



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 12:13 PM UTC

PDB ID : 2A06 / pdb_00002a06
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2005-06-16
Resolution : 2.10 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)
Xtrriage (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

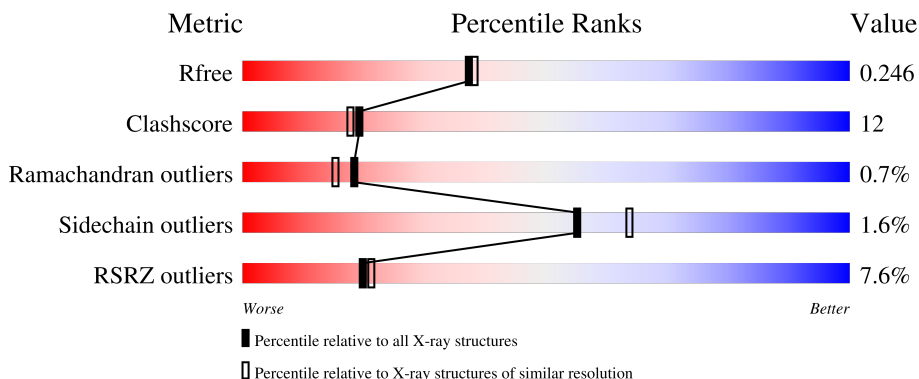
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	 4% 80% 18% ..
1	N	446	 7% 78% 20% ..
2	B	439	 4% 74% 21% ..
2	O	439	 11% 72% 22% ..
3	C	379	 2% 77% 18% ..

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Mol	Chain	Length	Quality of chain
3	P	379	
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	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

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	JZR	F	3012	-	-	-	X
12	PO4	A	2010	-	X	-	-
12	PO4	B	3009	-	X	-	-
12	PO4	D	4010	-	X	-	-
12	PO4	D	4011	-	X	-	-
12	PO4	I	4015	-	X	-	-
12	PO4	O	2009	-	X	-	-
12	PO4	P	3010	-	X	-	-
12	PO4	Q	4012	-	X	-	-
12	PO4	R	4013	-	X	-	-
12	PO4	R	4014	-	X	-	-
12	PO4	T	4016	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	AZI	A	4002	-	X	-	-
13	AZI	C	2005	-	X	-	-
13	AZI	G	4001	-	X	-	-
13	AZI	P	3005	-	X	-	-
14	UNL	O	4043	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33890 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
			Total	C	N	O	S			
1	A	443	3398	2118	602	658	20	10	0	1
1	N	443	3398	2118	602	658	20	10	0	1

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	3177	1996	562	612	7	0	0	1
2	O	424	3180	1998	562	613	7	0	0	0

- Molecule 3 is a protein called Cytochrome b, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	365	2897	1945	450	485	17	0	0	0
3	P	370	2936	1973	455	490	18	0	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0
4	Q	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	955	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- 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	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

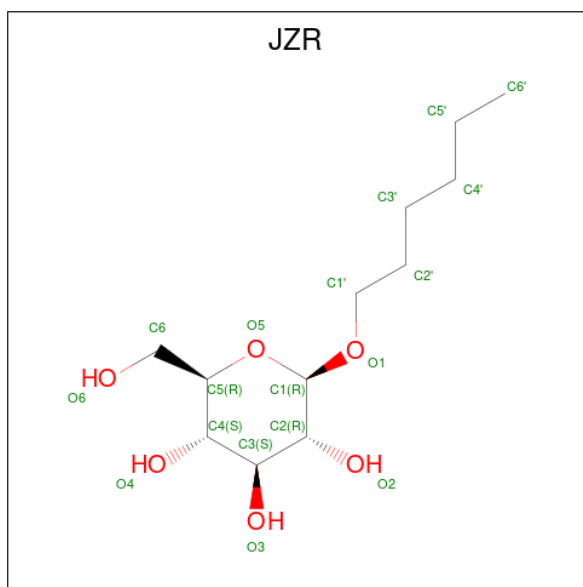
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

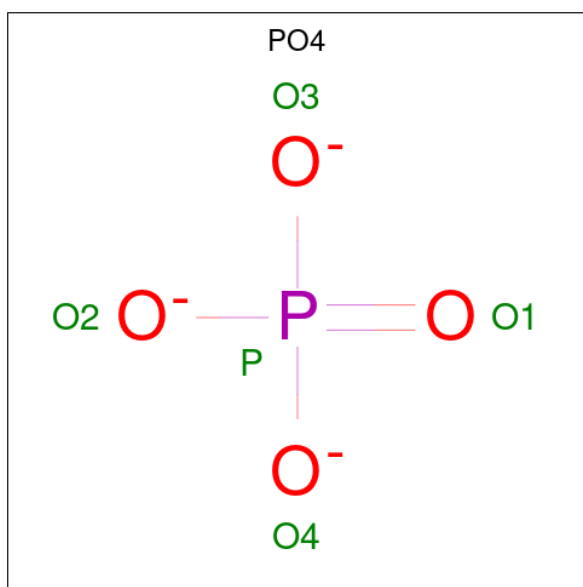
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: C₁₂H₂₄O₆).



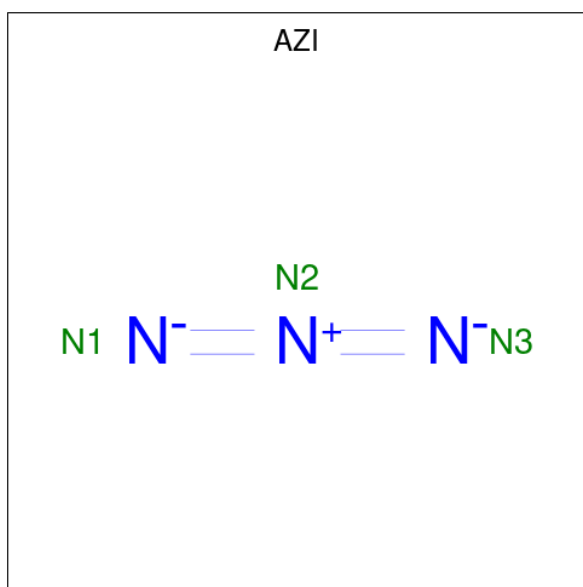
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	I	1	Total	O	P	0	0
			5	4	1		
12	O	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	Q	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 3 3	0	0
13	C	1	Total N 3 3	0	0
13	G	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

- Molecule 14 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

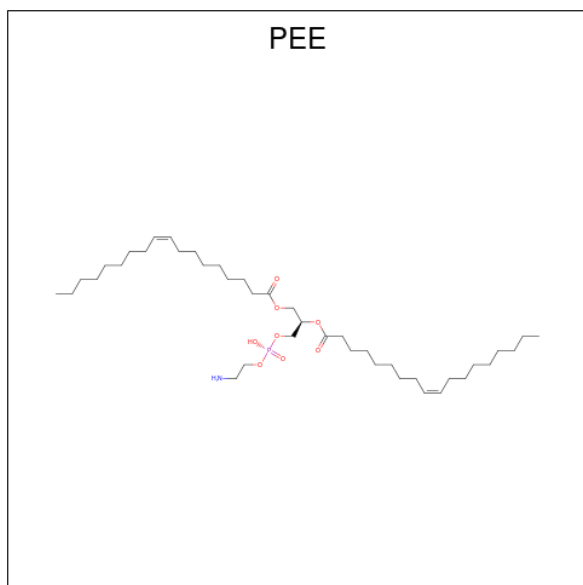
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	10	Total O 10 10	0	0
14	B	11	Total O 11 11	0	0
14	C	6	Total O 7 7	0	0
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	F	1	Total O 1 1	0	0
14	G	3	Total O 3 3	0	0
14	I	2	Total O 2 2	0	0

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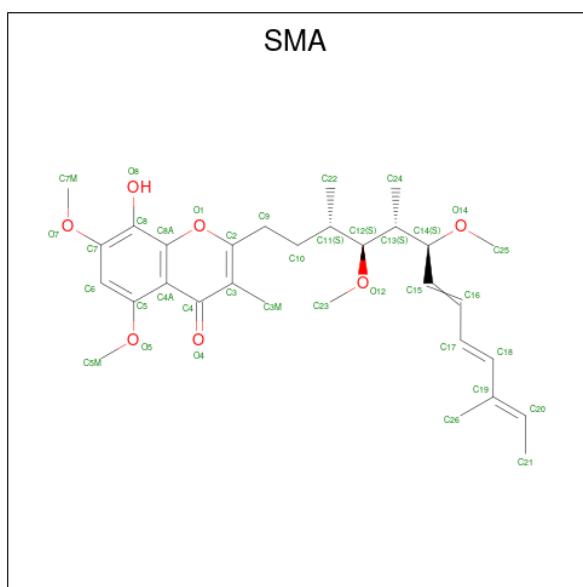
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	N	4	Total O 5 5	0	0
14	O	8	Total O 9 9	0	0
14	P	7	Total O 8 8	0	0
14	Q	1	Total O 1 1	0	0
14	R	2	Total O 2 2	0	0
14	S	1	Total O 1 1	0	0
14	T	2	Total O 2 2	0	0
14	U	2	Total O 2 2	0	0
14	V	4	Total O 4 4	0	0
14	W	1	Total O 1 1	0	0

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



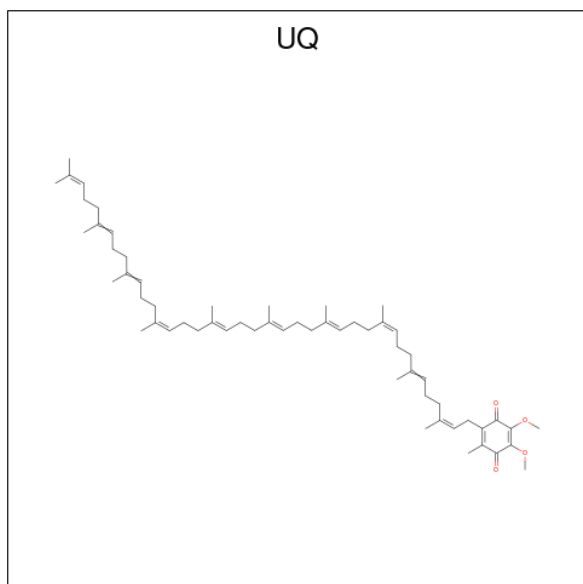
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total	C O	0	0
			37	30 7		
17	P	1	Total	C O	0	0
			37	30 7		

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



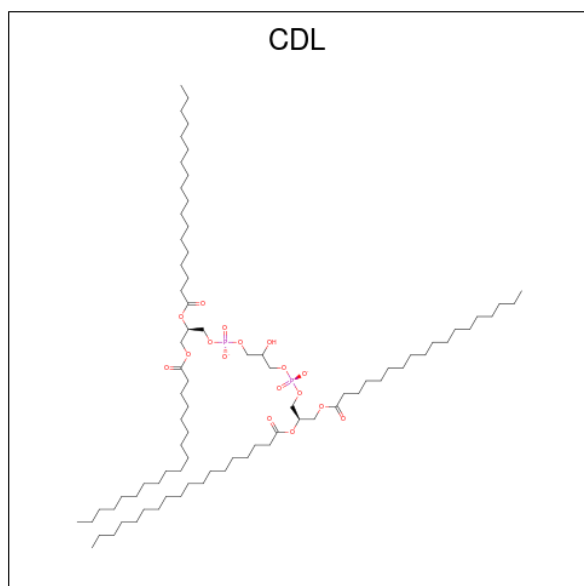
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	C O	0	0
			18	14 4		

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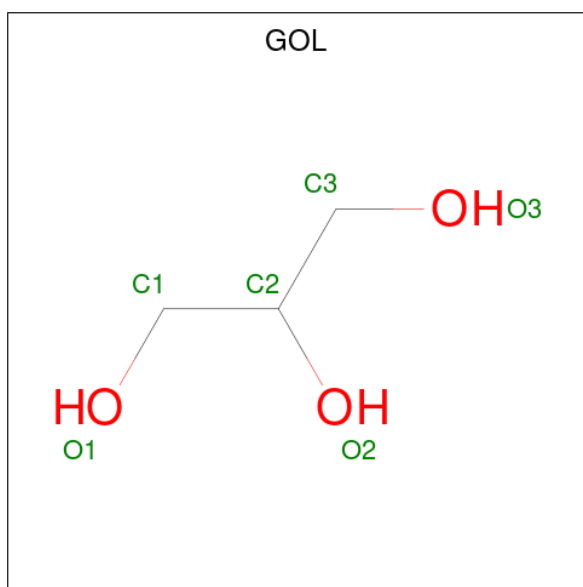
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	P	1	18	14	4	0	0

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



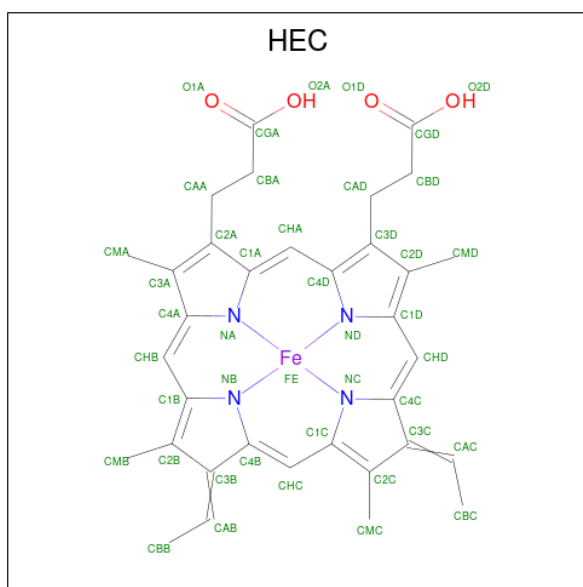
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
19	C	1	44	25	17	2	0	0
19	D	1	39	24	13	2	0	0
19	P	1	49	30	17	2	0	0
19	Q	1	39	24	13	2	0	0

- Molecule 20 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



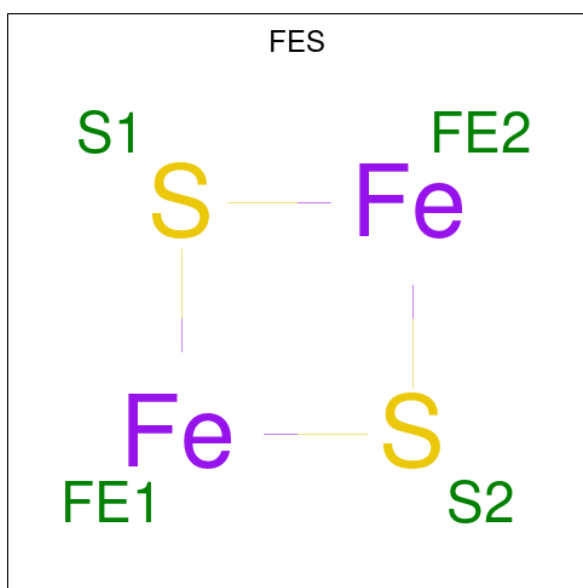
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	1	Total C O 6 3 3	0	0
20	C	1	Total C O 6 3 3	0	0
20	E	1	Total C O 6 3 3	0	0
20	E	1	Total C O 5 3 2	0	0
20	O	1	Total C O 6 3 3	0	0
20	P	1	Total C O 6 3 3	0	0
20	P	1	Total C O 6 3 3	0	0

- Molecule 21 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

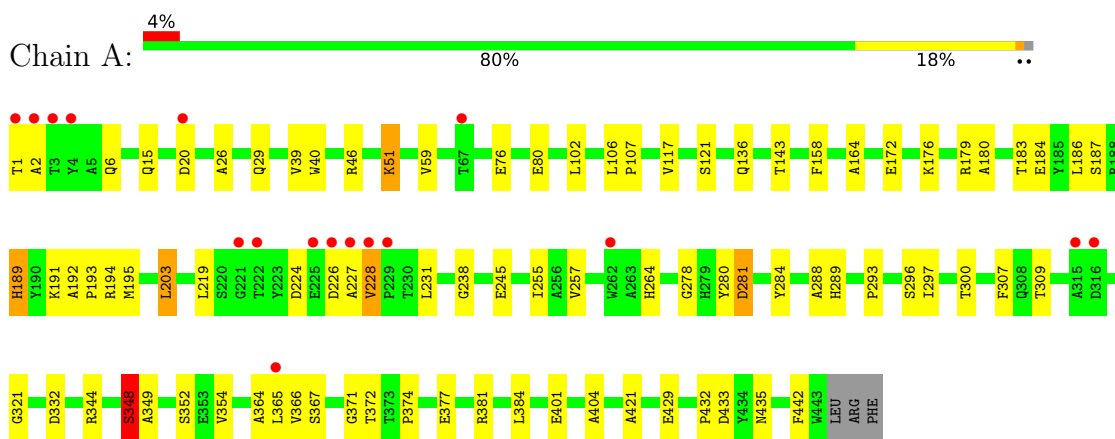
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	209	Total 209	O 209	0	0
23	B	170	Total 170	O 170	0	0
23	C	137	Total 137	O 137	0	0
23	D	133	Total 133	O 133	0	0
23	E	63	Total 63	O 63	0	0
23	F	68	Total 68	O 68	0	0
23	G	31	Total 31	O 31	0	0
23	H	15	Total 15	O 15	0	0
23	I	18	Total 18	O 18	0	0
23	J	7	Total 7	O 7	0	0
23	N	145	Total 145	O 145	0	0
23	O	136	Total 136	O 136	0	0
23	P	135	Total 135	O 135	0	0
23	Q	126	Total 126	O 126	0	0
23	R	77	Total 77	O 77	0	0
23	S	81	Total 81	O 81	0	0
23	T	17	Total 17	O 17	0	0
23	U	16	Total 16	O 16	0	0
23	V	16	Total 16	O 16	0	0
23	W	12	Total 12	O 12	0	0

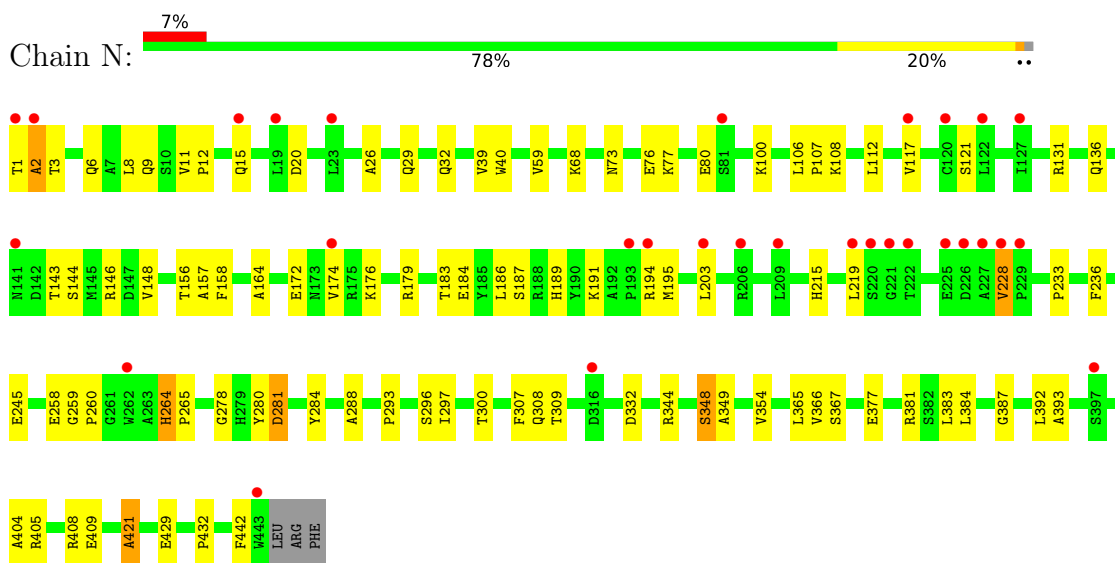
3 Residue-property plots [i](#)

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.

