-CBD-CGD
18	J	405	U10	C13-C14-C16-C17
18	V	404	U10	C44-C46-C47-C48
15	U	402	HEC	CAD-CBD-CGD-O1D
12	C	301	3PE	C32-C33-C34-C35
18	V	404	U10	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	U	402	HEC	CAD-CBD-CGD-O2D
12	U	401	3PE	C35-C36-C37-C38
17	J	403	PEE	C12-C13-C14-C15
16	J	401	HEM	C1A-C2A-CAA-CBA
11	Y	501	CDL	C71-C72-C73-C74
18	J	406	U10	C30-C29-C31-C32
18	V	403	U10	C33-C34-C36-C37
18	V	404	U10	C28-C29-C31-C32
11	G	101	CDL	C32-C33-C34-C35
18	V	403	U10	C11-C12-C13-C14
18	V	403	U10	C41-C42-C43-C44
12	C	303	3PE	O22-C21-O21-C2
18	V	404	U10	C26-C27-C28-C29
18	J	405	U10	C12-C11-C9-C8
18	J	406	U10	C13-C14-C16-C17
18	V	404	U10	C23-C24-C26-C27
11	J	404	CDL	C35-C36-C37-C38
11	J	404	CDL	C73-C74-C75-C76
19	P	302	PC1	C3A-C3B-C3C-C3D
18	V	404	U10	C36-C37-C38-C39
18	J	406	U10	C40-C39-C41-C42
14	D	101	PLX	C9-C10-C11-C12
16	V	401	HEM	CAA-CBA-CGA-O2A
11	T	101	CDL	C13-C14-C15-C16
11	H	402	CDL	CA4-CA6-OA8-CA7
12	L	501	3PE	C2-C3-O31-C31
11	V	406	CDL	OB5-CB3-CB4-OB6
18	J	406	U10	C15-C14-C16-C17
11	Y	501	CDL	C32-C33-C34-C35
18	V	404	U10	C6-C7-C8-C9
16	J	402	HEM	CAD-CBD-CGD-O2D
11	J	407	CDL	CA2-C1-CB2-OB2
11	V	406	CDL	OA5-CA3-CA4-CA6
11	Y	501	CDL	OA5-CA3-CA4-CA6
14	D	101	PLX	O6-C4-C5-O8
18	V	403	U10	C21-C22-C23-C24
11	A	101	CDL	C33-C34-C35-C36
12	C	303	3PE	C33-C34-C35-C36
16	V	401	HEM	CAA-CBA-CGA-O1A
12	V	405	3PE	C24-C25-C26-C27
11	J	404	CDL	CA3-CA4-OA6-CA5
11	J	404	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
11	J	407	CDL	CB3-CB4-OB6-CB5
11	J	407	CDL	CB6-CB4-OB6-CB5
18	V	403	U10	C16-C17-C18-C19
18	V	404	U10	C51-C52-C53-C54
16	J	402	HEM	CAD-CBD-CGD-O1D
19	P	302	PC1	C32-C33-C34-C35
11	V	406	CDL	C72-C71-CB7-OB8
18	J	406	U10	C27-C28-C29-C30
18	J	405	U10	C18-C19-C21-C22
11	G	101	CDL	C35-C36-C37-C38
11	U	403	CDL	C51-C52-C53-C54
11	J	407	CDL	C13-C14-C15-C16
15	H	401	HEC	CAD-CBD-CGD-O2D
11	H	402	CDL	C11-C12-C13-C14
12	V	405	3PE	C1-C2-C3-O31
18	V	403	U10	C34-C36-C37-C38
11	A	101	CDL	CA7-C31-C32-C33
18	J	405	U10	C5-C4-O4-C4M
11	A	101	CDL	C53-C54-C55-C56
11	J	404	CDL	OB6-CB4-CB6-OB8
17	J	403	PEE	O2-C2-C3-O3
11	V	406	CDL	C14-C15-C16-C17
11	H	402	CDL	OA5-CA3-CA4-CA6
11	A	101	CDL	C34-C35-C36-C37
14	T	102	PLX	C24-C25-C26-C27
17	J	403	PEE	C1-C2-O2-C10
18	J	406	U10	C3-C4-O4-C4M
14	T	102	PLX	C26-C27-C28-C29
18	V	404	U10	C16-C17-C18-C19
11	Y	501	CDL	C33-C34-C35-C36
11	V	406	CDL	OA5-CA3-CA4-OA6
18	V	403	U10	C5-C4-O4-C4M
12	U	401	3PE	C39-C3A-C3B-C3C
14	D	101	PLX	O9-C24-O8-C5
14	T	102	PLX	O9-C24-O8-C5
15	H	401	HEC	CAD-CBD-CGD-O1D
19	P	302	PC1	C25-C26-C27-C28
16	V	402	HEM	CAA-CBA-CGA-O2A
11	V	406	CDL	C72-C71-CB7-OB9
11	H	402	CDL	CB3-CB4-CB6-OB8
18	V	403	U10	C49-C51-C52-C53
18	V	404	U10	C11-C12-C13-C14

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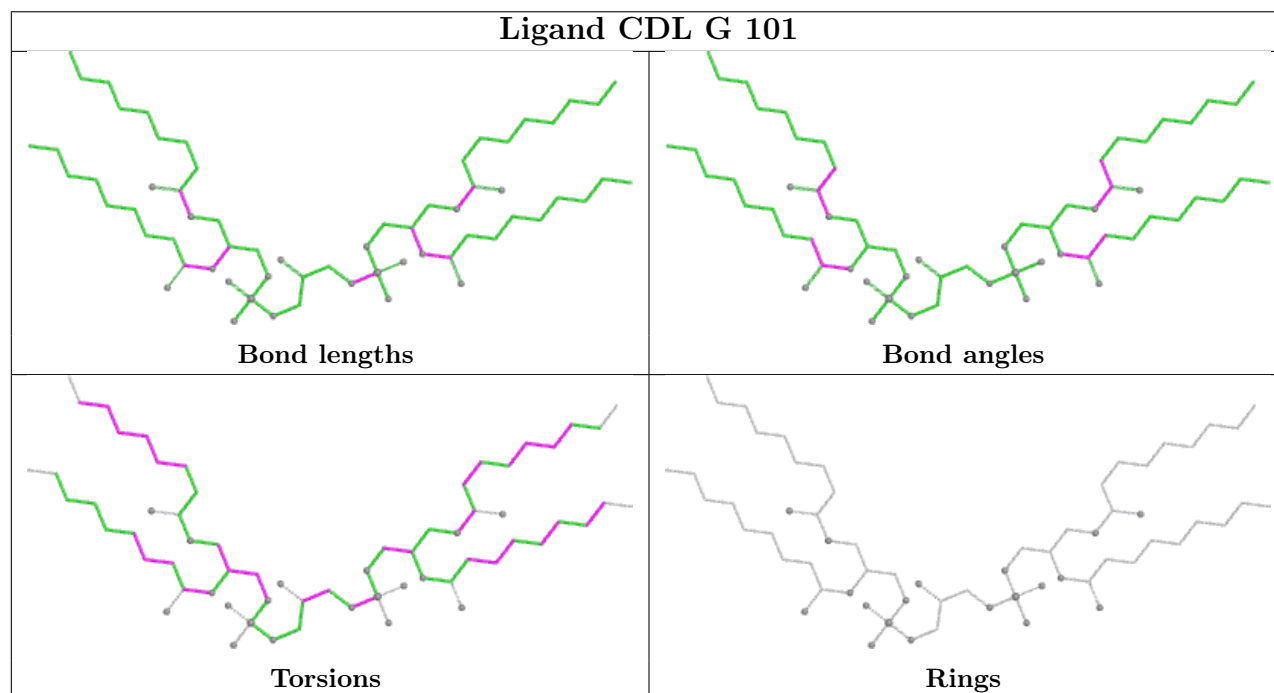
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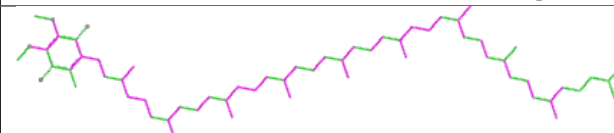
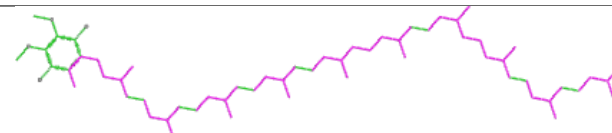
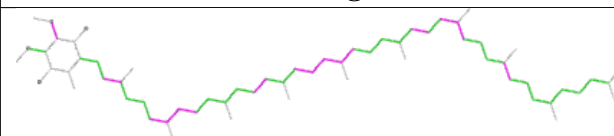
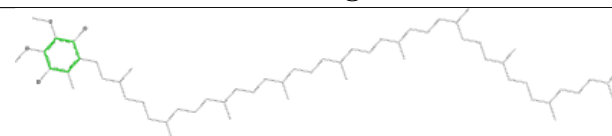
Mol	Chain	Res	Type	Atoms
12	U	401	3PE	C23-C24-C25-C26
16	V	402	HEM	CAA-CBA-CGA-O1A
18	V	403	U10	C51-C52-C53-C54
12	V	405	3PE	C33-C34-C35-C36
11	Y	501	CDL	C32-C31-CA7-OA8
11	T	101	CDL	C12-C13-C14-C15
17	J	403	PEE	C18-C19-C20-C21

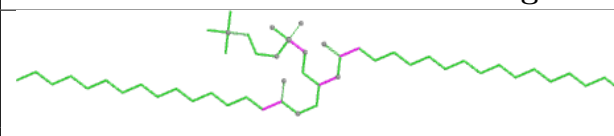
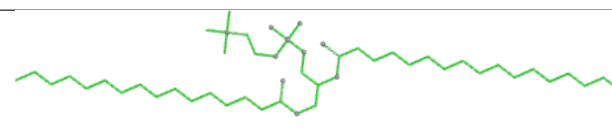
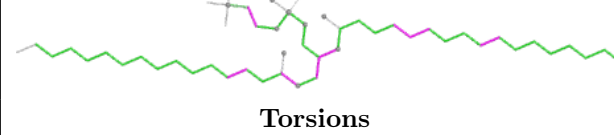
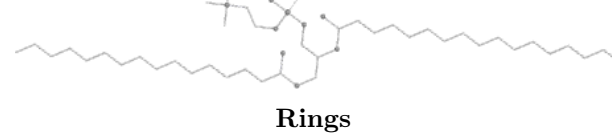
There are no ring outliers.

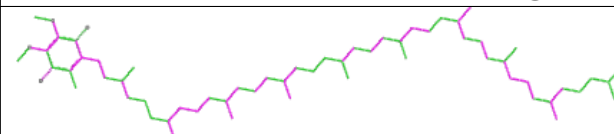
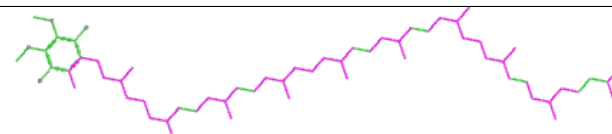
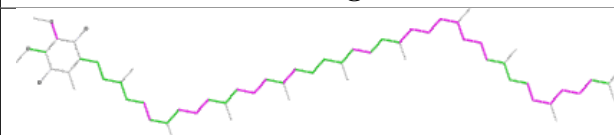
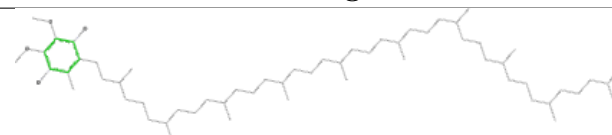
No monomer is involved in short contacts.

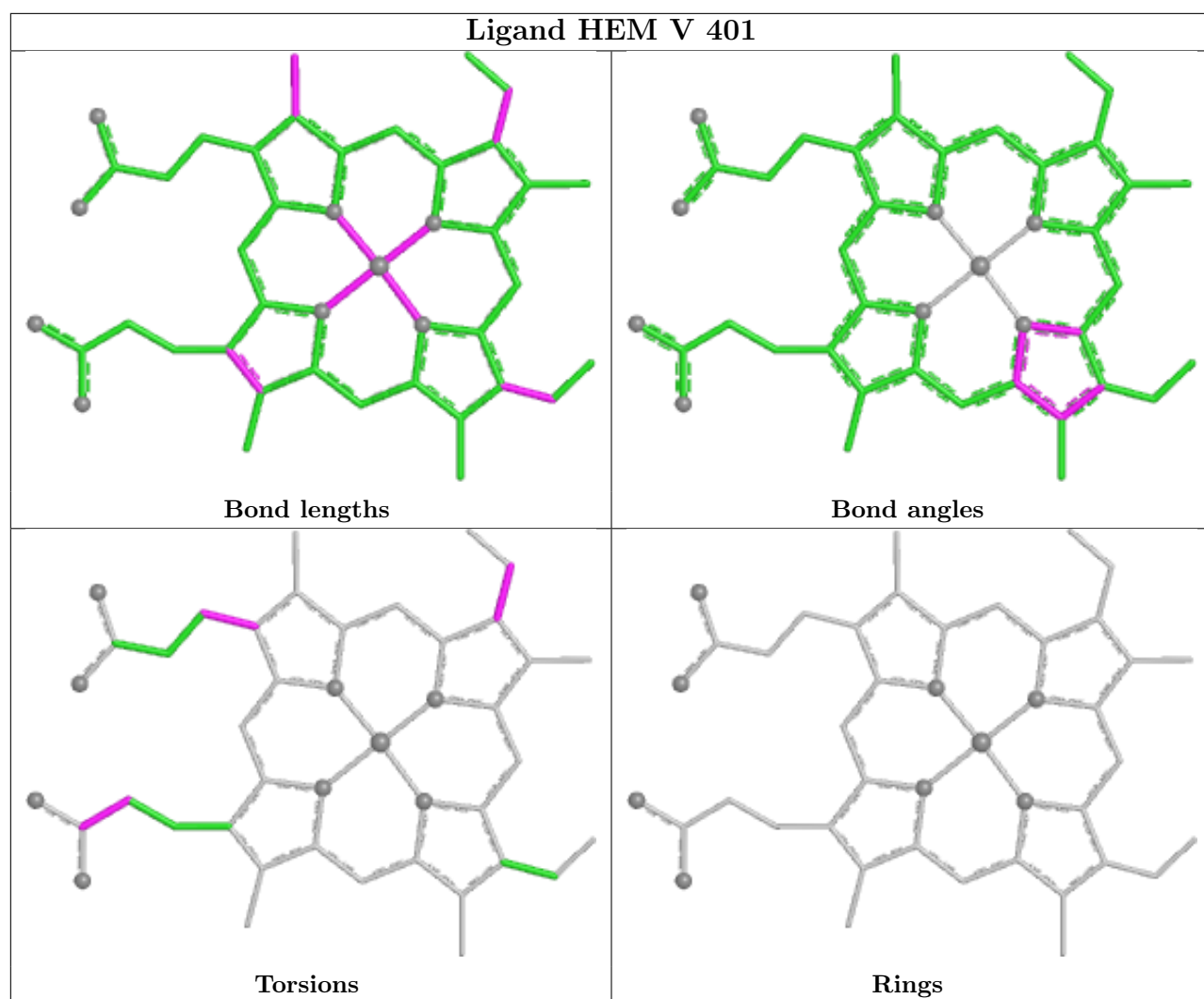
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

