



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 16, 2025 – 06:45 am GMT

PDB ID : 9GCX  
Title : Crystal structure of bovine Cytochrome bc1 in complex with inhibitor F8  
Authors : Pinthong, N.; Hong, W.; O'Neill, P.W.; Antonyuk, S.V.  
Deposited on : 2024-08-03  
Resolution : 3.52 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

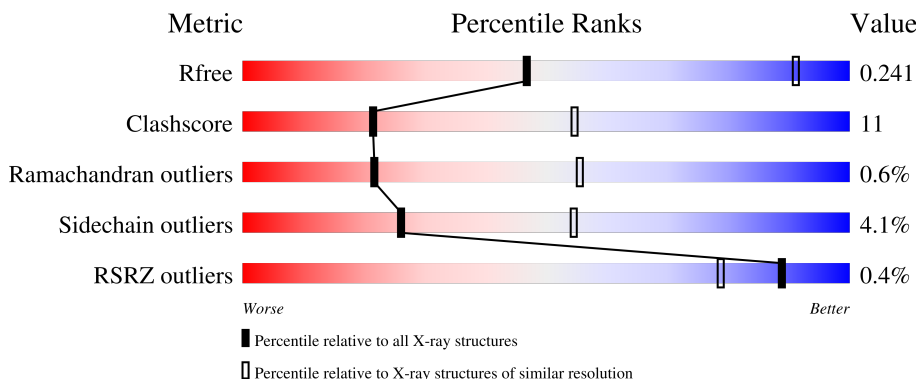
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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))
$R_{free}$	164625	1089 (3.58-3.46)
Clashscore	180529	1165 (3.58-3.46)
Ramachandran outliers	177936	1150 (3.58-3.46)
Sidechain outliers	177891	1151 (3.58-3.46)
RSRZ outliers	164620	1088 (3.58-3.46)

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  $\geq 3$ , 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	480	 70% 20% • 8%
2	B	453	 67% 23% • 9%
3	C	379	 74% 24% •
4	D	325	 55% 17% • 26%
5	E	274	 48% 22% • 28%

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Mol	Chain	Length	Quality of chain
5	I	274	
6	F	111	
7	G	82	
8	H	109	
9	J	64	
10	K	56	

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
12	CDL	A	502	-	-	X	-
14	A1IKG	C	505	X	-	-	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 16707 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3402	2129	600	653	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	1	0
			3112	1952	552	601	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	2	0
			3008	2019	470	500	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1901	1213	326	347	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1505	946	262	290	7			
5	I	27	Total	C	N	O	S	0	0	0
			191	117	38	35	1			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			860	547	155	156	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	405	116	98	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			529	321	96	107	5			

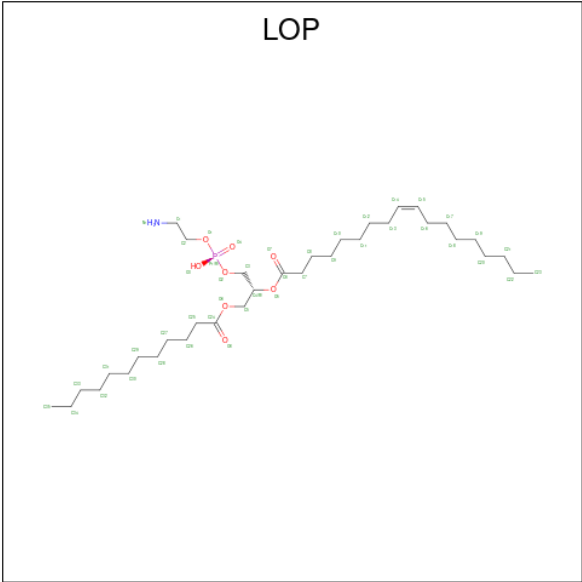
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	56	Total	C	N	O	S	0	0	0
			466	307	81	78				

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

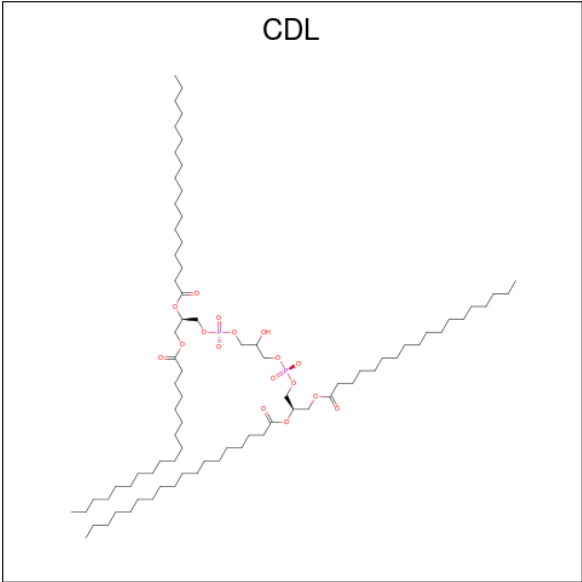
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	39	Total	C	N	O	S	0	0	0
			290	192	49	49				

- Molecule 11 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



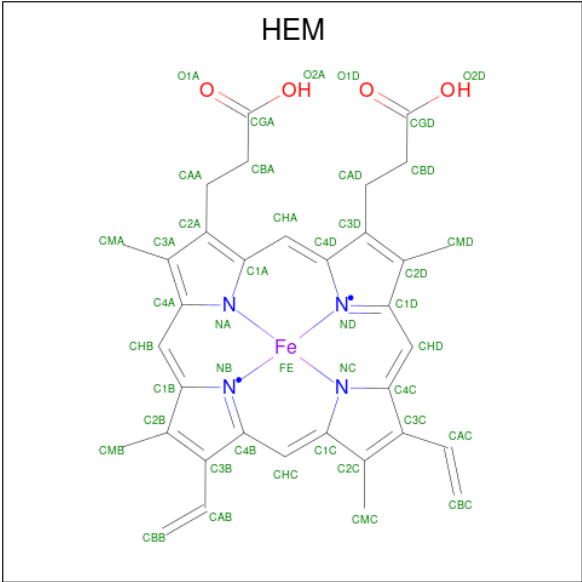
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	E	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
11	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



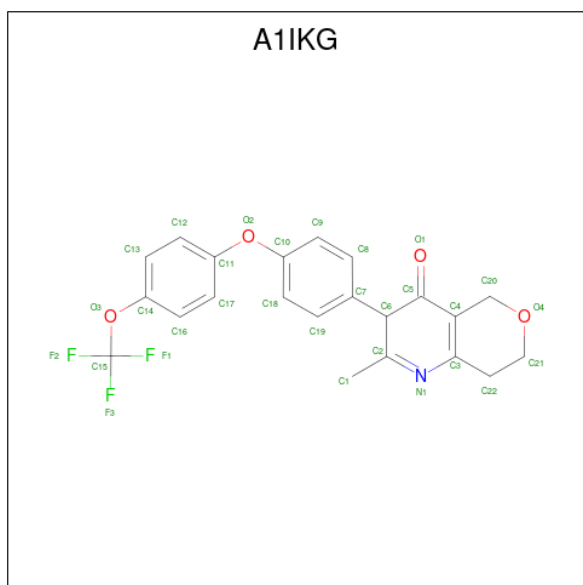
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			84	65	17	2		
12	C	1	Total	C	O	P	0	0
			100	81	17	2		
12	D	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



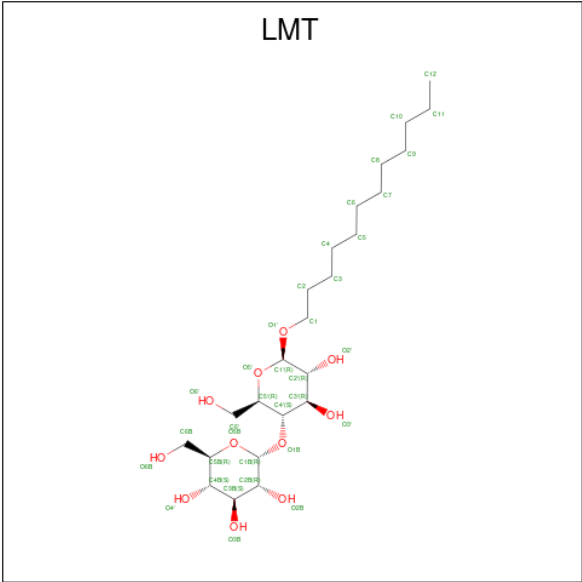
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is 2-methyl-3-(4-(4-(trifluoromethoxy)phenoxy)phenyl)-1,5,7,8-tetrahydro-4H-pyrano[4,3-b]pyridin-4-one (three-letter code: A1IKG) (formula: C<sub>22</sub>H<sub>18</sub>F<sub>3</sub>NO<sub>4</sub>).



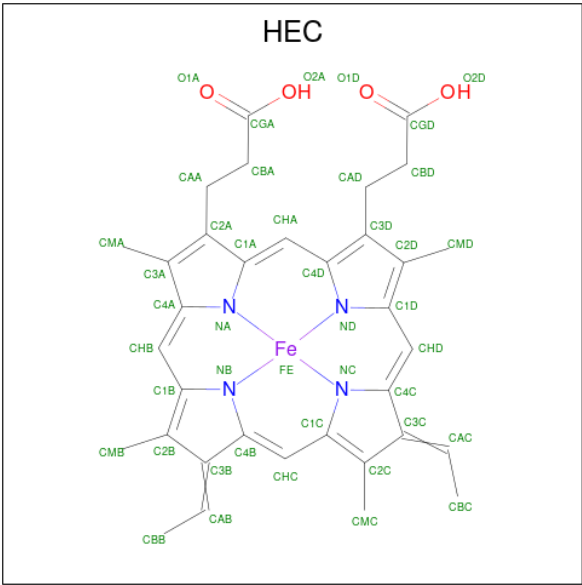
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	F	N	O	0	0
			30	22	3	1	4		

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



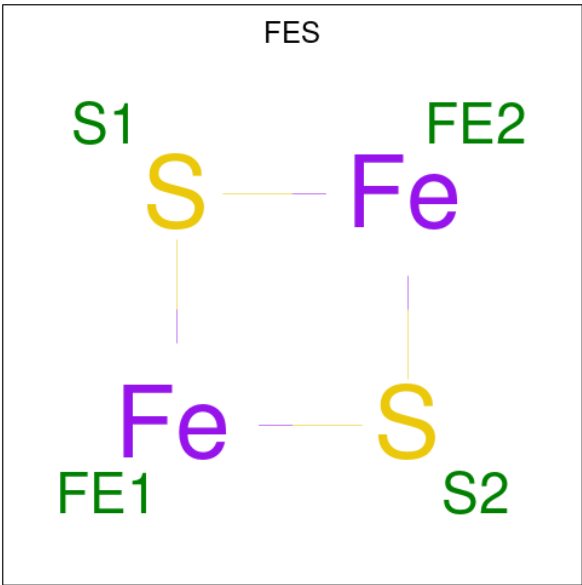
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