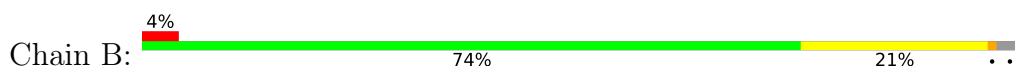
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

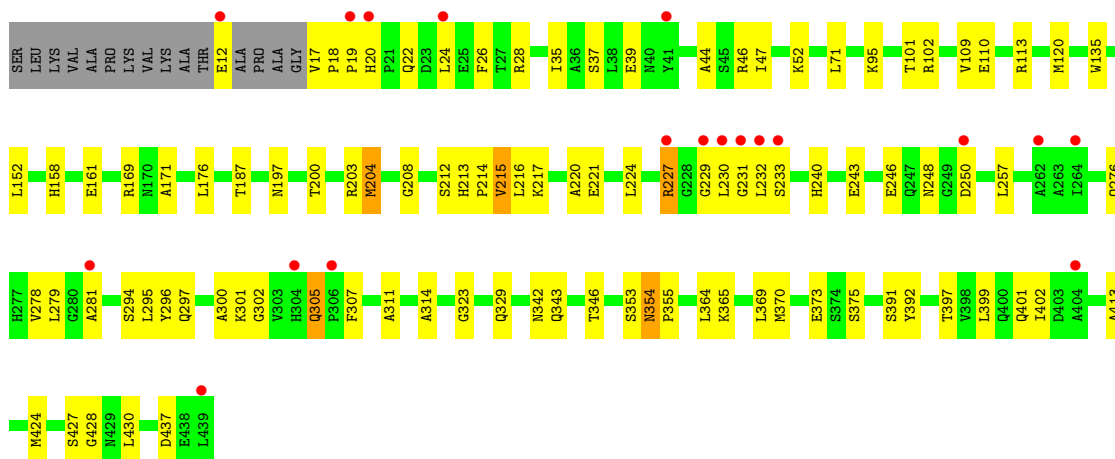


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

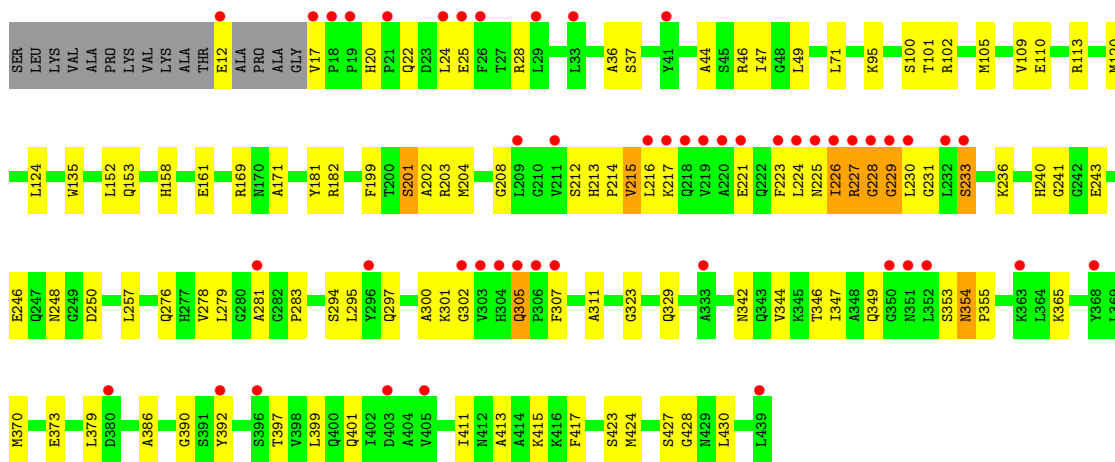
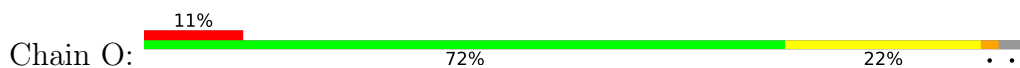


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

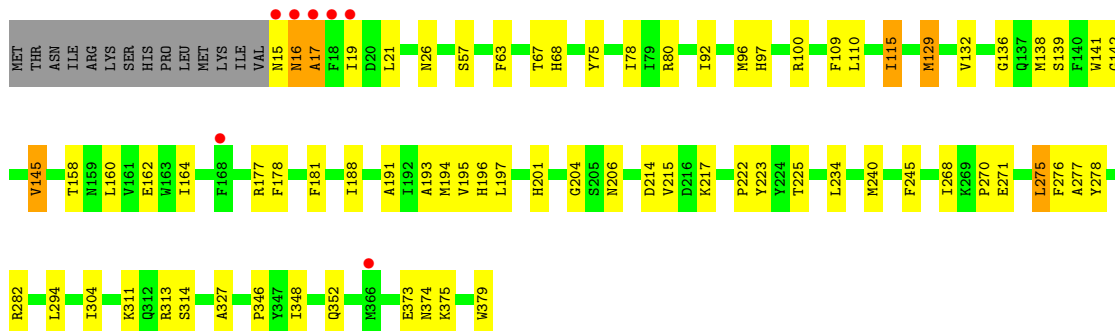
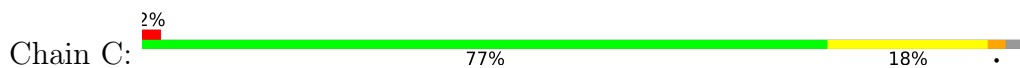




- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

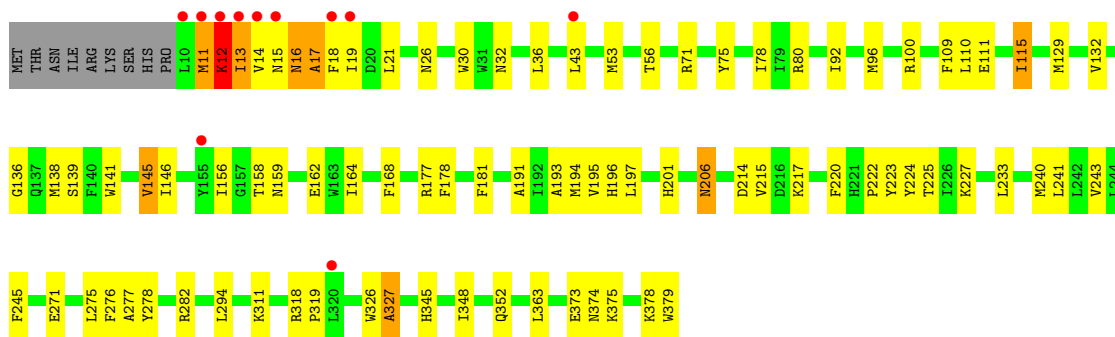


- Molecule 3: Cytochrome b, heme protein, mitochondrial

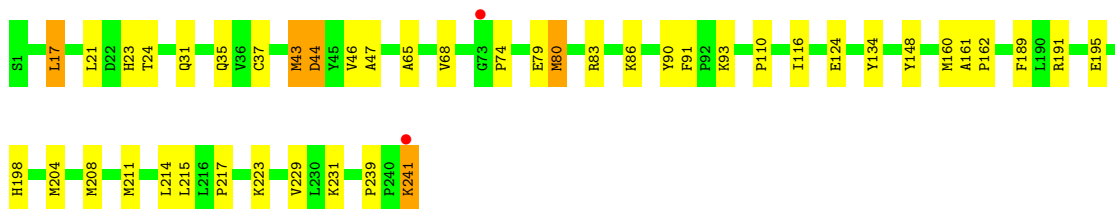
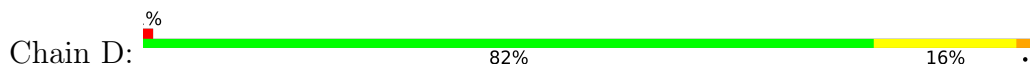


- Molecule 3: Cytochrome b, heme protein, mitochondrial

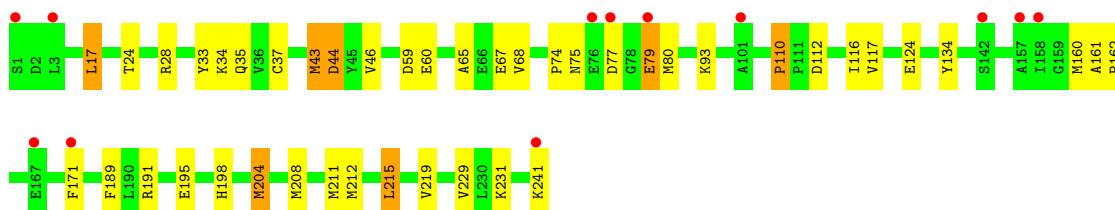
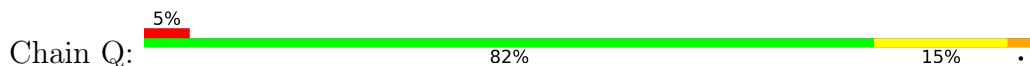




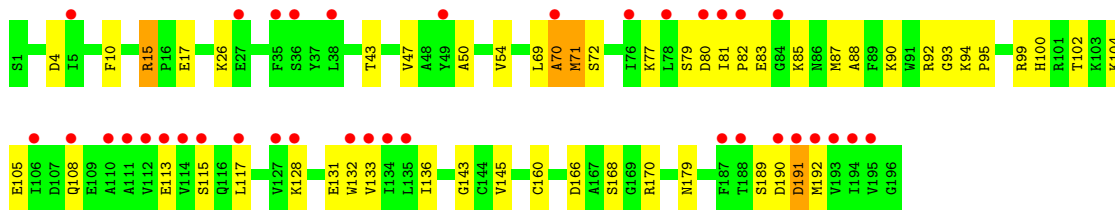
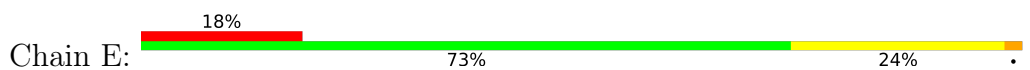
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



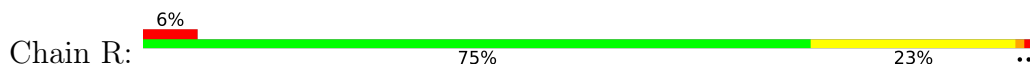
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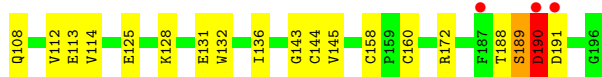


• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



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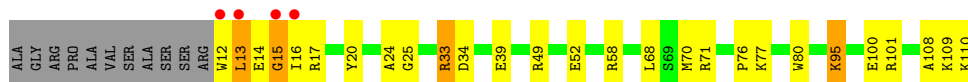




- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



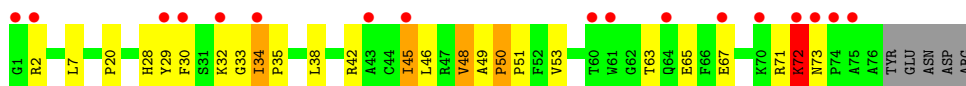
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



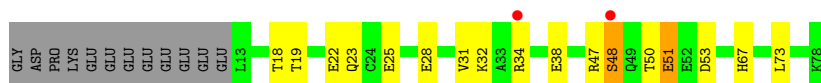
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



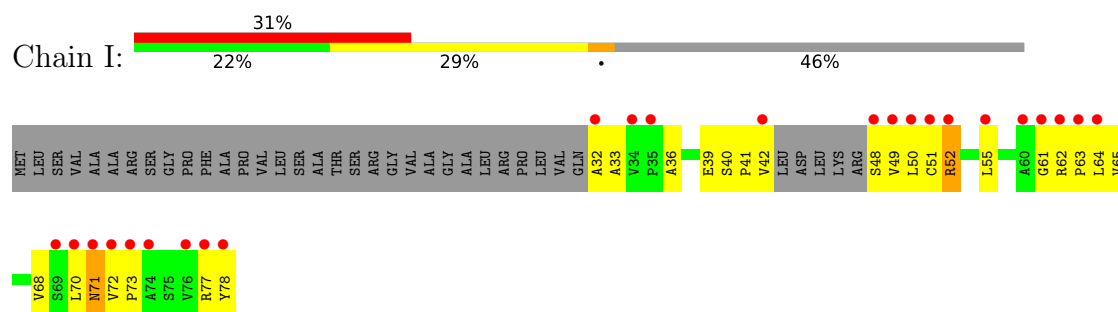
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



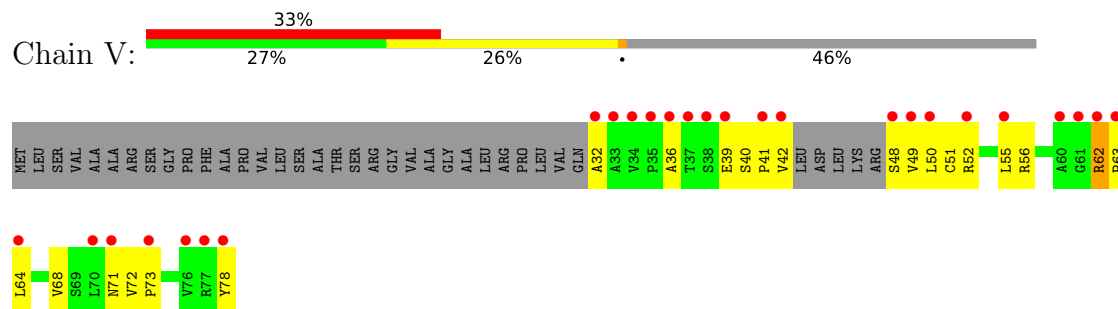
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



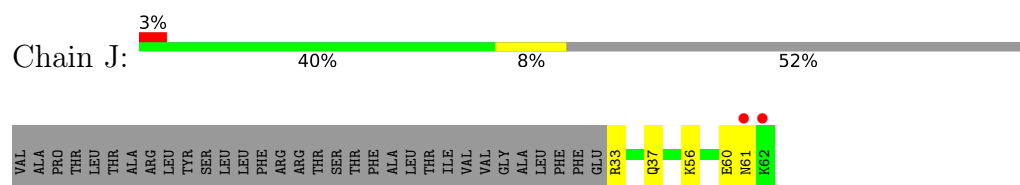
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



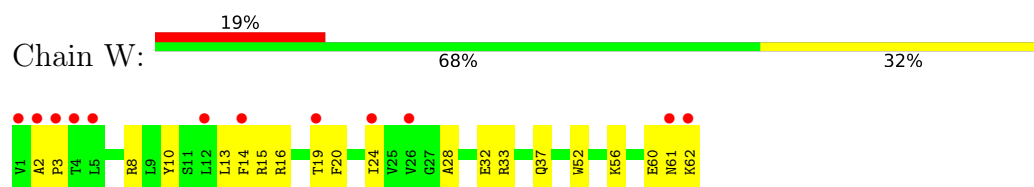
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



- 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	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 95.3 (37.87-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.258 0.212 , 0.246	Depositor DCC
R_{free} test set	15254 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, UNL, PO4, HEM, AZI, UQ, HEC, SMA, GOL, FES, JZR, 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	0.54	0/3467	0.96	10/4706 (0.2%)
1	N	0.46	0/3467	0.94	10/4706 (0.2%)
2	B	0.54	1/3235 (0.0%)	0.97	8/4387 (0.2%)
2	O	0.49	0/3239	0.99	11/4393 (0.3%)
3	C	0.60	1/2992 (0.0%)	0.99	18/4097 (0.4%)
3	P	0.56	0/3030	0.97	18/4145 (0.4%)
4	D	0.55	0/1978	0.96	6/2684 (0.2%)
4	Q	0.52	1/1978 (0.1%)	0.97	6/2684 (0.2%)
5	E	0.45	0/1553	1.12	14/2100 (0.7%)
5	R	0.51	0/1550	1.01	12/2094 (0.6%)
6	F	0.57	0/878	0.93	4/1175 (0.3%)
6	S	0.54	0/878	0.91	5/1175 (0.4%)
7	G	0.49	0/642	1.01	5/869 (0.6%)
7	T	0.44	0/647	1.02	7/876 (0.8%)
8	H	0.40	0/544	0.95	3/729 (0.4%)
8	U	0.38	0/544	0.88	0/729
9	I	0.72	0/285	1.33	3/384 (0.8%)
9	V	0.62	0/285	1.28	3/384 (0.8%)
10	J	0.44	0/252	0.83	0/333
10	W	0.41	0/520	0.91	1/699 (0.1%)
All	All	0.52	3/31964 (0.0%)	0.98	144/43349 (0.3%)

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
5	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	129	MET	SD-CE	-5.69	1.65	1.79
2	B	204	MET	SD-CE	-5.68	1.65	1.79
4	Q	204	MET	SD-CE	-5.64	1.65	1.79

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	228	GLY	N-CA-C	-11.53	97.33	115.08
5	E	70	ALA	CA-C-N	-10.57	104.57	122.33
5	E	70	ALA	C-N-CA	-10.57	104.57	122.33
5	E	69	LEU	CA-C-N	-9.66	108.53	123.13
5	E	69	LEU	C-N-CA	-9.66	108.53	123.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	70	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3398	0	3295	68	0
1	N	3398	0	3295	64	0
2	B	3177	0	3152	91	0
2	O	3180	0	3156	90	0
3	C	2897	0	2943	53	0
3	P	2936	0	2994	80	0
4	D	1919	0	1868	44	0
4	Q	1919	0	1868	45	0
5	E	1519	0	1503	38	0
5	R	1517	0	1498	40	0
6	F	861	0	854	24	0
6	S	861	0	854	31	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	539	0	524	20	0
9	I	285	0	288	41	0
9	V	285	0	288	32	0
10	J	245	0	229	3	0
10	W	507	0	513	22	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	4	0
11	P	18	0	24	0	0
11	S	18	0	24	6	0
12	A	5	0	0	0	0
12	B	5	0	0	0	0
12	D	10	0	0	0	0
12	I	5	0	0	1	0
12	O	5	0	0	0	0
12	P	5	0	0	0	0
12	Q	5	0	0	1	0
12	R	10	0	0	0	0
12	T	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	G	3	0	0	1	0
13	P	3	0	0	0	0
14	A	10	0	0	0	0
14	B	11	0	0	0	0
14	C	7	0	0	0	0
14	D	7	0	0	1	0
14	E	2	0	0	0	0
14	F	1	0	0	0	0
14	G	3	0	0	0	0
14	I	2	0	0	0	0
14	N	5	0	0	0	0
14	O	9	0	0	2	0
14	P	8	0	0	0	0
14	Q	1	0	0	0	0
14	R	2	0	0	0	0
14	S	1	0	0	0	0
14	T	2	0	0	0	0
14	U	2	0	0	0	0
14	V	4	0	0	0	0
14	W	1	0	0	0	0
15	B	8	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	49	0	72	1	0
15	D	51	0	82	3	0
15	P	49	0	72	3	0
15	Q	51	0	82	7	0
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	2	0
17	P	37	0	42	2	0
18	C	18	0	14	3	0
18	P	18	0	14	4	0
19	C	44	0	32	0	0
19	D	39	0	39	1	0
19	P	49	0	42	0	0
19	Q	39	0	39	0	0
20	C	12	0	16	0	0
20	E	11	0	13	0	0
20	O	6	0	8	0	0
20	P	12	0	16	2	0
21	D	43	0	30	3	0
21	Q	43	0	30	3	0
22	E	4	0	0	0	0
22	R	4	0	0	0	0
23	A	209	0	0	4	0
23	B	170	0	0	2	0
23	C	137	0	0	7	0
23	D	133	0	0	0	0
23	E	63	0	0	0	0
23	F	68	0	0	4	0
23	G	31	0	0	2	0
23	H	15	0	0	0	0
23	I	18	0	0	4	0
23	J	7	0	0	0	0
23	N	145	0	0	3	0
23	O	136	0	0	6	0
23	P	135	0	0	8	0
23	Q	126	0	0	0	0
23	R	77	0	0	1	0
23	S	81	0	0	2	0
23	T	17	0	0	0	0
23	U	16	0	0	0	0
23	V	16	0	0	0	0
23	W	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33890	0	31860	751	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 12.

