



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 04:20 AM BST

PDB ID : 2A06  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

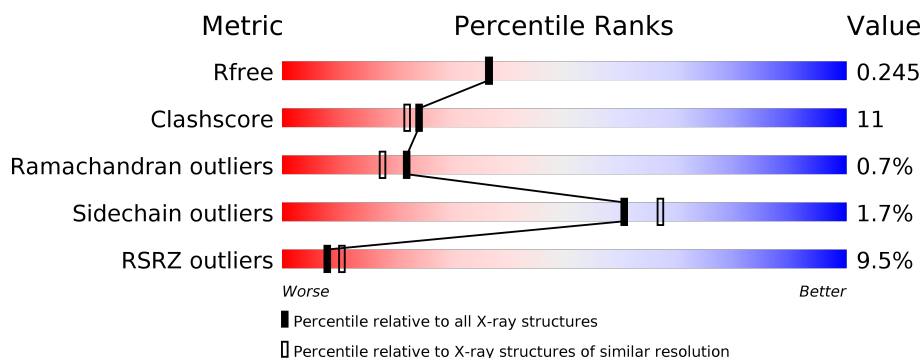
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	N	446	<div> <div>7%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	B	439	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	O	439	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
3	C	379	<div> <div>5%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
3	P	379	<div> <div>6%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
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	C	2011	-	-	-	X
11	JZR	F	3012	-	-	-	X
11	JZR	F	4003	-	-	-	X
11	JZR	P	3011	-	-	-	X
11	JZR	S	2012	-	-	-	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	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PO4	R	4013	-	X	-	-
12	PO4	R	4014	-	X	-	X
12	PO4	T	4016	-	X	-	-
13	AZI	A	4002	-	-	-	X
14	UNL	A	4035	-	-	-	X
14	UNL	A	4038	-	-	-	X
14	UNL	A	4076	-	-	-	X
14	UNL	A	4081	-	-	-	X
14	UNL	A	4091	-	-	-	X
14	UNL	B	4025	-	-	-	X
14	UNL	B	4026	-	-	-	X
14	UNL	B	4034	-	-	-	X
14	UNL	B	4057	-	-	-	X
14	UNL	B	4080	-	-	-	X
14	UNL	C	4045	-	-	-	X
14	UNL	C	4068	-	-	-	X
14	UNL	D	4059	-	-	-	X
14	UNL	D	4083	-	-	-	X
14	UNL	I	4072	-	-	-	X
14	UNL	N	4022	-	-	-	X
14	UNL	N	4029	-	-	-	X
14	UNL	O	4037	-	-	-	X
14	UNL	O	4043	-	-	X	-
14	UNL	O	4071	-	-	-	X
14	UNL	Q	4044	-	-	-	X
14	UNL	U	4049	-	-	-	X
14	UNL	U	4056	-	-	-	X
14	UNL	V	4024	-	-	-	X
14	UNL	V	4088	-	-	-	X
15	PEE	B	4017	-	-	-	X
20	GOL	E	4007	-	-	-	X
20	GOL	O	4005	-	-	-	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
1	A	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			
1	N	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			

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

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

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

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

- 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
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- 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			

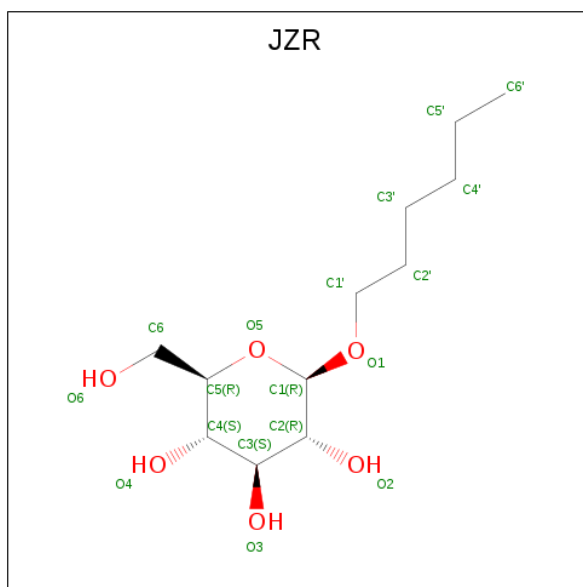
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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.

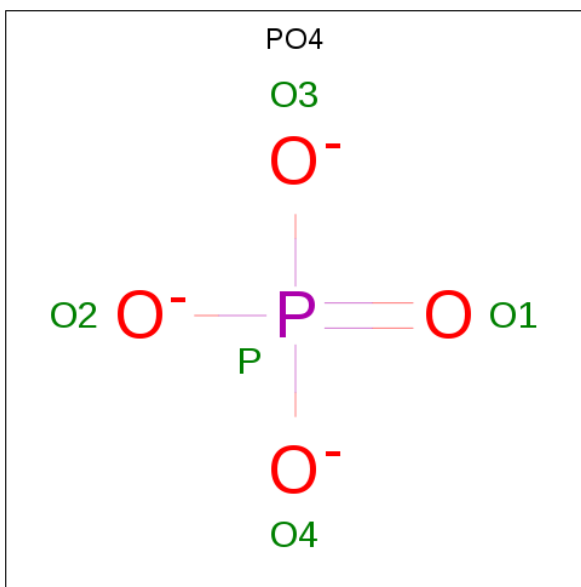
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).



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		

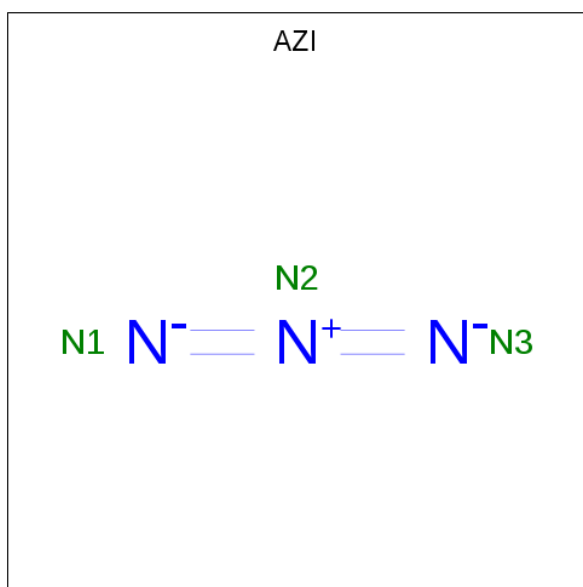
- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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 (three-letter code: AZI) (formula: N<sub>3</sub>).





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 (three-letter code: UNL) (formula: ).

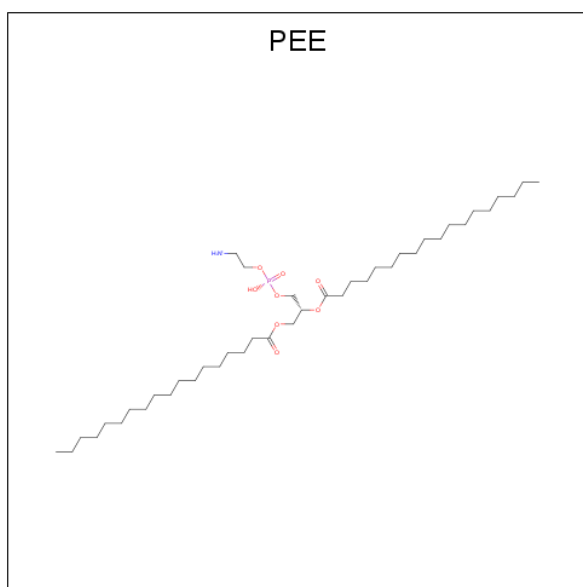
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	P	7	Total O 8 8	0	0
14	G	3	Total O 3 3	0	0
14	Q	1	Total O 1 1	0	0
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	B	11	Total O 11 11	0	0
14	I	2	Total O 2 2	0	0
14	C	6	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	V	4	Total	O	0	0
			4	4		
14	W	1	Total	O	0	0
			1	1		
14	A	10	Total	O	0	0
			10	10		
14	T	2	Total	O	0	0
			2	2		
14	N	4	Total	O	0	0
			5	5		
14	U	2	Total	O	0	0
			2	2		
14	O	8	Total	O	0	0
			9	9		
14	R	2	Total	O	0	0
			2	2		
14	S	1	Total	O	0	0
			1	1		
14	F	1	Total	O	0	0
			1	1		

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



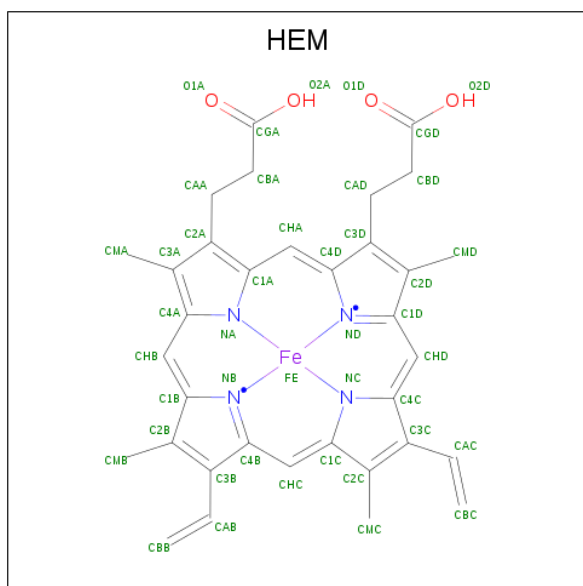
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			8	6	2		

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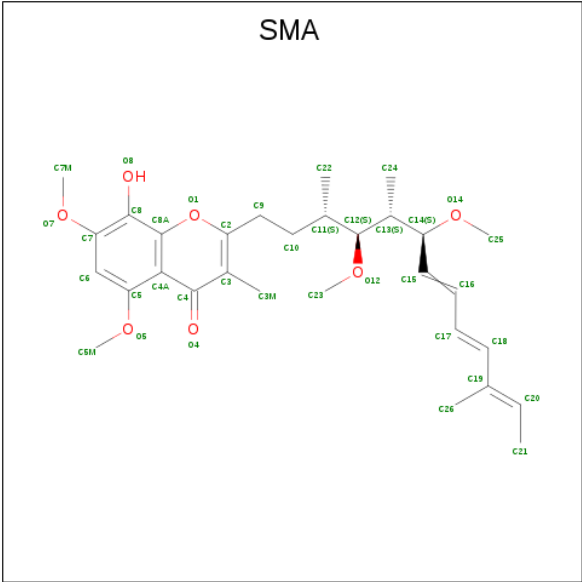
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



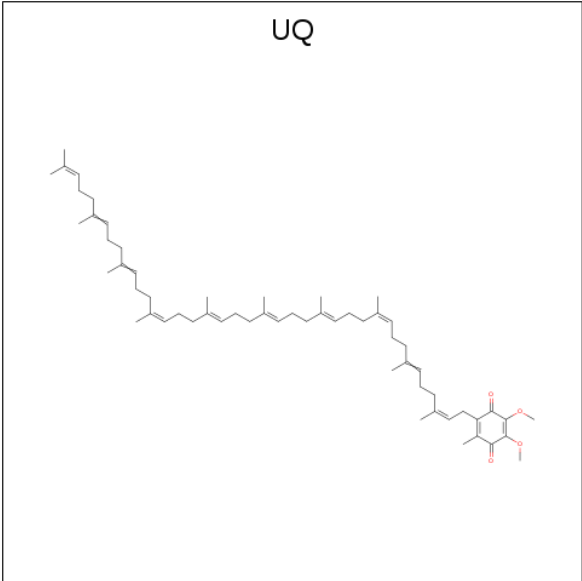
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).



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 (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



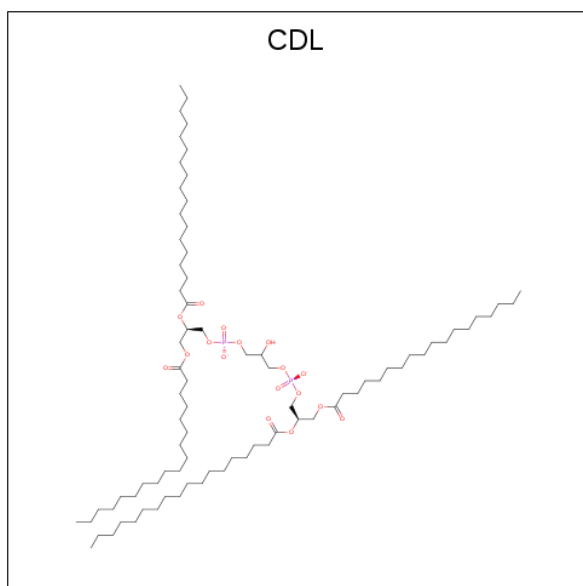
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		

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

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



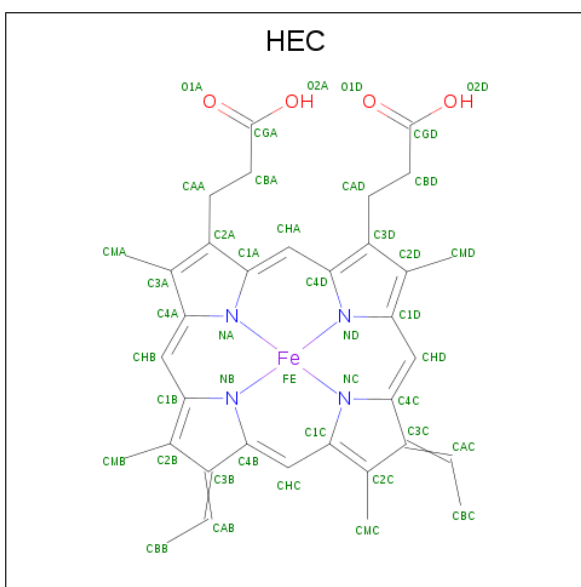
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	1	Total	C	O	P	0	0
			49	30	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		

- Molecule 20 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



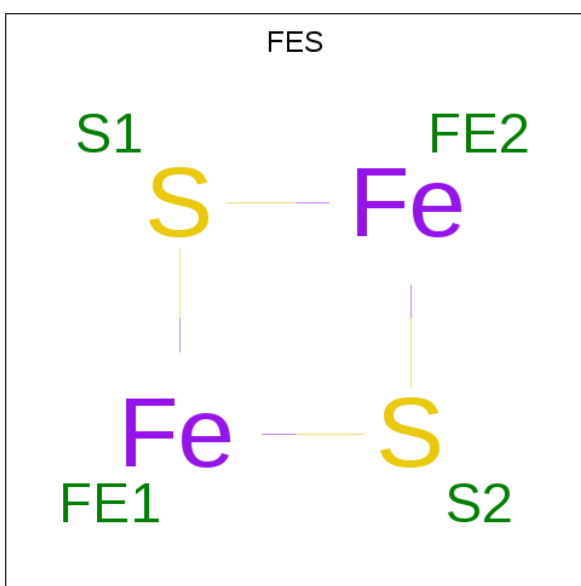
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	C	O	0	0
			6	3	3		
20	C	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			5	3	2		
20	O	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 21 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

- Molecule 23 is water.

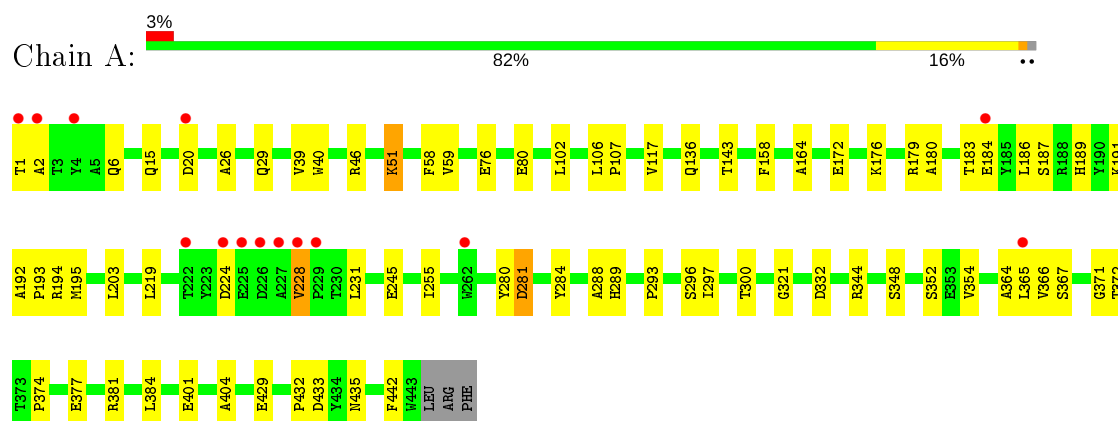
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	209	Total 209	O 209	0	0
23	B	170	Total 170	O 170	0	0
23	C	137	Total 137	O 137	0	0
23	D	133	Total 133	O 133	0	0
23	E	63	Total 63	O 63	0	0
23	F	68	Total 68	O 68	0	0
23	G	31	Total 31	O 31	0	0
23	H	15	Total 15	O 15	0	0
23	I	18	Total 18	O 18	0	0
23	J	7	Total 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



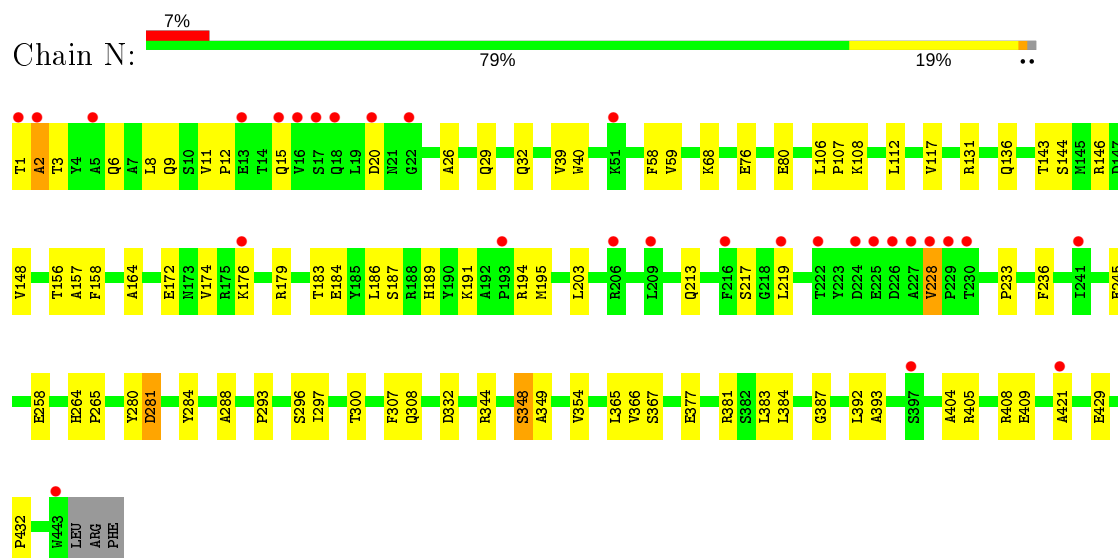
### 3 Residue-property plots [i](#)

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.