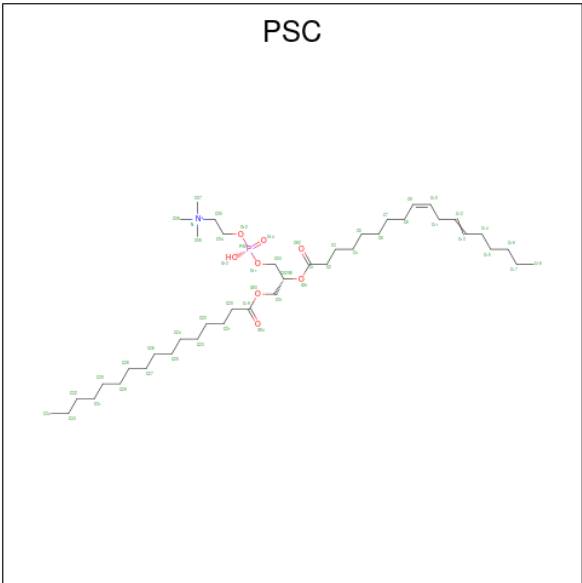
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



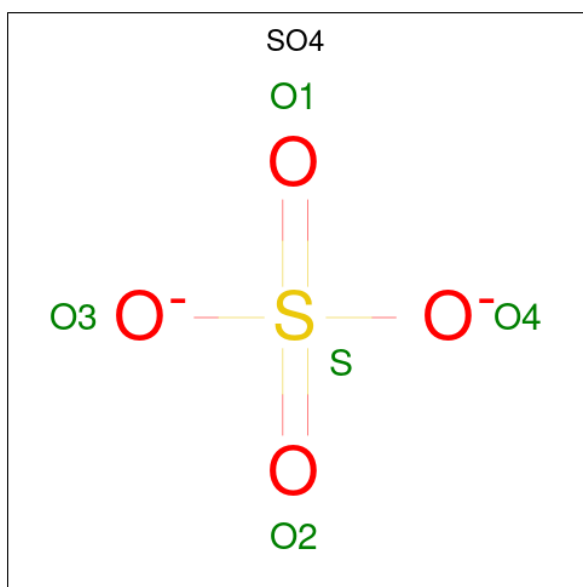
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 18 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	E	1	Total	C	N	O	0	0
			52	42	1	8		

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		

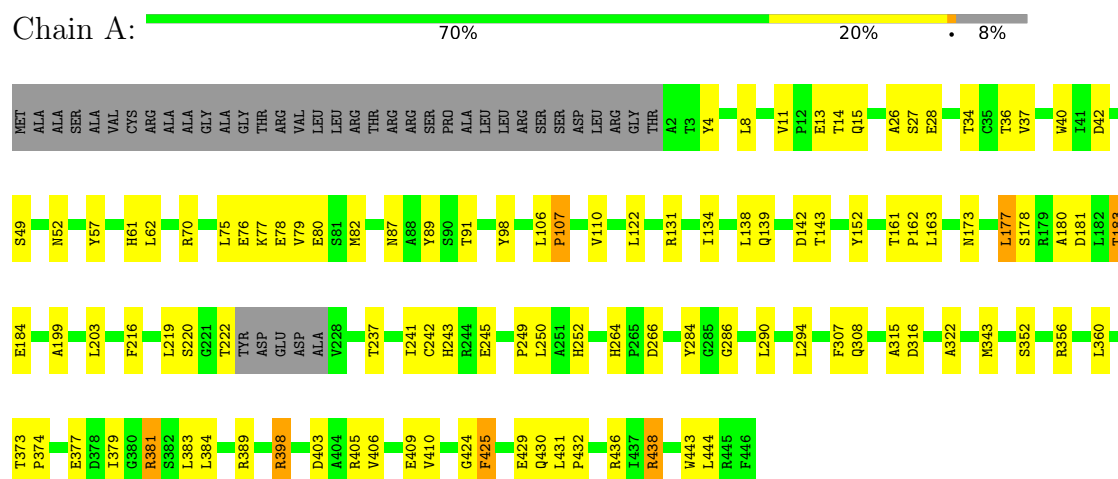
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	3	Total	O	0	0
			3	3		
20	B	1	Total	O	0	0
			1	1		
20	C	4	Total	O	0	0
			4	4		
20	E	1	Total	O	0	0
			1	1		
20	F	1	Total	O	0	0
			1	1		

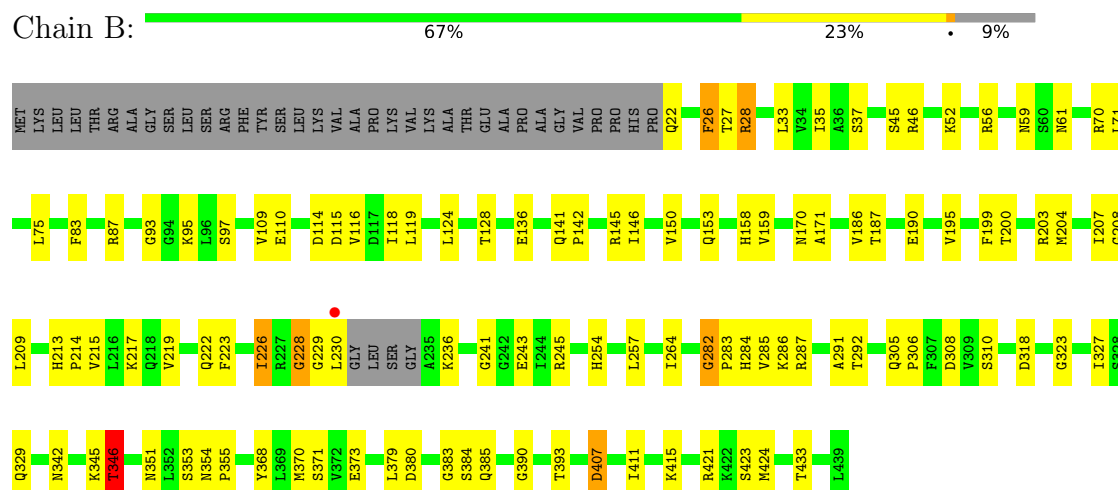
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

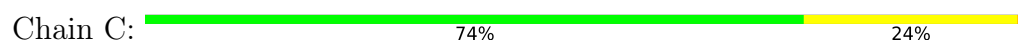
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



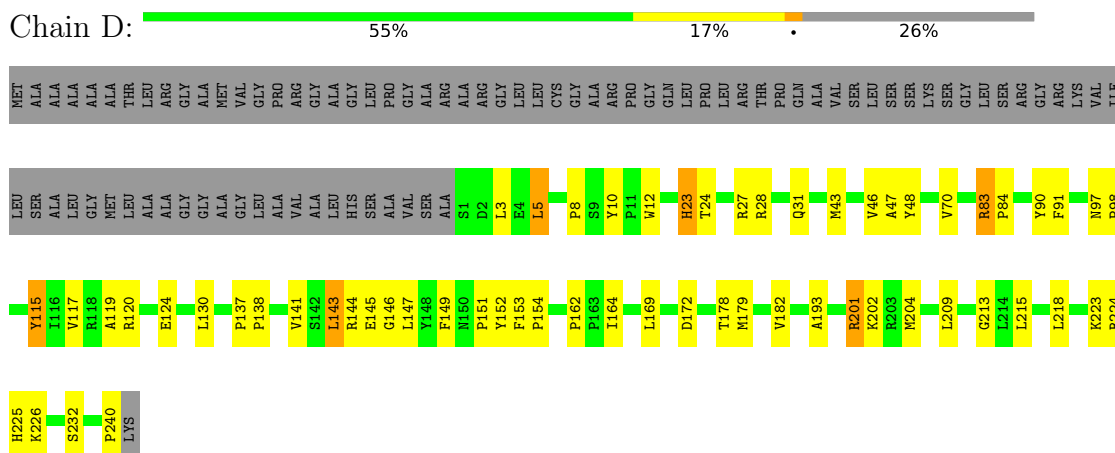
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



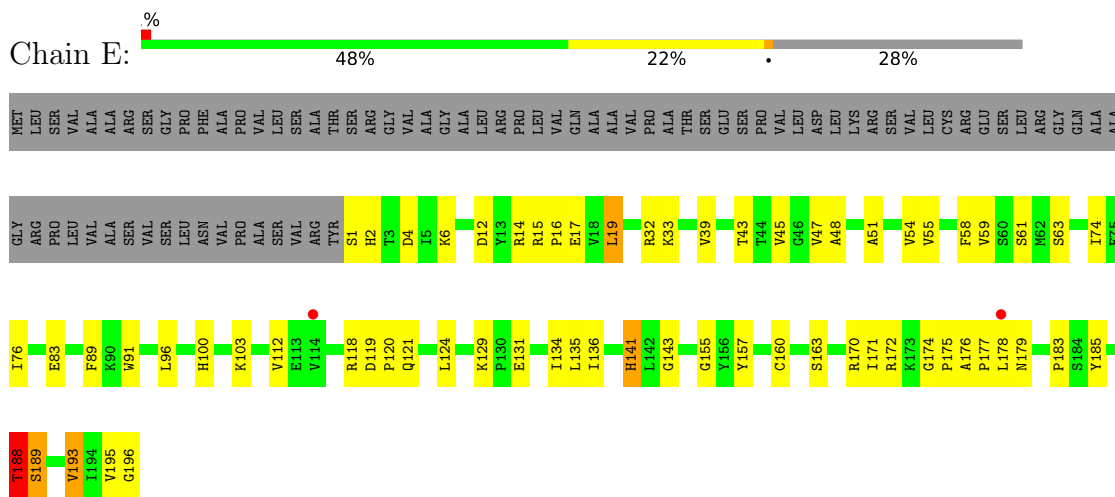
- Molecule 3: Cytochrome b



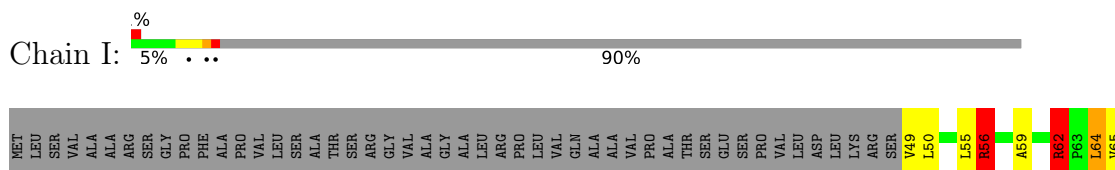
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

