



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 06:21 AM EDT

PDB ID : 3L74 / pdb_00003L74
Title : Cytochrome BC1 complex from chicken with famoxadone bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-28
Resolution : 2.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

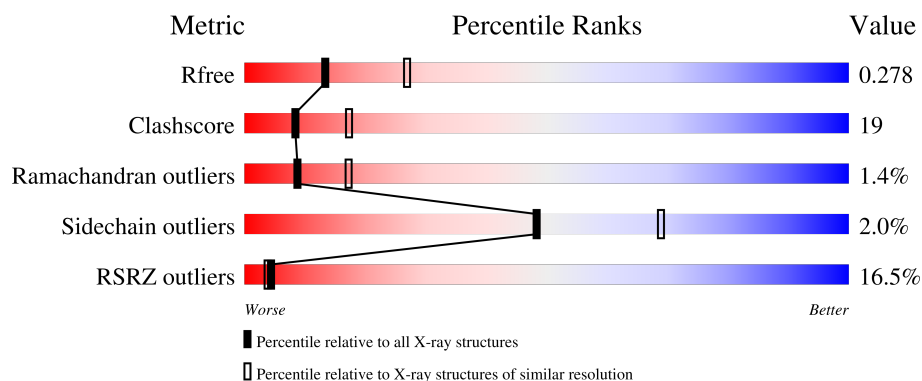
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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.



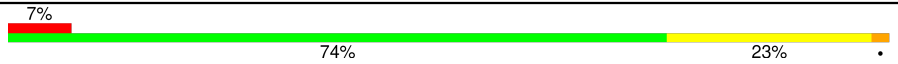
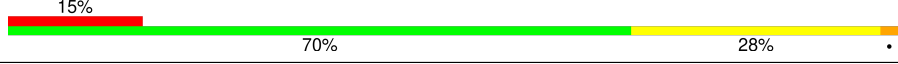
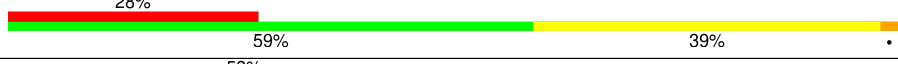
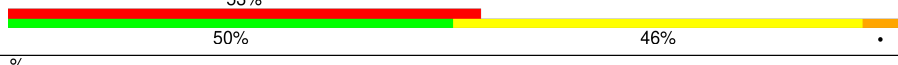
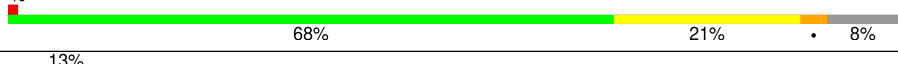
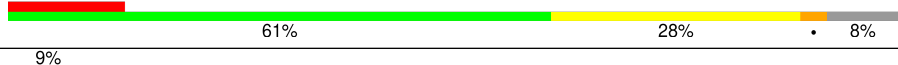
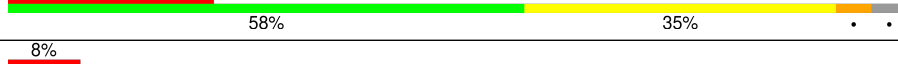
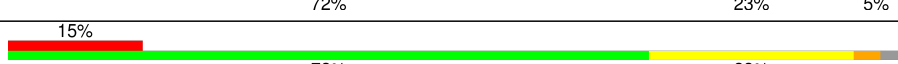
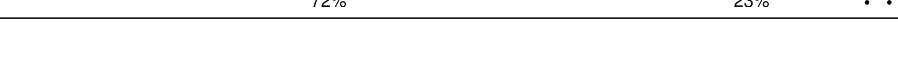
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	
1	N	446	
2	B	441	
2	O	441	
3	C	380	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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
11	PEE	N	3008	-	X	-	-
12	UNL	P	3048	-	-	-	X
16	AZI	C	2011	-	X	-	-
16	AZI	P	3011	-	X	-	-
17	BOG	D	2091	-	-	-	X
17	BOG	P	2010	-	-	-	X
18	HEC	D	501	X	-	-	-
18	HEC	Q	501	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32703 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1512	952	262	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	78	Total	C	N	O	0	0	0
			654	428	116	110			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

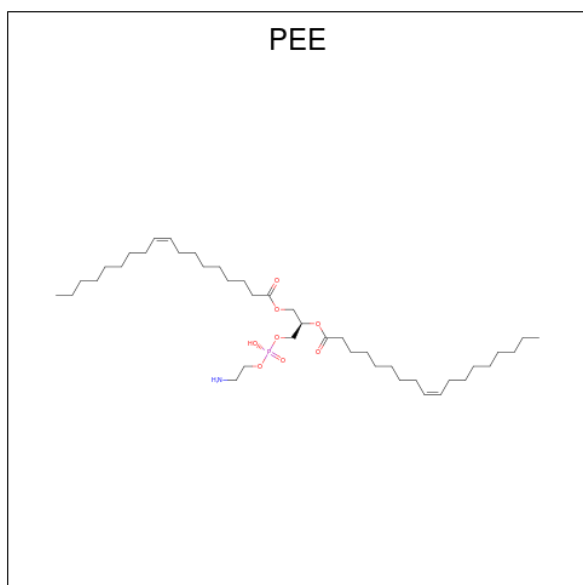
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			288	172	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
11	C	1	Total	C	O	P		0	0
			21	12	8	1			
11	N	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

- Molecule 12 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total 1 O 1	0	0

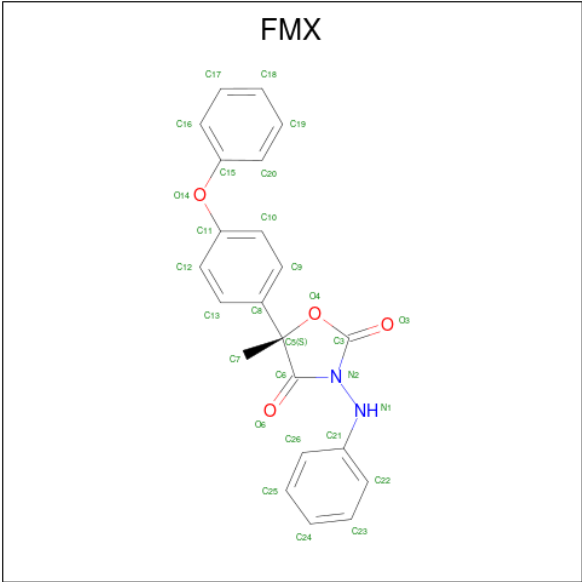
Continued on next page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	3	Total O 5 5	0	0
12	E	1	Total O 2 2	0	0
12	P	5	Total O 7 7	0	0
12	Q	1	Total O 1 1	0	0

- # HEM

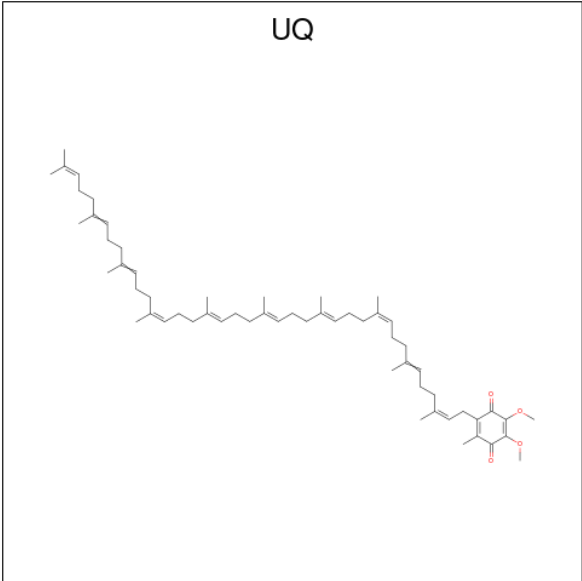
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			28	22	2	4		
14	P	1	Total	C	N	O	0	0
			28	22	2	4		

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



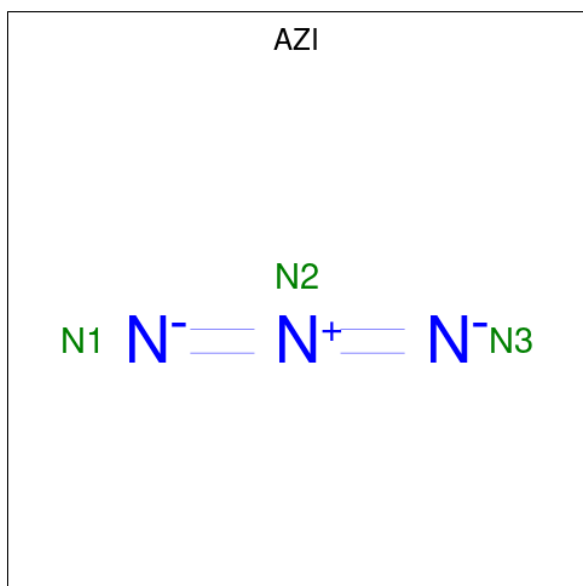
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

Continued on next page...

Continued from previous page...

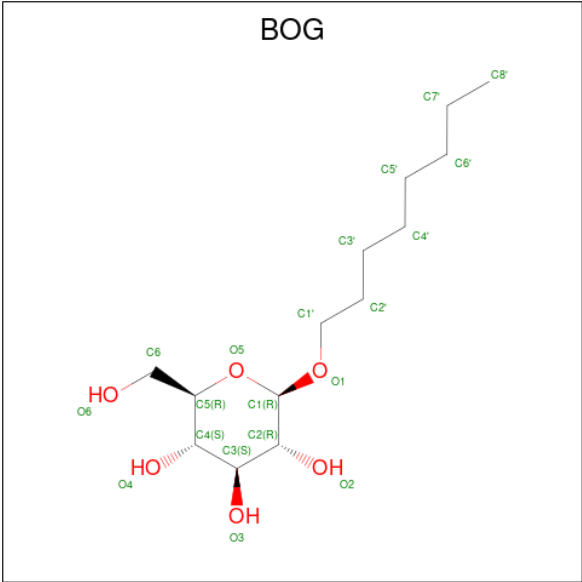
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 16 is AZIDE ION (CCD ID: AZI) (formula: N_3).



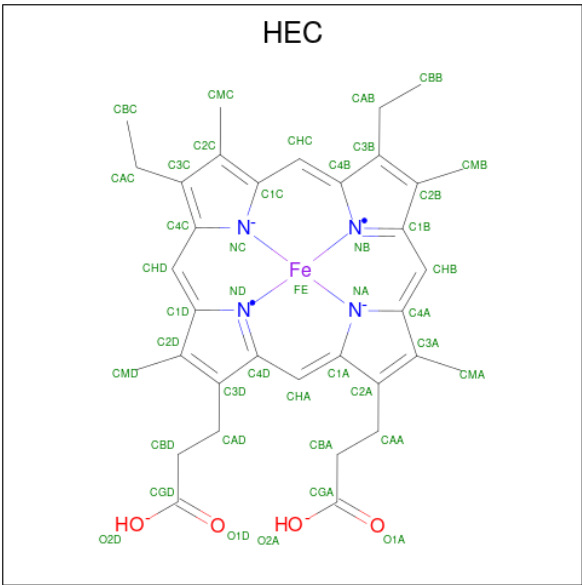
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	N	0	0
			3	3		
16	P	1	Total	N	0	0
			3	3		

- Molecule 17 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $\text{C}_{14}\text{H}_{28}\text{O}_6$).



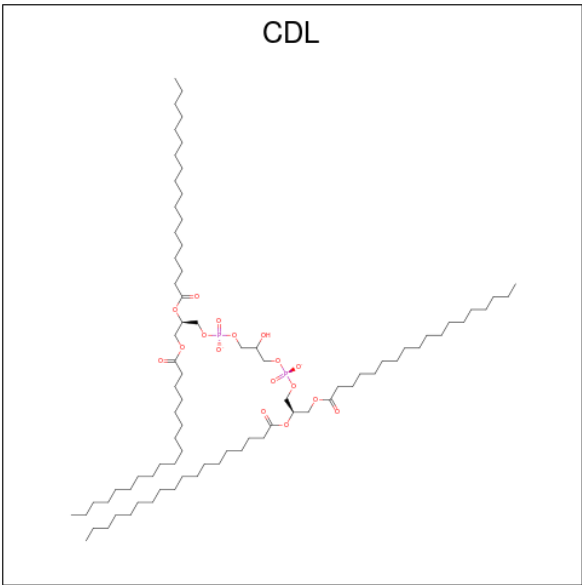
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			12	10	2		
17	D	1	Total	C	O	0	0
			20	14	6		
17	D	1	Total	C	O	0	0
			20	14	6		
17	P	1	Total	C	O	0	0
			19	13	6		
17	Q	1	Total	C	O	0	0
			20	14	6		
17	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
18	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



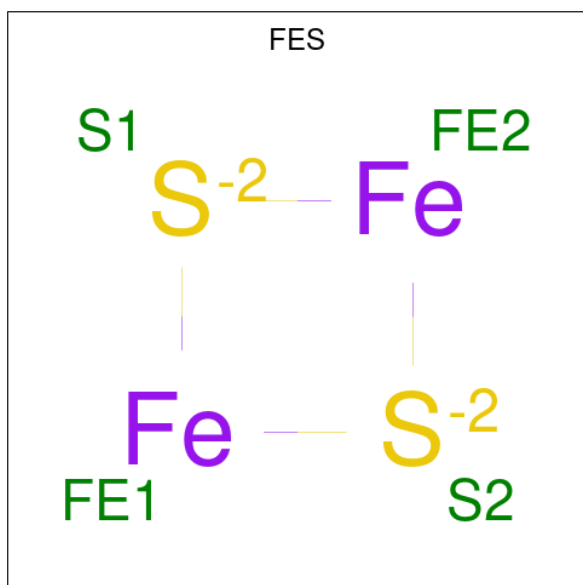
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			42	23	17	2		
19	G	1	Total	C	O	P	0	0
			40	21	17	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	Q	1	Total	C	O	P	0	0
			42	23	17	2		
19	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	E	1	Total	Fe	S	0	0
			4	2	2		
20	R	1	Total	Fe	S	0	0
			4	2	2		

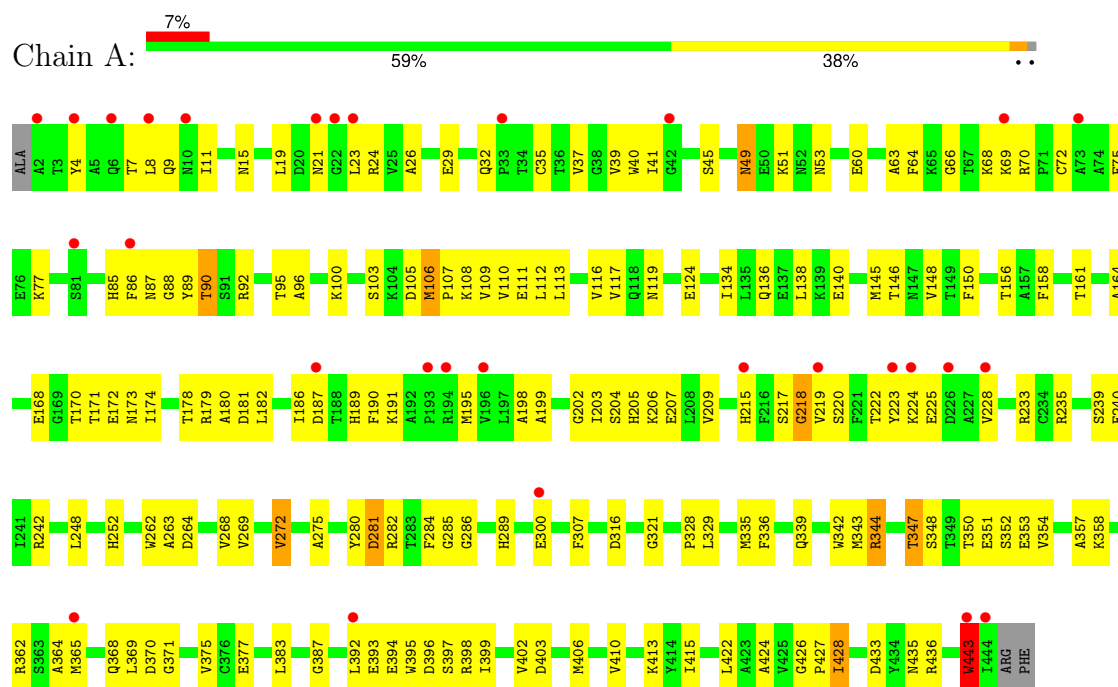
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	O	0	0
			2	2		
21	C	9	Total	O	0	0
			9	9		
21	E	1	Total	O	0	0
			1	1		
21	P	12	Total	O	0	0
			12	12		
21	R	4	Total	O	0	0
			4	4		

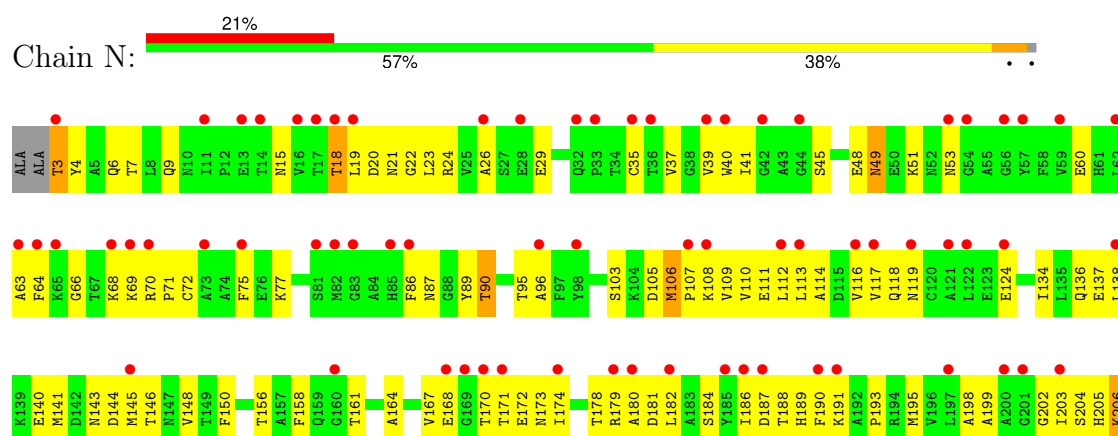
3 Residue-property plots [i](#)

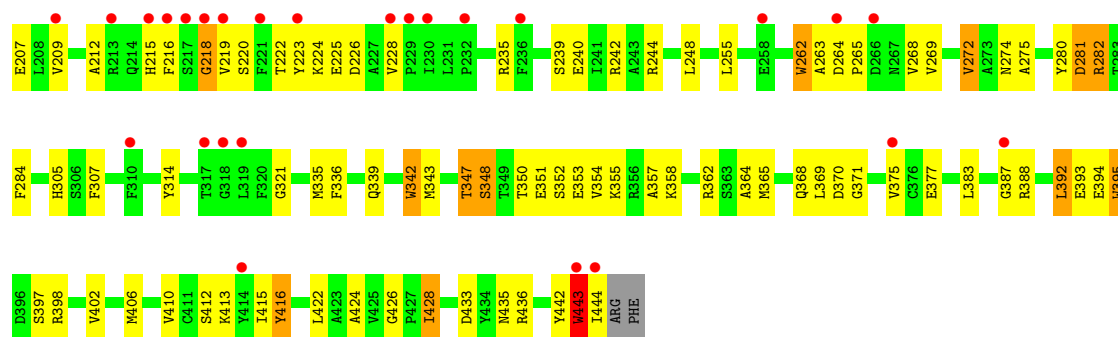
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