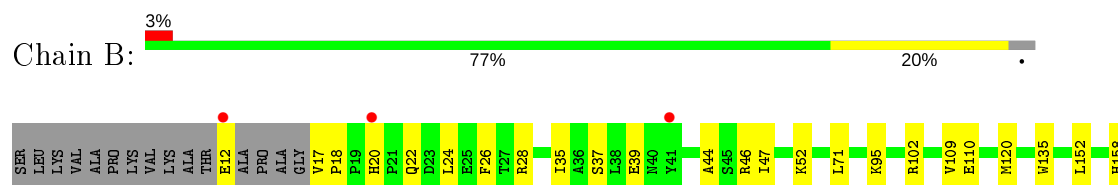
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

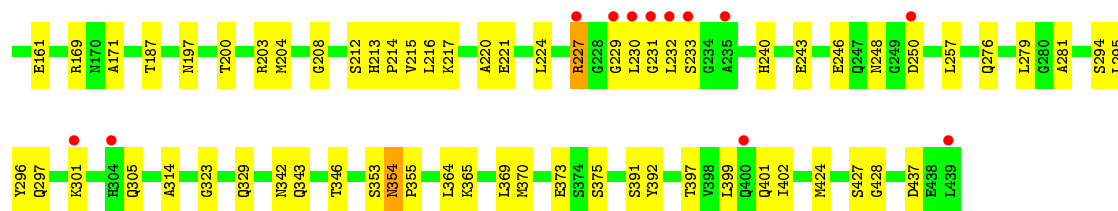


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

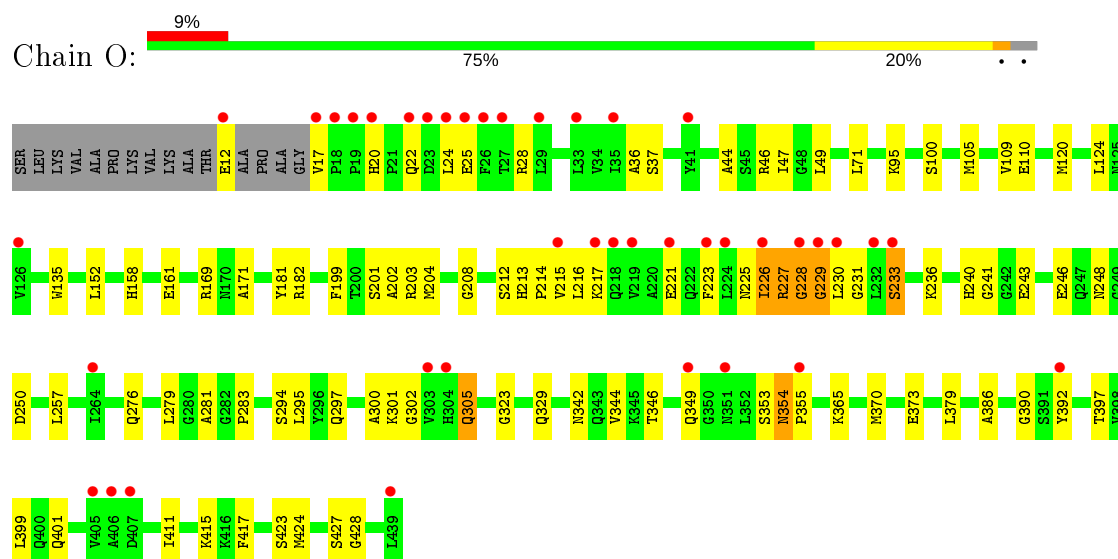


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

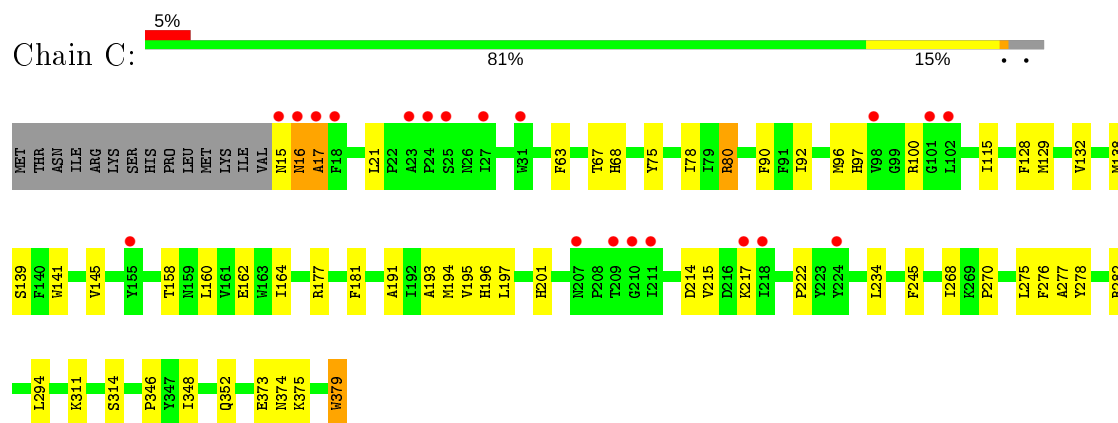




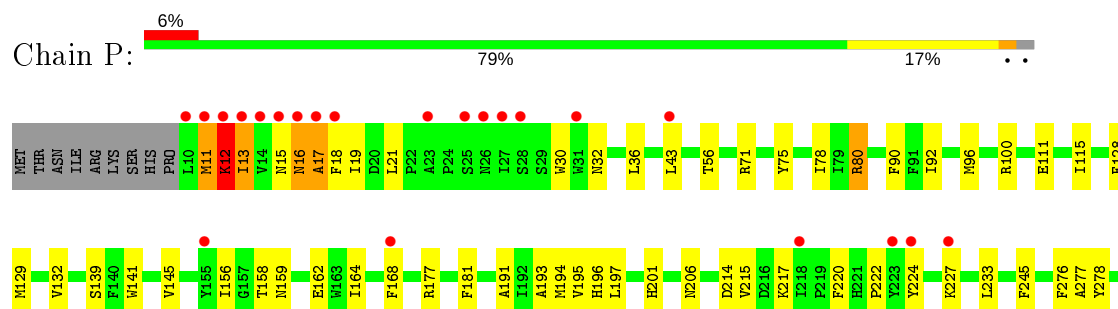
• Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

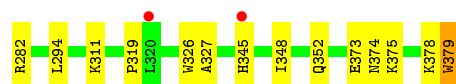


• Molecule 3: Cytochrome b, heme protein, mitochondrial

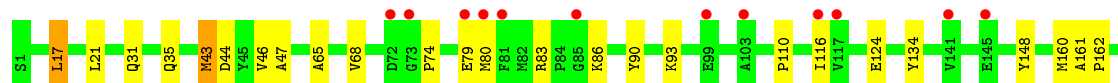
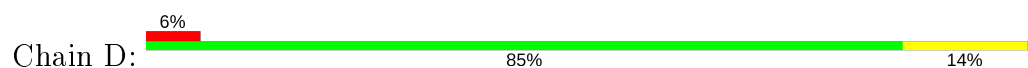


• Molecule 3: Cytochrome b, heme protein, mitochondrial

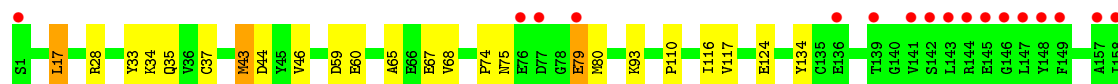
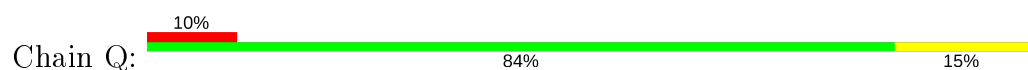




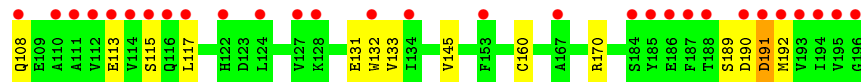
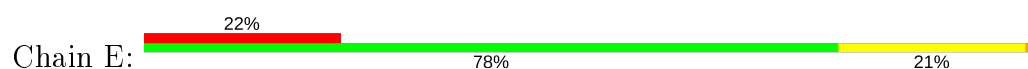
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



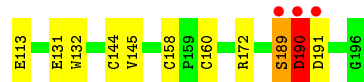
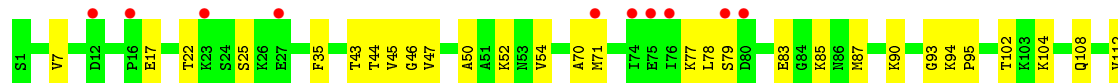
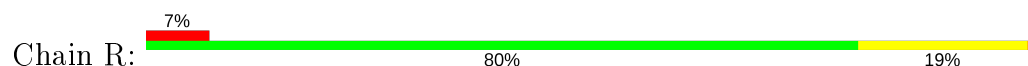
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



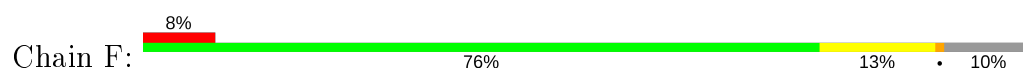
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



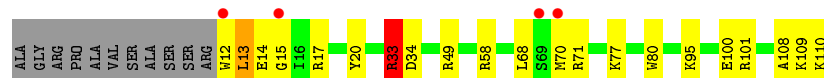
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



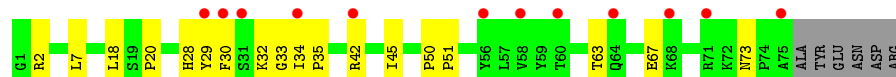
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



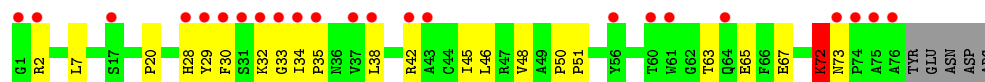
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



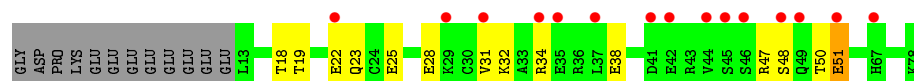
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



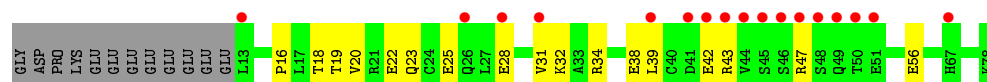
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



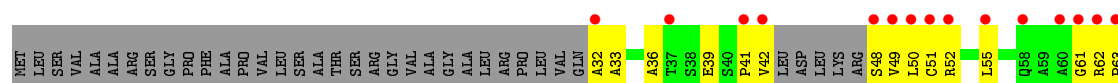
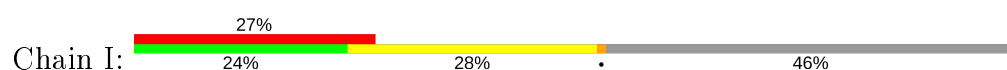
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

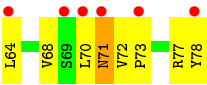


- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

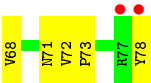
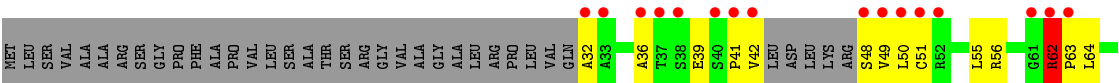
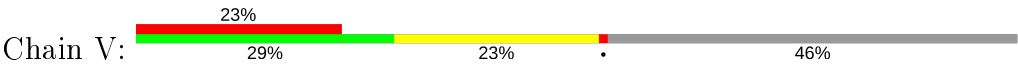


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

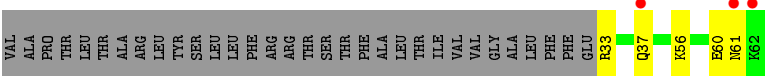
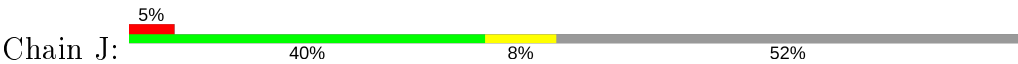




● Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



● 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, $\alpha$ , $\beta$ , $\gamma$	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 91.8 (37.87-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.258 0.212 , 0.245	Depositor DCC
$R_{free}$ test set	15254 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 69.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AZI, GOL, CDL, UNL, PO4, UQ, FES, HEC, HEM, PEE, JZR, SMA

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	0.44	0/3467	0.67	0/4706
1	N	0.38	0/3467	0.64	0/4706
2	B	0.42	0/3235	0.65	0/4387
2	O	0.39	0/3239	0.65	1/4393 (0.0%)
3	C	0.48	0/2992	0.66	0/4097
3	P	0.44	0/3030	0.64	0/4145
4	D	0.44	0/1978	0.64	0/2684
4	Q	0.41	0/1978	0.62	0/2684
5	E	0.35	0/1553	0.70	3/2100 (0.1%)
5	R	0.41	0/1550	0.69	0/2094
6	F	0.45	0/878	0.66	0/1175
6	S	0.44	0/878	0.68	1/1175 (0.1%)
7	G	0.42	0/642	0.63	0/869
7	T	0.39	0/647	0.65	0/876
8	H	0.34	0/544	0.61	0/729
8	U	0.34	0/544	0.56	0/729
9	I	0.60	0/285	0.96	0/384
9	V	0.50	0/285	0.94	1/384 (0.3%)
10	J	0.38	0/252	0.56	0/333
10	W	0.36	0/520	0.59	0/699
All	All	0.42	0/31964	0.66	6/43349 (0.0%)

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	70	ALA	C-N-CA	-6.85	104.57	121.70
2	O	228	GLY	N-CA-C	-6.31	97.33	113.10
5	E	71	MET	C-N-CA	-6.26	106.05	121.70
6	S	33	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	V	62	ARG	NE-CZ-NH2	5.70	123.15	120.30

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	88	0
2	O	3180	0	3156	87	0
3	C	2897	0	2943	47	0
3	P	2936	0	2994	74	0
4	D	1919	0	1868	38	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	34	0
5	R	1517	0	1498	38	0
6	F	861	0	854	20	0
6	S	861	0	854	26	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	17	0
8	U	539	0	524	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
15	C	49	0	72	0	0
15	D	51	0	82	2	0
15	P	49	0	72	3	0
15	Q	51	0	82	5	0
16	C	86	0	60	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	86	0	60	3	0
17	C	37	0	42	3	0
17	P	37	0	42	3	0
18	C	18	0	14	4	0
18	P	18	0	14	5	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	4	0
21	Q	43	0	30	5	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	6	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
All	All	33890	0	31860	708	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 11.

The worst 5 of 708 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
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
5:R:90:LYS:HE2	5:R:93:GLY:HA2	1.39	1.03

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%)	29	26
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	29	26
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	47	49
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	13	8
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	25	21
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	11	6
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%)	29	26
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	15	11
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%)	11	6
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	2	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	5	2
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	3	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	22	18

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 ⓘ

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%)	57	63
1	N	363/370 (98%)	355 (98%)	8 (2%)	52	57
2	B	332/343 (97%)	330 (99%)	2 (1%)	86	90
2	O	332/343 (97%)	329 (99%)	3 (1%)	78	84
3	C	313/327 (96%)	307 (98%)	6 (2%)	57	63
3	P	317/327 (97%)	311 (98%)	6 (2%)	57	63
4	D	206/206 (100%)	203 (98%)	3 (2%)	65	71
4	Q	206/206 (100%)	202 (98%)	4 (2%)	57	63
5	E	168/168 (100%)	167 (99%)	1 (1%)	86	90
5	R	168/168 (100%)	165 (98%)	3 (2%)	59	65
6	F	90/98 (92%)	89 (99%)	1 (1%)	73	79
6	S	90/98 (92%)	88 (98%)	2 (2%)	52	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	66/71 (93%)	64 (97%)	2 (3%)	41	44
7	T	66/71 (93%)	63 (96%)	3 (4%)	27	27
8	H	63/74 (85%)	61 (97%)	2 (3%)	39	41
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	35	36
9	V	28/60 (47%)	26 (93%)	2 (7%)	14	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%)	3280 (98%)	56 (2%)	60	67

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	20	ASP
1	N	348	SER
7	T	45	ILE
1	N	32	GLN
1	N	184	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	73	ASN
1	N	136	GLN
4	Q	35	GLN
1	N	9	GLN
1	N	32	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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
12	PO4	T	4016	-	4,4,4	1.39	1 (25%)	6,6,6	5.79	5 (83%)
12	PO4	A	2010	-	4,4,4	1.42	1 (25%)	6,6,6	5.79	5 (83%)
11	JZR	F	3012	-	18,18,18	1.89	5 (27%)	23,23,23	0.73	0
20	GOL	P	4009	-	5,5,5	1.08	0	5,5,5	0.53	0
15	PEE	C	2007	-	48,48,50	1.08	5 (10%)	51,53,55	0.85	4 (7%)
12	PO4	P	3010	-	4,4,4	1.33	1 (25%)	6,6,6	5.79	5 (83%)
22	FES	R	501	5	0,4,4	0.00	-	-	-	-
12	PO4	D	4011	-	4,4,4	1.33	1 (25%)	6,6,6	5.82	5 (83%)
20	GOL	E	4007	-	3,4,5	1.10	0	1,4,5	0.42	0
15	PEE	D	2006	-	50,50,50	1.24	5 (10%)	53,55,55	0.85	4 (7%)
15	PEE	P	3007	-	48,48,50	1.11	4 (8%)	51,53,55	0.85	4 (7%)
16	HEM	C	501	3	27,50,50	1.84	7 (25%)	17,82,82	1.73	5 (29%)
22	FES	E	501	5	0,4,4	0.00	-	-	-	-
20	GOL	C	4008	-	5,5,5	1.23	0	5,5,5	0.56	0
20	GOL	C	2008	-	5,5,5	1.28	0	5,5,5	0.67	0
15	PEE	B	4017	-	4,7,50	0.50	0	3,7,55	0.41	0
12	PO4	O	2009	-	4,4,4	1.37	0	6,6,6	5.78	5 (83%)
13	AZI	C	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
11	JZR	A	4004	-	18,18,18	1.36	4 (22%)	23,23,23	0.58	0
20	GOL	P	3008	-	5,5,5	1.23	0	5,5,5	0.53	0
19	CDL	C	2004	-	43,43,99	1.14	3 (6%)	49,55,111	1.23	4 (8%)
20	GOL	O	4005	-	5,5,5	1.29	0	5,5,5	0.63	0
11	JZR	C	2011	-	18,18,18	1.84	5 (27%)	23,23,23	0.70	0
12	PO4	I	4015	-	4,4,4	1.37	1 (25%)	6,6,6	5.82	5 (83%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	UQ	C	2002	-	18,18,63	2.45	9 (50%)	19,24,79	0.84	1 (5%)
11	JZR	S	2012	-	18,18,18	1.88	6 (33%)	23,23,23	0.70	0
17	SMA	C	2001	-	35,38,38	1.35	5 (14%)	46,52,52	1.82	8 (17%)
17	SMA	P	3001	-	35,38,38	1.41	5 (14%)	46,52,52	1.70	6 (13%)
12	PO4	B	3009	-	4,4,4	1.37	1 (25%)	6,6,6	5.80	5 (83%)
20	GOL	E	4006	-	5,5,5	1.31	0	5,5,5	0.64	0
15	PEE	Q	3006	-	50,50,50	1.22	6 (12%)	53,55,55	0.84	4 (7%)
16	HEM	P	502	3	27,50,50	1.69	6 (22%)	17,82,82	1.75	6 (35%)
19	CDL	P	3004	-	48,48,99	1.12	2 (4%)	54,60,111	1.11	3 (5%)
13	AZI	A	4002	-	0,2,2	0.00	-	0,1,1	0.00	-
16	HEM	P	501	3	27,50,50	1.74	6 (22%)	17,82,82	1.65	4 (23%)
12	PO4	D	4010	-	4,4,4	1.38	1 (25%)	6,6,6	5.80	5 (83%)
16	HEM	C	502	3	27,50,50	1.55	5 (18%)	17,82,82	1.78	6 (35%)
19	CDL	Q	3003	-	38,38,99	1.08	3 (7%)	43,47,111	1.04	3 (6%)
18	UQ	P	3002	-	18,18,63	2.26	9 (50%)	19,24,79	0.76	1 (5%)
19	CDL	D	2003	-	38,38,99	1.04	1 (2%)	43,47,111	1.08	3 (6%)
11	JZR	P	3011	-	18,18,18	1.84	5 (27%)	23,23,23	0.70	0
21	HEC	Q	501	4	26,50,50	1.80	6 (23%)	18,82,82	1.02	1 (5%)
21	HEC	D	501	4	26,50,50	1.98	5 (19%)	18,82,82	0.99	1 (5%)
12	PO4	R	4014	-	4,4,4	1.40	1 (25%)	6,6,6	5.80	5 (83%)
11	JZR	F	4003	-	18,18,18	1.85	5 (27%)	23,23,23	0.67	0
13	AZI	G	4001	-	0,2,2	0.00	-	0,1,1	0.00	-
13	AZI	P	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
12	PO4	R	4013	-	4,4,4	1.41	1 (25%)	6,6,6	5.80	5 (83%)
12	PO4	Q	4012	-	4,4,4	1.50	1 (25%)	6,6,6	5.80	5 (83%)

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
19	CDL	D	2003	-	-	21/43/43/110	-
20	GOL	P	4009	-	-	2/4/4/4	-
15	PEE	C	2007	-	-	21/52/52/54	-
22	FES	R	501	5	-	-	0/1/1/1
15	PEE	D	2006	-	-	23/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	P	3007	-	-	22/52/52/54	-
16	HEM	C	501	3	-	0/6/54/54	-
22	FES	E	501	5	-	-	0/1/1/1
20	GOL	C	4008	-	-	0/4/4/4	-
20	GOL	C	2008	-	-	2/4/4/4	-
15	PEE	B	4017	-	-	1/3/5/54	-
11	JZR	A	4004	-	-	1/9/29/29	0/1/1/1
20	GOL	P	3008	-	-	0/4/4/4	-
19	CDL	C	2004	-	-	30/52/52/110	-
20	GOL	O	4005	-	-	3/4/4/4	-
11	JZR	C	2011	-	-	4/9/29/29	0/1/1/1
20	GOL	E	4007	-	-	2/2/2/4	-
18	UQ	C	2002	-	-	1/9/33/87	0/1/1/1
11	JZR	S	2012	-	-	5/9/29/29	0/1/1/1
17	SMA	C	2001	-	-	1/33/34/34	0/2/2/2
17	SMA	P	3001	-	-	3/33/34/34	0/2/2/2
15	PEE	Q	3006	-	-	23/54/54/54	-
16	HEM	P	502	3	-	0/6/54/54	-
19	CDL	P	3004	-	-	27/57/57/110	-
16	HEM	P	501	3	-	0/6/54/54	-
16	HEM	C	502	3	-	0/6/54/54	-
19	CDL	Q	3003	-	-	22/43/43/110	-
18	UQ	P	3002	-	-	3/9/33/87	0/1/1/1
11	JZR	F	3012	-	-	2/9/29/29	0/1/1/1
11	JZR	P	3011	-	-	3/9/29/29	0/1/1/1
21	HEC	Q	501	4	-	0/6/54/54	-
21	HEC	D	501	4	-	0/6/54/54	-
11	JZR	F	4003	-	-	4/9/29/29	0/1/1/1
20	GOL	E	4006	-	-	4/4/4/4	-

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3B-C2B	-6.39	1.34	1.40
21	Q	501	HEC	C3B-C2B	-5.19	1.35	1.40
21	D	501	HEC	C3C-C2C	-4.98	1.35	1.40
11	S	2012	JZR	O1-C1	4.81	1.48	1.40
11	F	3012	JZR	O1-C1	4.79	1.48	1.40



The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	2009	PO4	O4-P-O1	-8.18	80.98	110.89
12	R	4013	PO4	O4-P-O1	-8.15	81.06	110.89
12	I	4015	PO4	O4-P-O1	-8.12	81.16	110.89
12	D	4010	PO4	O4-P-O1	-8.12	81.18	110.89
12	T	4016	PO4	O4-P-O1	-8.10	81.25	110.89

There are no chirality outliers.