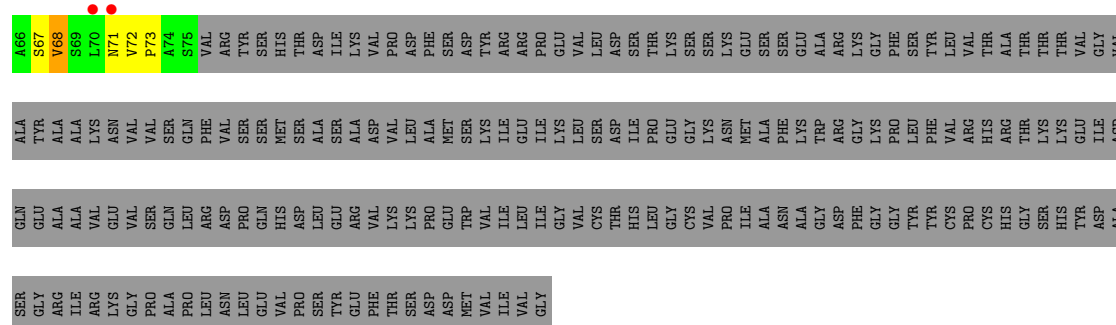


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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





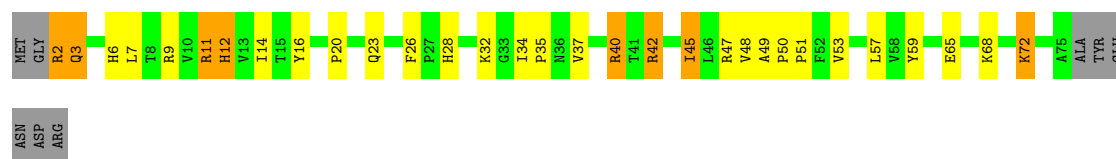
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F: 75% 12% 12%



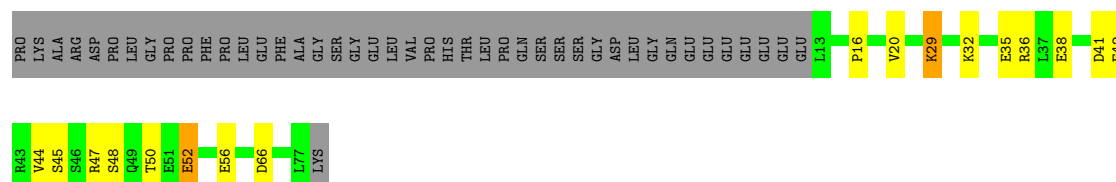
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 52% 28% 10% 10%



• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 44% 14% 40%



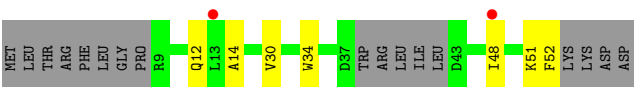
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain J: 62% 23% 12%



• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain K: 4% 57% 12% 30%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.08Å 210.08Å 344.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.52 30.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.52) 98.9 (30.00-3.52)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.188 , 0.241 0.188 , 0.241	Depositor DCC
$R_{free}$ test set	2846 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PSC, FES, LMT, HEC, SO4, A1IKG, LOP, 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	0.40	0/3473	1.05	14/4713 (0.3%)
2	B	0.41	0/3167	1.03	7/4297 (0.2%)
3	C	0.38	0/3111	1.01	12/4259 (0.3%)
4	D	0.39	0/1960	1.01	5/2665 (0.2%)
5	E	0.39	0/1538	0.99	3/2082 (0.1%)
5	I	0.69	0/192	1.57	5/260 (1.9%)
6	F	0.40	0/879	1.16	5/1180 (0.4%)
7	G	0.45	0/641	1.27	7/869 (0.8%)
8	H	0.37	0/534	1.29	6/718 (0.8%)
9	J	0.42	0/478	1.08	3/644 (0.5%)
10	K	0.44	0/300	1.00	0/414
All	All	0.40	0/16273	1.06	67/22101 (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
1	A	0	2
2	B	0	2
4	D	0	2
5	E	0	1
5	I	0	1
6	F	0	2
7	G	0	3
9	J	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194[A]	MET	CG-SD-CE	12.18	119.69	100.20
3	C	194[B]	MET	CG-SD-CE	12.18	119.69	100.20
5	I	64	LEU	CB-CG-CD1	10.04	128.07	111.00
8	H	52	GLU	CB-CA-C	-8.43	93.53	110.40
7	G	2	ARG	CA-CB-CG	8.26	131.57	113.40

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Sidechain
1	A	398	ARG	Sidechain
2	B	282	GLY	Peptide
2	B	421	ARG	Sidechain
4	D	83	ARG	Sidechain

## 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	3402	0	3306	62	0
2	B	3112	0	3078	75	1
3	C	3008	0	3074	71	0
4	D	1901	0	1833	44	0
5	E	1505	0	1478	37	1
5	I	191	0	203	12	0
6	F	860	0	851	4	0
7	G	620	0	619	22	0
8	H	529	0	511	8	0
9	J	466	0	469	18	0
10	K	290	0	260	8	0
11	A	45	0	67	11	0
11	C	135	0	201	10	0
11	E	45	0	67	5	0
11	G	45	0	67	4	0
12	A	84	0	121	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	100	0	156	11	0
12	D	94	0	141	12	0
13	C	86	0	60	8	0
14	C	30	0	0	0	0
15	C	35	0	46	3	0
16	D	43	0	30	2	0
17	E	4	0	0	0	0
18	E	52	0	80	5	0
19	F	5	0	0	0	0
19	G	10	0	0	0	0
20	A	3	0	0	0	0
20	B	1	0	0	1	0
20	C	4	0	0	0	0
20	E	1	0	0	0	0
20	F	1	0	0	0	0
All	All	16707	0	16718	357	1

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 357 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)
12:A:502:CDL:H162	3:C:11:MET:HE1	1.48	0.95
12:A:502:CDL:HA22	12:A:502:CDL:H112	1.50	0.93
12:A:502:CDL:H422	12:A:502:CDL:H341	1.54	0.89
1:A:406:VAL:O	1:A:410:VAL:HG23	1.71	0.89
12:D:502:CDL:H342	12:D:502:CDL:H171	1.52	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLN:NE2	5:E:112:VAL:O[5_555]	1.67	0.53

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/480 (91%)	423 (97%)	13 (3%)	0	100	100
2	B	411/453 (91%)	383 (93%)	26 (6%)	2 (0%)	25	59
3	C	378/379 (100%)	362 (96%)	16 (4%)	0	100	100
4	D	238/325 (73%)	227 (95%)	9 (4%)	2 (1%)	16	50
5	E	194/274 (71%)	174 (90%)	15 (8%)	5 (3%)	4	27
5	I	25/274 (9%)	21 (84%)	4 (16%)	0	100	100
6	F	96/111 (86%)	94 (98%)	2 (2%)	0	100	100
7	G	72/82 (88%)	66 (92%)	5 (7%)	1 (1%)	9	39
8	H	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
9	J	54/64 (84%)	54 (100%)	0	0	100	100
10	K	35/56 (62%)	28 (80%)	5 (14%)	2 (6%)	1	13
All	All	2002/2607 (77%)	1893 (95%)	97 (5%)	12 (1%)	22	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	228	GLY
5	E	141	HIS
5	E	143	GLY
5	E	155	GLY
10	K	12	GLN

### 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	364/394 (92%)	356 (98%)	8 (2%)	47	69
2	B	324/355 (91%)	316 (98%)	8 (2%)	42	67
3	C	327/327 (100%)	314 (96%)	13 (4%)	27	55
4	D	203/257 (79%)	195 (96%)	8 (4%)	27	56
5	E	165/228 (72%)	154 (93%)	11 (7%)	13	40
5	I	21/228 (9%)	14 (67%)	7 (33%)	0	1
6	F	90/99 (91%)	85 (94%)	5 (6%)	17	45
7	G	65/72 (90%)	60 (92%)	5 (8%)	10	34
8	H	62/99 (63%)	59 (95%)	3 (5%)	21	50
9	J	47/54 (87%)	46 (98%)	1 (2%)	48	70
10	K	25/46 (54%)	25 (100%)	0	100	100
All	All	1693/2159 (78%)	1624 (96%)	69 (4%)	26	54

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	72	LYS
8	H	35	GLU
5	I	65	VAL
3	C	281	LEU
3	C	254	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	164	HIS
7	G	28	HIS
2	B	385	GLN
3	C	201	HIS
3	C	267	HIS

