



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:38 AM UTC

PDB ID : 3H1I / pdb_00003h1i
Title : Stigmatellin and antimycin bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.;
Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on : 2009-04-12
Resolution : 3.53 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

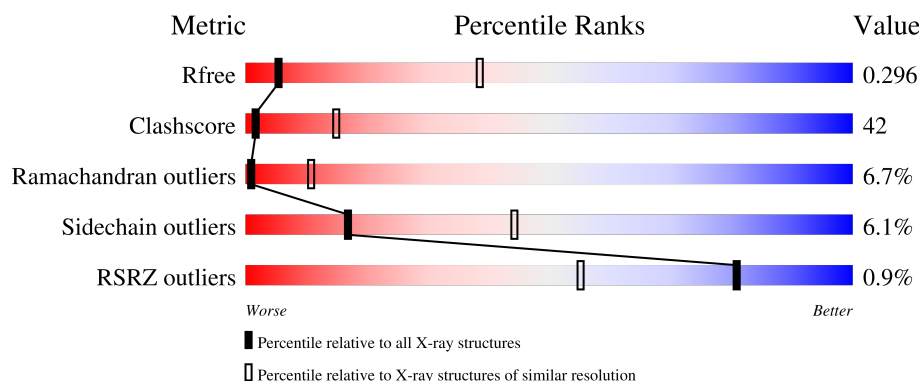
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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.



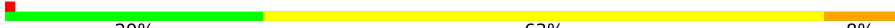
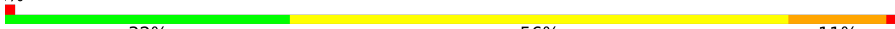
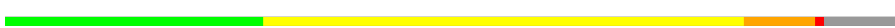
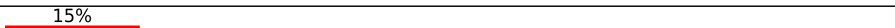
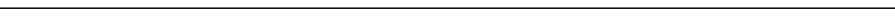
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	36% 54% 9% ..
1	N	446	% 34% 55% 9% ..
2	B	441	% 34% 51% 10% 5%
2	O	441	% 36% 49% 10% .
3	C	380	32% 58% 10% .

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	-	-
15	ANY	C	2002	X	-	-	-
15	ANY	P	3002	X	-	-	-
19	FES	E	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32701 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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL.

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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL.

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
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

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

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 Rieske, 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
			1513	952	263	292	6			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN.

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			

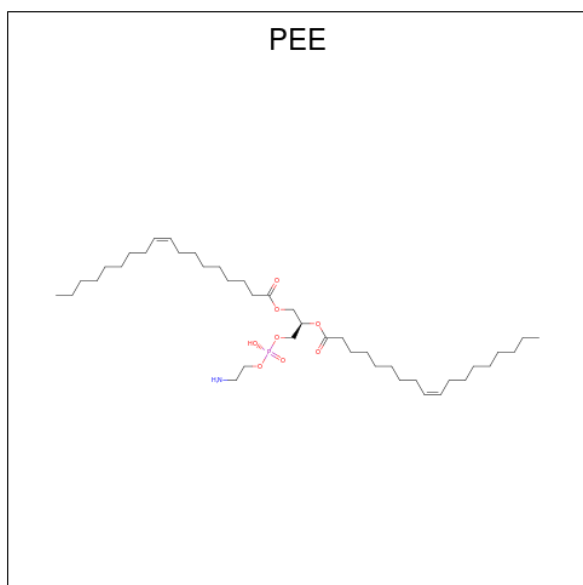
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

- Molecule 10 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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	59	Total	C	N	O	0	0	0
			478	311	85	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	O	P		0	0
			21	12	8	1			
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	E	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
			50	40	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			49	39	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

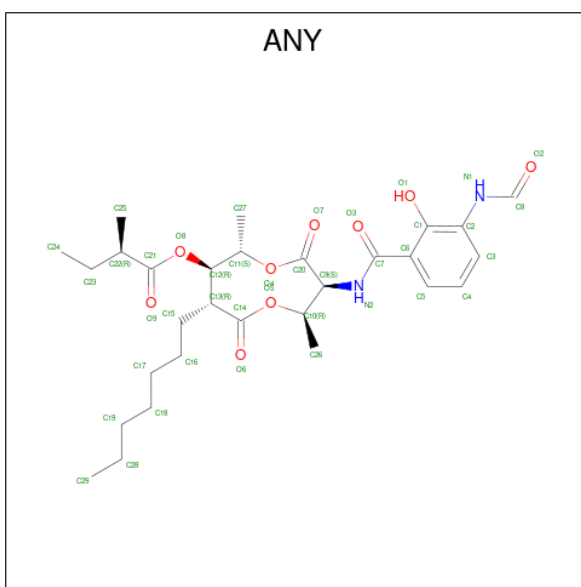
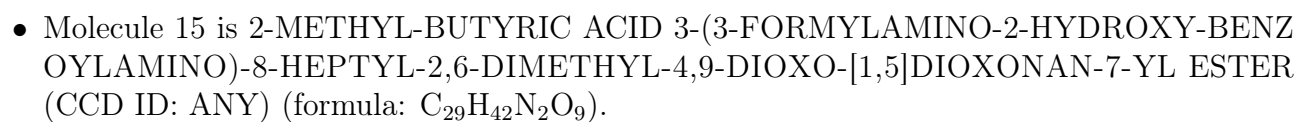
Continued on next page...

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

-
- The diagram shows the chemical structure of Heme (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl, methyl, and ethyl groups. The central heme group is shown in red, with labels O1A, O2A, O1D, and O2D indicating the positions of the oxygen atoms. The side chains are labeled with green text: CAA, CBA, CAD, CBD, CMA, C3A, C2A, C1A, C4A, C3B, C4B, C3C, C4C, C3D, C4D, C2D, C1D, C3E, C4E, C2E, C1E, C3F, C4F, C2F, C1F, C3G, C4G, C2G, C1G, C3H, C4H, C2H, C1H, C3I, C4I, C2I, C1I, C3J, C4J, C2J, C1J, C3K, C4K, C2K, C1K, C3L, C4L, C2L, C1L, C3M, C4M, C2M, C1M, C3N, C4N, C2N, C1N, C3O, C4O, C2O, C1O, C3P, C4P, C2P, C1P, C3Q, C4Q, C2Q, C1Q, C3R, C4R, C2R, C1R, C3S, C4S, C2S, C1S, C3T, C4T, C2T, C1T, C3U, C4U, C2U, C1U, C3V, C4V, C2V, C1V, C3W, C4W, C2W, C1W, C3X, C4X, C2X, C1X, C3Y, C4Y, C2Y, C1Y, C3Z, C4Z, C2Z, C1Z.

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

- 



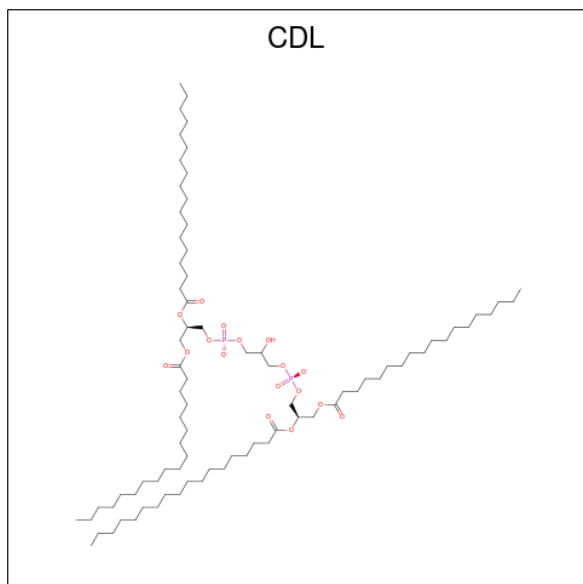
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	N	O	0	0
			37	26	2	9		

Continued on next page...

Continued from previous page...

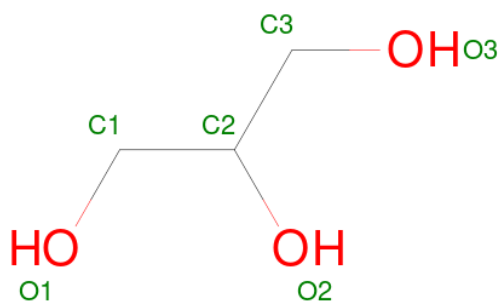
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	P	1	Total	C	N	O	0	0
			37	26	2	9		

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



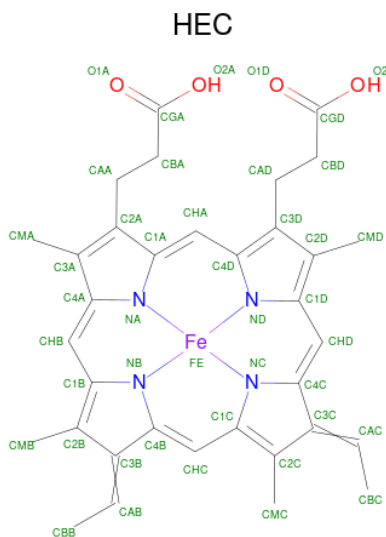
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O	P	0	0
			40	21	17	2		
16	D	1	Total	C	O	P	0	0
			50	31	17	2		
16	P	1	Total	C	O	P	0	0
			40	21	17	2		
16	Q	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 17 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



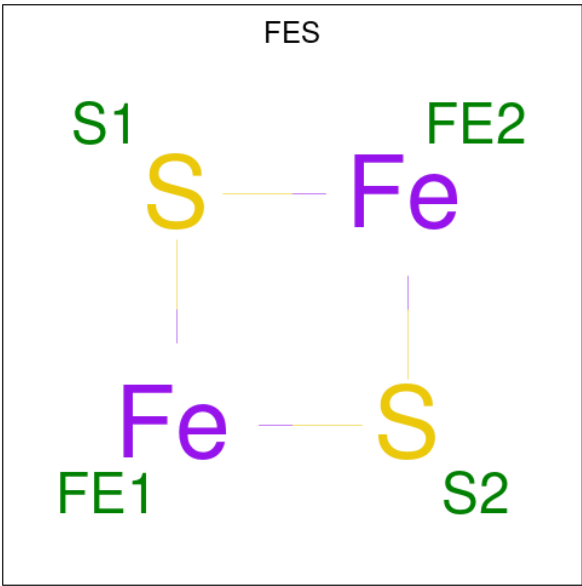
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total 6	C 3	O 3	0	0
17	P	1	Total 6	C 3	O 3	0	0

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



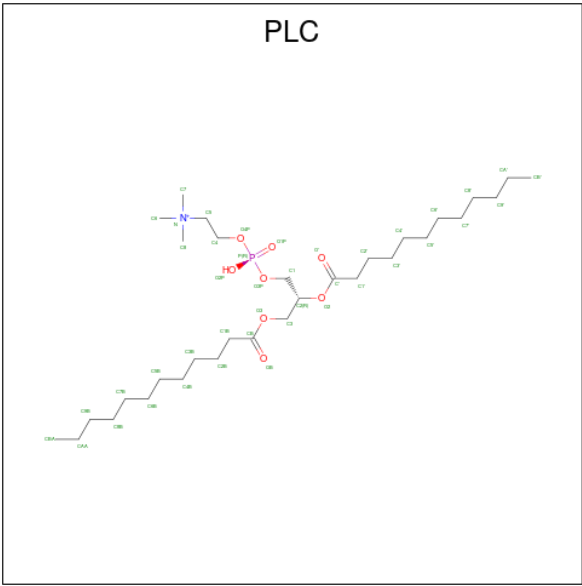
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
18	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

Continued on next page...

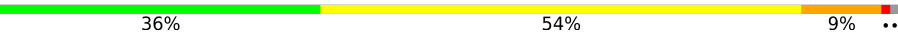
Continued from previous page...

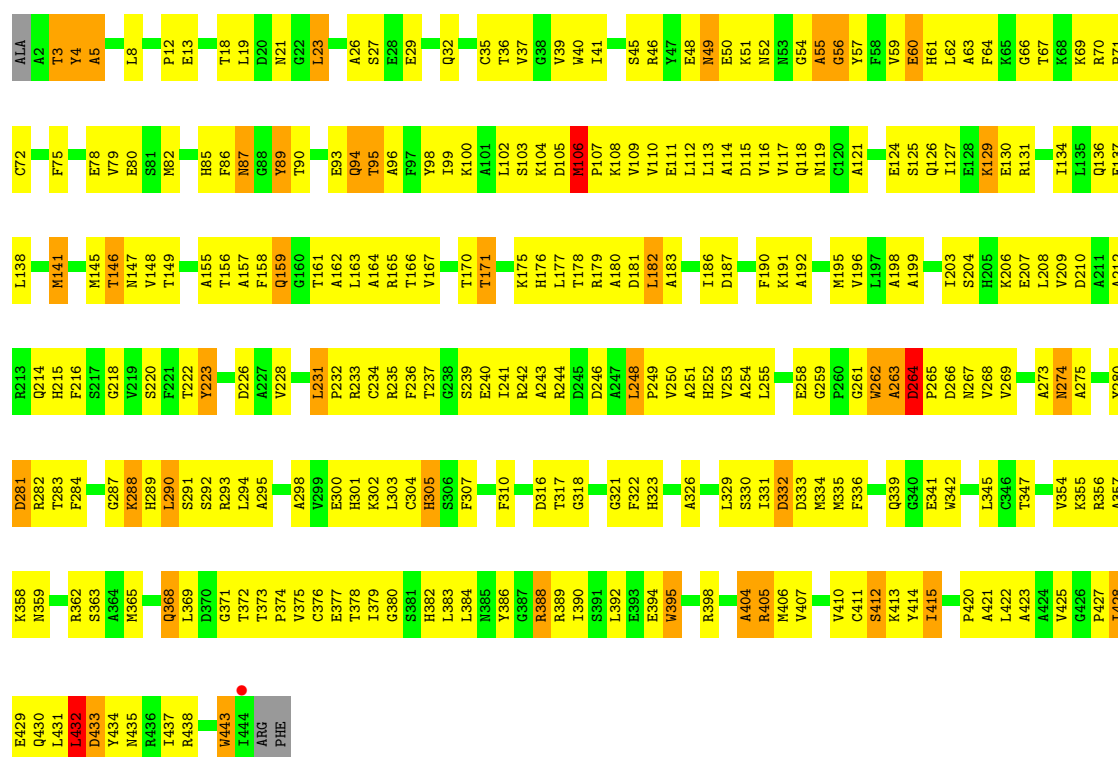
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

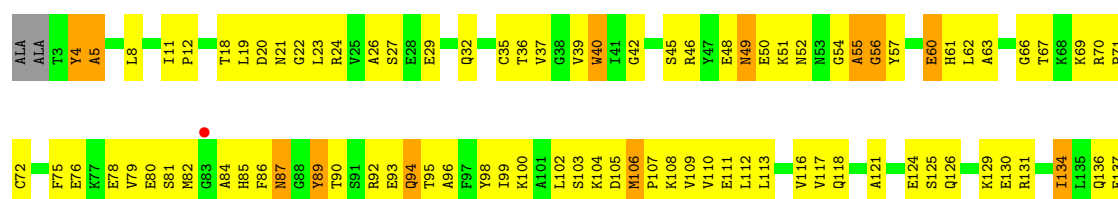
• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

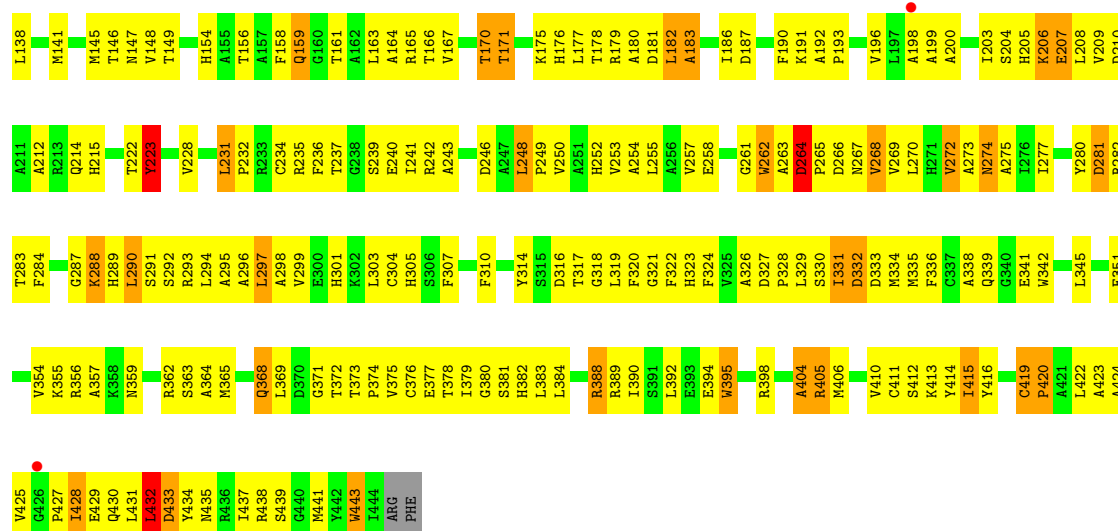
Chain A: 



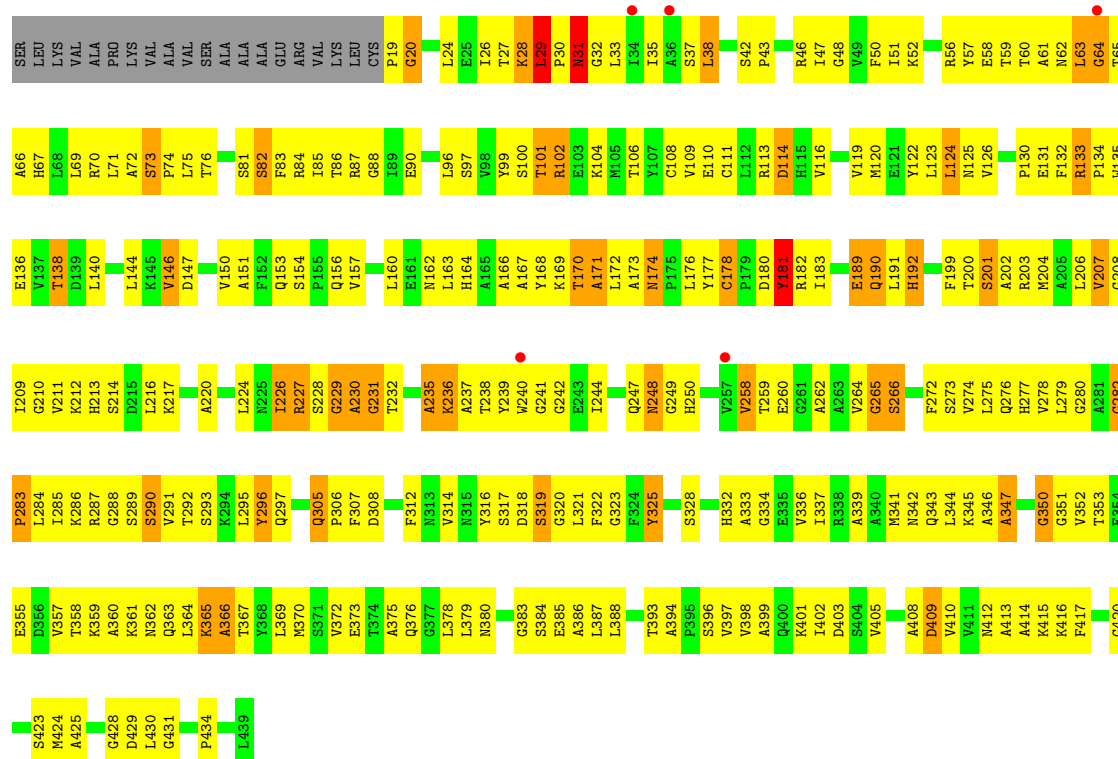
• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

Chain N: 