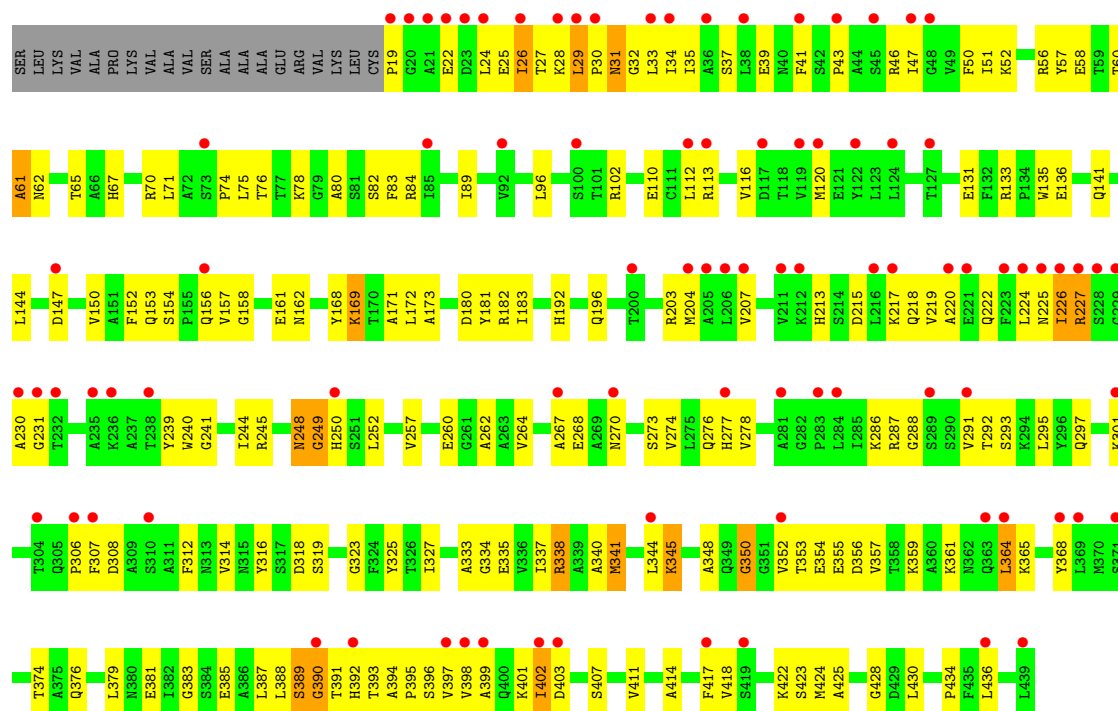


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

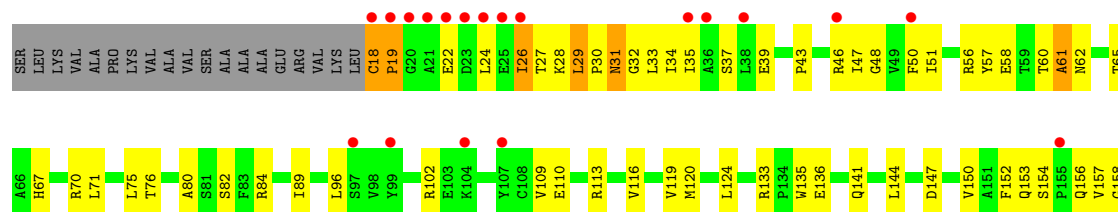


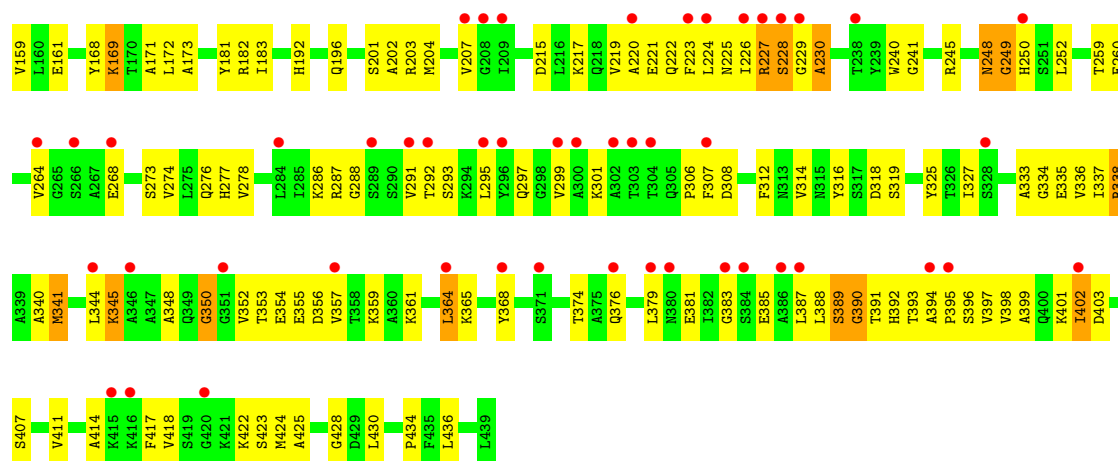


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

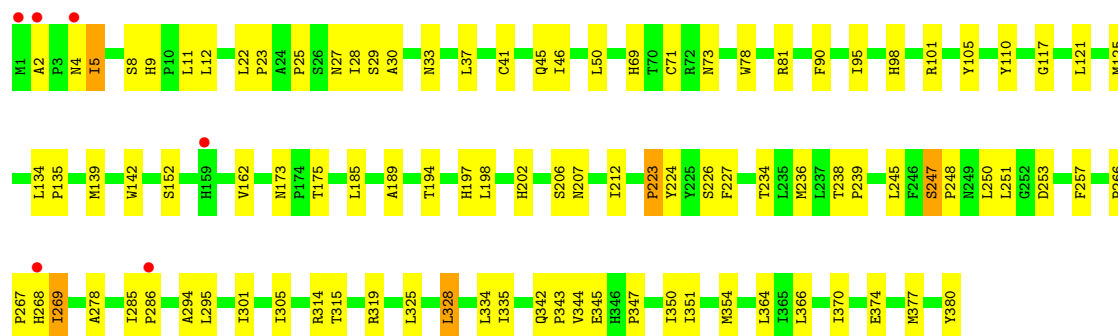
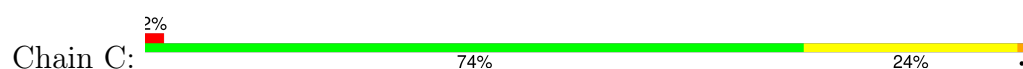


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

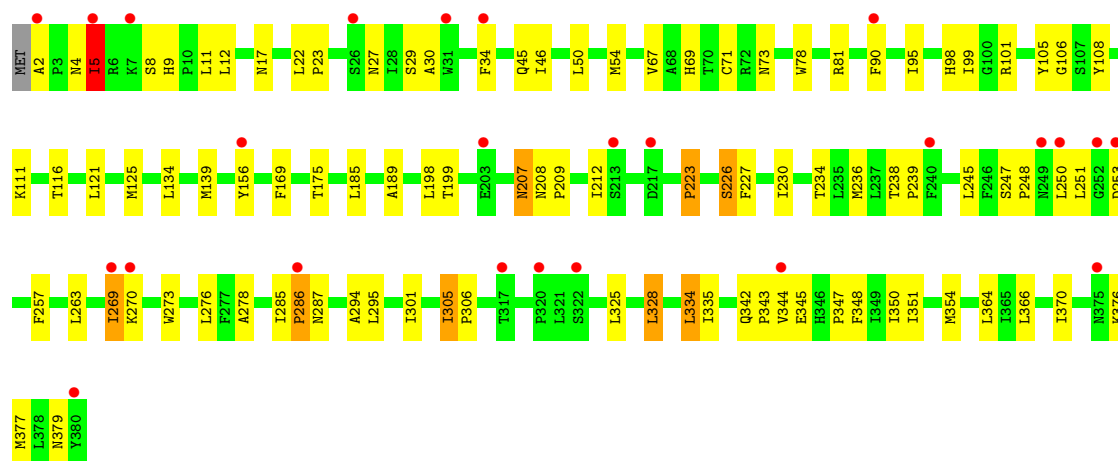
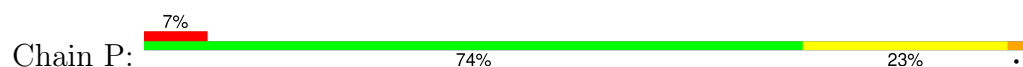




• Molecule 3: CYTOCHROME B

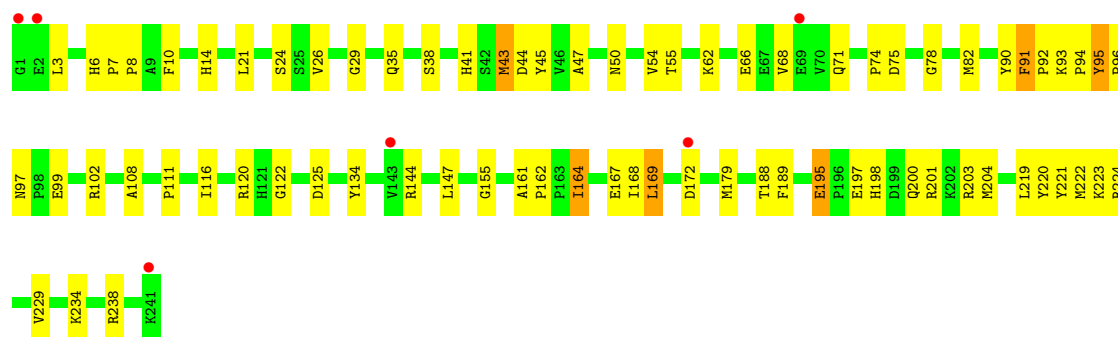


• Molecule 3: CYTOCHROME B

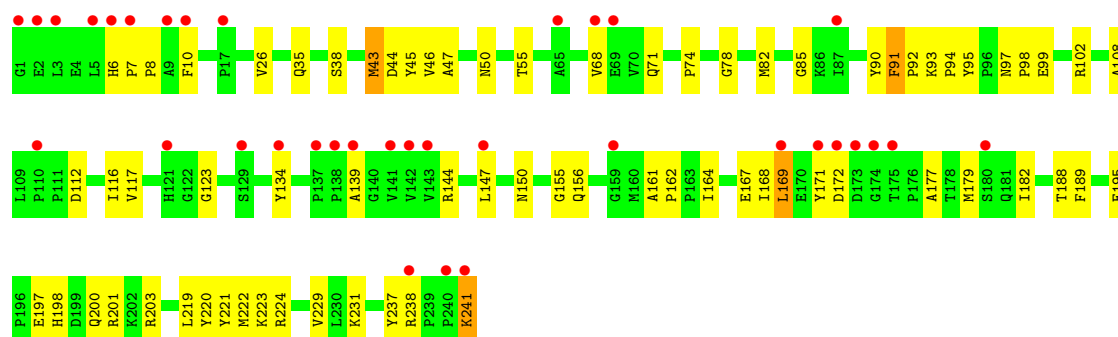


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

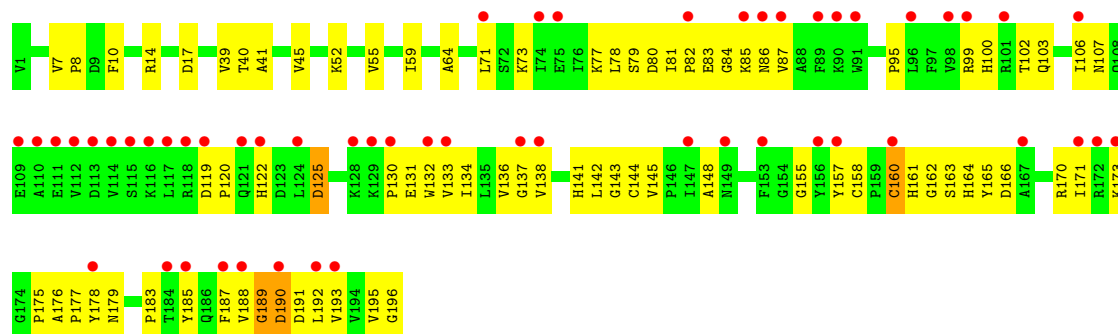




• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

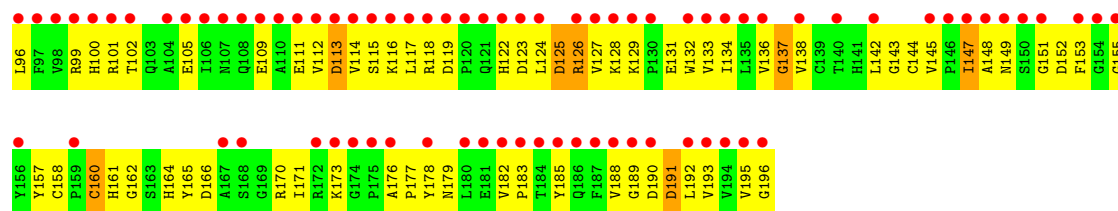


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

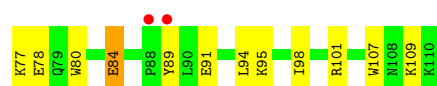
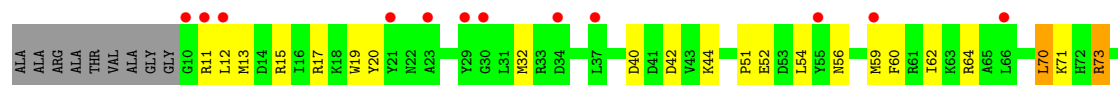




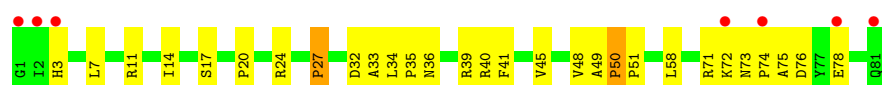
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



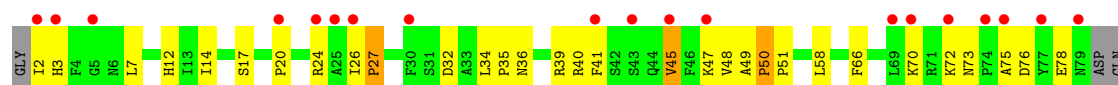
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

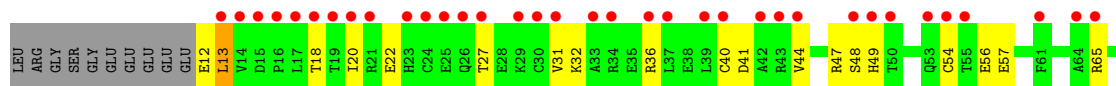


• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII





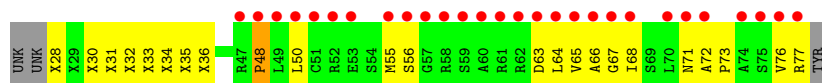
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



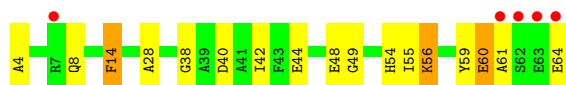
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



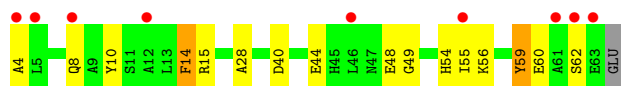
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.89Å 181.69Å 240.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.66 – 2.76 58.66 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.66-2.76) 98.0 (58.66-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.286 0.248 , 0.278	Depositor DCC
R_{free} test set	3886 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32703	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, FMX, UQ, AZI, BOG, PEE, HEM, UNL, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3511	0.97	15/4757 (0.3%)
1	N	0.48	0/3508	0.99	15/4753 (0.3%)
2	B	0.44	0/3196	0.93	8/4334 (0.2%)
2	O	0.47	0/3202	0.97	12/4343 (0.3%)
3	C	0.62	1/3119 (0.0%)	1.02	18/4270 (0.4%)
3	P	0.55	1/3114 (0.0%)	0.99	16/4263 (0.4%)
4	D	0.57	0/1956	1.03	14/2658 (0.5%)
4	Q	0.46	0/1956	1.00	12/2658 (0.5%)
5	E	0.47	0/1547	0.92	6/2103 (0.3%)
5	R	0.44	0/1545	0.90	4/2098 (0.2%)
6	F	0.61	0/911	0.94	2/1219 (0.2%)
6	S	0.45	0/911	0.93	3/1219 (0.2%)
7	G	0.54	0/698	1.05	3/946 (0.3%)
7	T	0.45	0/676	1.02	5/918 (0.5%)
8	H	0.51	0/582	0.89	1/779 (0.1%)
8	U	0.37	0/561	0.87	1/751 (0.1%)
9	I	0.49	0/218	1.01	1/293 (0.3%)
9	V	0.51	0/218	0.92	0/293
10	J	0.49	0/508	0.87	1/682 (0.1%)
10	W	0.49	0/490	0.85	1/660 (0.2%)
All	All	0.51	2/32427 (0.0%)	0.97	138/43997 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	125	MET	SD-CE	5.98	1.94	1.79
3	P	125	MET	SD-CE	5.30	1.92	1.79

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	18	CYS	CA-C-N	10.00	130.09	119.89
2	O	18	CYS	C-N-CA	10.00	130.09	119.89
2	O	227	ARG	N-CA-C	9.98	125.83	110.36
1	N	415	ILE	N-CA-C	8.84	119.16	111.56
1	N	428	ILE	N-CA-C	8.46	119.44	111.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	147	0
1	N	3437	0	3349	166	0
2	B	3141	0	3142	204	0
2	O	3147	0	3146	191	0
3	C	3017	0	3063	81	0
3	P	3012	0	3058	83	0
4	D	1898	0	1846	56	0
4	Q	1898	0	1846	56	0
5	E	1513	0	1478	65	0
5	R	1512	0	1476	88	0
6	F	891	0	893	19	0
6	S	891	0	893	29	0
7	G	676	0	659	27	0
7	T	654	0	641	25	0
8	H	574	0	548	14	0
8	U	553	0	535	18	0
9	I	288	0	253	43	0
9	V	278	0	253	32	0
10	J	497	0	490	14	0
10	W	479	0	478	11	0
11	A	50	0	77	0	0
11	C	69	0	83	0	0
11	N	55	0	77	0	0
11	P	48	0	70	0	0
12	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	5	0	0	0	0
12	E	2	0	0	0	0
12	P	7	0	0	0	0
12	Q	1	0	0	0	0
13	C	86	0	60	8	0
13	P	86	0	60	7	0
14	C	28	0	18	2	0
14	P	28	0	18	2	0
15	C	19	0	17	5	0
15	P	19	0	17	2	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0
17	C	12	0	18	0	0
17	D	40	0	56	3	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	2	0
18	Q	43	0	30	0	0
19	D	42	0	28	2	0
19	G	40	0	24	2	0
19	Q	42	0	28	3	0
19	T	40	0	24	1	0
20	E	4	0	0	1	0
20	R	4	0	0	1	0
21	A	2	0	0	0	0
21	C	9	0	0	2	0
21	E	1	0	0	0	0
21	P	12	0	0	2	0
21	R	4	0	0	0	0
All	All	32703	0	32215	1242	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 19.

The worst 5 of 1242 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)
1:A:344:ARG:HH11	1:A:344:ARG:HB2	1.04	1.10
1:A:344:ARG:HB2	1:A:344:ARG:NH1	1.69	1.08
1:N:178:THR:HG22	1:N:180:ALA:H	1.18	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.13	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:180:ALA:H	1.20	1.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	415 (94%)	21 (5%)	5 (1%)	11	22
1	N	440/446 (99%)	413 (94%)	21 (5%)	6 (1%)	9	17
2	B	419/441 (95%)	370 (88%)	40 (10%)	9 (2%)	5	11
2	O	420/441 (95%)	374 (89%)	38 (9%)	8 (2%)	6	12
3	C	378/380 (100%)	363 (96%)	14 (4%)	1 (0%)	36	56
3	P	377/380 (99%)	361 (96%)	15 (4%)	1 (0%)	36	56
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	30	50
5	E	194/196 (99%)	174 (90%)	13 (7%)	7 (4%)	2	4
5	R	192/196 (98%)	163 (85%)	22 (12%)	7 (4%)	2	4
6	F	99/110 (90%)	94 (95%)	4 (4%)	1 (1%)	12	24
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	18
7	T	76/81 (94%)	69 (91%)	7 (9%)	0	100	100
8	H	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	8	15
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	8	15
9	I	29/47 (62%)	25 (86%)	4 (14%)	0	100	100
9	V	29/47 (62%)	25 (86%)	3 (10%)	1 (3%)	3	5
10	J	59/61 (97%)	54 (92%)	3 (5%)	2 (3%)	3	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3 5
All	All	4000/4160 (96%)	3688 (92%)	258 (6%)	54 (1%)	9 17

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	226	ILE
2	B	227	ARG
2	B	389	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/368 (99%)	357 (98%)	8 (2%)	45 67
1	N	365/368 (99%)	352 (96%)	13 (4%)	31 55
2	B	332/347 (96%)	326 (98%)	6 (2%)	51 71
2	O	333/347 (96%)	327 (98%)	6 (2%)	51 71
3	C	328/329 (100%)	325 (99%)	3 (1%)	70 82
3	P	328/329 (100%)	323 (98%)	5 (2%)	57 74
4	D	200/200 (100%)	197 (98%)	3 (2%)	57 74
4	Q	200/200 (100%)	196 (98%)	4 (2%)	48 69
5	E	166/166 (100%)	166 (100%)	0	100 100
5	R	165/166 (99%)	163 (99%)	2 (1%)	63 78
6	F	93/96 (97%)	89 (96%)	4 (4%)	26 47
6	S	93/96 (97%)	89 (96%)	4 (4%)	26 47
7	G	71/71 (100%)	70 (99%)	1 (1%)	59 75
7	T	69/71 (97%)	67 (97%)	2 (3%)	37 61
8	H	65/71 (92%)	63 (97%)	2 (3%)	35 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	73
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	47
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	69
10	W	47/49 (96%)	46 (98%)	1 (2%)	47	67
All	All	3378/3446 (98%)	3311 (98%)	67 (2%)	48	69