5 of 230 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	O4P-C4-C5-N
15	D	2006	PEE	C1-O3P-P-O2P
15	D	2006	PEE	C4-O4P-P-O2P
19	C	2004	CDL	CA3-OA5-PA1-OA3
19	C	2004	CDL	CA3-OA5-PA1-OA4

There are no ring outliers.

23 monomers are involved in 58 short contacts:

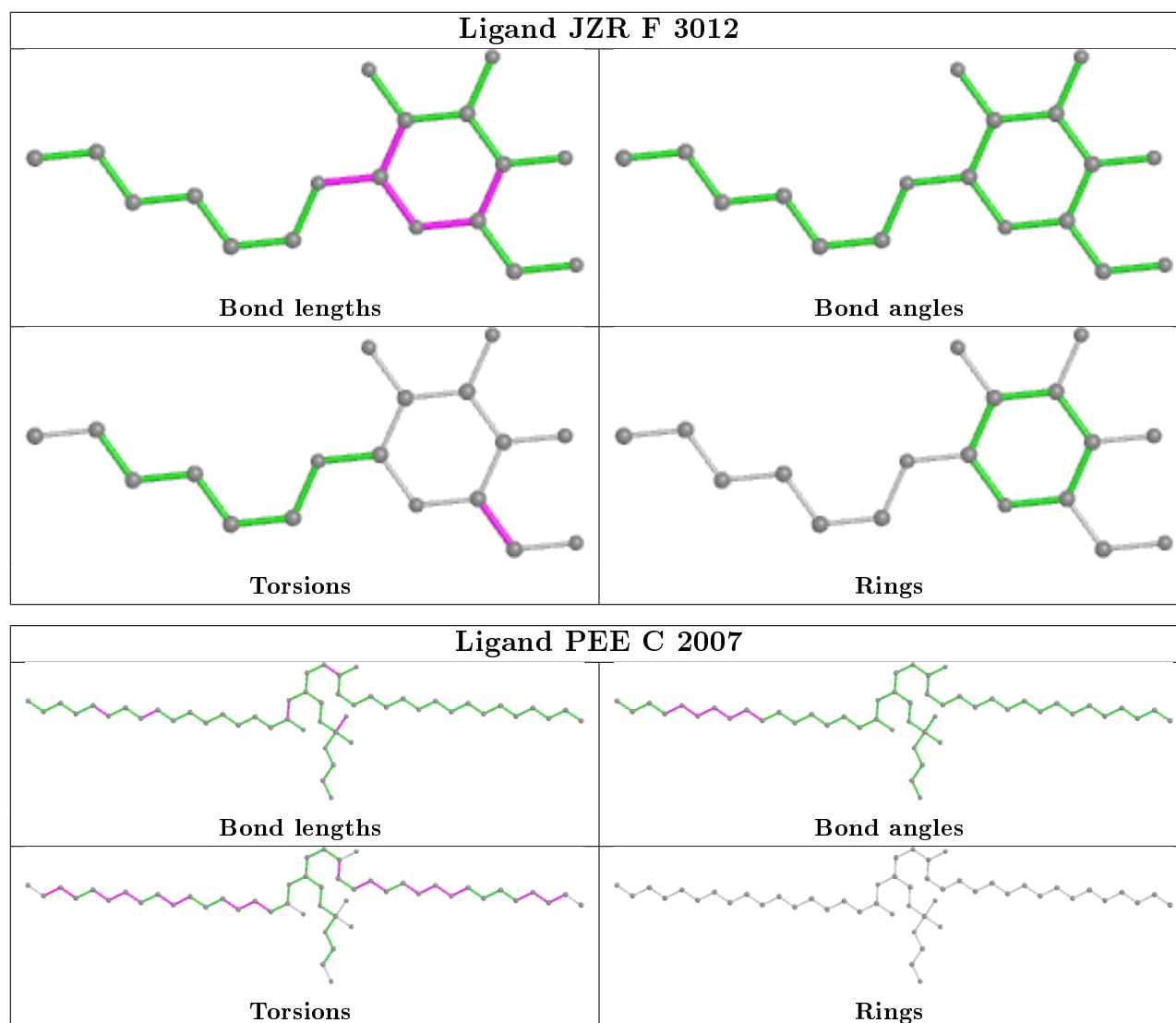
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	3012	JZR	3	0
20	P	4009	GOL	2	0
15	D	2006	PEE	2	0
15	P	3007	PEE	3	0
16	C	501	HEM	1	0
15	B	4017	PEE	1	0
11	A	4004	JZR	1	0
12	I	4015	PO4	1	0
18	C	2002	UQ	4	0
11	S	2012	JZR	6	0
17	C	2001	SMA	3	0
17	P	3001	SMA	3	0
15	Q	3006	PEE	5	0
16	P	502	HEM	2	0
16	P	501	HEM	1	0
16	C	502	HEM	4	0
18	P	3002	UQ	5	0
19	D	2003	CDL	1	0
21	Q	501	HEC	5	0
21	D	501	HEC	4	0
11	F	4003	JZR	1	0

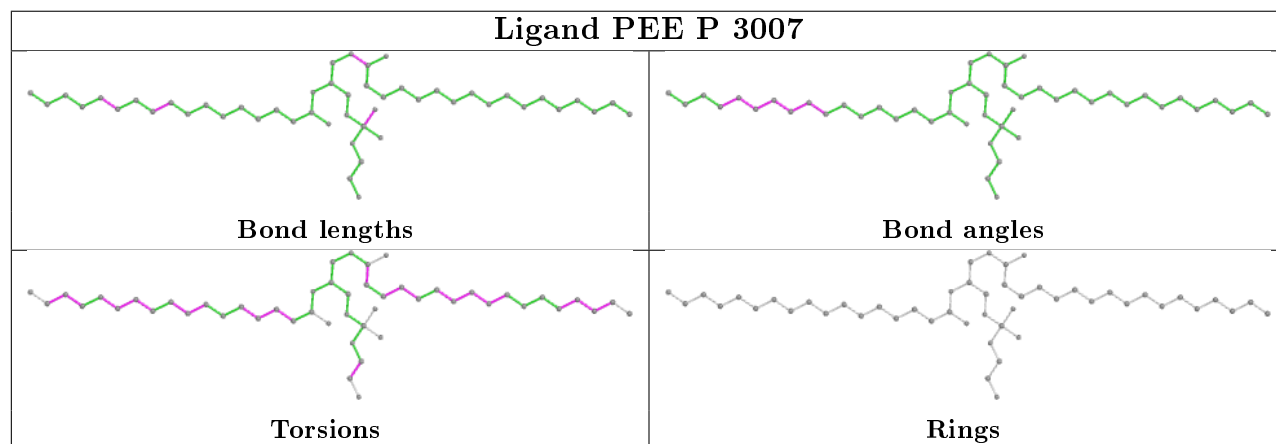
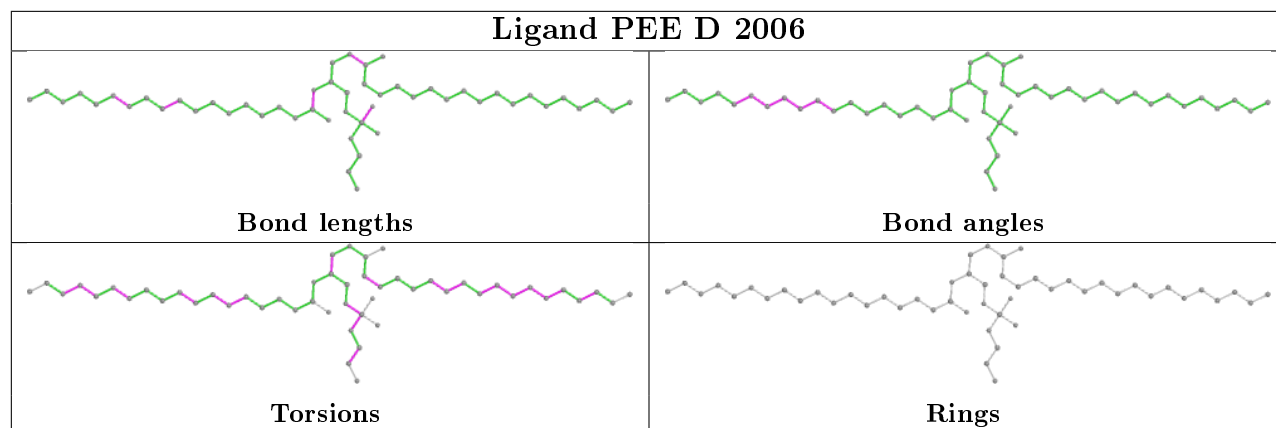
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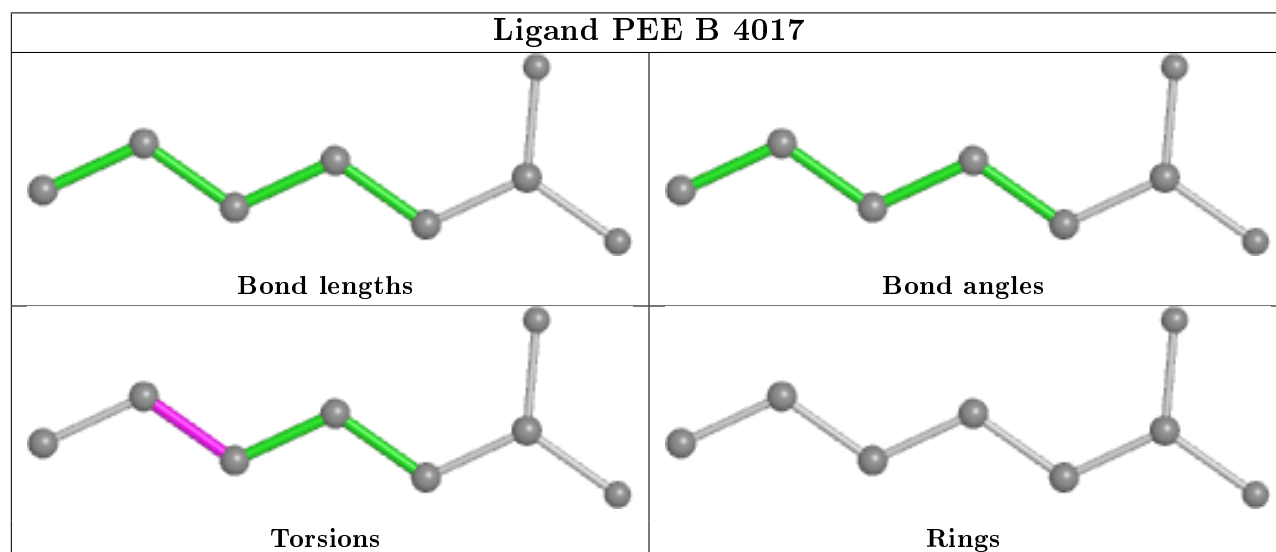
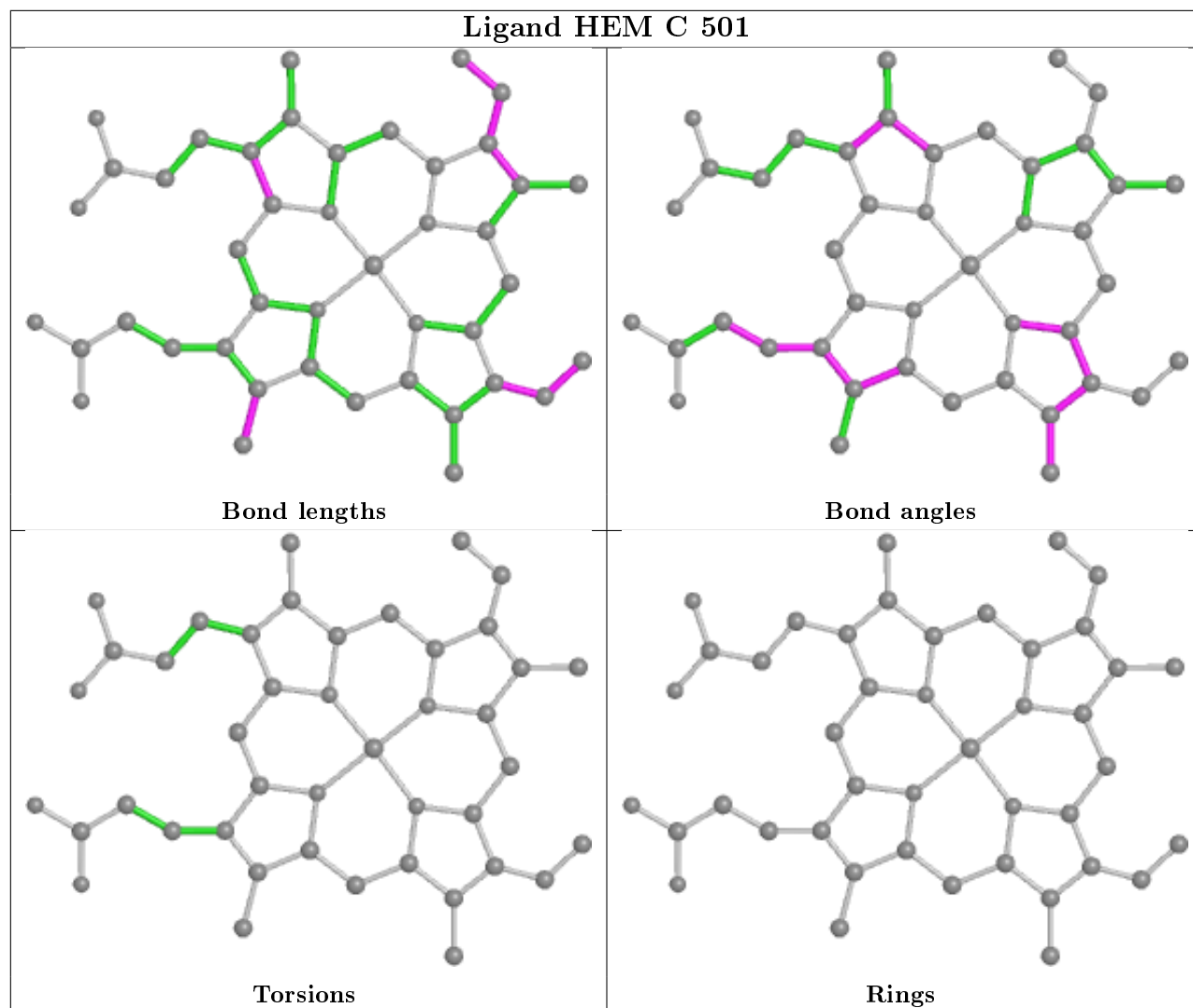
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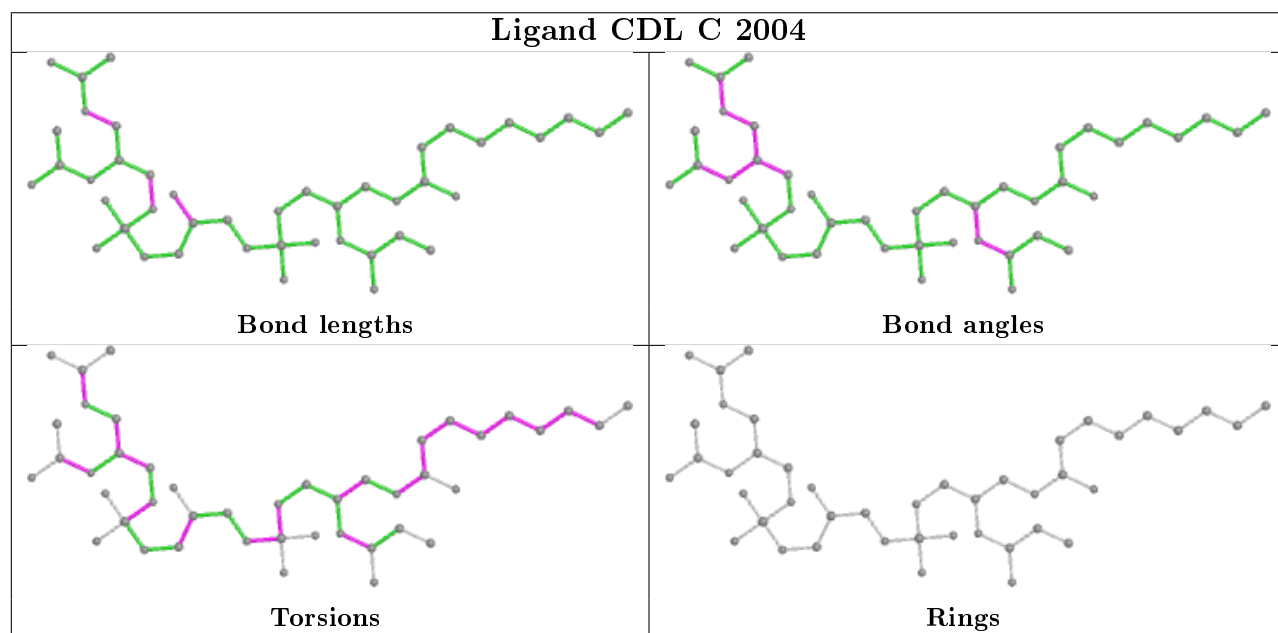
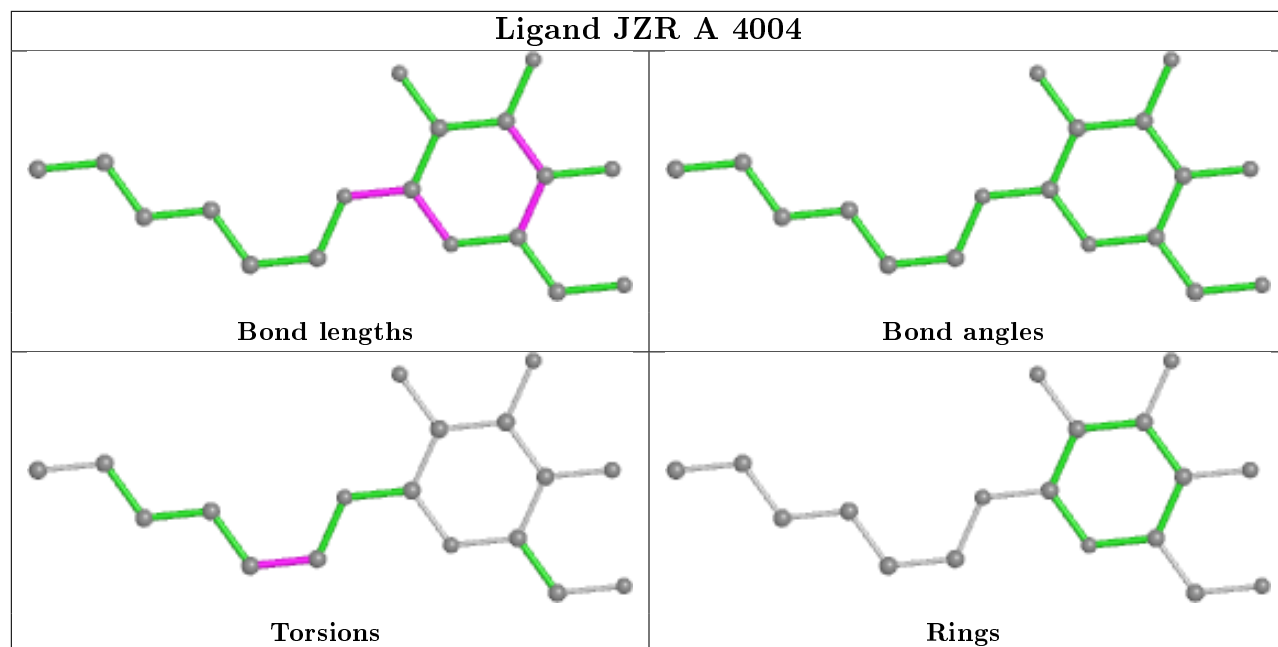
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	4001	AZI	1	0
12	Q	4012	PO4	1	0