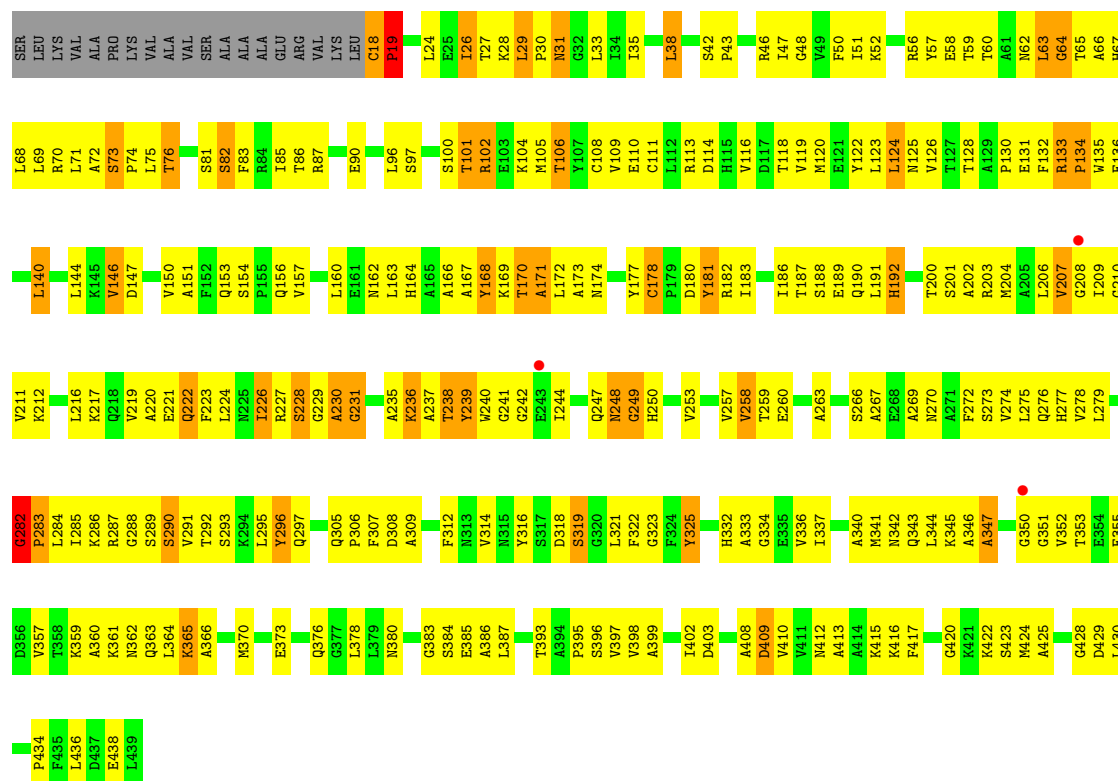


• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL



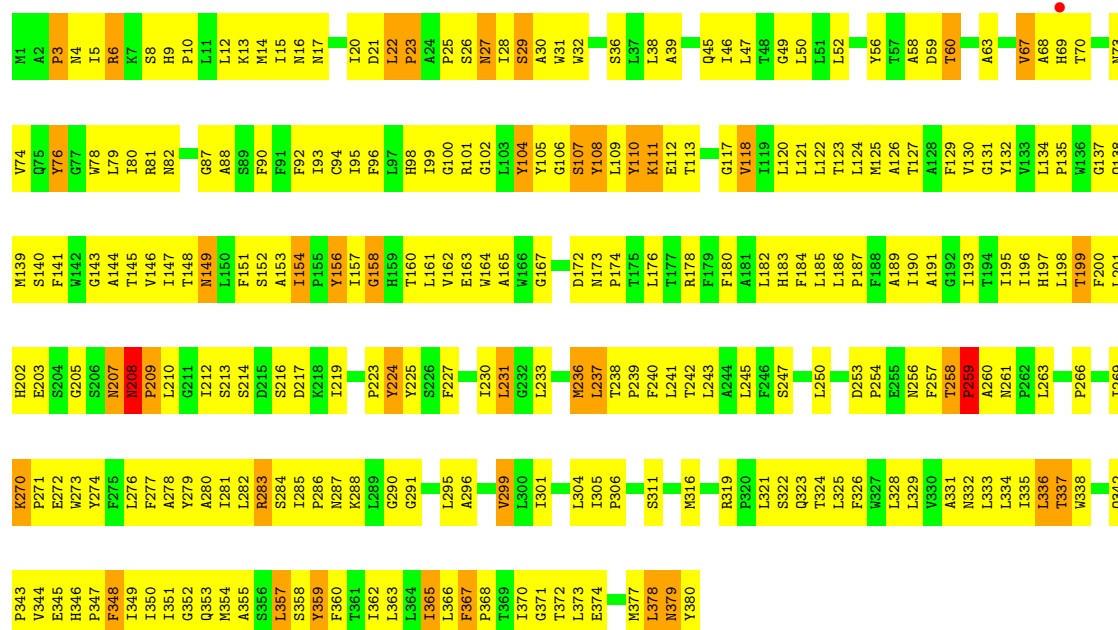
• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL





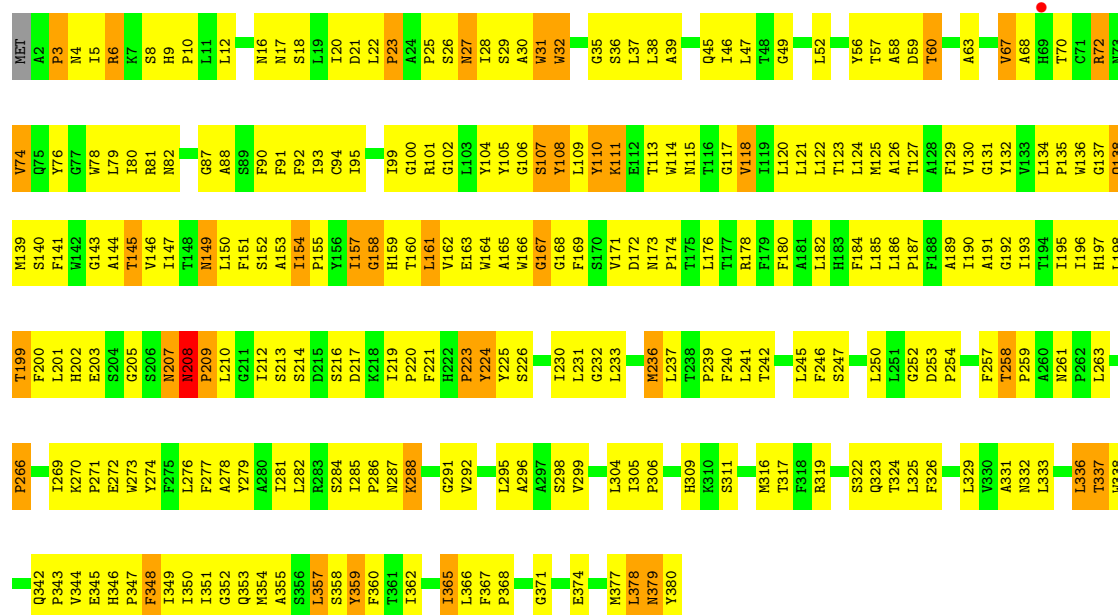
• Molecule 3: Cytochrome b

Chain C: 32% 58% 10%



• Molecule 3: Cytochrome b

Chain P: 32% 57% 11%



R224
H225
K226
W227
S228
V229
L230
K231
S232
R233
K234
M235
A236
Y237
R238
P240
K241

• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 29% 63% 8%

V1 H2 N3 T6 V7 F10 R14 D17 V18 H19 D20 A21 T22 T23 T24 S25 Q26 S29 E30 R32 D31 R32 R33 K33 F35 S36 Y37 L38 Y39 T40 T42 A41 T42 T42 A43 C44 V45 A46 T47 A48 A51 K52 N53 V54 V55 T56 Q57 F58 F59 S60 S61 L62 S63 A64 S65 L69

A70 L71 S72 K73 I74 K77 L78 D80 E83 G84 K85 N86 V87 A88 V91 R92 G93 K94 P95 L96 F97 V98 R99 H100 R101 T102 Q103 A104 L106 T107 Q108 A109 A110 E111 D112 V114 S115 L116 L117 N118 D119 H122 D123 L124 D125 R126 G127 L128 K129 P130 E131 W132 V133

I134 L135 V136 G137 V138 T140 H141 L142 G143 C144 A148 M149 S150 V151 D152 F153 G154 G155 Y156 Y157 C158 P159 H161 G162 S163 H164 Y165 D166 A167 S168 G169 H170 T171 I172 R173 A176 P177 Y178 N179 K180 E181 V182 P183 T184 Y185 Q186 V187 V188 P189 S190 E191 S192 F193 V194 G195

• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R: 32% 56% 11%

V1 H2 N3 T6 V7 P8 D9 F10 R14 D17 V18 H19 D20 A21 T22 T23 S29 E30 D31 R32 K33 G34 F35 S36 Y37 L38 Y39 T40 A41 T42 A43 C44 V45 A46 T47 A48 Y49 A51 K52 N53 V54 V55 Q57 F58 I59 S60 S61 L62 S63 A64 S65 L69 A70

L71 S72 K73 I74 K77 L78 S79 E83 G84 K85 N86 V87 A88 V91 R92 G93 K94 P95 L96 F97 H100 R101 T102 Q103 A104 E105 Q108 E109 A110 E111 V112 D113 V114 S115 D119 P120 Q121 H122 D123 V127 K128 P130 E131 W132 V133 L134 V136 G137 C138 T140

H141 L142 G143 C144 I147 A148 M149 S150 D152 F153 G154 G155 Y156 Y157 C158 H161 G162 S163 H164 Y165 D166 A167 S168 G169 H170 T171 I172 R173 A176 P177 Y178 N179 K180 E181 V182 P183 T184 Y185 Q186 V187 V188 P189 S190 E191 S192 F193 V194 G195

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

Chain F: 29% 54% 8%

ALA ALA ARG THR VAL ALA GLY G10 R11 L12 I16 R17 K18 Y19 Y20 Y21 N22 A23 F26 N27 L31 M32 R33 D34 D35 T36 L37 T38 E39 D40 D41 D42 V43 K44 A46 R49 L50 P51 E52 D53 Y54 Y55 N56 E57 R58 M59 F60 F61 T62 K63 R64 A65 L66

D67 L68 S69 L70 H71 K72 R73 I74 L75 P76 K77 E78 Q79 W80 V81 E84 K87 P88 Y89 L90 E91 L94 K95 E96 Y97 L98 R99 E100 R101 L102 R104 N108 K109 K110

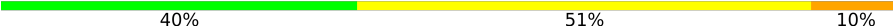
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN

Chain S: 29% 54% 8%

ALA ALA ARG THR VAL ALA GLY G10 R11 L12 M13 D14 R15 K16 R17 K18 Y19 Y20 Y21 N22 F26 N27 L31 M32 R33 D34 D35 T36 L37 Y38 E39 D40 D41 D42 V43 K44 A46 R49 L50 P51 E52 D53 N56 E57 R58 M59 F60 F61 T62 K63 R64 A65 L66

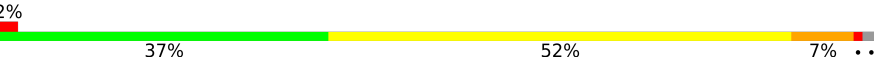
D67 L68 S69 L70 H71 K72 R73 I74 L75 P76 K77 E78 Q79 W80 V81 E84 K87 P88 Y89 L90 E91 E96 V97 E100 R101 R104 N108 K109 K110

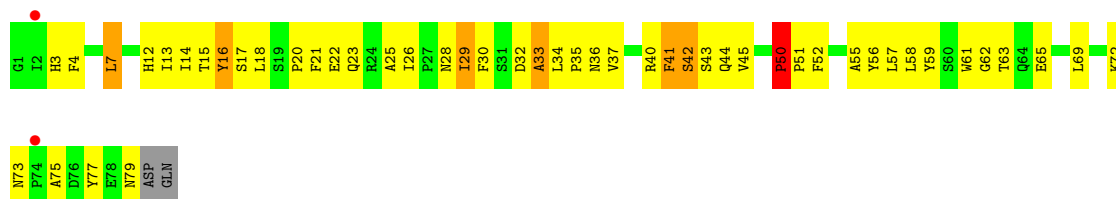
● Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



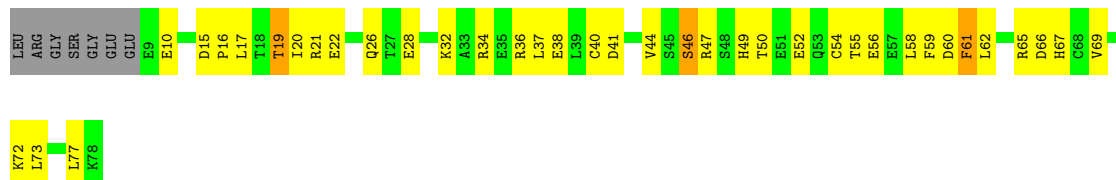
● Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



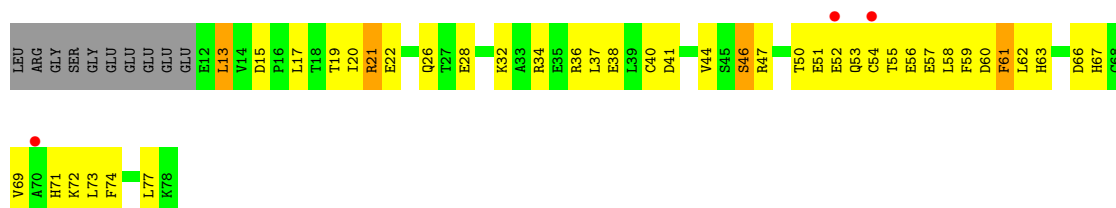
● Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

Chain H: 



● Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

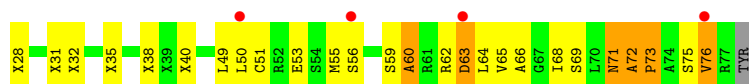
Chain U: 



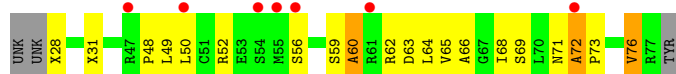
● Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 

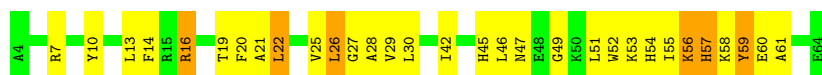




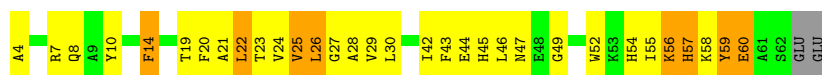
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



- Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 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	174.69Å 181.67Å 240.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.53 19.99 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.99-3.53) 90.1 (19.99-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.306 0.253 , 0.296	Depositor DCC
R_{free} test set	2560 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32701	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: HEM, CDL, GOL, PEE, UNL, ANY, PLC, SMA, FES, HEC

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	0.58	0/3511	1.07	26/4757 (0.5%)
1	N	0.58	0/3508	1.06	30/4753 (0.6%)
2	B	0.52	0/3196	1.04	19/4334 (0.4%)
2	O	0.55	0/3202	1.03	15/4343 (0.3%)
3	C	0.74	0/3122	1.11	23/4273 (0.5%)
3	P	0.64	0/3114	1.09	21/4263 (0.5%)
4	D	0.64	0/1956	1.13	21/2658 (0.8%)
4	Q	0.56	0/1956	1.12	21/2658 (0.8%)
5	E	0.51	0/1547	1.08	12/2103 (0.6%)
5	R	0.56	0/1547	1.05	11/2103 (0.5%)
6	F	0.64	0/911	0.99	5/1219 (0.4%)
6	S	0.55	0/911	0.99	4/1219 (0.3%)
7	G	0.65	0/698	1.03	0/946
7	T	0.57	0/680	0.97	1/923 (0.1%)
8	H	0.54	0/582	0.85	1/779 (0.1%)
8	U	0.44	0/561	0.84	1/751 (0.1%)
9	I	0.65	0/218	1.06	2/293 (0.7%)
9	V	0.65	0/218	0.93	0/293
10	J	0.58	0/508	0.89	0/682
10	W	0.54	0/489	0.89	0/658
All	All	0.59	0/32435	1.06	213/44008 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	LEU	N-CA-C	12.09	127.03	110.35
5	E	71	LEU	N-CA-C	11.95	126.84	110.35
4	Q	36	VAL	N-CA-C	9.27	118.94	111.62
1	N	415	ILE	N-CA-C	8.18	118.53	111.90
1	N	66	GLY	N-CA-C	7.99	123.36	112.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	104	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	293	0
1	N	3437	0	3349	298	0
2	B	3141	0	3142	300	0
2	O	3147	0	3146	319	0
3	C	3020	0	3070	287	0
3	P	3012	0	3058	311	0
4	D	1898	0	1846	166	0
4	Q	1898	0	1846	178	0
5	E	1513	0	1478	144	0
5	R	1513	0	1478	129	0
6	F	891	0	893	74	0
6	S	891	0	893	78	0
7	G	676	0	659	61	0
7	T	658	0	647	67	0
8	H	574	0	548	30	0
8	U	553	0	535	43	0
9	I	285	0	239	30	0
9	V	275	0	238	30	0
10	J	497	0	490	31	0
10	W	478	0	478	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	21	0	13	0	0
11	C	49	0	72	2	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0
11	P	99	0	149	6	0
12	A	1	0	0	0	0
12	C	3	0	0	0	0
12	E	2	0	0	0	0
12	P	3	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	20	0
13	P	86	0	60	22	0
14	C	37	0	42	3	0
14	P	37	0	42	4	0
15	C	37	0	28	3	0
15	P	37	0	29	1	0
16	C	40	0	24	2	0
16	D	50	0	44	1	0
16	P	40	0	24	2	0
16	Q	50	0	44	5	0
17	C	6	0	8	1	0
17	P	6	0	8	0	0
18	D	43	0	30	6	0
18	Q	43	0	30	5	0
19	E	4	0	0	2	0
19	R	4	0	0	1	0
20	E	32	0	38	2	0
20	R	32	0	38	3	0
All	All	32701	0	32246	2697	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 42.