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	125	ASP
6	S	64	ARG
8	U	72	LYS
7	G	27	PRO
6	F	84	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	31	ASN
3	P	69	HIS
2	O	156	GLN
2	O	329	GLN
3	P	268	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 41 ligands modelled in this entry, 11 are unknown - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BOG	Q	3009	-	20,20,20	0.95	1 (5%)	25,25,25	0.86	1 (4%)
17	BOG	D	2009	-	20,20,20	1.01	1 (5%)	25,25,25	0.89	2 (8%)
13	HEM	C	502	3	50,50,50	1.68	7 (14%)	67,82,82	1.53	10 (14%)
11	PEE	C	2007	-	47,47,50	1.33	7 (14%)	50,52,55	0.81	3 (6%)
19	CDL	Q	3003	-	41,41,99	1.19	2 (4%)	47,53,111	1.07	3 (6%)
20	FES	E	501	5	0,4,4	-	-	-	-	-
14	FMX	C	2001	-	30,31,31	1.25	2 (6%)	36,44,44	1.18	3 (8%)
11	PEE	C	2008	-	20,20,50	1.66	5 (25%)	23,25,55	0.67	0
17	BOG	D	2091	-	20,20,20	1.11	2 (10%)	25,25,25	1.02	1 (4%)
15	UQ	C	2002	-	19,19,63	2.57	10 (52%)	24,26,79	1.00	2 (8%)
19	CDL	D	2003	-	41,41,99	1.18	1 (2%)	47,53,111	1.07	4 (8%)
19	CDL	T	3004	-	39,39,99	1.20	3 (7%)	45,51,111	1.07	3 (6%)
17	BOG	P	2010	-	18,18,20	1.07	3 (16%)	22,22,25	0.57	0
19	CDL	G	2004	-	39,39,99	1.20	2 (5%)	45,51,111	1.06	3 (6%)
15	UQ	P	3002	-	19,19,63	2.43	10 (52%)	24,26,79	1.06	2 (8%)
17	BOG	Q	3091	-	20,20,20	1.11	2 (10%)	25,25,25	0.89	1 (4%)
13	HEM	P	502	3	50,50,50	1.43	4 (8%)	67,82,82	1.22	5 (7%)
18	HEC	Q	501	4	50,50,50	1.25	6 (12%)	68,82,82	1.52	13 (19%)
13	HEM	P	501	3	50,50,50	1.35	4 (8%)	67,82,82	1.27	5 (7%)
11	PEE	N	3008	-	4,4,50	3.75	4 (100%)	6,6,55	0.58	0
16	AZI	P	3011	-	2,2,2	3.31	2 (100%)	0,1,1	-	-
20	FES	R	501	5	0,4,4	-	-	-	-	-
11	PEE	P	3007	-	47,47,50	1.36	5 (10%)	50,52,55	0.78	2 (4%)
11	PEE	A	2005	-	49,49,50	1.46	9 (18%)	52,54,55	0.83	3 (5%)
17	BOG	C	3010	-	11,11,20	1.07	2 (18%)	10,11,25	1.02	1 (10%)
14	FMX	P	3001	-	30,31,31	1.17	2 (6%)	36,44,44	1.17	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	AZI	C	2011	-	2,2,2	2.88	2 (100%)	0,1,1	-	-
18	HEC	D	501	4	50,50,50	1.05	2 (4%)	68,82,82	1.61	11 (16%)
13	HEM	C	501	3	50,50,50	1.43	6 (12%)	67,82,82	1.48	9 (13%)
11	PEE	N	3005	-	49,49,50	1.44	9 (18%)	52,54,55	0.82	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BOG	Q	3009	-	-	6/11/31/31	0/1/1/1
17	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
13	HEM	C	502	3	-	6/14/54/54	-
11	PEE	C	2007	-	-	22/51/51/54	-
19	CDL	Q	3003	-	-	21/51/51/110	-
20	FES	E	501	5	-	-	0/1/1/1
14	FMX	C	2001	-	-	4/14/33/33	0/4/4/4
11	PEE	C	2008	-	-	10/24/24/54	-
17	BOG	D	2091	-	-	7/11/31/31	0/1/1/1
15	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
19	CDL	D	2003	-	-	22/51/51/110	-
19	CDL	T	3004	-	-	25/49/49/110	-
17	BOG	P	2010	-	-	1/6/26/31	0/1/1/1
19	CDL	G	2004	-	-	23/49/49/110	-
15	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
17	BOG	Q	3091	-	-	5/11/31/31	0/1/1/1
18	HEC	Q	501	4	1/1/3/7	10/14/54/54	-
13	HEM	P	502	3	-	6/14/54/54	-
13	HEM	P	501	3	-	4/14/54/54	-
20	FES	R	501	5	-	-	0/1/1/1
11	PEE	P	3007	-	-	22/51/51/54	-
11	PEE	A	2005	-	-	30/53/53/54	-
17	BOG	C	3010	-	-	4/9/9/31	-
14	FMX	P	3001	-	-	2/14/33/33	0/4/4/4
18	HEC	D	501	4	1/1/3/7	9/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	C	501	3	-	4/14/54/54	-
11	PEE	N	3005	-	-	31/53/53/54	-

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	502	HEM	CBB-CAB	5.37	1.56	1.30
11	N	3008	PEE	P-O1P	5.10	1.62	1.50
15	C	2002	UQ	C6-C5	5.08	1.44	1.35
13	C	502	HEM	CBB-CAB	5.01	1.54	1.30
15	P	3002	UQ	C6-C5	4.83	1.43	1.35

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	HEM	CAD-C3D-C4D	5.43	134.16	124.70
13	C	501	HEM	CAD-C3D-C4D	5.13	133.63	124.70
18	D	501	HEC	CAA-C2A-C3A	-4.88	118.72	127.87
18	Q	501	HEC	CAA-C2A-C3A	-4.66	119.15	127.87
13	C	502	HEM	C3B-C4B-NB	4.31	112.56	109.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	D	501	HEC	NA
18	Q	501	HEC	NA

5 of 282 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2005	PEE	C11-C10-O2-C2
11	A	2005	PEE	C4-O4P-P-O3P
11	A	2005	PEE	C4-O4P-P-O2P
11	A	2005	PEE	C4-O4P-P-O1P
11	A	2005	PEE	O4P-C4-C5-N

There are no ring outliers.

19 monomers are involved in 43 short contacts:

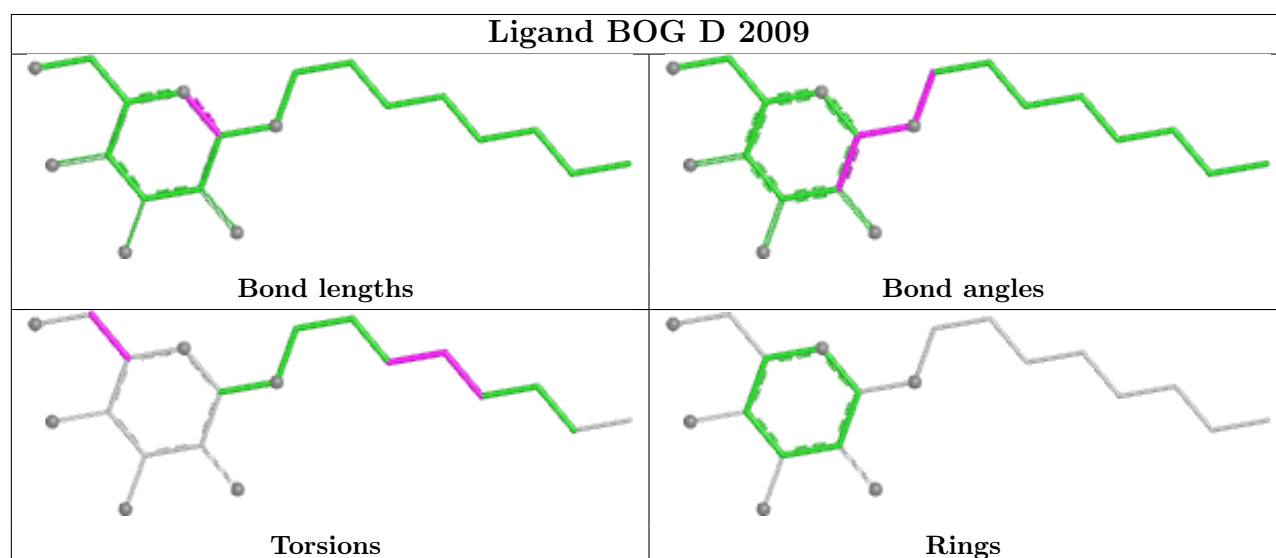
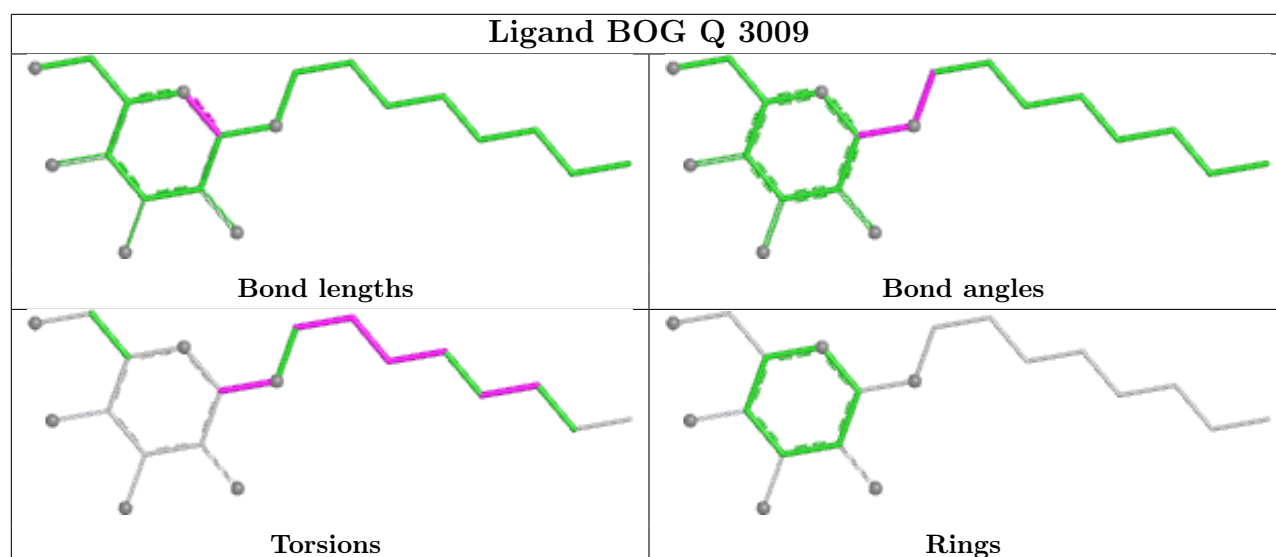
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	2009	BOG	1	0

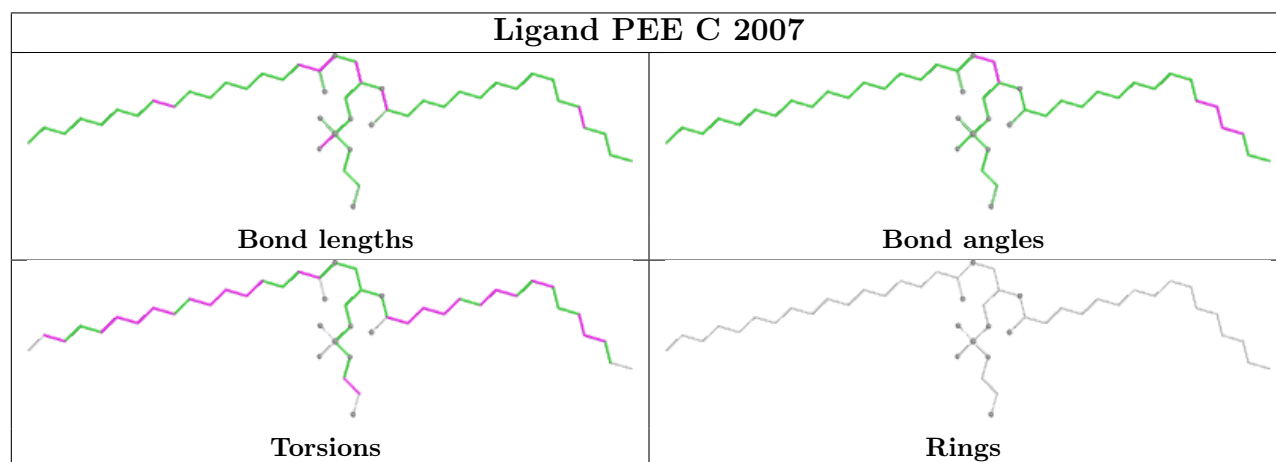
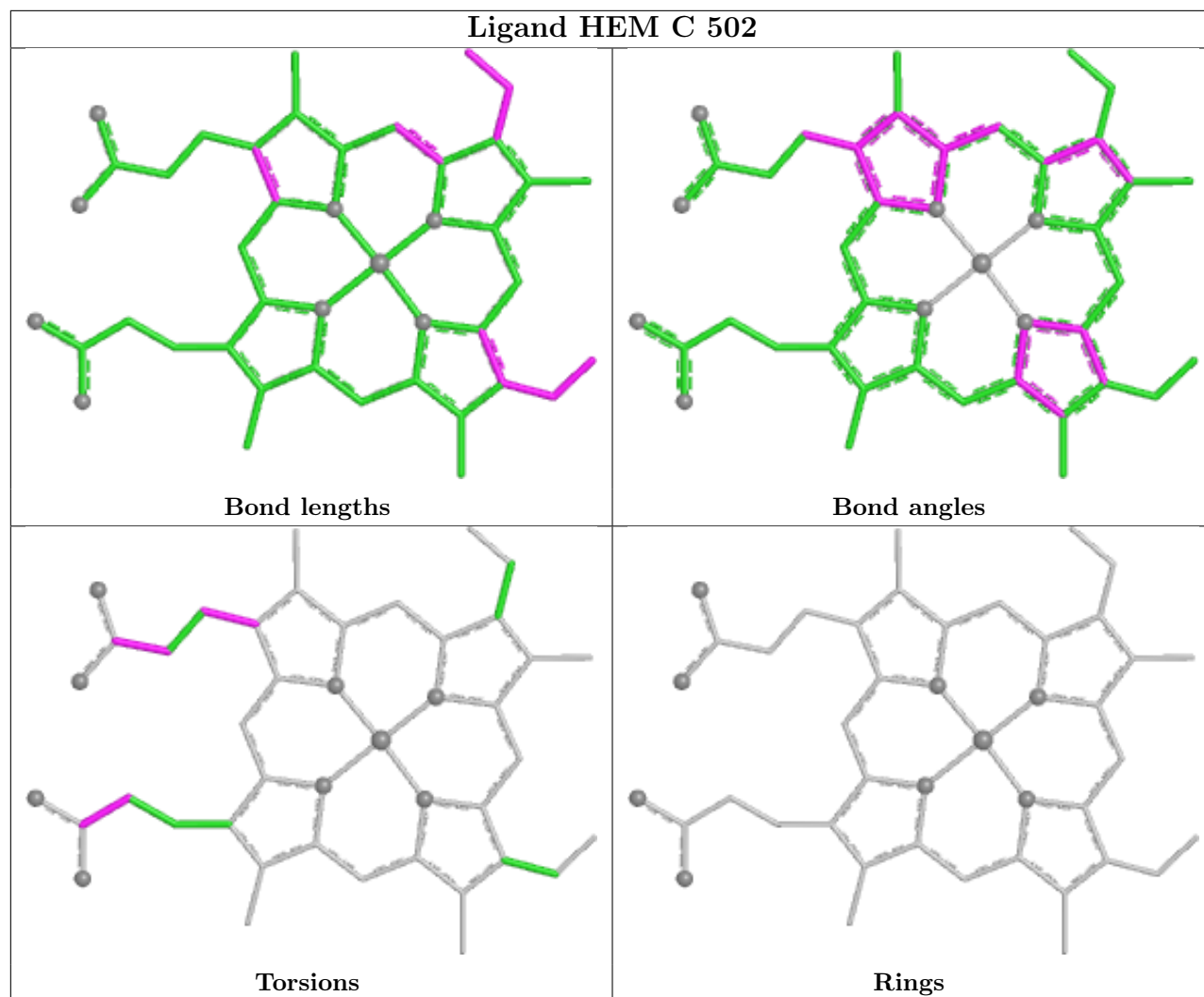
Continued on next page...

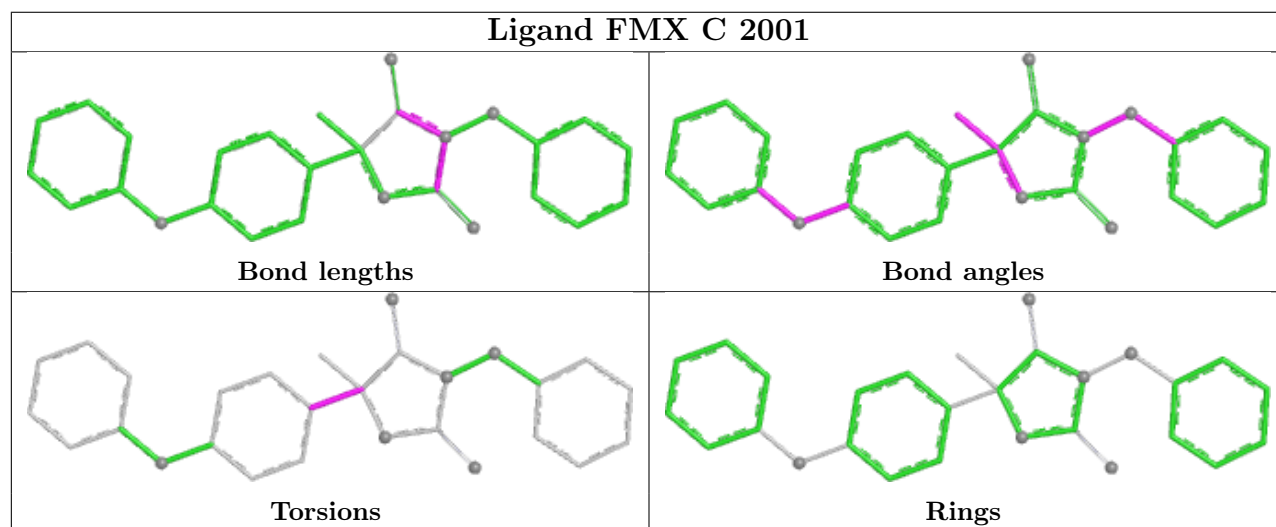
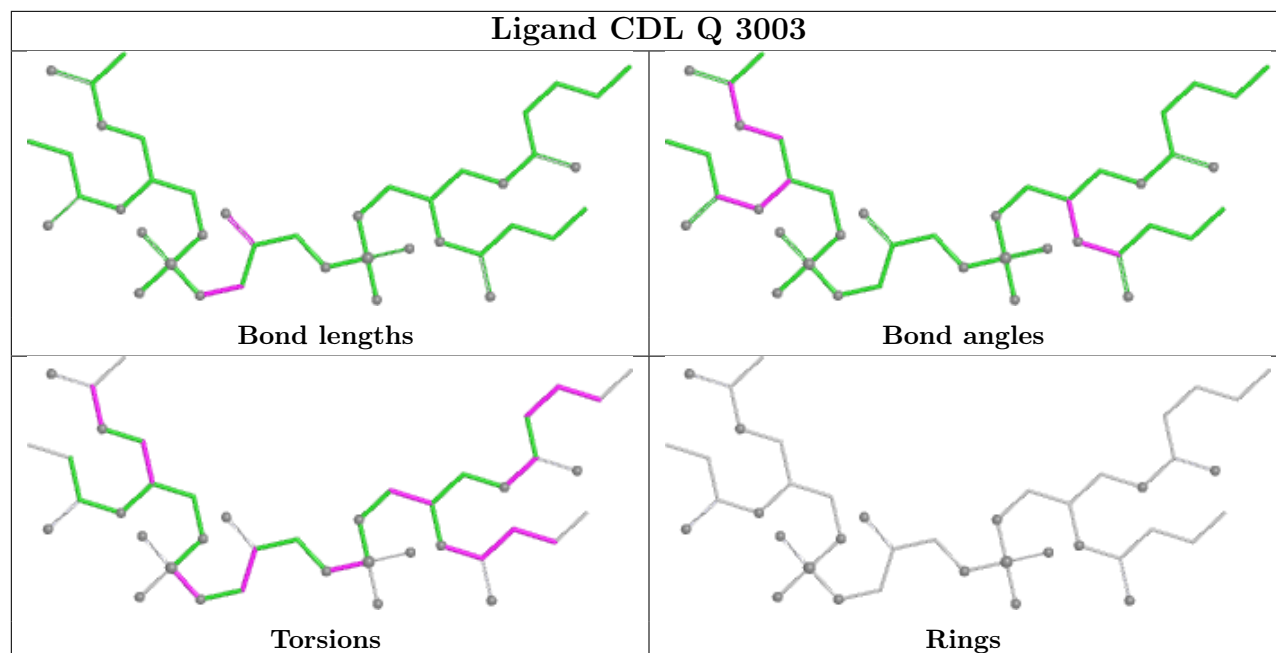
Continued from previous page...