### 5.3.3 RNA ⓘ

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](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	HEC	D	501	4	32,50,50	2.05	9 (28%)	24,82,82	2.51	11 (45%)
13	HEM	C	502	3	41,50,50	1.59	6 (14%)	45,82,82	1.66	10 (22%)
12	CDL	A	502	-	83,83,99	0.52	0	89,95,111	0.87	3 (3%)
11	LOP	C	506	-	44,44,44	0.62	0	47,49,49	0.90	1 (2%)
15	LMT	C	508	-	36,36,36	0.52	0	47,47,47	0.84	2 (4%)
18	PSC	E	203	-	51,51,51	0.56	0	57,59,59	1.28	4 (7%)
11	LOP	G	101	-	44,44,44	0.44	0	47,49,49	1.25	3 (6%)
11	LOP	C	503	-	44,44,44	0.56	0	47,49,49	0.95	3 (6%)
12	CDL	C	504	-	99,99,99	0.43	0	105,111,111	0.79	2 (1%)
11	LOP	E	202	-	44,44,44	0.45	0	47,49,49	0.92	2 (4%)
14	A1IKG	C	505	-	32,33,33	1.57	6 (18%)	40,48,48	1.46	7 (17%)
11	LOP	C	507	-	44,44,44	0.56	0	47,49,49	0.76	2 (4%)
19	SO4	G	102	-	4,4,4	0.34	0	6,6,6	0.12	0
11	LOP	A	501	-	44,44,44	0.49	0	47,49,49	0.80	0
12	CDL	D	502	-	93,93,99	0.44	0	99,105,111	0.63	0
13	HEM	C	501	3	41,50,50	1.51	7 (17%)	45,82,82	2.11	14 (31%)
19	SO4	F	201	-	4,4,4	0.30	0	6,6,6	0.17	0
19	SO4	G	103	-	4,4,4	0.28	0	6,6,6	0.11	0
17	FES	E	201	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LOP	A	501	-	-	22/48/48/48	-
11	LOP	C	506	-	-	21/48/48/48	-
12	CDL	D	502	-	-	49/104/104/110	-
15	LMT	C	508	-	-	7/21/61/61	0/2/2/2
16	HEC	D	501	4	-	2/10/54/54	-
13	HEM	C	501	3	-	4/12/54/54	-
14	A1IKG	C	505	-	1/1/6/6	0/13/40/40	0/4/4/4
18	PSC	E	203	-	-	28/55/55/55	-
13	HEM	C	502	3	-	4/12/54/54	-
11	LOP	C	507	-	-	33/48/48/48	-
12	CDL	A	502	-	-	52/93/93/110	-
11	LOP	G	101	-	-	27/48/48/48	-
17	FES	E	201	5	-	-	0/1/1/1
11	LOP	C	503	-	-	17/48/48/48	-
12	CDL	C	504	-	-	54/110/110/110	-
11	LOP	E	202	-	-	23/48/48/48	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3C-C2C	7.01	1.48	1.40
14	C	505	A1IKG	C6-C2	-6.04	1.42	1.52
13	C	502	HEM	C1B-NB	-5.33	1.31	1.40
16	D	501	HEC	C2B-C3B	3.61	1.44	1.40
14	C	505	A1IKG	C5-C4	-3.58	1.39	1.47

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	C1D-C2D-C3D	-7.22	101.98	107.00
18	E	203	PSC	O01-C1-C2	6.49	125.50	111.50
11	G	101	LOP	O5-C6-C7	6.29	125.06	111.50
13	C	501	HEM	CBA-CAA-C2A	-5.87	102.60	112.62
14	C	505	A1IKG	C7-C6-C2	5.26	123.16	111.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	A1IKG	C6

5 of 343 torsion outliers are listed below:

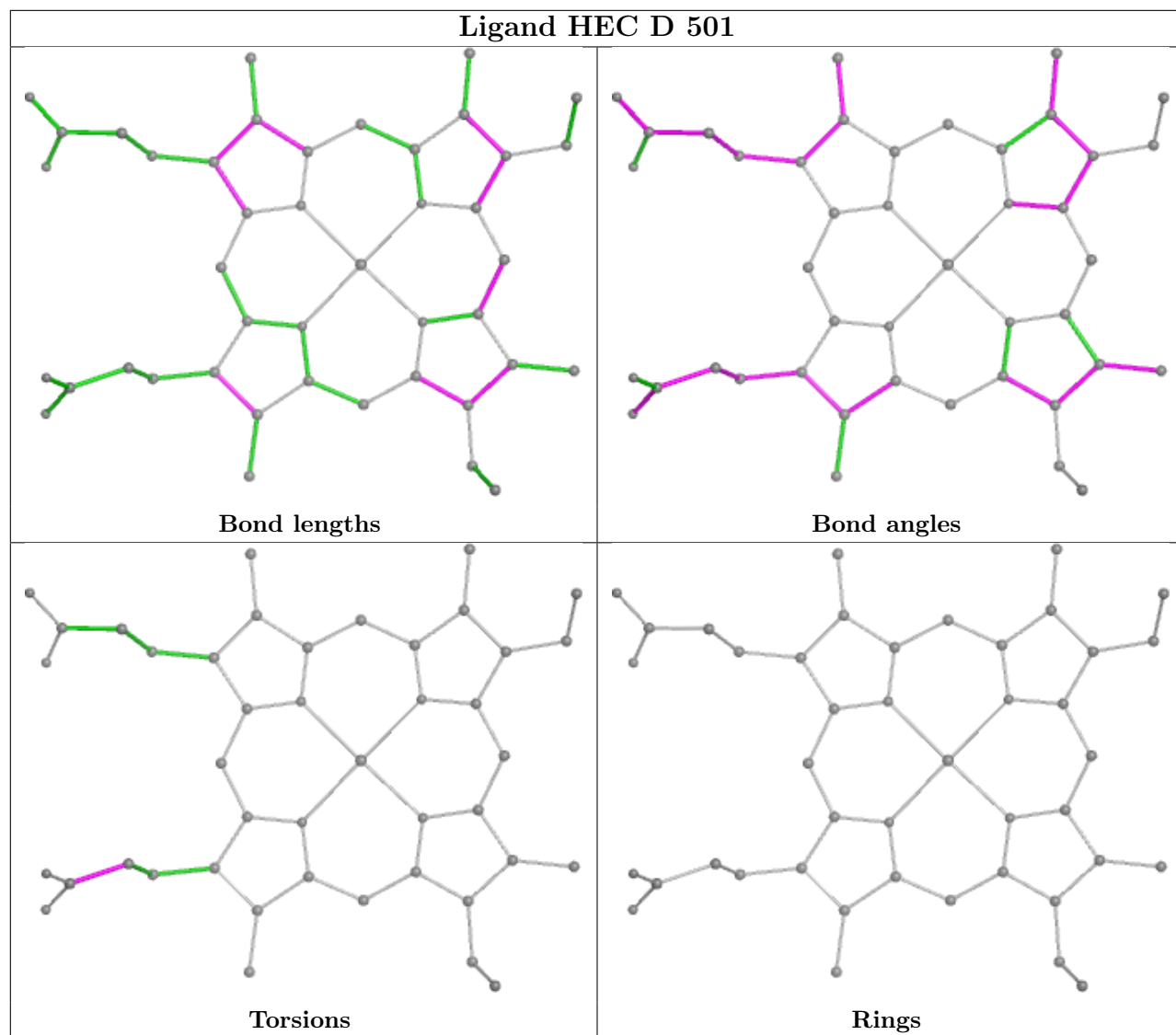
Mol	Chain	Res	Type	Atoms
11	A	501	LOP	N1-C1-C2-O1
11	A	501	LOP	C2-O1-P1-O4
11	C	507	LOP	N1-C1-C2-O1
11	C	507	LOP	C2-O1-P1-O2
11	C	507	LOP	C2-O1-P1-O3

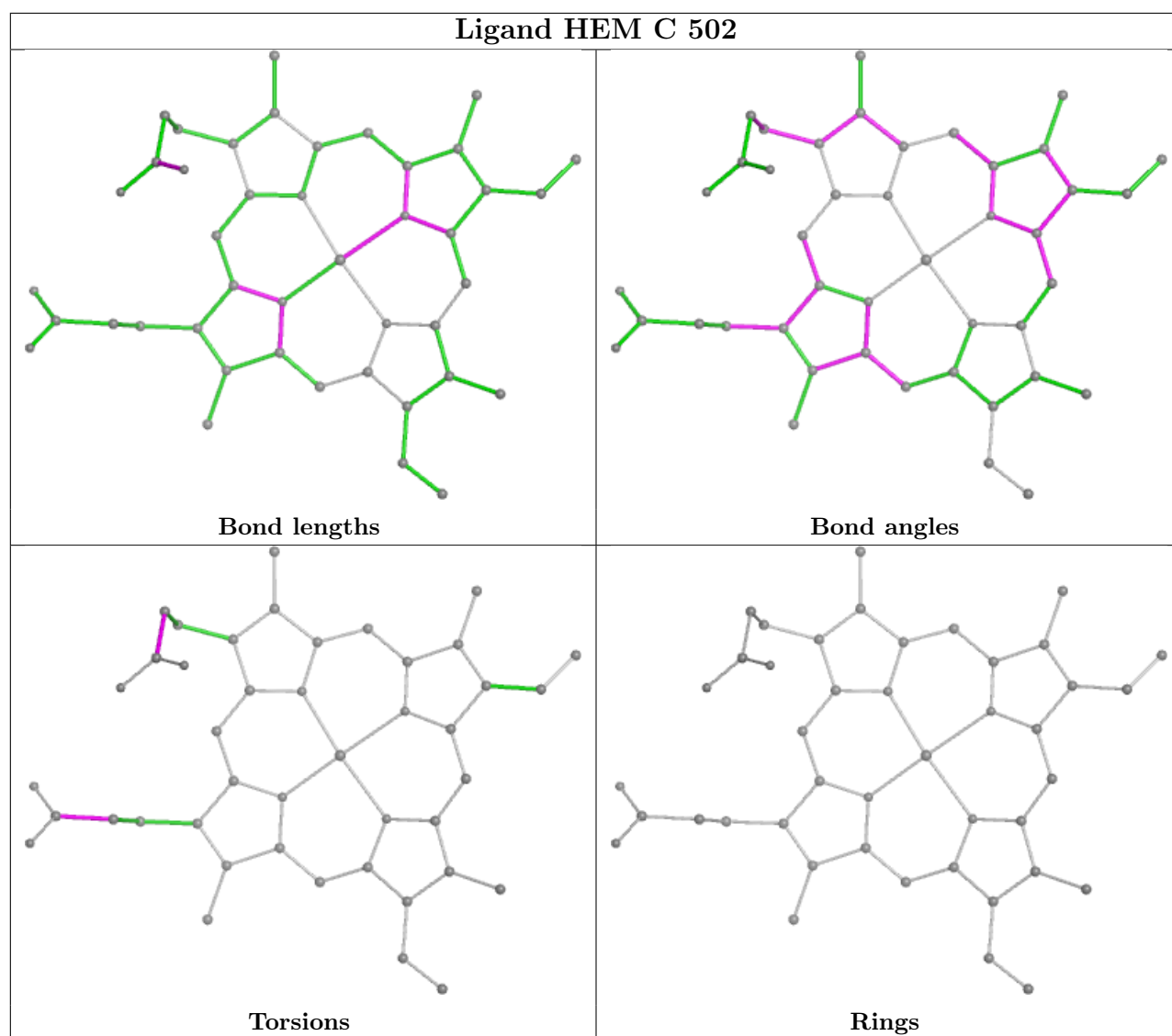
There are no ring outliers.