The worst 5 of 751 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)
2:O:226:ILE:HG13	14:O:4043:UNL:O1	1.38	1.23
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.17	1.08
9:I:32:ALA:N	9:I:71:ASN:HB2	1.70	1.05
2:B:12:GLU:HG2	2:B:17:VAL:H	1.16	1.04
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.34	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%)	427 (97%)	12 (3%)	2 (0%)	24 22
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	24 22
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	43 44
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	10 7
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	21 18
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	9 5
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100 100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100 100
5	E	194/196 (99%)	179 (92%)	14 (7%)	1 (0%)	24 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	12	9
6	F	97/110 (88%)	97 (100%)	0	0	100	100
6	S	97/110 (88%)	95 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	9	5
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	1	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	4	1
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	2	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	18	15

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO
10	J	61	ASN
1	N	2	ALA
2	O	226	ILE
2	O	233	SER

5.3.2 Protein sidechains [i](#)

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	363/370 (98%)	356 (98%)	7 (2%)	50	58
1	N	363/370 (98%)	356 (98%)	7 (2%)	50	58
2	B	332/343 (97%)	329 (99%)	3 (1%)	70	78
2	O	332/343 (97%)	328 (99%)	4 (1%)	63	72
3	C	313/327 (96%)	311 (99%)	2 (1%)	78	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	317/327 (97%)	315 (99%)	2 (1%)	78	86
4	D	206/206 (100%)	203 (98%)	3 (2%)	57	65
4	Q	206/206 (100%)	202 (98%)	4 (2%)	50	58
5	E	168/168 (100%)	168 (100%)	0	100	100
5	R	168/168 (100%)	166 (99%)	2 (1%)	63	72
6	F	90/98 (92%)	86 (96%)	4 (4%)	25	26
6	S	90/98 (92%)	85 (94%)	5 (6%)	19	18
7	G	66/71 (93%)	64 (97%)	2 (3%)	36	41
7	T	66/71 (93%)	63 (96%)	3 (4%)	24	25
8	H	63/74 (85%)	61 (97%)	2 (3%)	34	38
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	26 (93%)	2 (7%)	13	11
9	V	28/60 (47%)	26 (93%)	2 (7%)	13	11
10	J	23/52 (44%)	23 (100%)	0	100	100
10	W	51/52 (98%)	51 (100%)	0	100	100
All	All	3336/3538 (94%)	3282 (98%)	54 (2%)	55	64

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	245	GLU
2	O	354	ASN
7	T	45	ILE
1	N	281	ASP
2	O	215	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	165	GLN
2	O	104	ASN
8	U	71	HIS
5	R	57	GLN
1	N	213	GLN

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 123 ligands modelled in this entry, 74 are unknown - leaving 49 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	JZR	S	2012	-	18,18,18	1.89	4 (22%)	23,23,23	0.71	0
22	FES	R	501	5	0,4,4	-	-	-		
12	PO4	B	3009	-	4,4,4	1.43	1 (25%)	6,6,6	5.99	5 (83%)
15	PEE	Q	3006	-	50,50,50	1.31	7 (14%)	53,55,55	0.74	2 (3%)
13	AZI	C	2005	-	2,2,2	2.43	2 (100%)	0,1,1	-	-
18	UQ	C	2002	-	18,18,63	2.44	9 (50%)	23,24,79	0.90	1 (4%)
12	PO4	P	3010	-	4,4,4	1.40	1 (25%)	6,6,6	5.98	5 (83%)
16	HEM	C	501	3	50,50,50	1.56	8 (16%)	67,82,82	1.28	7 (10%)
20	GOL	C	2008	-	5,5,5	1.32	0	5,5,5	0.69	0
21	HEC	D	501	4	46,50,50	1.59	4 (8%)	58,82,82	1.82	4 (6%)
19	CDL	C	2004	-	43,43,99	1.16	3 (6%)	49,55,111	1.27	4 (8%)
15	PEE	D	2006	-	50,50,50	1.34	5 (10%)	53,55,55	0.74	2 (3%)
20	GOL	P	4009	-	5,5,5	1.11	0	5,5,5	0.54	0
17	SMA	C	2001	-	38,38,38	1.35	5 (13%)	47,52,52	0.92	2 (4%)
21	HEC	Q	501	4	46,50,50	1.50	3 (6%)	58,82,82	1.98	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	FES	E	501	5	0,4,4	-	-	-	-	-
16	HEM	P	502	3	50,50,50	1.42	6 (12%)	67,82,82	1.17	4 (5%)
15	PEE	C	2007	-	48,48,50	1.20	5 (10%)	51,53,55	0.73	2 (3%)
12	PO4	D	4010	-	4,4,4	1.44	1 (25%)	6,6,6	5.99	5 (83%)
18	UQ	P	3002	-	18,18,63	2.26	9 (50%)	23,24,79	0.83	1 (4%)
20	GOL	E	4007	-	4,4,5	1.38	0	4,4,5	0.55	0
11	JZR	F	3012	-	18,18,18	1.89	5 (27%)	23,23,23	0.74	0
19	CDL	P	3004	-	48,48,99	1.14	3 (6%)	54,60,111	1.15	5 (9%)
11	JZR	F	4003	-	18,18,18	1.86	5 (27%)	23,23,23	0.68	0
12	PO4	R	4013	-	4,4,4	1.48	1 (25%)	6,6,6	5.98	5 (83%)
13	AZI	A	4002	-	2,2,2	2.82	2 (100%)	0,1,1	-	-
12	PO4	T	4016	-	4,4,4	1.45	1 (25%)	6,6,6	5.98	5 (83%)
16	HEM	P	501	3	50,50,50	1.42	7 (14%)	67,82,82	1.15	6 (8%)
12	PO4	R	4014	-	4,4,4	1.46	1 (25%)	6,6,6	5.99	5 (83%)
20	GOL	E	4006	-	5,5,5	1.35	1 (20%)	5,5,5	0.66	0
12	PO4	A	2010	-	4,4,4	1.49	1 (25%)	6,6,6	5.97	5 (83%)
11	JZR	C	2011	-	18,18,18	1.85	5 (27%)	23,23,23	0.71	0
20	GOL	C	4008	-	5,5,5	1.27	0	5,5,5	0.57	0
11	JZR	P	3011	-	18,18,18	1.84	5 (27%)	23,23,23	0.72	0
12	PO4	I	4015	-	4,4,4	1.43	1 (25%)	6,6,6	6.01	5 (83%)
13	AZI	P	3005	-	2,2,2	2.97	2 (100%)	0,1,1	-	-
16	HEM	C	502	3	50,50,50	1.42	6 (12%)	67,82,82	1.07	4 (5%)
20	GOL	P	3008	-	5,5,5	1.27	0	5,5,5	0.54	0
19	CDL	Q	3003	-	38,38,99	1.10	2 (5%)	42,47,111	1.04	3 (7%)
12	PO4	D	4011	-	4,4,4	1.39	1 (25%)	6,6,6	6.01	5 (83%)
20	GOL	O	4005	-	5,5,5	1.33	0	5,5,5	0.64	0
12	PO4	Q	4012	-	4,4,4	1.57	2 (50%)	6,6,6	5.98	5 (83%)
15	PEE	B	4017	-	7,7,50	1.51	2 (28%)	7,7,55	0.33	0
19	CDL	D	2003	-	38,38,99	1.06	1 (2%)	42,47,111	1.07	3 (7%)
15	PEE	P	3007	-	48,48,50	1.22	4 (8%)	51,53,55	0.73	2 (3%)
12	PO4	O	2009	-	4,4,4	1.44	1 (25%)	6,6,6	5.96	5 (83%)
17	SMA	P	3001	-	38,38,38	1.38	7 (18%)	47,52,52	0.90	2 (4%)
11	JZR	A	4004	-	18,18,18	1.36	4 (22%)	23,23,23	0.58	0
13	AZI	G	4001	-	2,2,2	3.30	2 (100%)	0,1,1	-	-

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	JZR	S	2012	-	-	5/9/29/29	0/1/1/1
22	FES	R	501	5	-	-	0/1/1/1
15	PEE	Q	3006	-	-	25/54/54/54	-
18	UQ	C	2002	-	-	1/9/33/87	0/1/1/1
16	HEM	C	501	3	-	4/14/54/54	-
20	GOL	C	2008	-	-	2/4/4/4	-
19	CDL	C	2004	-	-	30/52/52/110	-
15	PEE	D	2006	-	-	23/54/54/54	-
20	GOL	P	4009	-	-	2/4/4/4	-
17	SMA	C	2001	-	-	4/34/34/34	0/2/2/2
21	HEC	Q	501	4	-	8/14/54/54	-
22	FES	E	501	5	-	-	0/1/1/1
16	HEM	P	502	3	-	2/14/54/54	-
15	PEE	C	2007	-	-	19/52/52/54	-
18	UQ	P	3002	-	-	3/9/33/87	0/1/1/1
20	GOL	E	4007	-	-	2/2/2/4	-
11	JZR	F	3012	-	-	2/9/29/29	0/1/1/1
19	CDL	P	3004	-	-	26/57/57/110	-
11	JZR	F	4003	-	-	4/9/29/29	0/1/1/1
16	HEM	P	501	3	-	4/14/54/54	-
20	GOL	E	4006	-	-	4/4/4/4	-
20	GOL	C	4008	-	-	0/4/4/4	-
11	JZR	C	2011	-	-	4/9/29/29	0/1/1/1
11	JZR	P	3011	-	-	3/9/29/29	0/1/1/1
16	HEM	C	502	3	-	2/14/54/54	-
20	GOL	P	3008	-	-	0/4/4/4	-
19	CDL	Q	3003	-	-	22/43/43/110	-
20	GOL	O	4005	-	-	3/4/4/4	-
19	CDL	D	2003	-	-	21/43/43/110	-
15	PEE	B	4017	-	-	3/5/5/54	-
15	PEE	P	3007	-	-	22/52/52/54	-
21	HEC	D	501	4	-	8/14/54/54	-
17	SMA	P	3001	-	-	4/34/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	JZR	A	4004	-	-	1/9/29/29	0/1/1/1

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	CAB-C3B	6.21	1.55	1.35
21	Q	501	HEC	CAB-C3B	5.52	1.52	1.35
21	D	501	HEC	CAC-C3C	5.49	1.52	1.35
21	Q	501	HEC	CAC-C3C	5.18	1.51	1.35
11	S	2012	JZR	O1-C1	4.93	1.48	1.40

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	501	HEC	CBB-CAB-C3B	-8.96	109.52	127.43
21	D	501	HEC	CBC-CAC-C3C	-8.85	109.75	127.43
12	O	2009	PO4	O4-P-O1	-8.48	80.98	110.95
12	R	4013	PO4	O4-P-O1	-8.45	81.06	110.95
12	I	4015	PO4	O4-P-O1	-8.42	81.16	110.95

There are no chirality outliers.

5 of 263 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	C1-O3P-P-O2P
15	D	2006	PEE	C1-O3P-P-O4P
15	D	2006	PEE	C4-O4P-P-O2P
15	D	2006	PEE	O4P-C4-C5-N
15	Q	3006	PEE	C1-O3P-P-O2P

There are no ring outliers.

24 monomers are involved in 55 short contacts:

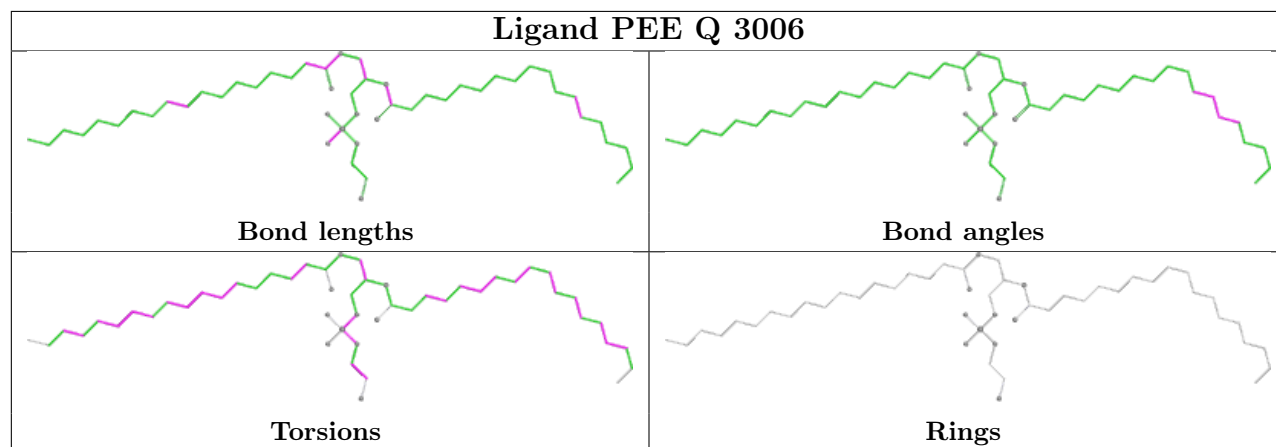
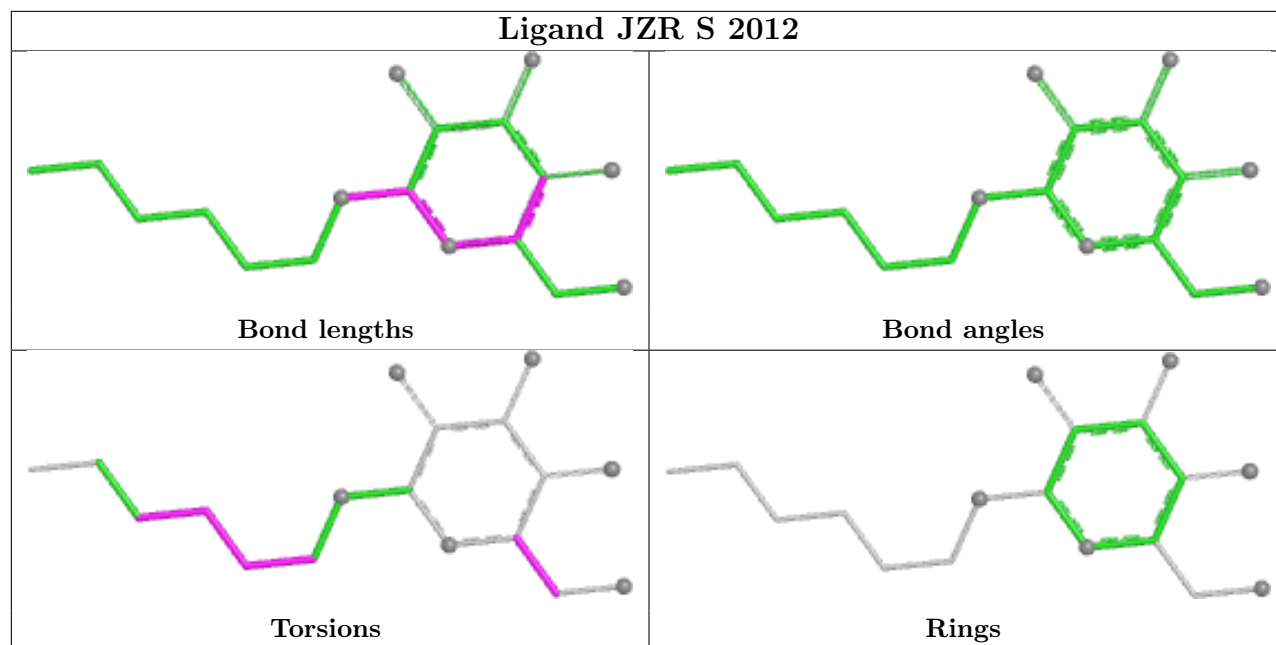
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	2012	JZR	6	0
15	Q	3006	PEE	7	0
18	C	2002	UQ	3	0
16	C	501	HEM	1	0
21	D	501	HEC	3	0
15	D	2006	PEE	3	0
20	P	4009	GOL	2	0

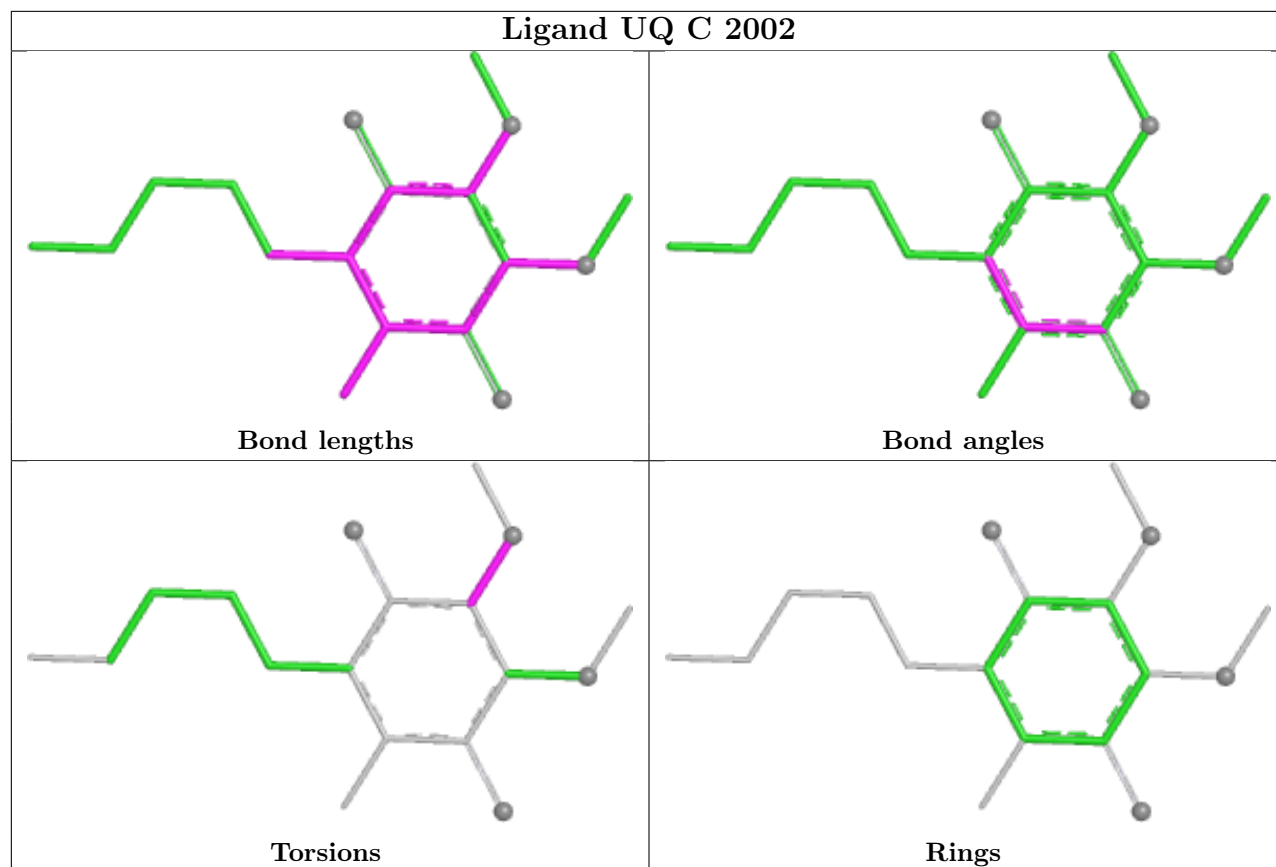
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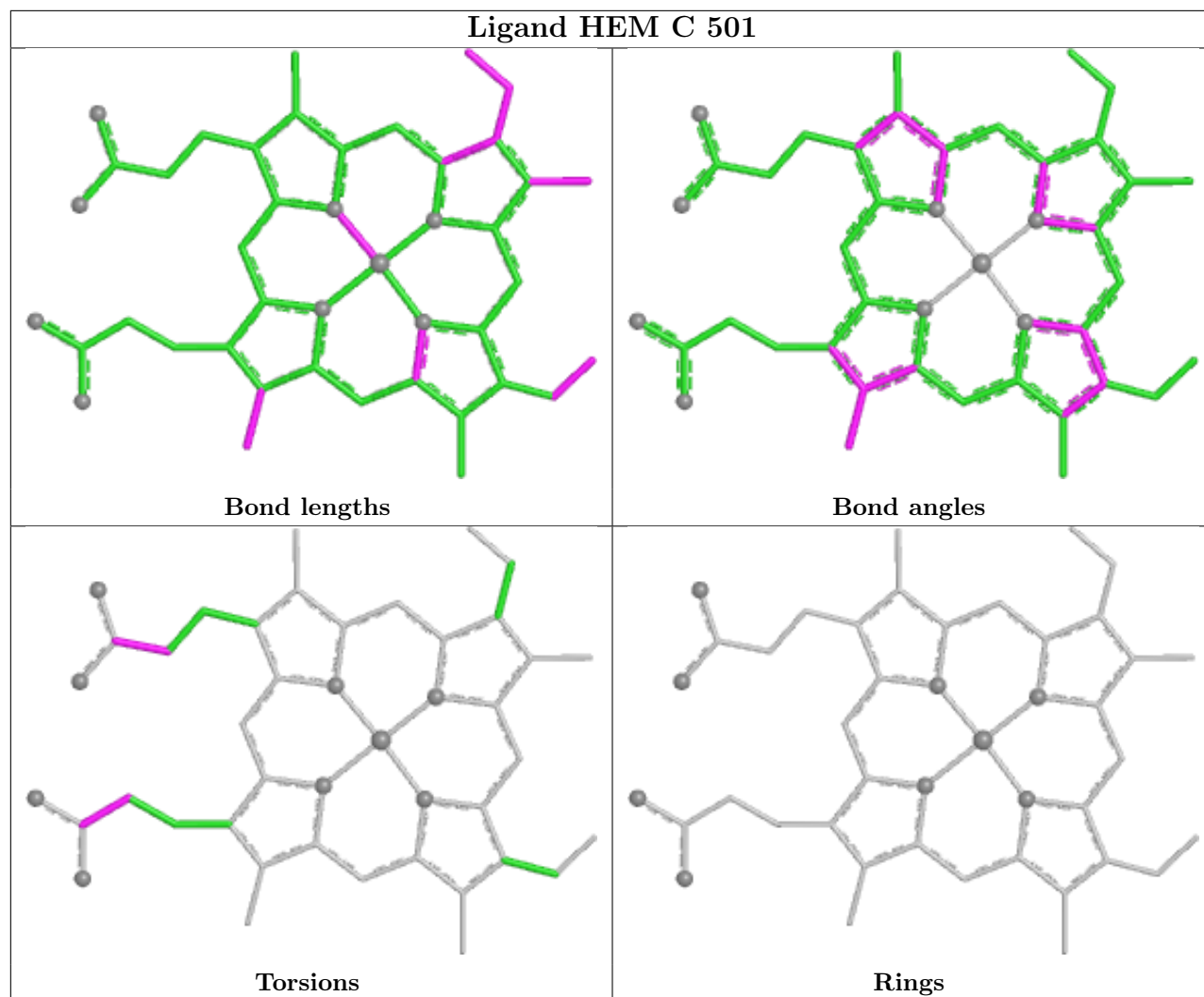
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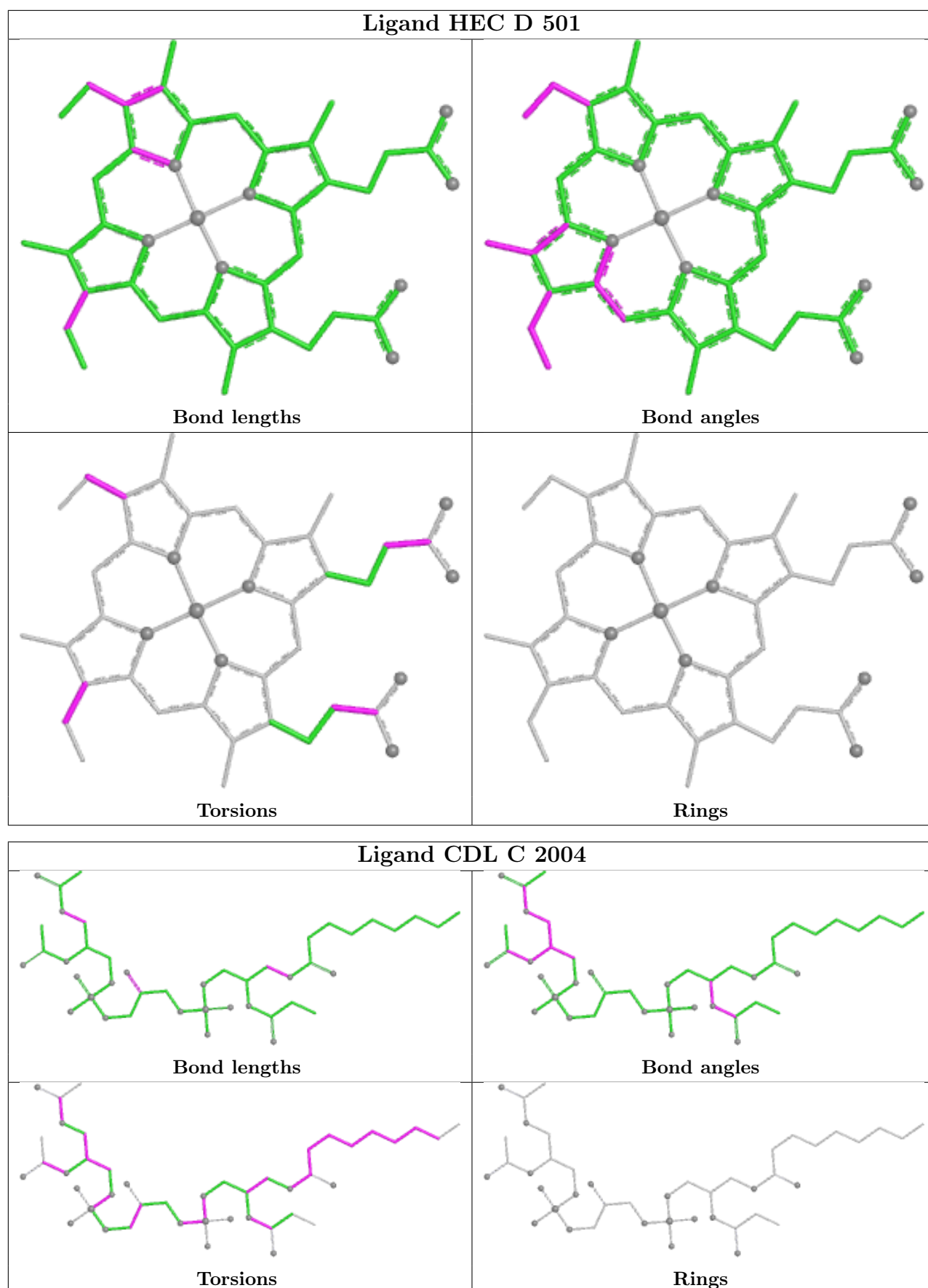
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	2001	SMA	2	0
21	Q	501	HEC	3	0
16	P	502	HEM	2	0
15	C	2007	PEE	1	0
18	P	3002	UQ	4	0
11	F	3012	JZR	3	0
11	F	4003	JZR	1	0
16	P	501	HEM	1	0
12	I	4015	PO4	1	0
16	C	502	HEM	4	0
12	Q	4012	PO4	1	0
15	B	4017	PEE	1	0
19	D	2003	CDL	1	0
15	P	3007	PEE	3	0
17	P	3001	SMA	2	0
11	A	4004	JZR	1	0
13	G	4001	AZI	1	0