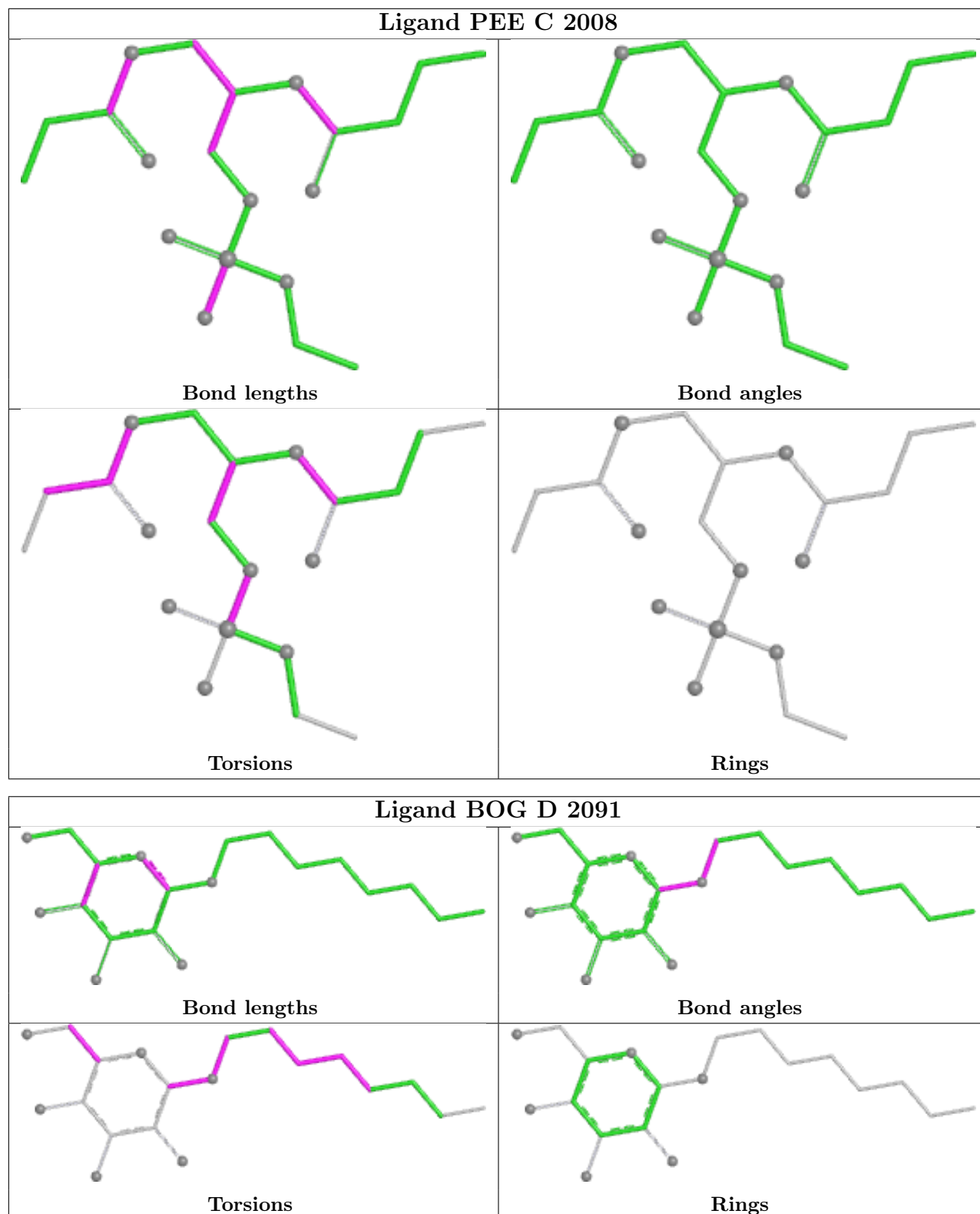
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	502	HEM	4	0
19	Q	3003	CDL	3	0
20	E	501	FES	1	0
14	C	2001	FMX	2	0
17	D	2091	BOG	2	0
15	C	2002	UQ	5	0
19	D	2003	CDL	2	0
19	T	3004	CDL	1	0
17	P	2010	BOG	1	0
19	G	2004	CDL	2	0
15	P	3002	UQ	2	0
17	Q	3091	BOG	1	0
13	P	502	HEM	4	0
13	P	501	HEM	3	0
20	R	501	FES	1	0
14	P	3001	FMX	2	0
18	D	501	HEC	2	0
13	C	501	HEM	4	0

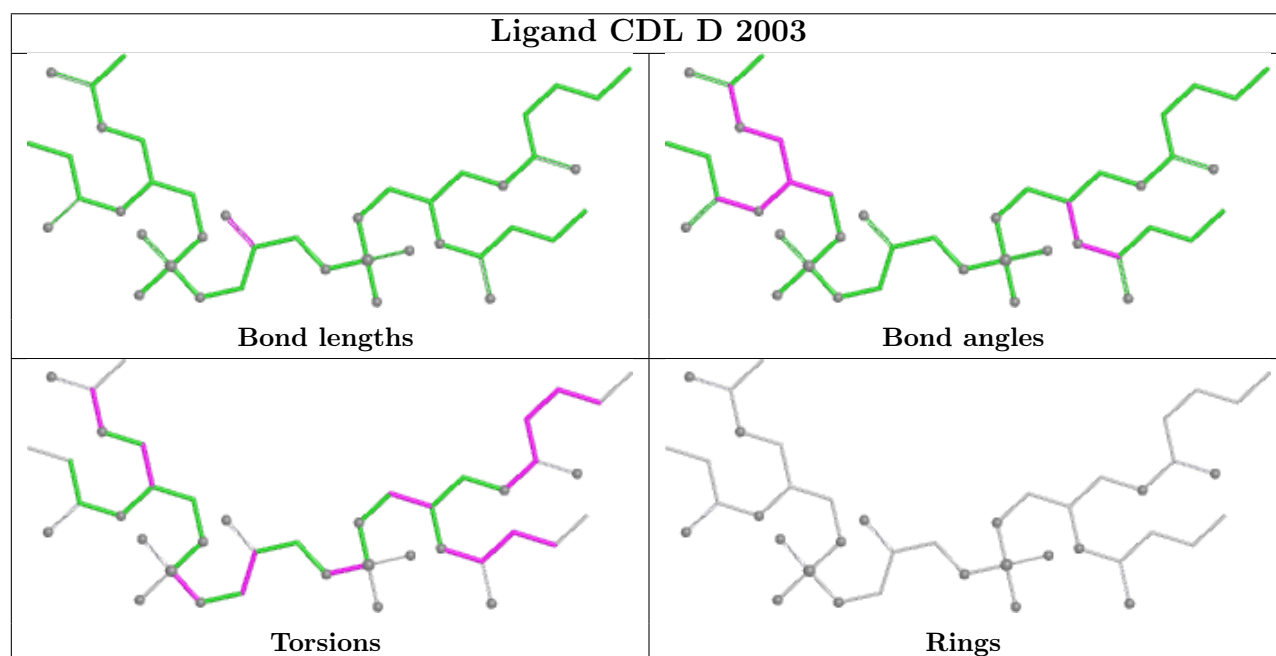
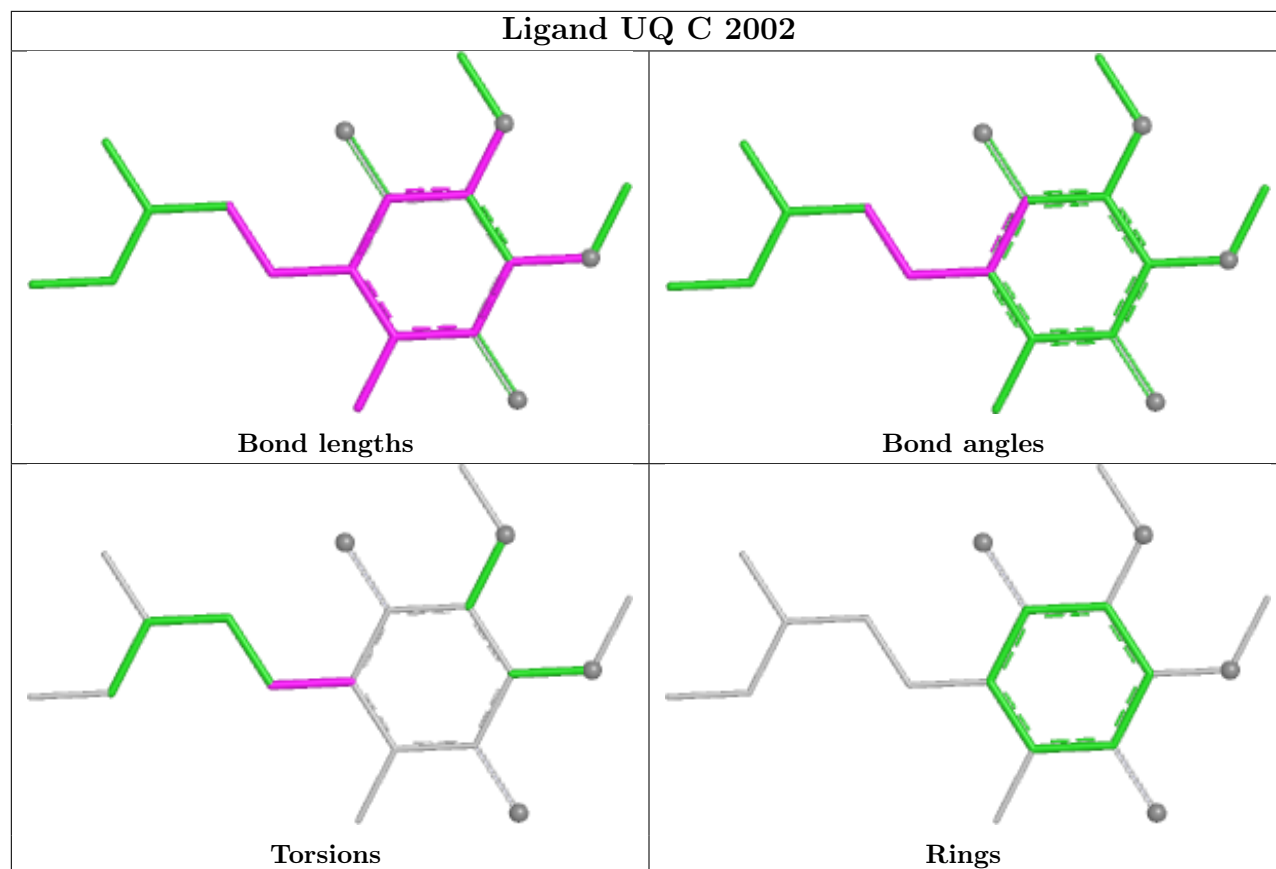
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