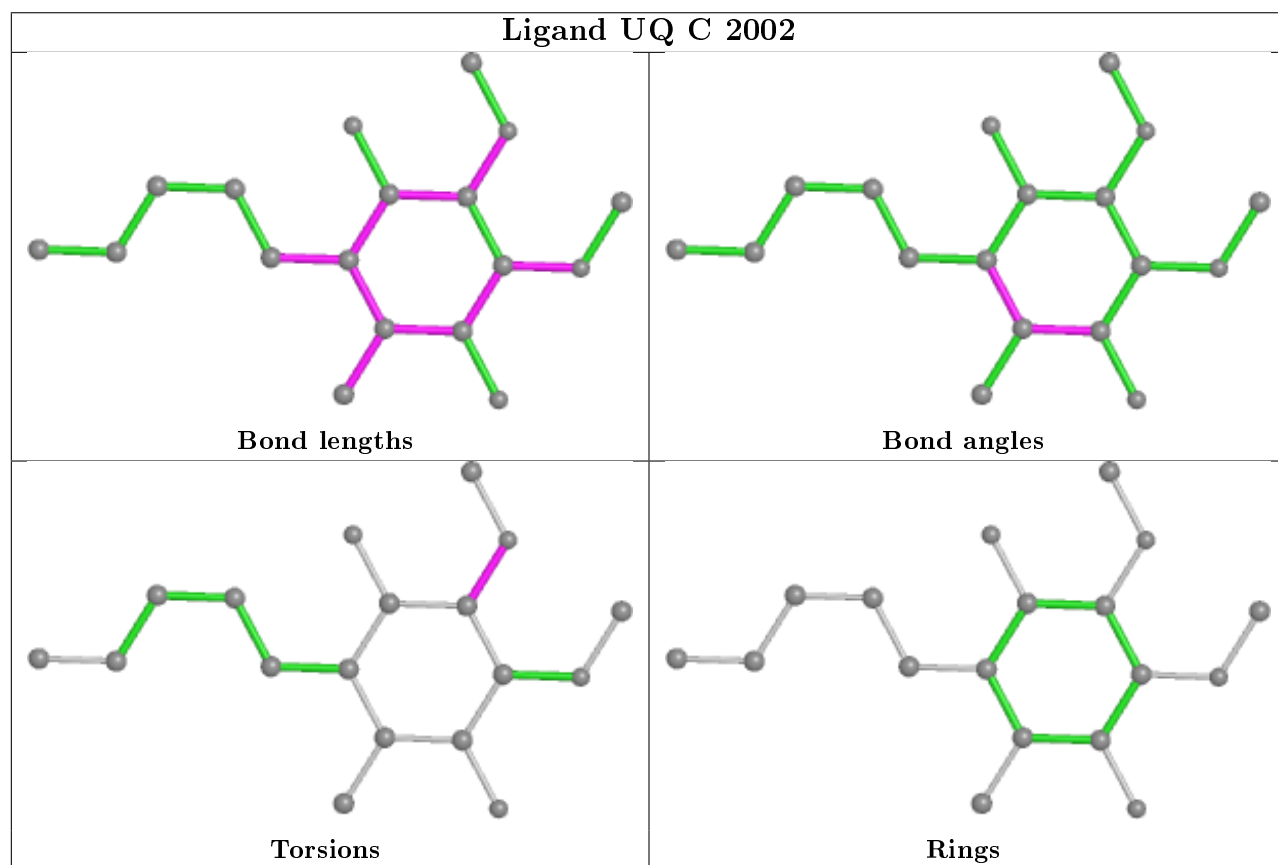
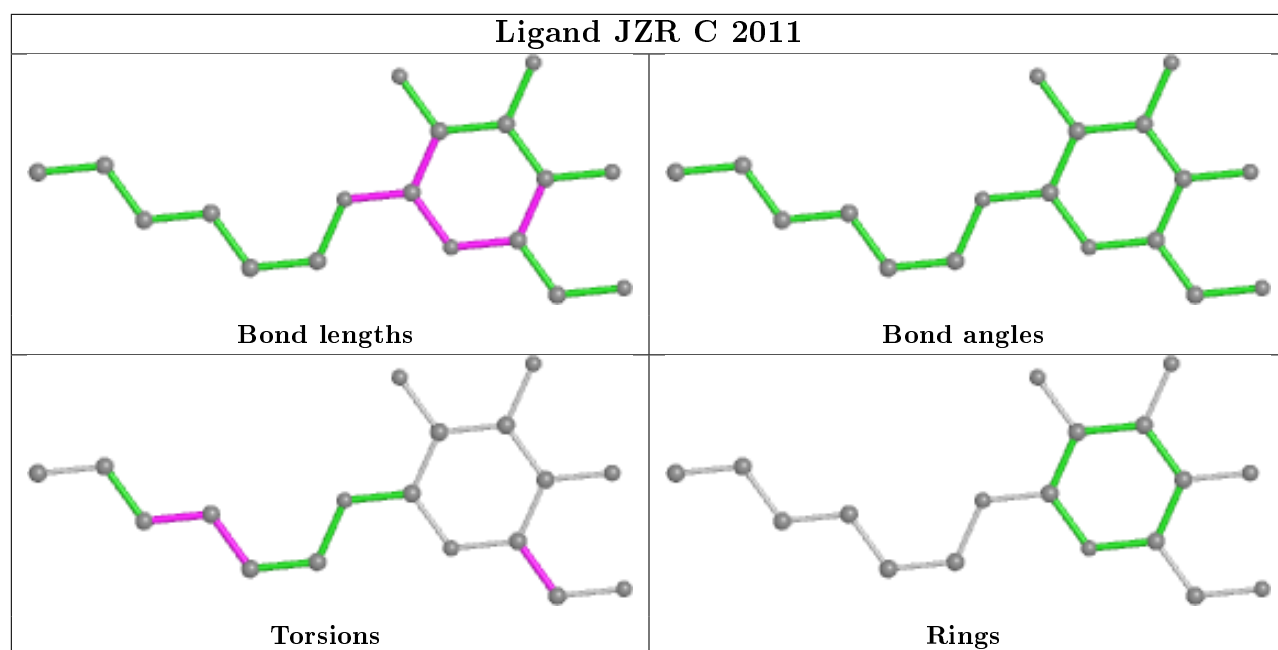
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

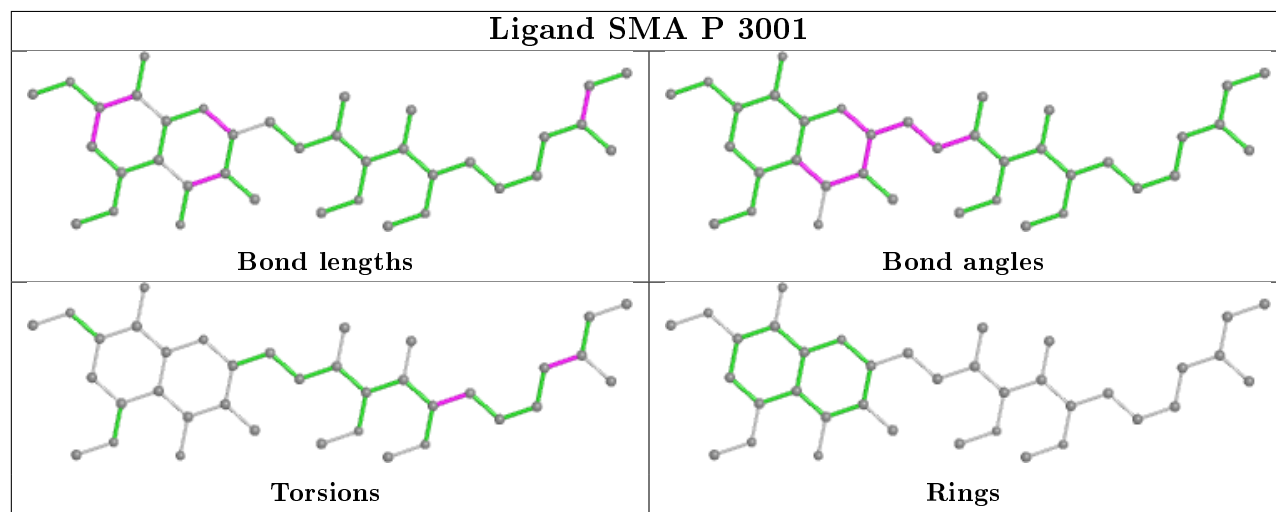
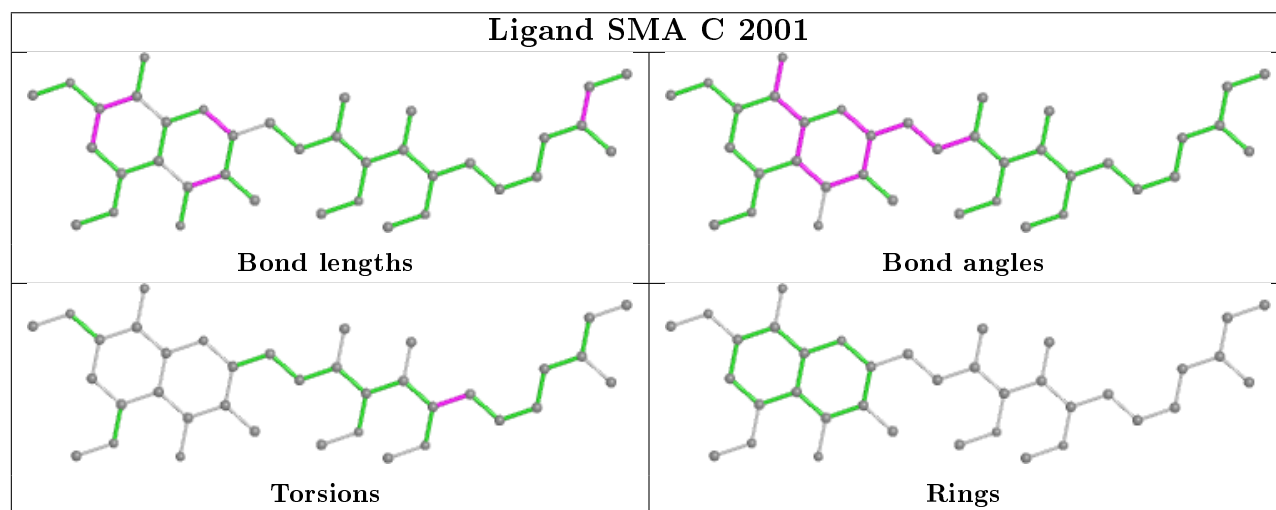
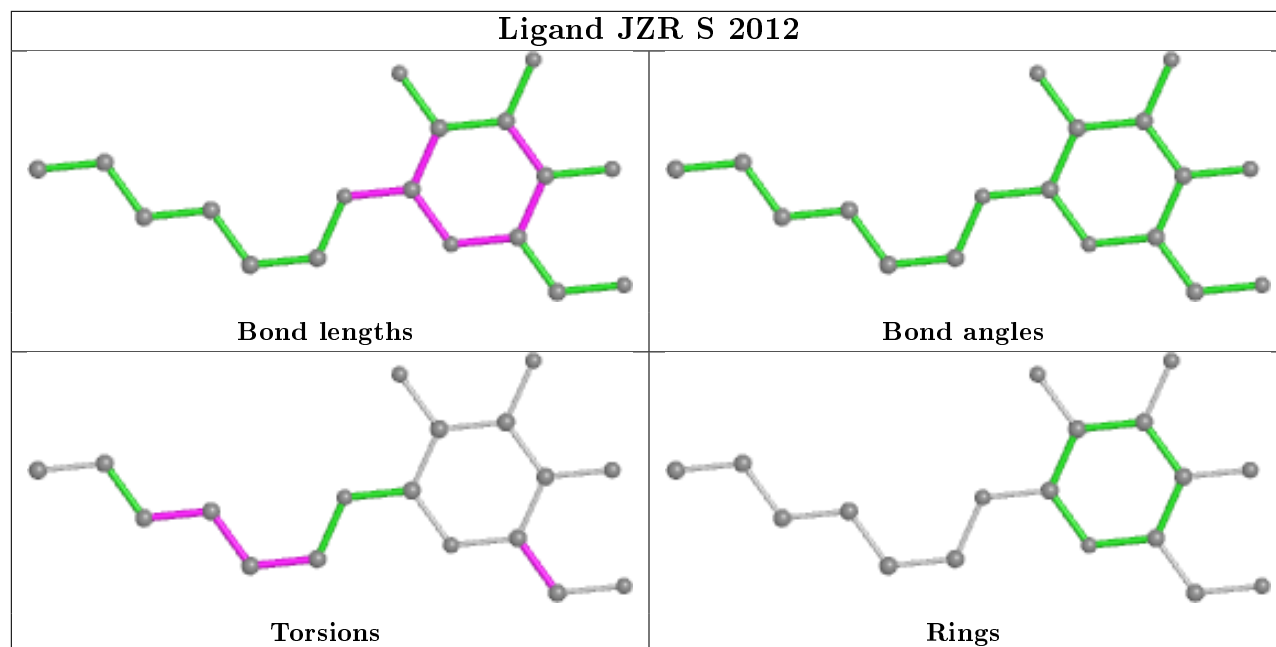


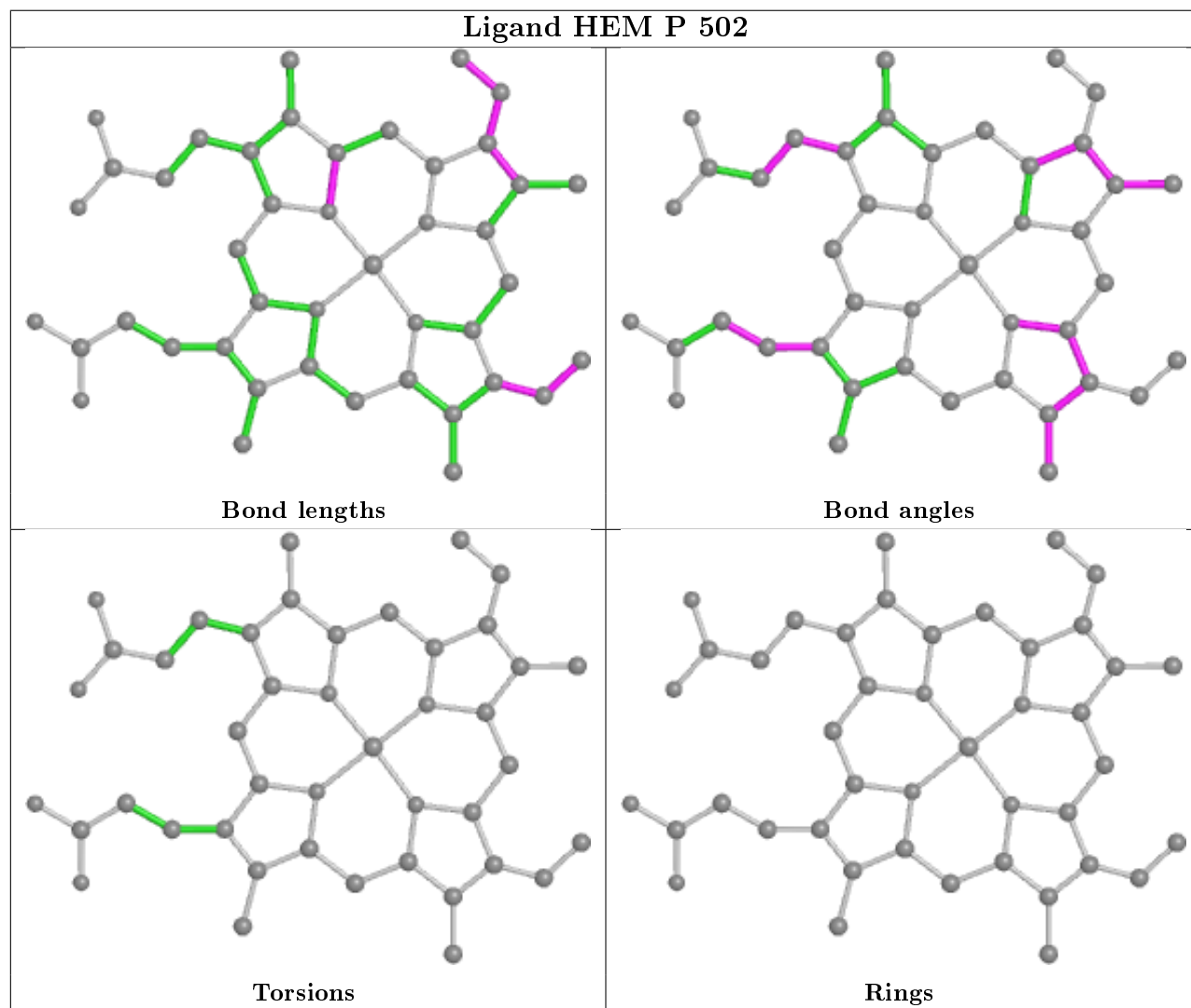
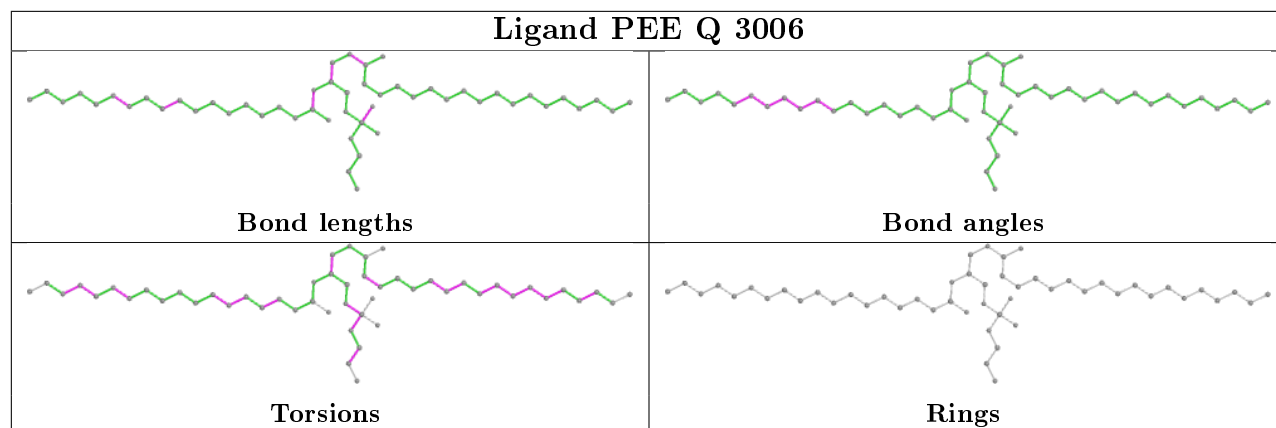