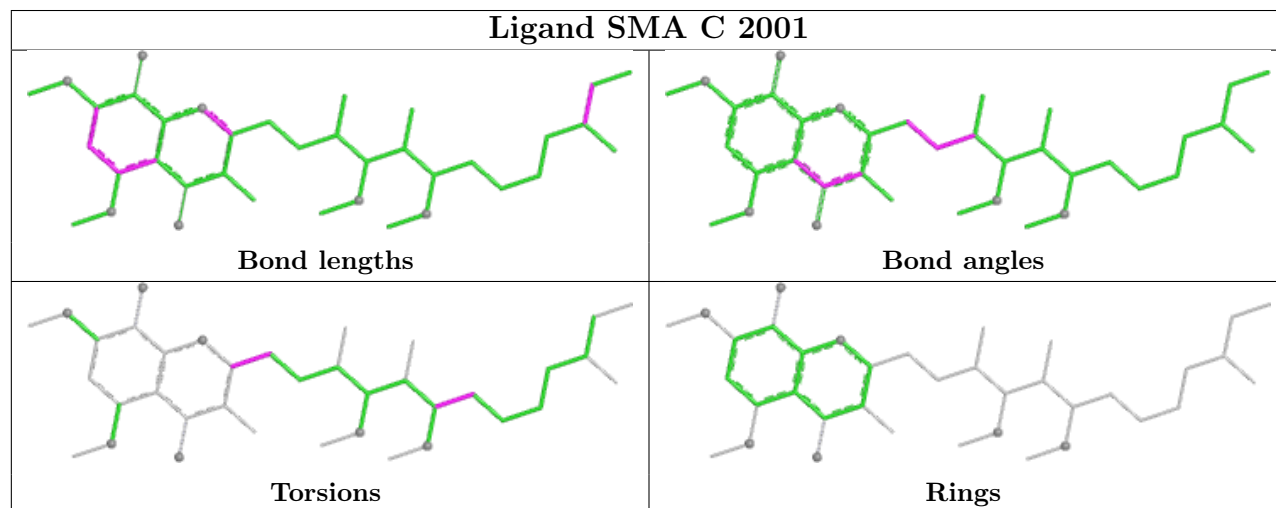
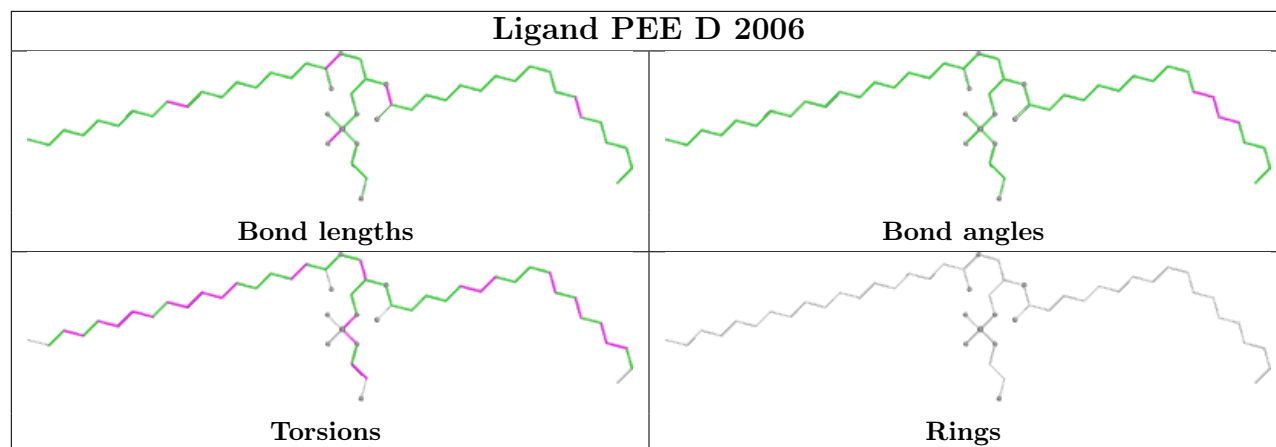
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

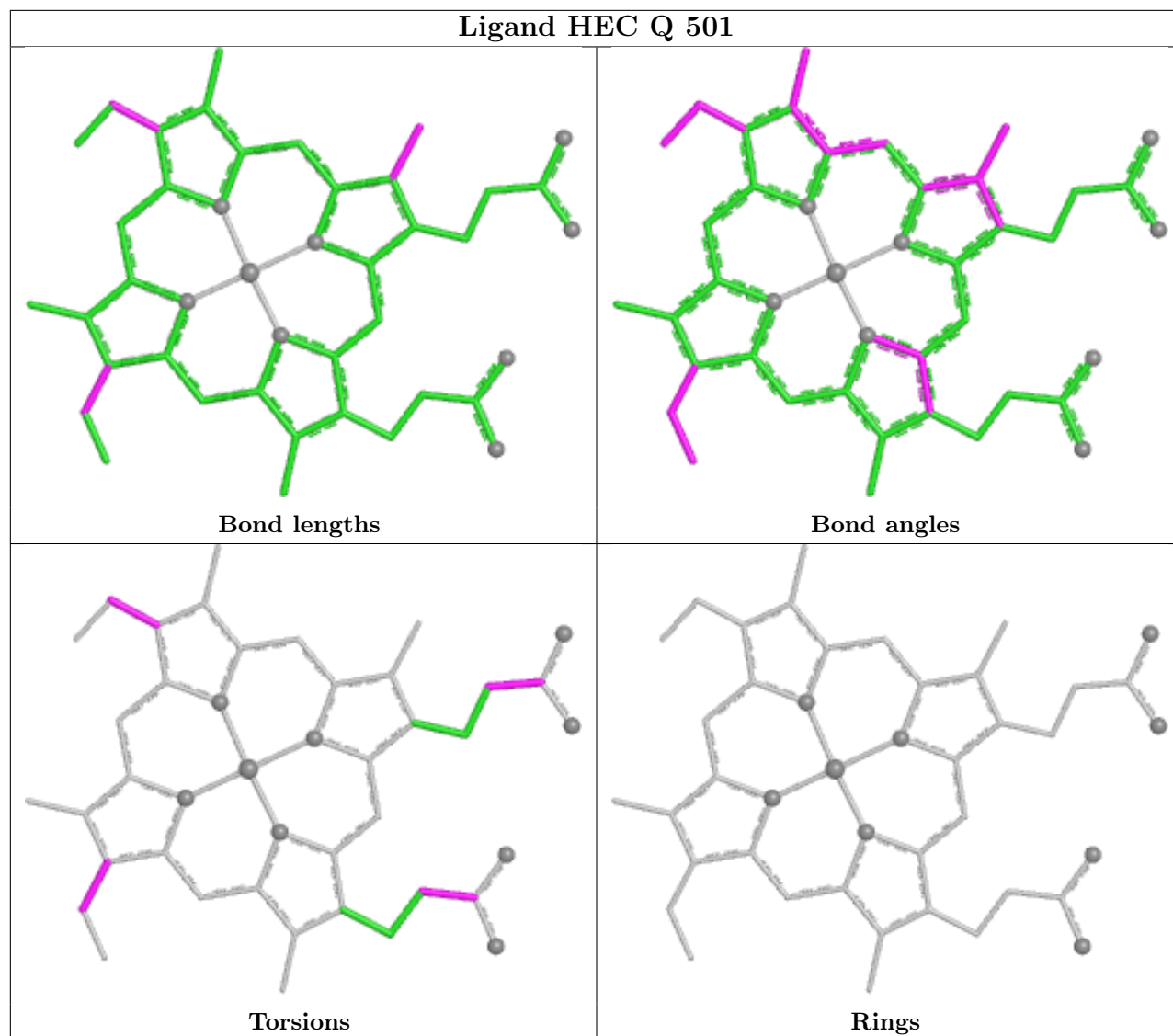


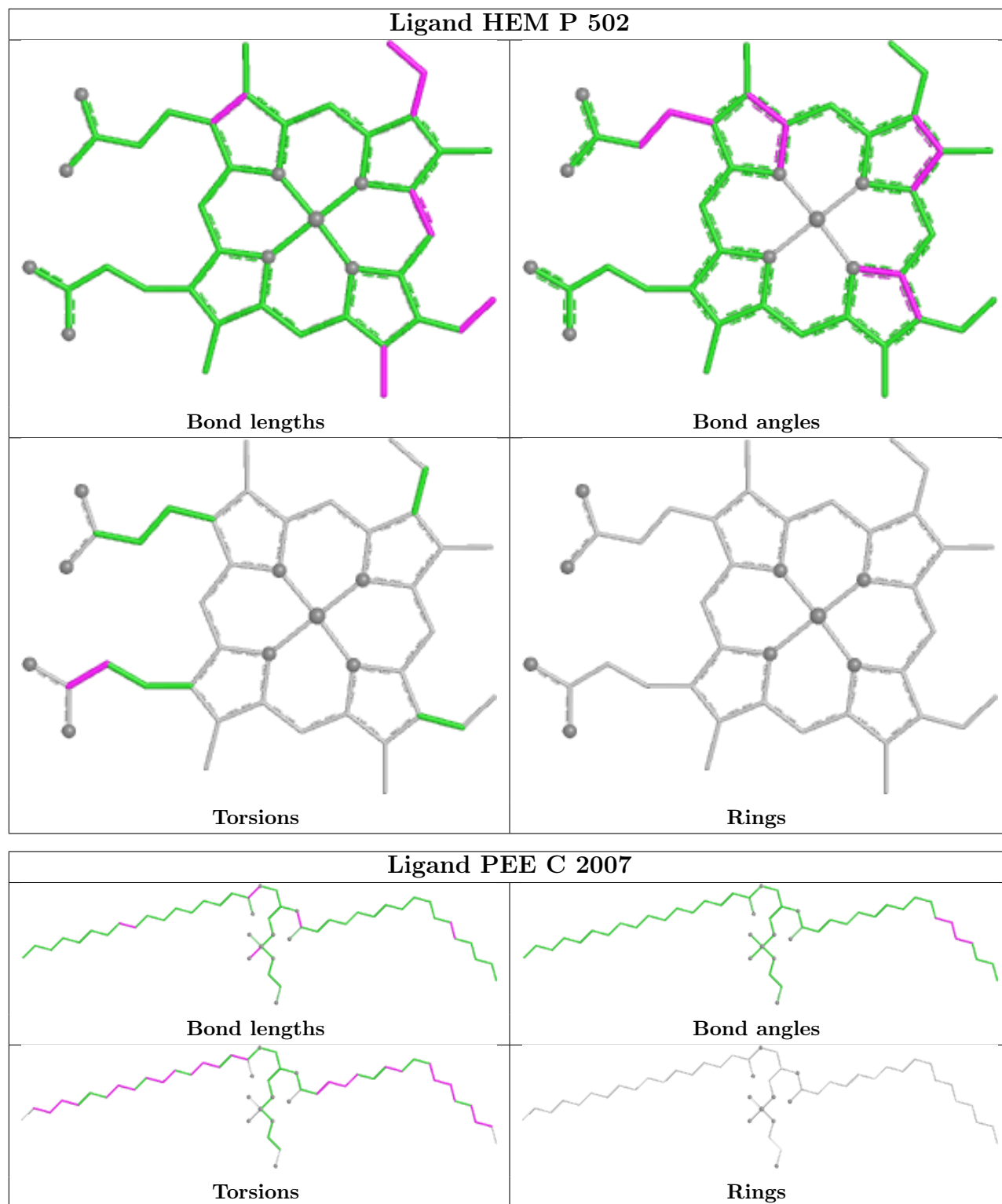


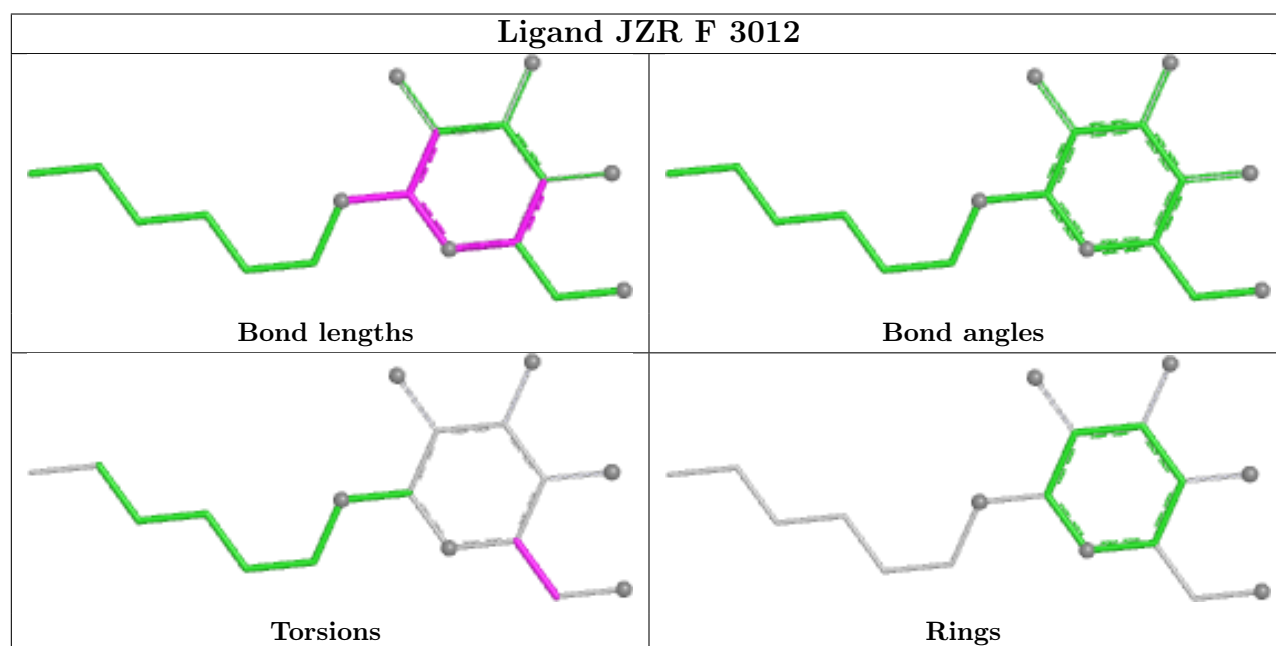
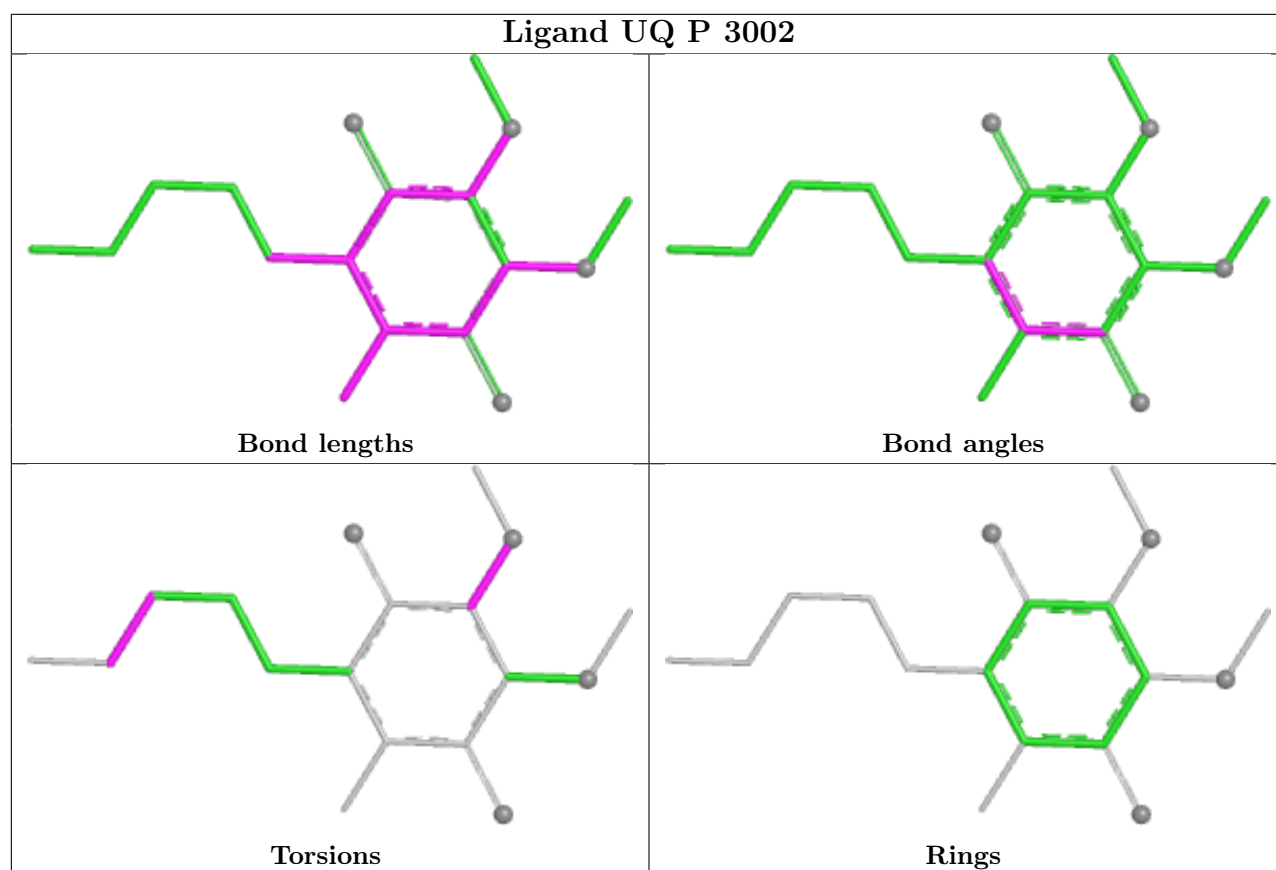