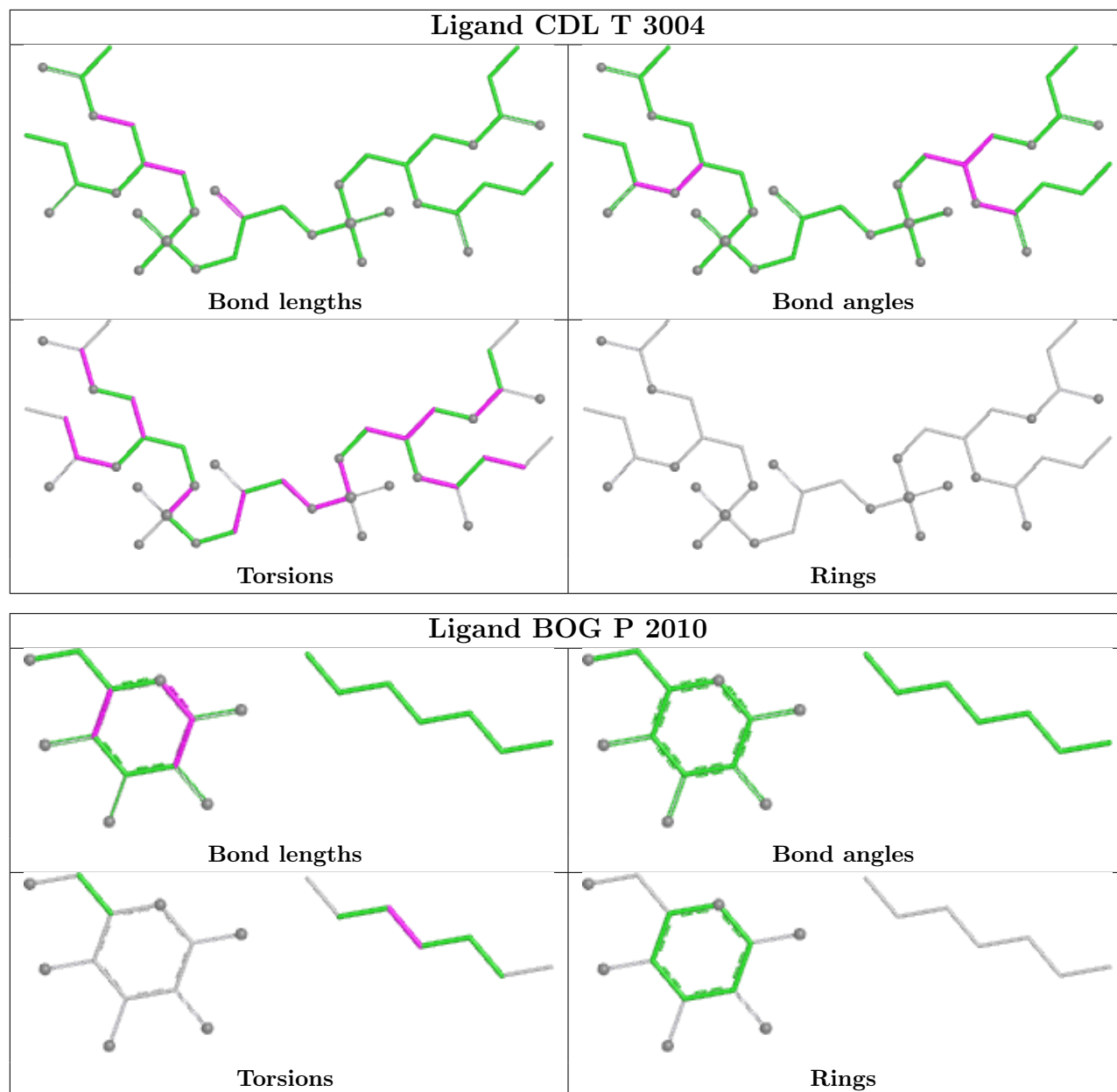




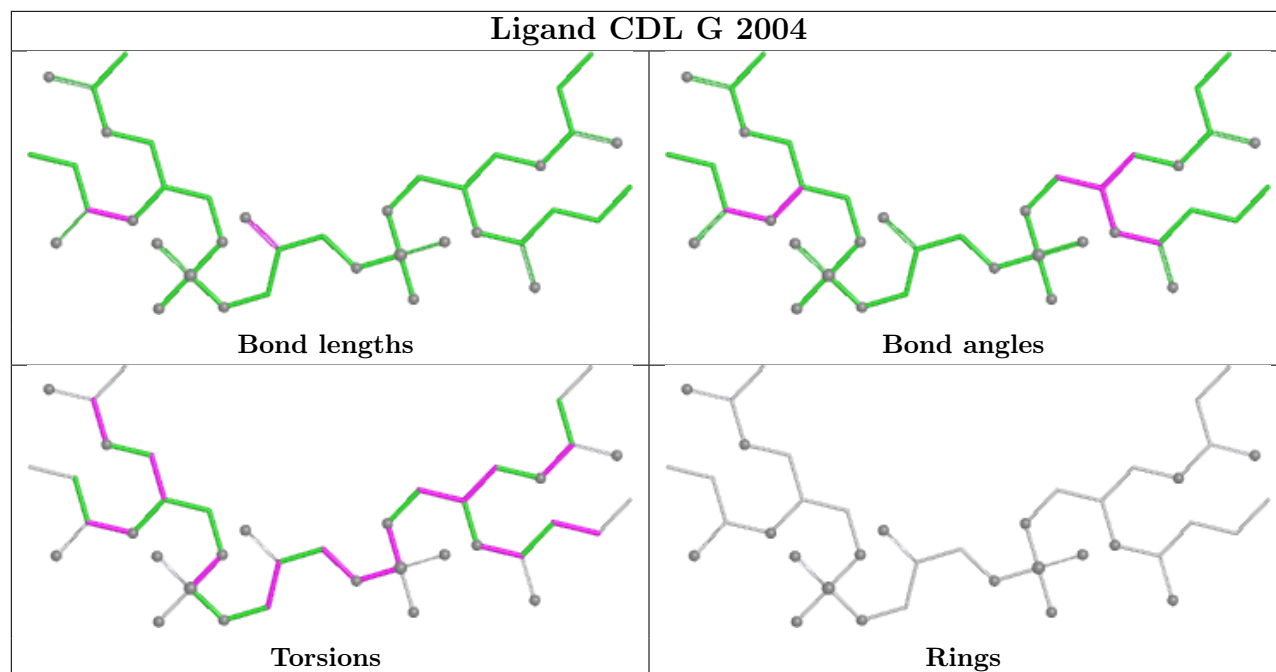




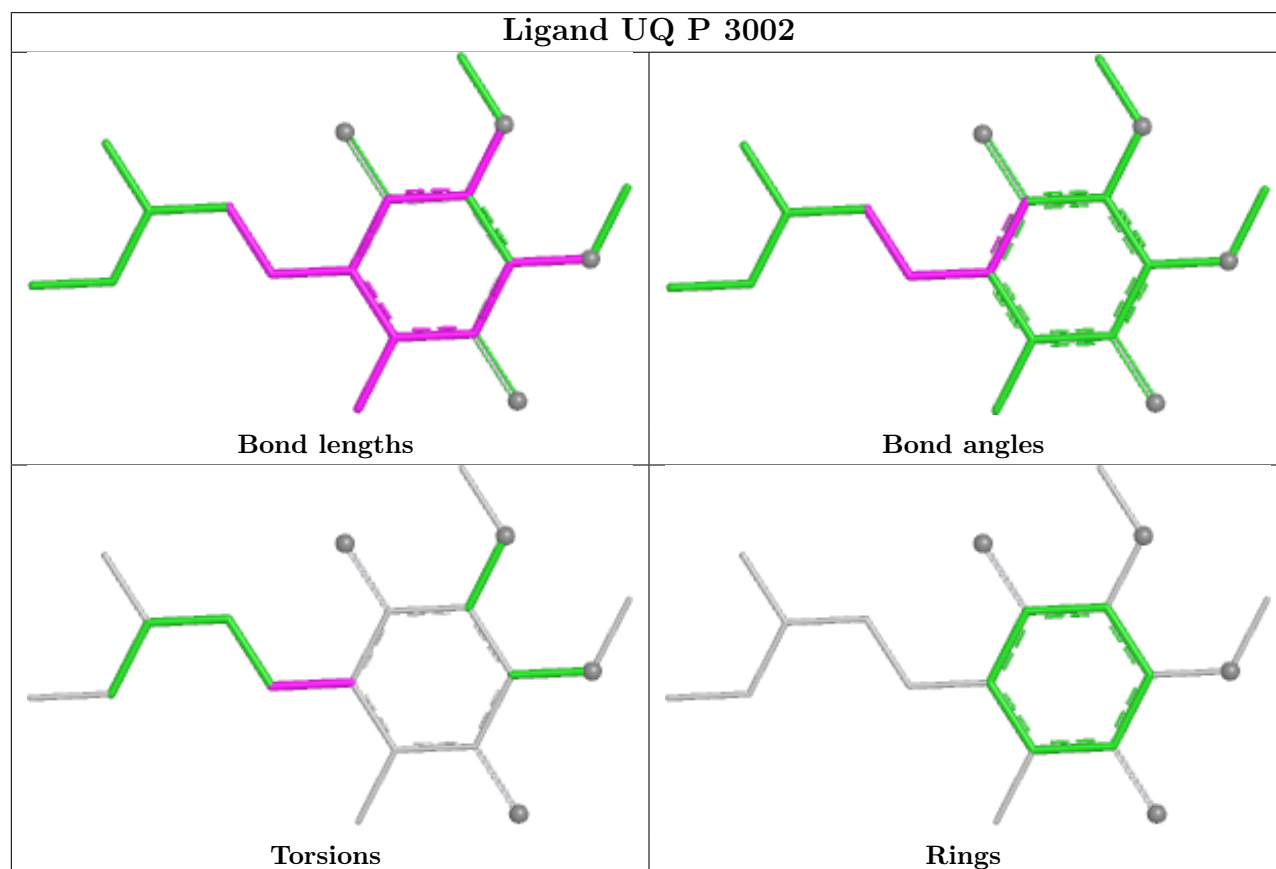


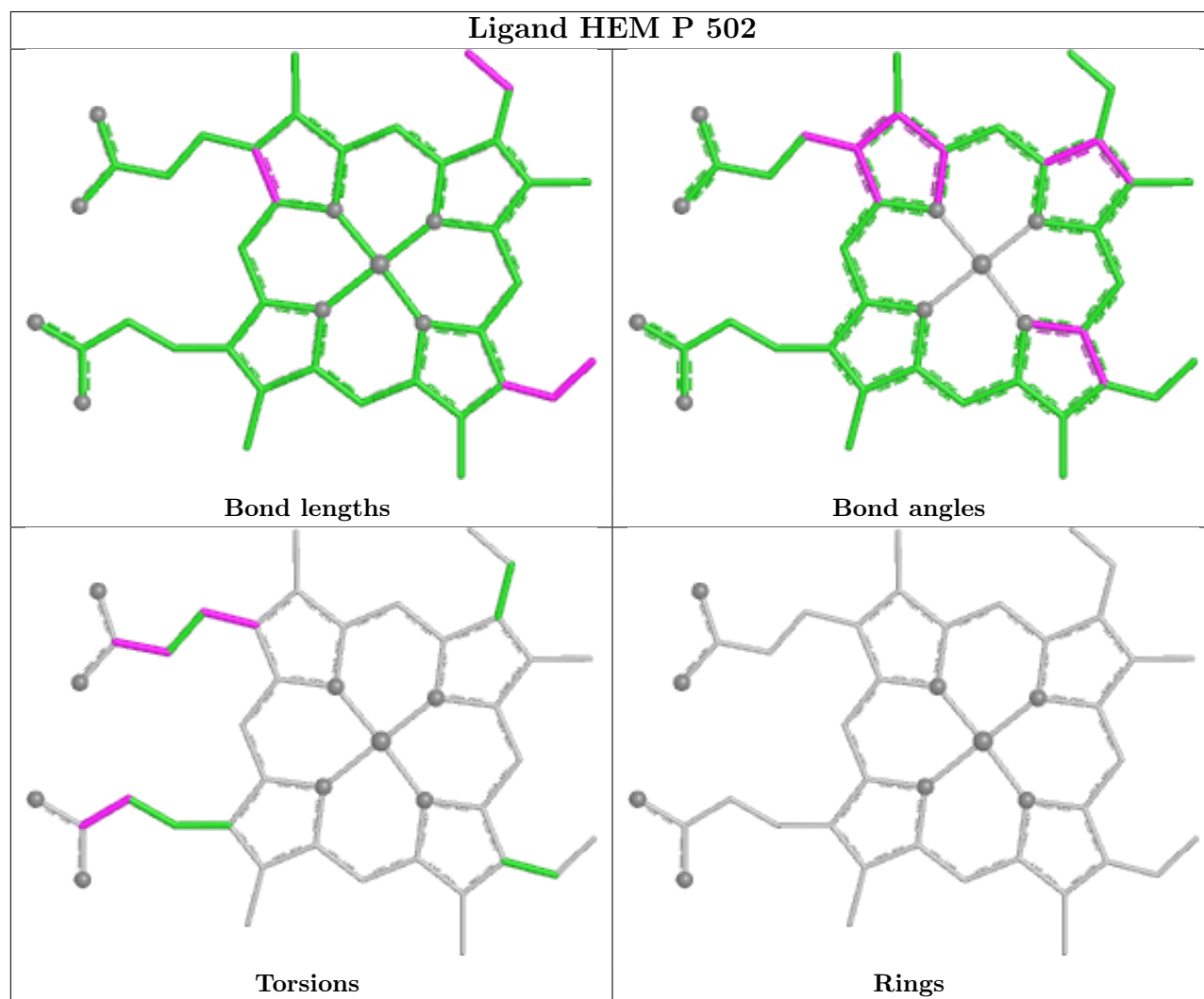
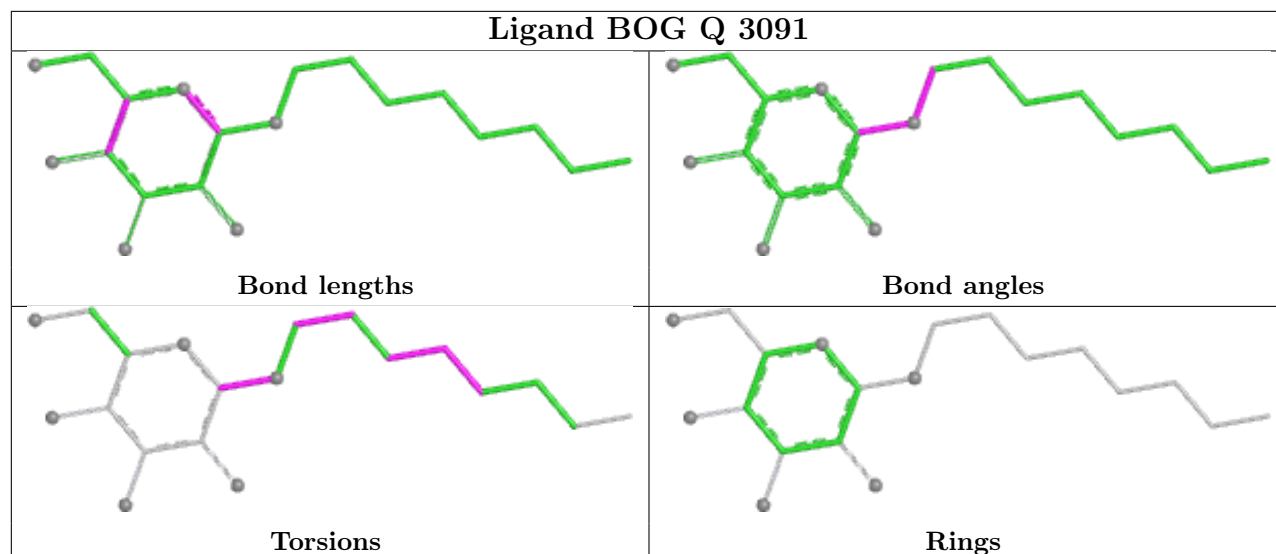


Ligand CDL G 2004

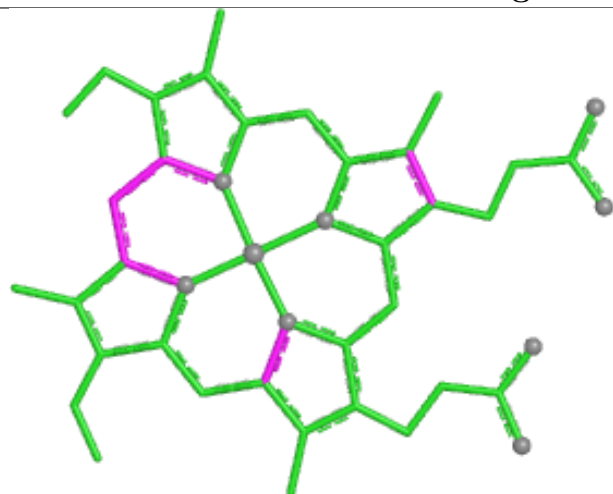


Ligand UQ P 3002

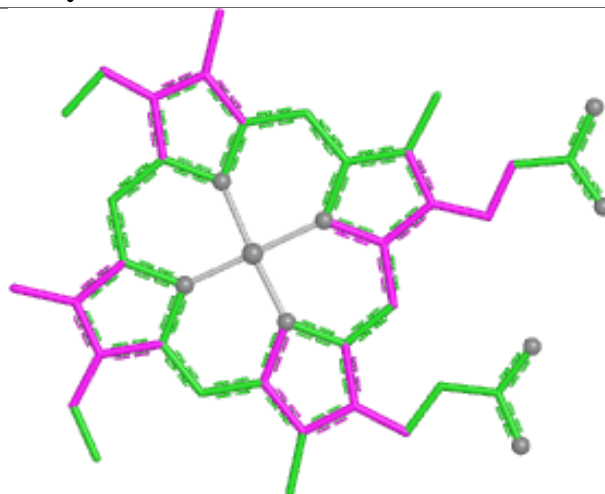




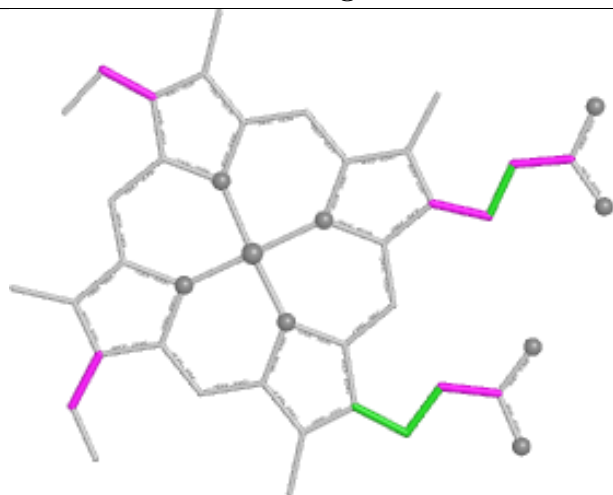
Ligand HEC Q 501



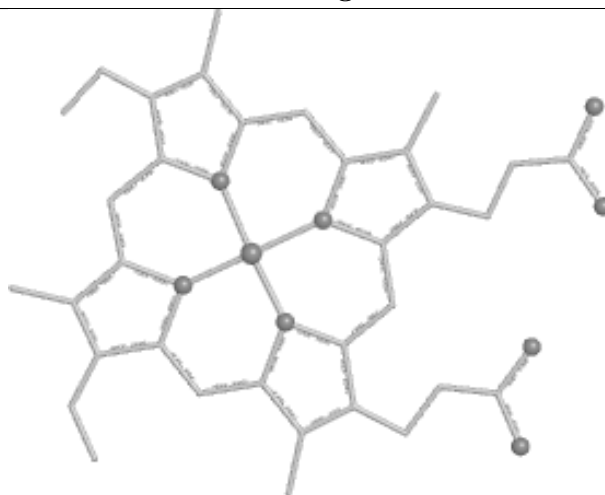
Bond lengths



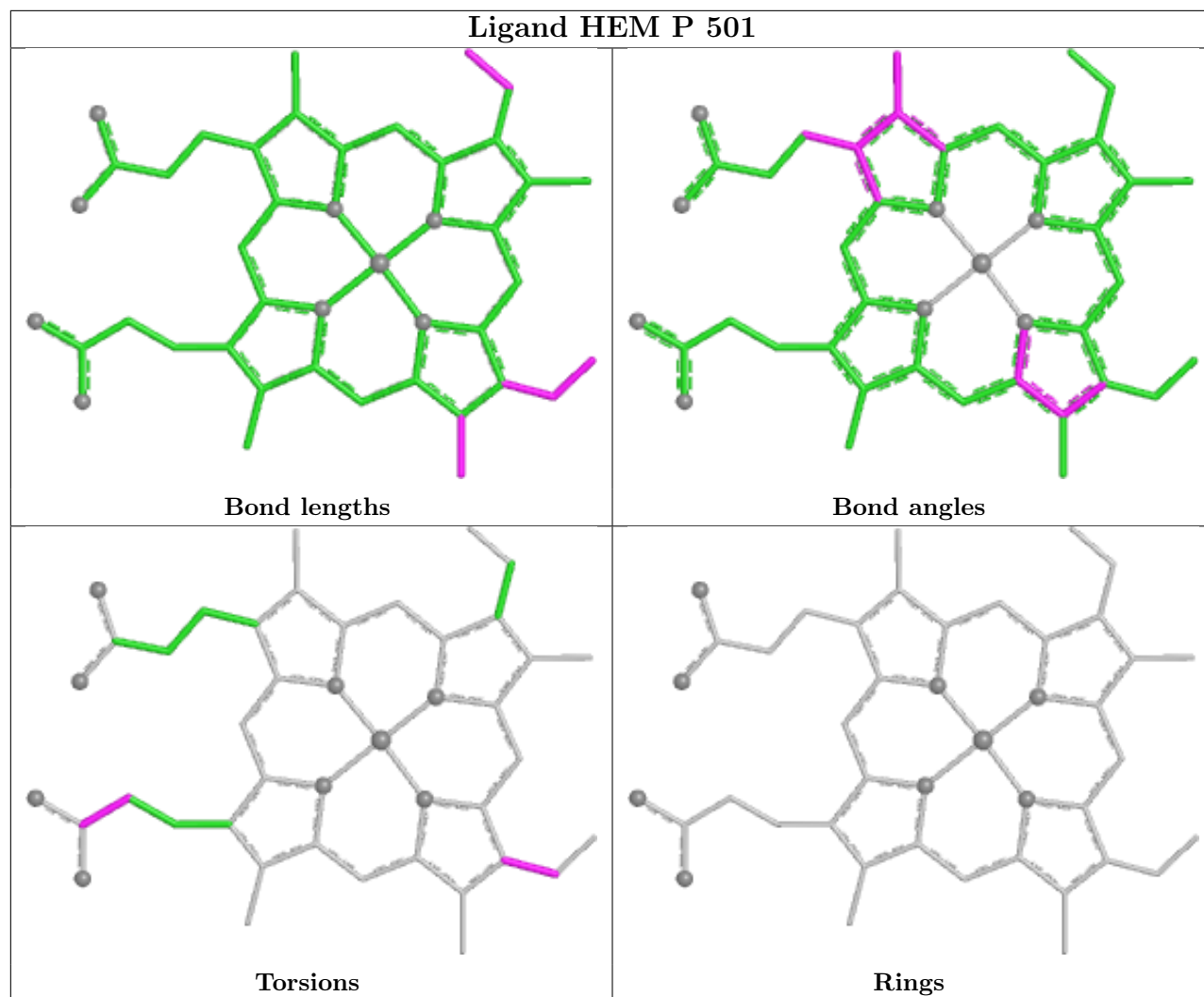
Bond angles

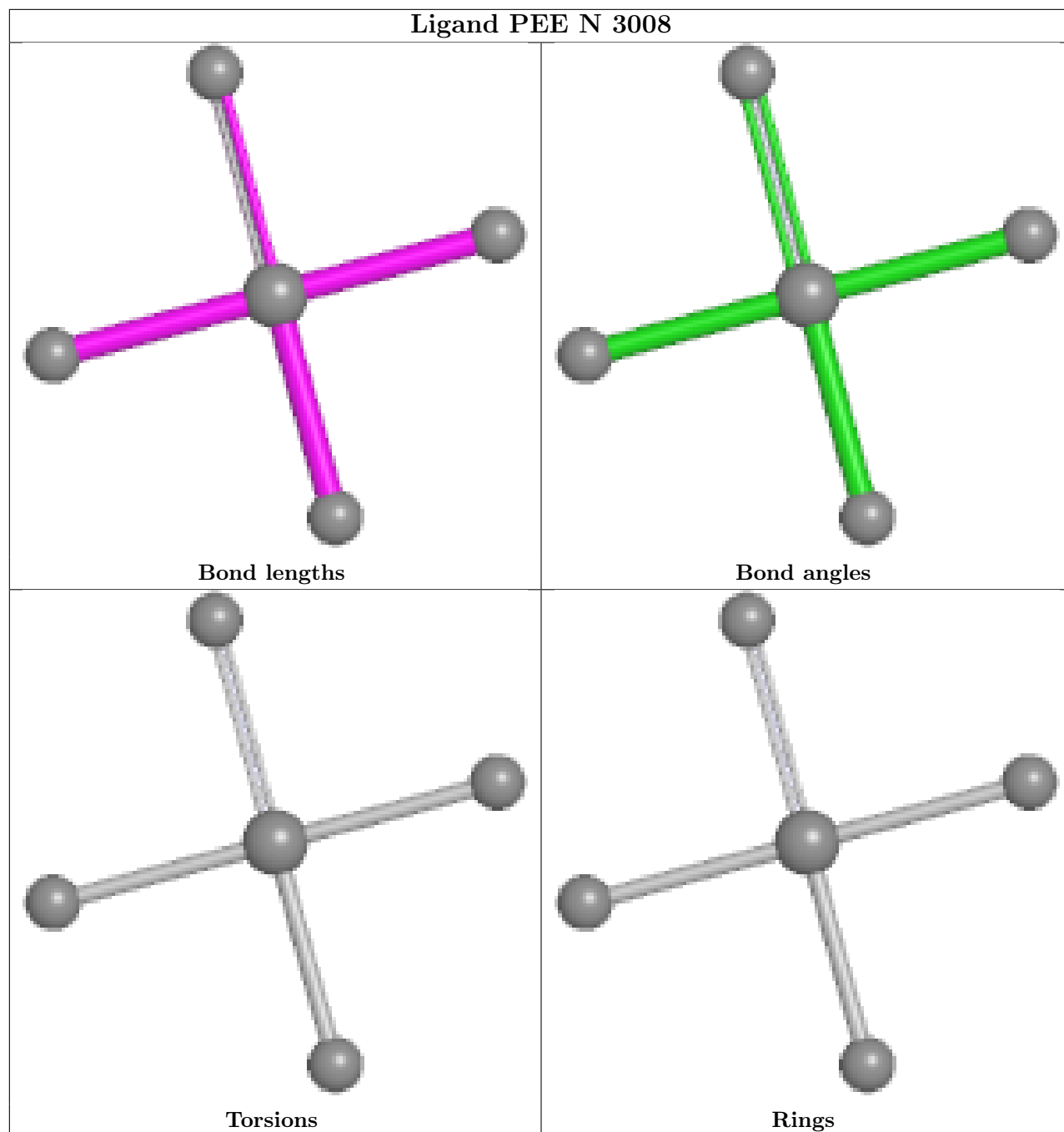


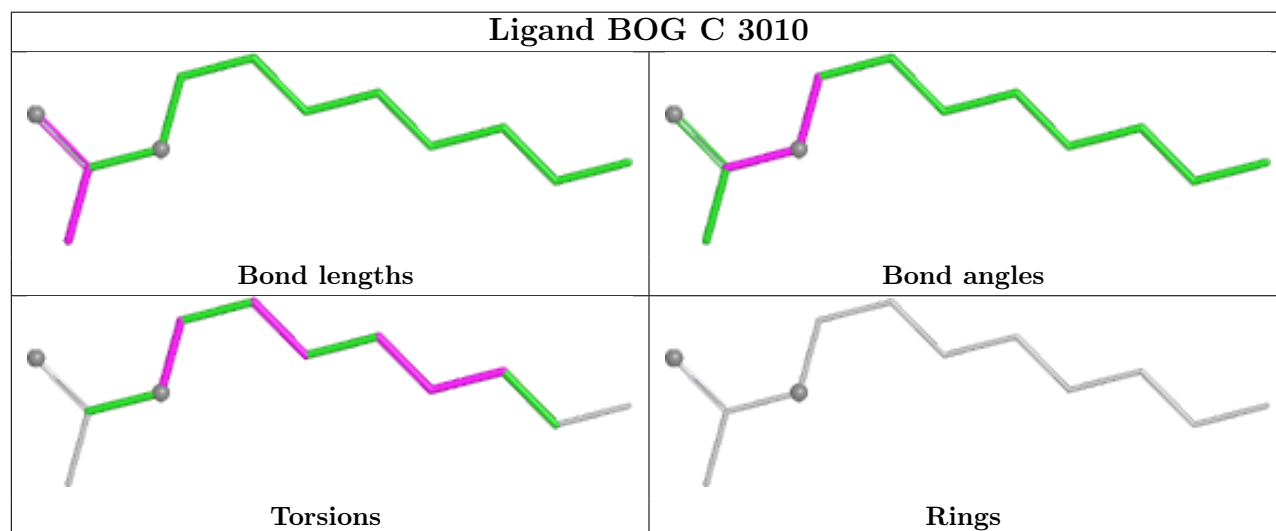
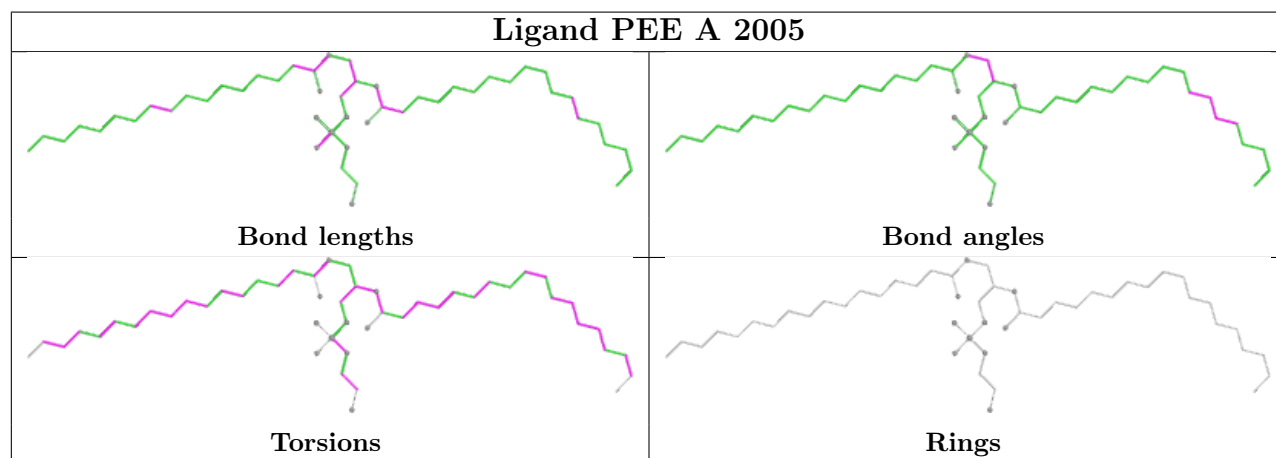
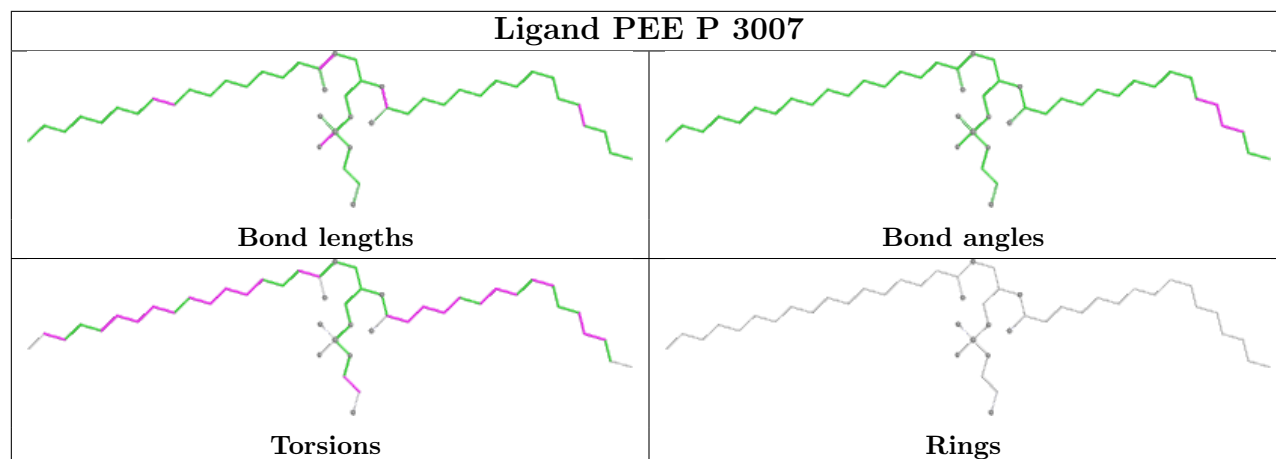
Torsions