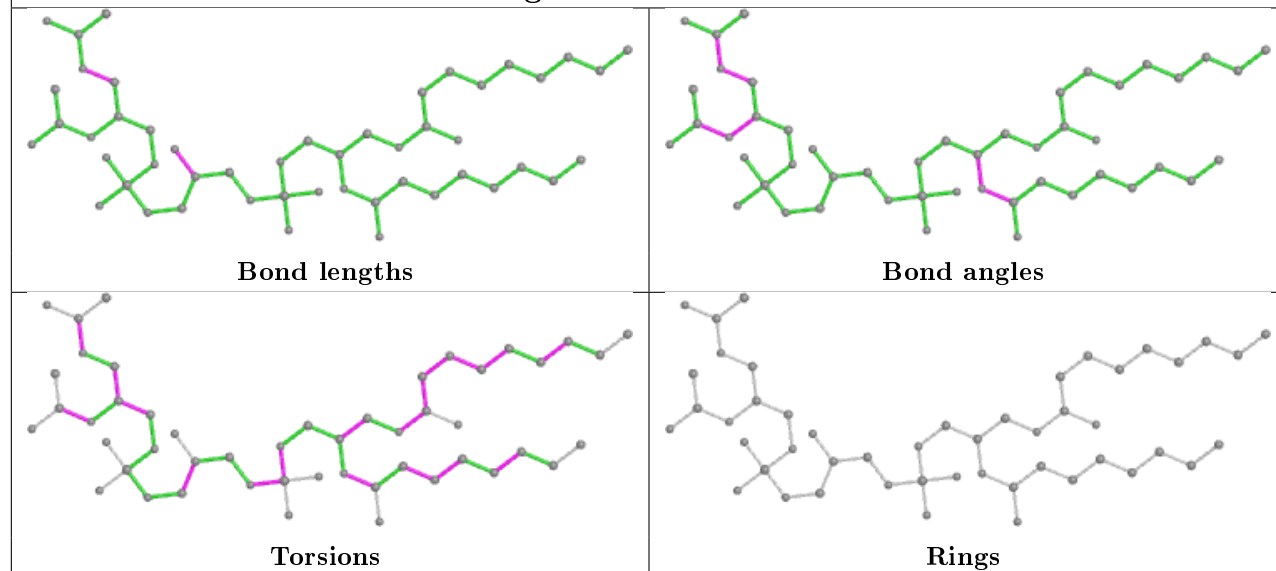




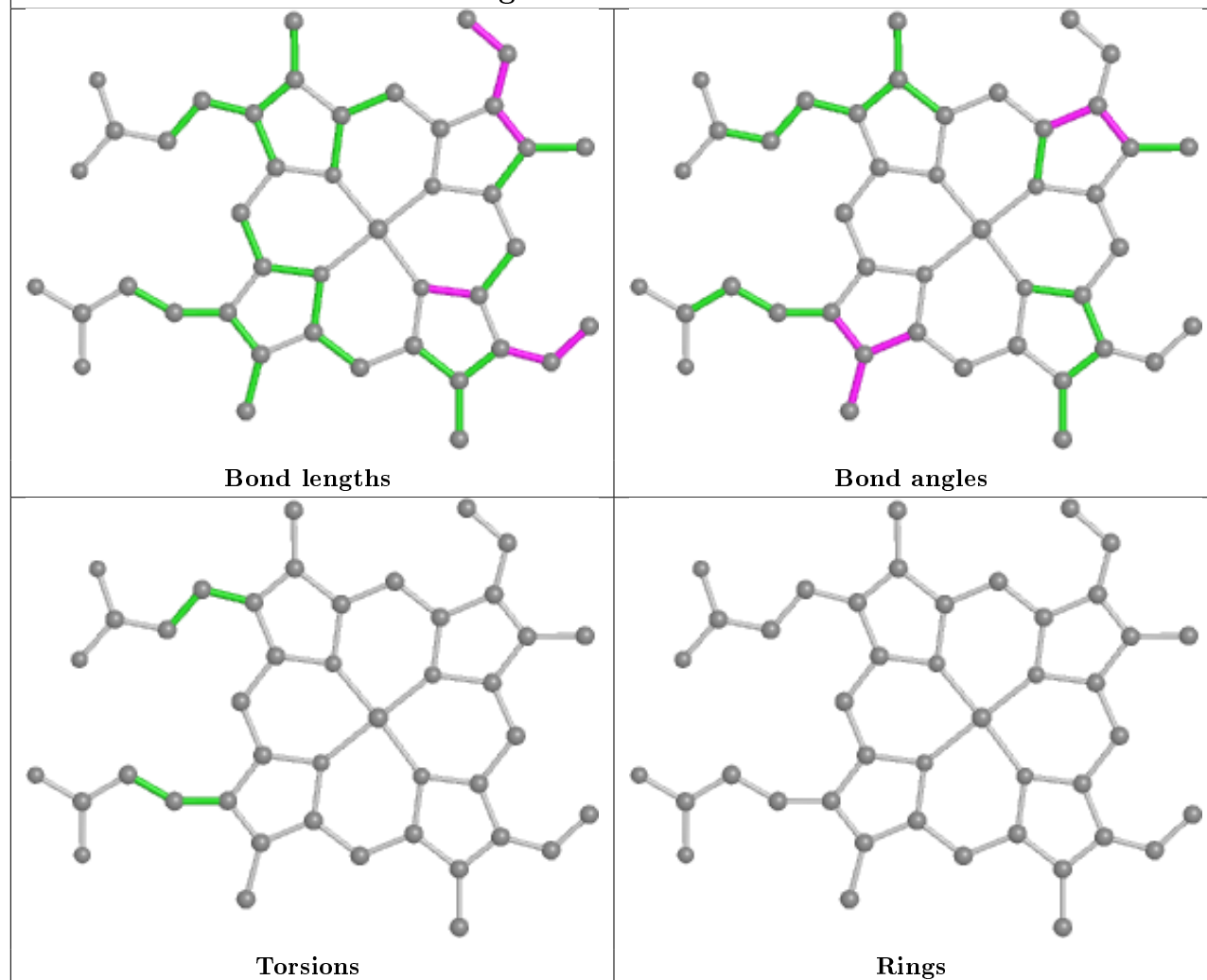


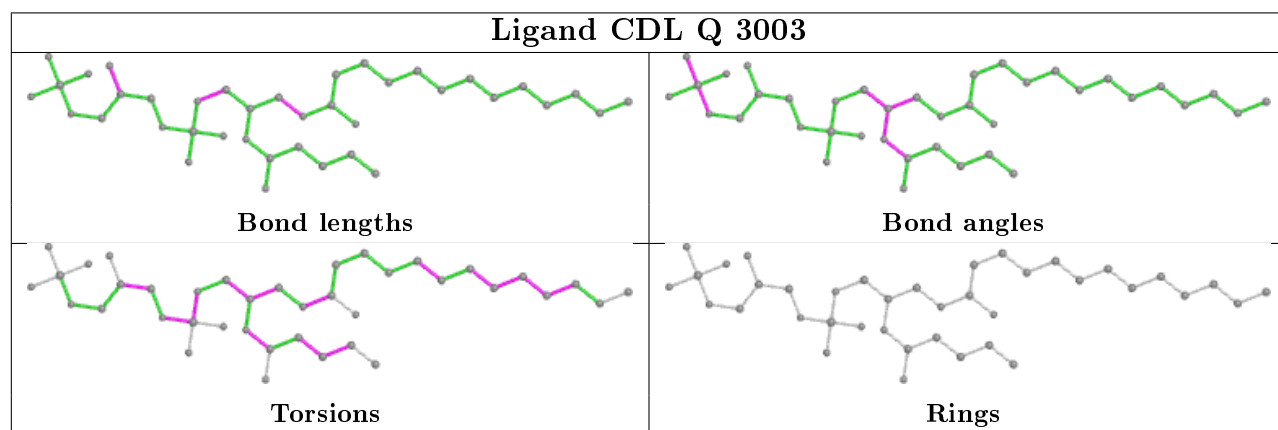
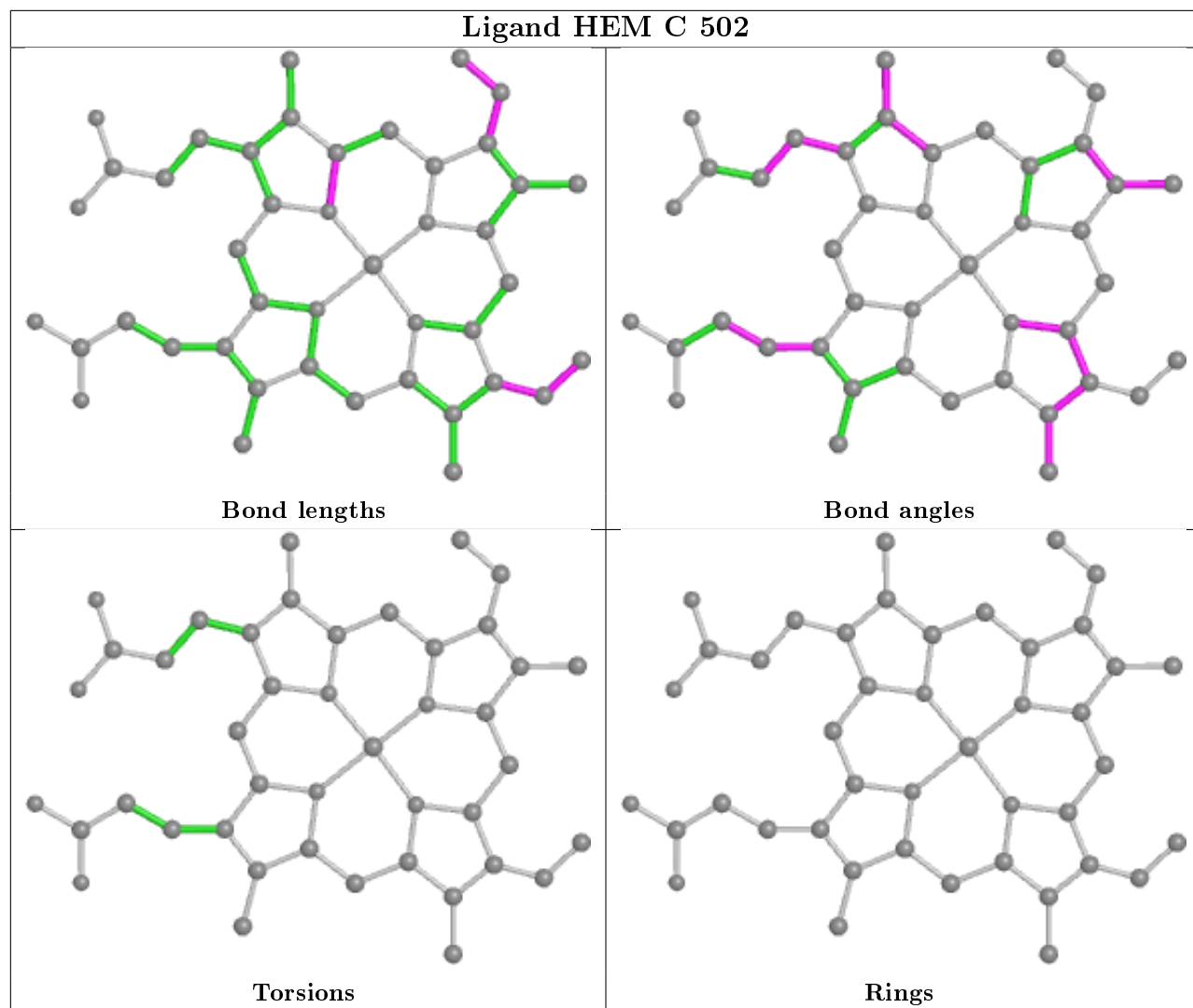


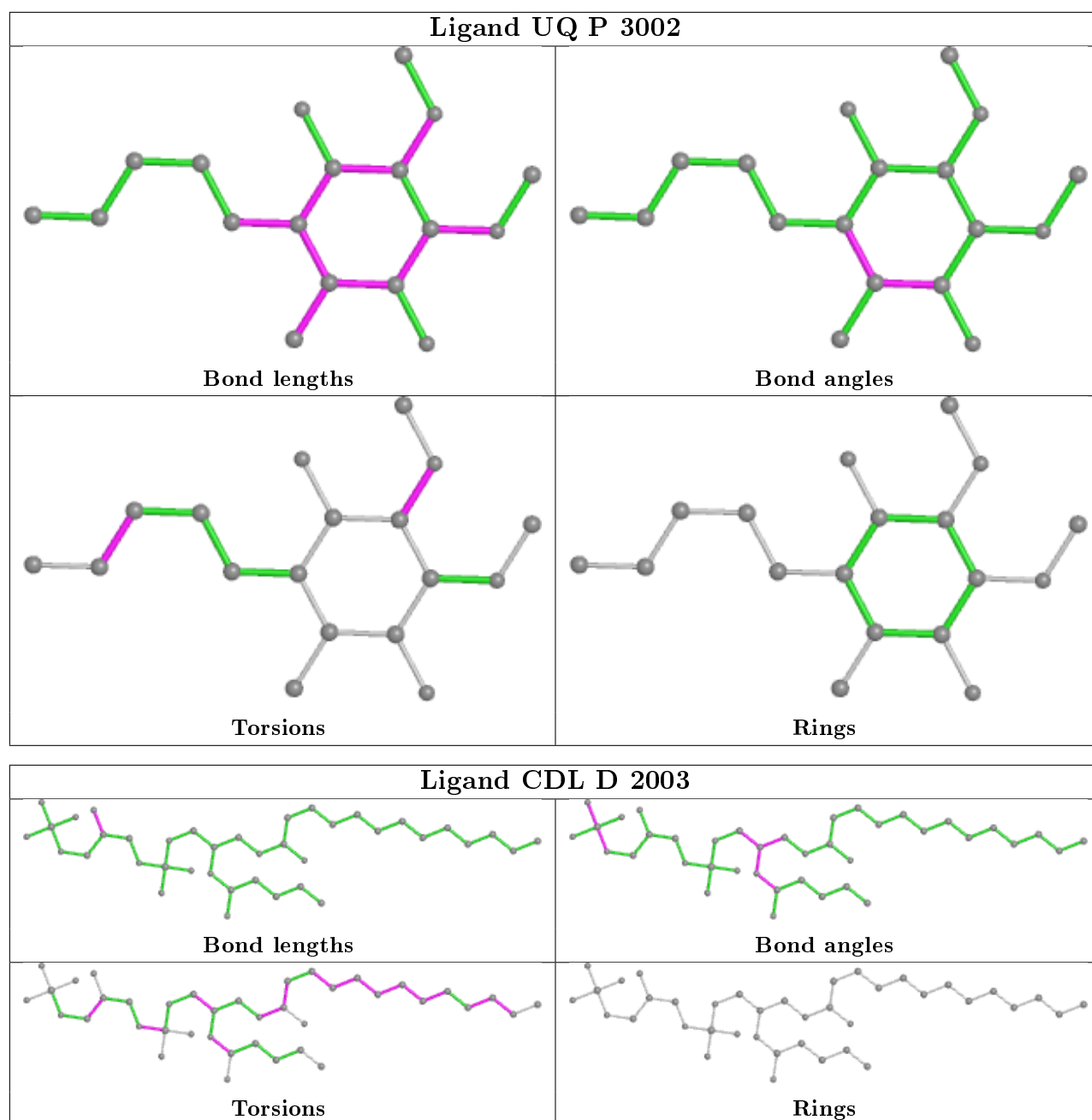
## Ligand CDL P 3004

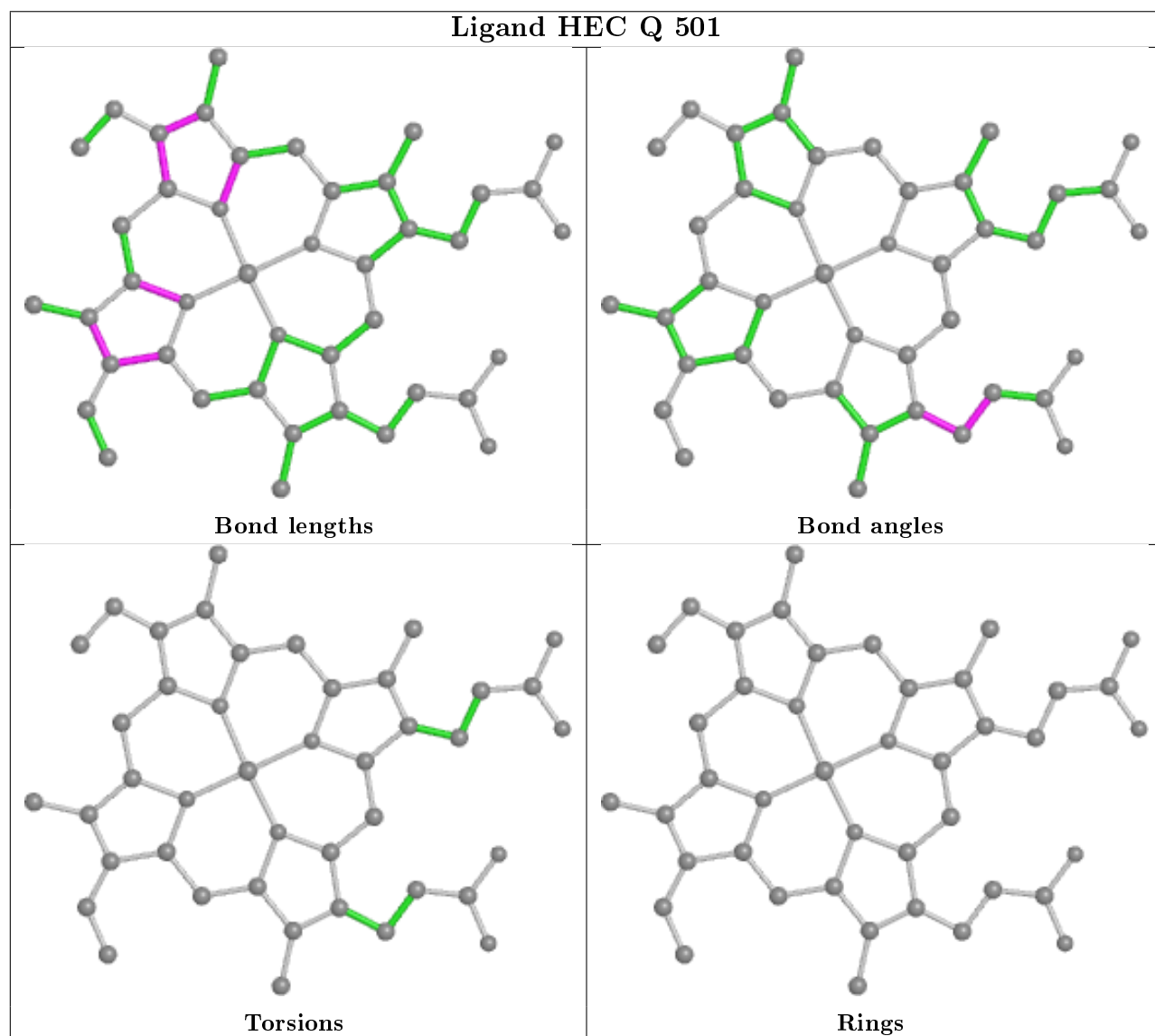
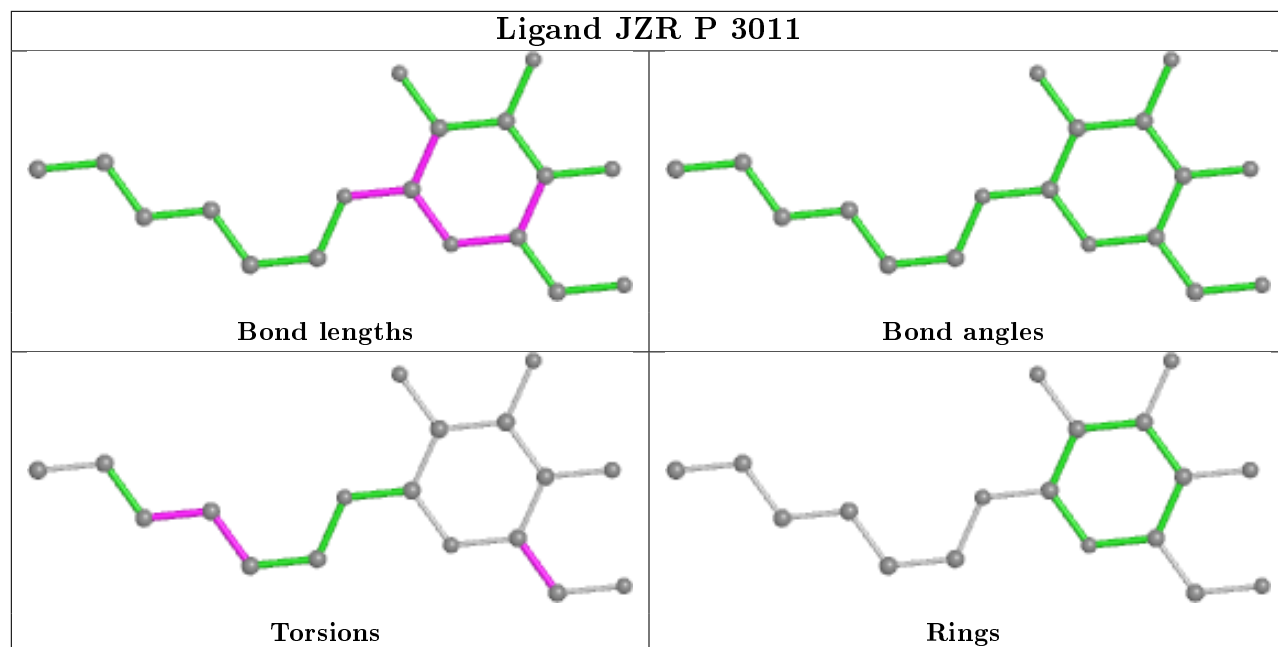