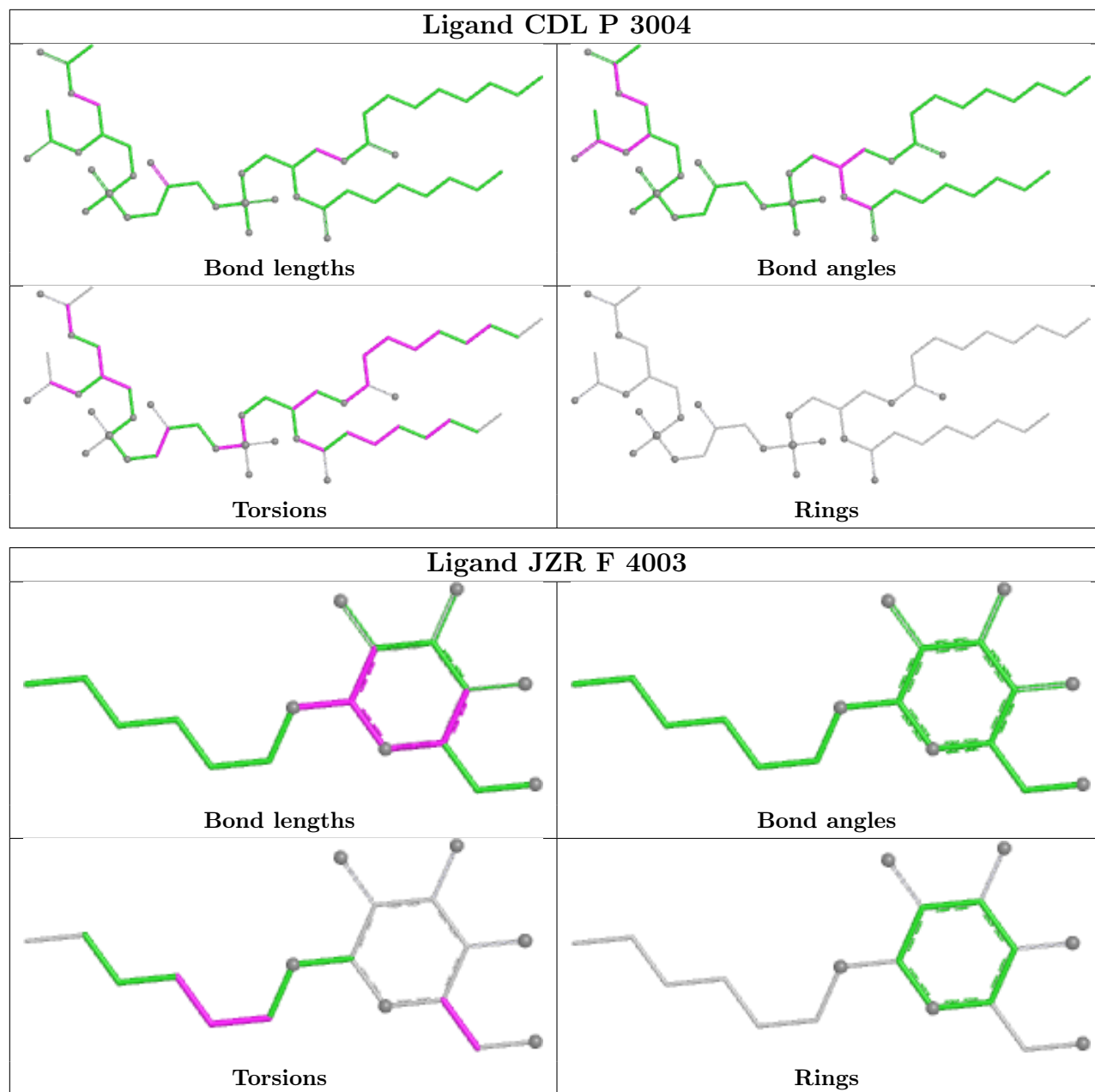


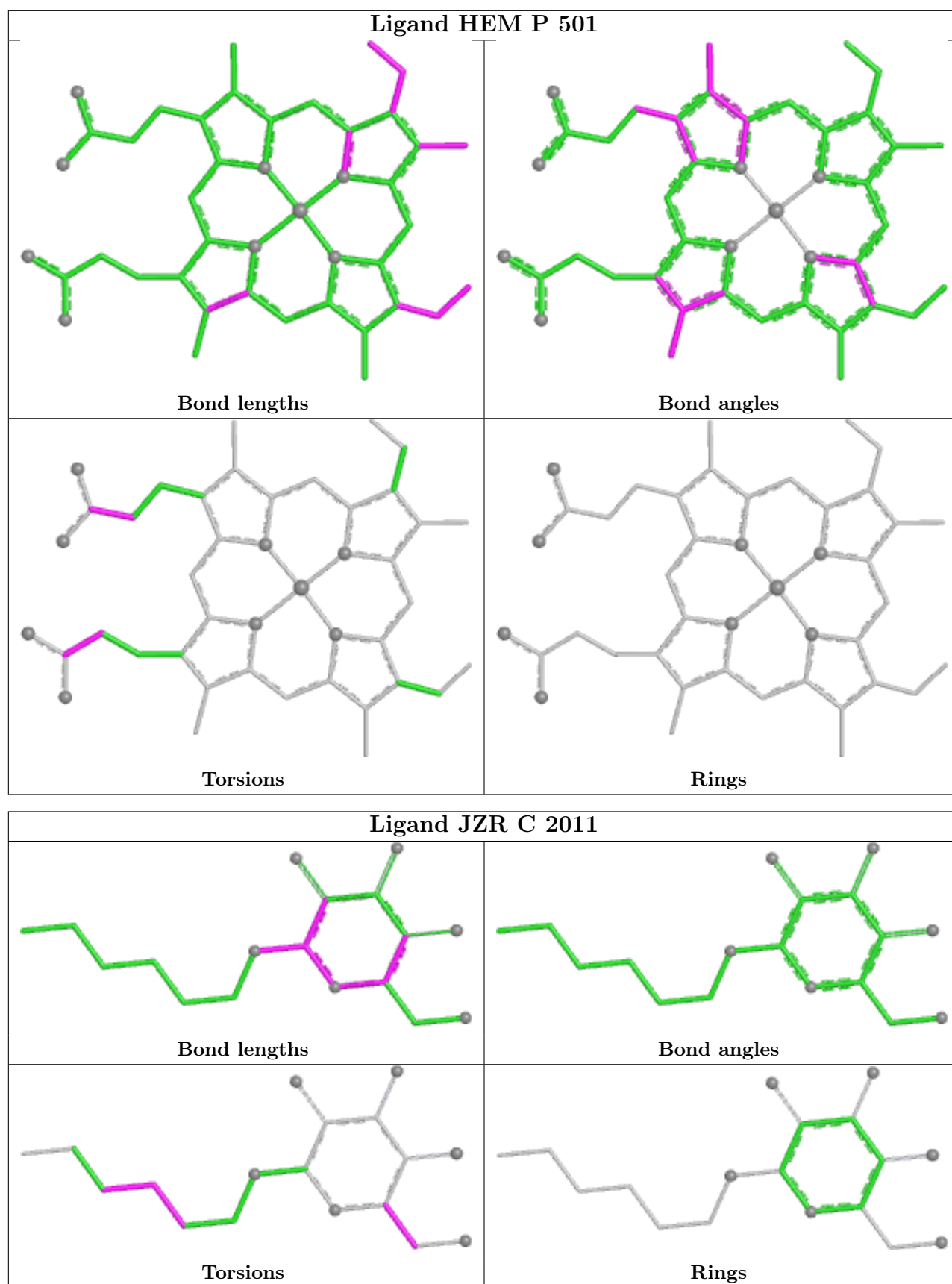


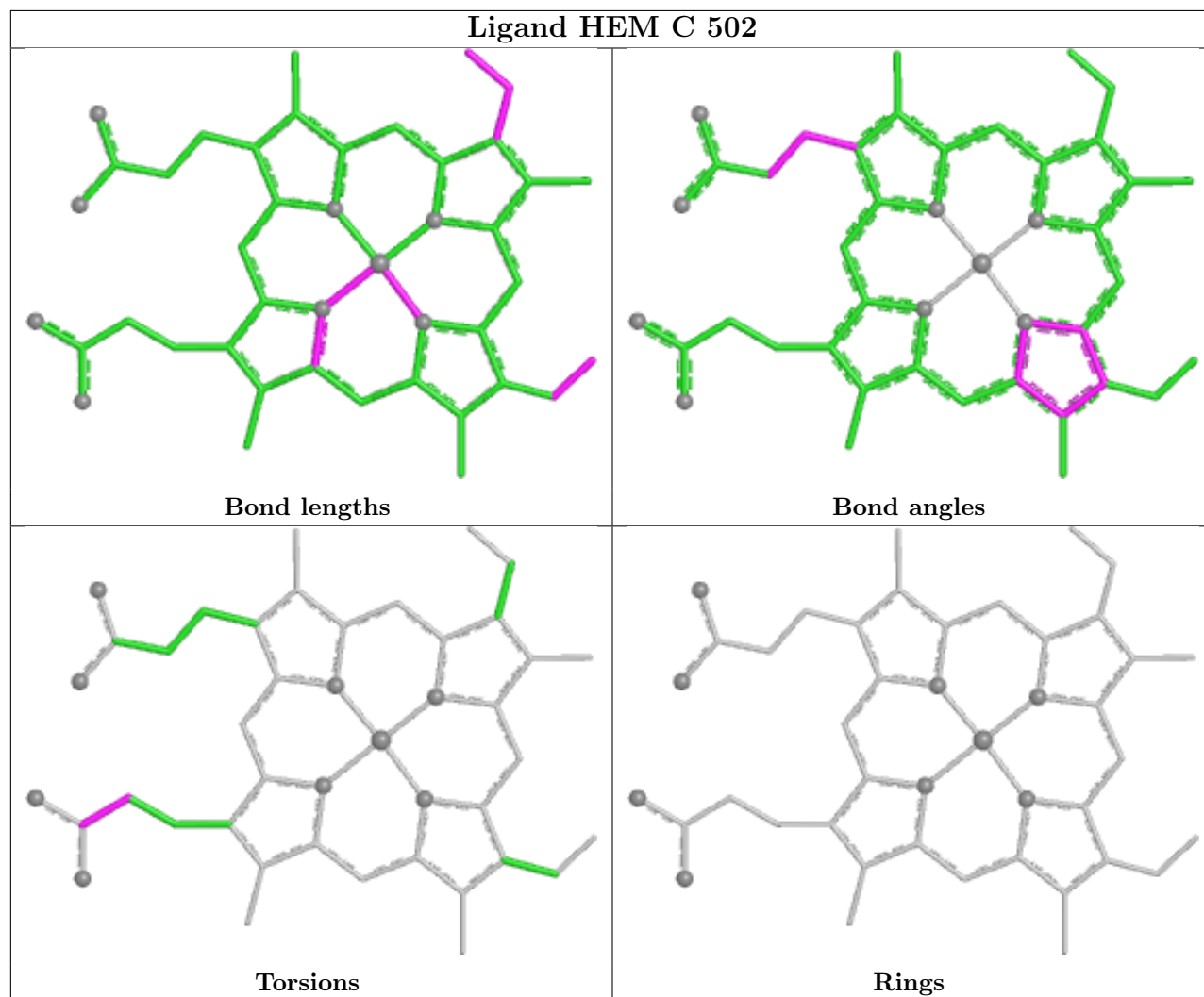
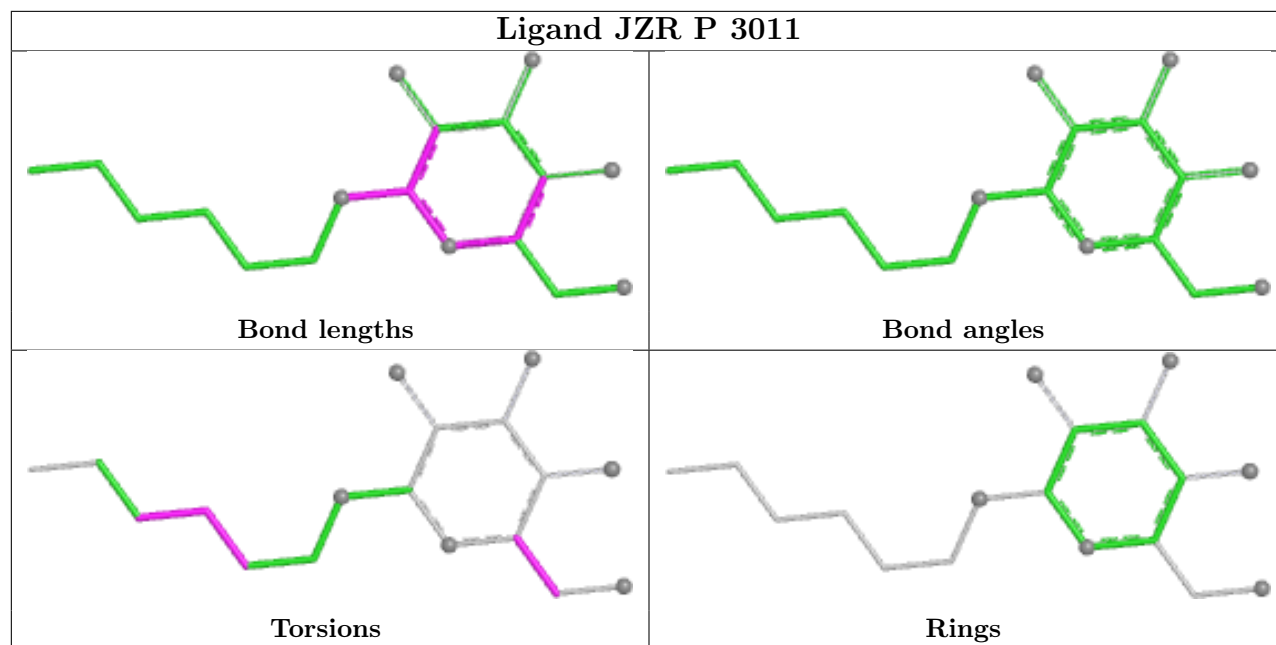


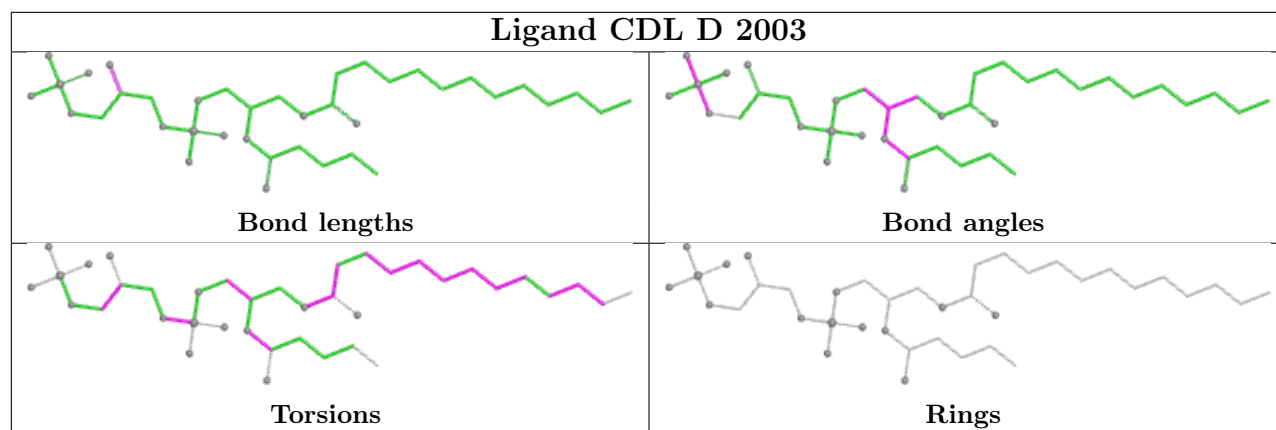
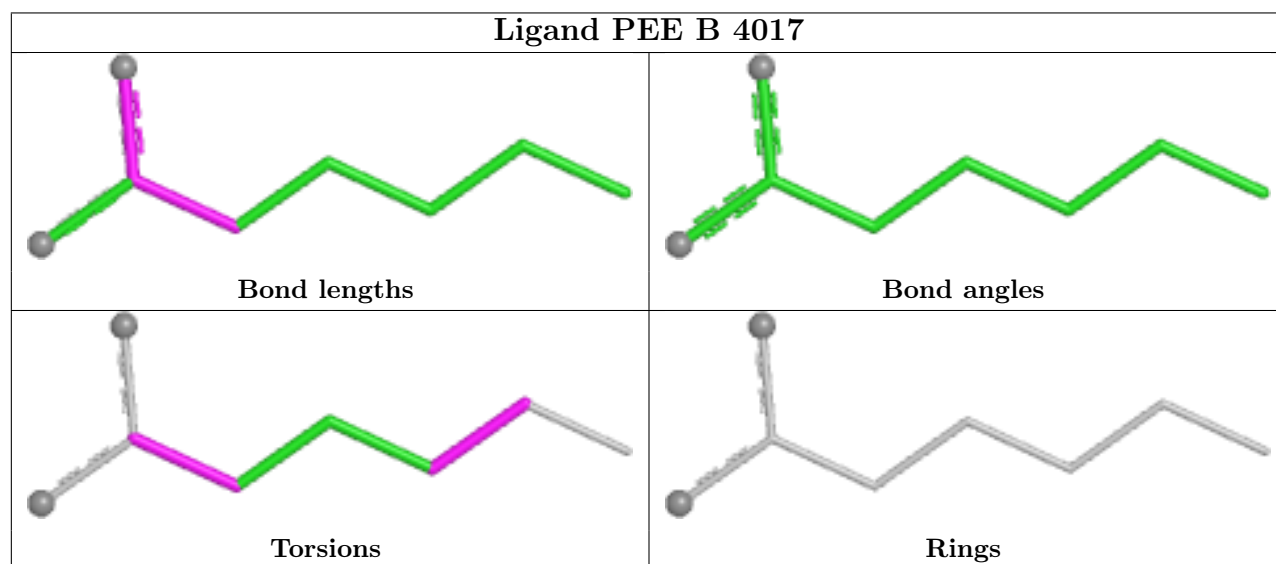
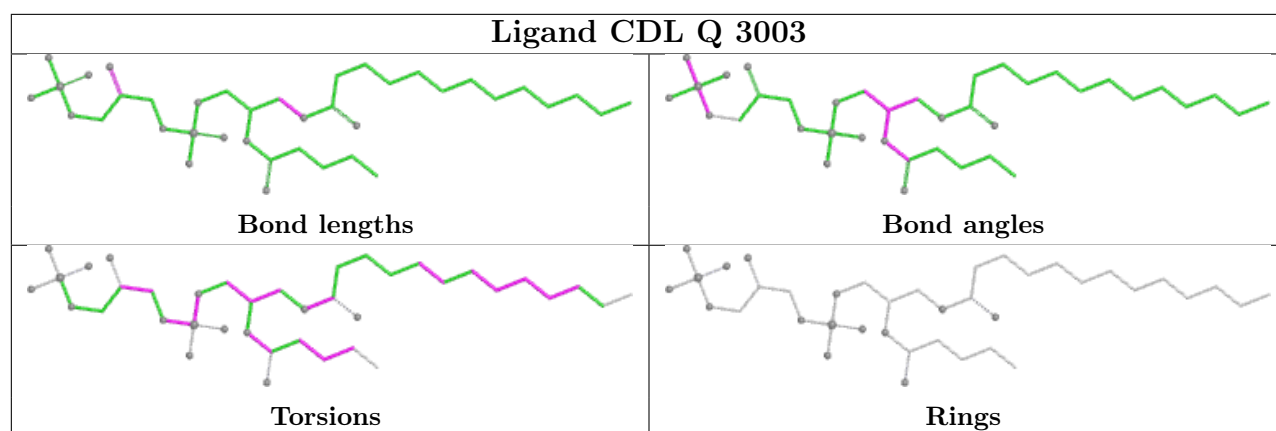