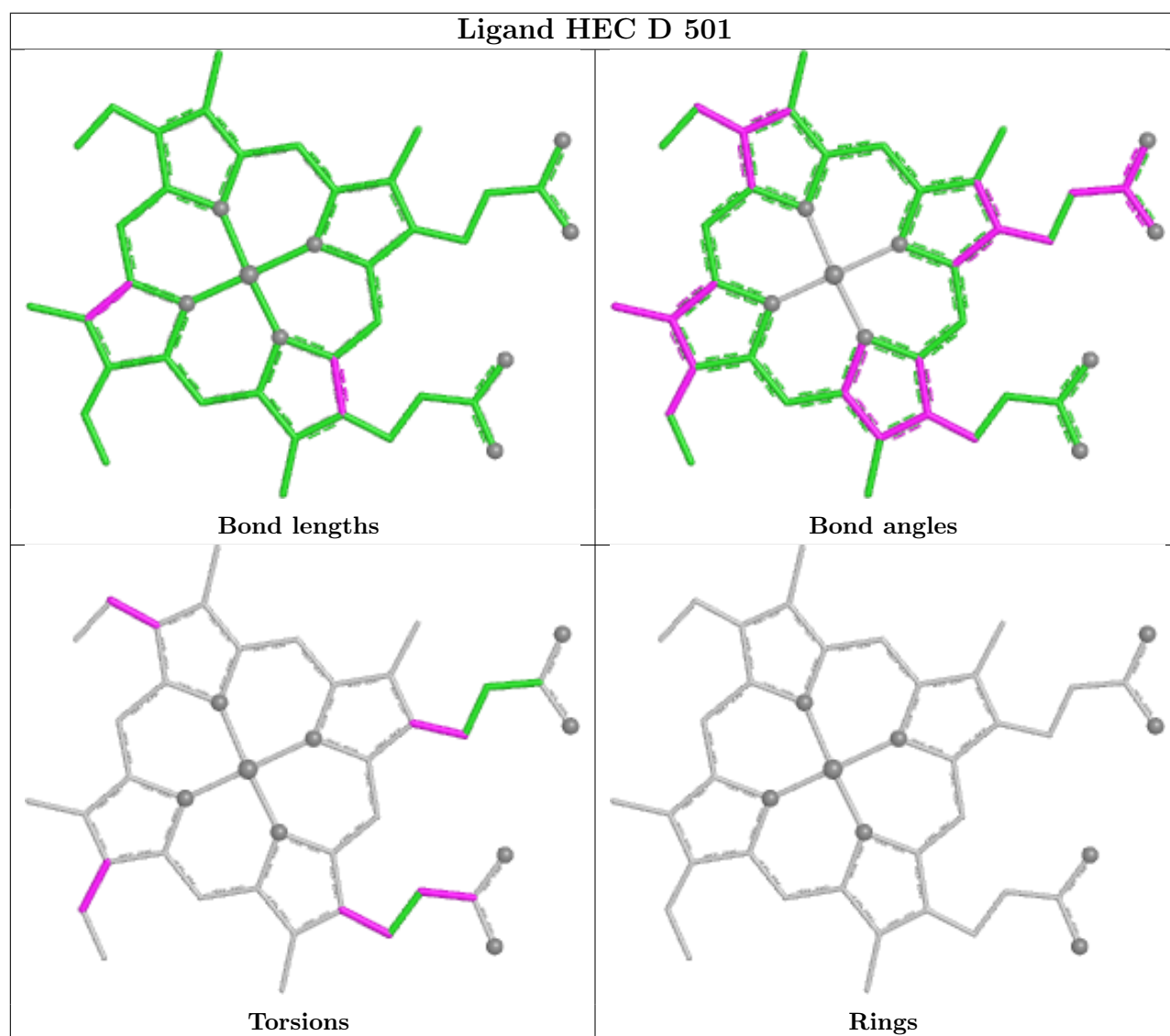
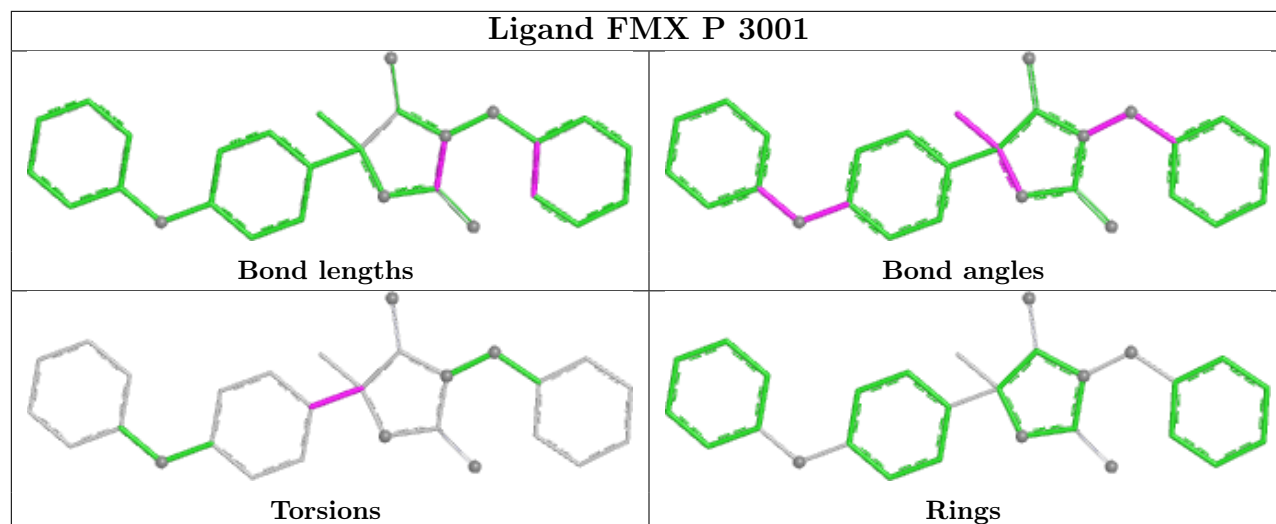


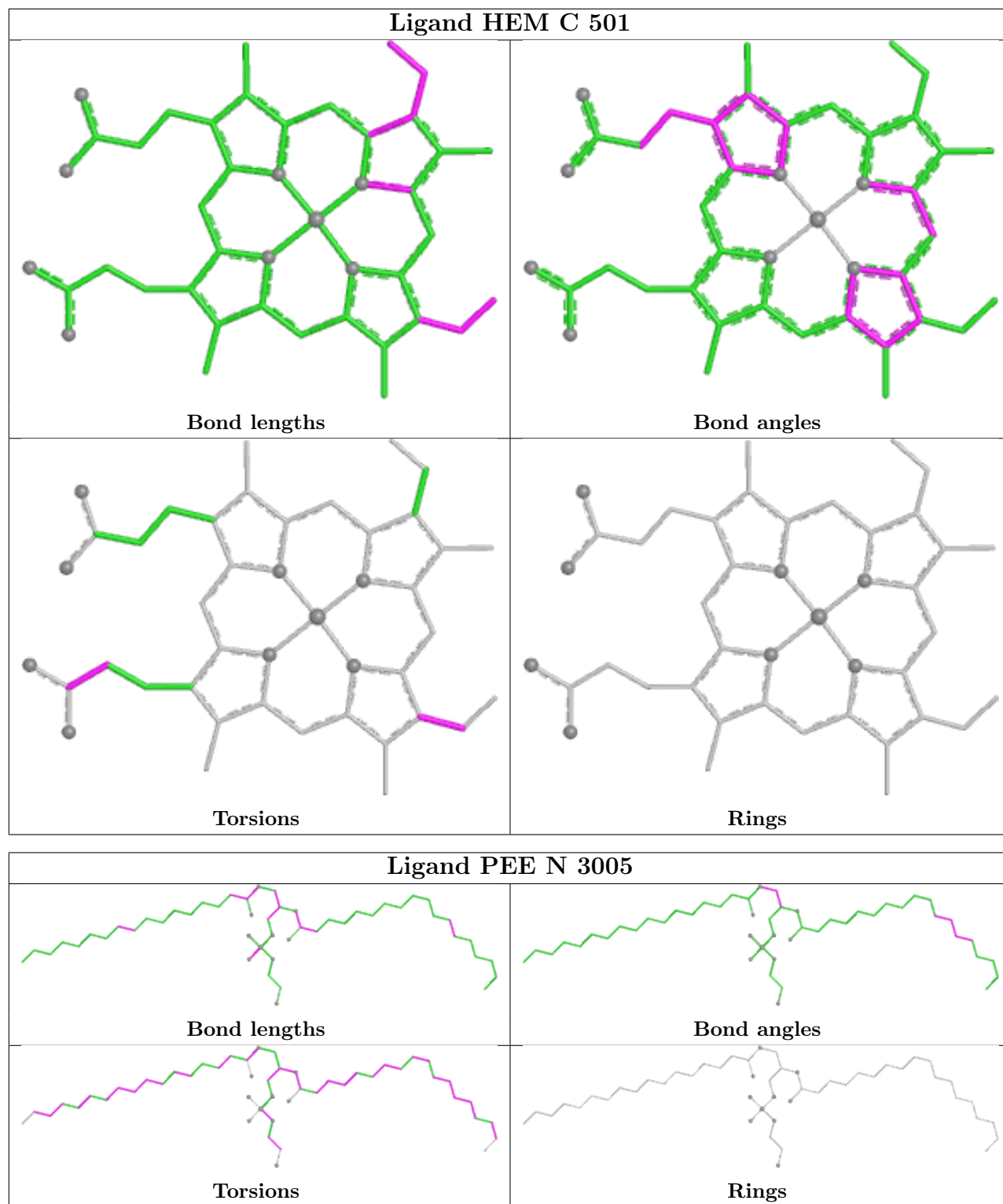
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.66	29 (6%) 25 24	29, 57, 82, 98	0
1	N	442/446 (99%)	1.21	95 (21%) 2 2	33, 64, 89, 98	0
2	B	421/441 (95%)	1.30	89 (21%) 2 2	44, 74, 109, 136	0
2	O	422/441 (95%)	1.13	67 (15%) 5 4	32, 69, 100, 114	0
3	C	380/380 (100%)	-0.15	6 (1%) 70 69	18, 33, 63, 102	0
3	P	379/380 (99%)	0.66	25 (6%) 24 24	26, 56, 76, 85	0
4	D	241/241 (100%)	-0.14	6 (2%) 58 56	25, 36, 70, 88	0
4	Q	241/241 (100%)	1.07	35 (14%) 6 5	39, 65, 91, 114	0
5	E	196/196 (100%)	1.27	54 (27%) 1 1	33, 76, 107, 114	0
5	R	196/196 (100%)	2.56	104 (53%) 0 0	32, 98, 147, 152	0
6	F	101/110 (91%)	-0.19	1 (0%) 79 79	19, 35, 54, 85	0
6	S	101/110 (91%)	1.10	14 (13%) 6 5	52, 65, 106, 131	0
7	G	81/81 (100%)	0.44	7 (8%) 16 16	28, 46, 82, 97	0
7	T	78/81 (96%)	1.59	19 (24%) 2 1	43, 77, 139, 156	0
8	H	70/77 (90%)	0.56	6 (8%) 16 16	34, 51, 75, 115	0
8	U	67/77 (87%)	2.45	42 (62%) 0 0	87, 108, 130, 134	0
9	I	31/47 (65%)	3.80	27 (87%) 0 0	80, 102, 120, 121	0
9	V	31/47 (65%)	3.91	28 (90%) 0 0	65, 105, 136, 138	0
10	J	61/61 (100%)	0.44	5 (8%) 17 18	40, 53, 85, 124	0
10	W	60/61 (98%)	1.24	9 (15%) 5 5	52, 70, 96, 105	0
All	All	4042/4160 (97%)	0.94	668 (16%) 4 4	18, 61, 107, 156	0

The worst 5 of 668 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	195	VAL	9.6
5	R	194	VAL	9.2
9	V	63	ASP	9.0
5	R	114	VAL	8.8
5	R	193	VAL	8.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	UNL	P	3048	2/-	0.39	0.88	93,93,93,95	0
17	BOG	Q	3091	20/20	0.48	0.39	172,179,180,180	0
17	BOG	D	2091	20/20	0.65	0.54	171,182,183,184	0
17	BOG	P	2010	19/20	0.73	0.43	97,177,178,178	0
12	UNL	P	3046	2/-	0.77	0.27	85,85,85,86	0
12	UNL	C	2048	2/-	0.78	0.31	41,41,41,45	0
19	CDL	T	3004	40/100	0.78	0.27	85,89,100,101	0
19	CDL	Q	3003	42/100	0.81	0.28	114,118,123,124	0
11	PEE	C	2008	21/51	0.82	0.24	89,103,110,111	0
19	CDL	D	2003	42/100	0.82	0.20	60,75,87,88	0
15	UQ	C	2002	19/63	0.83	0.29	80,84,86,86	0
12	UNL	P	3047	1/-	0.85	0.12	45,45,45,45	0
12	UNL	P	3014	1/-	0.85	0.19	55,55,55,55	0
12	UNL	E	2012	2/-	0.86	0.20	51,51,51,51	0
11	PEE	N	3005	50/51	0.86	0.27	64,92,98,98	0
15	UQ	P	3002	19/63	0.86	0.36	132,136,138,138	0
12	UNL	Q	3012	1/-	0.87	0.20	33,33,33,33	0
19	CDL	G	2004	40/100	0.87	0.17	48,63,77,78	0
17	BOG	Q	3009	20/20	0.87	0.19	69,80,83,84	0

Continued on next page...

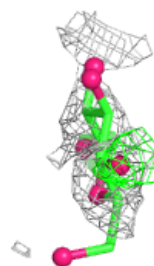
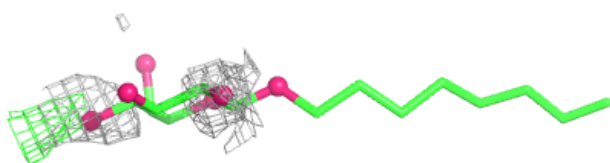
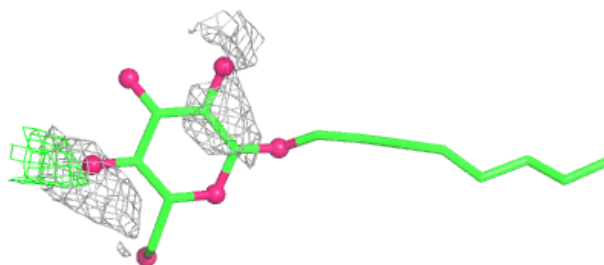
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	PEE	N	3008	5/51	0.87	0.11	74,74,75,76	0
17	BOG	D	2009	20/20	0.88	0.14	47,57,61,61	0
12	UNL	P	3013	1/-	0.88	0.29	72,72,72,72	0
11	PEE	A	2005	50/51	0.88	0.25	74,85,89,90	0
12	UNL	C	2046	2/-	0.89	0.21	78,78,78,80	0
14	FMX	P	3001	28/28	0.90	0.17	55,65,70,71	0
11	PEE	P	3007	48/51	0.90	0.23	71,83,98,100	0
14	FMX	C	2001	28/28	0.91	0.14	31,49,61,62	0
16	AZI	C	2011	3/3	0.91	0.20	62,62,63,64	0
17	BOG	C	3010	12/20	0.91	0.22	78,81,83,84	0
12	UNL	A	3015	1/-	0.94	0.06	45,45,45,45	0
12	UNL	C	2047	1/-	0.95	0.12	28,28,28,28	0
16	AZI	P	3011	3/3	0.95	0.17	66,66,68,68	0
11	PEE	C	2007	48/51	0.95	0.14	33,49,72,72	0
18	HEC	Q	501	43/43	0.96	0.11	40,49,58,60	0
20	FES	E	501	4/4	0.97	0.07	72,73,74,74	0
20	FES	R	501	4/4	0.97	0.14	85,85,86,86	0
13	HEM	P	502	43/43	0.98	0.07	32,38,50,56	0
18	HEC	D	501	43/43	0.98	0.07	14,25,29,32	0
13	HEM	P	501	43/43	0.98	0.09	37,41,52,56	0
13	HEM	C	501	43/43	0.99	0.07	17,27,37,40	0
13	HEM	C	502	43/43	0.99	0.06	15,20,28,32	0

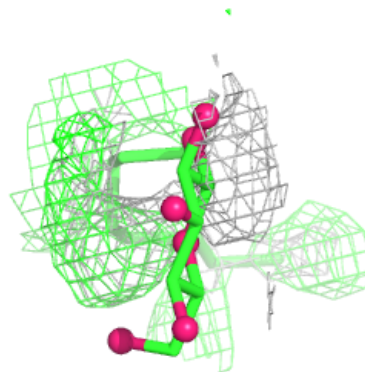
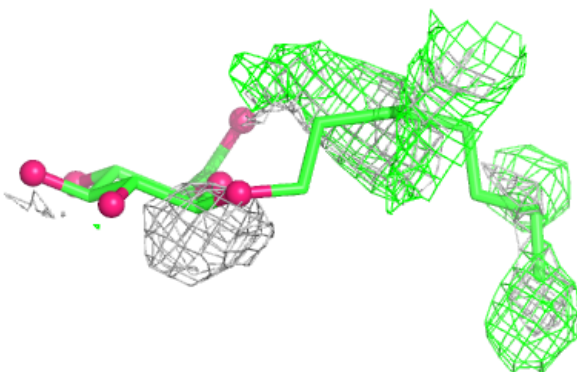
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG Q 3091:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

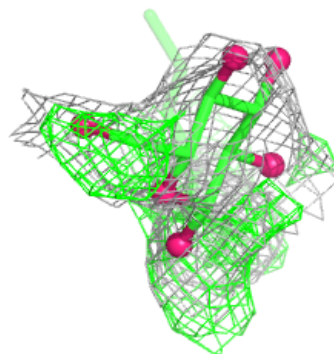
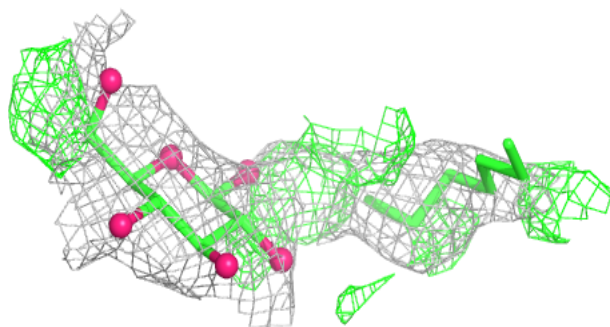
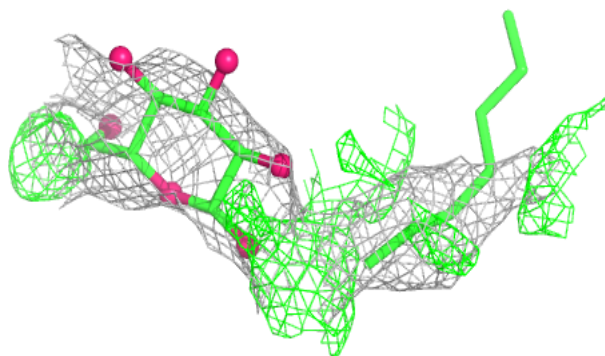
**Electron density around BOG D 2091:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



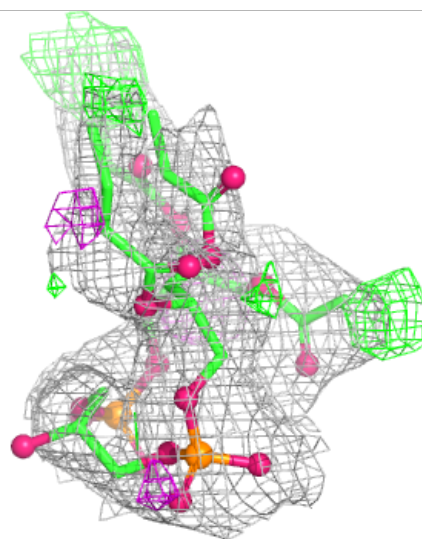
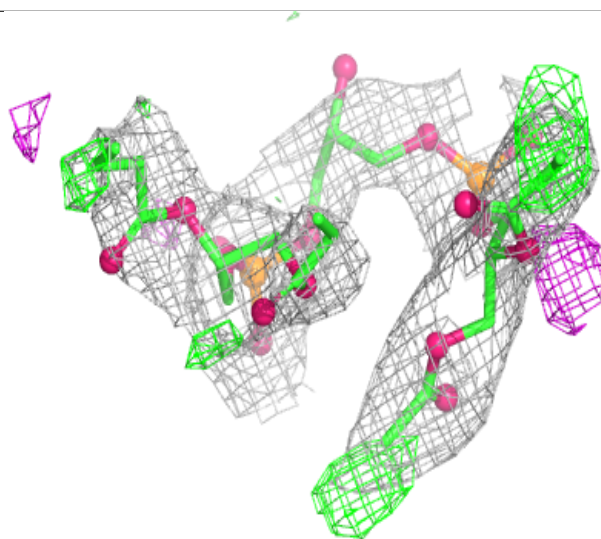
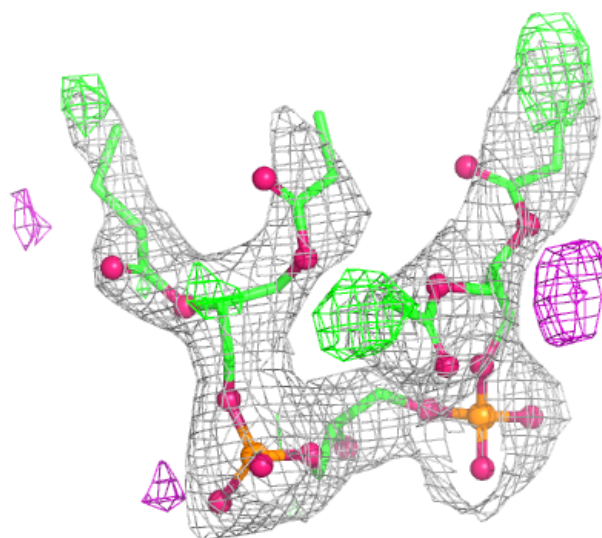
Electron density around BOG P 2010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