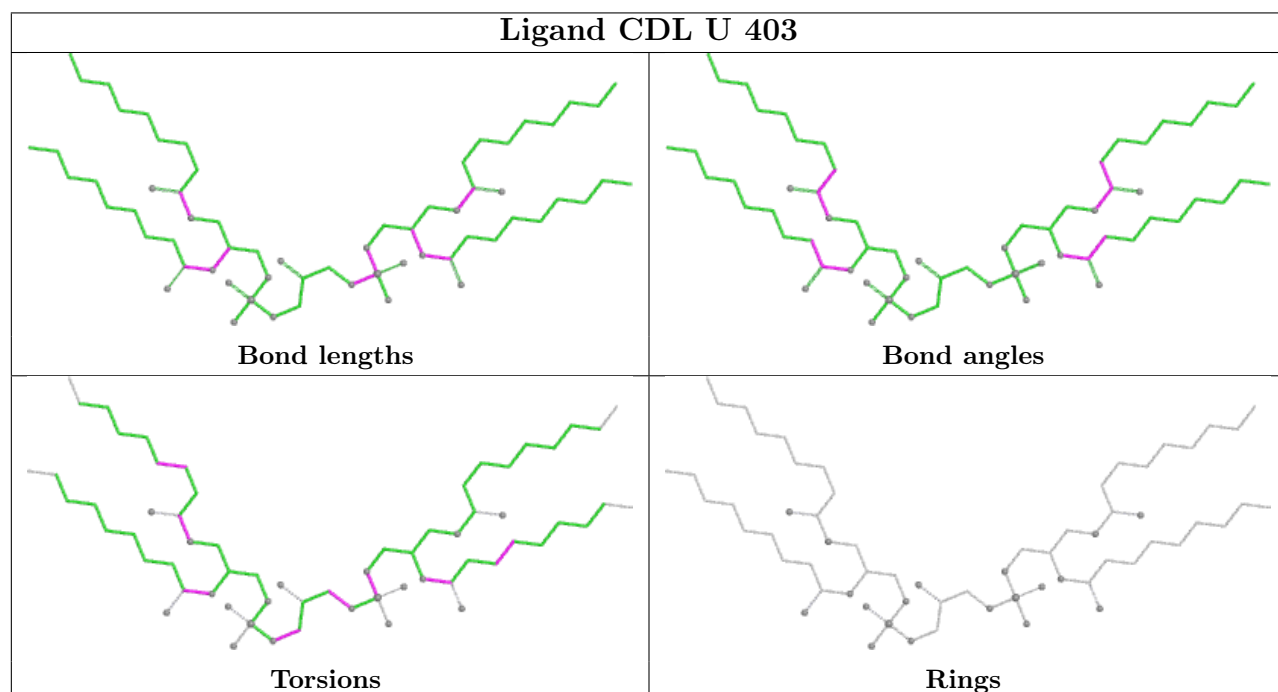
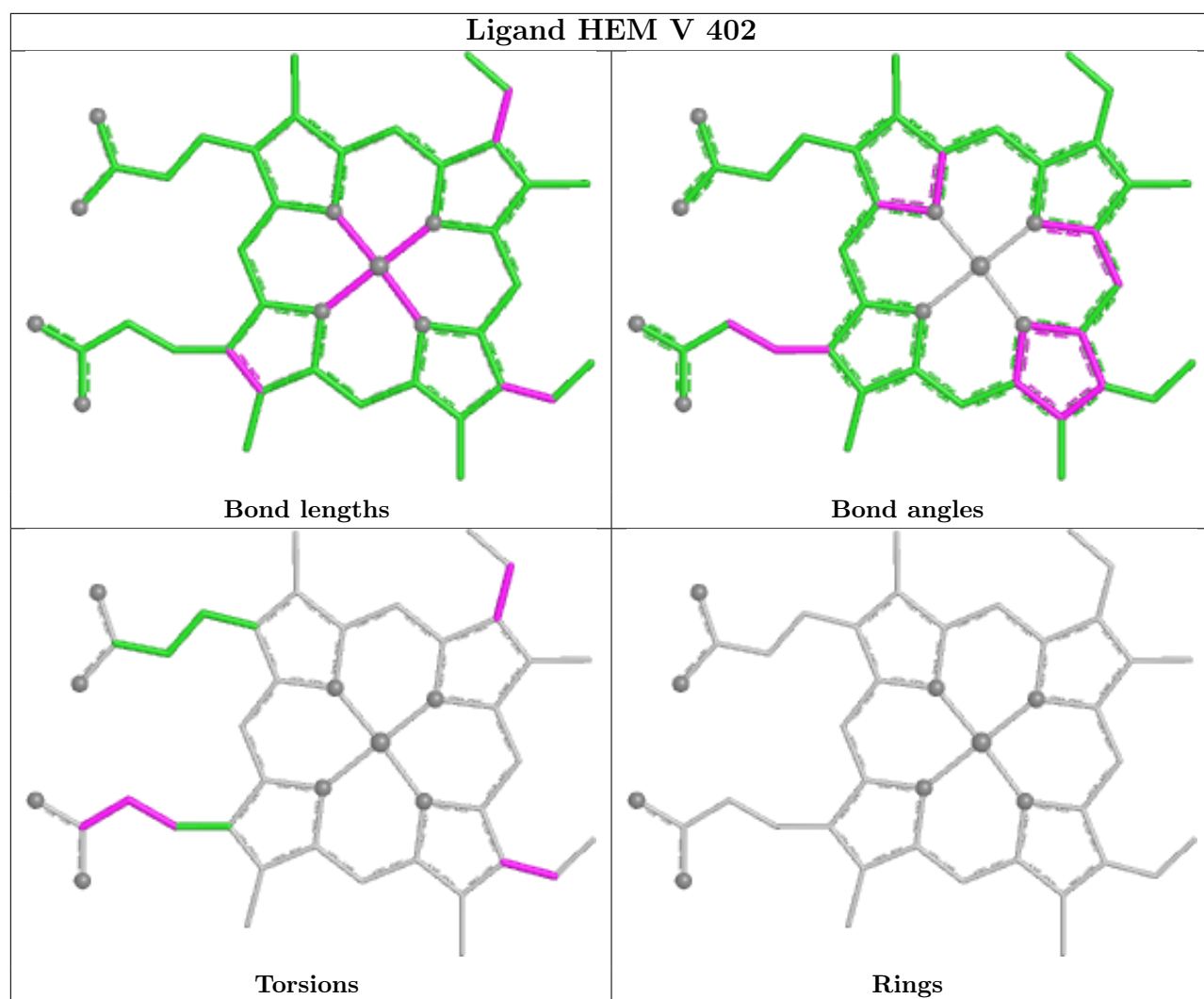


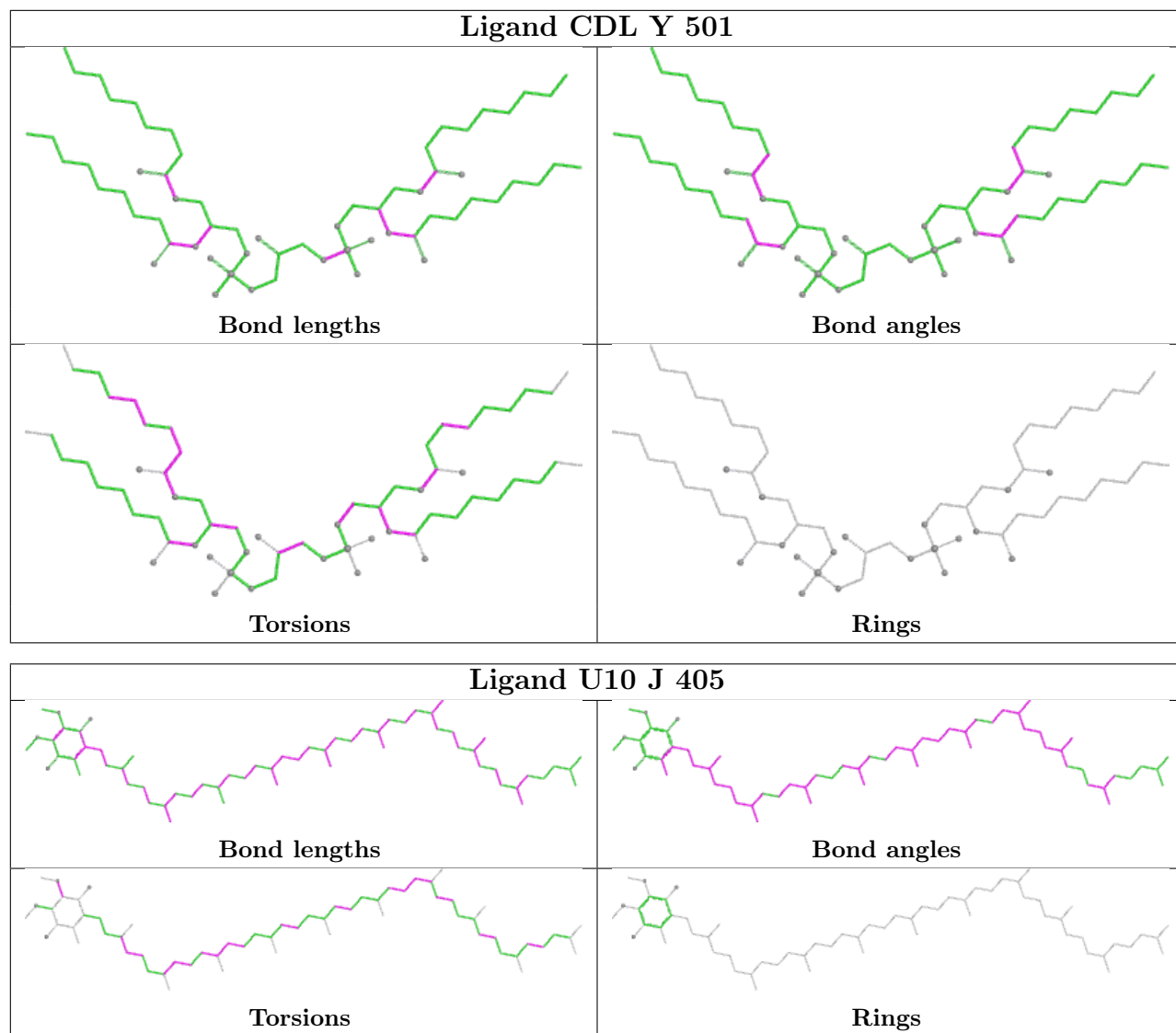
Ligand U10 J 406	
	Bond lengths
	Bond angles
	Torsions
	Rings

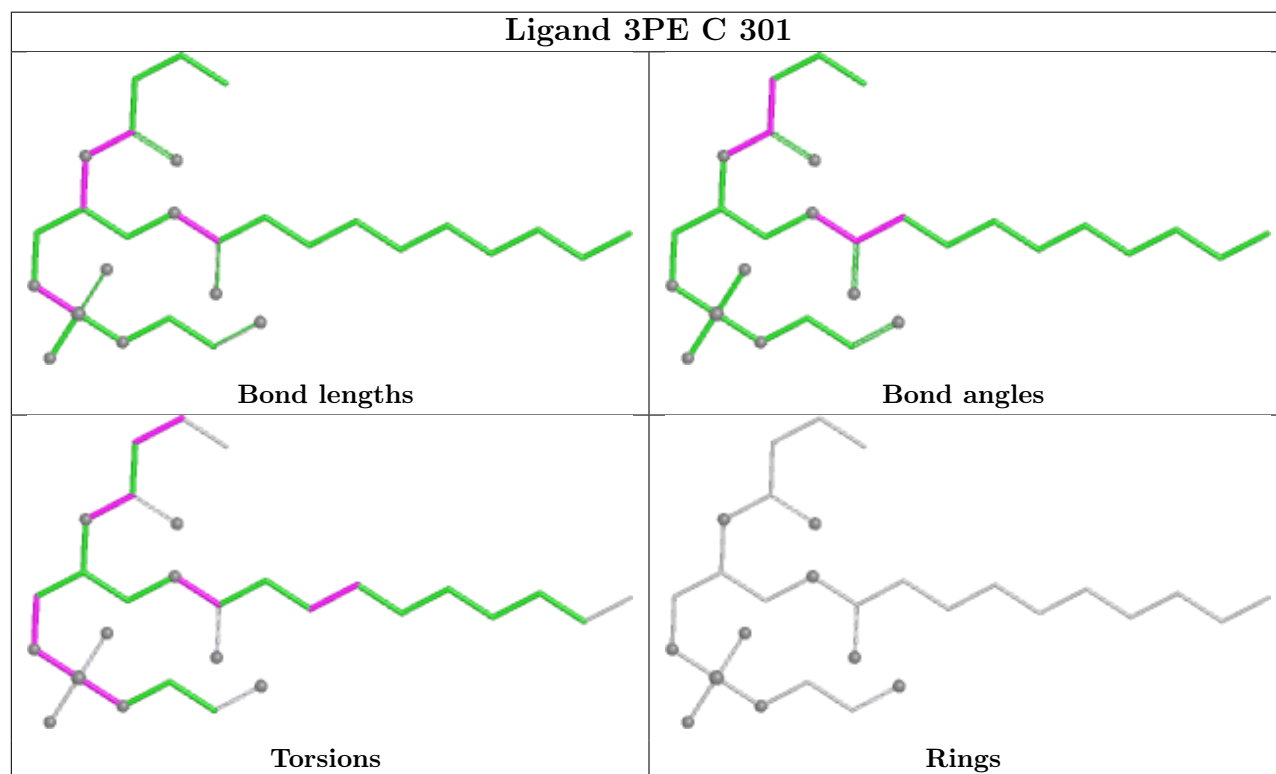
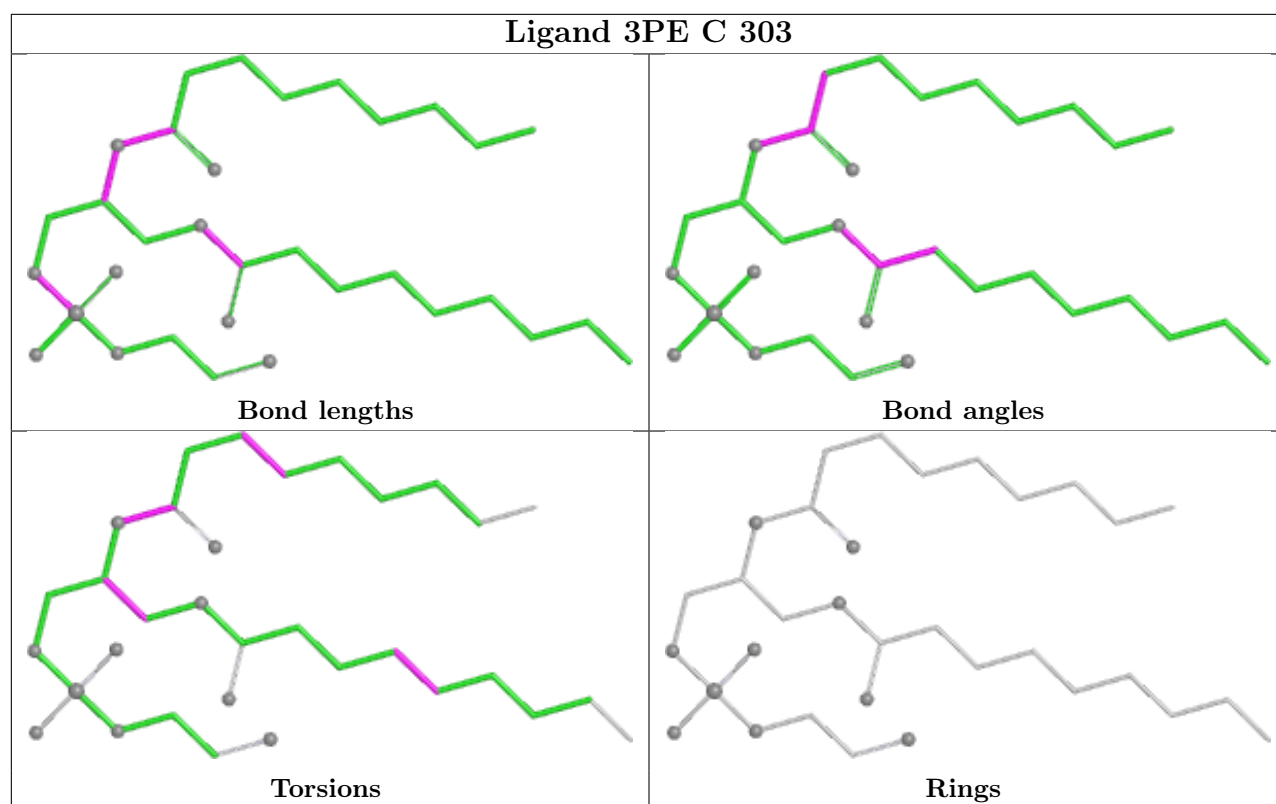
Ligand PLX D 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand U10 V 403	
	Bond lengths
	Bond angles
	Torsions
	Rings