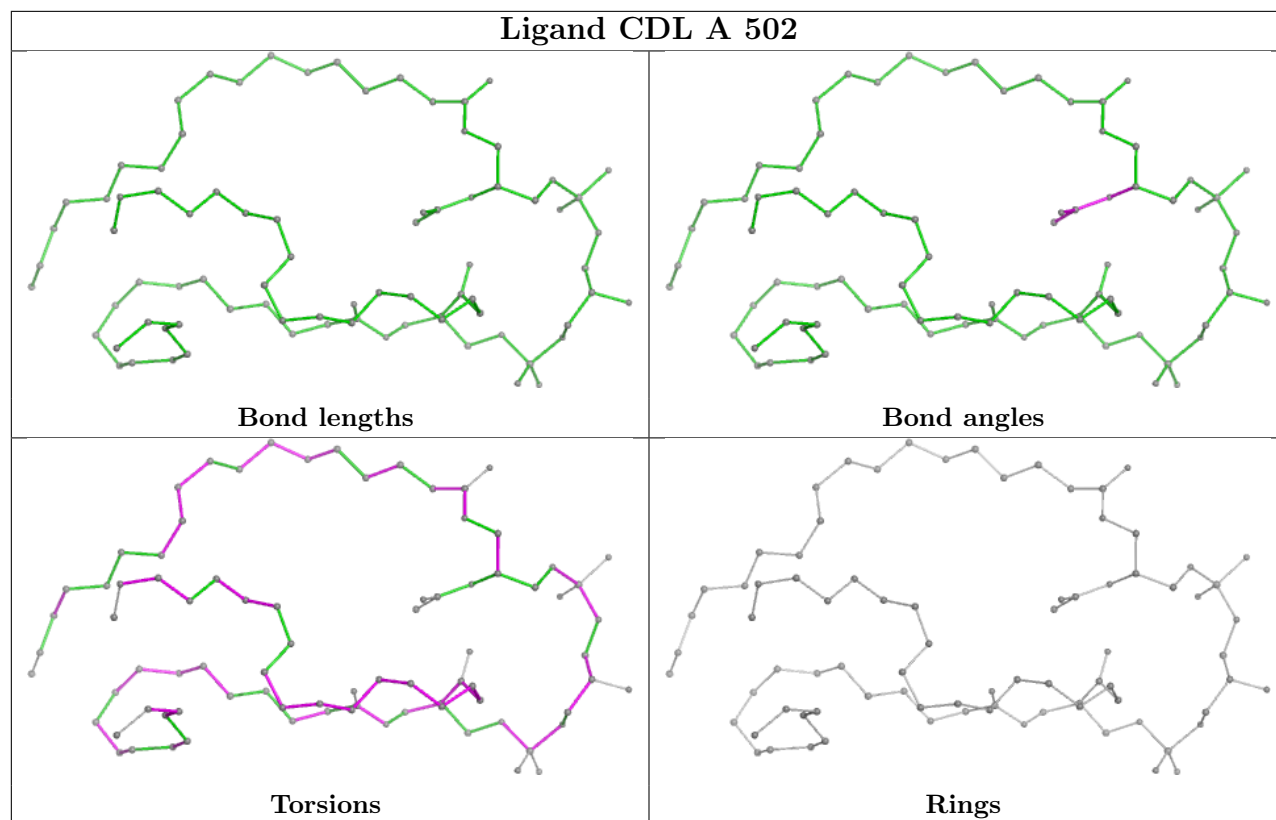
13 monomers are involved in 84 short contacts:

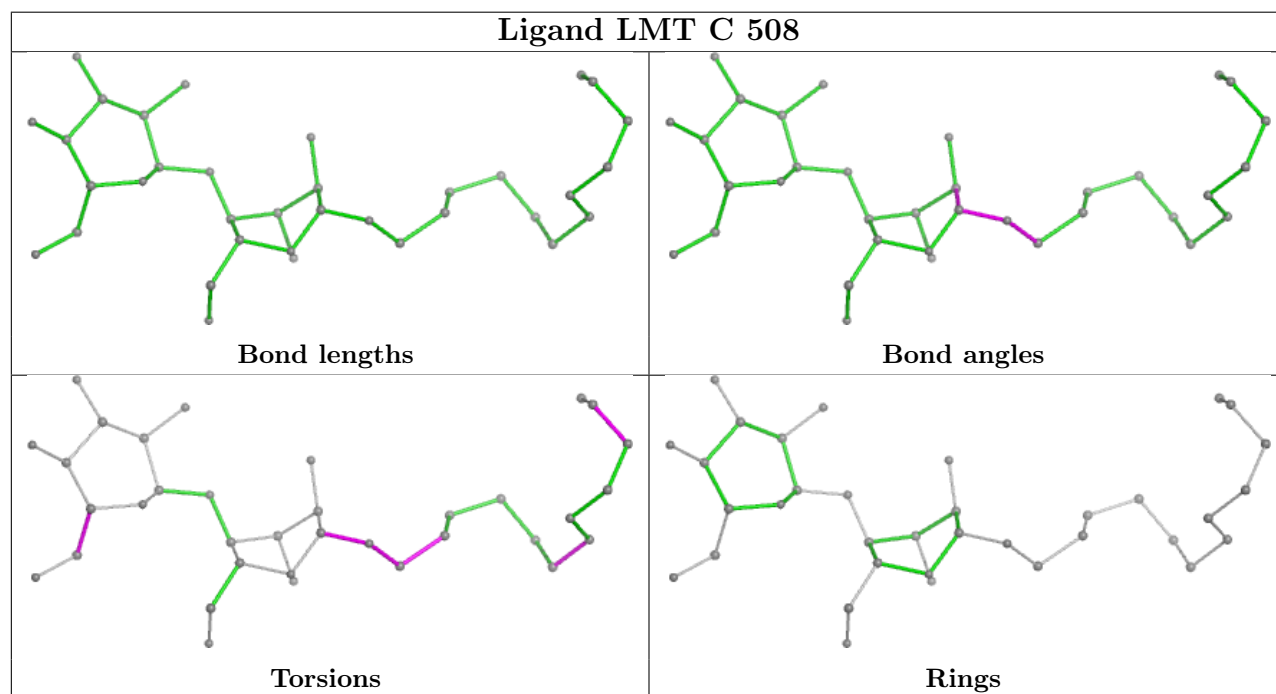
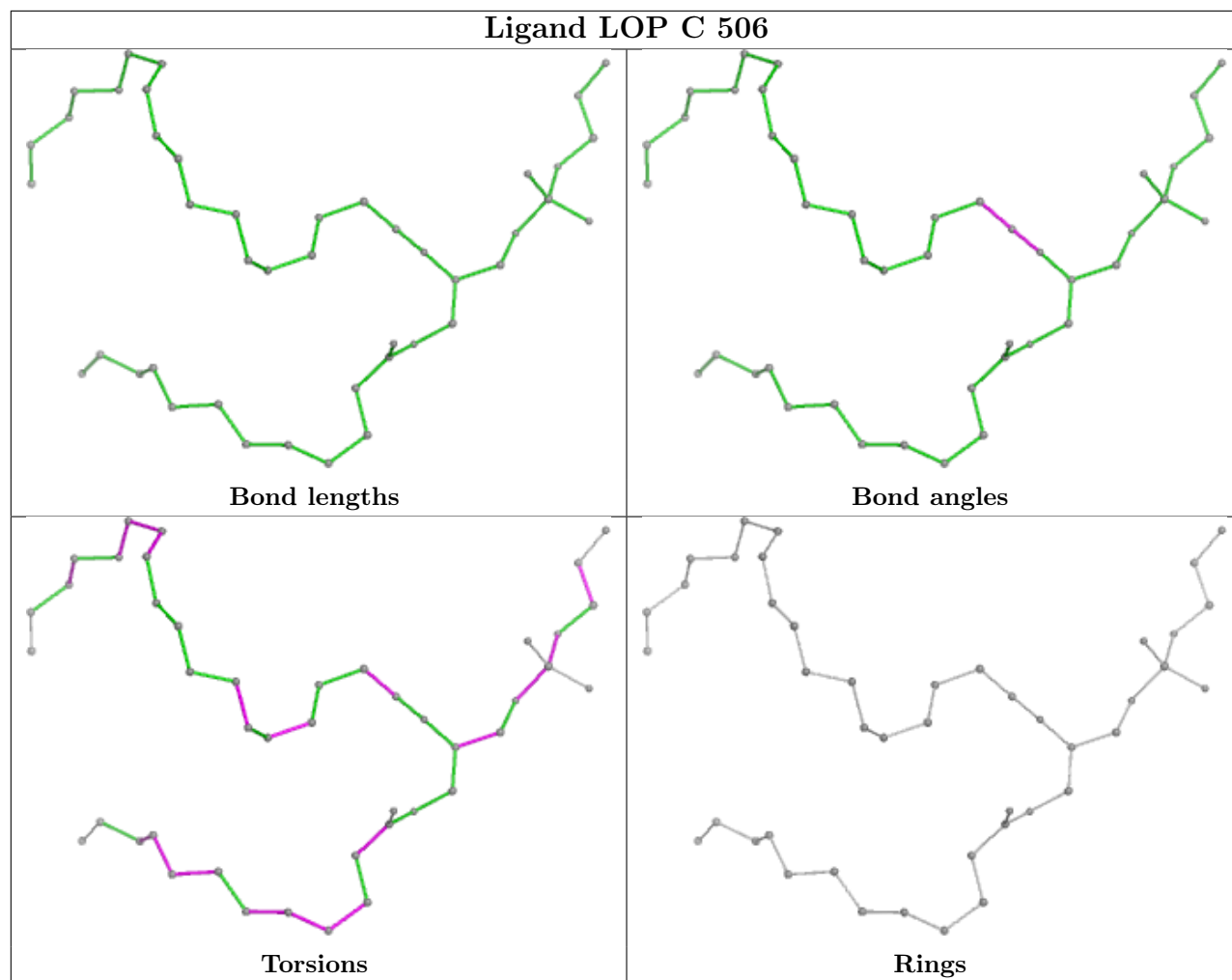
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	501	HEC	2	0
13	C	502	HEM	5	0
12	A	502	CDL	22	0
11	C	506	LOP	4	0
15	C	508	LMT	3	0
18	E	203	PSC	5	0
11	G	101	LOP	4	0
11	C	503	LOP	6	0
12	C	504	CDL	11	0
11	E	202	LOP	5	0
11	A	501	LOP	11	0
12	D	502	CDL	12	0
13	C	501	HEM	3	0