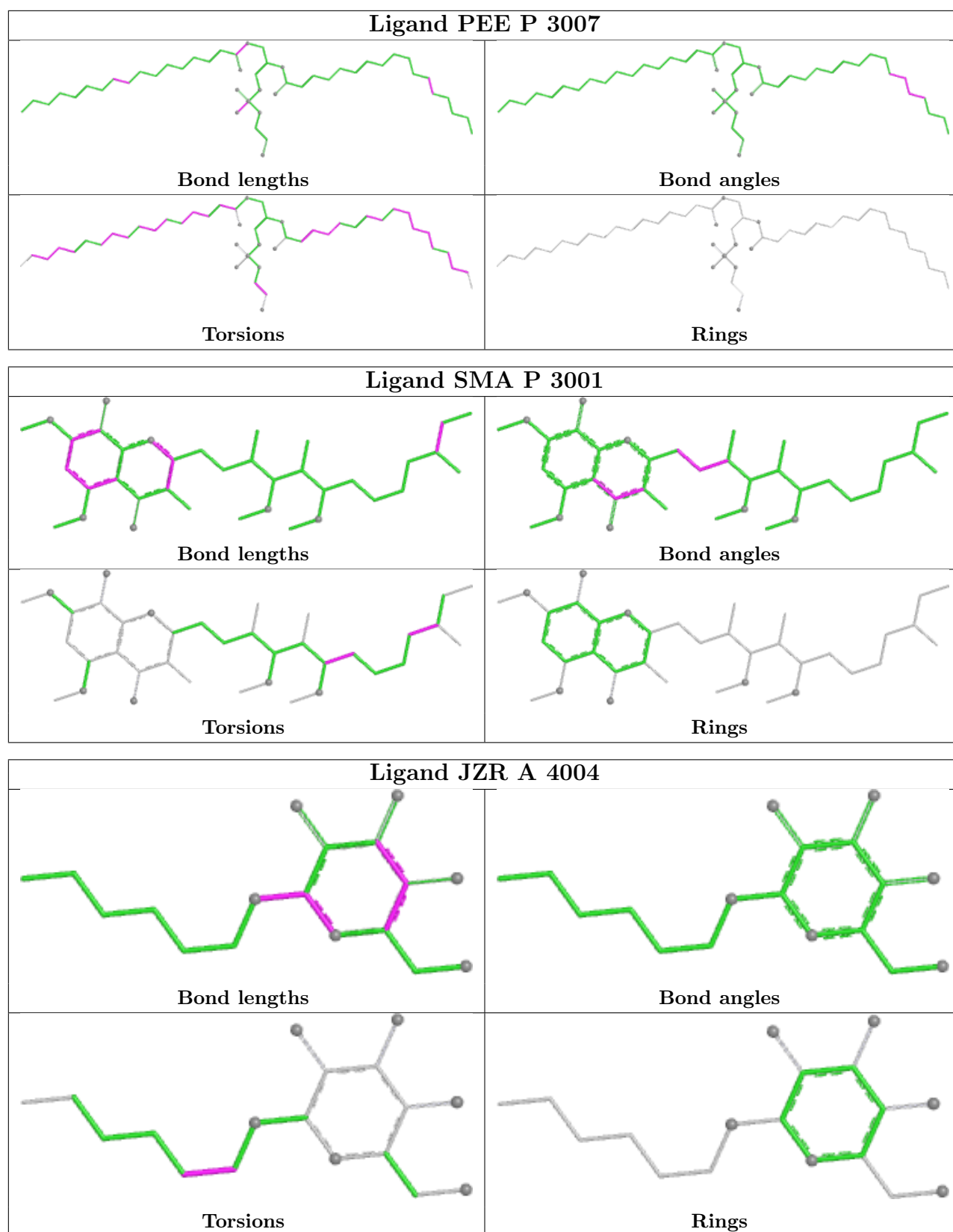












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	442/446 (99%)	0.18	17 (3%) 44 46	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.63	30 (6%) 23 25	31, 49, 76, 132	1 (0%)
2	B	424/439 (96%)	0.30	19 (4%) 38 40	28, 41, 66, 102	0
2	O	424/439 (96%)	0.71	49 (11%) 9 10	31, 48, 87, 185	0
3	C	365/379 (96%)	0.03	7 (1%) 66 69	24, 34, 48, 108	0
3	P	370/379 (97%)	0.12	11 (2%) 52 55	28, 37, 52, 218	0
4	D	241/241 (100%)	0.13	2 (0%) 82 84	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.45	12 (4%) 34 36	31, 45, 67, 87	0
5	E	196/196 (100%)	1.02	36 (18%) 3 3	32, 57, 105, 117	0
5	R	196/196 (100%)	0.49	11 (5%) 30 32	27, 46, 71, 99	0
6	F	99/110 (90%)	0.24	7 (7%) 22 23	24, 39, 70, 83	0
6	S	99/110 (90%)	0.35	4 (4%) 42 44	28, 40, 67, 88	0
7	G	75/81 (92%)	0.77	5 (6%) 24 25	26, 49, 77, 86	0
7	T	76/81 (93%)	0.94	17 (22%) 2 2	32, 55, 98, 114	0
8	H	66/78 (84%)	0.72	2 (3%) 52 55	40, 56, 73, 78	0
8	U	66/78 (84%)	1.11	9 (13%) 7 7	44, 63, 94, 104	0
9	I	42/78 (53%)	2.49	24 (57%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.47	26 (61%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.95	2 (6%) 24 25	40, 52, 80, 109	0
10	W	62/62 (100%)	1.30	12 (19%) 3 3	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.48	302 (7%) 20 21	24, 43, 80, 218	2 (0%)

The worst 5 of 302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	THR	10.5
1	N	222	THR	9.6
3	P	18	PHE	7.8
6	S	12	TRP	7.4
3	P	13	ILE	7.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
11	JZR	F	4003	18/18	0.53	0.25	176,180,181,181	0
12	PO4	D	4010	5/5	0.53	0.10	169,169,170,170	0
14	UNL	I	4072	1/-	0.55	0.11	93,93,93,93	0
12	PO4	A	2010	5/5	0.57	0.15	133,133,134,134	0
14	UNL	V	4078	1/-	0.59	0.13	94,94,94,94	0
14	UNL	D	4062	1/-	0.61	0.13	90,90,90,90	0
18	UQ	C	2002	18/63	0.64	0.28	61,73,76,76	0
14	UNL	V	4024	1/-	0.65	0.17	96,96,96,96	0
14	UNL	R	4055	1/-	0.66	0.12	73,73,73,73	0
20	GOL	E	4007	5/6	0.66	0.27	97,100,101,102	0
12	PO4	P	3010	5/5	0.67	0.15	115,115,115,116	0
11	JZR	F	3012	18/18	0.67	0.44	159,162,164,164	0
12	PO4	I	4015	5/5	0.68	0.18	122,122,123,123	0
13	AZI	P	3005	3/3	0.69	0.25	54,54,59,63	0
12	PO4	D	4011	5/5	0.69	0.18	130,130,130,131	0
14	UNL	D	4083	1/-	0.69	0.15	82,82,82,82	0
14	UNL	I	4033	1/-	0.69	0.18	69,69,69,69	0
12	PO4	R	4014	5/5	0.69	0.11	173,174,174,174	0
14	UNL	N	4029	1/-	0.71	0.19	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	UNL	U	4056	1/-	0.71	0.21	101,101,101,101	0
13	AZI	C	2005	3/3	0.72	0.20	41,41,55,60	0
11	JZR	S	2012	18/18	0.73	0.26	89,103,106,107	0
18	UQ	P	3002	18/63	0.74	0.23	60,82,85,86	0
14	UNL	V	4090	1/-	0.74	0.09	74,74,74,74	0
20	GOL	O	4005	6/6	0.74	0.29	166,167,167,168	0
14	UNL	A	4091	1/-	0.75	0.20	72,72,72,72	0
14	UNL	C	4045	1/-	0.75	0.17	71,71,71,71	0
14	UNL	V	4088	1/-	0.75	0.20	80,80,80,80	0
14	UNL	N	4022	1/-	0.75	0.13	81,81,81,81	0
14	UNL	O	4020	2/-	0.76	0.11	96,96,96,97	0
13	AZI	A	4002	3/3	0.76	0.27	48,48,58,65	0
15	PEE	B	4017	8/51	0.76	0.32	85,88,91,92	0
14	UNL	U	4049	1/-	0.76	0.21	77,77,77,77	0
14	UNL	A	4081	1/-	0.76	0.18	71,71,71,71	0
12	PO4	T	4016	5/5	0.76	0.11	107,108,108,108	0
14	UNL	F	4028	1/-	0.76	0.13	82,82,82,82	0
11	JZR	C	2011	18/18	0.77	0.26	106,118,123,125	0
14	UNL	G	4053	1/-	0.78	0.17	77,77,77,77	0
14	UNL	A	4085	1/-	0.78	0.10	56,56,56,56	0
14	UNL	N	4073	1/-	0.78	0.28	69,69,69,69	0
14	UNL	B	4042	1/-	0.78	0.14	81,81,81,81	0
11	JZR	P	3011	18/18	0.79	0.22	99,107,109,109	0
14	UNL	R	4069	1/-	0.80	0.19	62,62,62,62	0
14	UNL	D	4036	1/-	0.80	0.18	83,83,83,83	0
14	UNL	E	4061	1/-	0.81	0.06	79,79,79,79	0
14	UNL	O	4037	1/-	0.81	0.44	62,62,62,62	0
12	PO4	Q	4012	5/5	0.81	0.13	108,109,110,110	0
19	CDL	D	2003	39/100	0.81	0.20	64,84,106,107	0
14	UNL	B	4051	1/-	0.81	0.10	78,78,78,78	0
12	PO4	R	4013	5/5	0.81	0.20	114,114,116,116	0
14	UNL	A	4032	1/-	0.82	0.25	65,65,65,65	0
14	UNL	A	4035	1/-	0.82	0.19	69,69,69,69	0
14	UNL	C	4063	1/-	0.82	0.35	74,74,74,74	0
12	PO4	B	3009	5/5	0.83	0.10	97,99,100,101	0
14	UNL	O	4084	1/-	0.83	0.19	67,67,67,67	0
15	PEE	D	2006	51/51	0.83	0.24	85,98,115,118	0
14	UNL	B	4025	1/-	0.83	0.11	93,93,93,93	0
14	UNL	G	4064	1/-	0.84	0.31	56,56,56,56	0
14	UNL	S	4047	1/-	0.84	0.18	71,71,71,71	0
14	UNL	P	4040	1/-	0.84	0.19	73,73,73,73	0
14	UNL	Q	4044	1/-	0.84	0.36	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	UNL	B	4034	1/-	0.84	0.28	87,87,87,87	0
14	UNL	D	4054	1/-	0.85	0.13	76,76,76,76	0
14	UNL	B	4030	1/-	0.86	0.13	70,70,70,70	0
14	UNL	A	4075	1/-	0.86	0.08	64,64,64,64	0
19	CDL	Q	3003	39/100	0.86	0.16	54,90,96,96	0
14	UNL	G	4070	1/-	0.86	0.11	67,67,67,67	0
14	UNL	O	4031	1/-	0.86	0.10	86,86,86,86	0
14	UNL	D	4059	1/-	0.87	0.14	57,57,57,57	0
19	CDL	C	2004	44/100	0.87	0.17	54,83,104,106	0
13	AZI	G	4001	3/3	0.87	0.19	47,47,57,59	0
14	UNL	C	4018	2/-	0.87	0.14	74,74,74,76	0
12	PO4	O	2009	5/5	0.87	0.09	76,79,81,81	0
14	UNL	O	4071	1/-	0.87	0.17	70,70,70,70	0
14	UNL	C	4068	1/-	0.88	0.20	72,72,72,72	0
14	UNL	O	4043	1/-	0.88	0.10	80,80,80,80	0
14	UNL	A	4048	1/-	0.88	0.15	72,72,72,72	0
14	UNL	E	4050	1/-	0.88	0.19	65,65,65,65	0
14	UNL	P	4021	2/-	0.88	0.14	71,71,71,73	0
14	UNL	B	4026	1/-	0.88	0.20	92,92,92,92	0
14	UNL	P	4058	1/-	0.88	0.09	61,61,61,61	0
20	GOL	E	4006	6/6	0.88	0.14	67,71,72,75	0
14	UNL	P	4060	1/-	0.88	0.14	88,88,88,88	0
14	UNL	B	4079	1/-	0.88	0.19	66,66,66,66	0
14	UNL	B	4052	1/-	0.89	0.09	60,60,60,60	0
20	GOL	C	2008	6/6	0.89	0.14	60,63,63,70	0
14	UNL	A	4076	1/-	0.89	0.20	68,68,68,68	0
14	UNL	P	4089	1/-	0.89	0.13	63,63,63,63	0
15	PEE	Q	3006	51/51	0.89	0.18	53,65,110,110	0
20	GOL	P	3008	6/6	0.89	0.25	83,84,85,88	0
14	UNL	C	4023	1/-	0.90	0.11	55,55,55,55	0
14	UNL	A	4038	1/-	0.90	0.23	85,85,85,85	0
14	UNL	D	4067	1/-	0.90	0.14	58,58,58,58	0
19	CDL	P	3004	49/100	0.90	0.17	54,81,117,120	0
14	UNL	N	4019	2/-	0.90	0.11	76,76,76,76	0
14	UNL	T	4065	1/-	0.91	0.27	66,66,66,66	0
14	UNL	T	4066	1/-	0.91	0.11	70,70,70,70	0
14	UNL	B	4080	1/-	0.91	0.30	67,67,67,67	0
14	UNL	W	4077	1/-	0.91	0.13	60,60,60,60	0
14	UNL	C	4086	1/-	0.91	0.10	50,50,50,50	0
14	UNL	D	4027	1/-	0.91	0.20	87,87,87,87	0
20	GOL	P	4009	6/6	0.91	0.14	67,70,71,72	0
14	UNL	P	4074	1/-	0.92	0.09	59,59,59,59	0

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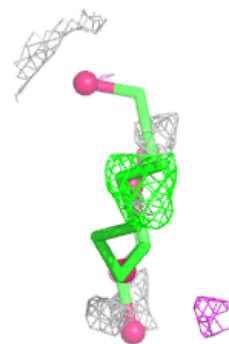
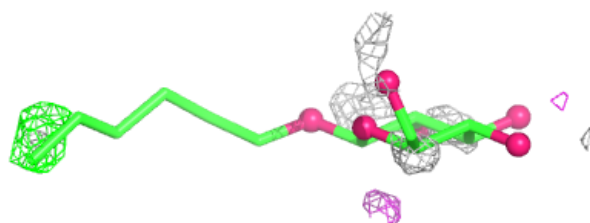
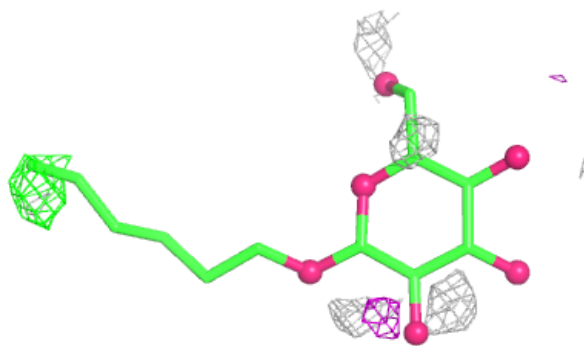
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	PEE	P	3007	49/51	0.92	0.15	35,58,75,76	0
14	UNL	O	4082	1/-	0.92	0.12	73,73,73,73	0
14	UNL	B	4039	1/-	0.92	0.10	73,73,73,73	0
14	UNL	B	4057	1/-	0.92	0.17	57,57,57,57	0
20	GOL	C	4008	6/6	0.93	0.10	53,55,60,60	0
14	UNL	A	4087	1/-	0.93	0.21	60,60,60,60	0
14	UNL	O	4041	1/-	0.94	0.10	71,71,71,71	0
15	PEE	C	2007	49/51	0.94	0.13	33,58,74,74	0
11	JZR	A	4004	18/18	0.94	0.09	29,36,42,44	0
17	SMA	C	2001	37/37	0.95	0.07	25,33,44,46	0
14	UNL	P	4046	1/-	0.95	0.20	65,65,65,65	0
17	SMA	P	3001	37/37	0.96	0.08	30,39,47,52	0
16	HEM	C	501	43/43	0.98	0.06	21,27,34,38	0
16	HEM	C	502	43/43	0.98	0.06	23,26,33,36	0
16	HEM	P	501	43/43	0.98	0.07	22,26,33,40	0
21	HEC	D	501	43/43	0.98	0.07	26,33,37,38	0
21	HEC	Q	501	43/43	0.98	0.06	29,36,41,45	0
22	FES	E	501	4/4	0.98	0.04	38,39,40,40	0
16	HEM	P	502	43/43	0.99	0.05	23,27,37,39	0
22	FES	R	501	4/4	0.99	0.03	27,29,30,30	0

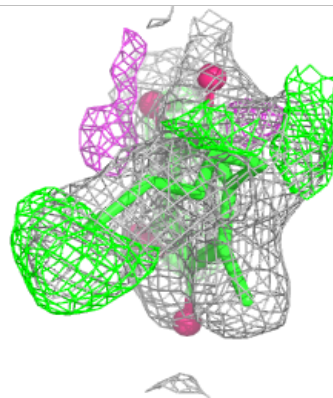
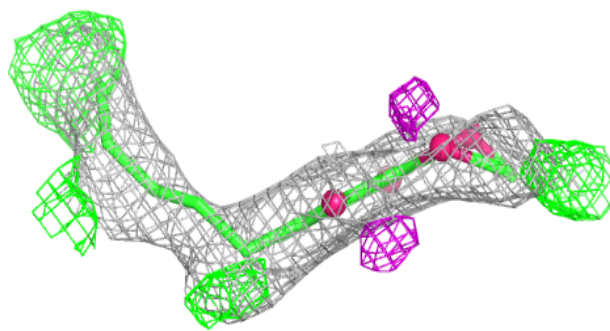
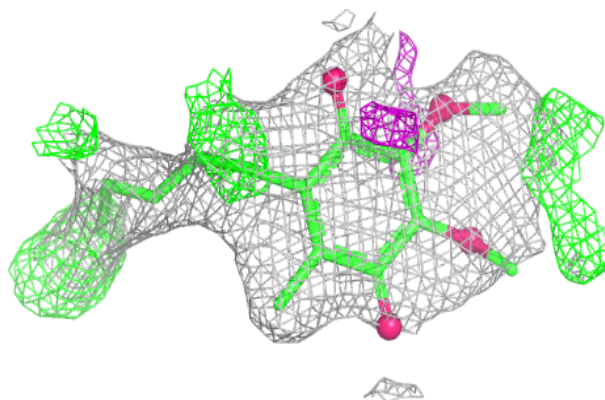
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZR F 4003:

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

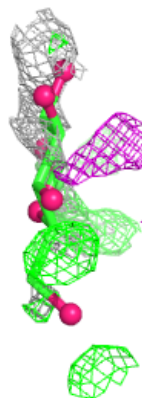
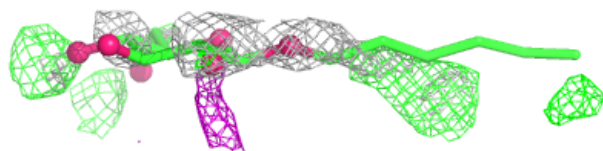
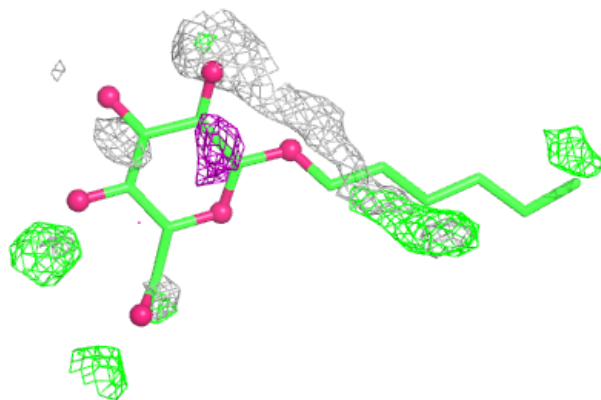
**Electron density around UQ C 2002:**