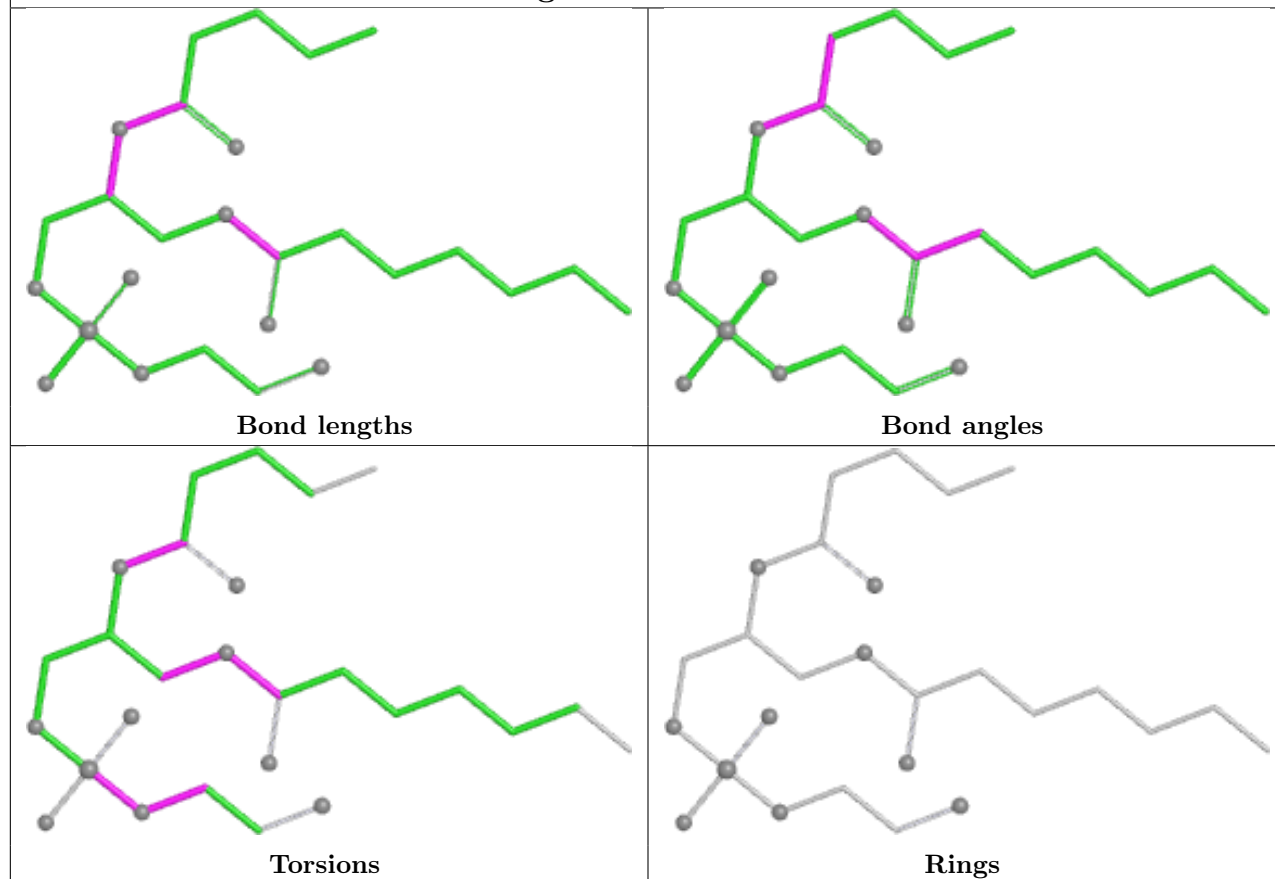




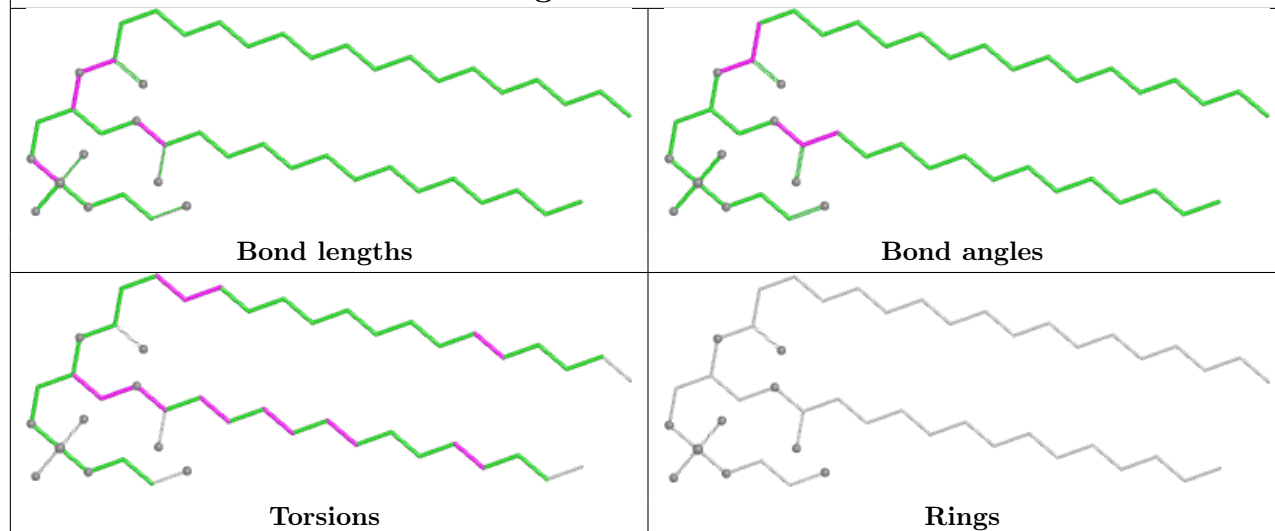


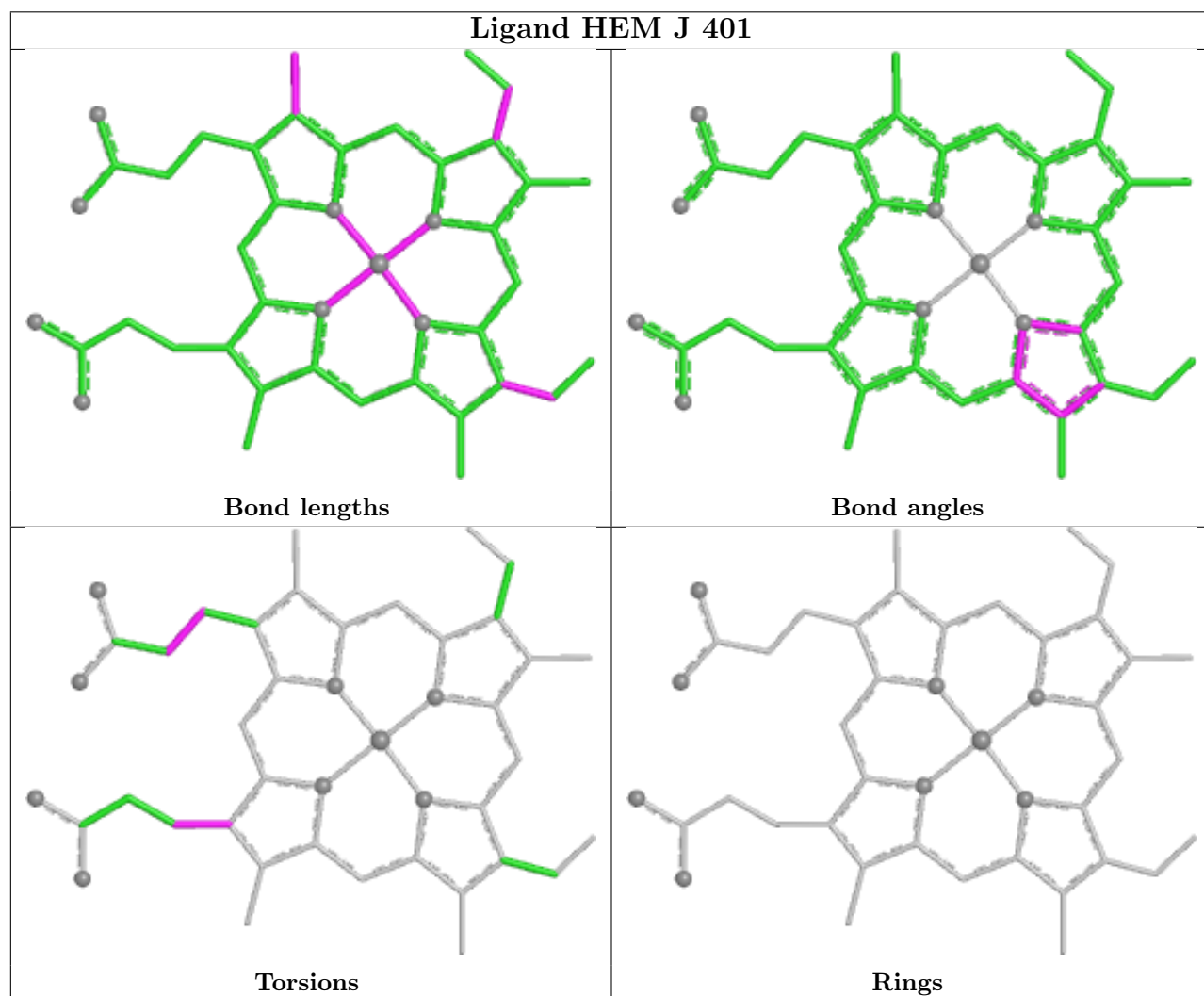
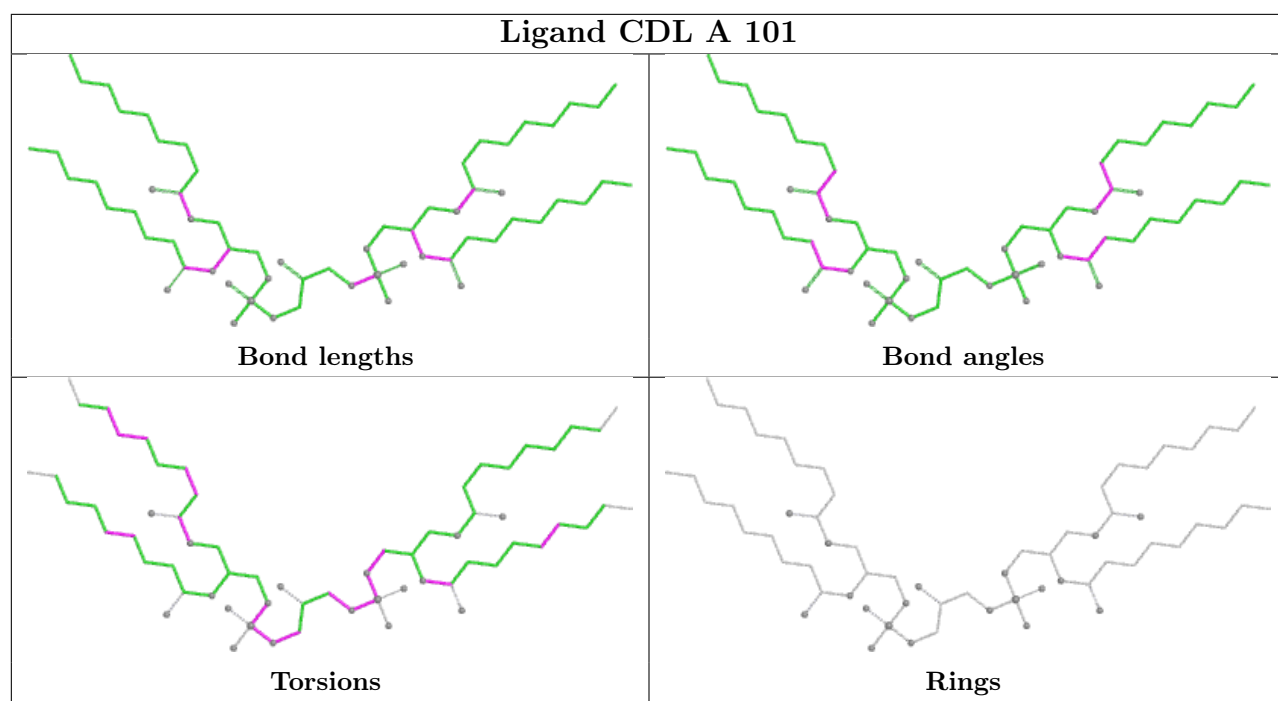