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

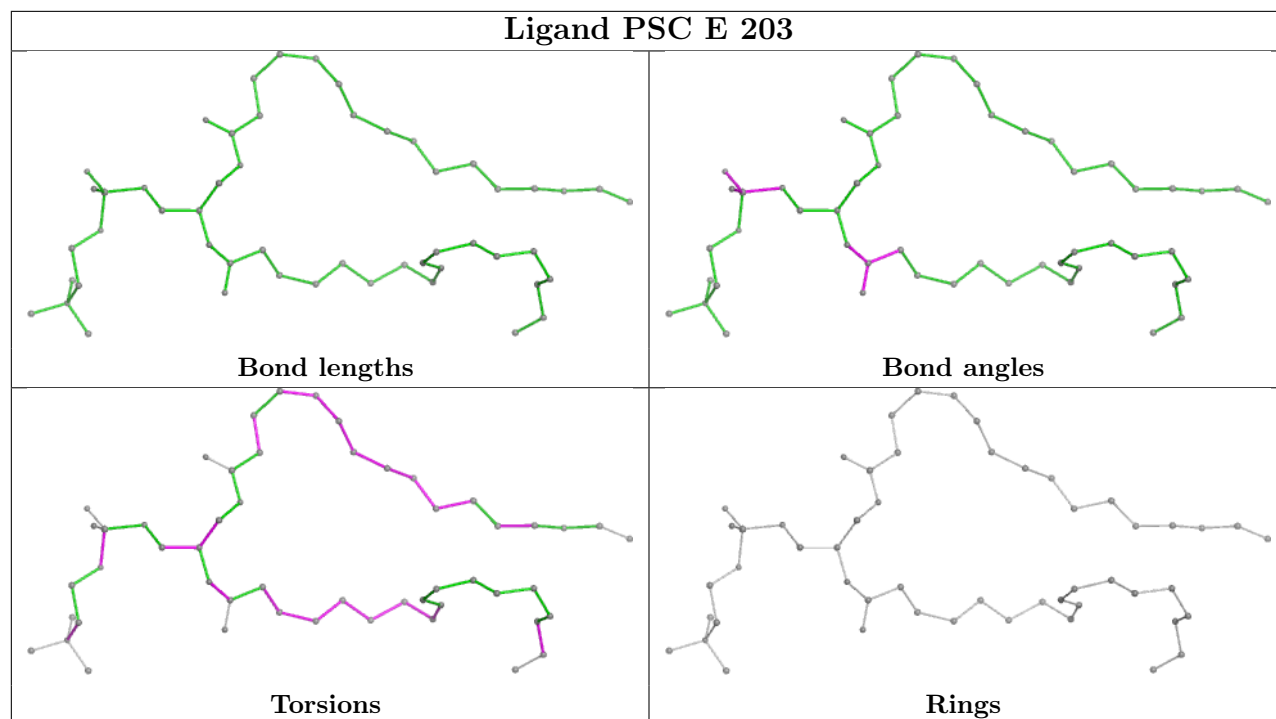




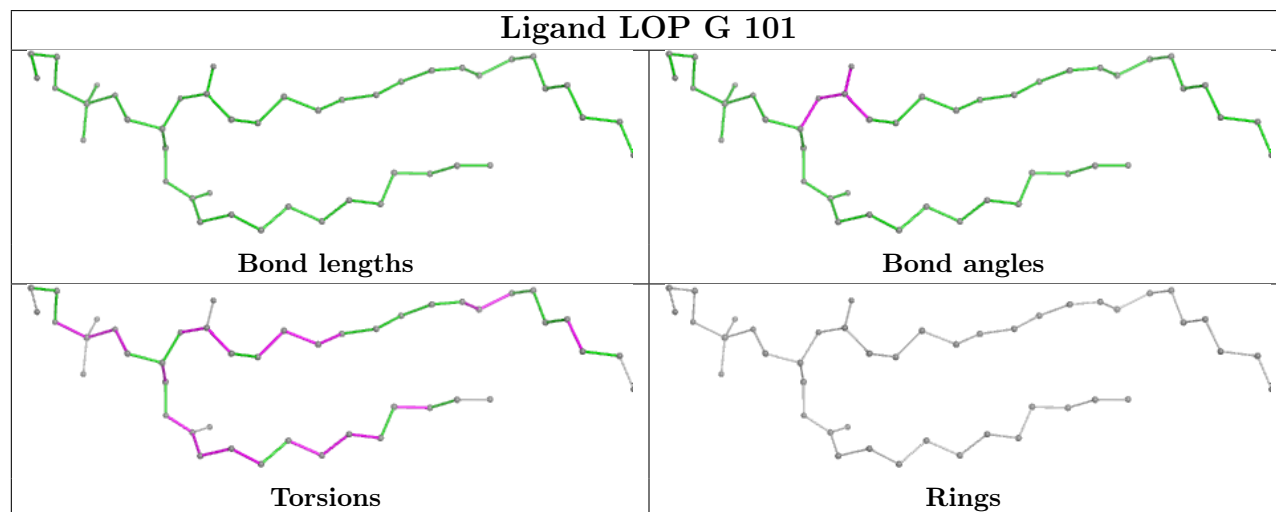




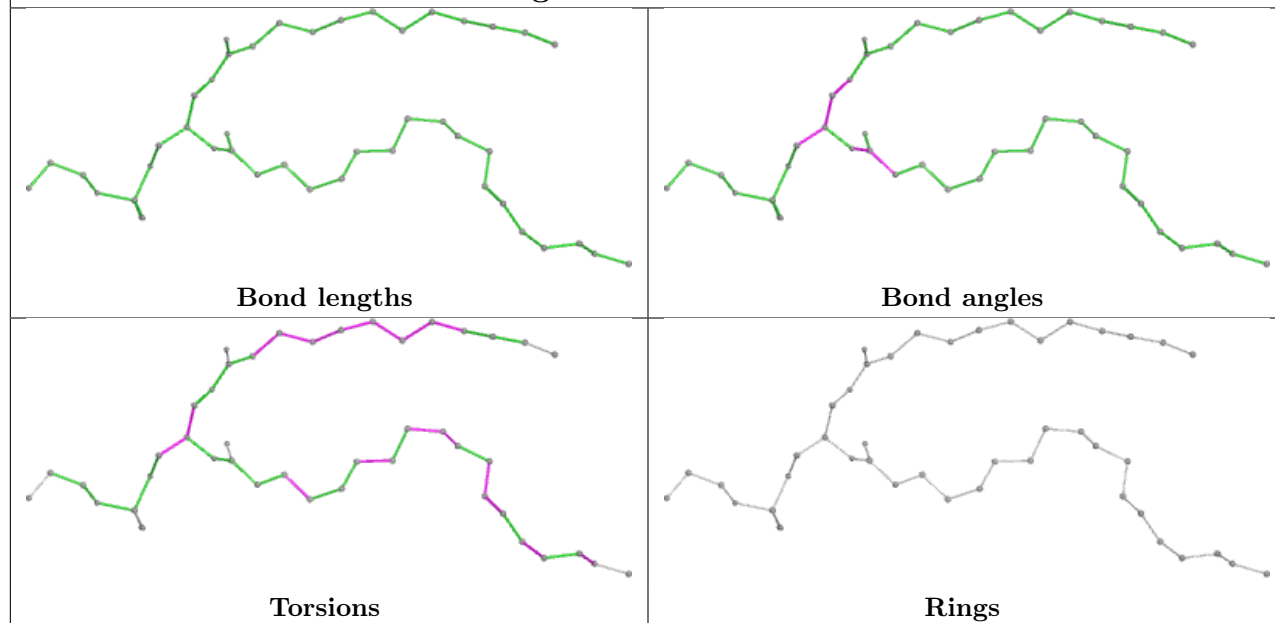
## Ligand PSC E 203



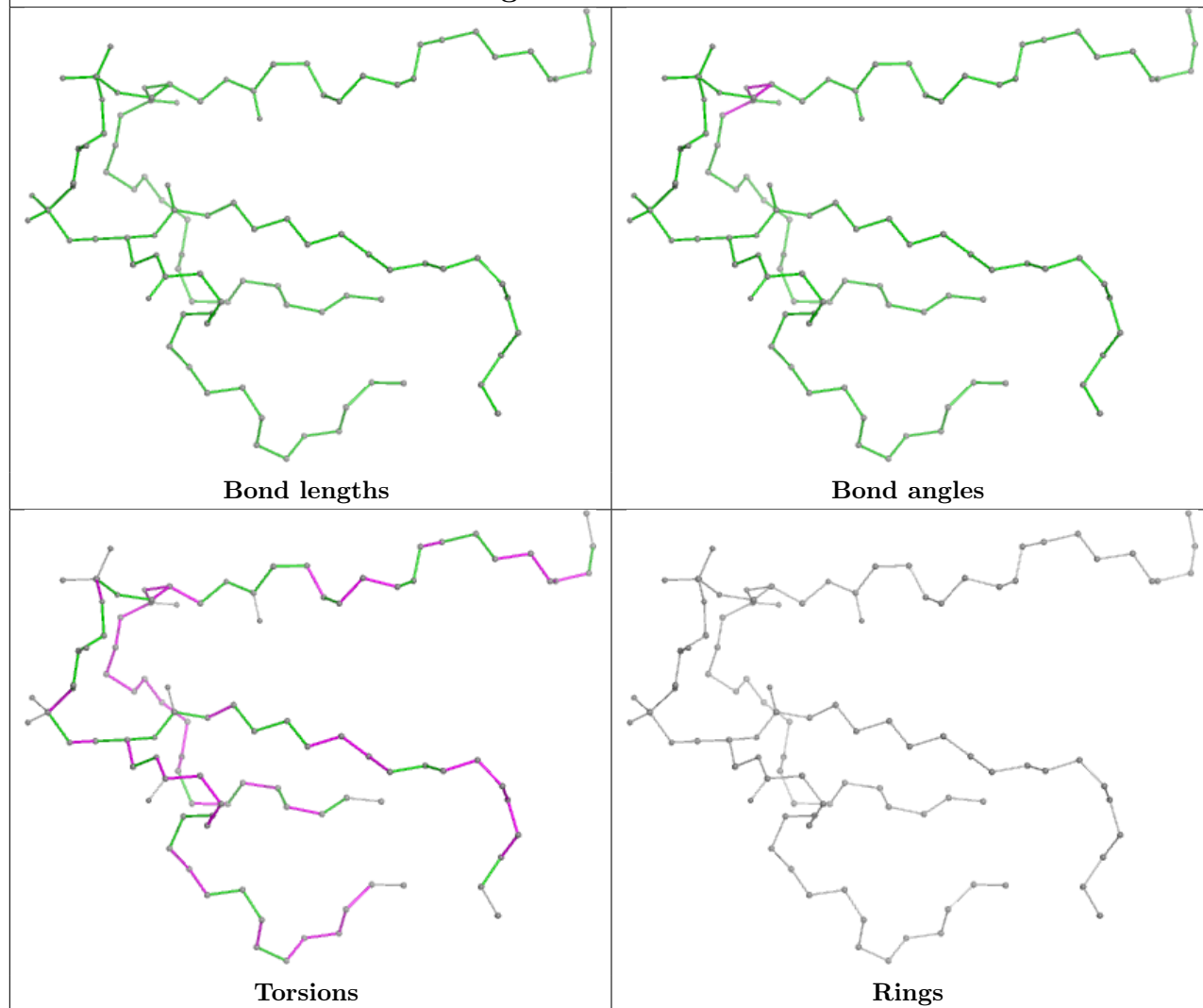