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

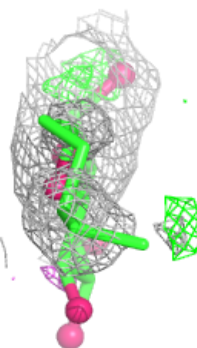
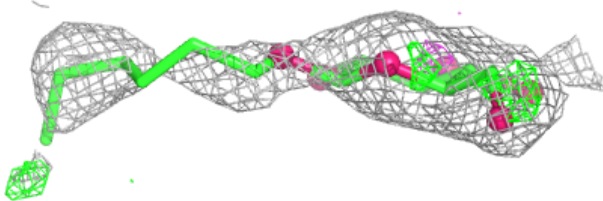
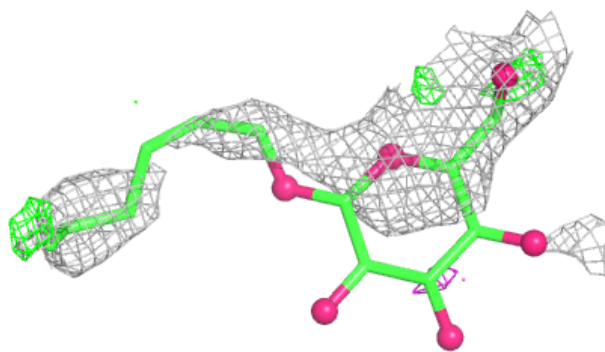


Electron density around JZR F 3012:

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

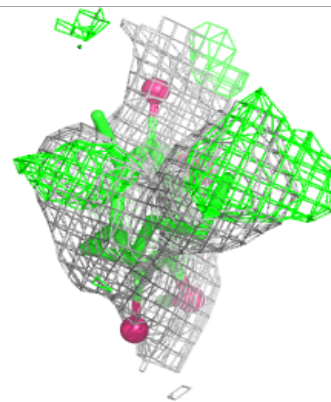
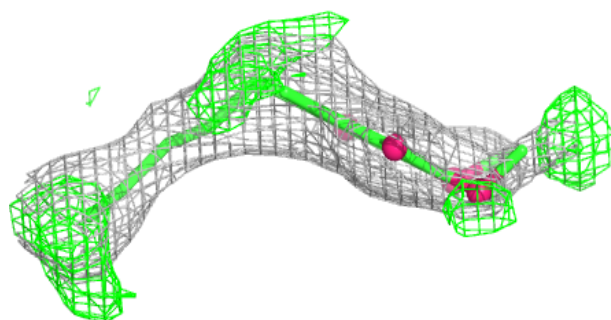
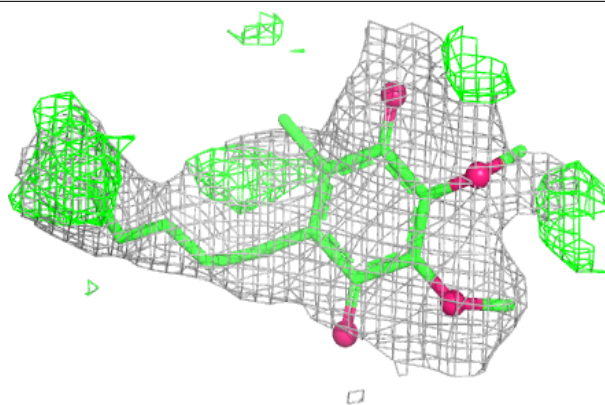
**Electron density around JZR S 2012:**

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

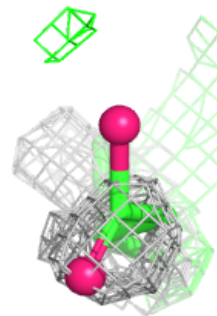
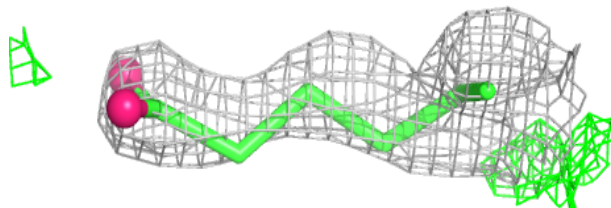
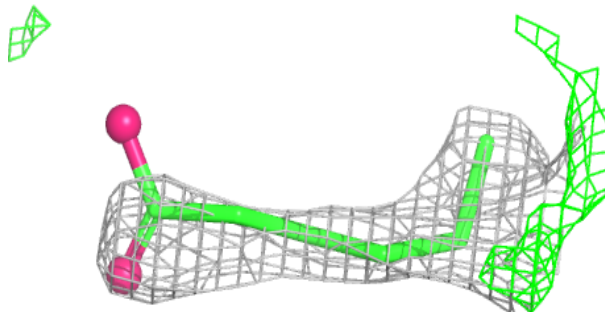


Electron density around UQ P 3002:

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

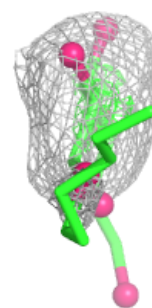
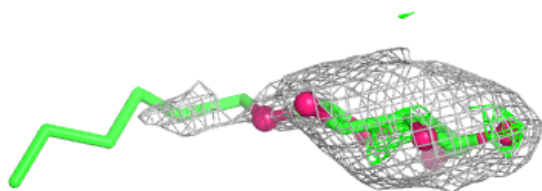
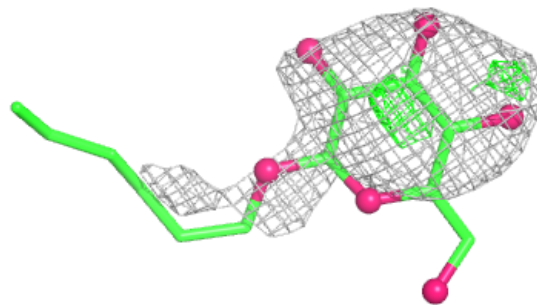
**Electron density around PEE B 4017:**

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

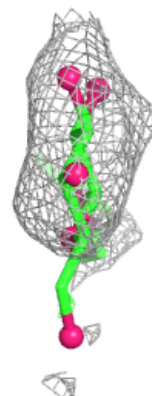
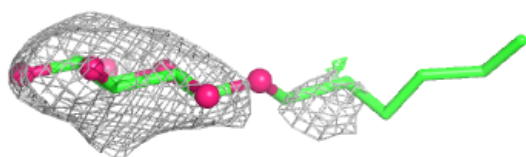
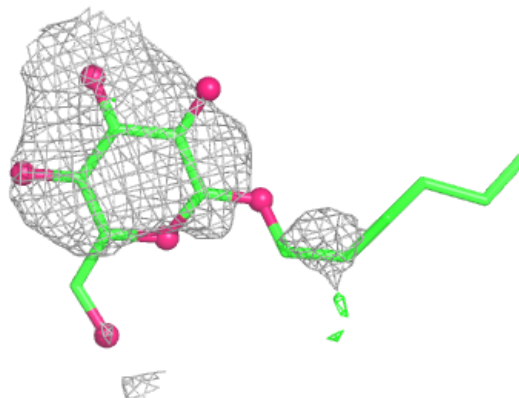


Electron density around JZR C 2011:

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

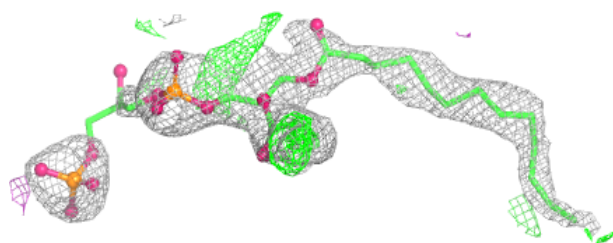
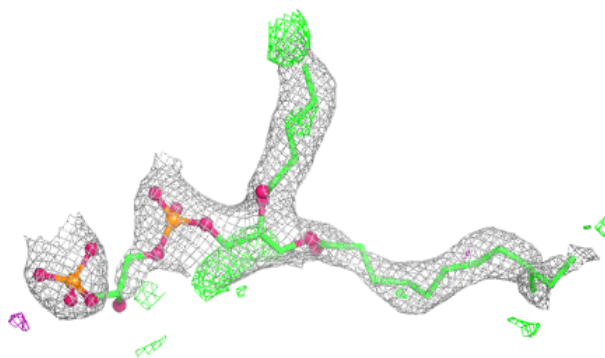
**Electron density around JZR P 3011:**

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

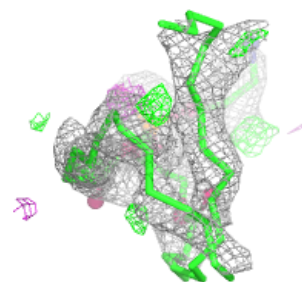
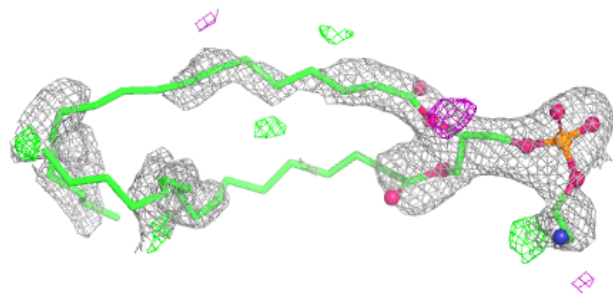
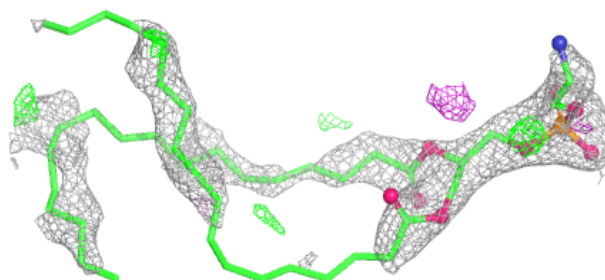


Electron density around CDL D 2003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

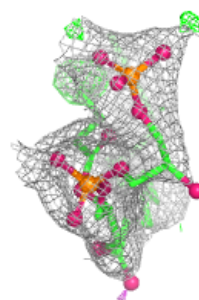
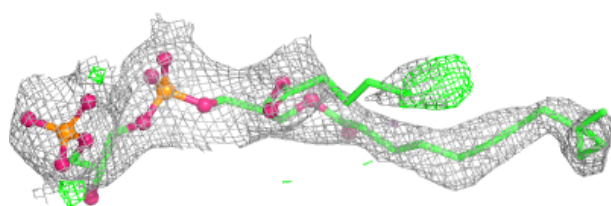
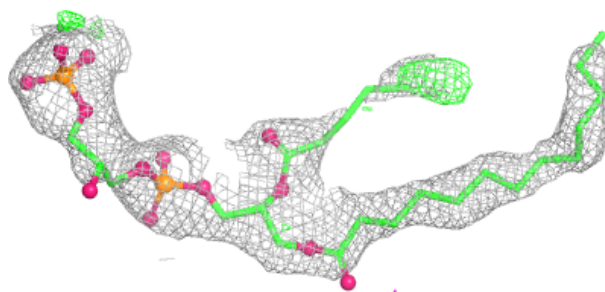
**Electron density around PEE D 2006:**

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

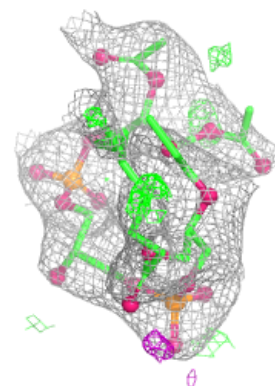
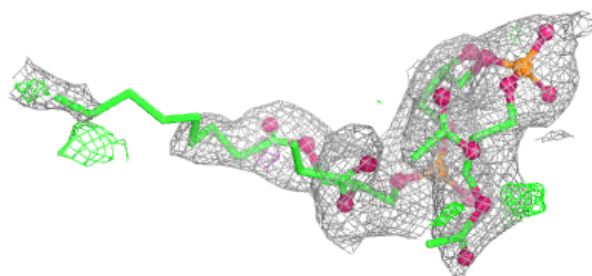
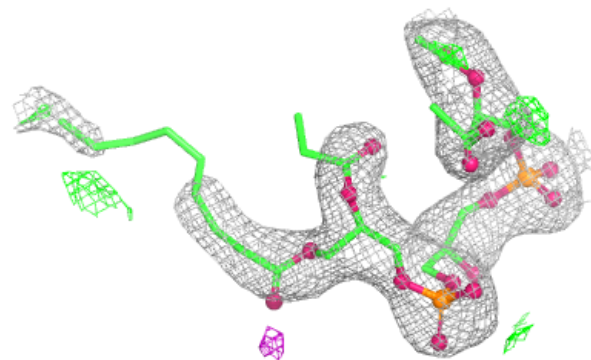


Electron density around CDL Q 3003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

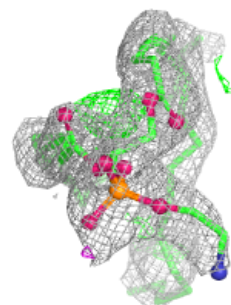
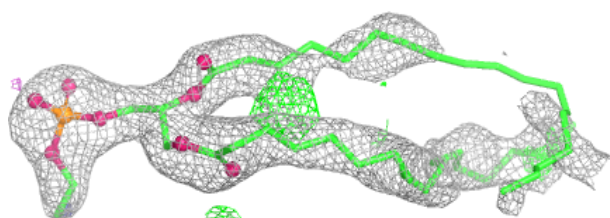
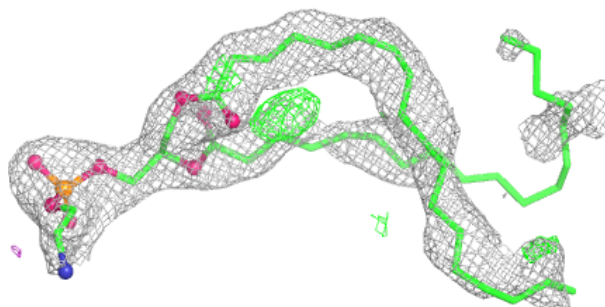
**Electron density around CDL C 2004:**

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

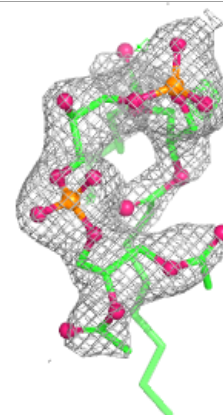
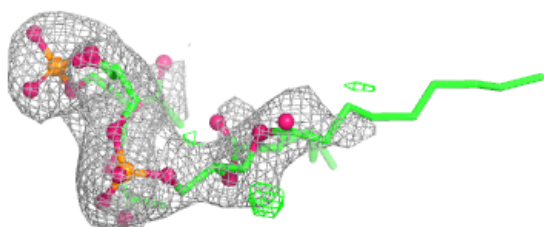
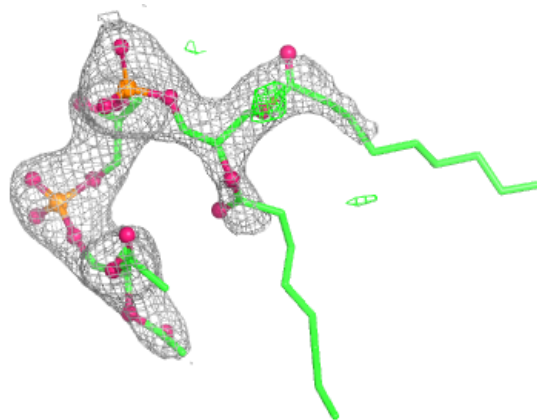


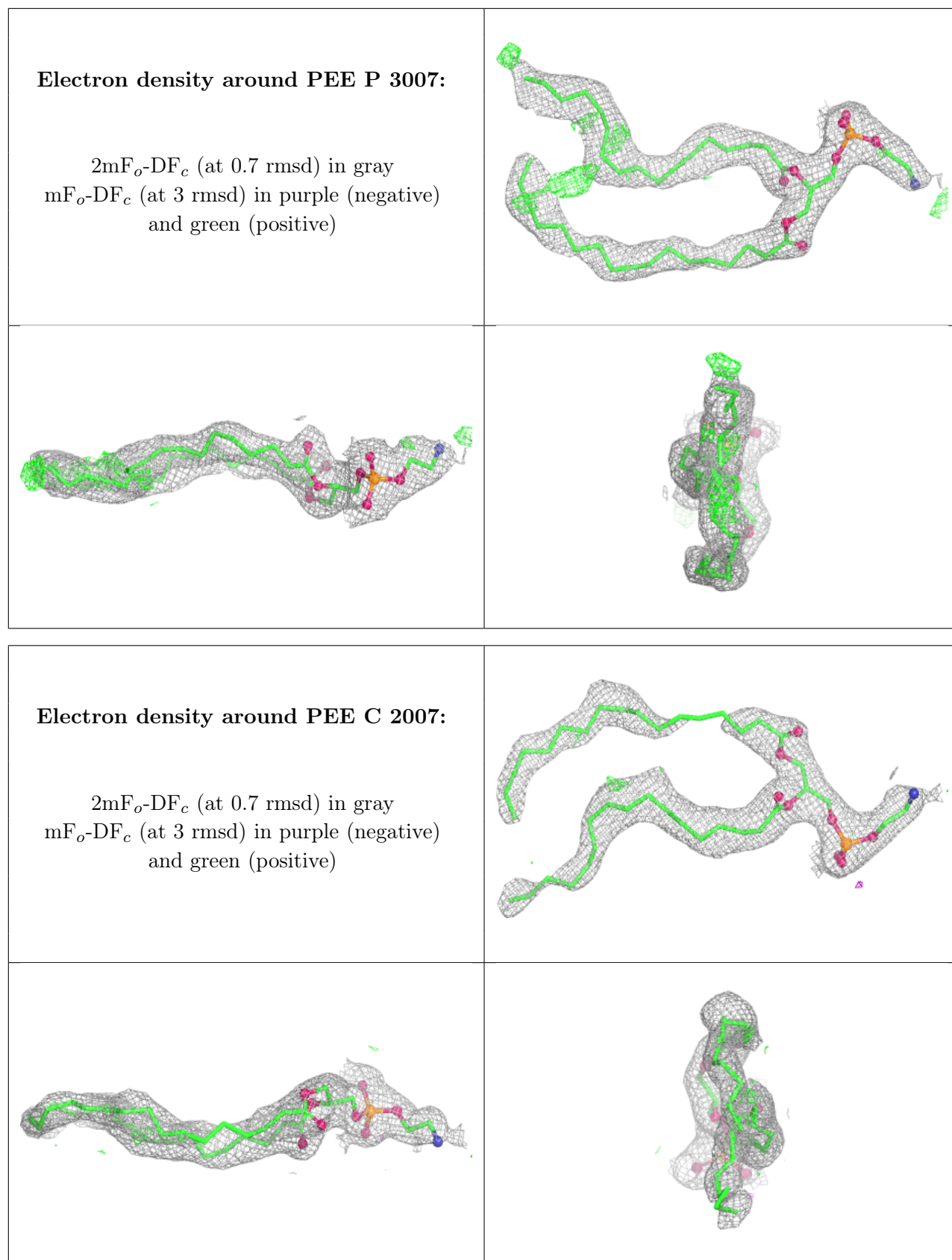
Electron density around PEE Q 3006:

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

**Electron density around CDL P 3004:**

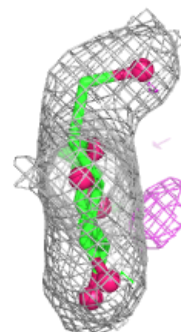
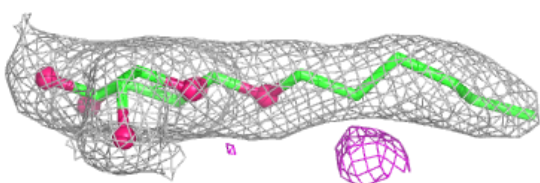
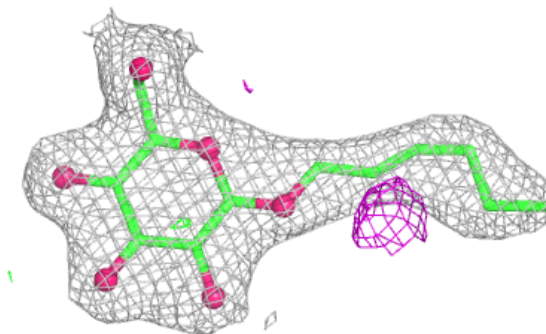
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



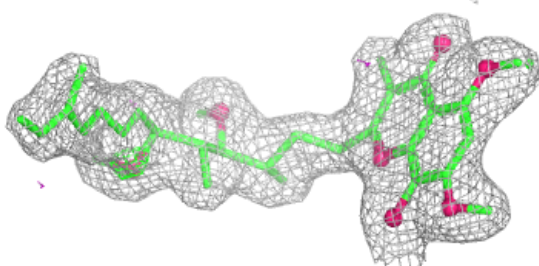
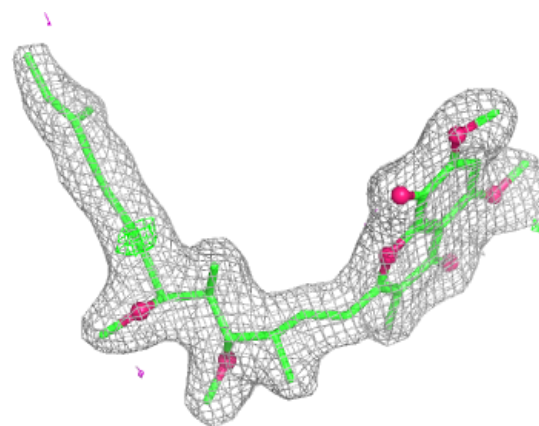