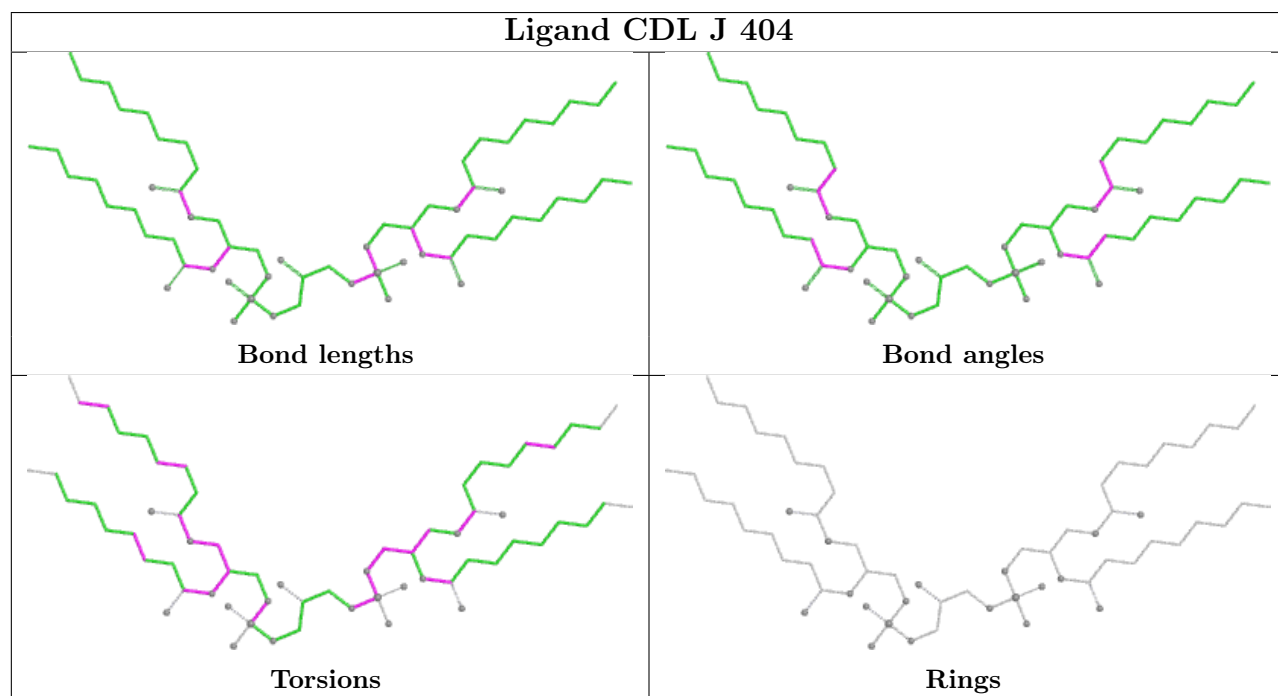
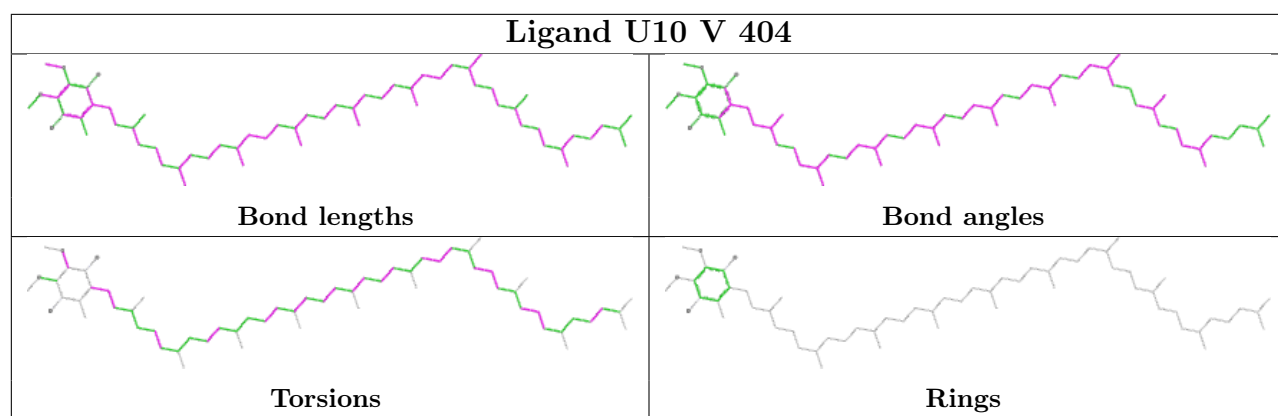
Ligand 3PE L 501

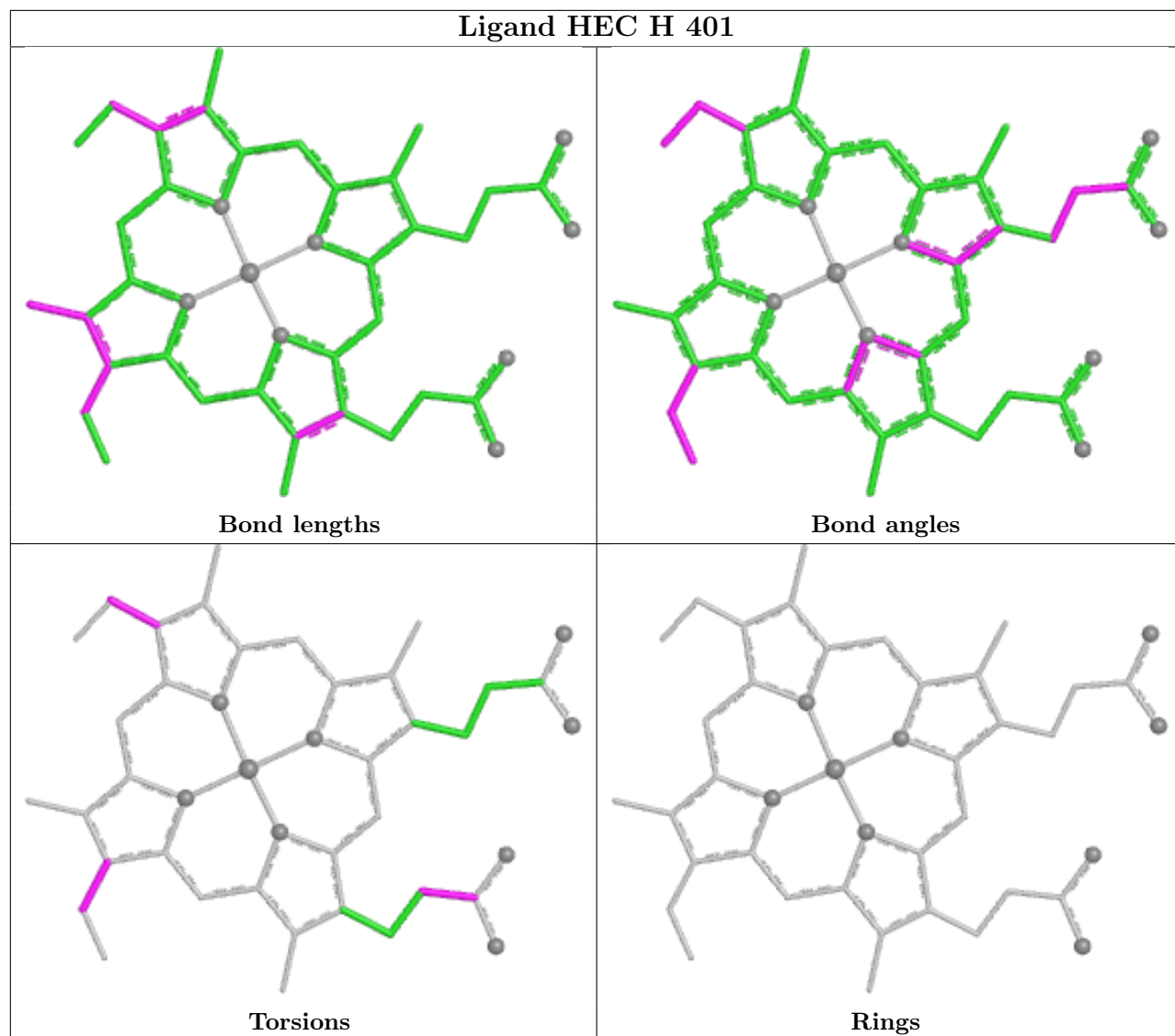


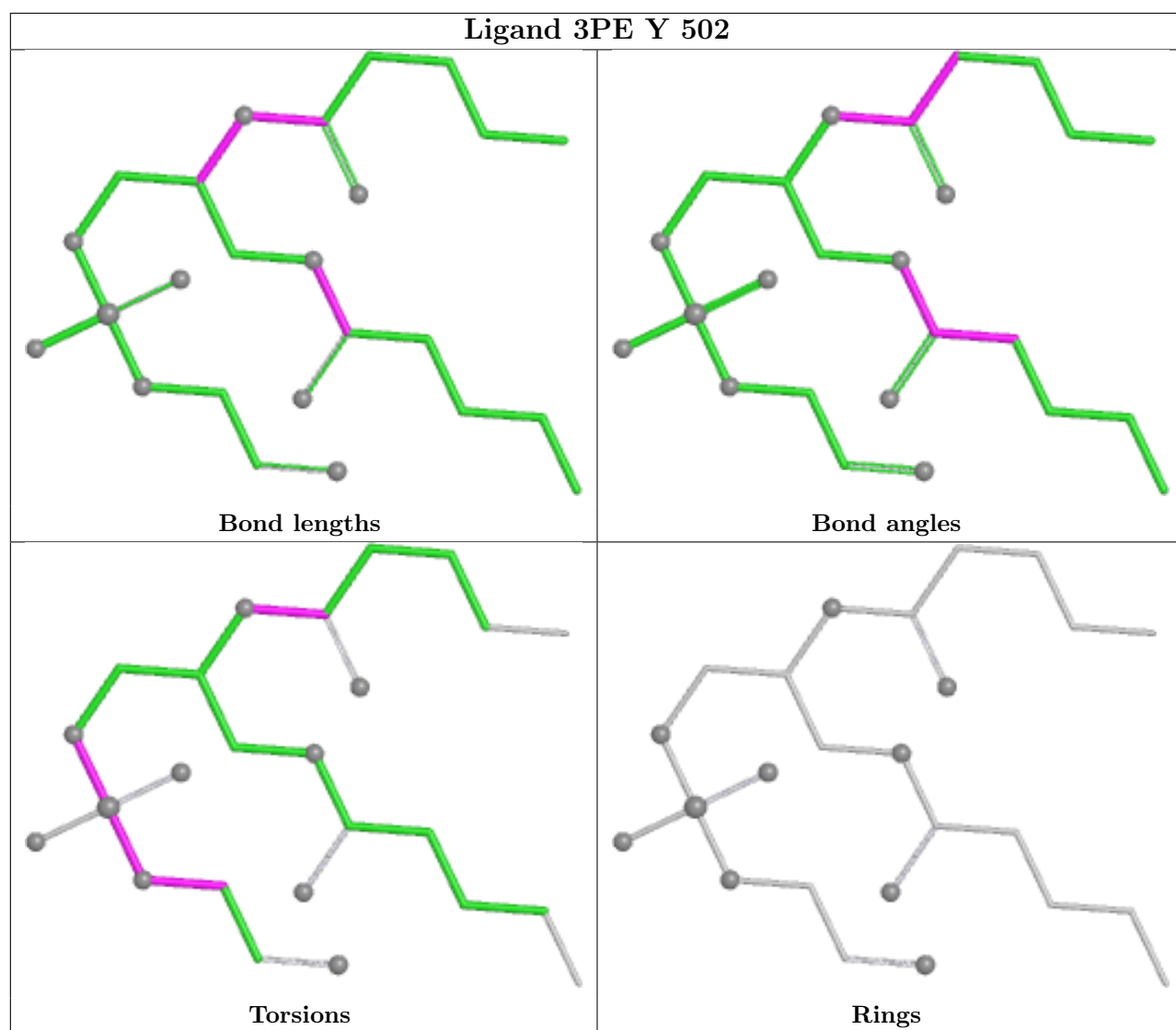
Ligand 3PE U 401

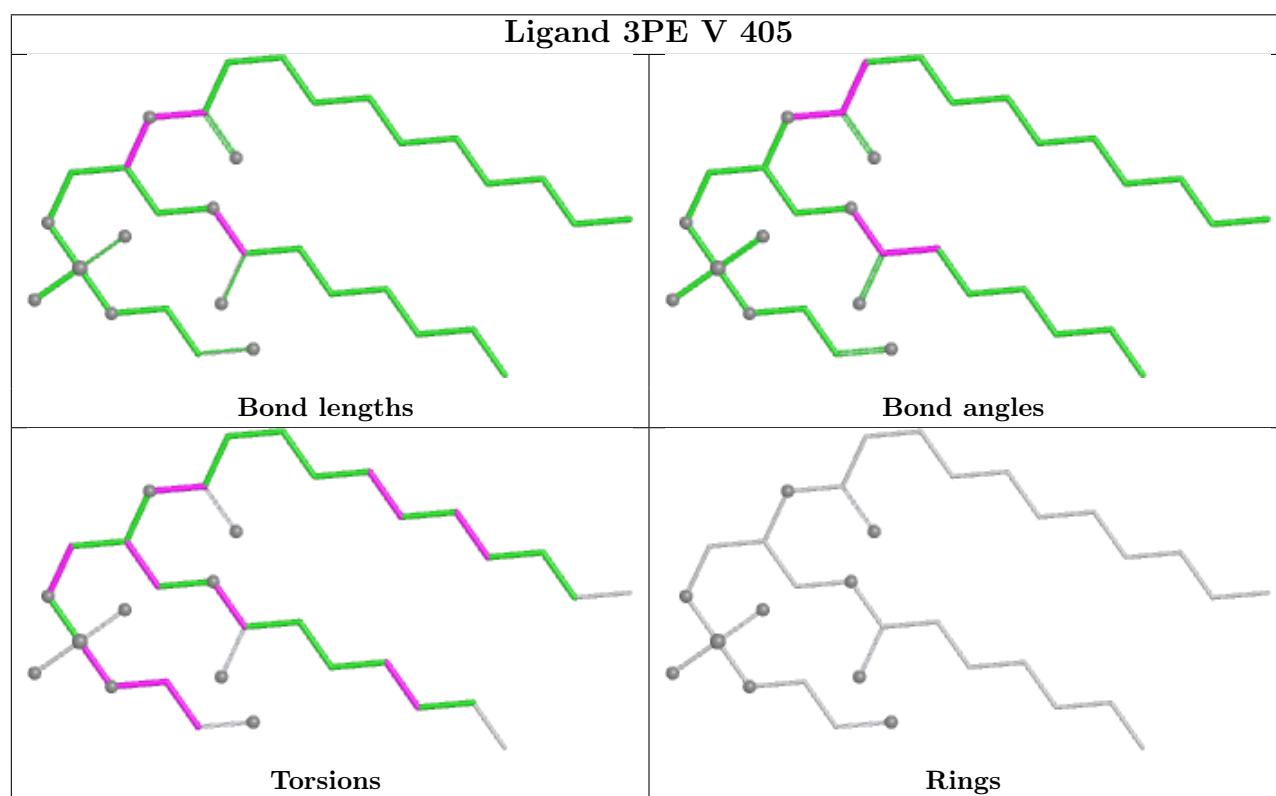
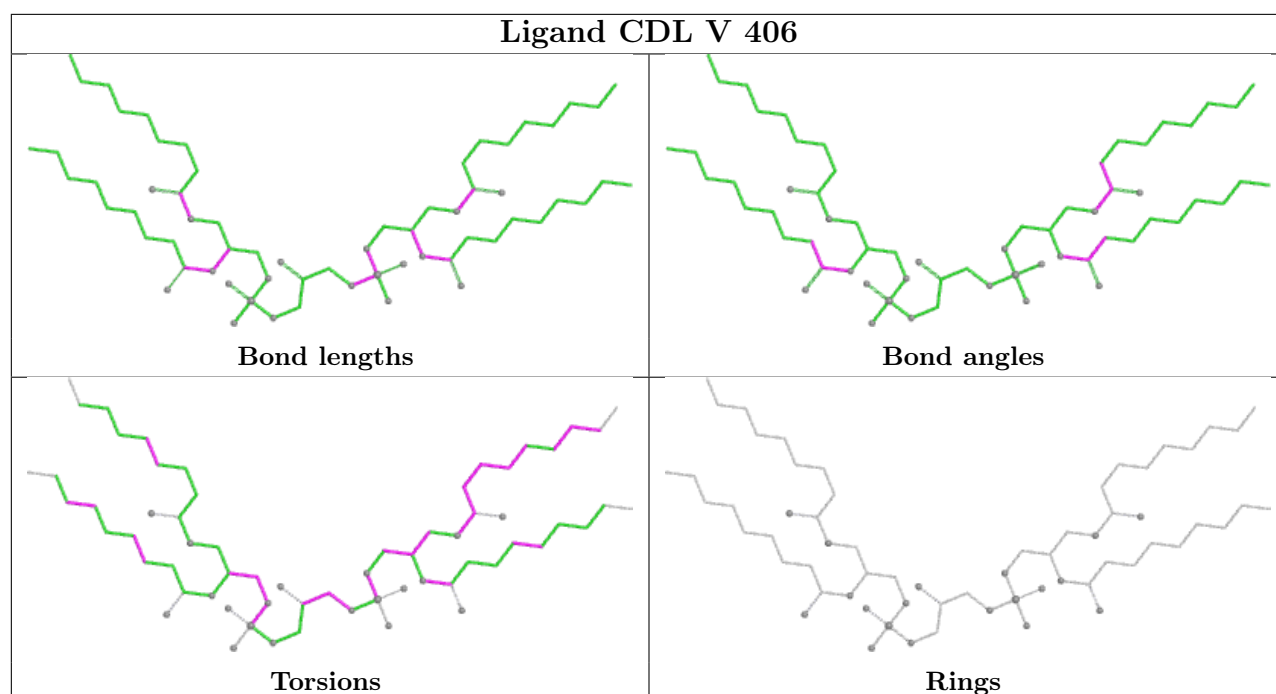