The worst 5 of 2697 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:157:ILE:HG13	3:P:158:GLY:H	1.04	1.15
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.19	1.12
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.16	1.12
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.29	1.07
5:E:119:ASP:HB3	5:E:179:ASN:ND2	1.67	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	323 (73%)	94 (21%)	24 (5%)	1	13
1	N	440/446 (99%)	320 (73%)	95 (22%)	25 (6%)	1	13
2	B	419/441 (95%)	302 (72%)	77 (18%)	40 (10%)	0	6
2	O	420/441 (95%)	302 (72%)	85 (20%)	33 (8%)	1	8
3	C	378/380 (100%)	284 (75%)	72 (19%)	22 (6%)	1	12
3	P	377/380 (99%)	284 (75%)	73 (19%)	20 (5%)	1	14
4	D	239/241 (99%)	188 (79%)	37 (16%)	14 (6%)	1	12
4	Q	239/241 (99%)	186 (78%)	40 (17%)	13 (5%)	1	13
5	E	194/196 (99%)	136 (70%)	42 (22%)	16 (8%)	0	8
5	R	194/196 (99%)	136 (70%)	36 (19%)	22 (11%)	0	4
6	F	99/110 (90%)	73 (74%)	24 (24%)	2 (2%)	6	32
6	S	99/110 (90%)	73 (74%)	23 (23%)	3 (3%)	3	25
7	G	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	9
7	T	77/81 (95%)	52 (68%)	20 (26%)	5 (6%)	1	11
8	H	68/77 (88%)	46 (68%)	18 (26%)	4 (6%)	1	12
8	U	65/77 (84%)	41 (63%)	20 (31%)	4 (6%)	1	12
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0	3
9	V	29/47 (62%)	21 (72%)	4 (14%)	4 (14%)	0	3
10	J	59/61 (97%)	41 (70%)	16 (27%)	2 (3%)	3	23
10	W	57/61 (93%)	36 (63%)	17 (30%)	4 (7%)	1	10
All	All	4002/4160 (96%)	2919 (73%)	816 (20%)	267 (7%)	1	11

5 of 267 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	72	CYS
1	A	94	GLN
1	A	159	GLN
1	A	282	ARG

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%)	344 (94%)	21 (6%)	18	45
1	N	365/368 (99%)	343 (94%)	22 (6%)	17	44
2	B	332/347 (96%)	316 (95%)	16 (5%)	23	49
2	O	333/347 (96%)	315 (95%)	18 (5%)	20	47
3	C	329/329 (100%)	307 (93%)	22 (7%)	15	41
3	P	328/329 (100%)	305 (93%)	23 (7%)	14	40
4	D	200/200 (100%)	191 (96%)	9 (4%)	24	51
4	Q	200/200 (100%)	191 (96%)	9 (4%)	24	51
5	E	166/166 (100%)	156 (94%)	10 (6%)	17	44
5	R	166/166 (100%)	156 (94%)	10 (6%)	17	44
6	F	93/96 (97%)	83 (89%)	10 (11%)	6	28
6	S	93/96 (97%)	83 (89%)	10 (11%)	6	28
7	G	71/71 (100%)	65 (92%)	6 (8%)	10	34
7	T	69/71 (97%)	64 (93%)	5 (7%)	13	39
8	H	65/71 (92%)	62 (95%)	3 (5%)	24	50
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	49
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	34
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	35
10	W	47/49 (96%)	43 (92%)	4 (8%)	10	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3380/3446 (98%)	3173 (94%)	207 (6%)	17 44

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	274	ASN
3	P	23	PRO
7	T	63	THR
1	N	388	ARG
2	O	102	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	118	GLN
2	O	222	GLN
7	T	12	HIS
1	N	159	GLN
2	O	31	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 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
11	PEE	C	2007	-	48,48,50	1.48	9 (18%)	51,53,55	0.84	3 (5%)
17	GOL	P	3011	-	5,5,5	1.25	0	5,5,5	0.60	0
13	HEM	C	502	3	50,50,50	1.83	13 (26%)	67,82,82	1.87	13 (19%)
16	CDL	C	2004	-	39,39,99	1.27	5 (12%)	45,51,111	1.16	3 (6%)
14	SMA	P	3001	-	38,38,38	1.57	8 (21%)	47,52,52	0.80	1 (2%)
16	CDL	P	3004	-	39,39,99	1.26	5 (12%)	45,51,111	1.16	2 (4%)
14	SMA	C	2001	-	38,38,38	1.34	4 (10%)	47,52,52	0.82	3 (6%)
11	PEE	N	3008	-	4,4,50	3.72	4 (100%)	6,6,55	0.70	0
18	HEC	Q	501	4	46,50,50	1.83	8 (17%)	58,82,82	2.39	7 (12%)
13	HEM	C	501	3	50,50,50	1.73	9 (18%)	67,82,82	1.87	17 (25%)
15	ANY	C	2002	-	38,38,41	1.58	5 (13%)	32,52,55	2.27	8 (25%)
11	PEE	A	2008	-	20,20,50	1.82	6 (30%)	23,25,55	0.73	1 (4%)
15	ANY	P	3002	-	38,38,41	1.87	8 (21%)	32,52,55	2.29	7 (21%)
18	HEC	D	501	4	46,50,50	1.69	7 (15%)	58,82,82	2.58	11 (18%)
20	PLC	E	2009	-	31,31,41	1.74	6 (19%)	37,39,49	0.73	1 (2%)
13	HEM	P	502	3	50,50,50	1.61	8 (16%)	67,82,82	1.53	11 (16%)
20	PLC	R	3009	-	31,31,41	1.65	9 (29%)	37,39,49	0.61	0
16	CDL	Q	3003	-	49,49,99	1.16	3 (6%)	55,61,111	0.96	2 (3%)
11	PEE	P	3005	-	49,49,50	1.57	10 (20%)	52,54,55	0.87	3 (5%)
16	CDL	D	2003	-	49,49,99	1.20	4 (8%)	55,61,111	0.94	1 (1%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
13	HEM	P	501	3	50,50,50	1.73	9 (18%)	67,82,82	1.74	17 (25%)
17	GOL	C	2011	-	5,5,5	1.29	0	5,5,5	0.62	0
11	PEE	E	2005	-	49,49,50	1.46	8 (16%)	52,54,55	0.87	3 (5%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
11	PEE	P	3007	-	48,48,50	1.46	7 (14%)	51,53,55	0.83	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
11	PEE	C	2007	-	-	29/52/52/54	-
17	GOL	P	3011	-	-	2/4/4/4	-
13	HEM	C	502	3	-	7/14/54/54	-
16	CDL	C	2004	-	-	23/49/49/110	-
14	SMA	P	3001	-	-	15/34/34/34	0/2/2/2
16	CDL	P	3004	-	-	22/49/49/110	-
14	SMA	C	2001	-	-	15/34/34/34	0/2/2/2
18	HEC	Q	501	4	-	10/14/54/54	-
15	ANY	C	2002	-	1/1/10/13	1/37/52/56	0/1/2/2
15	ANY	P	3002	-	1/1/10/13	1/37/52/56	0/1/2/2
11	PEE	A	2008	-	-	14/24/24/54	-
13	HEM	C	501	3	-	8/14/54/54	-
18	HEC	D	501	4	-	8/14/54/54	-
20	PLC	E	2009	-	-	13/35/35/45	-
13	HEM	P	502	3	-	6/14/54/54	-
20	PLC	R	3009	-	-	12/35/35/45	-
16	CDL	Q	3003	-	-	28/59/59/110	-
11	PEE	P	3005	-	-	27/53/53/54	-
16	CDL	D	2003	-	-	29/59/59/110	-
19	FES	R	501	5	-	-	0/1/1/1
13	HEM	P	501	3	-	8/14/54/54	-
17	GOL	C	2011	-	-	1/4/4/4	-
11	PEE	E	2005	-	-	28/53/53/54	-
19	FES	E	501	5	-	-	0/1/1/1
11	PEE	P	3007	-	-	28/52/52/54	-

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	CAC-C3C	6.07	1.54	1.35
15	P	3002	ANY	C8-N1	5.85	1.42	1.34
15	C	2002	ANY	C8-N1	5.60	1.41	1.34
18	D	501	HEC	CAB-C3B	5.49	1.52	1.35
13	C	501	HEM	CBC-CAC	5.29	1.55	1.30

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	CBC-CAC-C3C	-13.57	100.31	127.43
18	Q	501	HEC	CBC-CAC-C3C	-12.77	101.91	127.43
15	P	3002	ANY	C25-C22-C21	8.07	135.38	110.94
15	C	2002	ANY	C25-C22-C21	7.87	134.77	110.94
18	D	501	HEC	CBB-CAB-C3B	-6.94	113.56	127.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	2002	ANY	C22
15	P	3002	ANY	C22

5 of 335 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	O3P-C1-C2-O2
11	C	2007	PEE	C1-O3P-P-O2P
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P

There are no ring outliers.

23 monomers are involved in 92 short contacts:

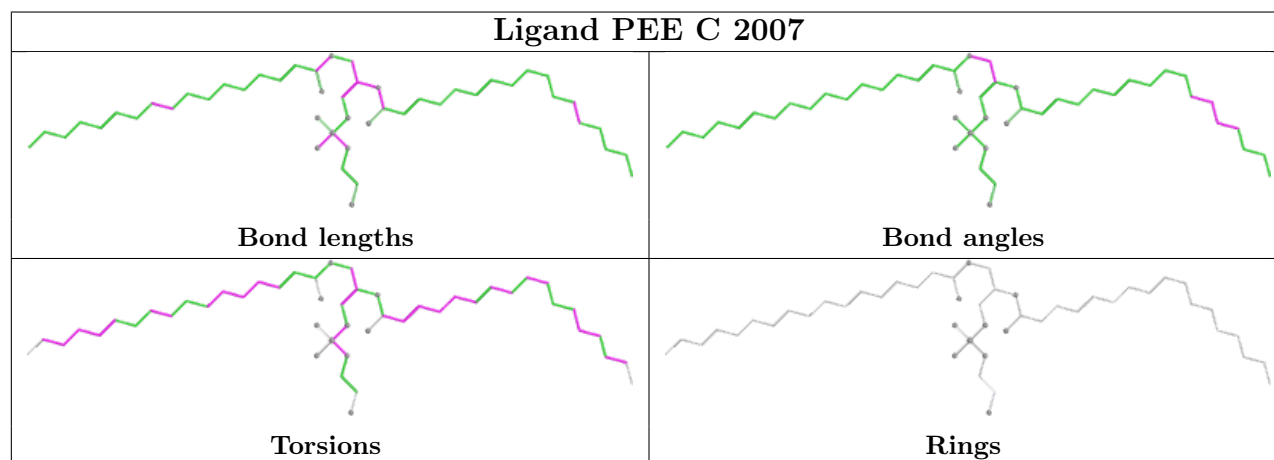
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	2007	PEE	2	0
13	C	502	HEM	9	0
16	C	2004	CDL	2	0
14	P	3001	SMA	4	0
16	P	3004	CDL	2	0
14	C	2001	SMA	3	0
18	Q	501	HEC	5	0
13	C	501	HEM	11	0
15	C	2002	ANY	3	0
15	P	3002	ANY	1	0
18	D	501	HEC	6	0
20	E	2009	PLC	2	0
13	P	502	HEM	11	0
20	R	3009	PLC	3	0
16	Q	3003	CDL	5	0
11	P	3005	PEE	3	0
16	D	2003	CDL	1	0
19	R	501	FES	1	0

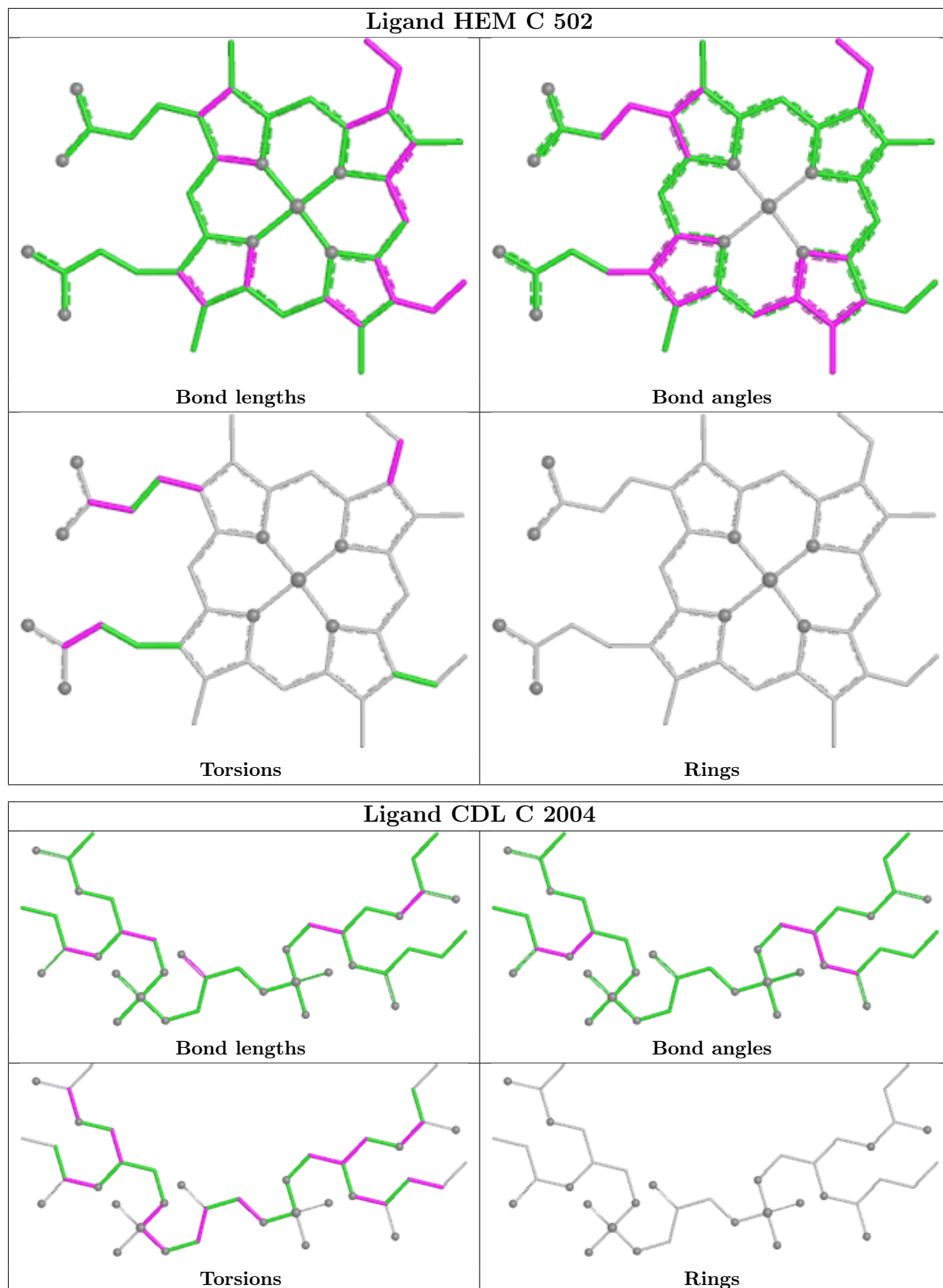
Continued on next page...

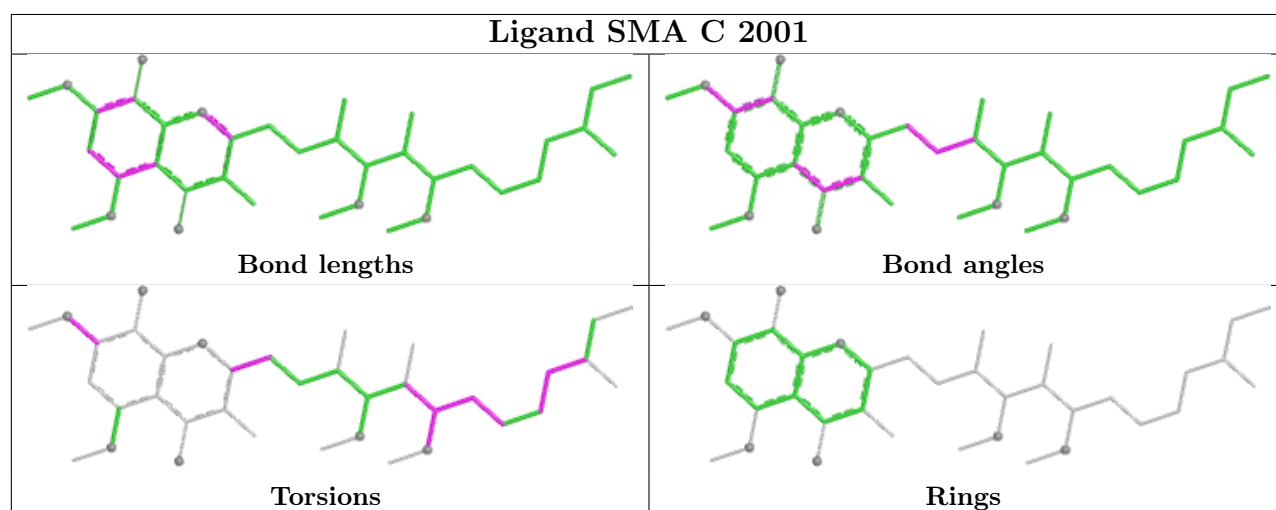
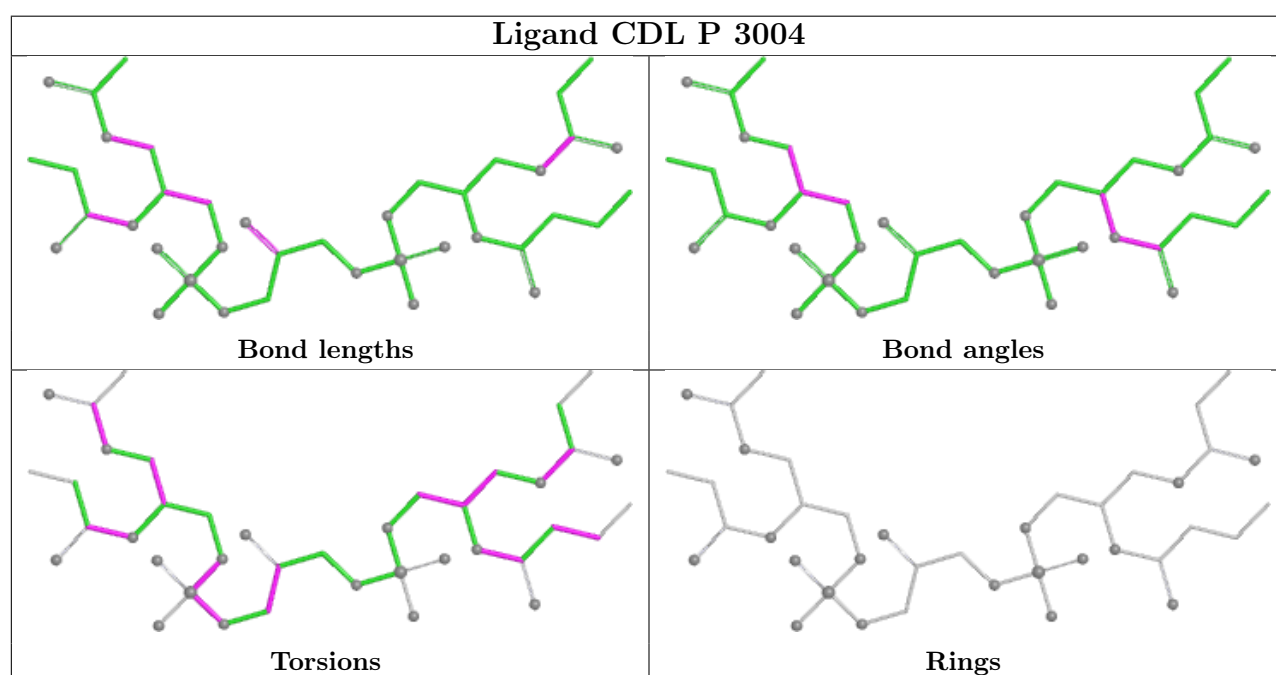
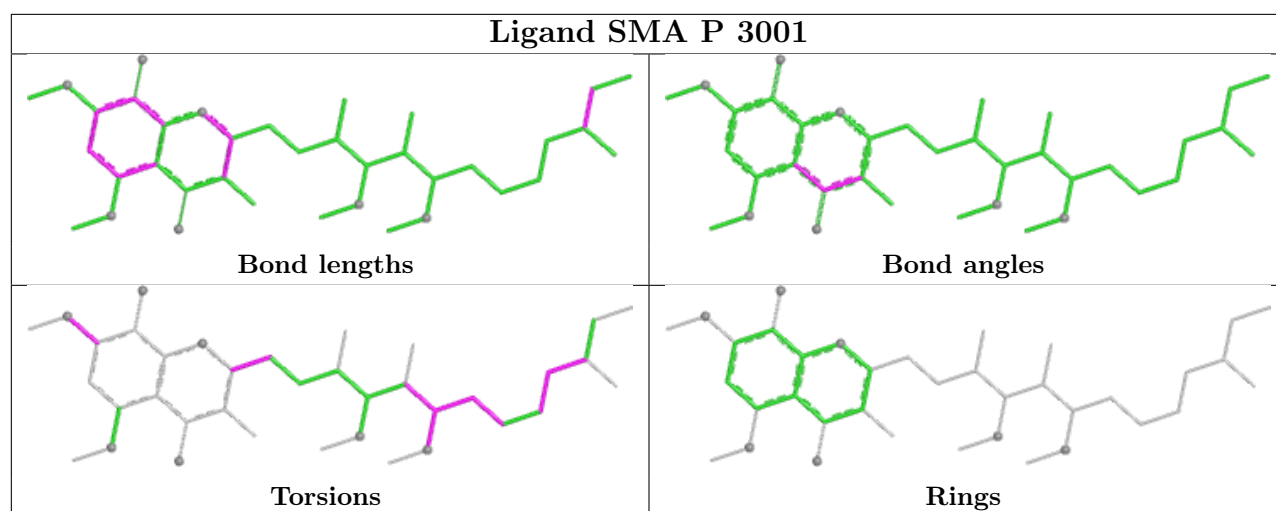
Continued from previous page...