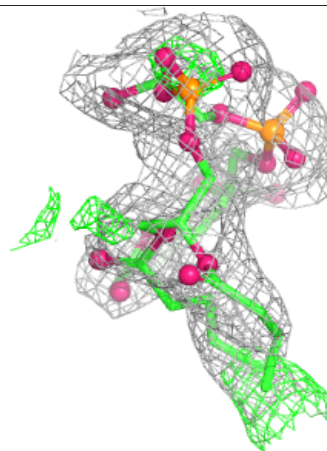
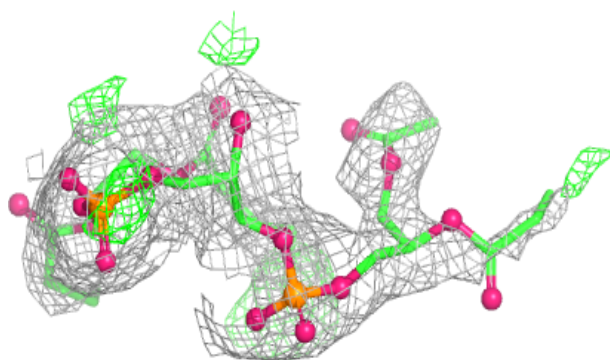
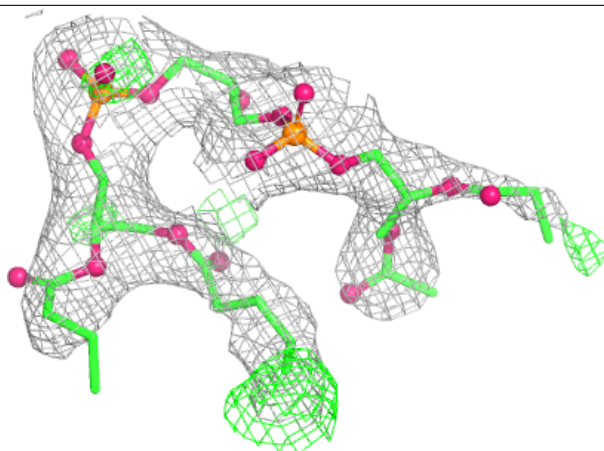
Electron density around CDL T 3004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



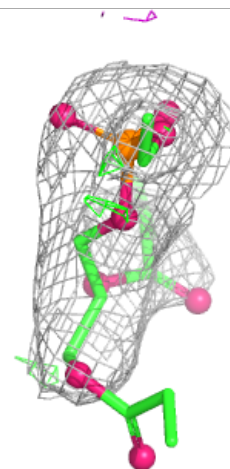
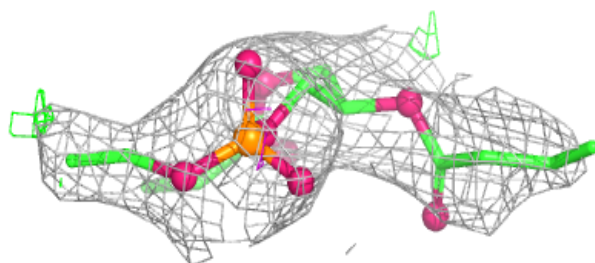
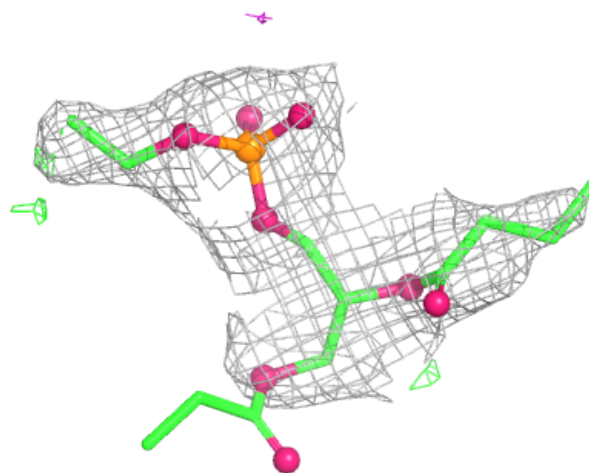
Electron density around CDL Q 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



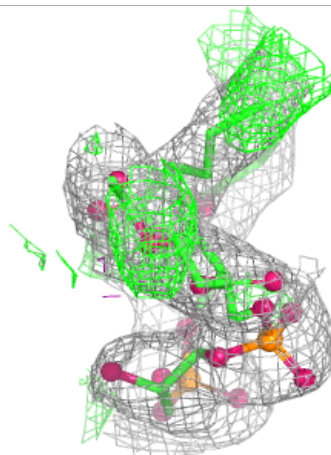
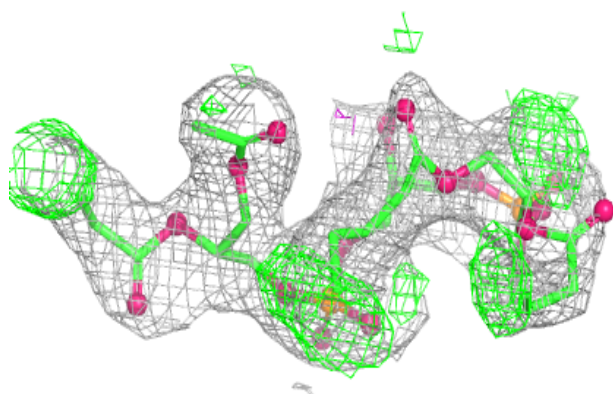
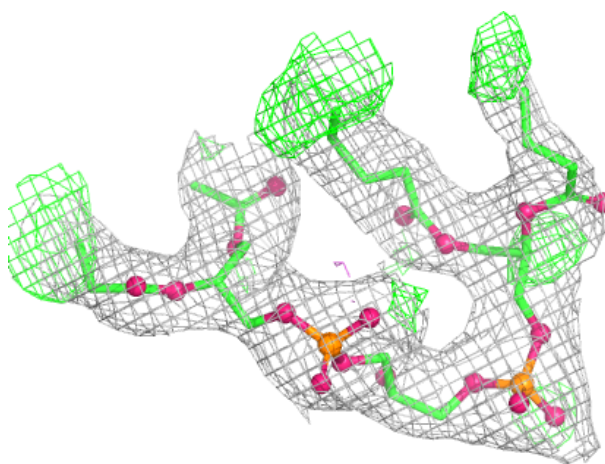
Electron density around PEE C 2008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



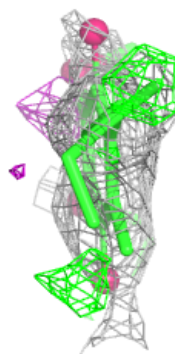
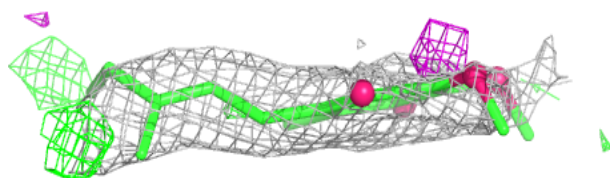
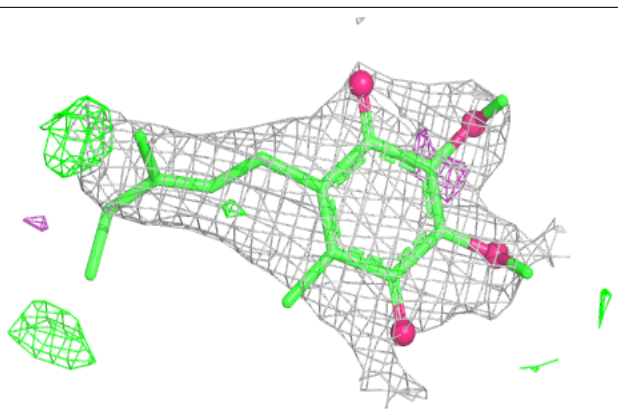
Electron density around CDL D 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

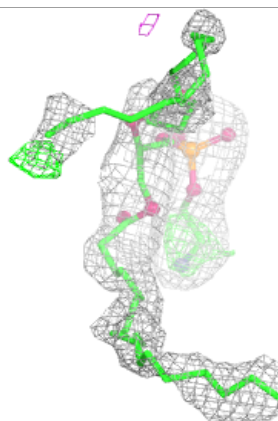
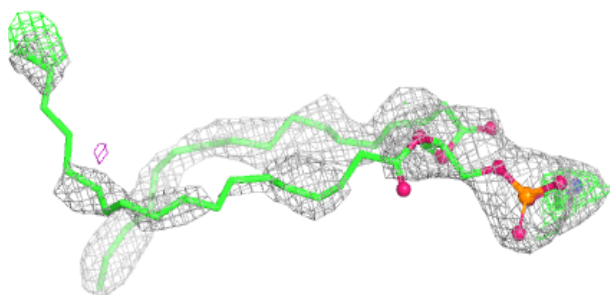
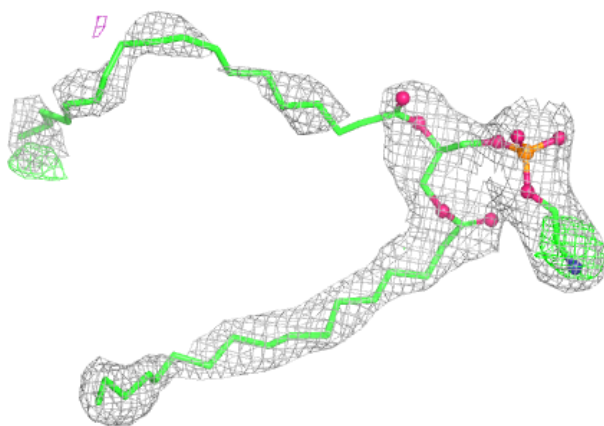


Electron density around UQ C 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

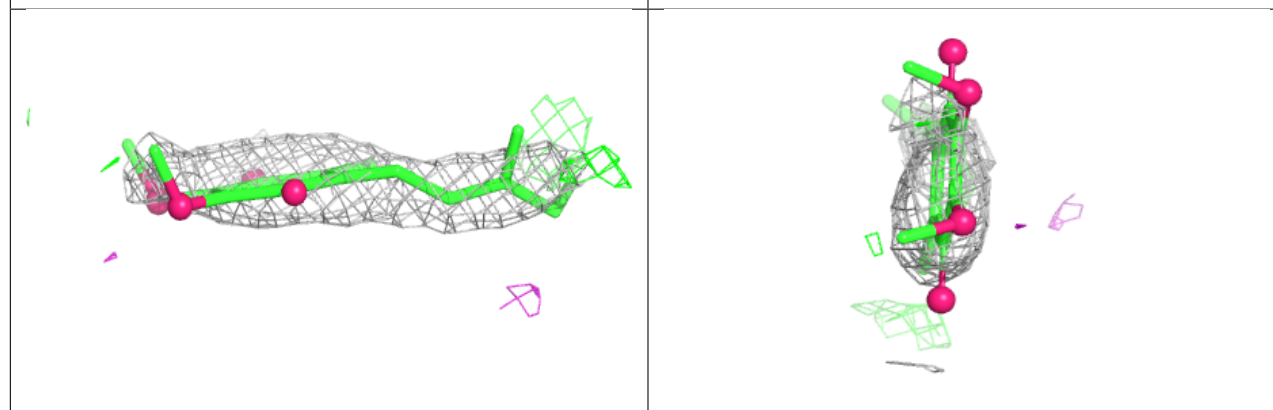
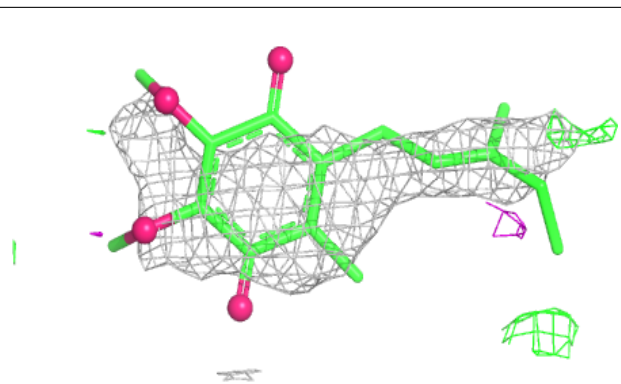
**Electron density around PEE N 3005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



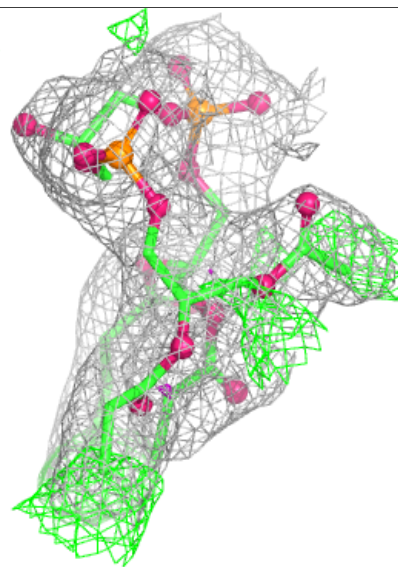
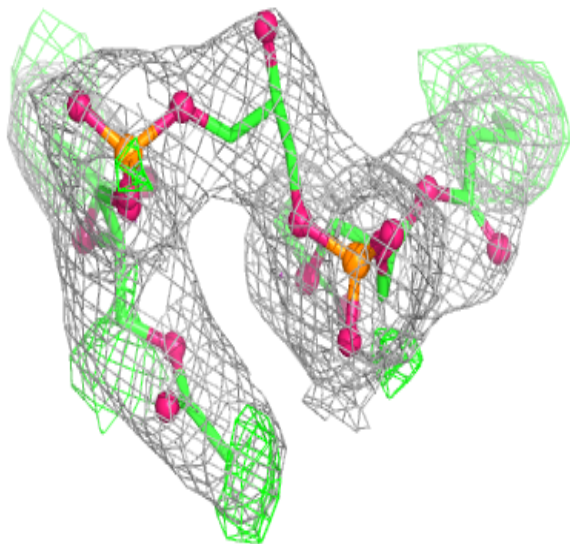
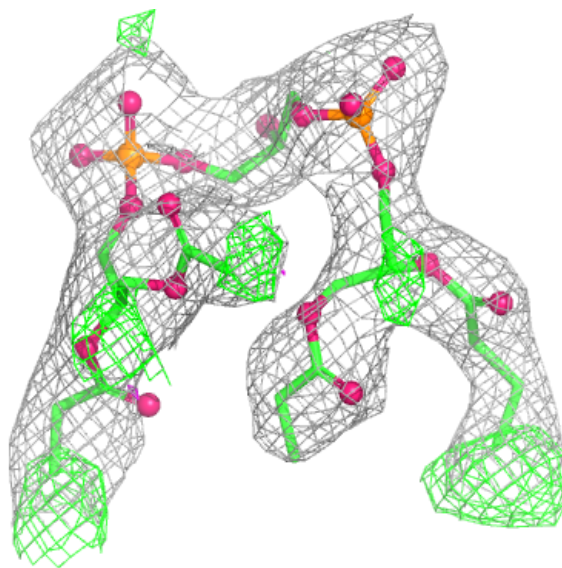
Electron density around UQ P 3002:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



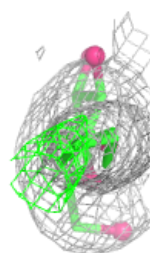
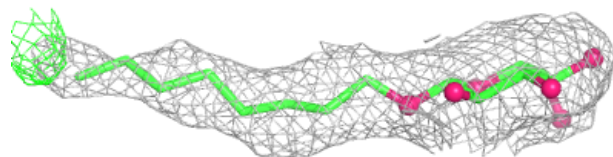
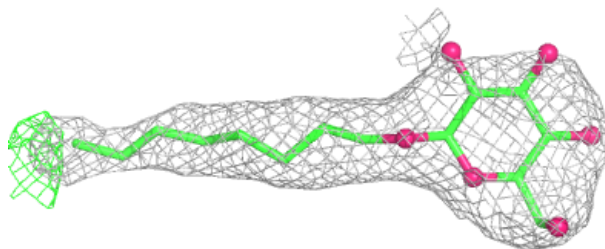
Electron density around CDL G 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



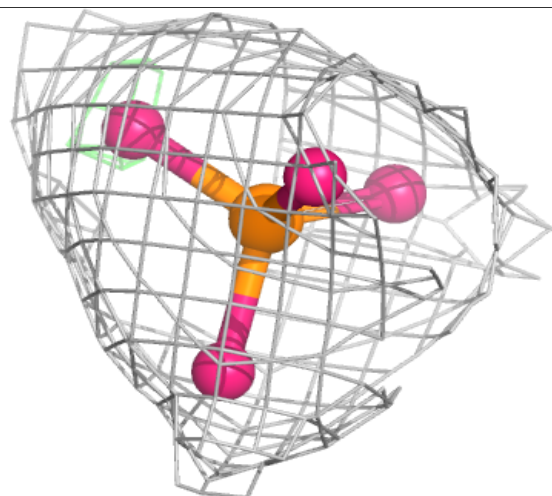
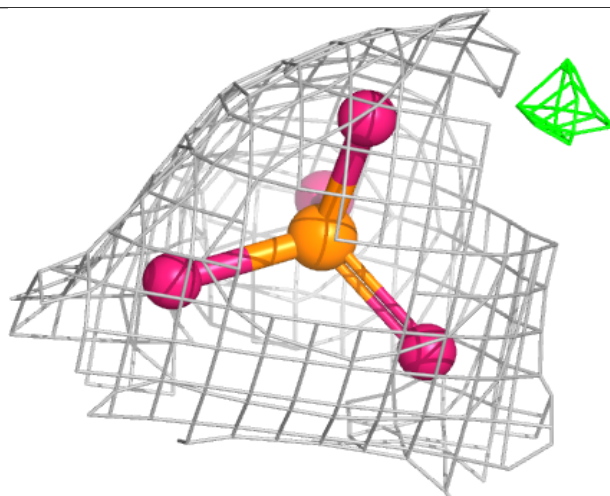
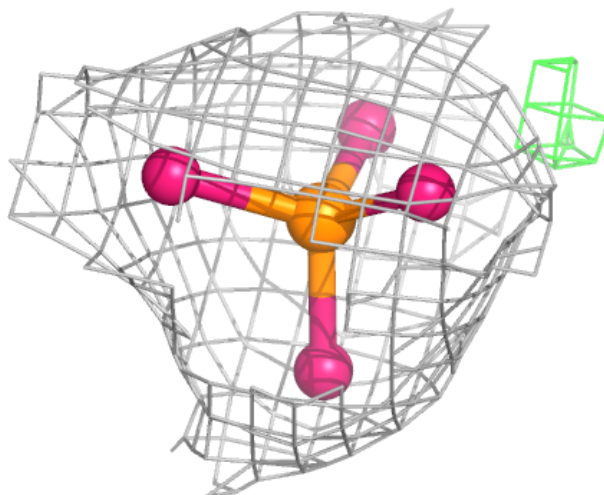
Electron density around BOG Q 3009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



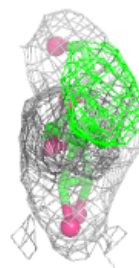
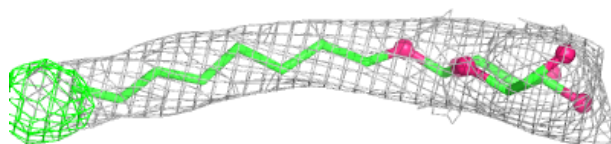
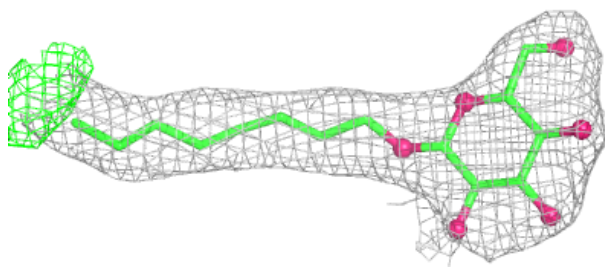
Electron density around PEE N 3008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

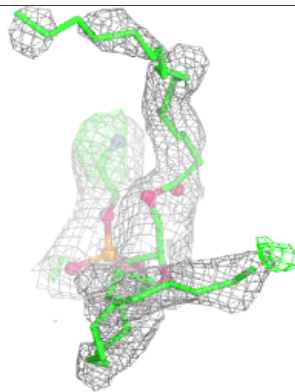
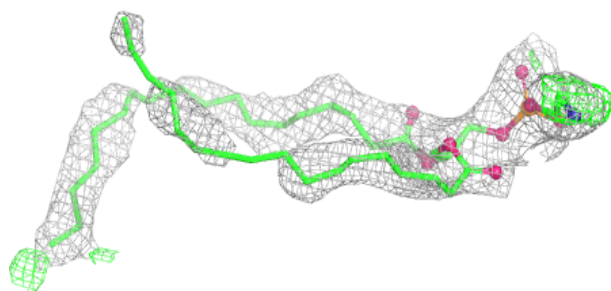
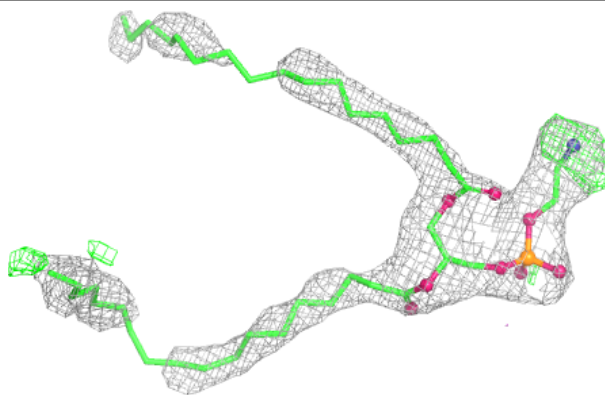