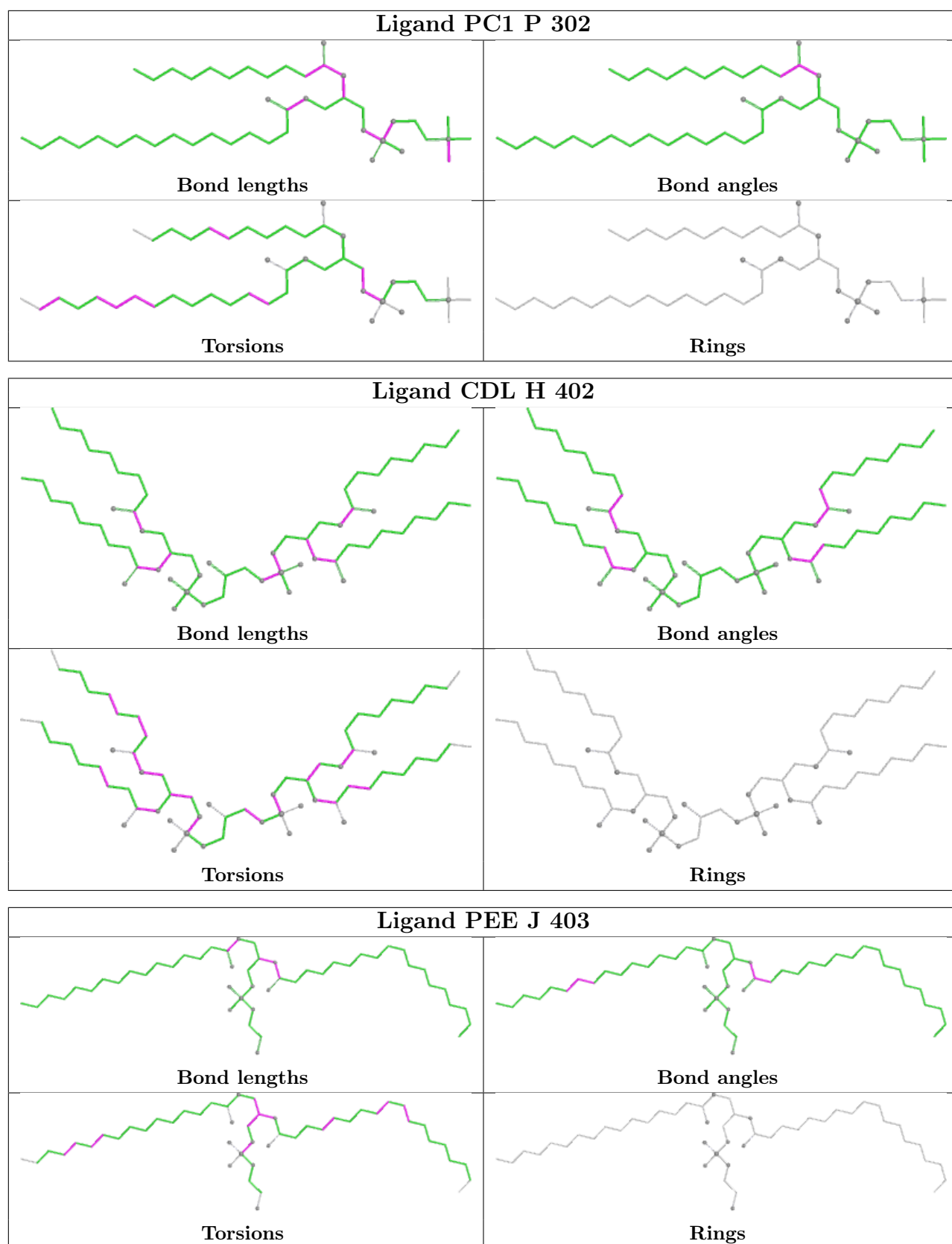




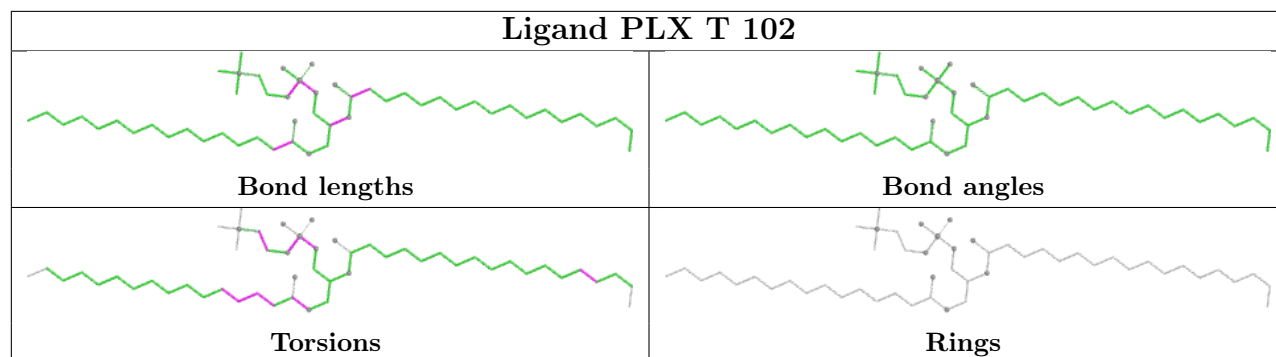




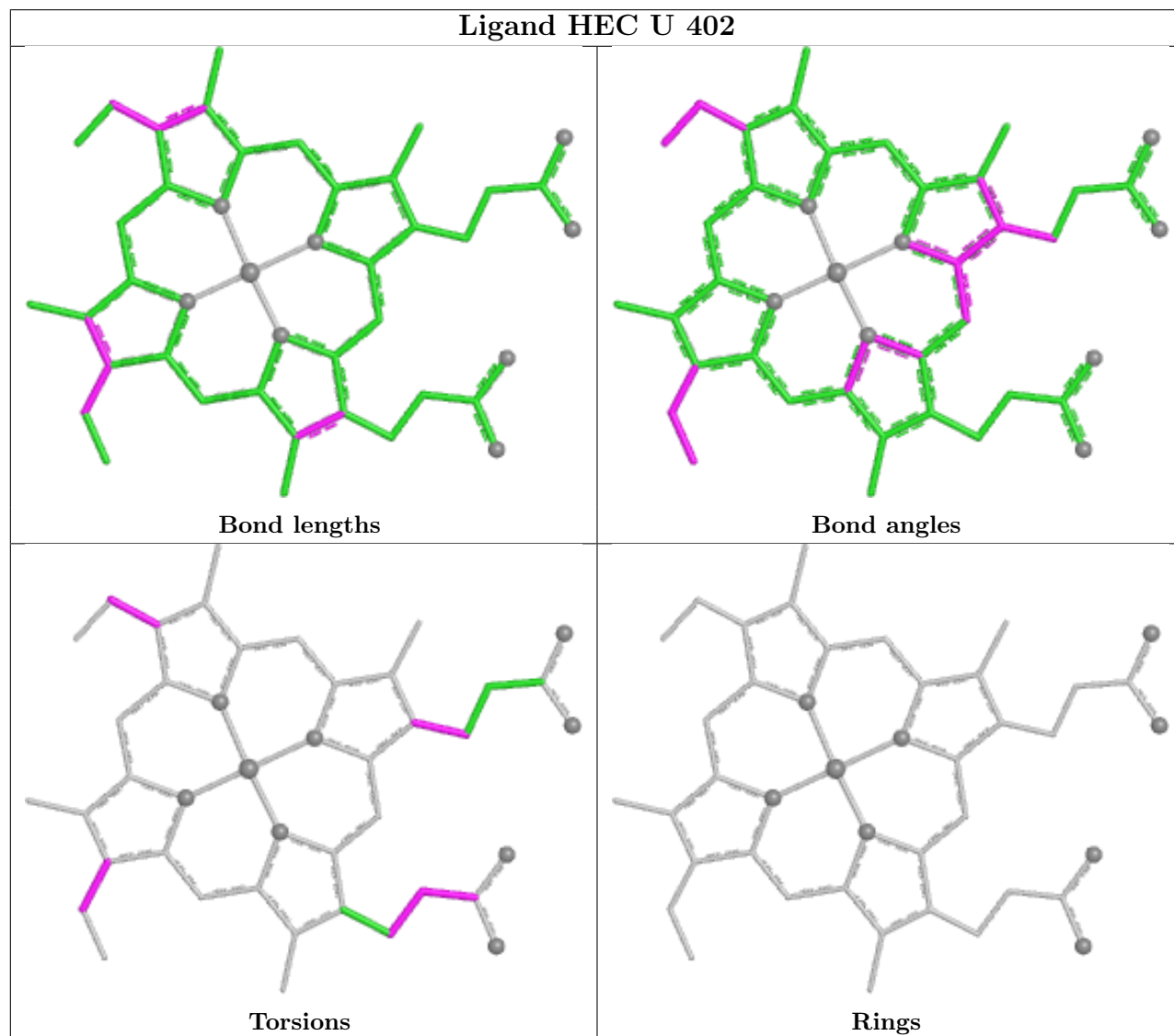


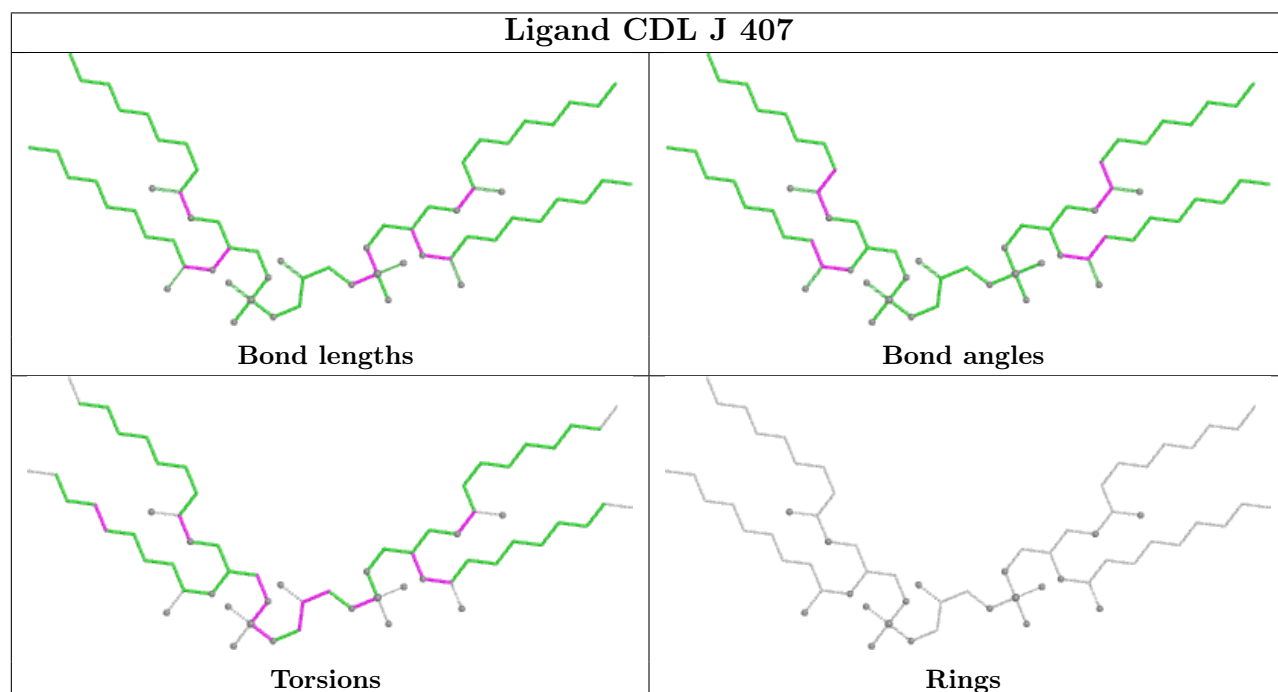
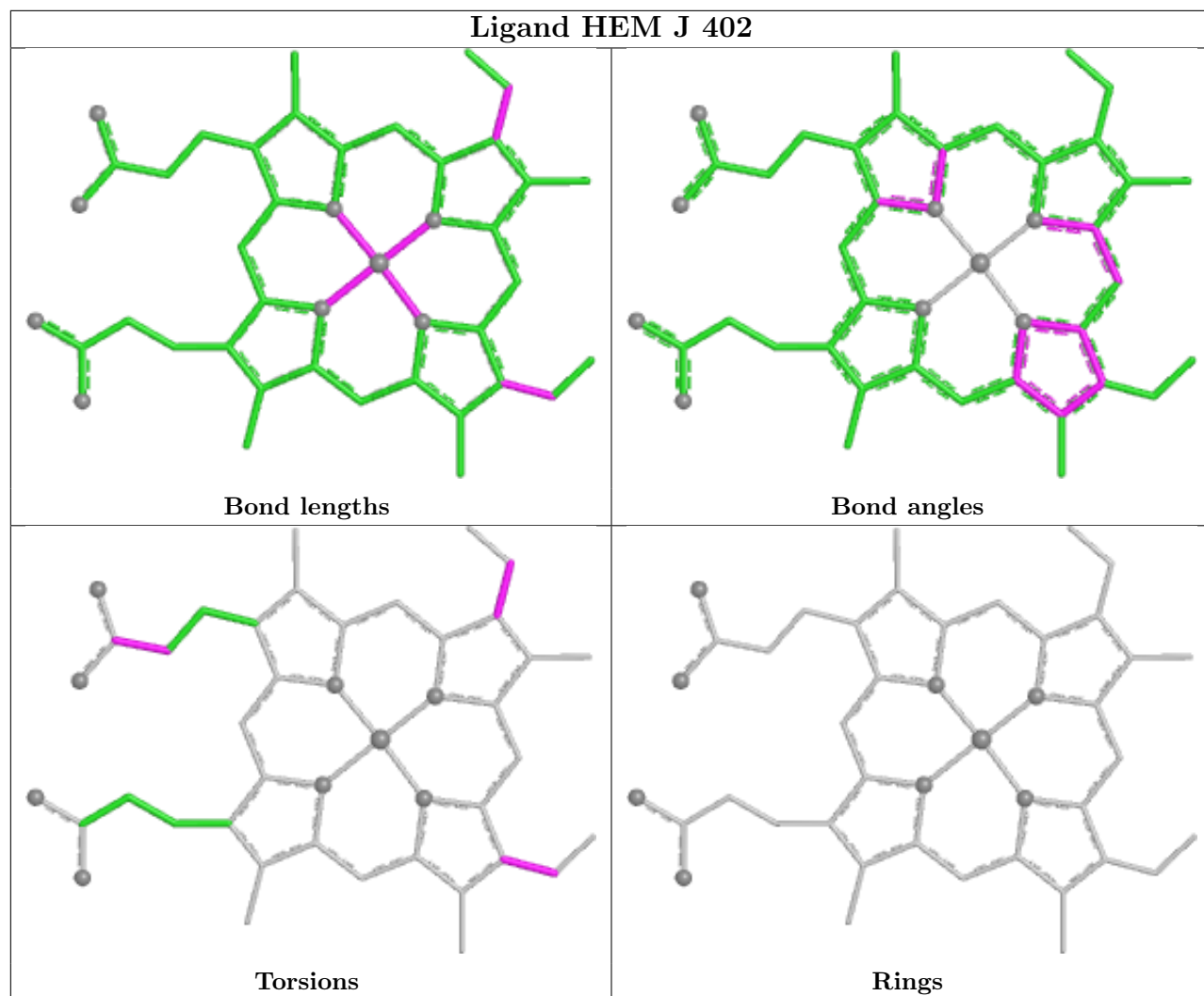