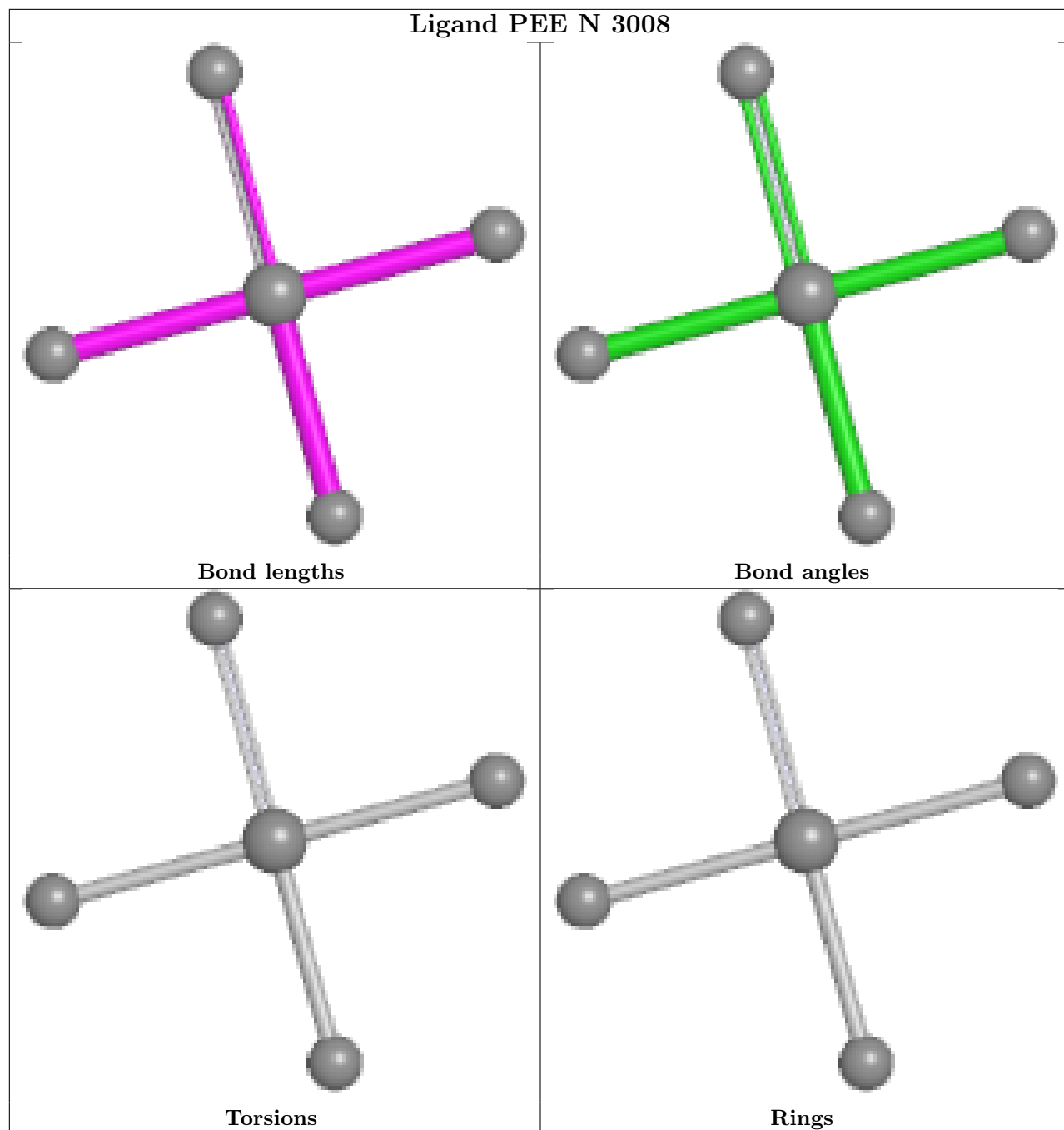
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	501	HEM	11	0
17	C	2011	GOL	1	0
11	E	2005	PEE	1	0
19	E	501	FES	2	0
11	P	3007	PEE	3	0

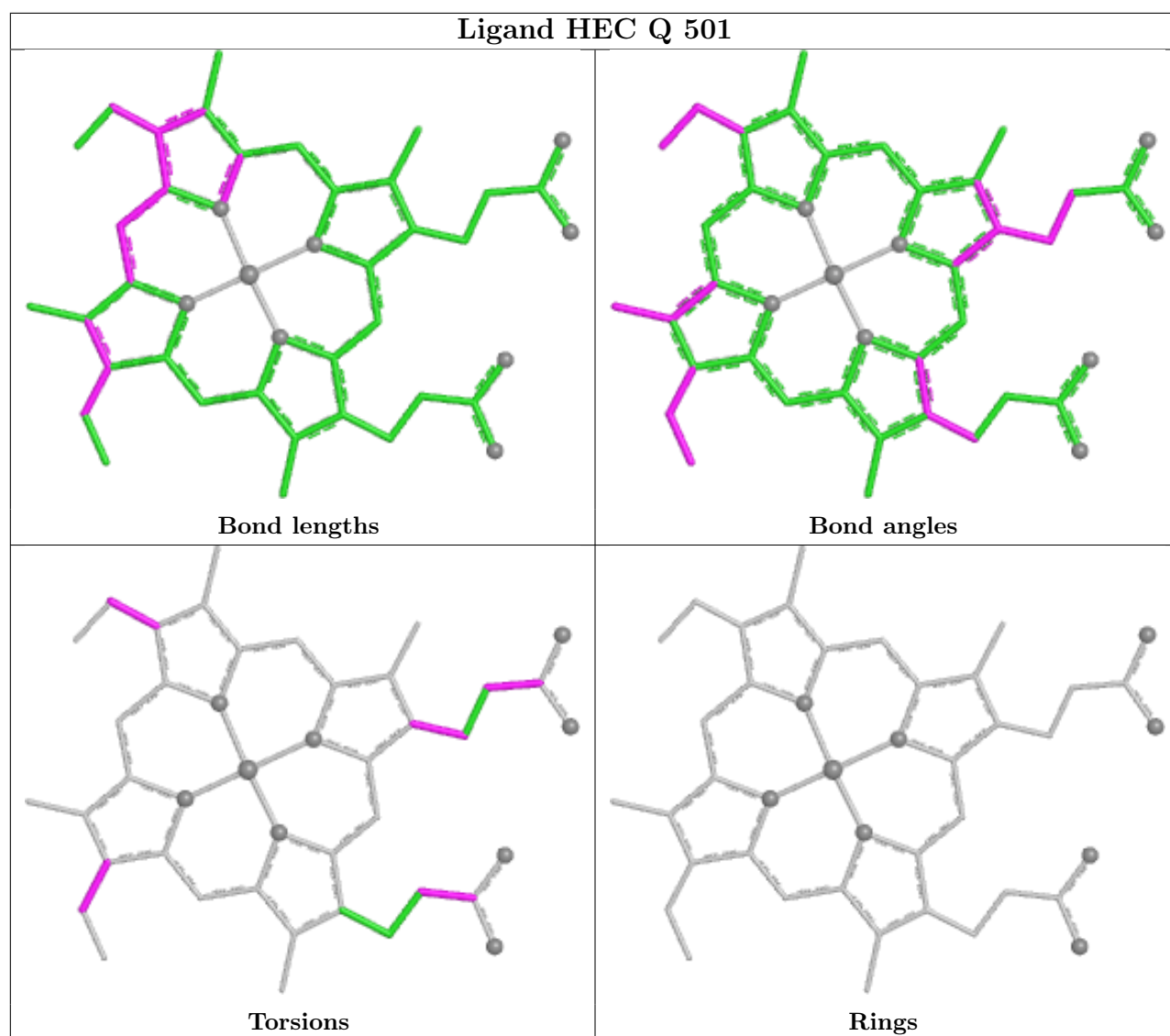
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