## Ligand LOP G 101



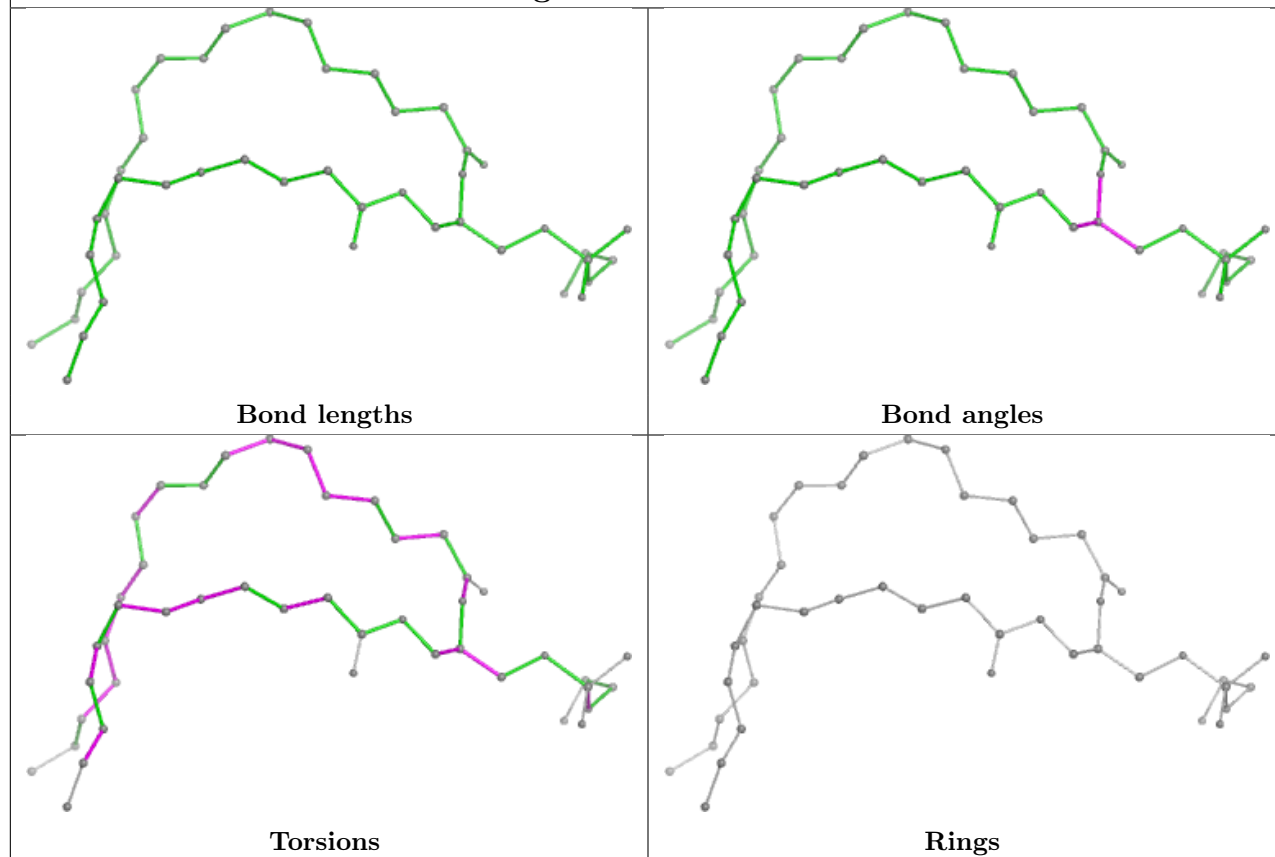
## Ligand LOP C 503



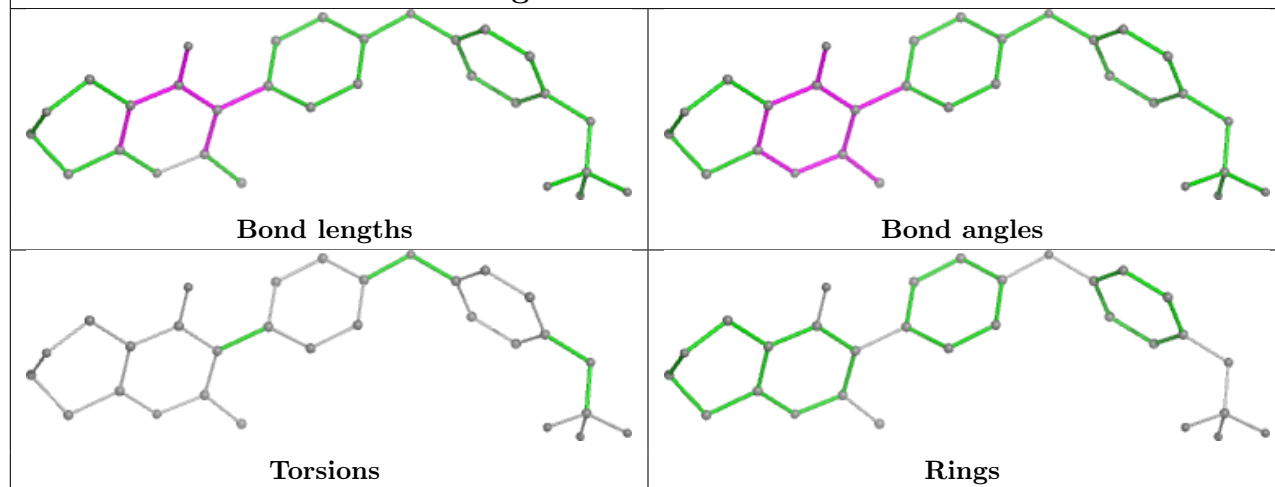
## Ligand CDL C 504

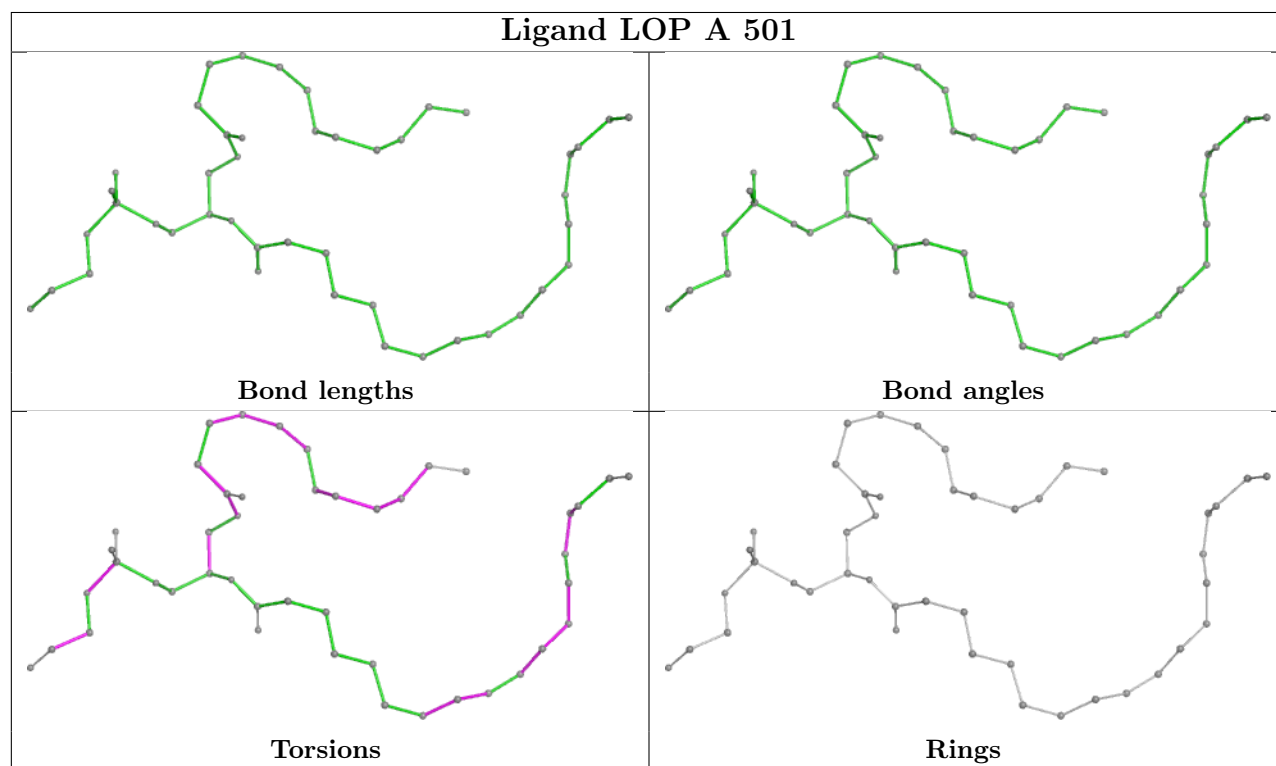
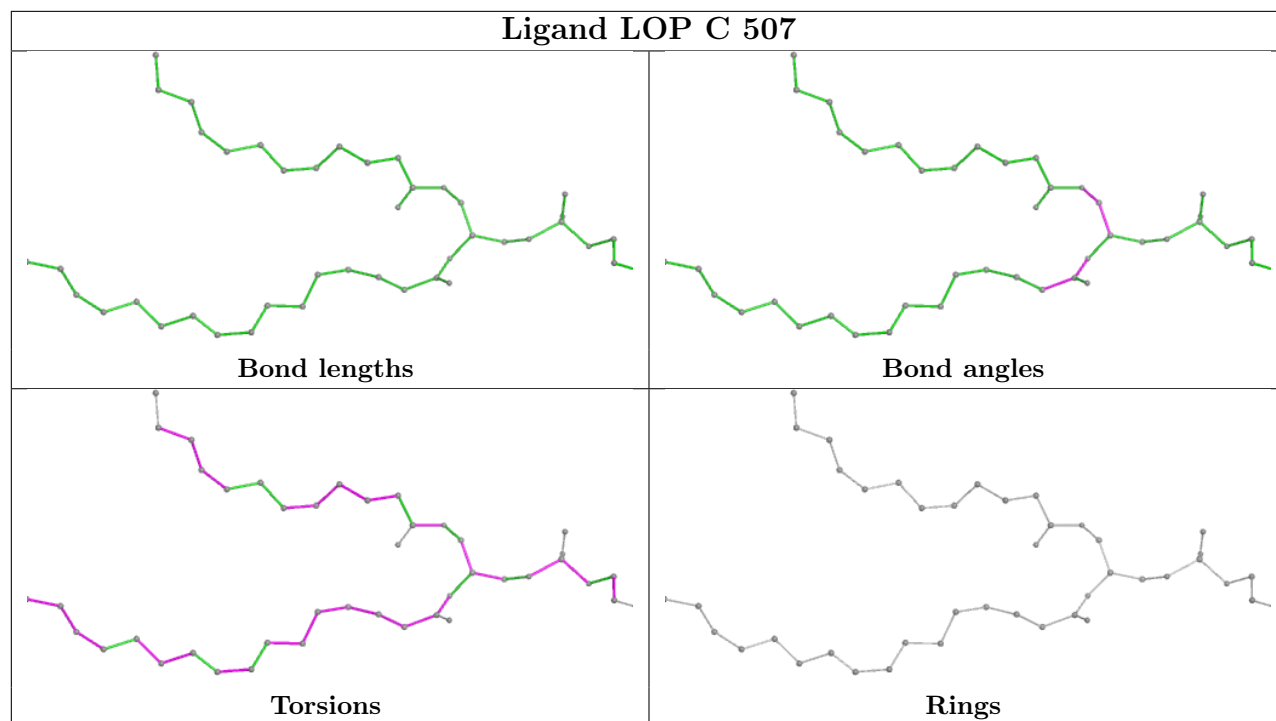