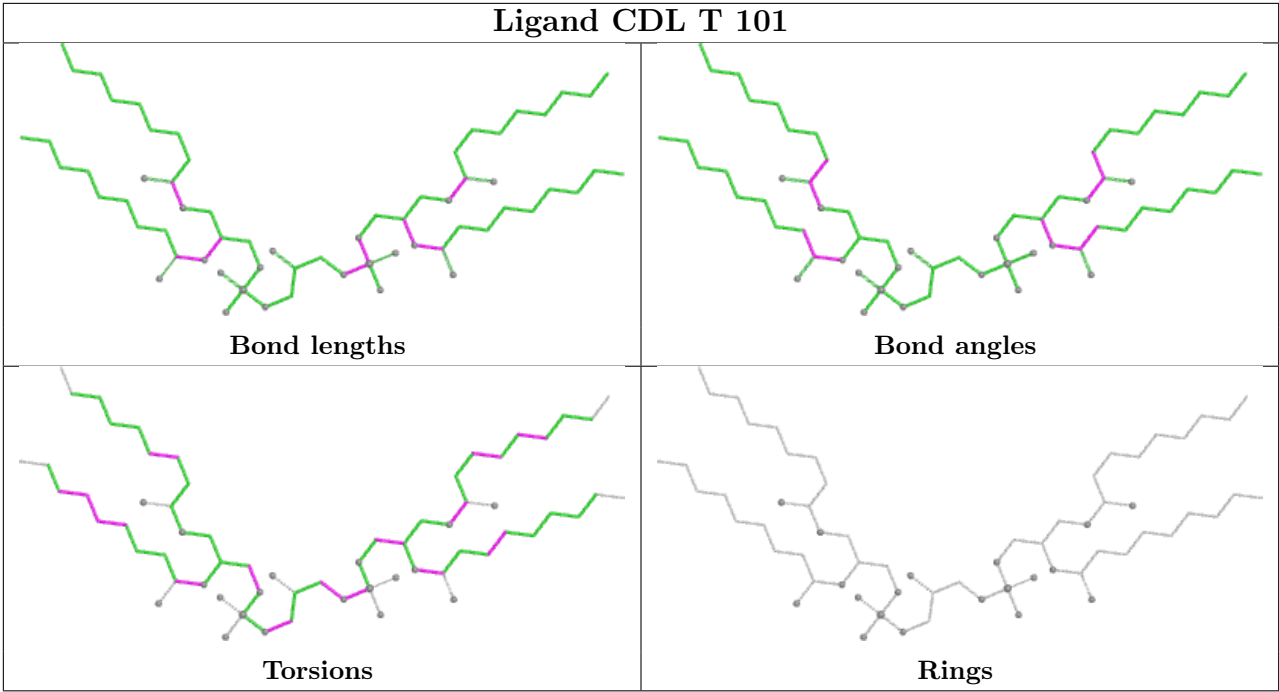
Ligand PLX T 102



Ligand HEC U 402







4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	52:PHE	C	57:LYS	N	3.00

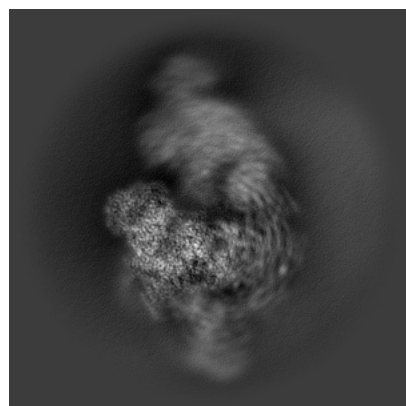
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52525. These allow visual inspection of the internal detail of the map and identification of artifacts.

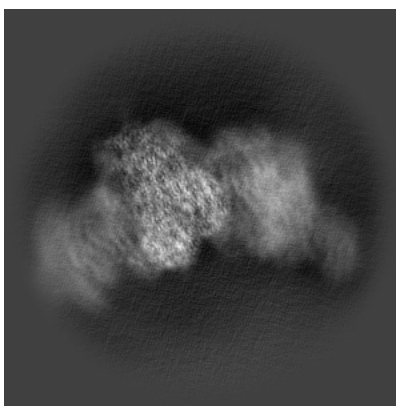
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

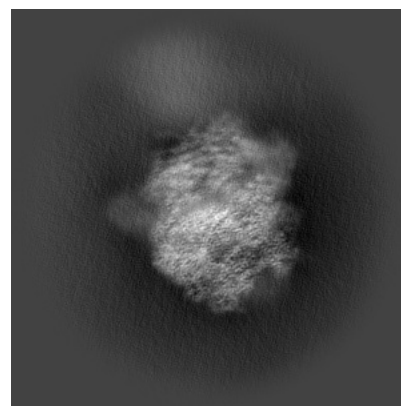
5.1.1 Primary map



X

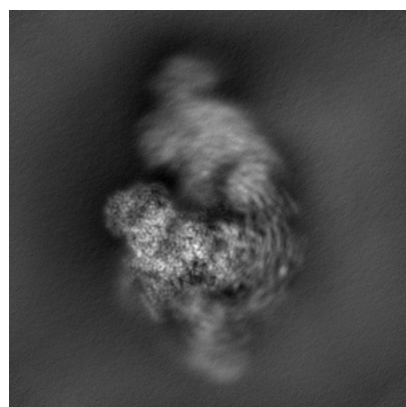


Y

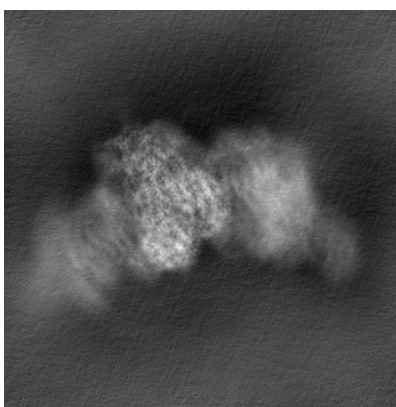


Z

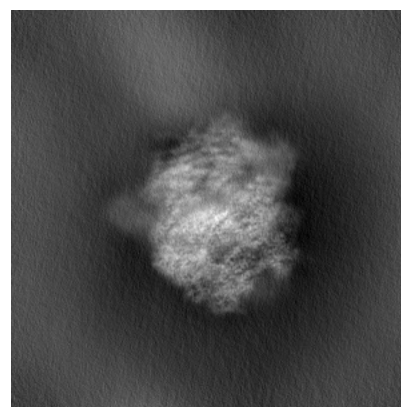
5.1.2 Raw map



X



Y

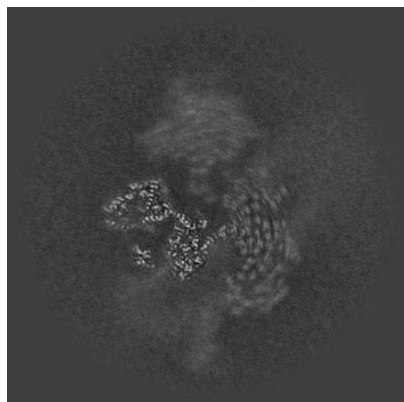


Z

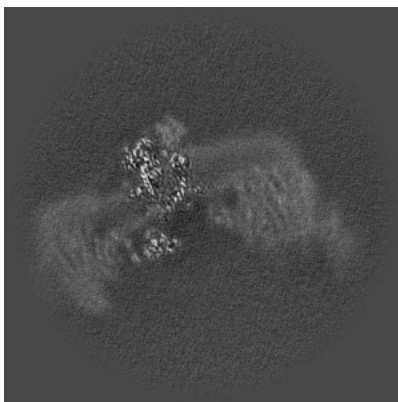
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

5.2.1 Primary map



X Index: 240

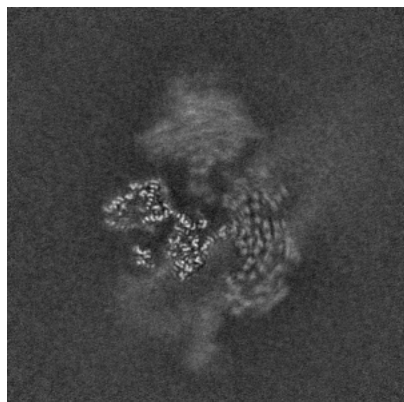


Y Index: 240

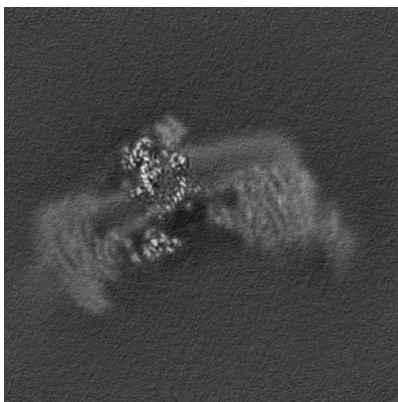


Z Index: 240

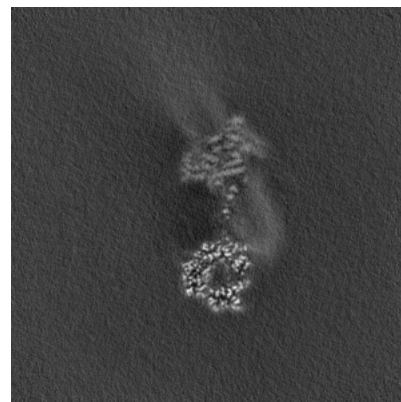
5.2.2 Raw map



X Index: 240



Y Index: 240

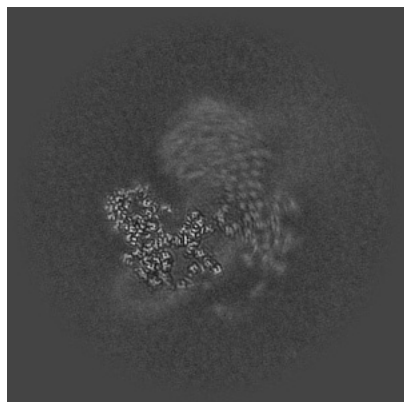


Z Index: 240

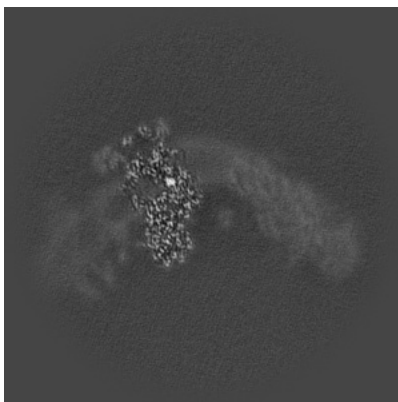
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

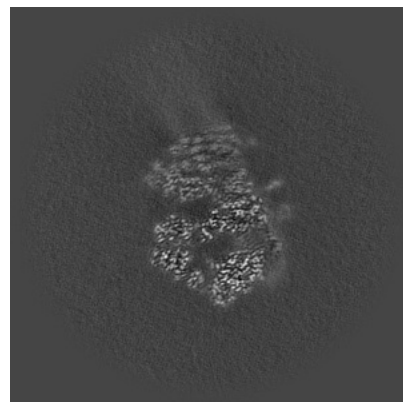
5.3.1 Primary map



X Index: 268

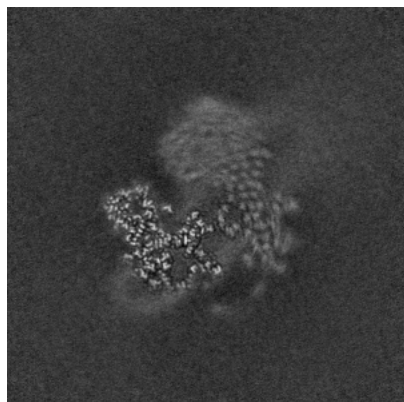


Y Index: 214

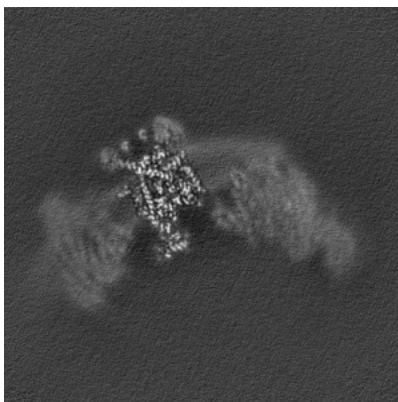


Z Index: 214

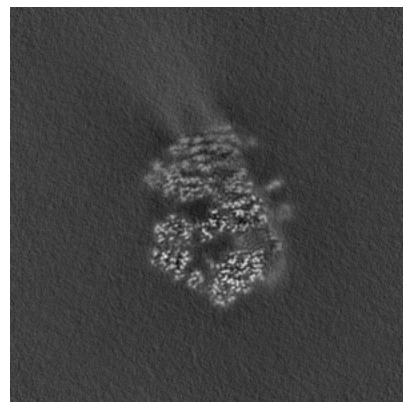
5.3.2 Raw map



X Index: 269



Y Index: 227

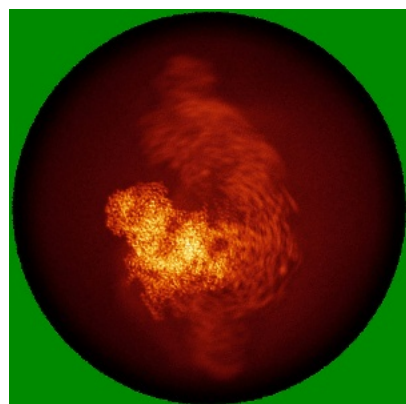


Z Index: 214

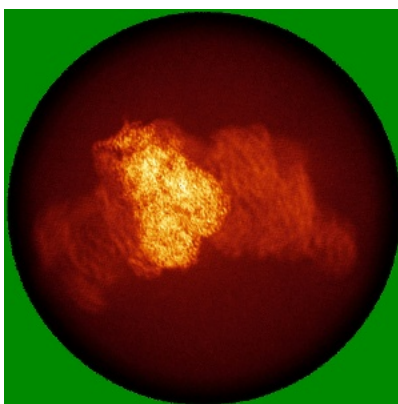
The images above show the largest variance slices of the map in three orthogonal directions.