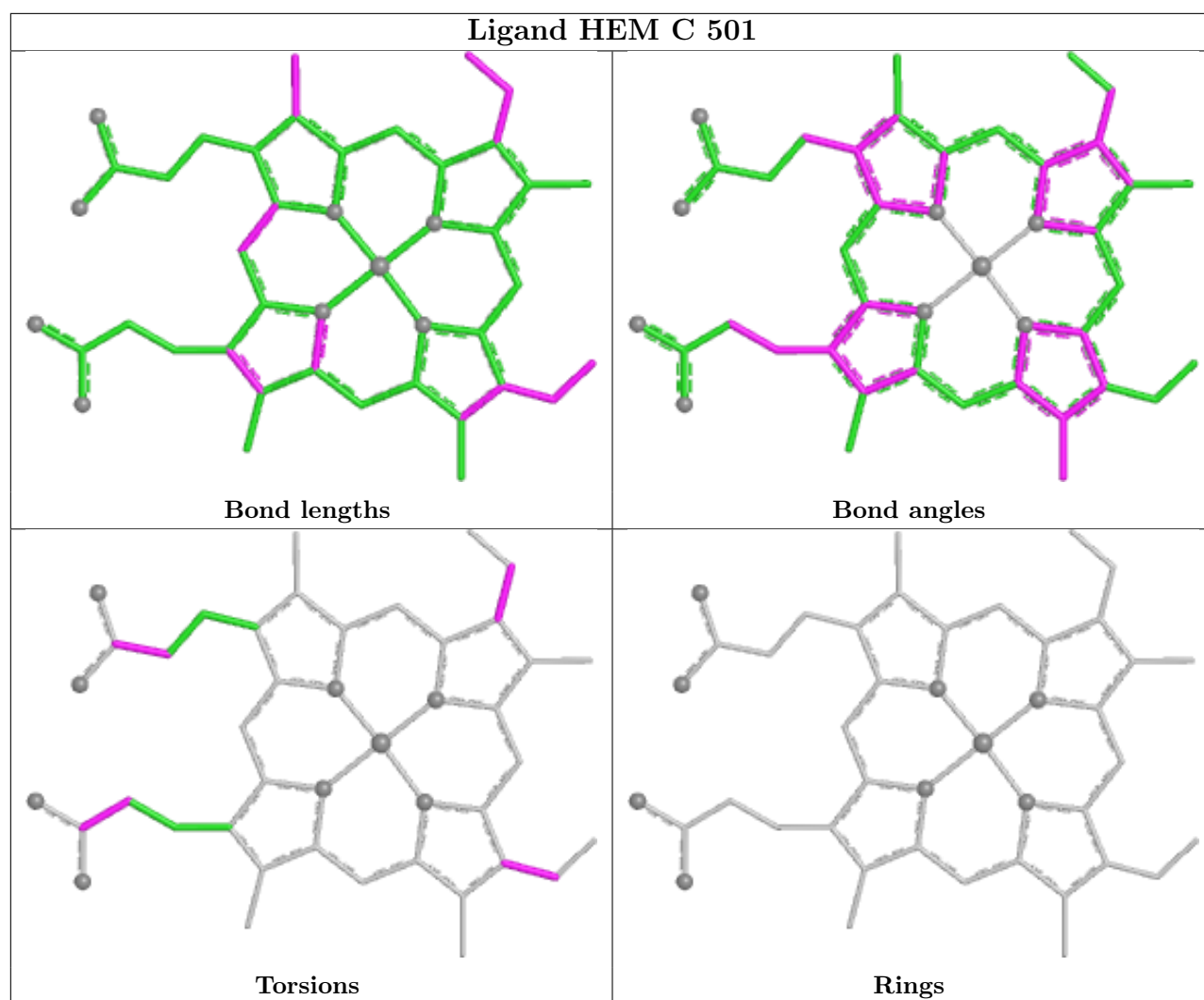


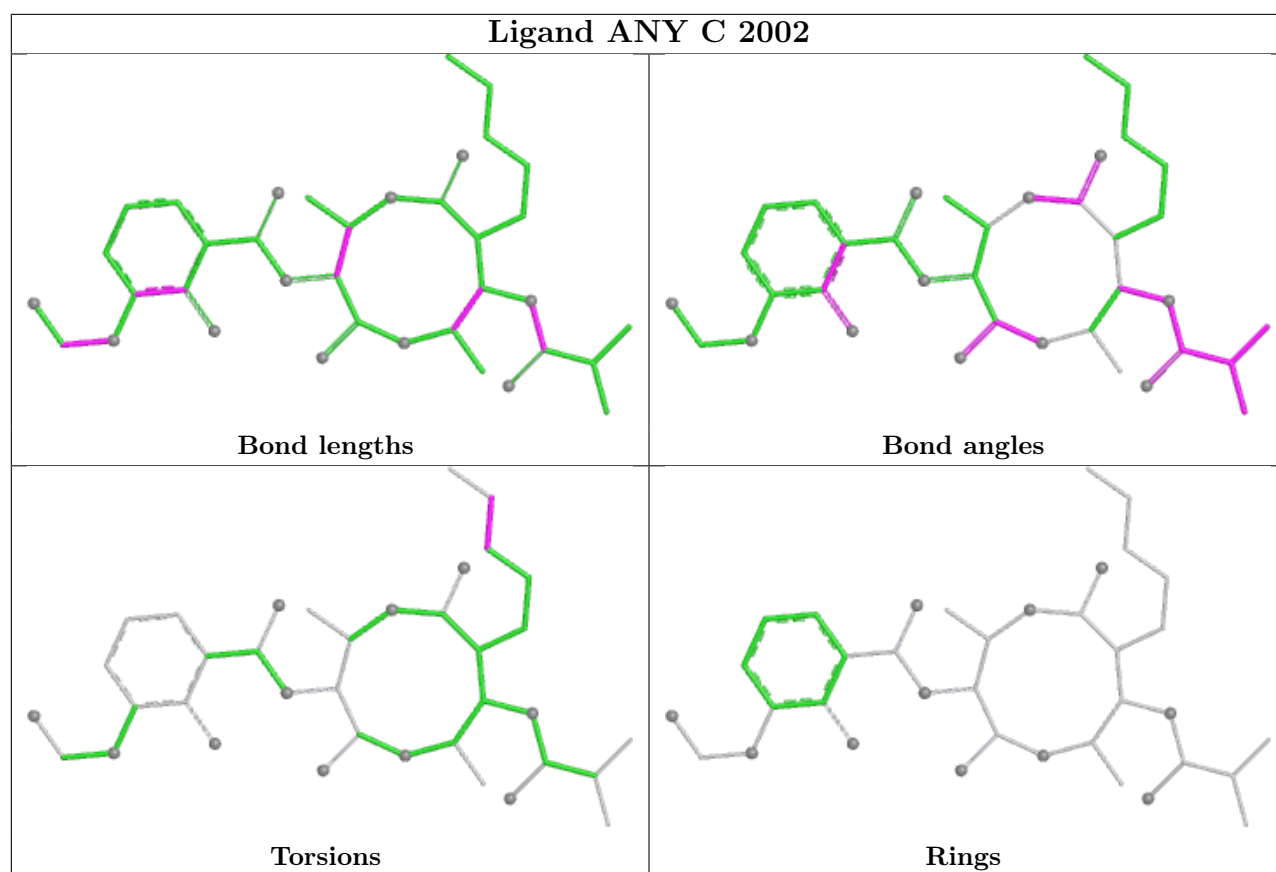


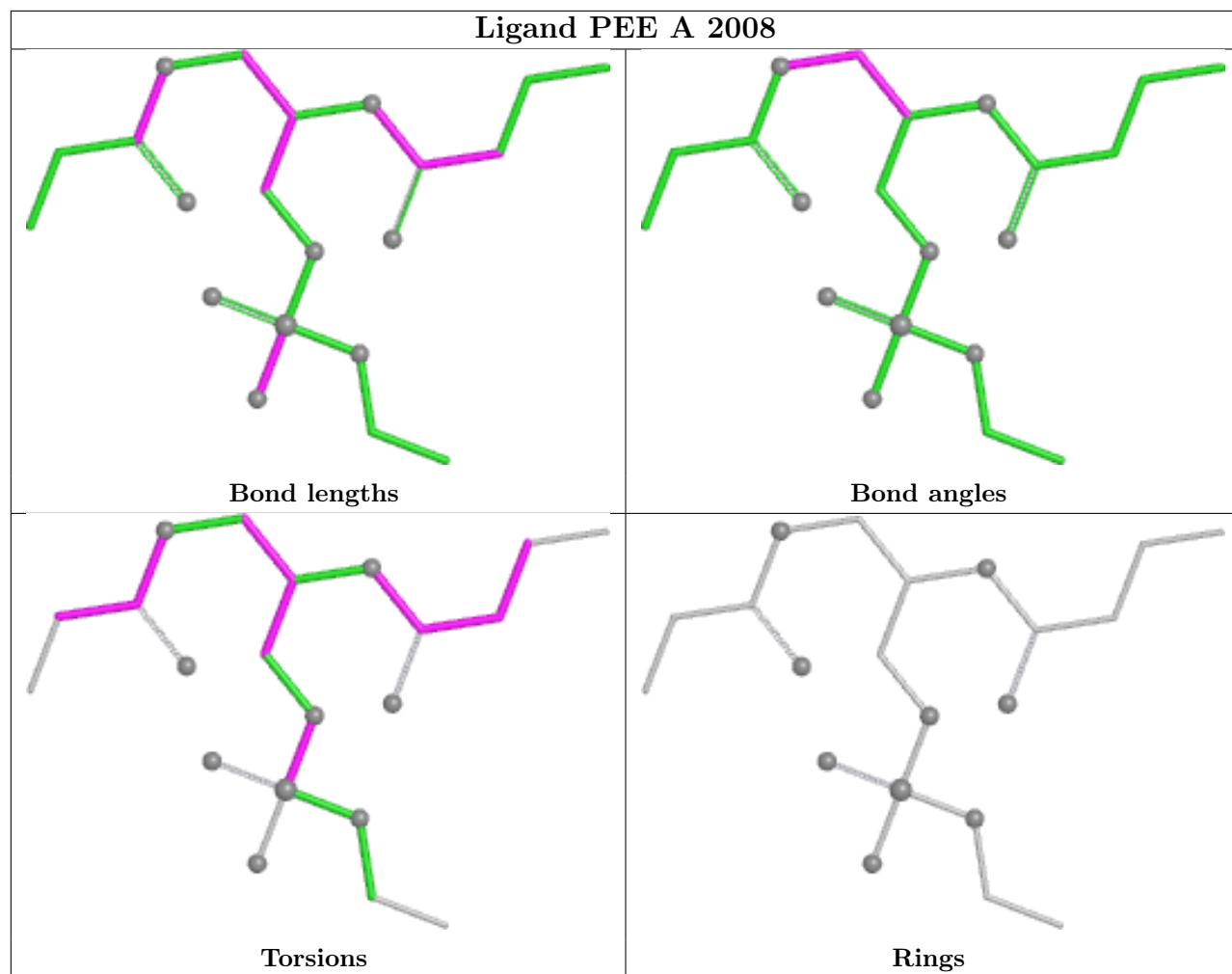


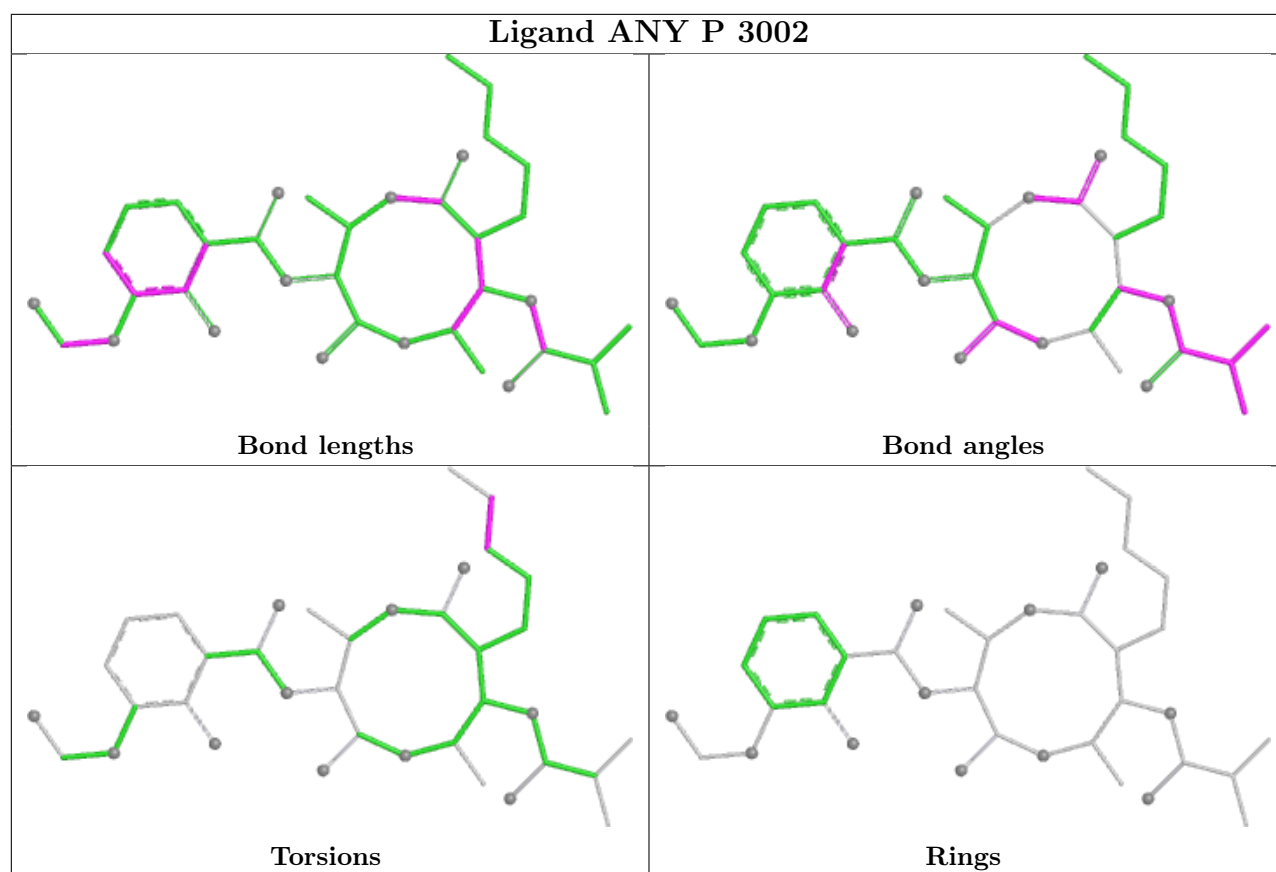




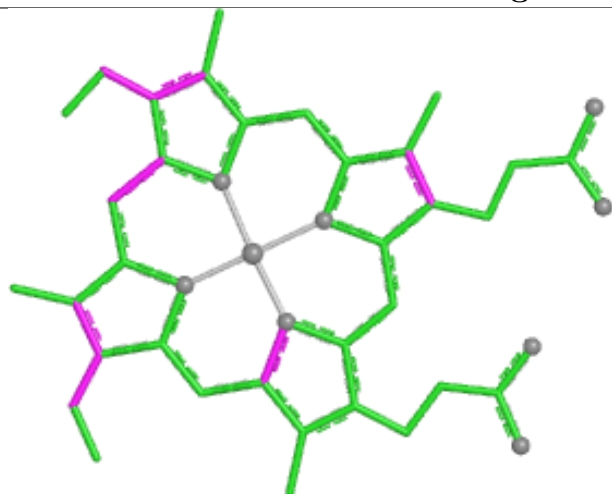




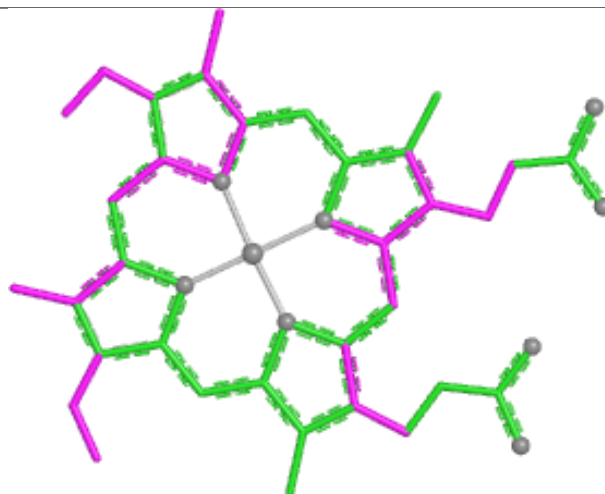




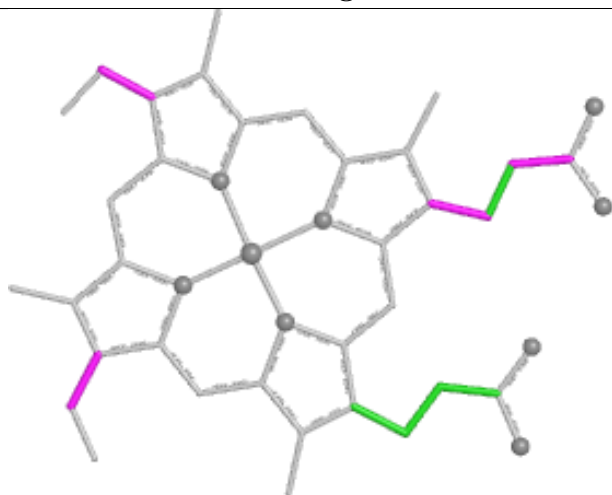
Ligand HEC D 501



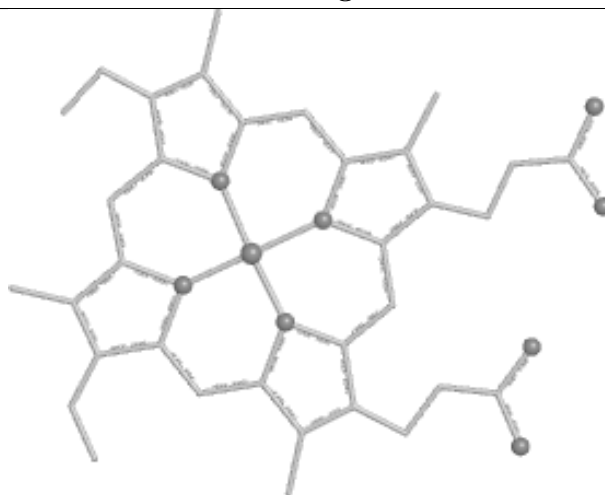
Bond lengths



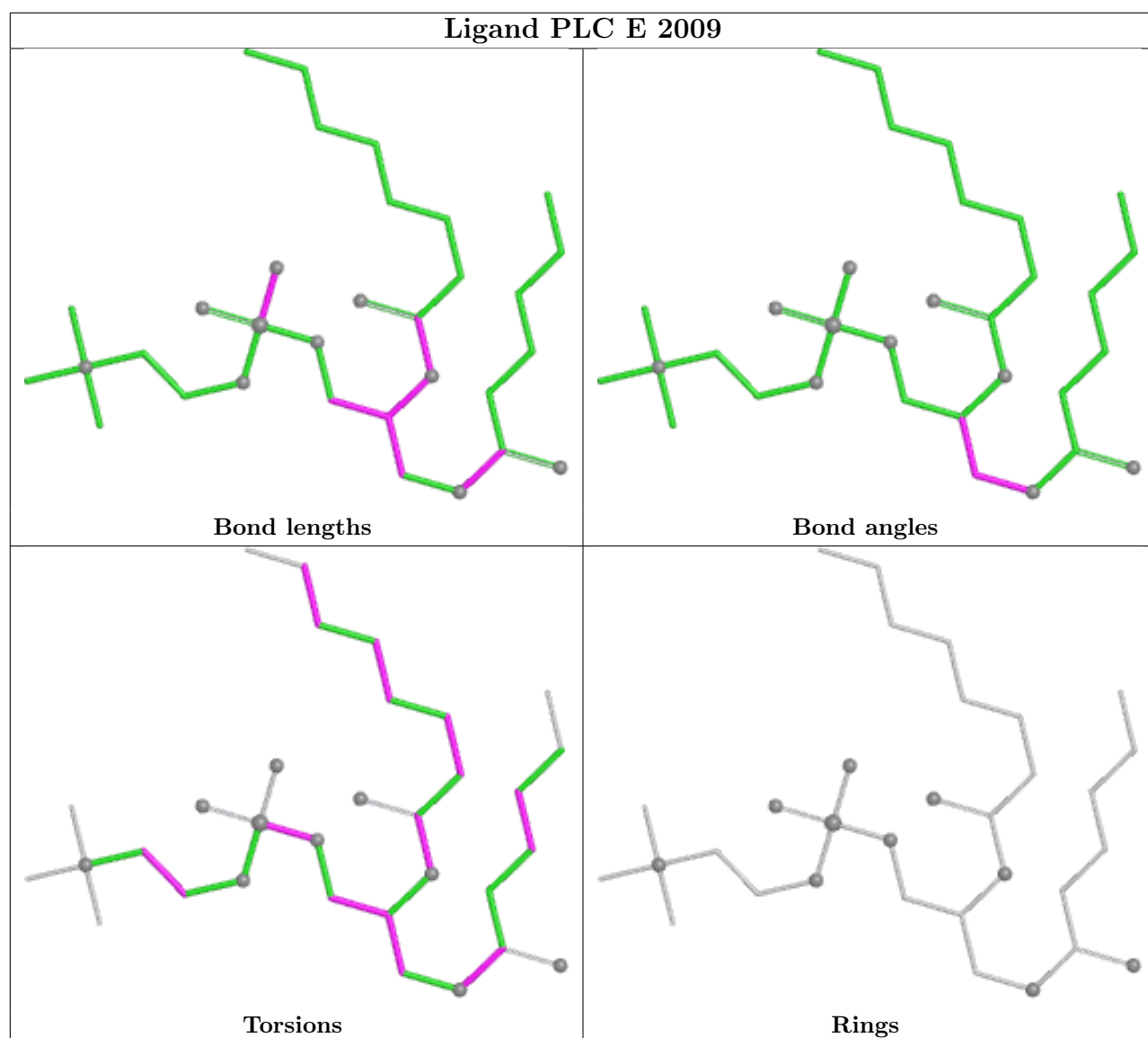
Bond angles

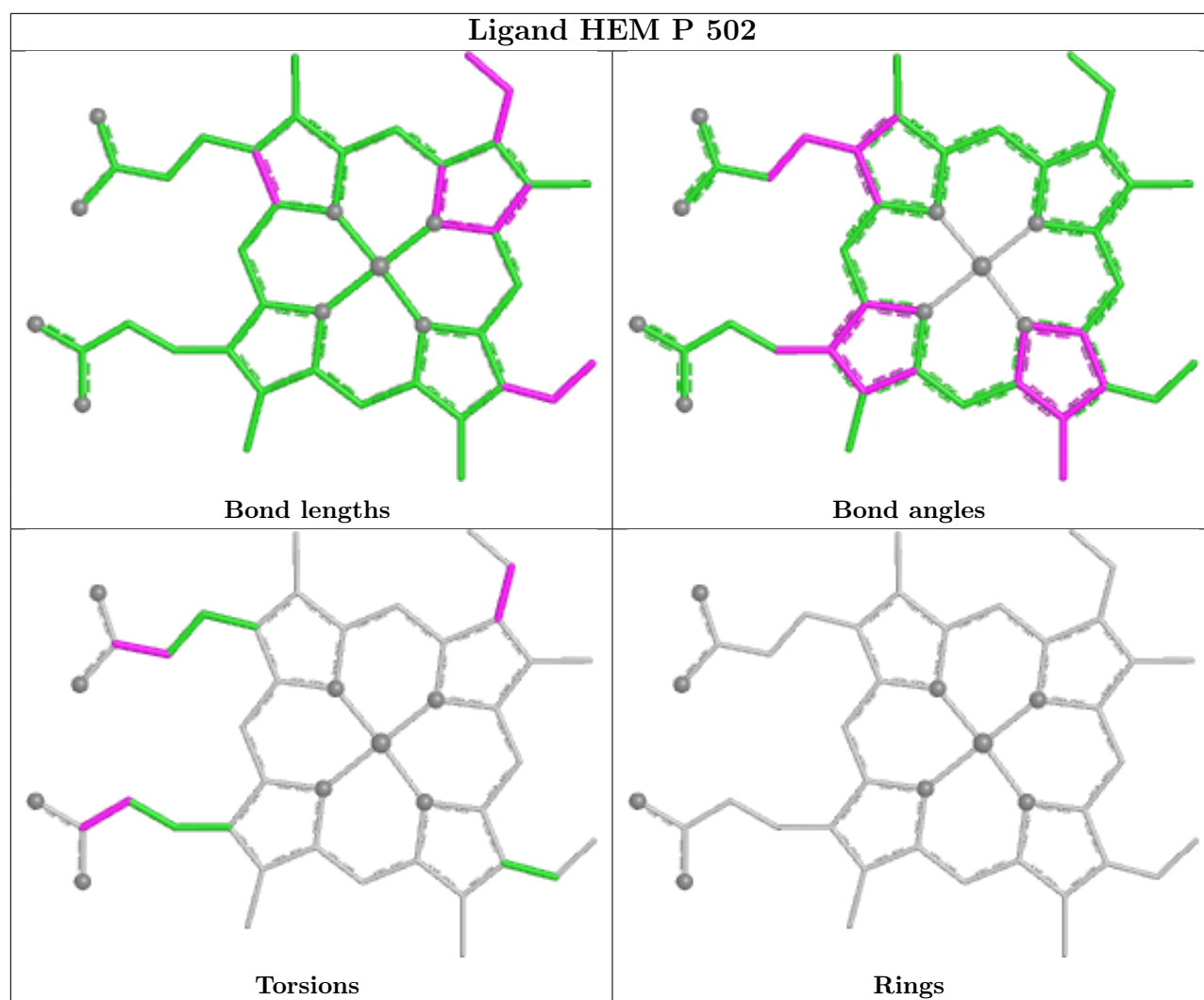


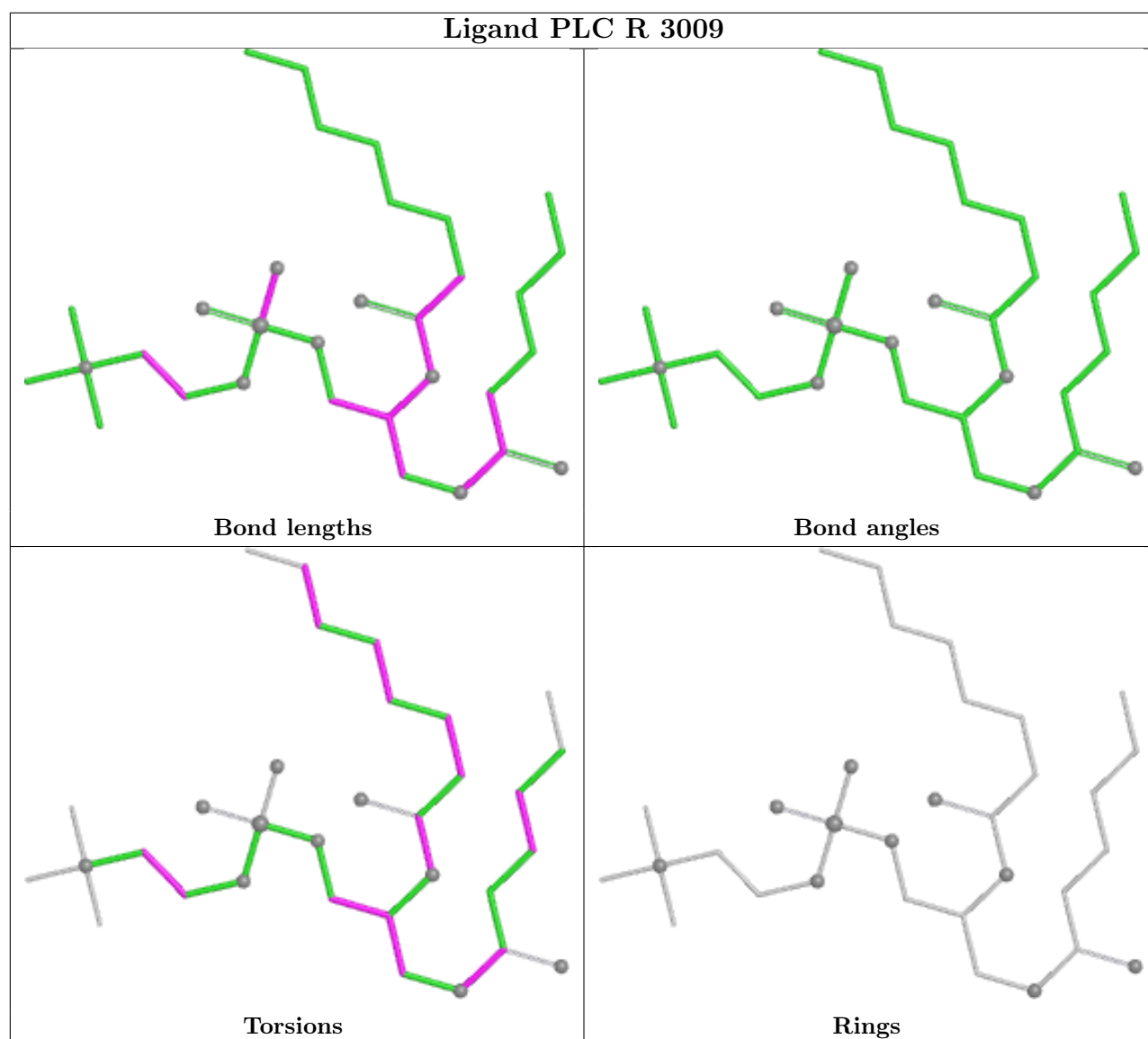
Torsions

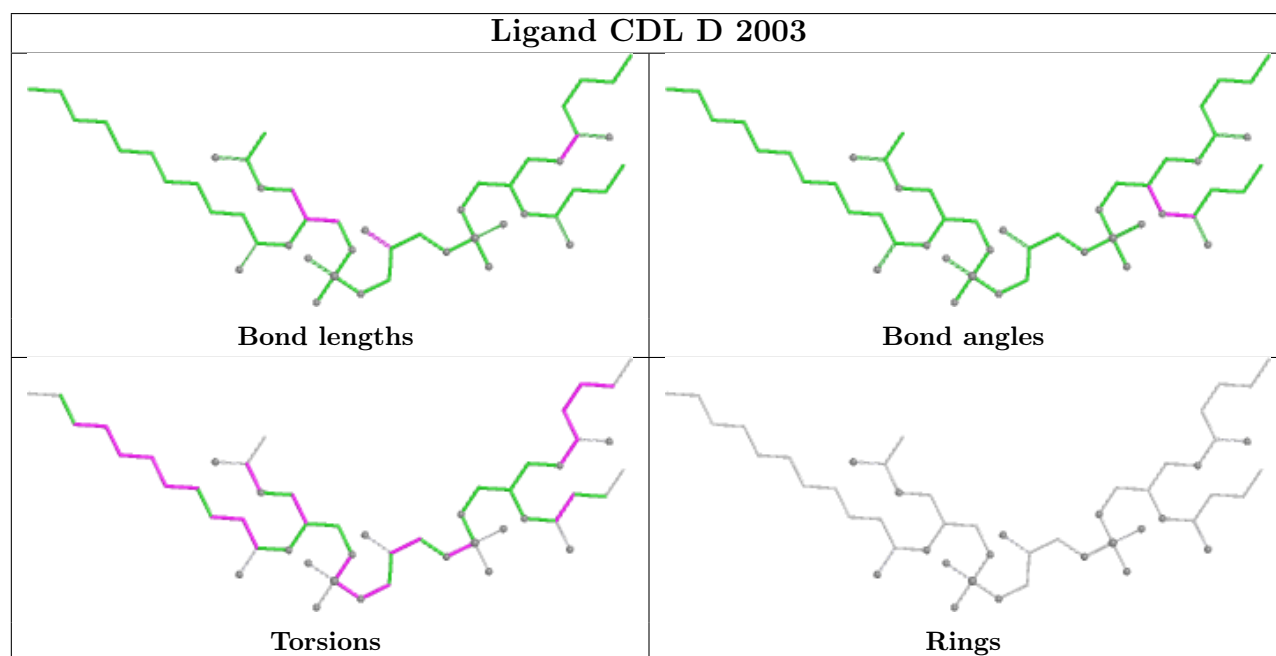
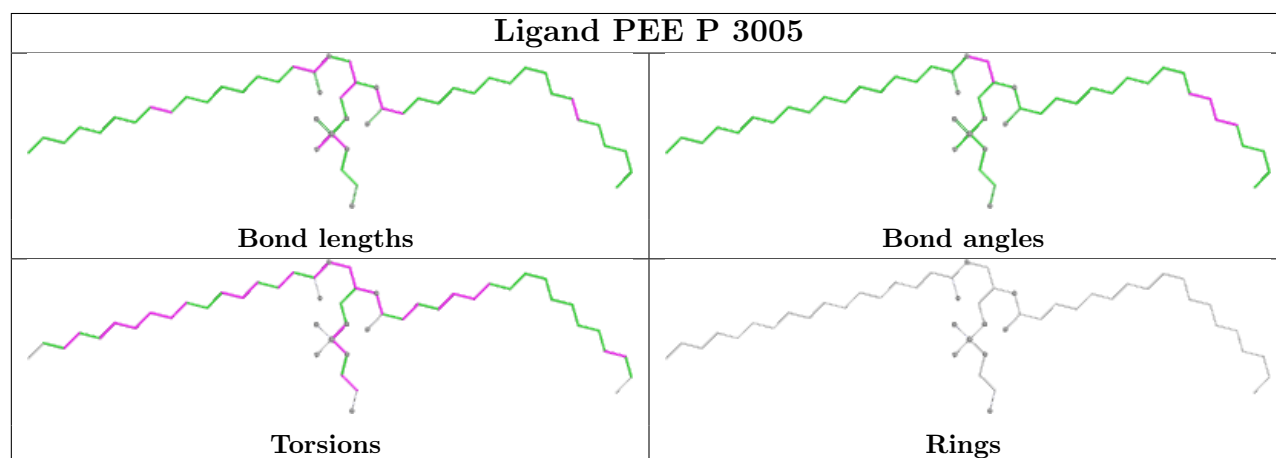
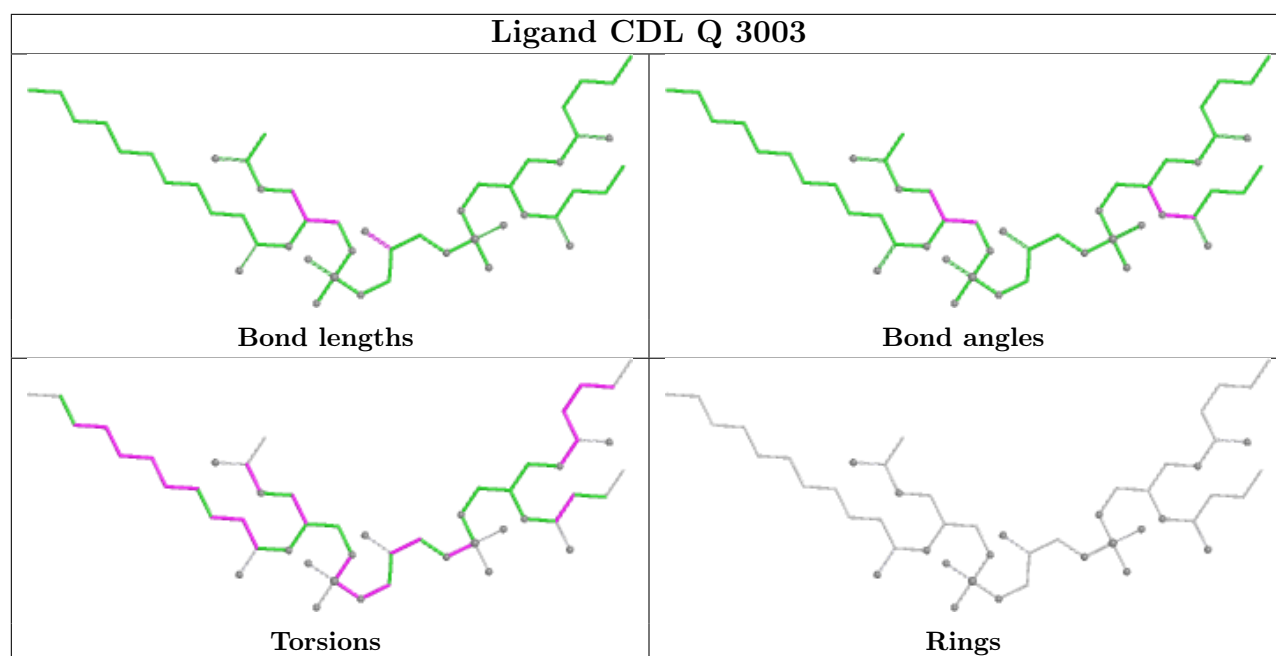


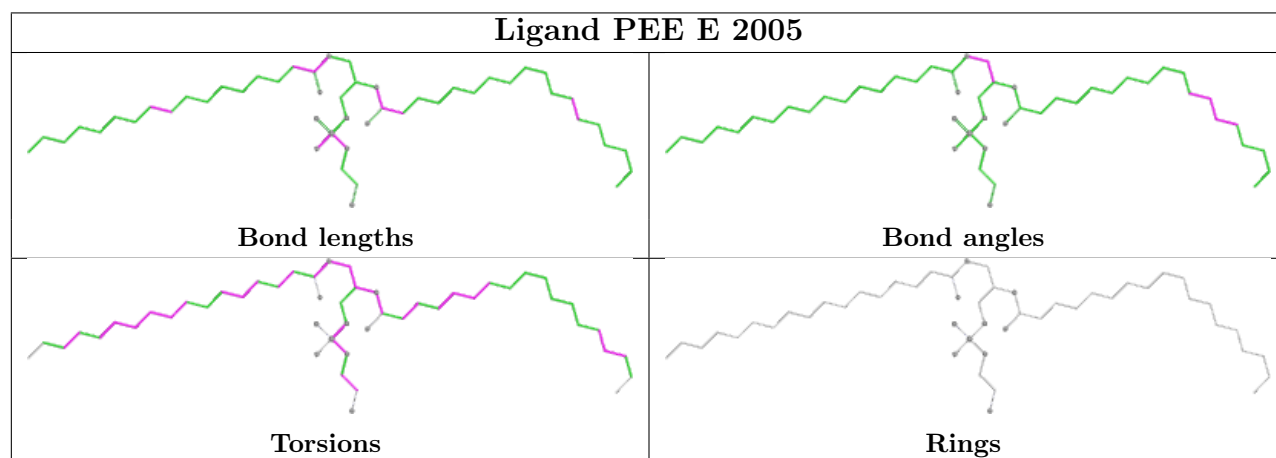
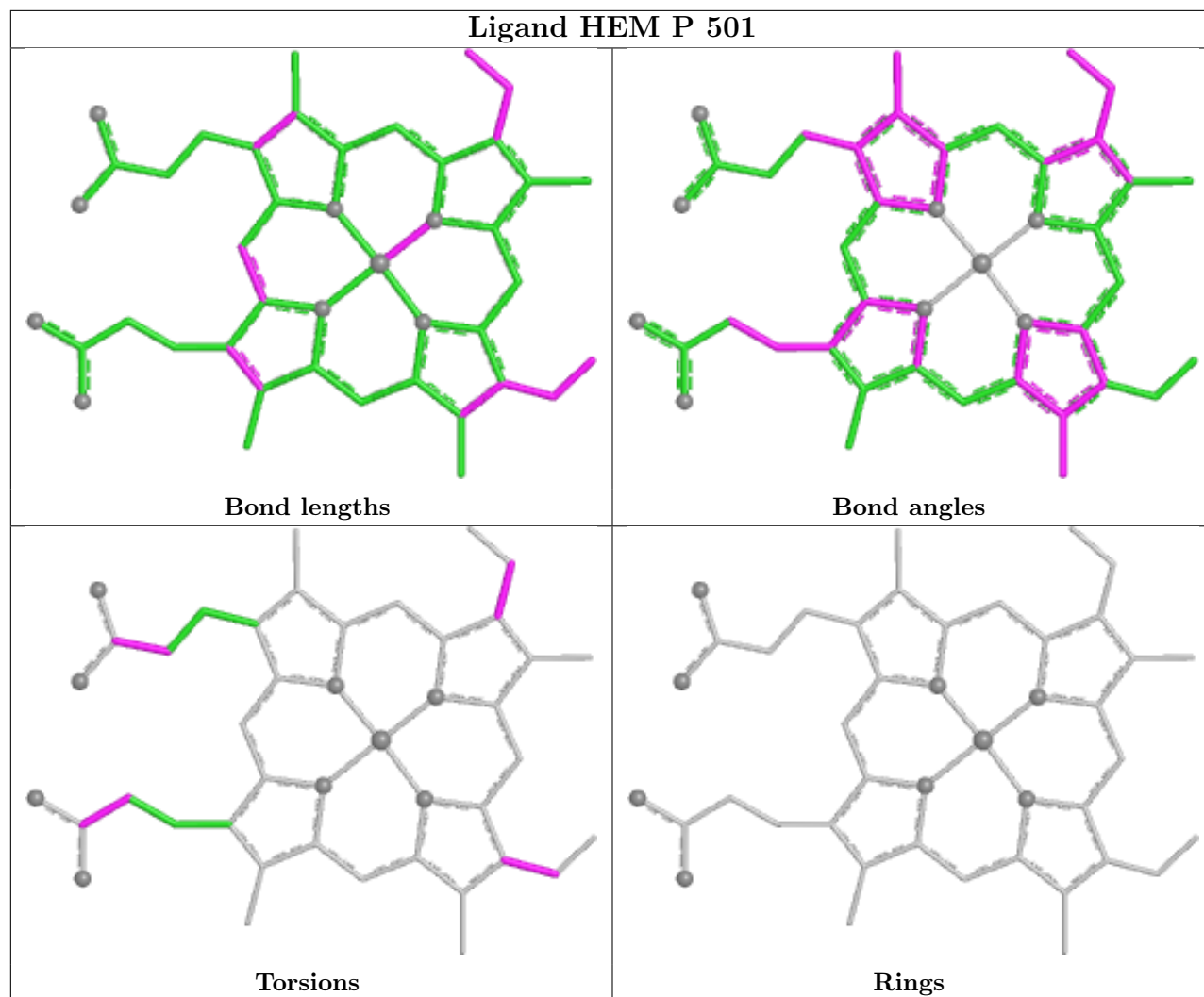
Rings

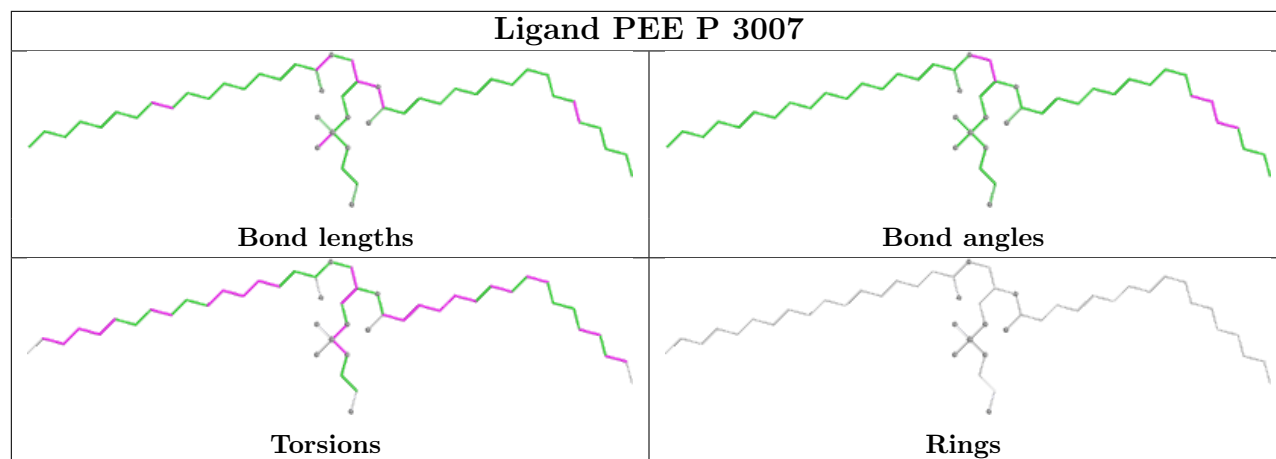












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.01	1 (0%) 91 80	40, 85, 131, 143	0
1	N	442/446 (99%)	0.17	3 (0%) 84 60	42, 91, 131, 143	0
2	B	421/441 (95%)	0.25	5 (1%) 76 49	63, 107, 145, 173	0
2	O	422/441 (95%)	0.14	3 (0%) 84 60	50, 97, 140, 150	0
3	C	380/380 (100%)	-0.64	1 (0%) 90 74	17, 40, 73, 122	0
3	P	379/380 (99%)	-0.25	1 (0%) 90 74	20, 71, 106, 136	0
4	D	241/241 (100%)	-0.44	0 100 100	28, 55, 105, 118	0
4	Q	241/241 (100%)	0.01	2 (0%) 82 57	51, 93, 136, 148	0
5	E	196/196 (100%)	0.23	1 (0%) 87 66	36, 123, 175, 180	0
5	R	196/196 (100%)	0.15	1 (0%) 87 66	50, 97, 152, 159	0
6	F	101/110 (91%)	-0.58	0 100 100	32, 57, 80, 112	0
6	S	101/110 (91%)	0.09	1 (0%) 79 53	67, 103, 138, 161	0
7	G	81/81 (100%)	-0.14	0 100 100	38, 66, 112, 123	0
7	T	79/81 (97%)	0.49	2 (2%) 58 32	62, 112, 176, 184	0
8	H	70/77 (90%)	-0.11	0 100 100	50, 90, 109, 132	0
8	U	67/77 (87%)	0.66	3 (4%) 38 19	129, 151, 171, 173	0
9	I	31/47 (65%)	1.05	4 (12%) 7 5	100, 143, 177, 178	0
9	V	31/47 (65%)	1.46	7 (22%) 2 2	107, 152, 194, 197	0
10	J	61/61 (100%)	-0.23	0 100 100	57, 72, 124, 165	0
10	W	59/61 (96%)	-0.10	0 100 100	62, 89, 125, 148	0
All	All	4042/4160 (97%)	-0.01	35 (0%) 81 55	17, 87, 148, 197	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	2	ILE	4.1