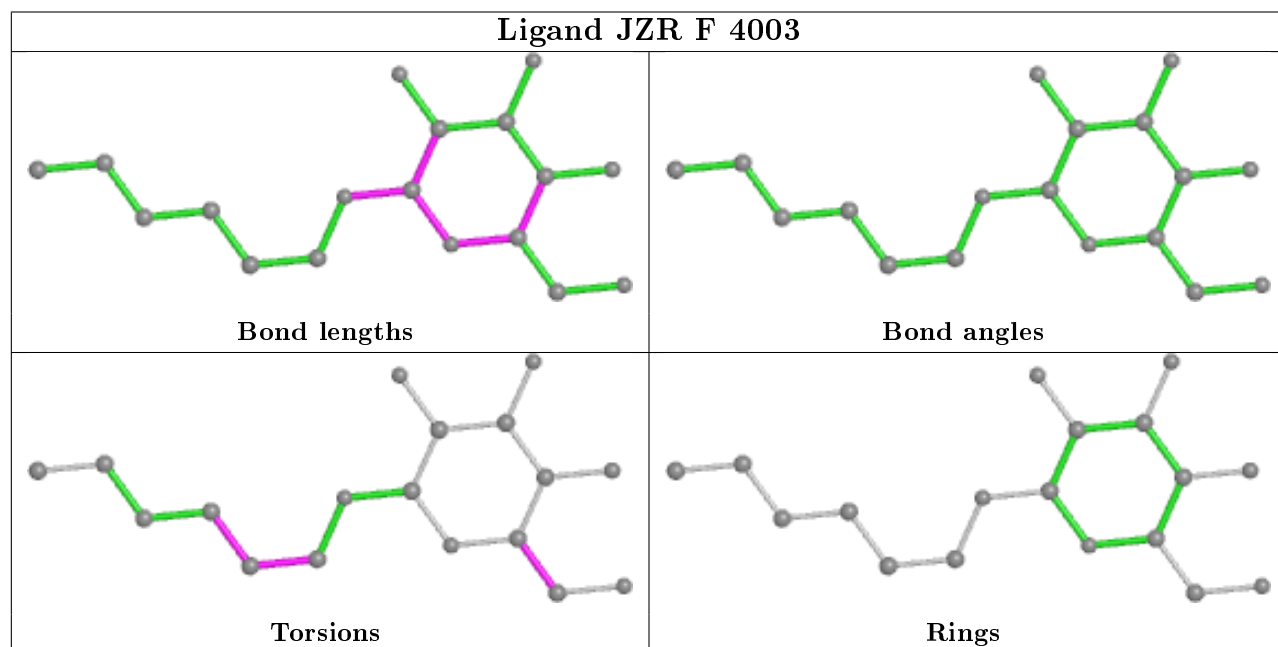
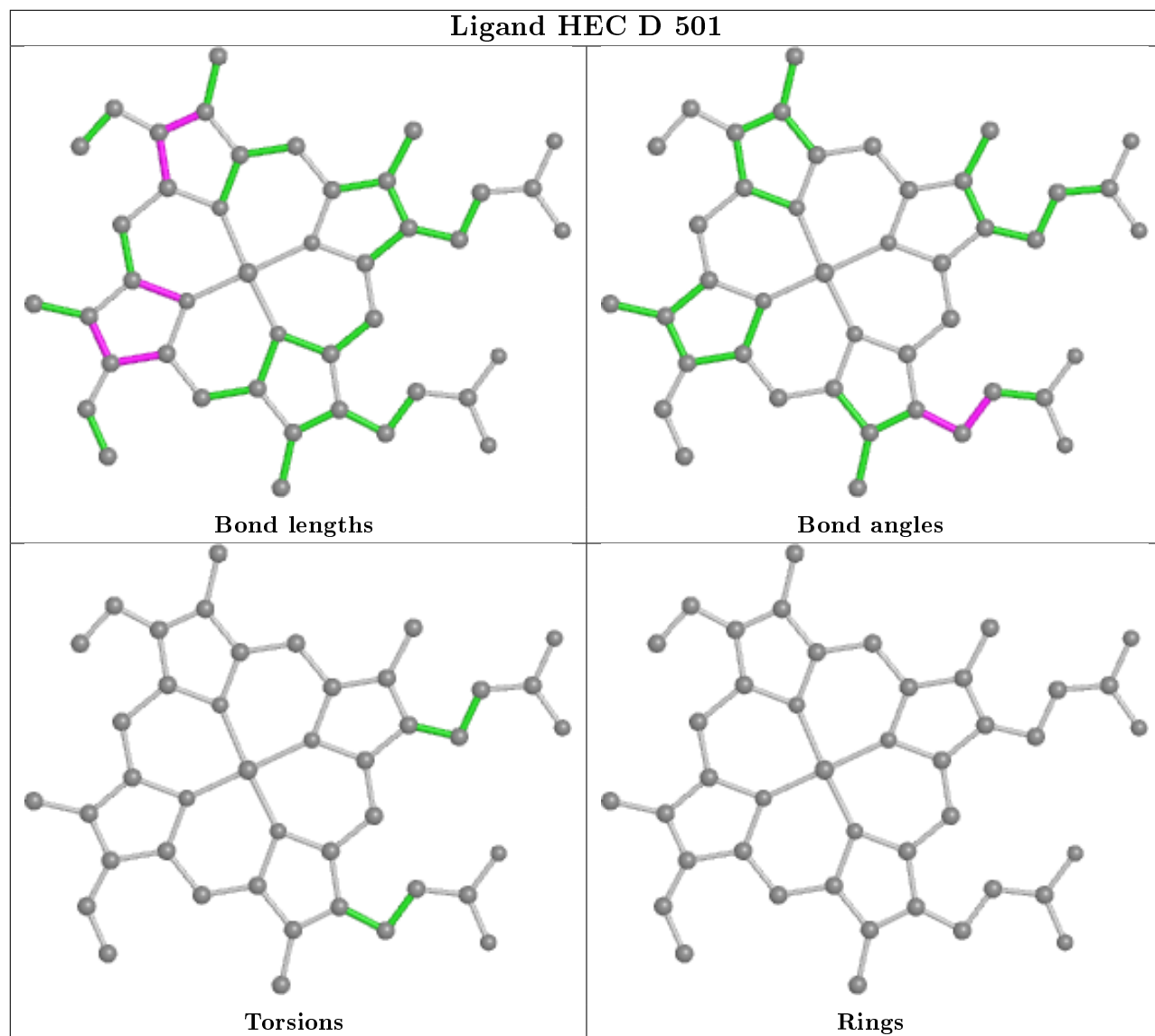
## Ligand HEM P 501











## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/446 (99%)	0.08	14 (3%) 47 54	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.48	29 (6%) 18 23	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.19	15 (3%) 44 50	28, 41, 66, 102	0
2	O	424/439 (96%)	0.48	40 (9%) 8 11	31, 48, 87, 185	0
3	C	365/379 (96%)	0.35	20 (5%) 25 31	24, 34, 48, 108	0
3	P	370/379 (97%)	0.46	24 (6%) 18 23	28, 37, 52, 218	0
4	D	241/241 (100%)	0.42	15 (6%) 20 25	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.58	24 (9%) 7 9	31, 45, 67, 87	0
5	E	196/196 (100%)	1.09	43 (21%) 0 0	32, 57, 105, 117	0
5	R	196/196 (100%)	0.30	13 (6%) 18 23	27, 46, 71, 99	0
6	F	99/110 (90%)	0.38	9 (9%) 9 12	24, 39, 71, 83	0
6	S	99/110 (90%)	0.27	4 (4%) 38 44	28, 40, 67, 88	0
7	G	75/81 (92%)	0.91	12 (16%) 1 2	26, 49, 77, 86	0
7	T	76/81 (93%)	1.51	23 (30%) 0 0	32, 55, 98, 114	0
8	H	66/78 (84%)	1.08	15 (22%) 0 0	40, 56, 73, 78	0
8	U	66/78 (84%)	1.16	17 (25%) 0 0	44, 63, 94, 104	0
9	I	42/78 (53%)	2.19	21 (50%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.05	18 (42%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.81	3 (10%) 7 9	40, 52, 80, 109	0
10	W	62/62 (100%)	2.06	19 (30%) 0 0	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.52	378 (9%) 8 10	24, 43, 80, 218	2 (0%)

The worst 5 of 378 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	22.1
10	W	1	VAL	21.3
10	W	62	LYS	12.6
2	O	12	GLU	10.6
10	W	2	ALA	10.6

## 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 monosaccharides 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, 95<sup>th</sup> 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	JZR	F	3012	18/18	0.17	0.72	159,162,164,164	0
14	UNL	U	4056	1/-	0.24	1.01	101,101,101,101	0
20	GOL	O	4005	6/6	0.25	0.74	166,167,167,168	0
14	UNL	P	4060	1/-	0.32	0.34	88,88,88,88	0
11	JZR	S	2012	18/18	0.38	0.46	89,103,106,107	0
11	JZR	F	4003	18/18	0.39	0.66	176,180,181,181	0
14	UNL	I	4072	1/-	0.39	2.21	93,93,93,93	0
14	UNL	D	4036	1/-	0.44	0.35	83,83,83,83	0
14	UNL	B	4034	1/-	0.47	0.70	87,87,87,87	0
14	UNL	S	4047	1/-	0.52	0.38	71,71,71,71	0
14	UNL	C	4068	1/-	0.55	0.58	72,72,72,72	0
11	JZR	P	3011	18/18	0.56	0.40	99,107,109,109	0
20	GOL	E	4007	5/6	0.58	0.50	97,100,101,102	0
14	UNL	P	4040	1/-	0.58	0.30	73,73,73,73	0
14	UNL	V	4024	1/-	0.59	1.07	96,96,96,96	0
14	UNL	E	4061	1/-	0.60	0.19	79,79,79,79	0
11	JZR	C	2011	18/18	0.60	0.47	106,118,123,125	0
14	UNL	B	4080	1/-	0.60	0.68	67,67,67,67	0
14	UNL	O	4020	2/-	0.61	0.23	96,96,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	PO4	A	2010	5/5	0.61	0.23	133,133,134,134	0
14	UNL	G	4070	1/-	0.63	0.26	67,67,67,67	0
14	UNL	Q	4044	1/-	0.63	1.63	88,88,88,88	0
14	UNL	U	4049	1/-	0.64	0.69	77,77,77,77	0
14	UNL	B	4025	1/-	0.64	1.82	93,93,93,93	0
14	UNL	N	4022	1/-	0.64	0.51	81,81,81,81	0
18	UQ	C	2002	18/63	0.65	0.30	61,73,76,76	0
12	PO4	D	4010	5/5	0.65	0.30	169,169,170,170	0
14	UNL	O	4071	1/-	0.67	0.86	70,70,70,70	0
15	PEE	B	4017	8/51	0.67	0.42	85,88,91,92	0
14	UNL	V	4088	1/-	0.68	0.92	80,80,80,80	0
14	UNL	A	4076	1/-	0.69	0.44	68,68,68,68	0
14	UNL	A	4081	1/-	0.71	0.47	71,71,71,71	0
13	AZI	A	4002	3/3	0.71	0.49	48,48,58,65	0
14	UNL	D	4054	1/-	0.72	0.27	76,76,76,76	0
14	UNL	N	4029	1/-	0.72	1.40	94,94,94,94	0
14	UNL	O	4037	1/-	0.73	0.82	62,62,62,62	0
14	UNL	A	4038	1/-	0.73	0.60	85,85,85,85	0
14	UNL	B	4026	1/-	0.73	1.33	92,92,92,92	0
14	UNL	D	4027	1/-	0.74	0.29	87,87,87,87	0
14	UNL	R	4055	1/-	0.74	0.13	73,73,73,73	0
12	PO4	R	4014	5/5	0.75	0.43	173,174,174,174	0
14	UNL	D	4059	1/-	0.75	0.90	57,57,57,57	0
14	UNL	A	4091	1/-	0.75	0.75	72,72,72,72	0
14	UNL	A	4048	1/-	0.75	0.38	72,72,72,72	0
14	UNL	D	4083	1/-	0.76	0.55	82,82,82,82	0
14	UNL	B	4057	1/-	0.77	0.85	57,57,57,57	0
14	UNL	N	4019	2/-	0.77	0.31	76,76,76,76	0
15	PEE	D	2006	51/51	0.77	0.32	85,98,115,118	0
18	UQ	P	3002	18/63	0.78	0.24	60,82,85,86	0
13	AZI	P	3005	3/3	0.78	0.35	54,54,59,63	0
12	PO4	R	4013	5/5	0.78	0.25	114,114,116,116	0
14	UNL	G	4053	1/-	0.79	0.23	77,77,77,77	0
14	UNL	P	4074	1/-	0.79	0.17	59,59,59,59	0
14	UNL	C	4045	1/-	0.79	0.41	71,71,71,71	0
12	PO4	D	4011	5/5	0.79	0.31	130,130,130,131	0
14	UNL	N	4073	1/-	0.79	0.17	69,69,69,69	0
14	UNL	B	4042	1/-	0.80	0.42	81,81,81,81	0
13	AZI	C	2005	3/3	0.80	0.35	41,41,55,60	0
14	UNL	A	4035	1/-	0.80	0.99	69,69,69,69	0
14	UNL	B	4079	1/-	0.80	0.44	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	UNL	P	4021	2/-	0.80	0.18	71,71,71,73	0
14	UNL	O	4031	1/-	0.81	0.46	86,86,86,86	0
14	UNL	O	4082	1/-	0.81	0.14	73,73,73,73	0
14	UNL	B	4030	1/-	0.82	0.44	70,70,70,70	0
12	PO4	P	3010	5/5	0.83	0.18	115,115,115,116	0
14	UNL	C	4023	1/-	0.83	0.52	55,55,55,55	0
20	GOL	E	4006	6/6	0.83	0.25	67,71,72,75	0
14	UNL	F	4028	1/-	0.84	0.58	82,82,82,82	0
12	PO4	I	4015	5/5	0.84	0.31	122,122,123,123	0
14	UNL	B	4051	1/-	0.84	0.22	78,78,78,78	0
14	UNL	O	4043	1/-	0.84	0.29	80,80,80,80	0
14	UNL	P	4058	1/-	0.84	0.34	61,61,61,61	0
14	UNL	A	4032	1/-	0.84	0.71	65,65,65,65	0
14	UNL	O	4084	1/-	0.84	0.68	67,67,67,67	0
14	UNL	D	4067	1/-	0.84	0.58	58,58,58,58	0
14	UNL	T	4065	1/-	0.84	0.73	66,66,66,66	0
14	UNL	V	4078	1/-	0.85	1.63	94,94,94,94	0
14	UNL	D	4062	1/-	0.85	0.27	90,90,90,90	0
14	UNL	B	4052	1/-	0.85	0.17	60,60,60,60	0
14	UNL	W	4077	1/-	0.86	0.14	60,60,60,60	0
19	CDL	D	2003	39/100	0.86	0.20	64,84,106,107	0
14	UNL	A	4087	1/-	0.86	0.33	60,60,60,60	0
14	UNL	O	4041	1/-	0.87	0.36	71,71,71,71	0
14	UNL	B	4039	1/-	0.87	0.31	73,73,73,73	0
14	UNL	I	4033	1/-	0.87	0.87	69,69,69,69	0
12	PO4	Q	4012	5/5	0.87	0.18	108,109,110,110	0
14	UNL	A	4085	1/-	0.88	0.18	56,56,56,56	0
14	UNL	T	4066	1/-	0.88	0.07	70,70,70,70	0
14	UNL	G	4064	1/-	0.88	0.52	56,56,56,56	0
19	CDL	Q	3003	39/100	0.88	0.23	54,90,96,96	0
20	GOL	C	2008	6/6	0.88	0.31	60,63,63,70	0
12	PO4	B	3009	5/5	0.89	0.17	97,99,100,101	0
14	UNL	E	4050	1/-	0.89	0.38	65,65,65,65	0
20	GOL	P	3008	6/6	0.89	0.50	83,84,85,88	0
14	UNL	C	4018	2/-	0.90	0.35	74,74,74,76	0
19	CDL	P	3004	49/100	0.90	0.26	54,81,117,120	0
15	PEE	Q	3006	51/51	0.91	0.20	53,65,110,110	0
14	UNL	P	4089	1/-	0.91	0.47	63,63,63,63	0
19	CDL	C	2004	44/100	0.91	0.21	54,83,104,106	0
14	UNL	P	4046	1/-	0.91	0.48	65,65,65,65	0
15	PEE	P	3007	49/51	0.92	0.23	35,58,75,76	0
13	AZI	G	4001	3/3	0.92	0.15	47,47,57,59	0

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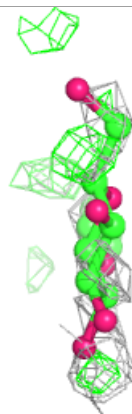
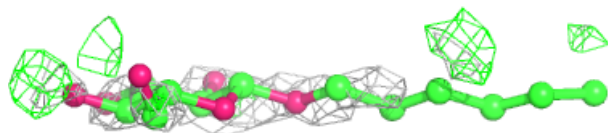
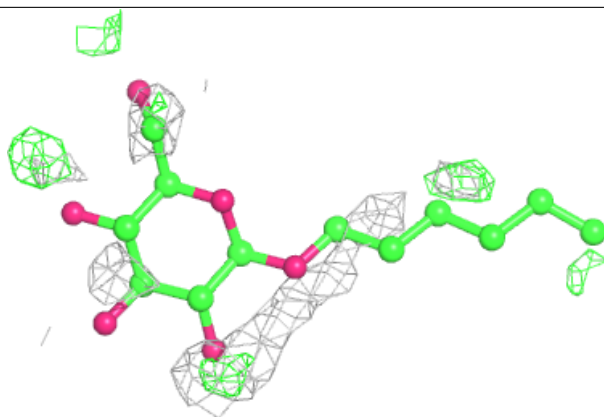
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	UNL	V	4090	1/-	0.92	0.98	74,74,74,74	0
15	PEE	C	2007	49/51	0.93	0.23	33,58,74,74	0
12	PO4	T	4016	5/5	0.93	0.09	107,108,108,108	0
14	UNL	R	4069	1/-	0.93	0.41	62,62,62,62	0
14	UNL	C	4086	1/-	0.93	0.24	50,50,50,50	0
14	UNL	A	4075	1/-	0.94	0.90	64,64,64,64	0
17	SMA	P	3001	37/37	0.95	0.16	30,39,47,52	0
20	GOL	P	4009	6/6	0.95	0.23	67,70,71,72	0
20	GOL	C	4008	6/6	0.95	0.20	53,55,60,60	0
17	SMA	C	2001	37/37	0.96	0.16	25,33,44,46	0
11	JZR	A	4004	18/18	0.96	0.13	29,36,42,44	0
14	UNL	C	4063	1/-	0.96	1.03	74,74,74,74	0
21	HEC	D	501	43/43	0.97	0.13	26,33,37,38	0
12	PO4	O	2009	5/5	0.97	0.09	76,79,81,81	0
21	HEC	Q	501	43/43	0.98	0.11	29,36,41,45	0
16	HEM	C	502	43/43	0.98	0.16	23,26,33,36	0
16	HEM	C	501	43/43	0.98	0.12	21,27,34,38	0
16	HEM	P	501	43/43	0.98	0.14	22,26,33,40	0
22	FES	R	501	4/4	0.99	0.12	27,29,30,30	0
22	FES	E	501	4/4	0.99	0.13	38,39,40,40	0
16	HEM	P	502	43/43	0.99	0.11	23,27,37,39	0

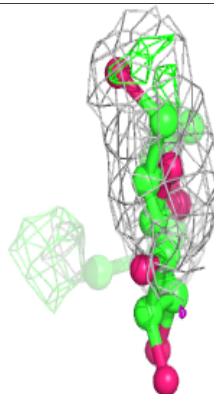
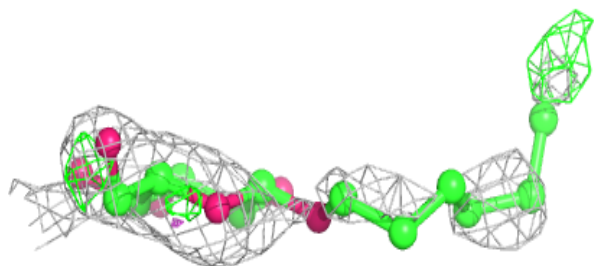
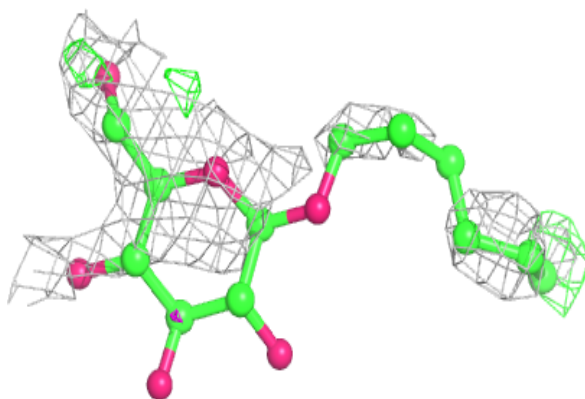
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around JZR F 3012:**