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

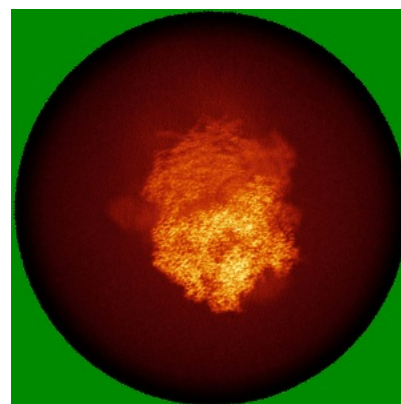
5.4.1 Primary map



X

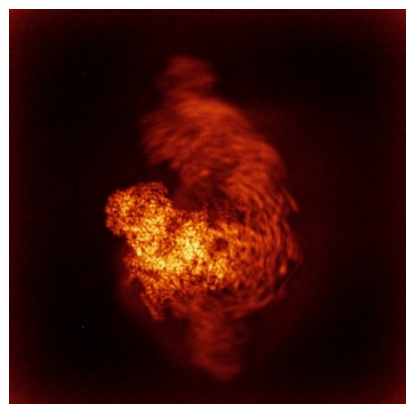


Y

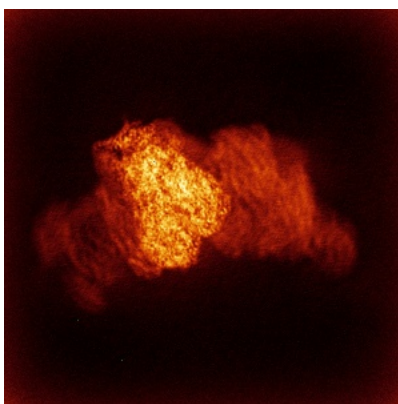


Z

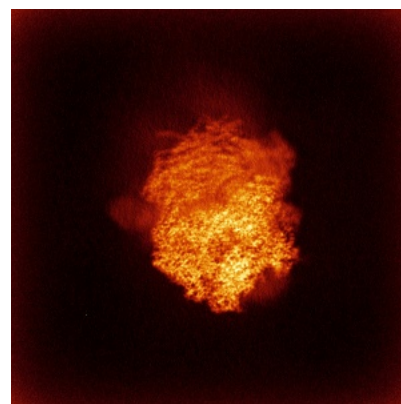
5.4.2 Raw map



X



Y



Z

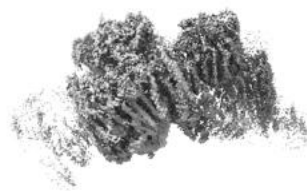
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



X



Y



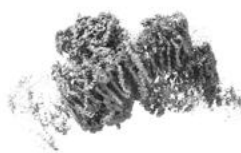
Z

The images above show the 3D surface view of the map at the recommended contour level 4.54. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



X



Y



Z

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

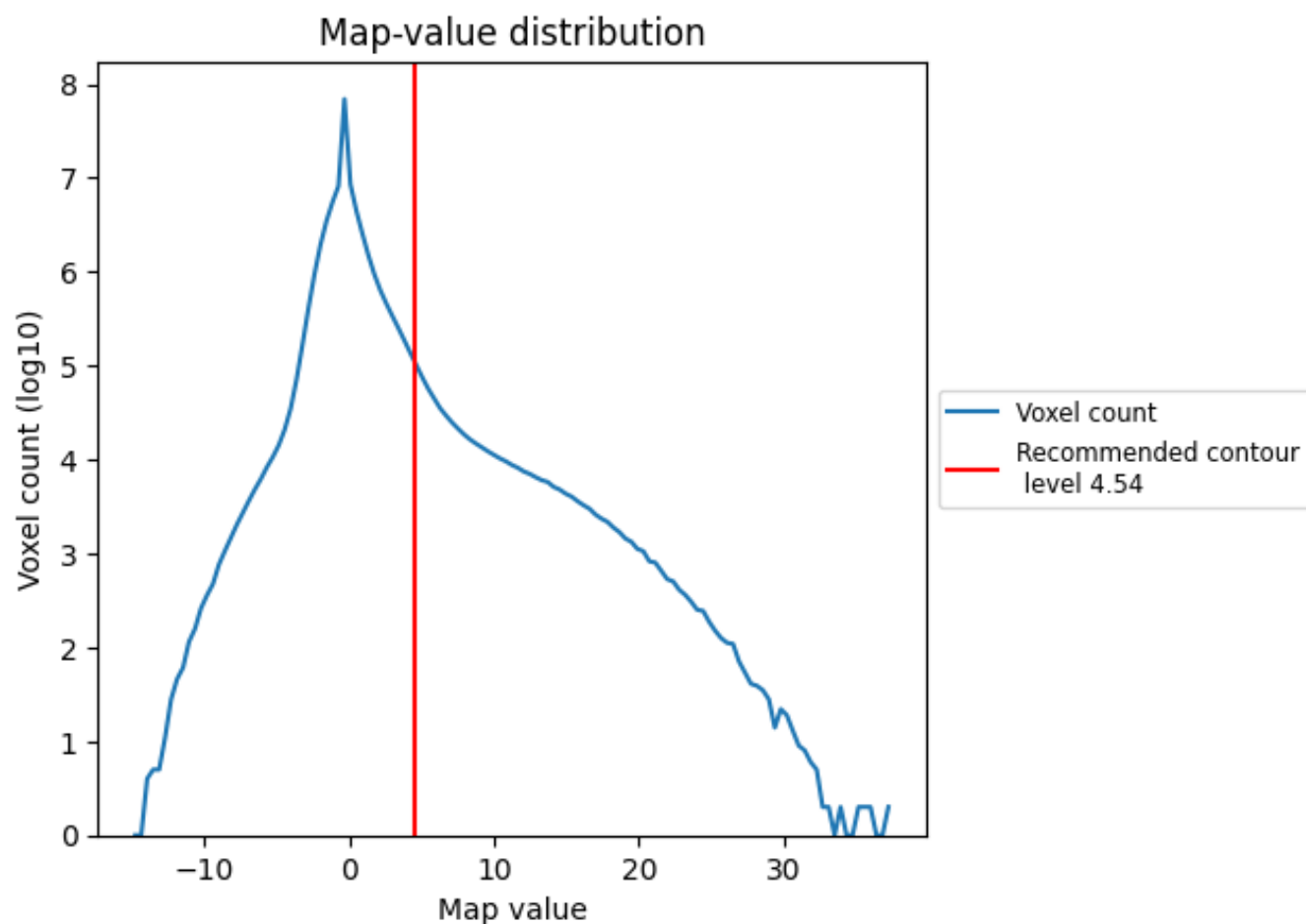
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

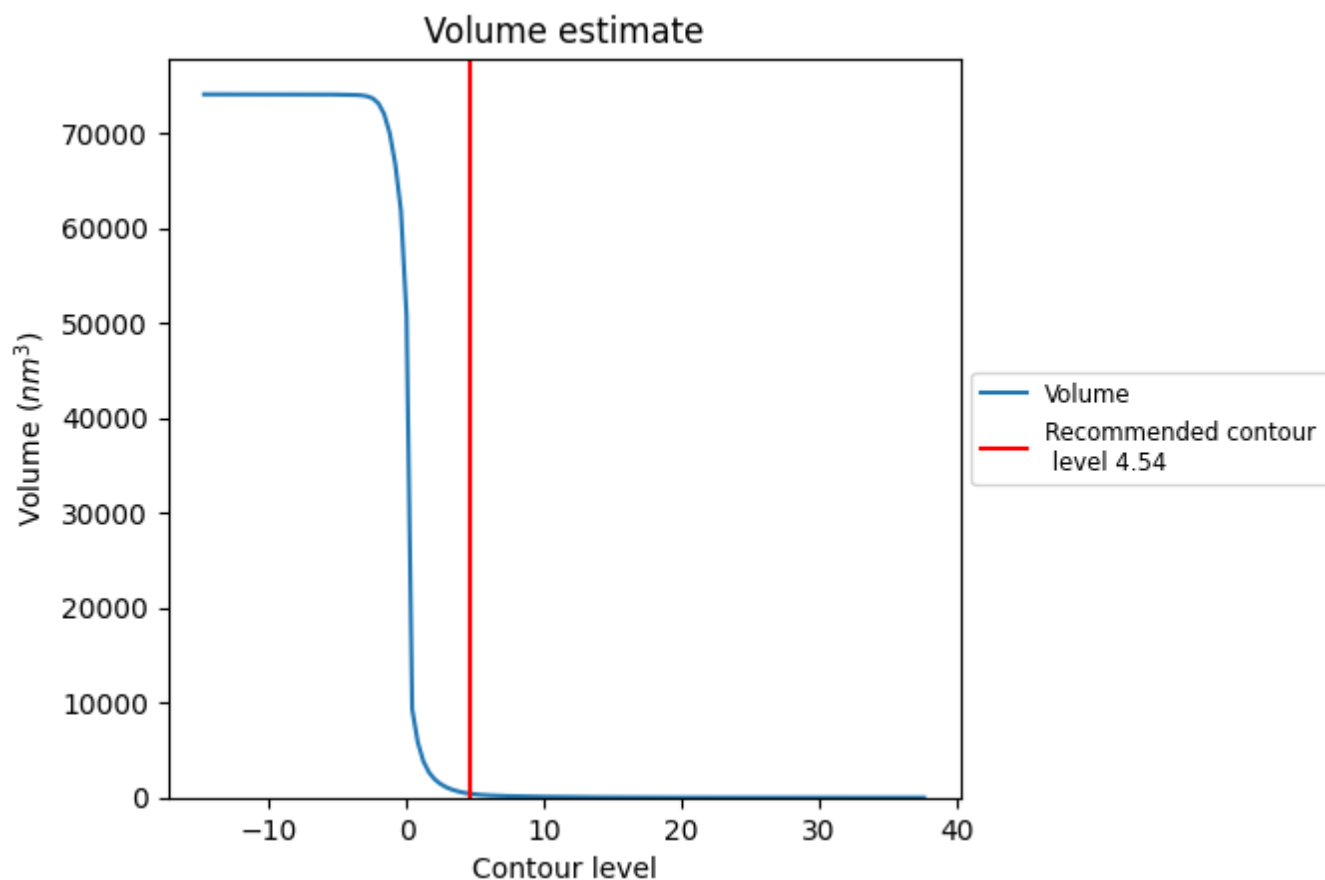
This section contains the results of statistical analysis of the map.

6.1 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.

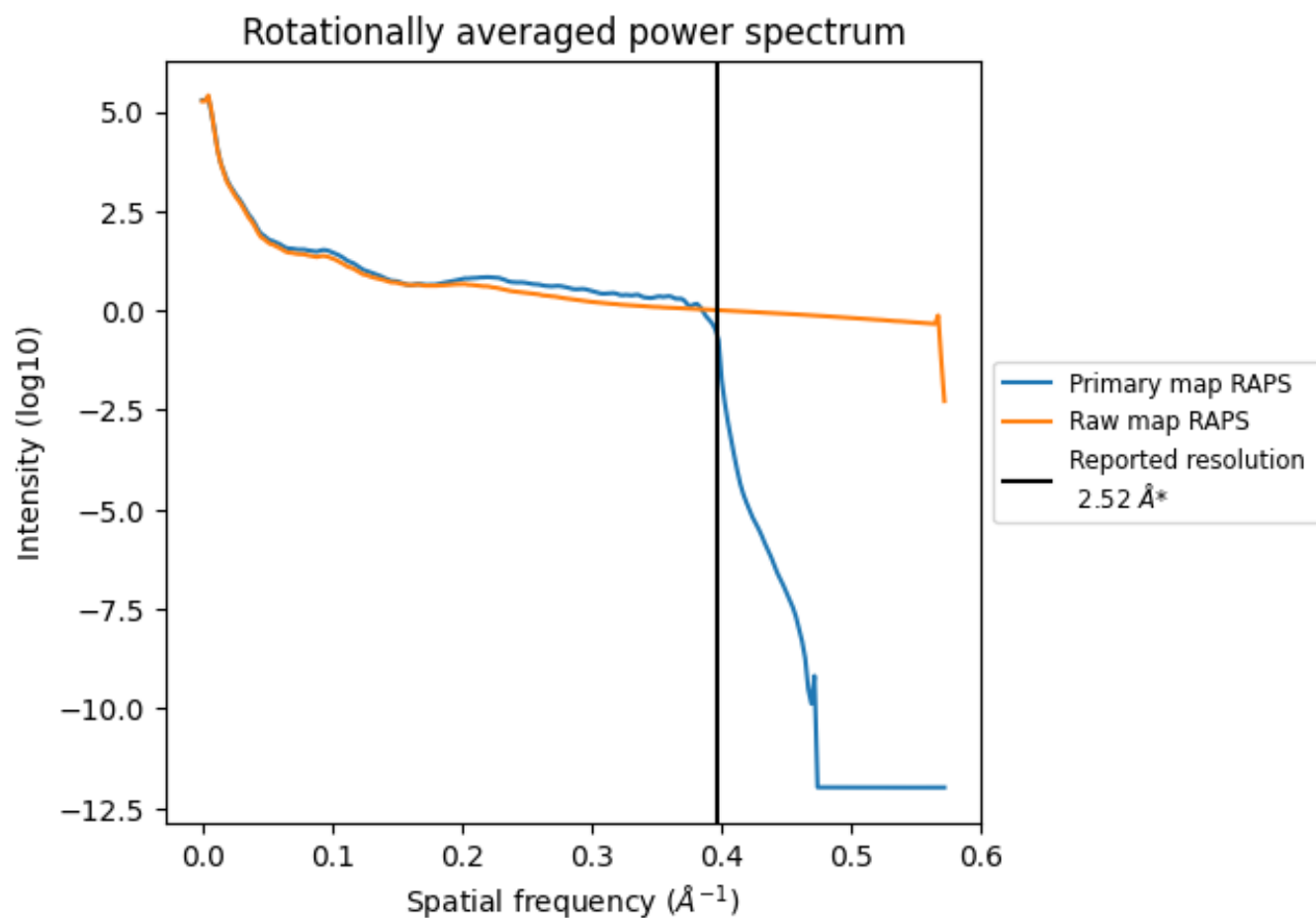
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 421 nm^3 ; this corresponds to an approximate mass of 380 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.