9	V	54	SER	4.0
1	A	444	ILE	3.9
9	V	72	ALA	3.7
9	V	56	SER	3.5

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($\text{\AA}^2$)	Q<0.9
11	PEE	A	2008	21/51	0.60	0.18	121,125,130,130	0
12	UNL	A	3016	1/-	0.75	0.09	10,10,10,10	0
16	CDL	Q	3003	50/100	0.79	0.26	116,149,158,158	0
16	CDL	D	2003	50/100	0.80	0.19	63,103,110,111	0
12	UNL	C	2010	1/-	0.80	0.13	24,24,24,24	0
11	PEE	N	3008	5/51	0.81	0.11	105,105,106,106	0
11	PEE	P	3005	50/51	0.81	0.25	75,97,113,115	0
16	CDL	P	3004	40/100	0.83	0.15	101,108,110,110	0
20	PLC	E	2009	32/42	0.84	0.19	37,60,94,95	0
20	PLC	R	3009	32/42	0.84	0.23	74,93,118,118	0
11	PEE	P	3007	49/51	0.85	0.17	63,96,134,135	0
16	CDL	C	2004	40/100	0.86	0.14	50,72,90,92	0
12	UNL	P	3104	1/-	0.86	0.10	42,42,42,42	0
12	UNL	R	2103	1/-	0.86	0.12	12,12,12,12	0
11	PEE	E	2005	50/51	0.87	0.19	66,86,100,101	0
12	UNL	P	3010	1/-	0.89	0.12	24,24,24,24	0
11	PEE	C	2007	49/51	0.90	0.14	44,56,90,91	0
12	UNL	E	2105	1/-	0.92	0.08	35,35,35,35	0
12	UNL	P	2015	1/-	0.93	0.07	25,25,25,25	0

Continued on next page...

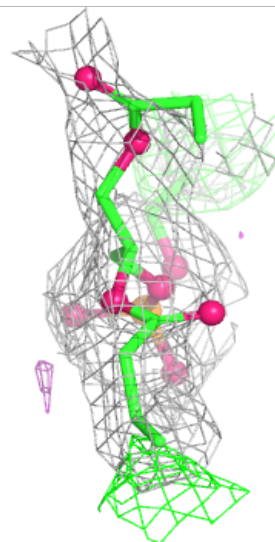
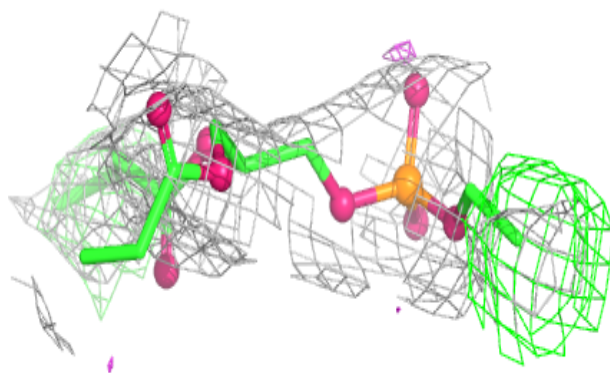
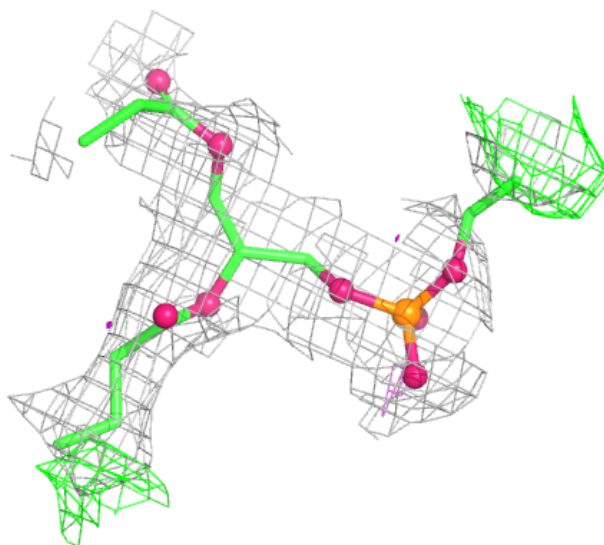
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	UNL	E	3103	1/-	0.93	0.10	32,32,32,32	0
14	SMA	P	3001	37/37	0.93	0.12	64,69,74,75	0
12	UNL	C	3015	1/-	0.95	0.13	32,32,32,32	0
12	UNL	C	2104	1/-	0.95	0.22	36,36,36,36	0
15	ANY	P	3002	37/40	0.95	0.12	65,69,82,82	0
15	ANY	C	2002	37/40	0.96	0.08	27,36,48,50	0
18	HEC	Q	501	43/43	0.97	0.09	64,68,72,76	0
13	HEM	P	502	43/43	0.97	0.10	49,52,70,77	0
17	GOL	P	3011	6/6	0.97	0.15	46,48,50,50	0
13	HEM	C	502	43/43	0.98	0.07	21,28,43,49	0
18	HEC	D	501	43/43	0.98	0.07	34,39,48,55	0
14	SMA	C	2001	37/37	0.98	0.06	20,30,37,39	0
19	FES	E	501	4/4	0.98	0.04	87,88,89,90	0
13	HEM	P	501	43/43	0.98	0.07	44,49,55,56	0
17	GOL	C	2011	6/6	0.98	0.14	67,70,71,73	0
13	HEM	C	501	43/43	0.99	0.07	24,32,36,39	0
19	FES	R	501	4/4	0.99	0.04	55,56,58,58	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.