Electron density around JZR A 4004:

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

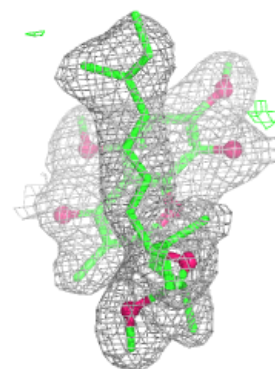
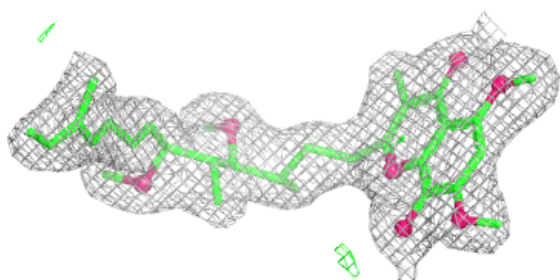
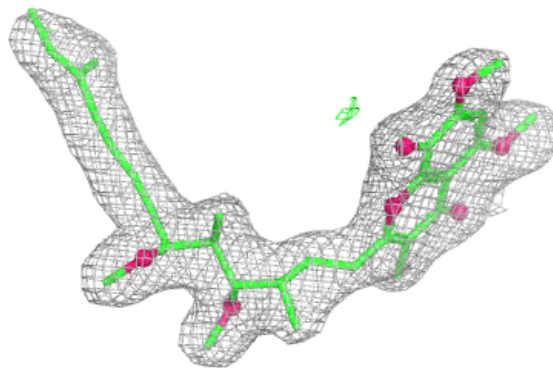
**Electron density around SMA C 2001:**

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



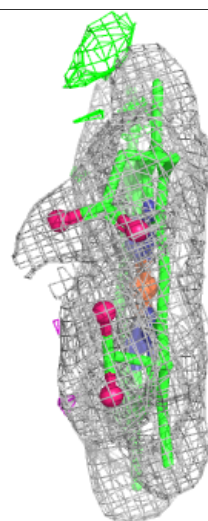
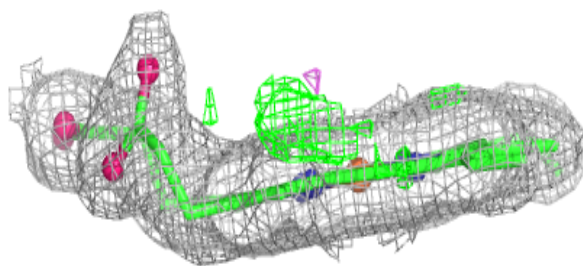
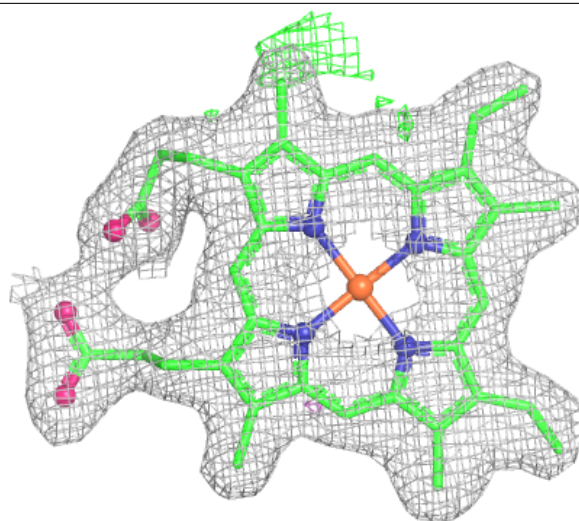
Electron density around SMA P 3001:

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



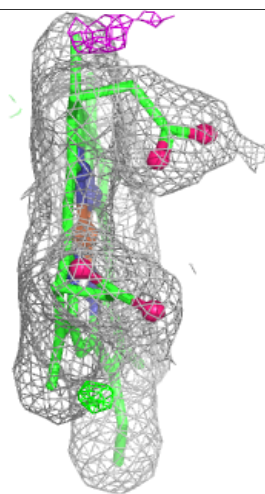
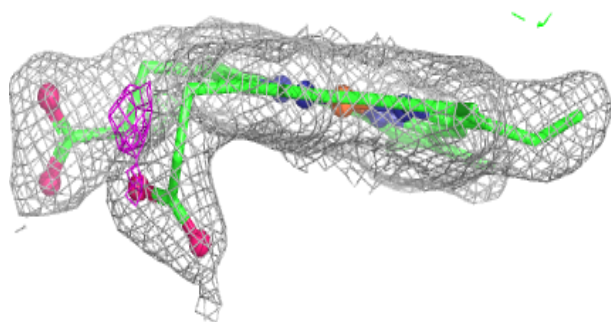
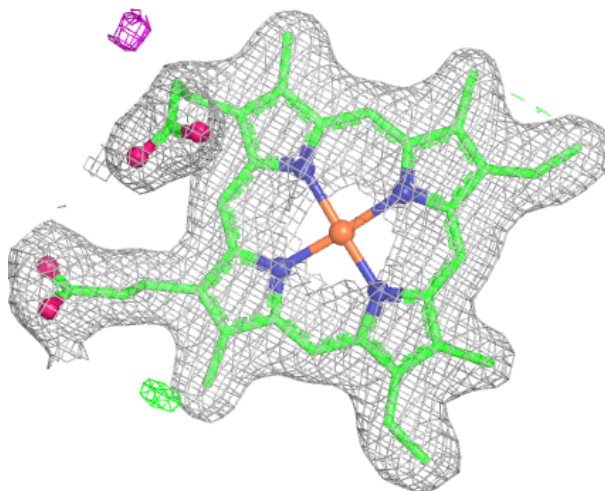
Electron density around HEM C 501:

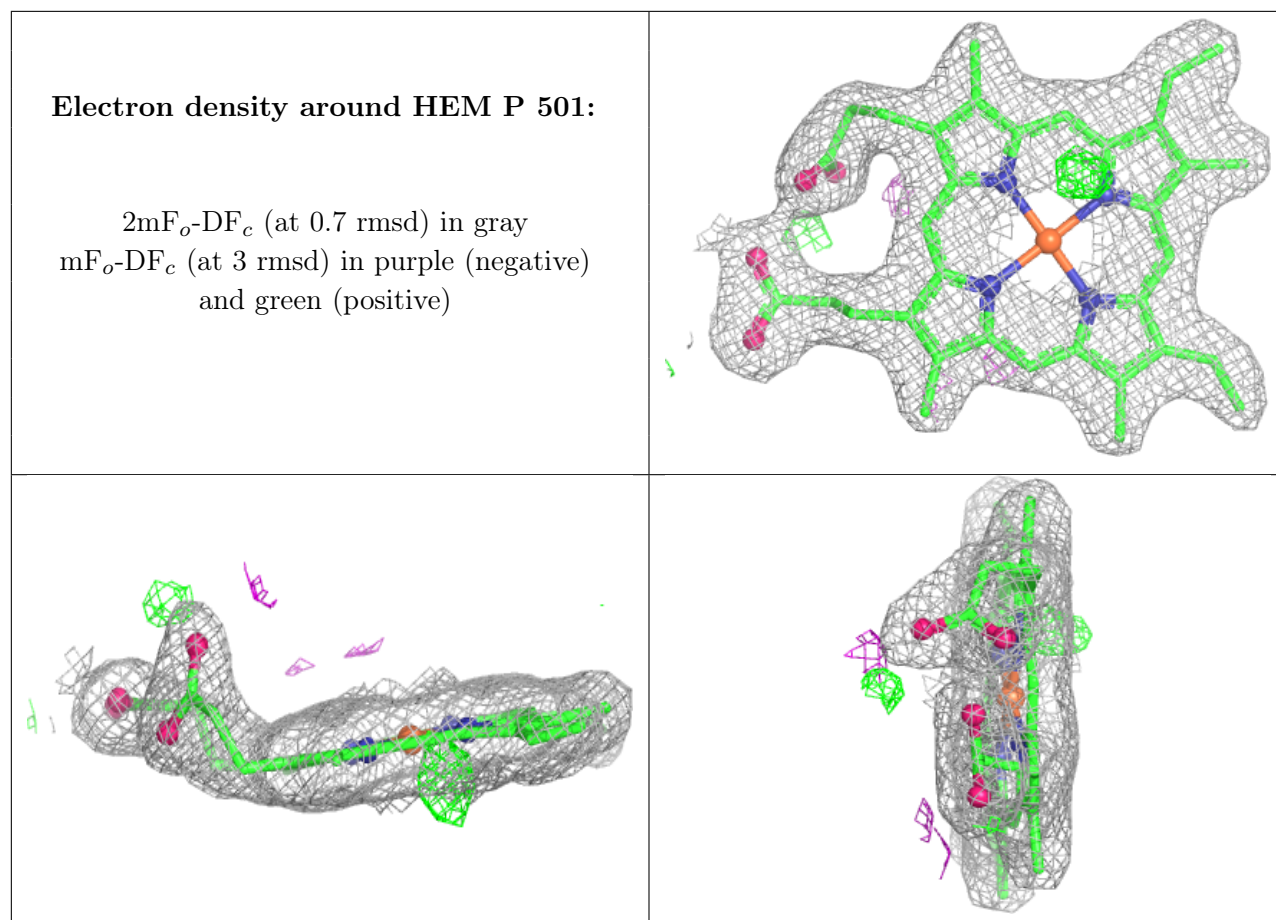
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

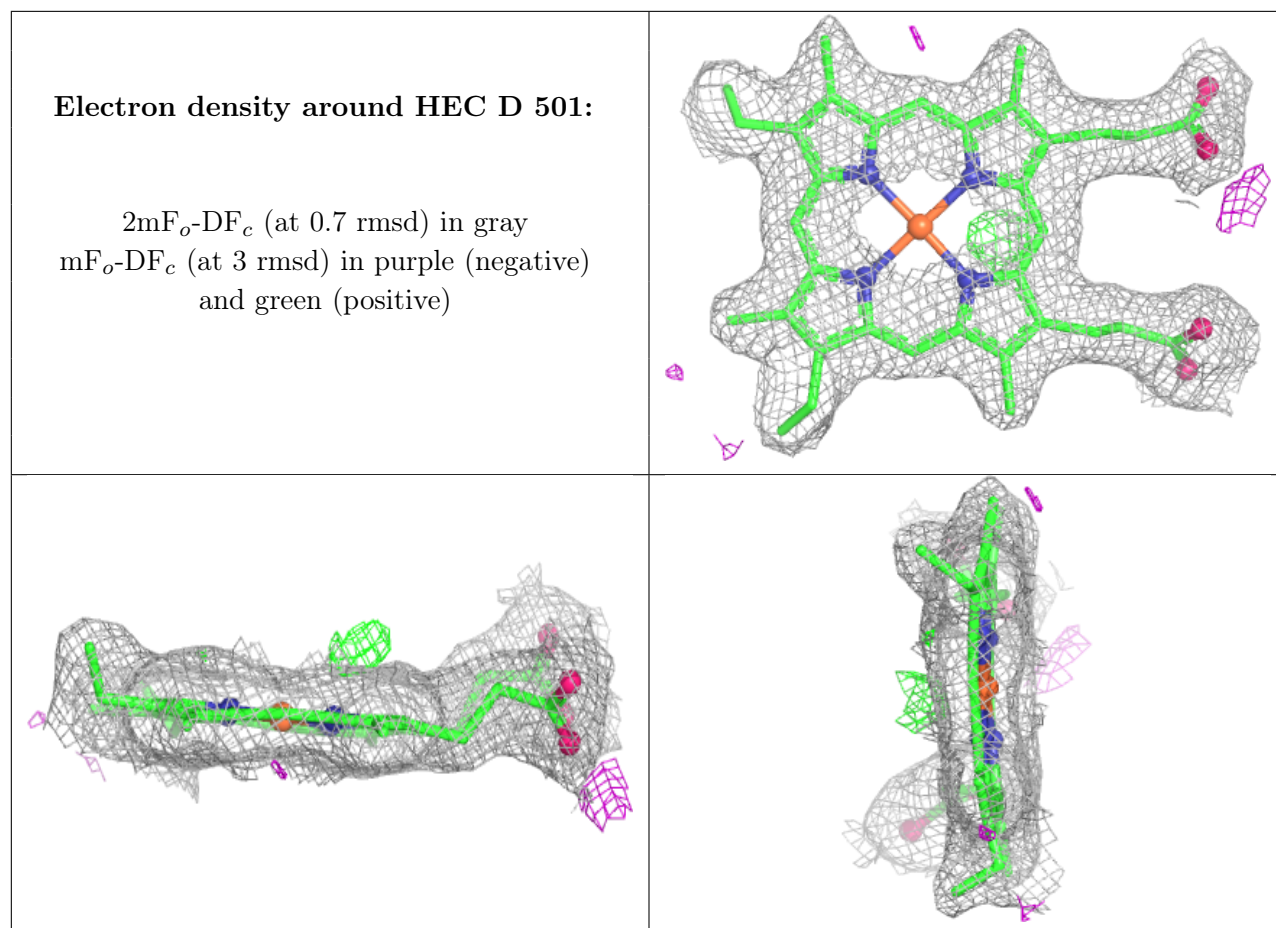


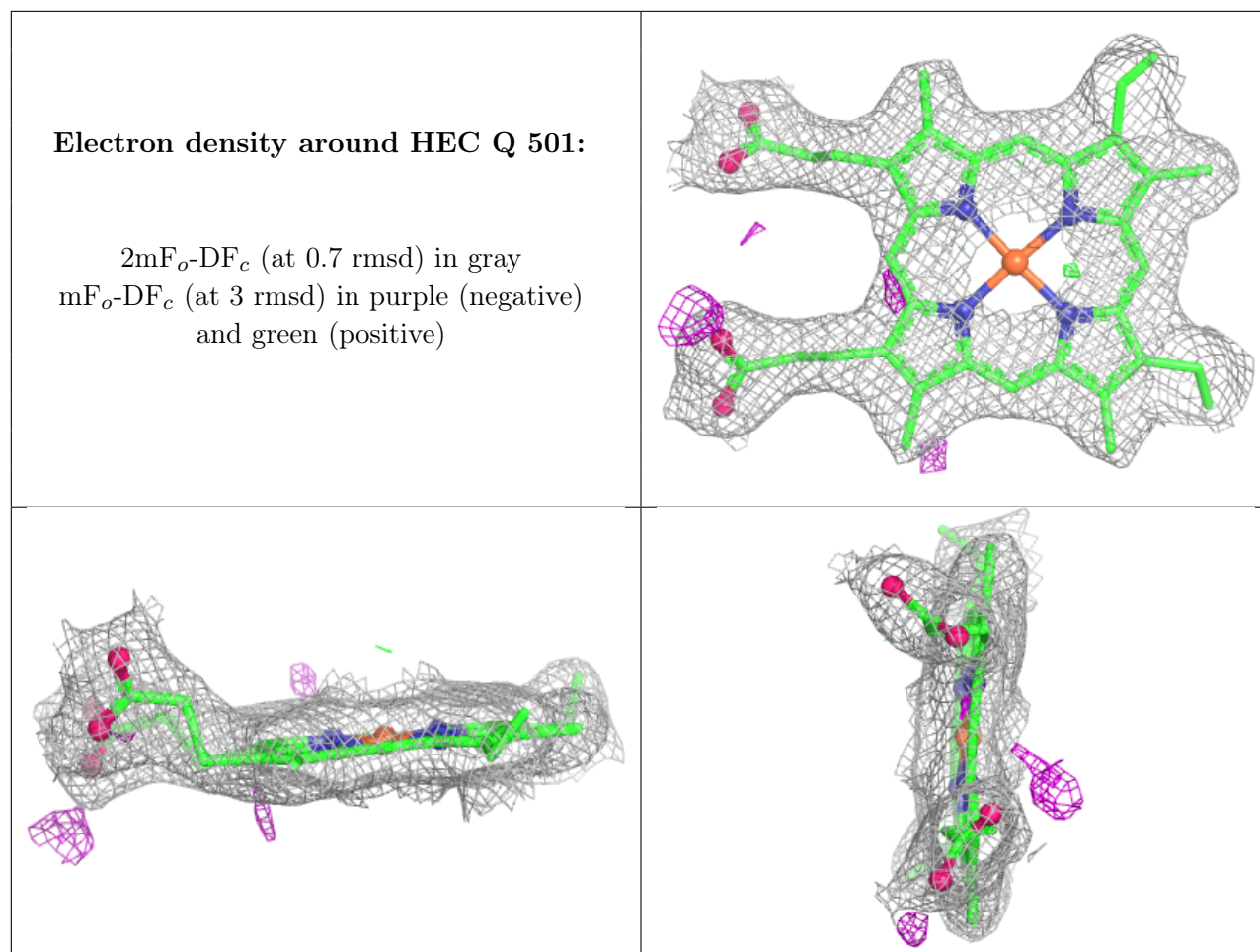
Electron density around HEM C 502:

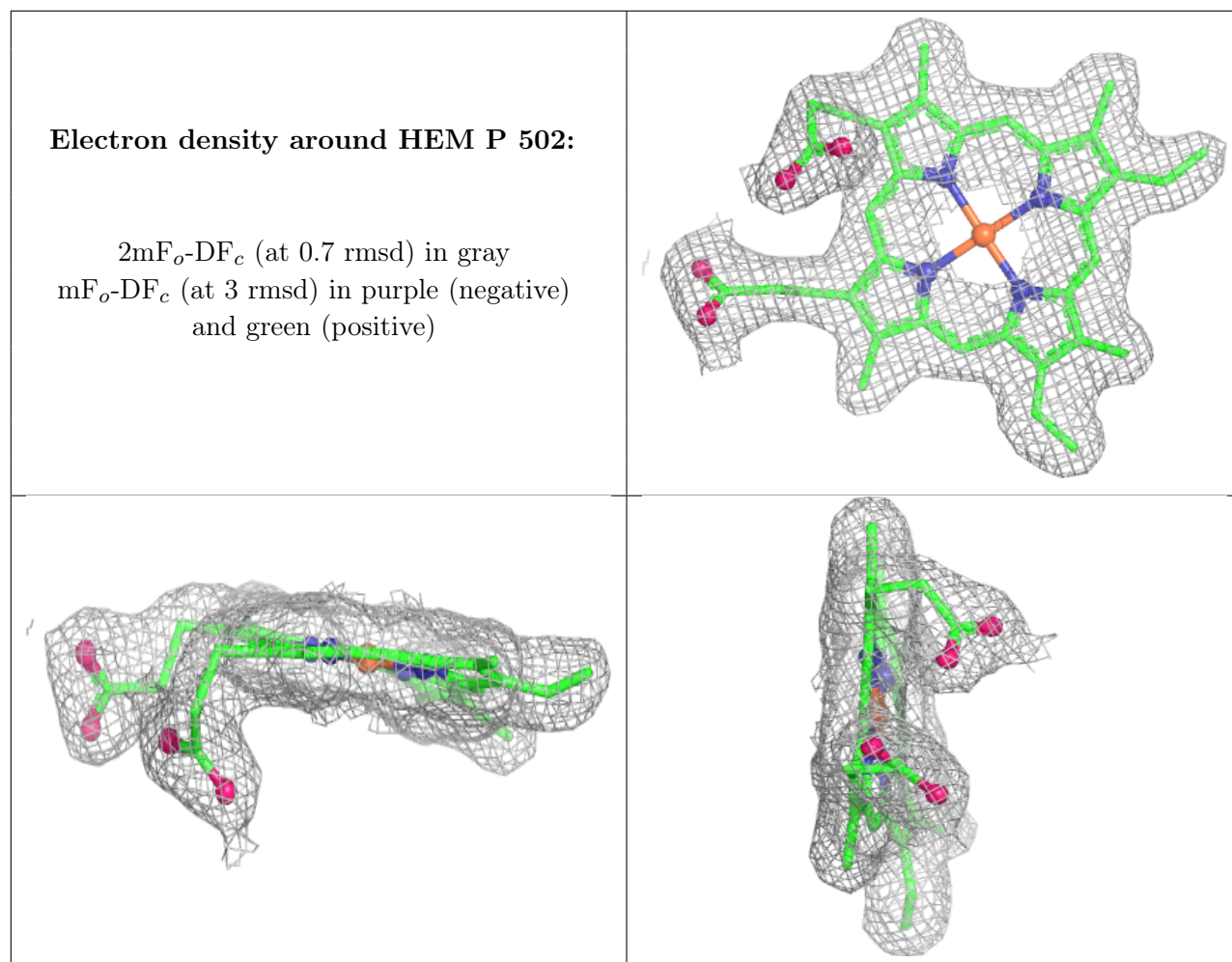
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)











6.5 Other polymers [i](#)

There are no such residues in this entry.