6.3 Rotationally averaged power spectrum ⓘ

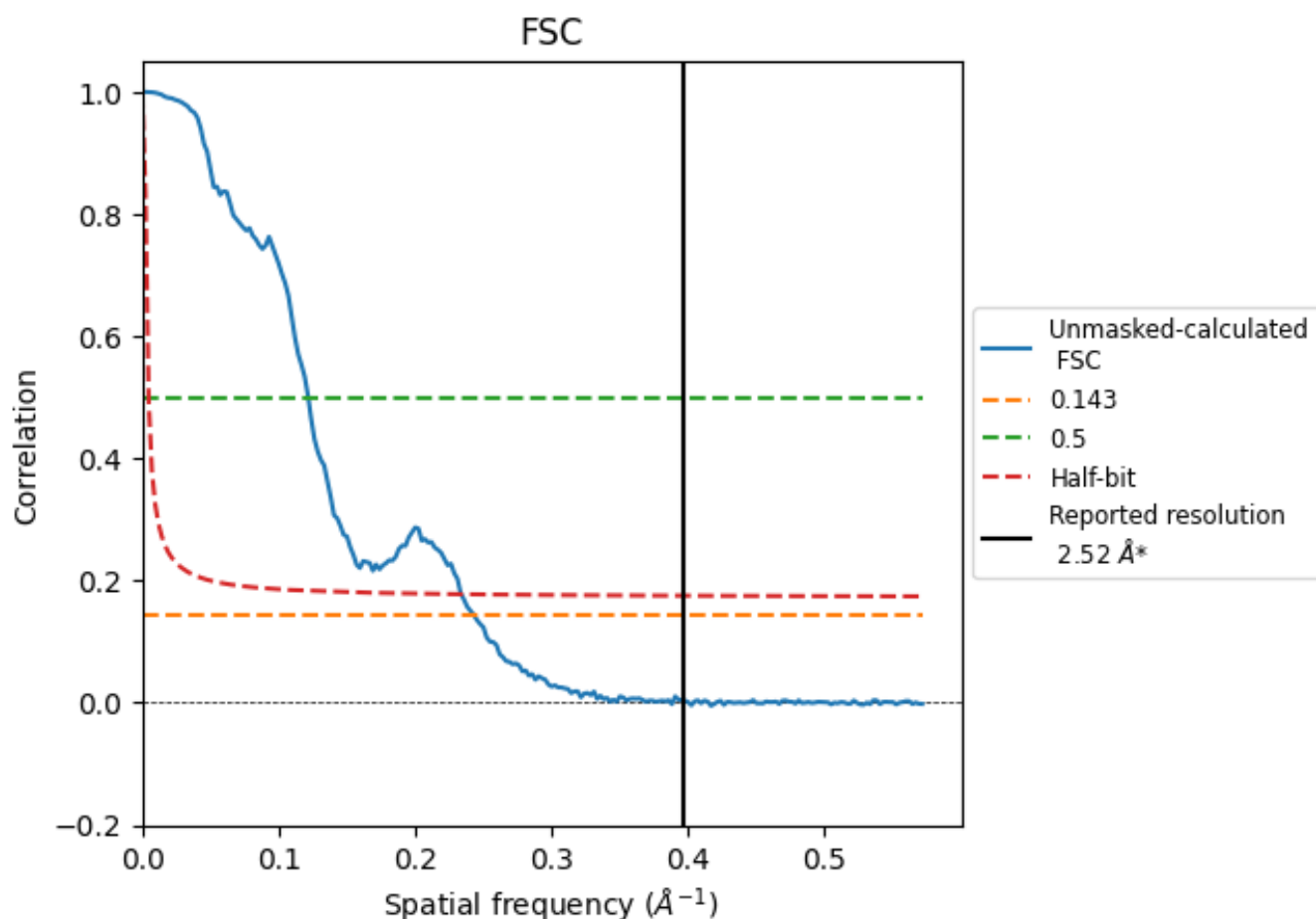


*Reported resolution corresponds to spatial frequency of 0.397 \AA^{-1}

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

7.2 Resolution estimates [i](#)

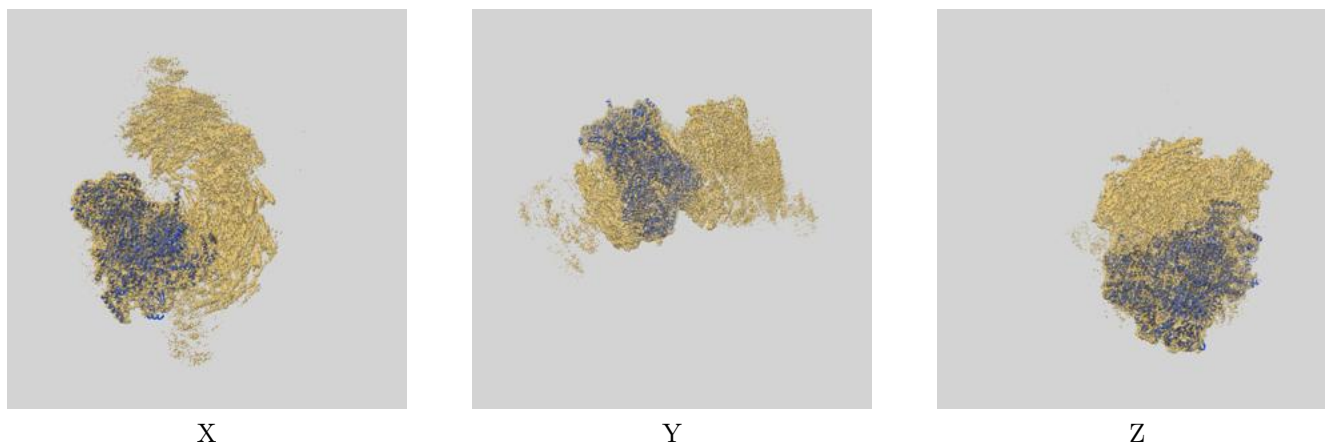
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	8.22	4.28

*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 4.11 differs from the reported value 2.52 by more than 10 %

8 Map-model fit [i](#)

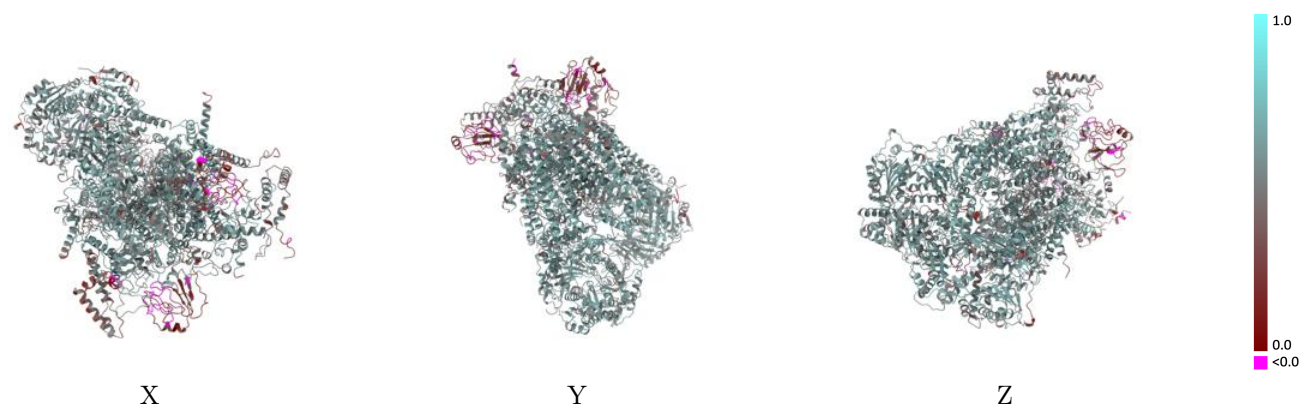
This section contains information regarding the fit between EMDB map EMD-52525 and PDB model 9HZL. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



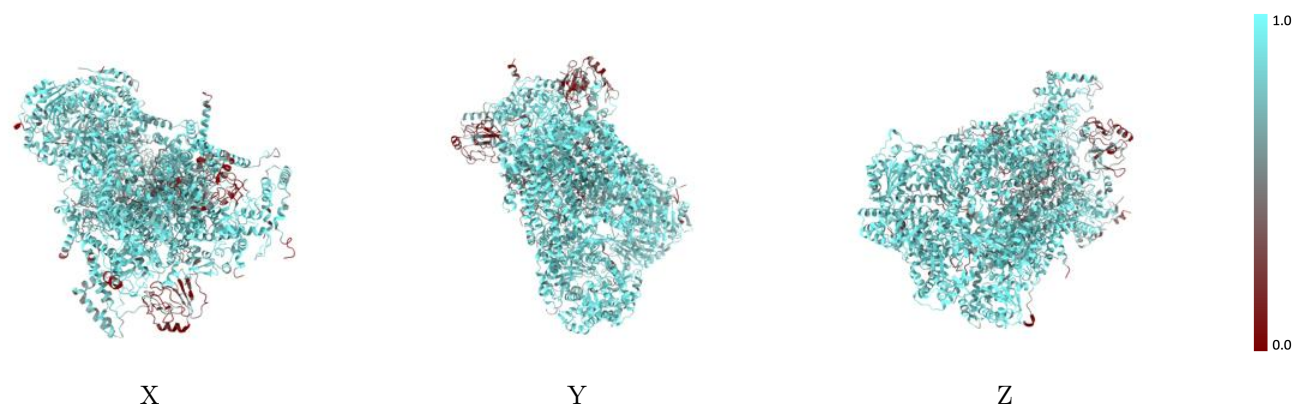
The images above show the 3D surface view of the map at the recommended contour level 4.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



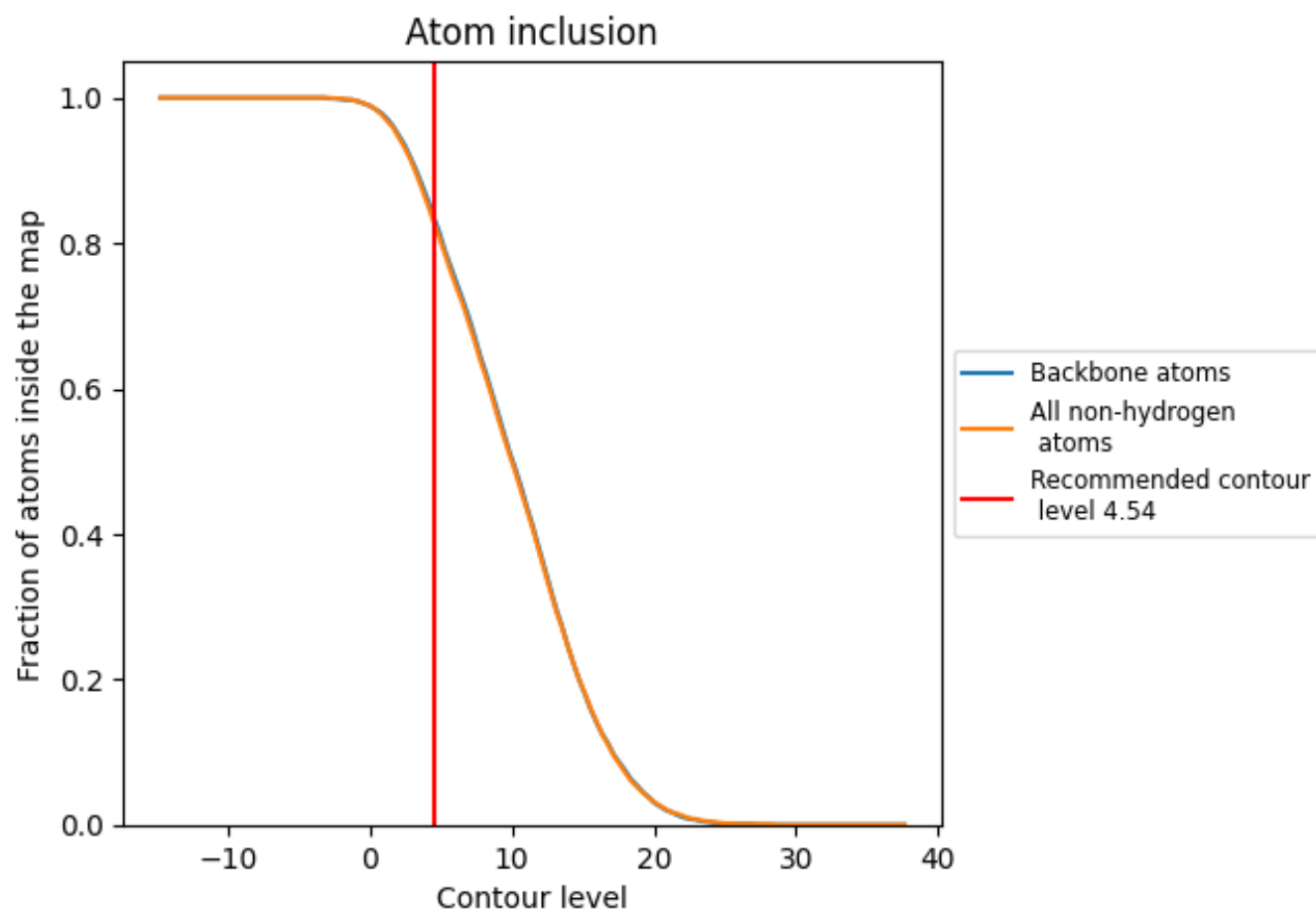
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (4.54).















































8.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5250
A	 0.8270	 0.5300
B	 0.4970	 0.3540
C	 0.5170	 0.3110
D	 0.8350	 0.5630
E	 0.7100	 0.4080
F	 0.8640	 0.5740
G	 0.7760	 0.5220
H	 0.8880	 0.5500
J	 0.8770	 0.5760
K	 0.8910	 0.5420
L	 0.9110	 0.5860
N	 0.8550	 0.5210
O	 0.4010	 0.2760
P	 0.5510	 0.3220
Q	 0.8140	 0.5010
R	 0.6720	 0.3410
S	 0.8700	 0.5620
T	 0.7520	 0.4890
U	 0.8610	 0.5420
V	 0.8710	 0.5780
W	 0.8930	 0.5620
Y	 0.8800	 0.5500