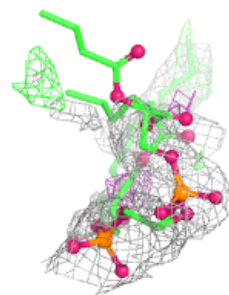
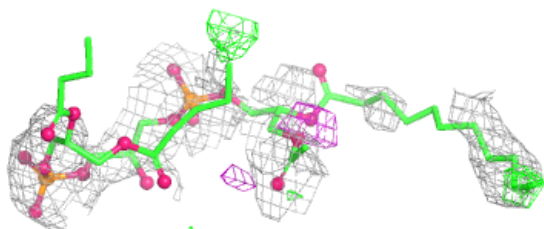
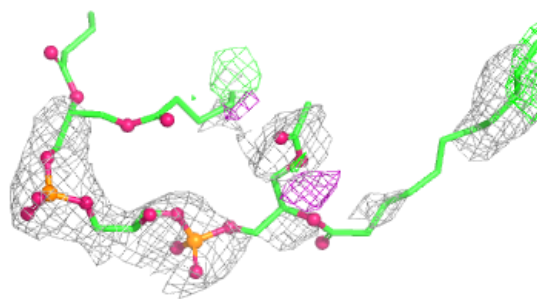
Electron density around PEE A 2008:

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

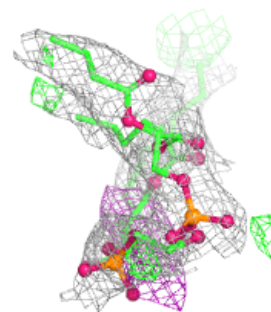
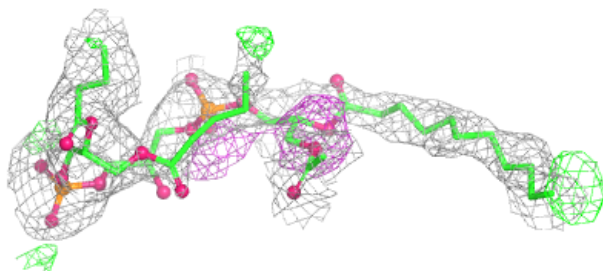
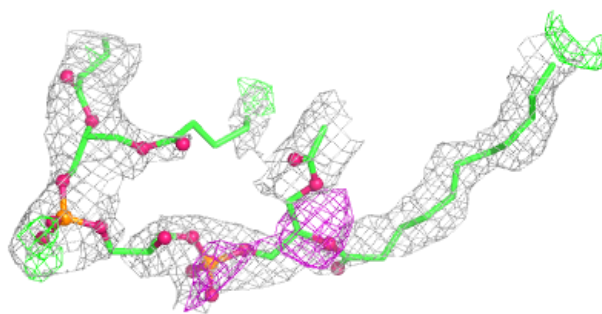


Electron density around CDL Q 3003:

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

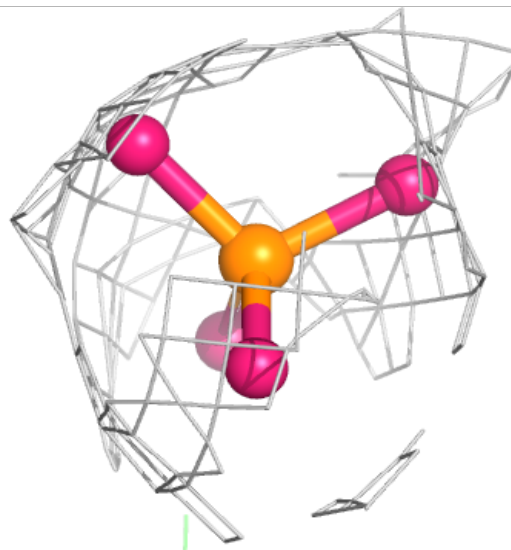
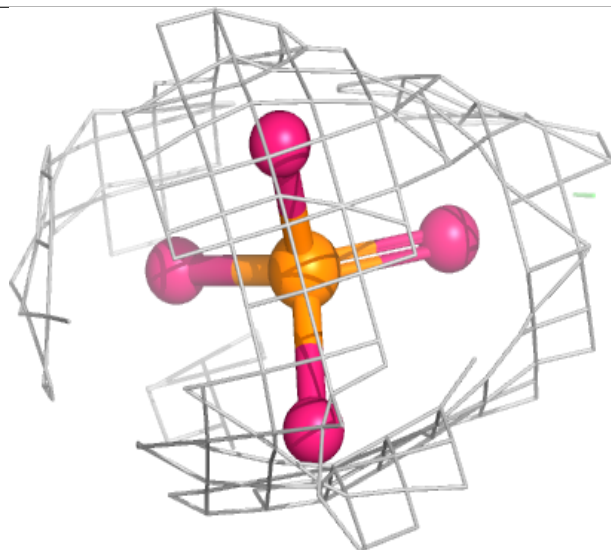
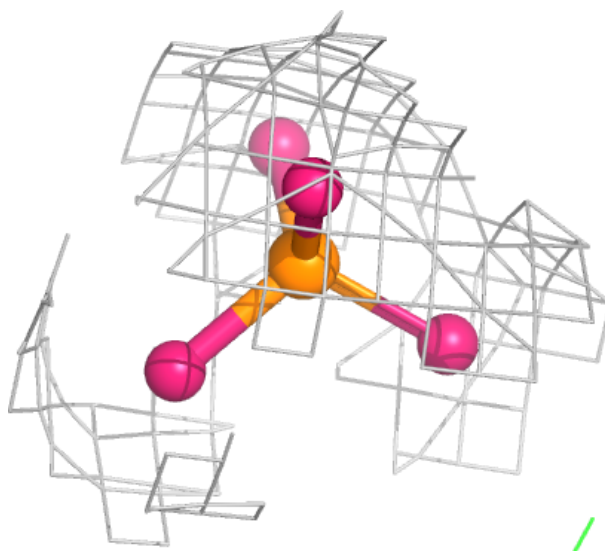
**Electron density around CDL D 2003:**

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



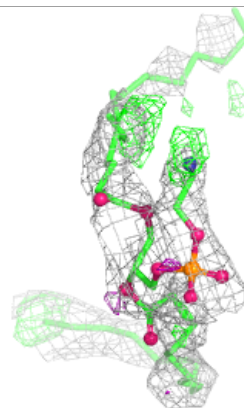
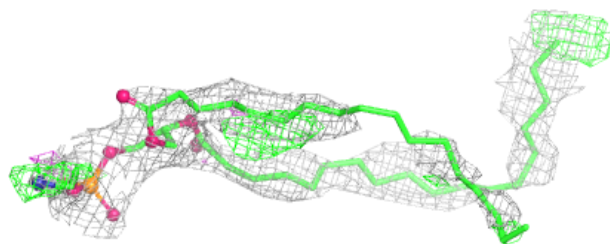
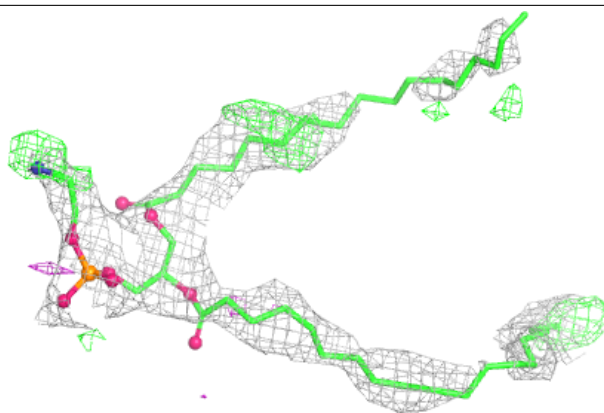
Electron density around PEE N 3008:

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



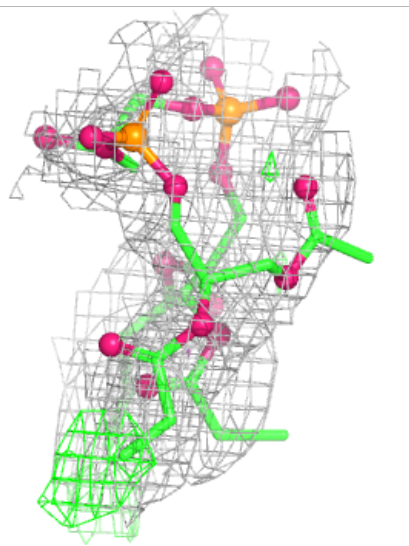
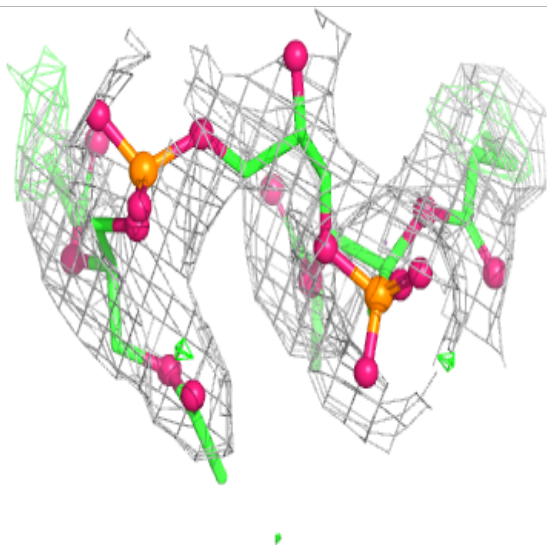
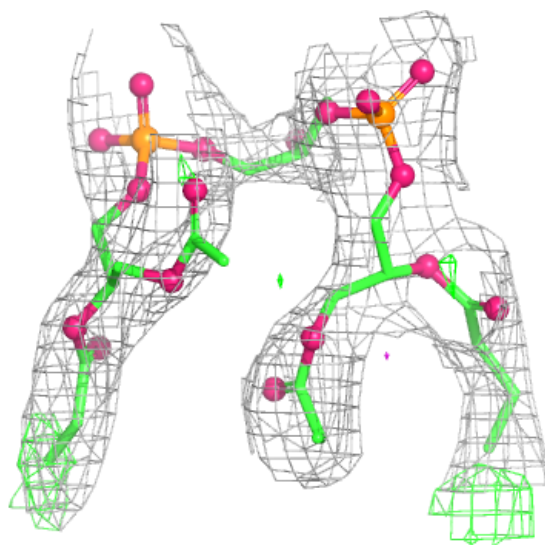
Electron density around PEE P 3005:

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



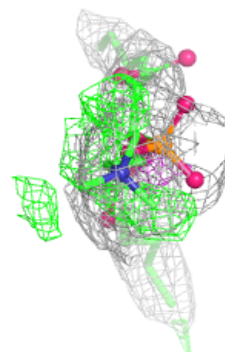
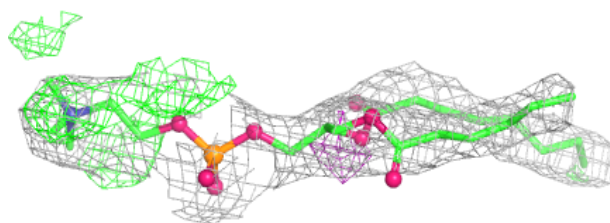
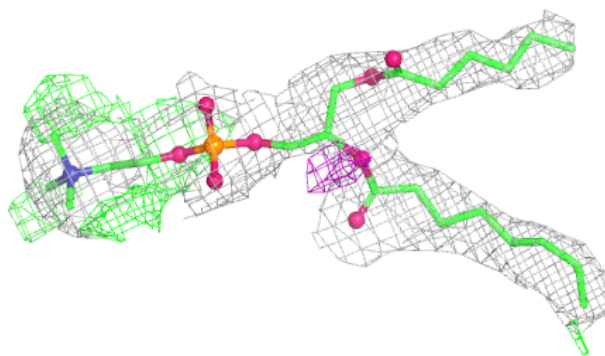
Electron density around CDL P 3004:

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

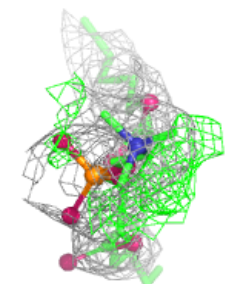
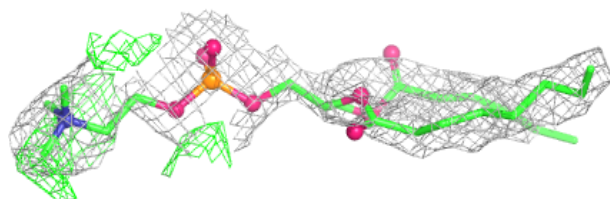
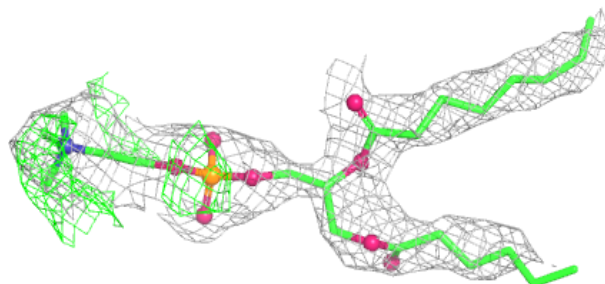


Electron density around PLC E 2009:

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

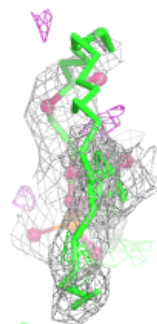
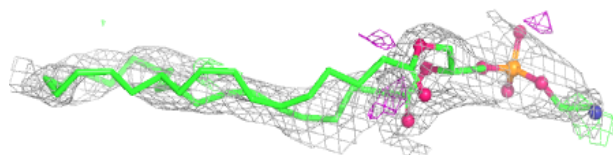
**Electron density around PLC R 3009:**

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



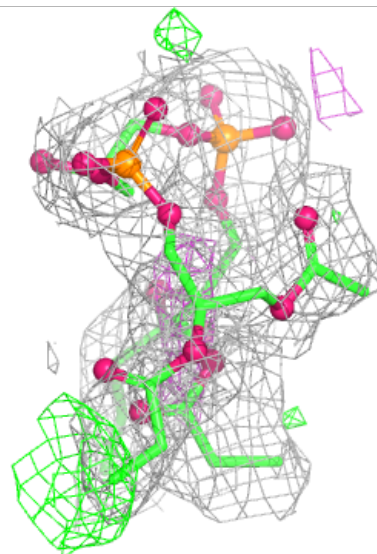
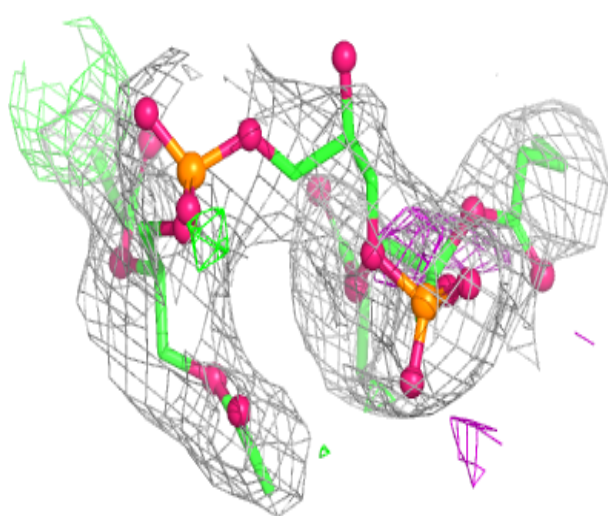
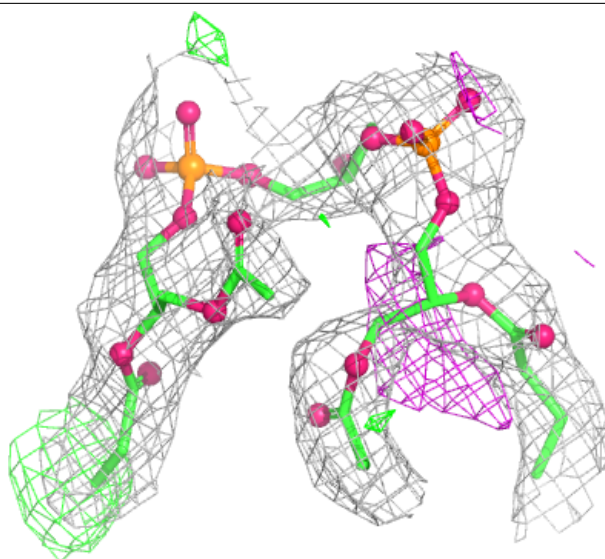
Electron density around PEE P 3007:

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



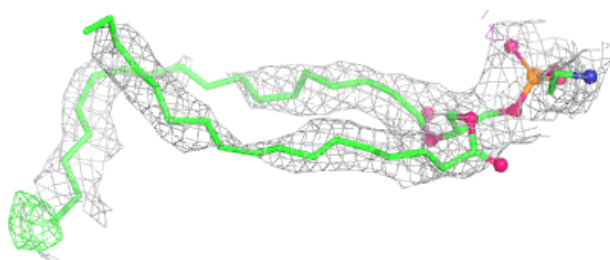
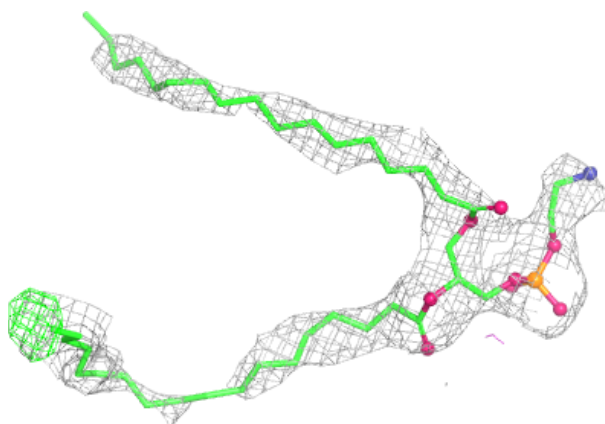
Electron density around CDL C 2004:

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

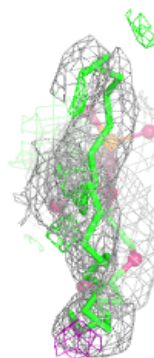
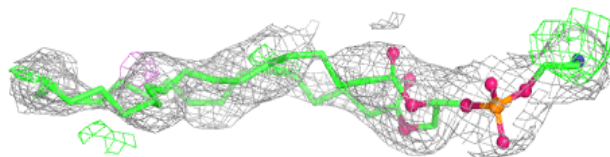
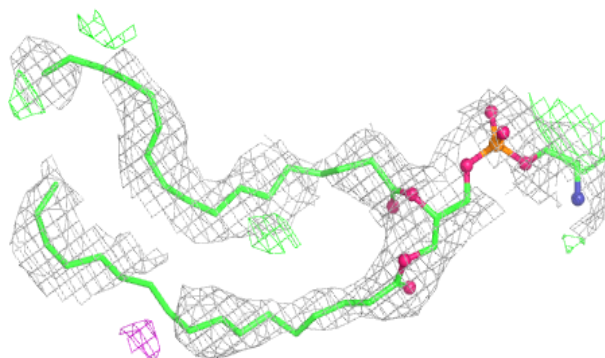