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

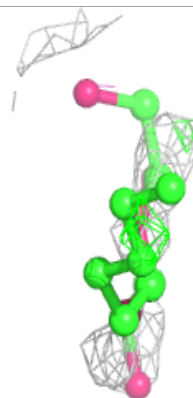
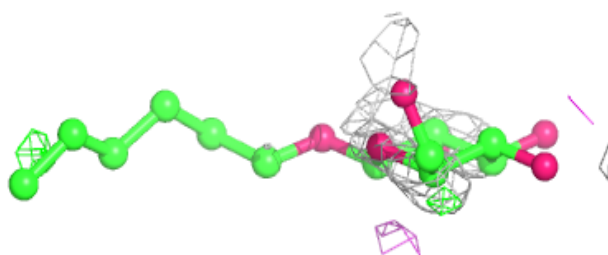
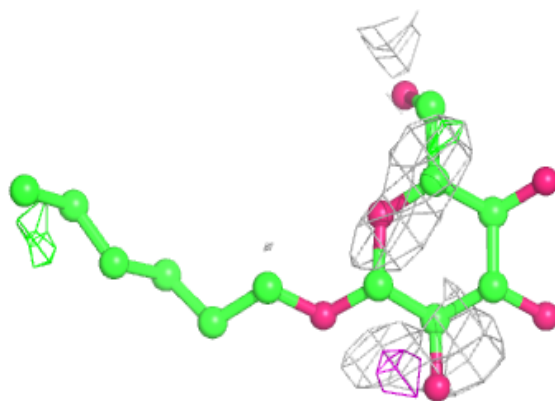
**Electron density around JZR S 2012:**

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

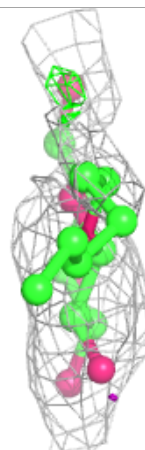
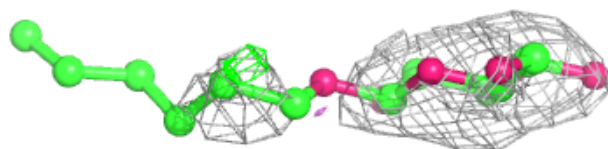
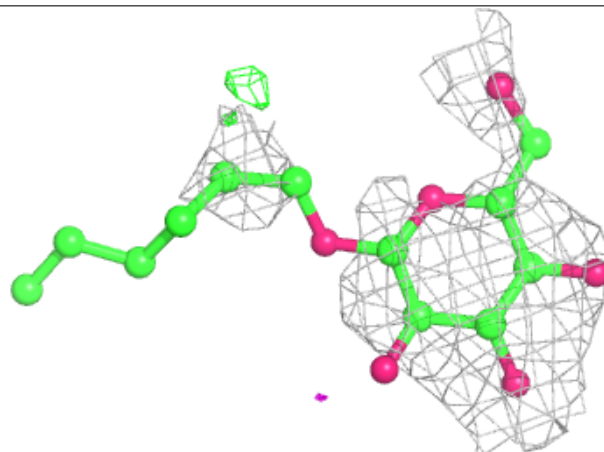


**Electron density around JZR F 4003:**

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

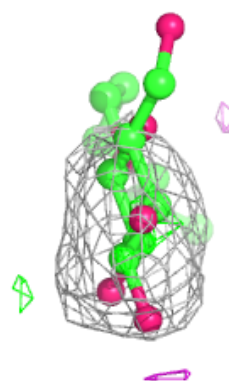
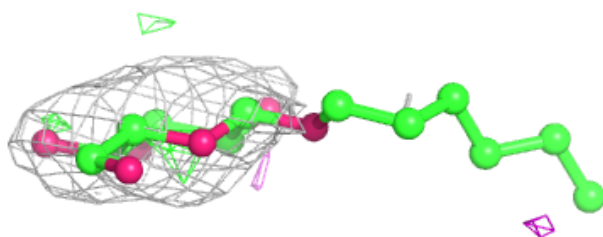
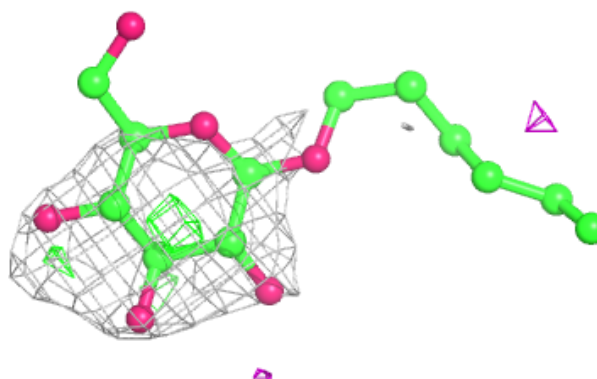
**Electron density around JZR P 3011:**

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

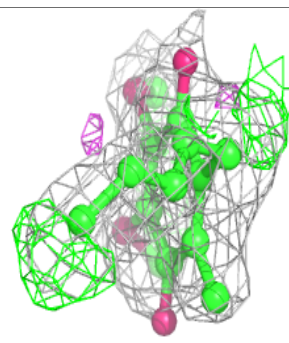
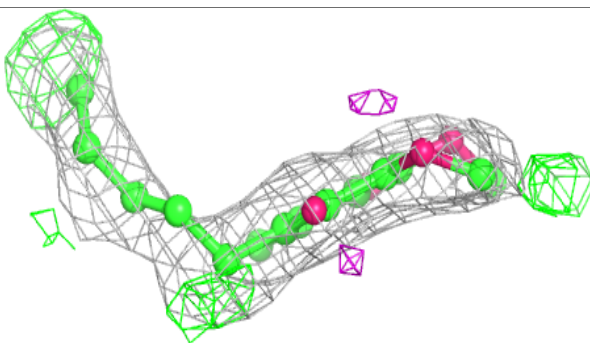
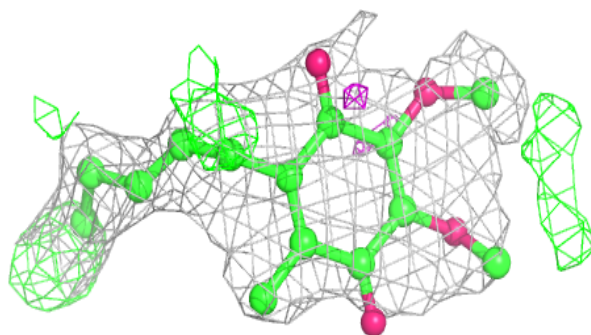


**Electron density around JZR C 2011:**

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

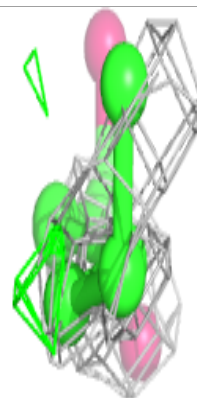
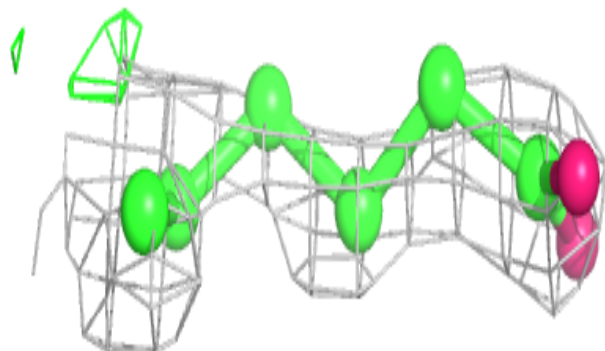
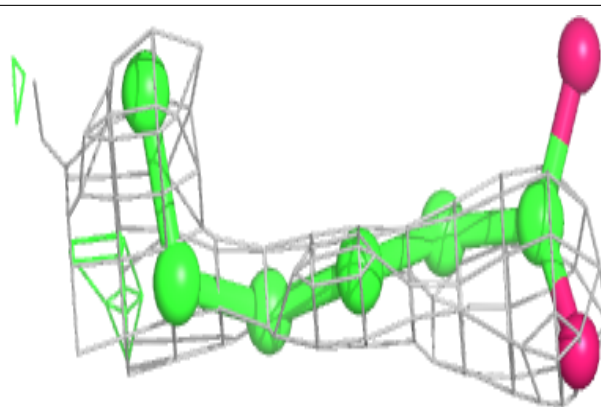
**Electron density around UQ C 2002:**

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

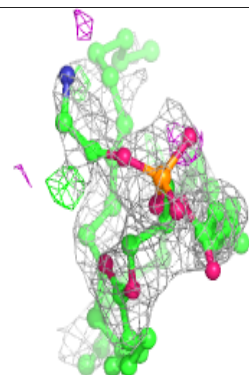
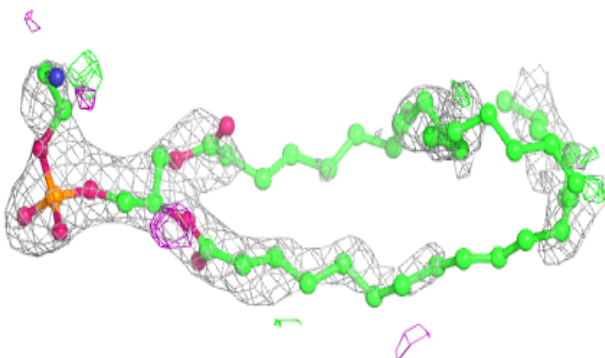
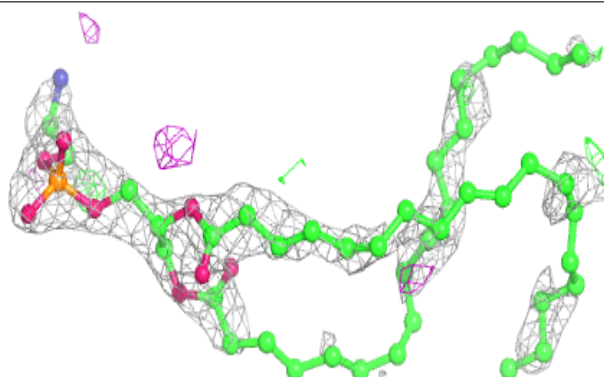


**Electron density around PEE B 4017:**

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

**Electron density around PEE D 2006:**

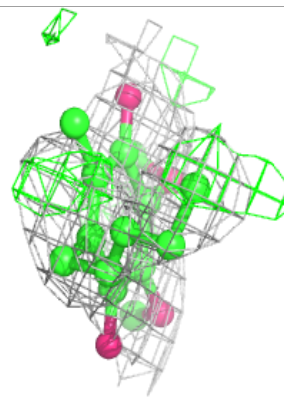
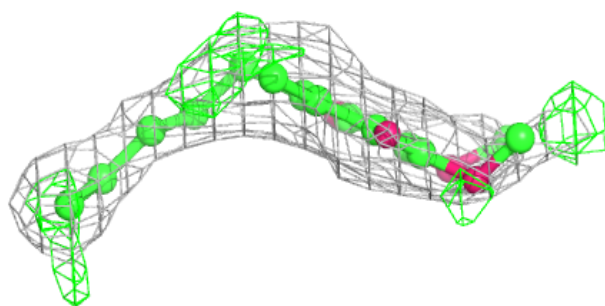
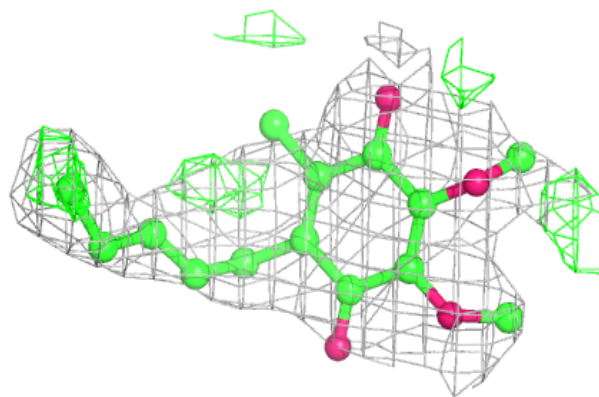
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



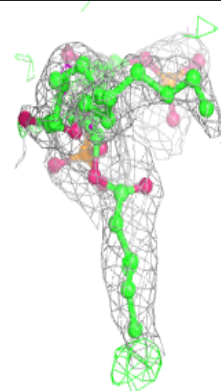
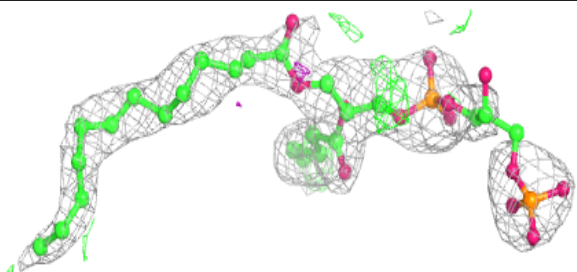
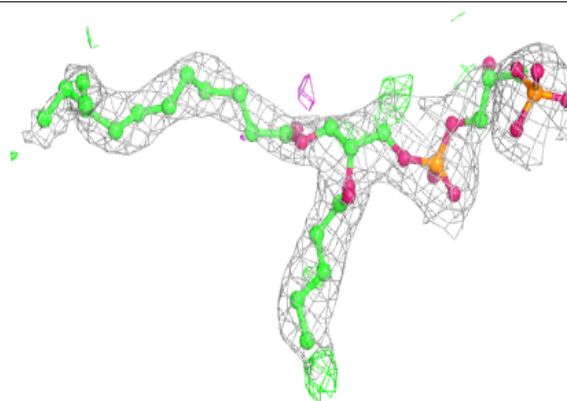


**Electron density around UQ P 3002:**

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

**Electron density around CDL D 2003:**

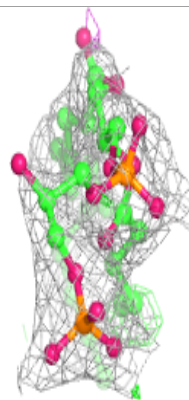
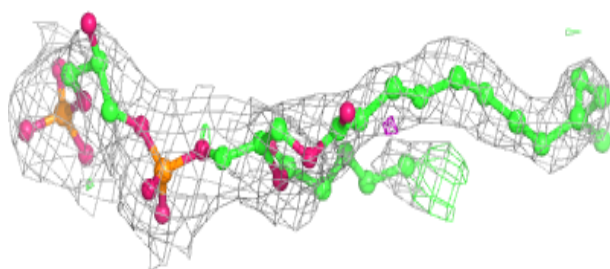
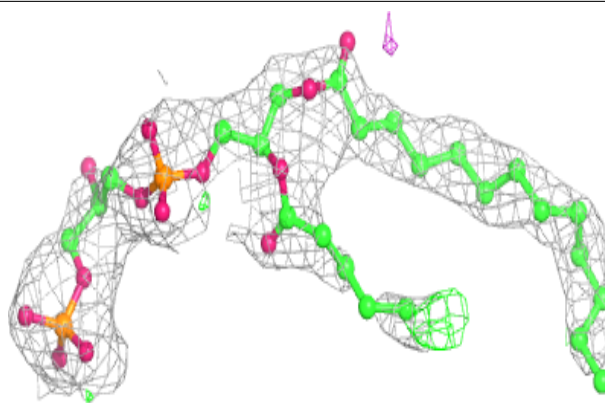
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



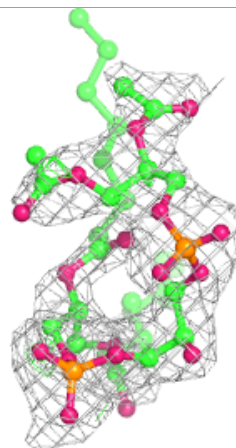
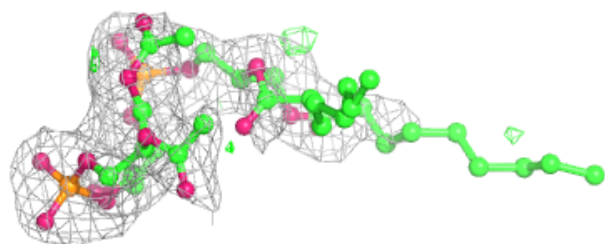
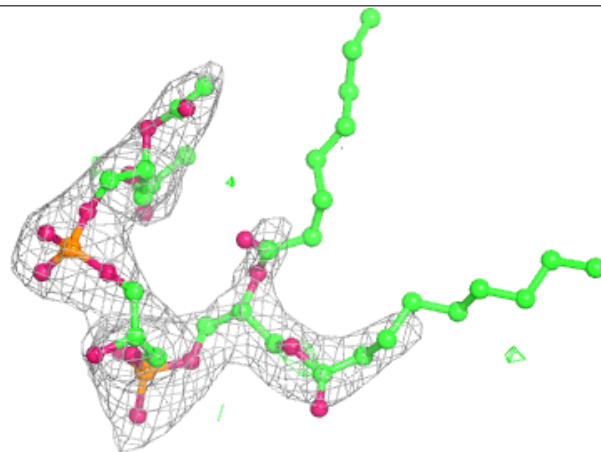


**Electron density around CDL Q 3003:**

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

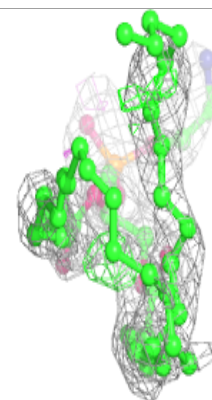
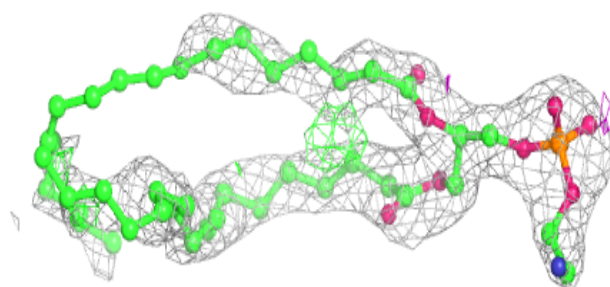
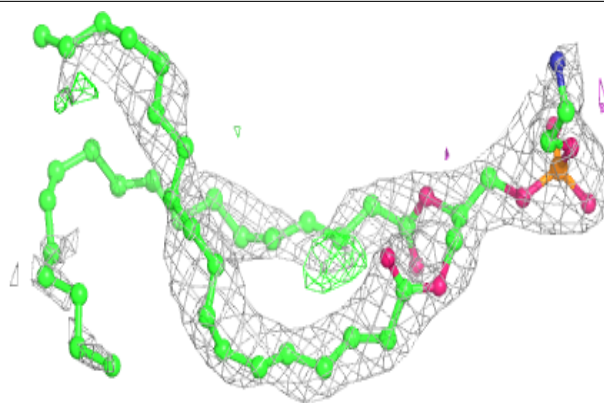
**Electron density around CDL P 3004:**

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

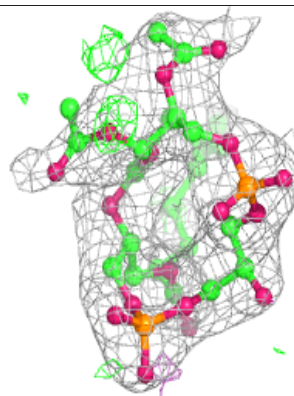
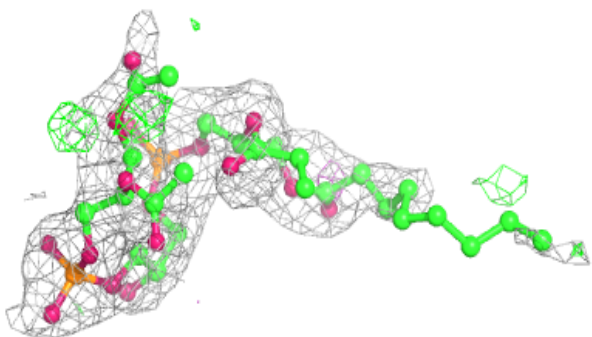
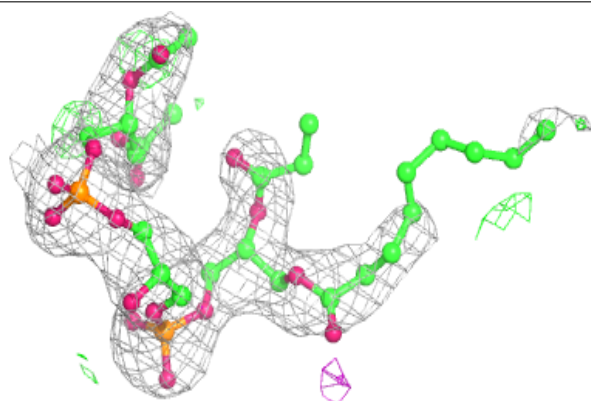