Electron density around BOG D 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

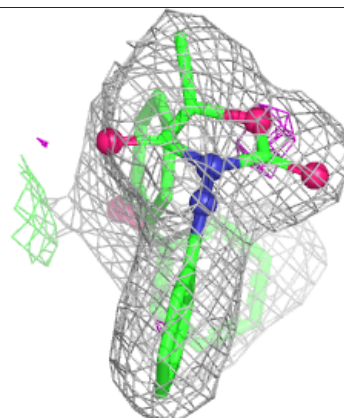
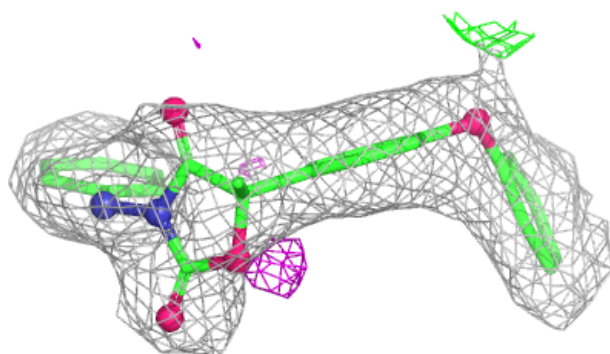
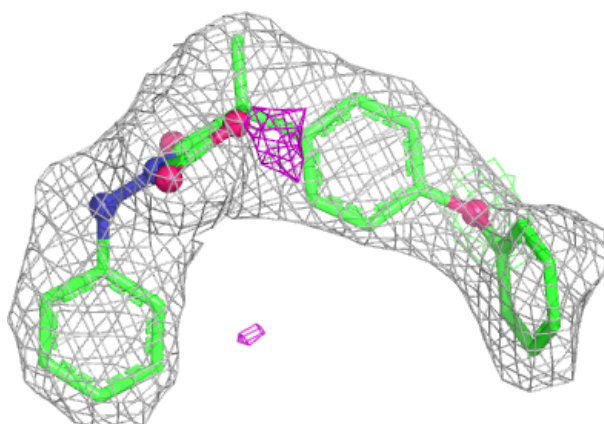
**Electron density around PEE A 2005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

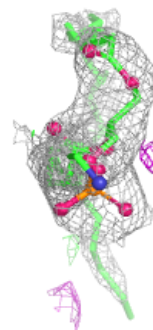
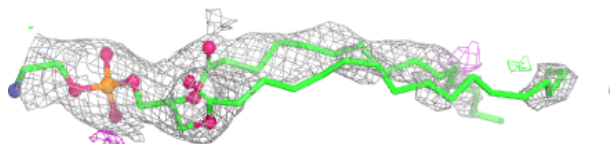
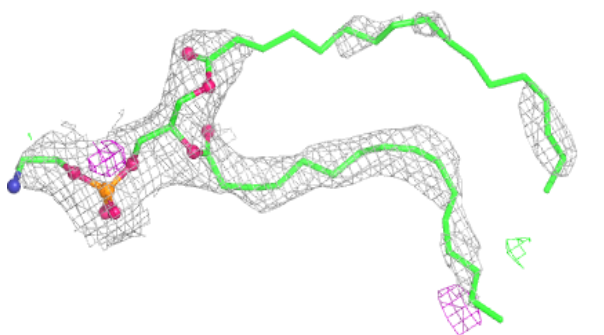


Electron density around FMX P 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

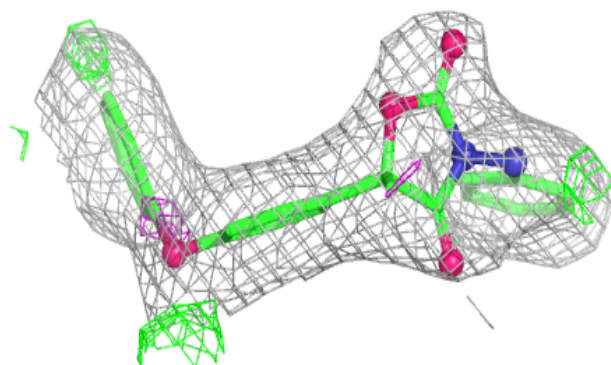
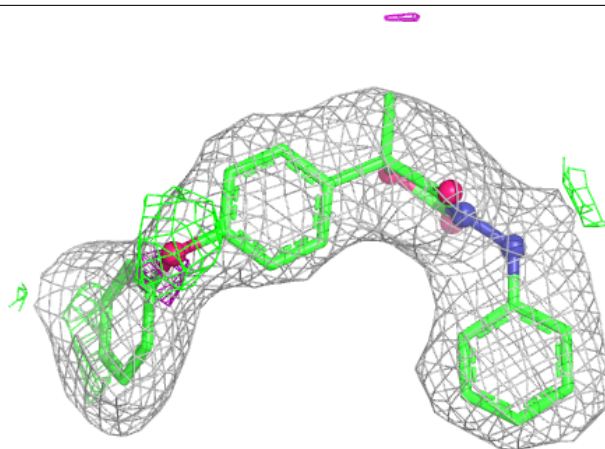
**Electron density around PEE P 3007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



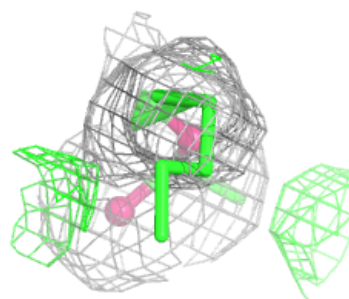
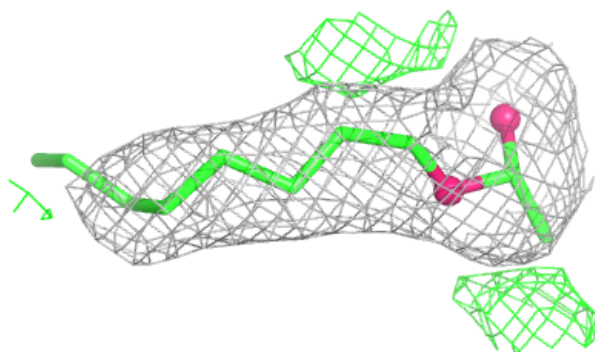
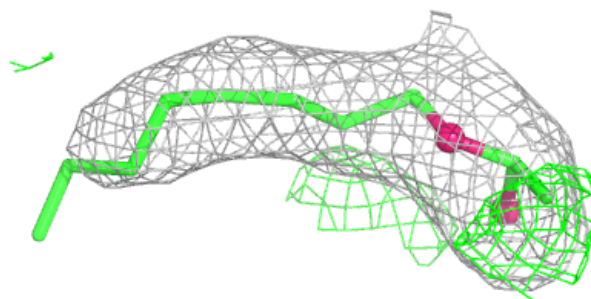
Electron density around FMX C 2001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

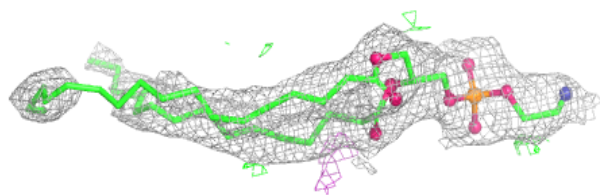
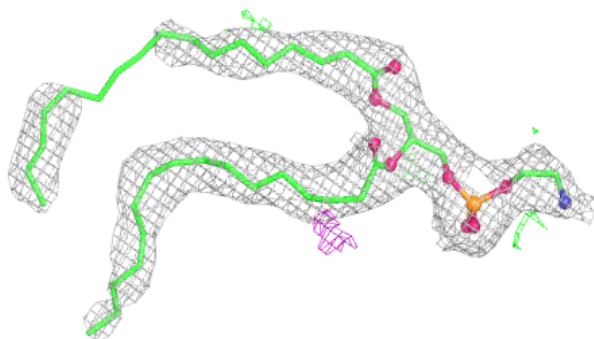


Electron density around BOG C 3010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

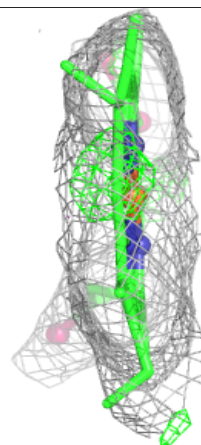
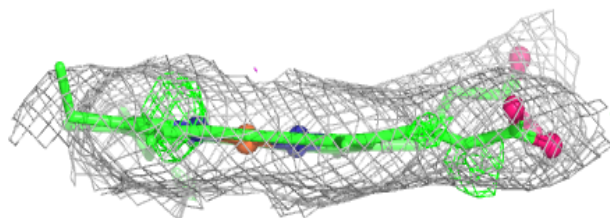
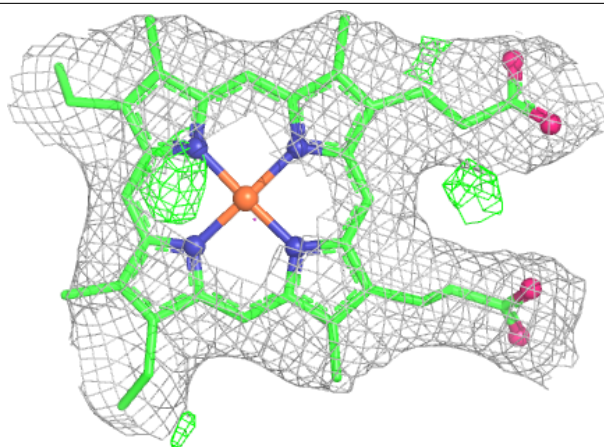
**Electron density around PEE C 2007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



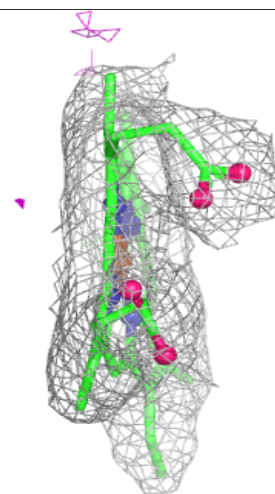
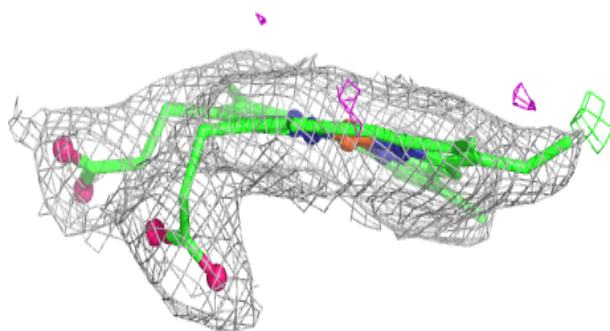
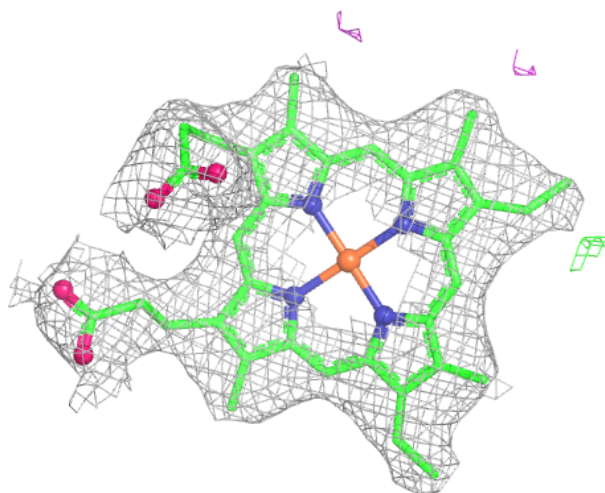
Electron density around HEC Q 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



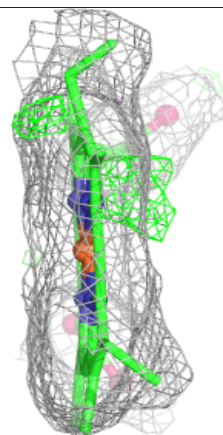
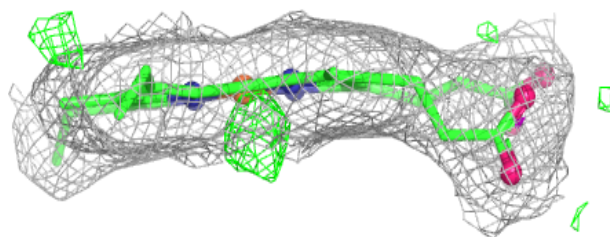
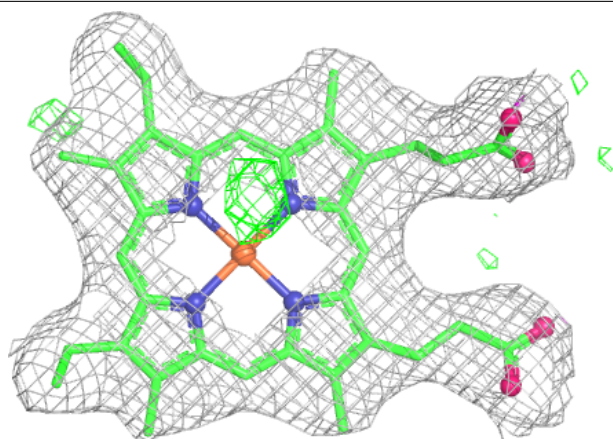
Electron density around HEM P 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



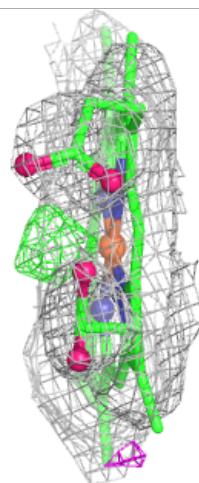
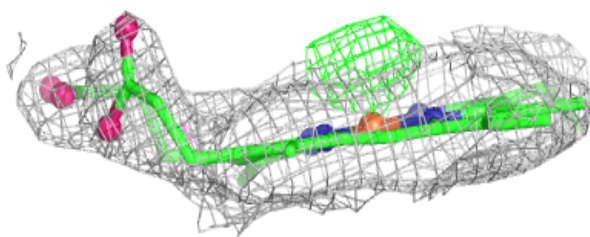
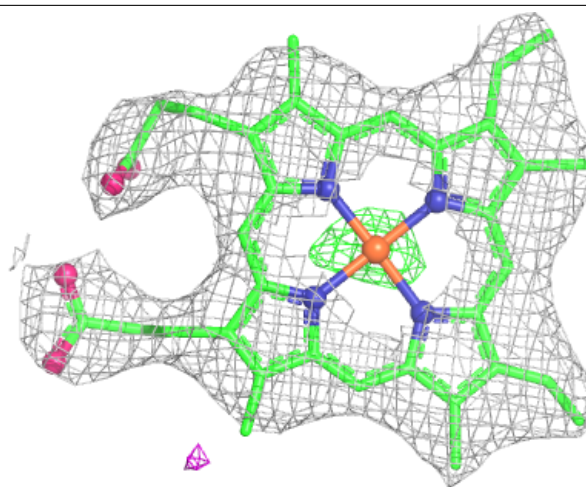
Electron density around HEC D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



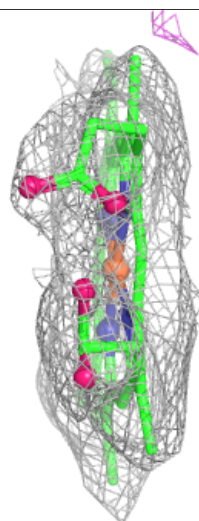
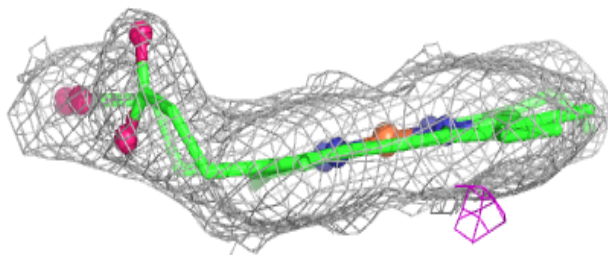
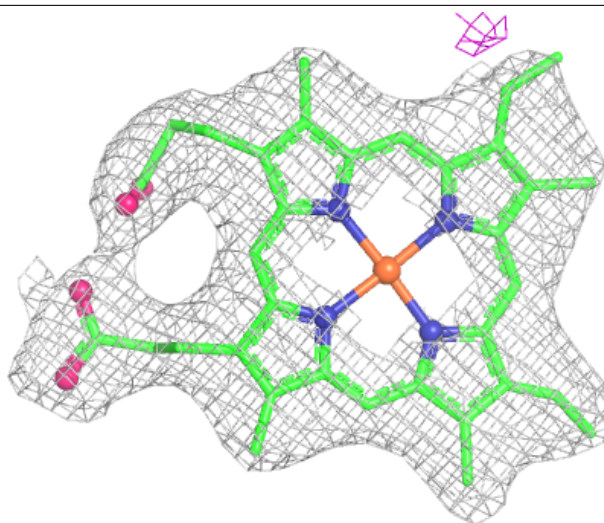
Electron density around HEM P 501:

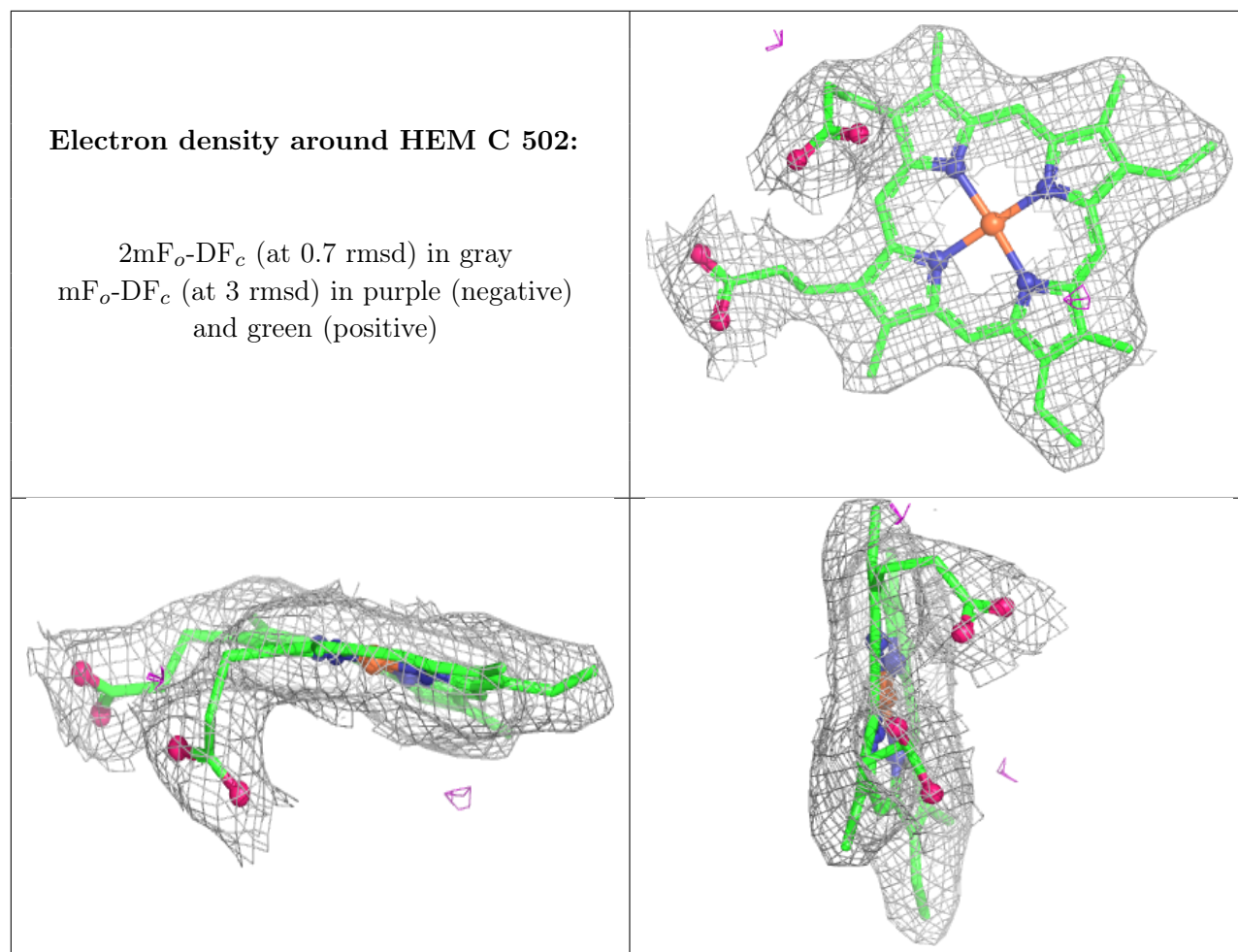
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.