Electron density around PEE E 2005:

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

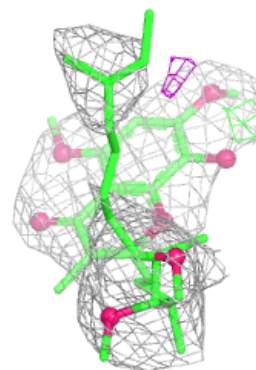
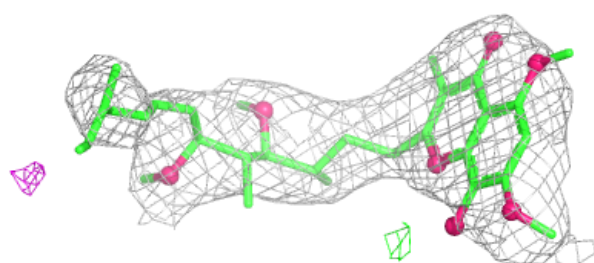
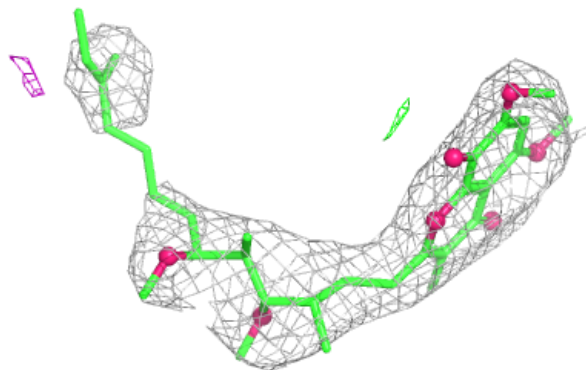
**Electron density around PEE C 2007:**

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

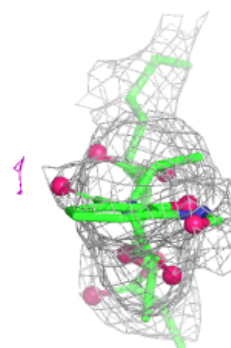
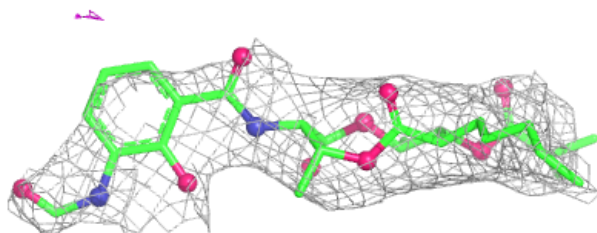
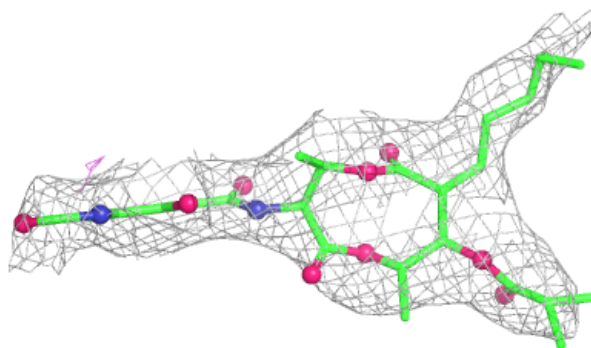


Electron density around SMA P 3001:

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

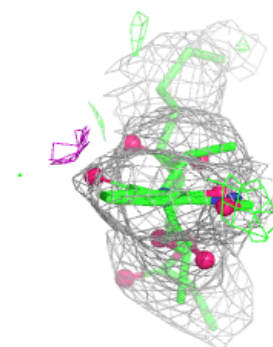
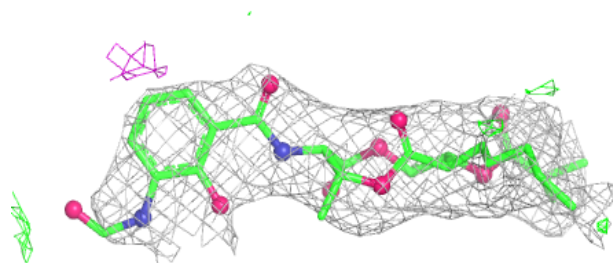
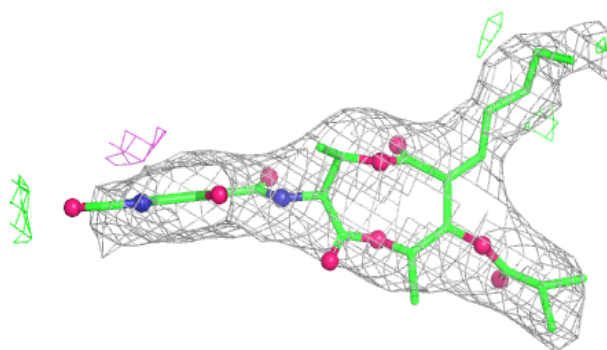
**Electron density around ANY P 3002:**

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

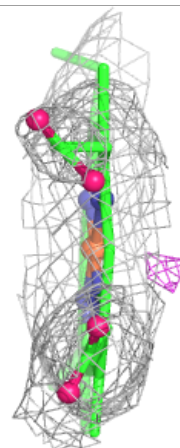
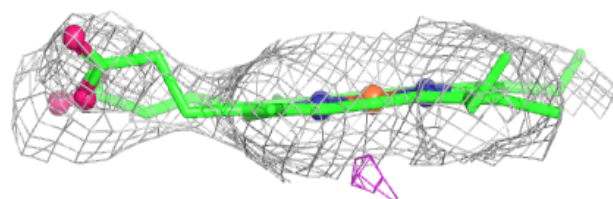
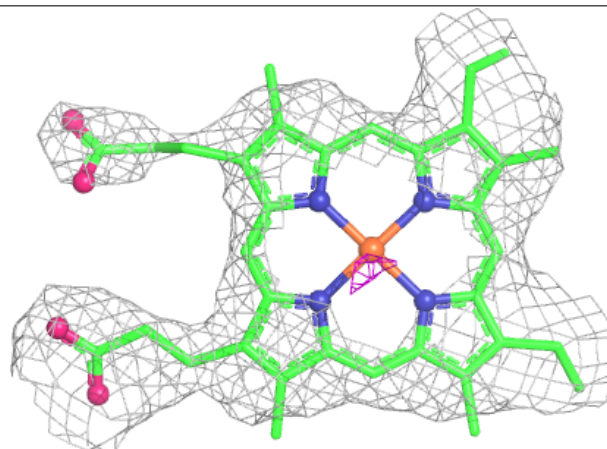


Electron density around ANY C 2002:

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

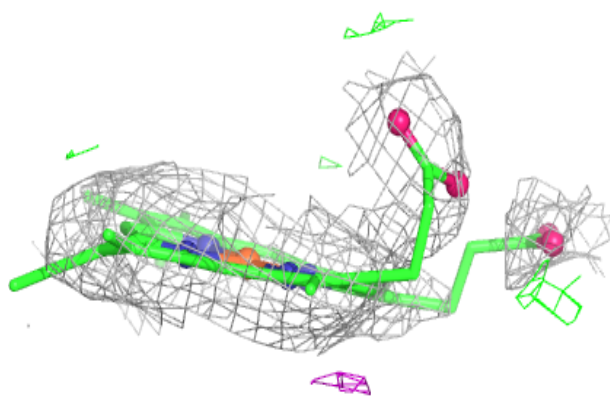
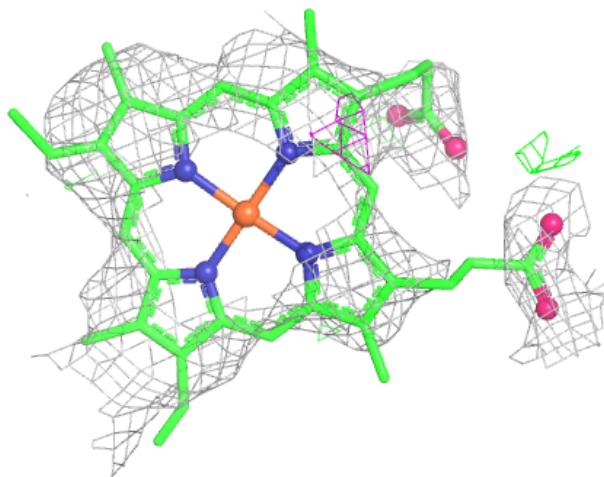
**Electron density around HEC Q 501:**

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



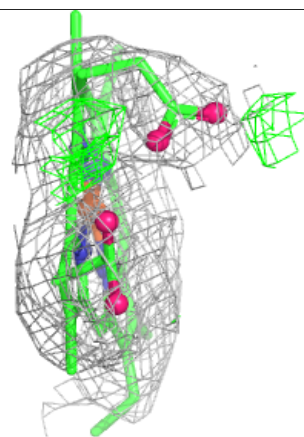
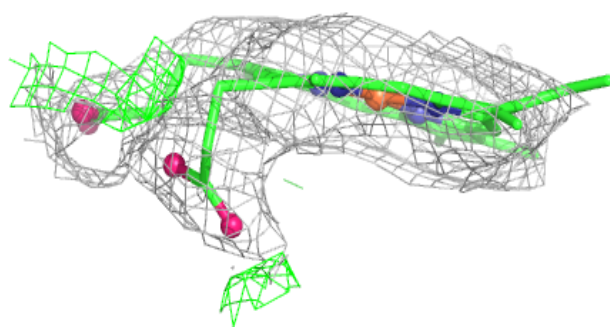
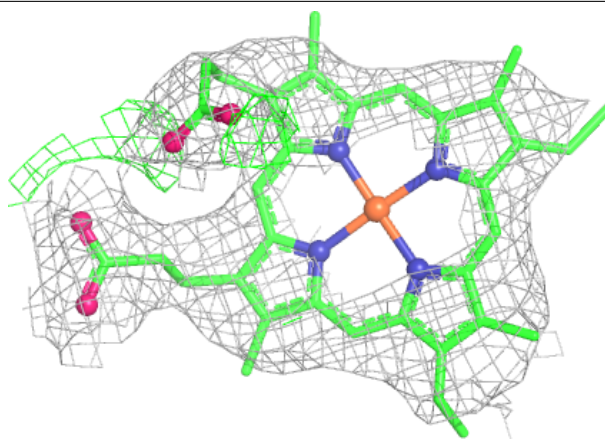
Electron density around HEM P 502:

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



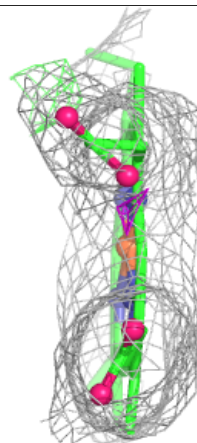
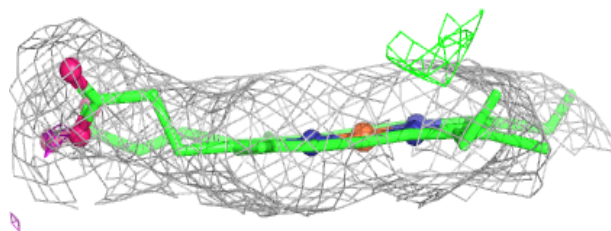
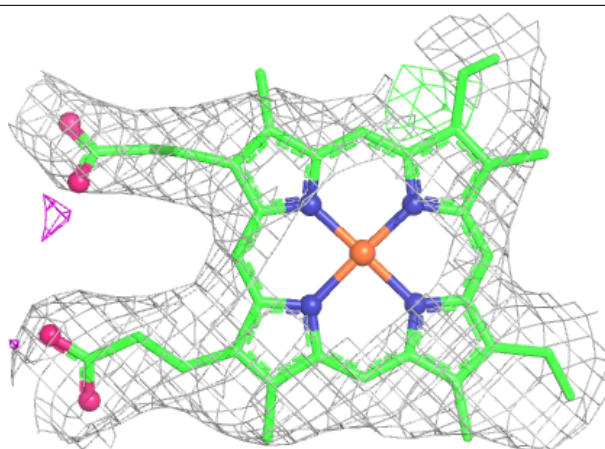
Electron density around HEM C 502:

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



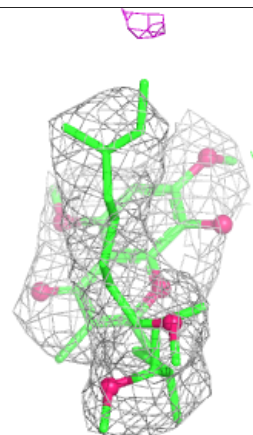
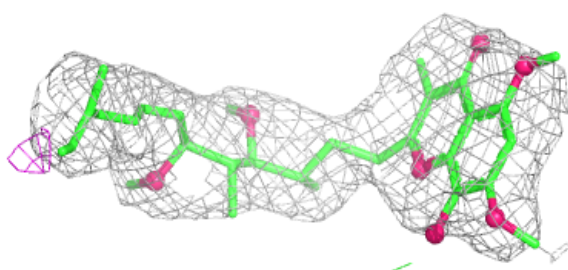
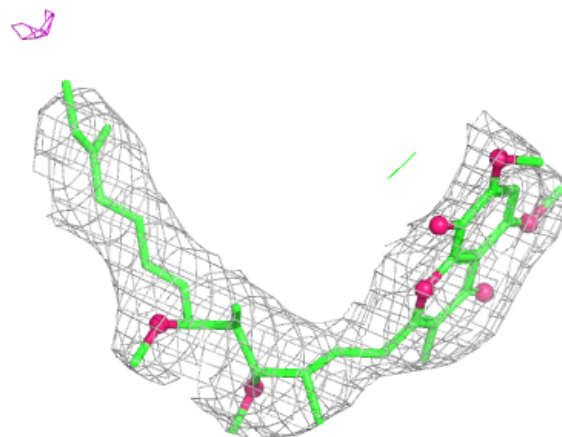
Electron density around HEC D 501:

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



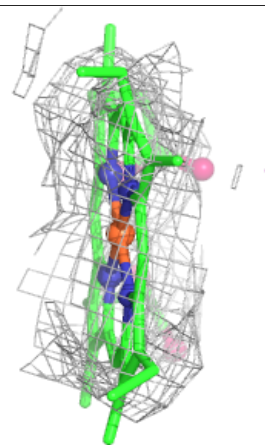
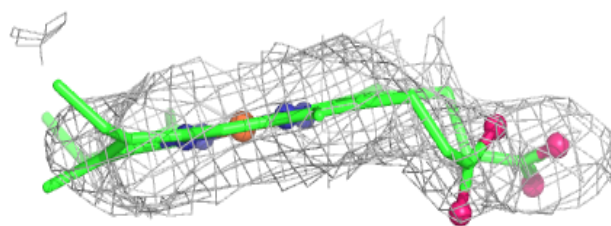
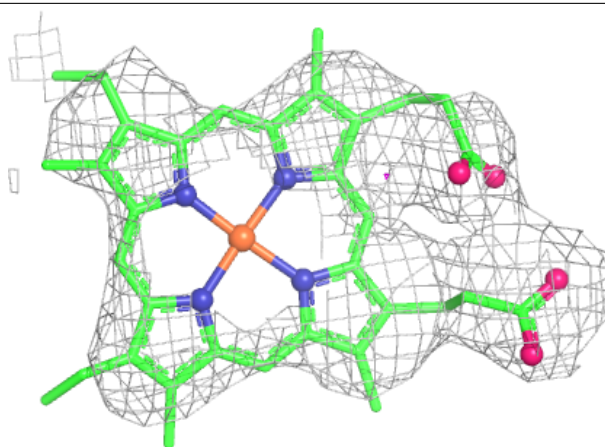
Electron density around SMA C 2001:

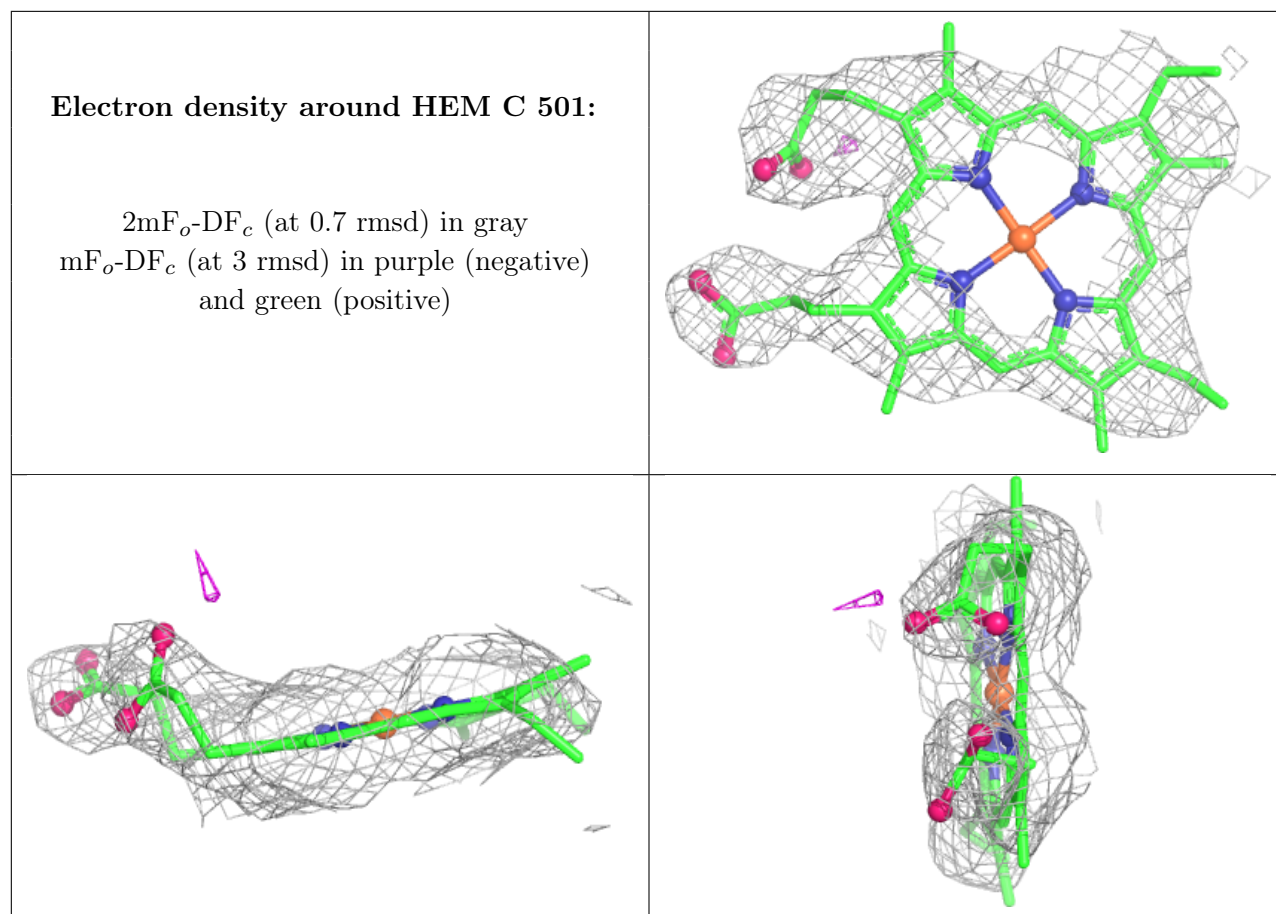
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.