**Electron density around PEE Q 3006:**

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

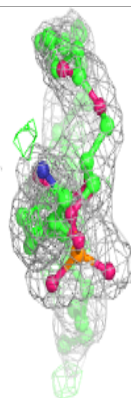
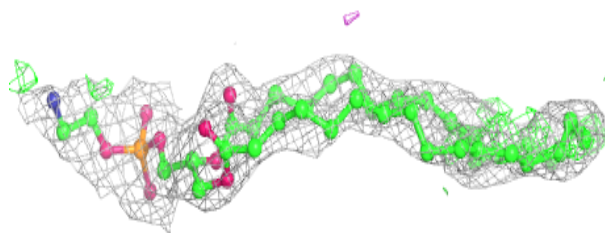
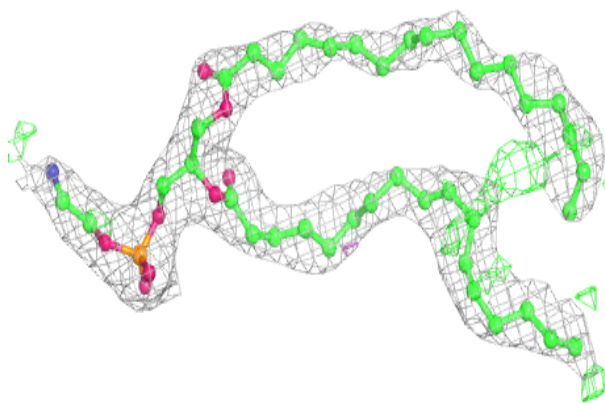
**Electron density around CDL C 2004:**

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

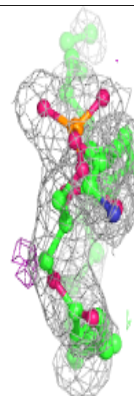
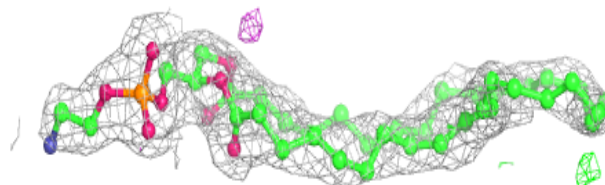
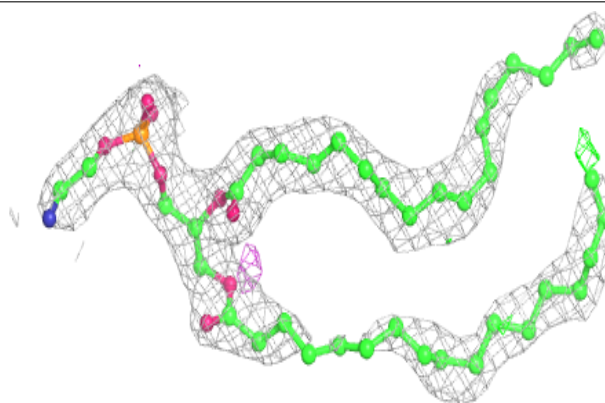


**Electron density around PEE P 3007:**

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

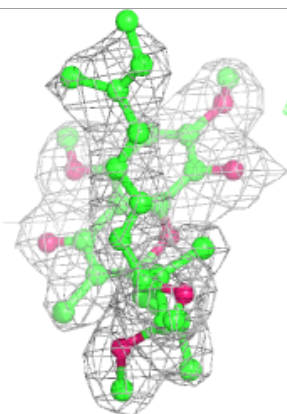
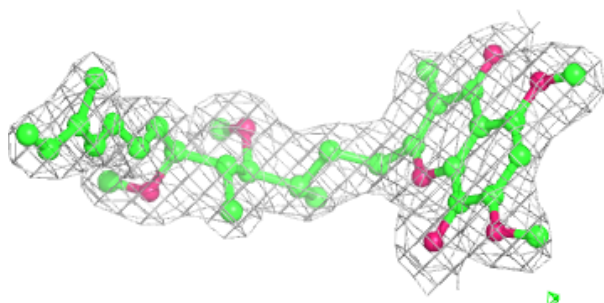
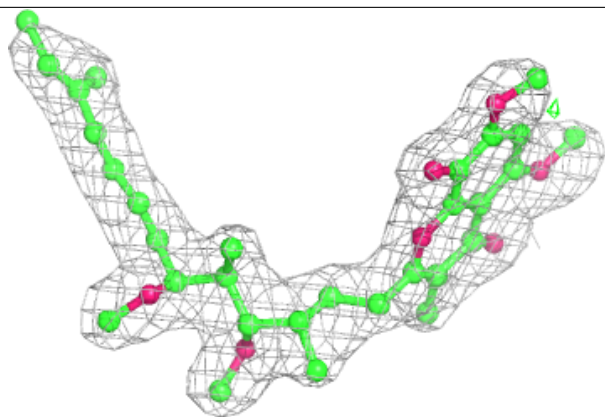
**Electron density around PEE C 2007:**

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

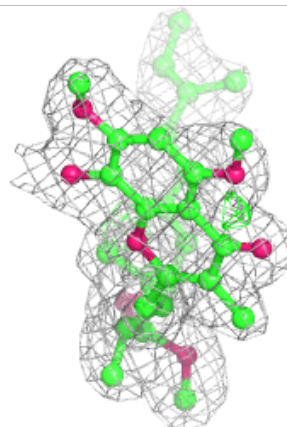
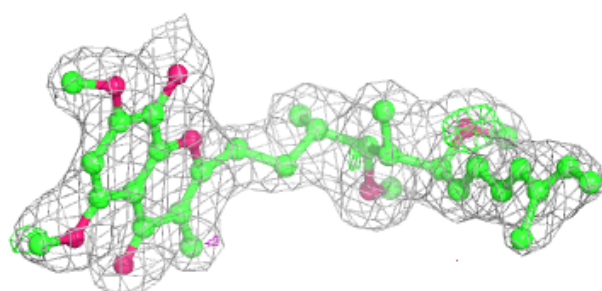
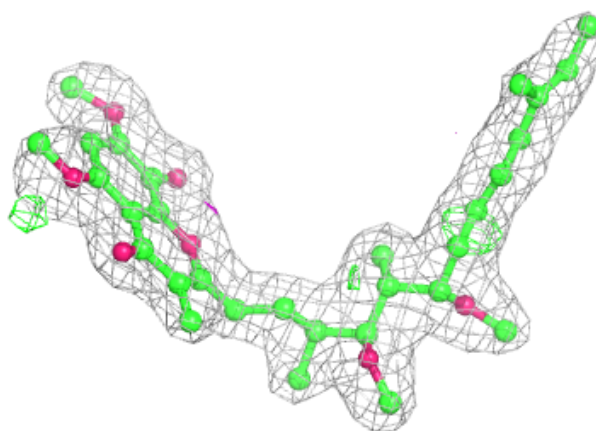


**Electron density around SMA P 3001:**

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

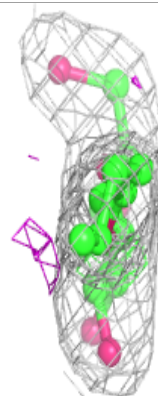
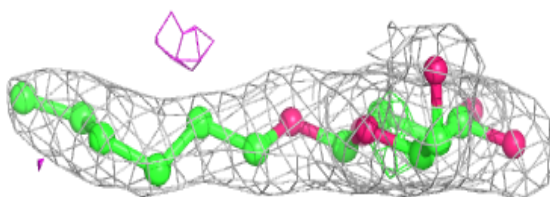
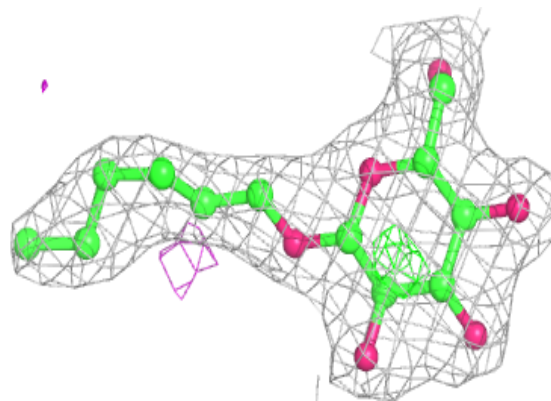
**Electron density around SMA C 2001:**

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



**Electron density around JZR A 4004:**

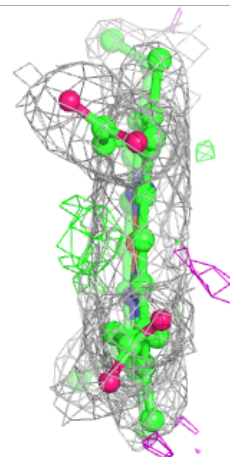
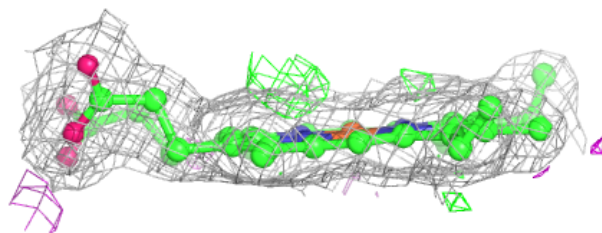
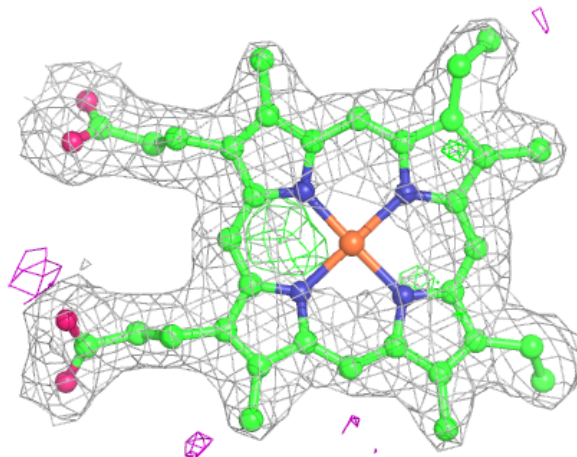
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





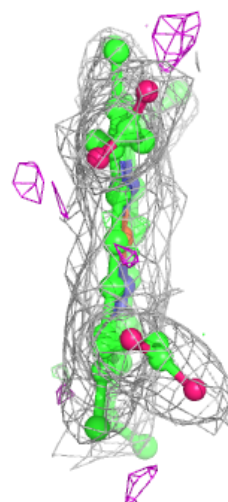
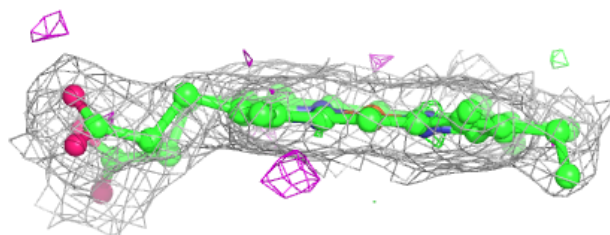
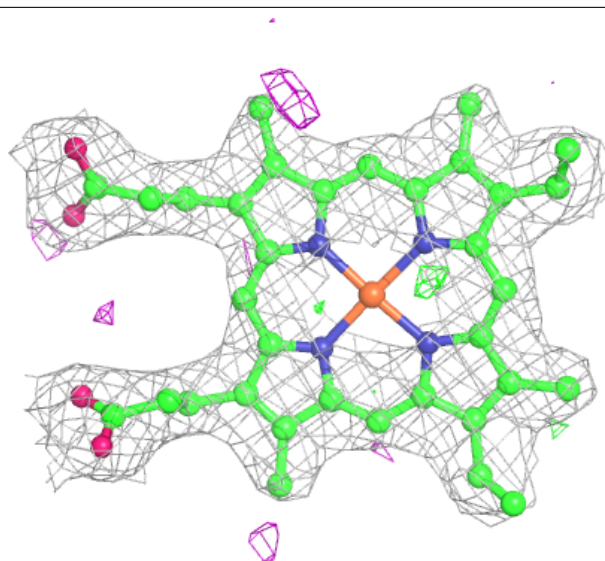
**Electron density around HEC D 501:**

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



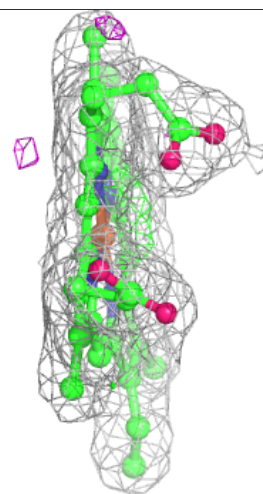
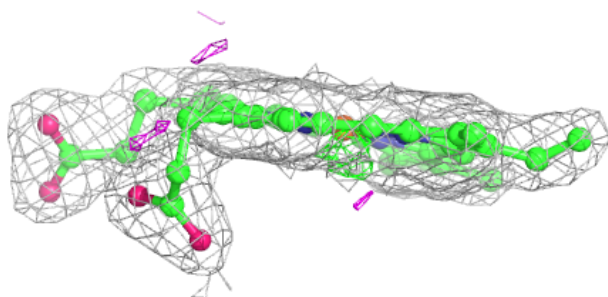
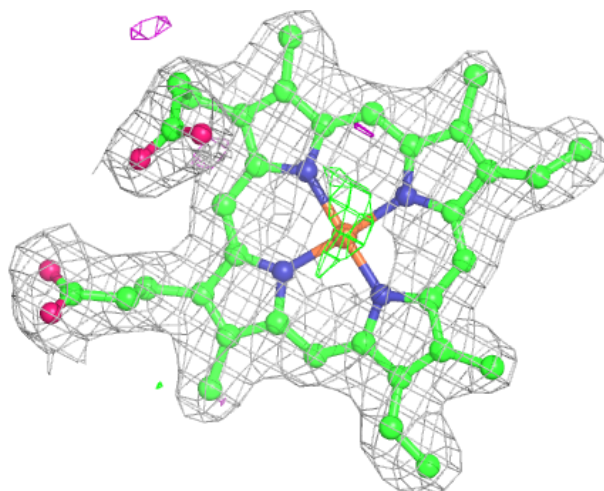
**Electron density around HEC Q 501:**

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



**Electron density around HEM C 502:**

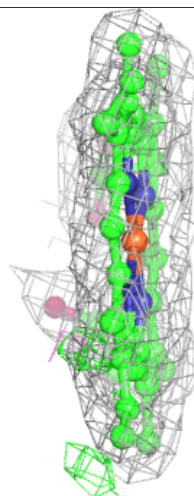
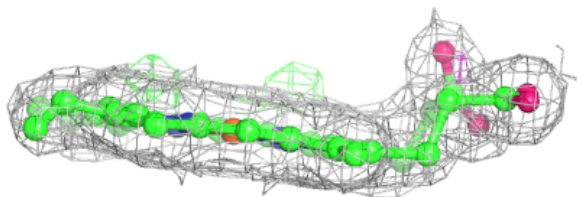
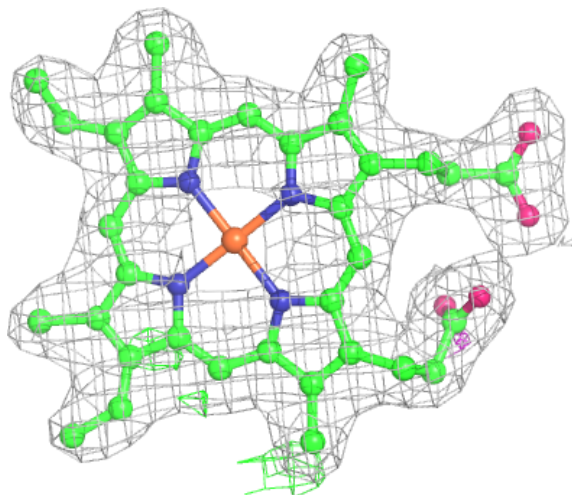
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





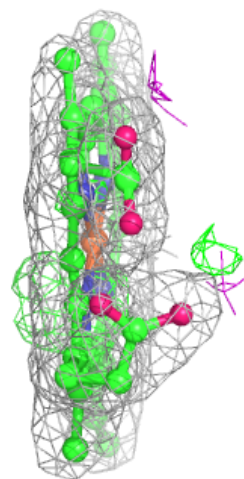
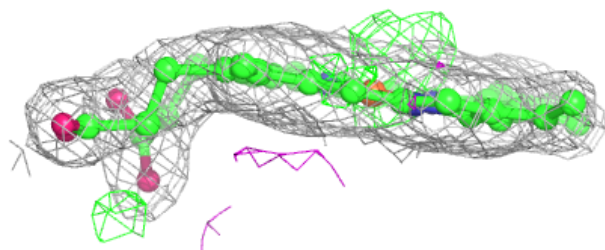
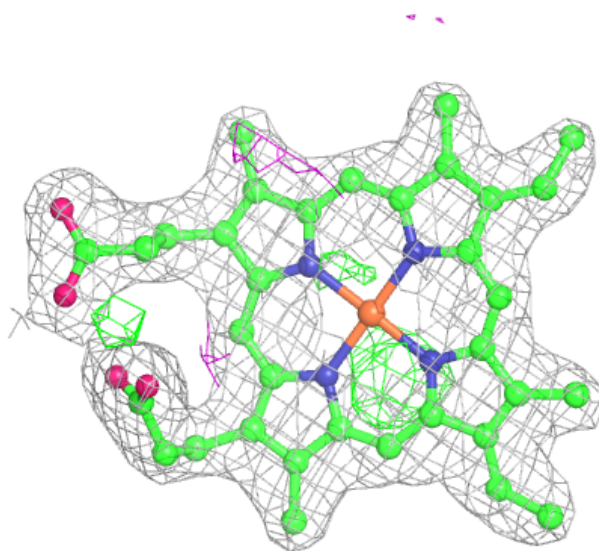
**Electron density around HEM C 501:**

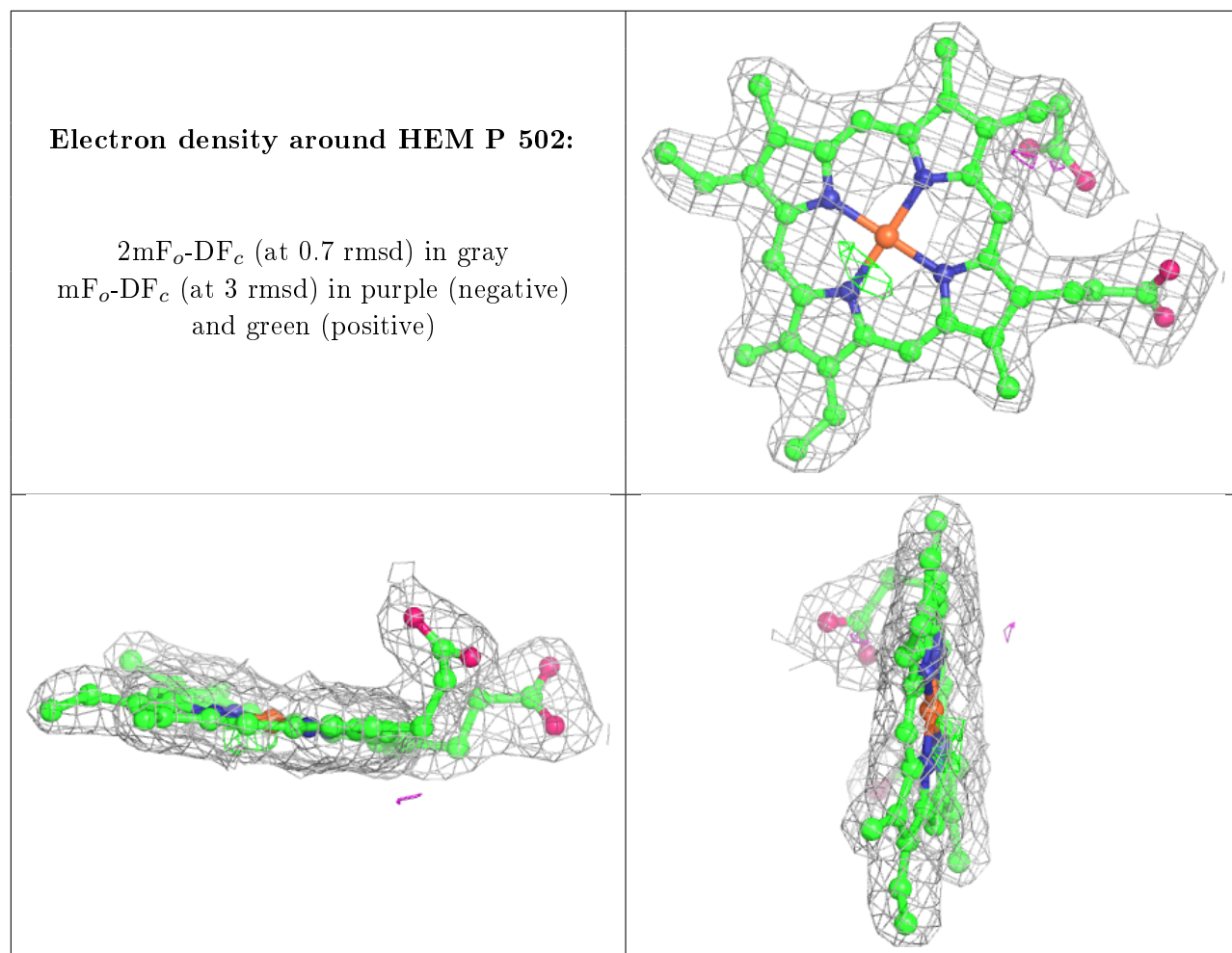
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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.