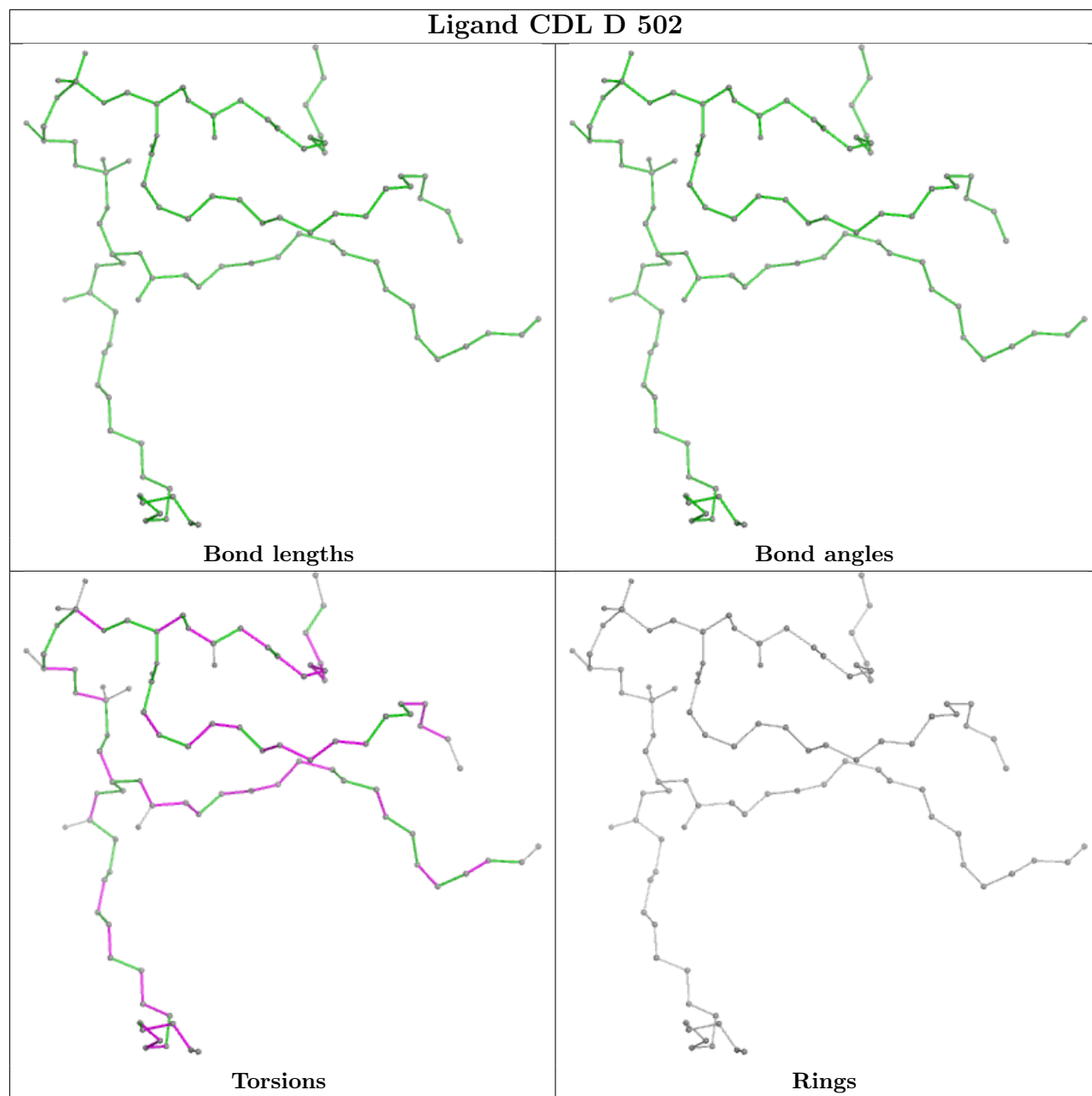
## Ligand LOP E 202

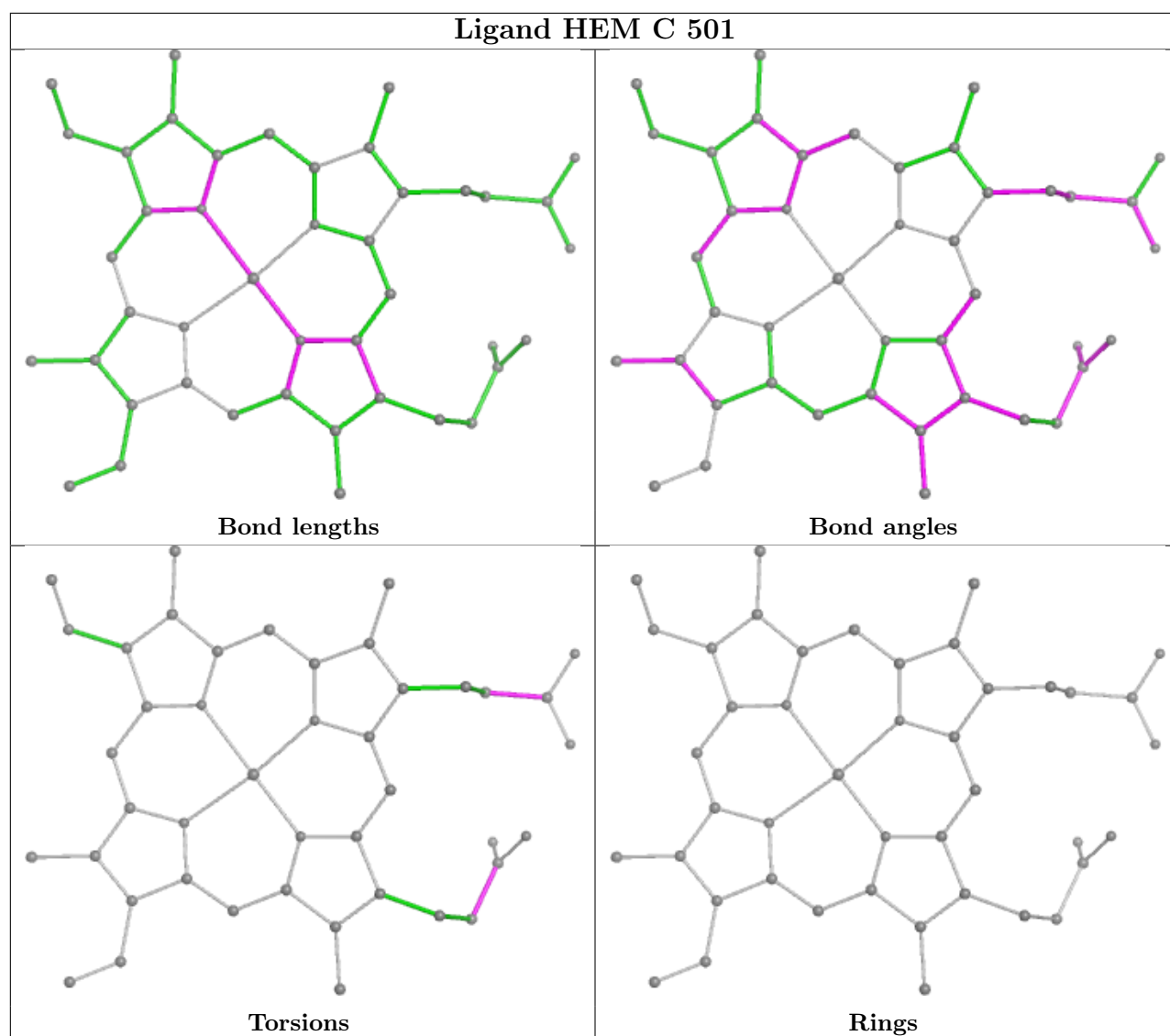


## Ligand A1IKG C 505









## 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	440/480 (91%)	-0.94	0	100   100	70, 111, 146, 195	0
2	B	414/453 (91%)	-0.86	1 (0%)	92   86	47, 112, 148, 230	1 (0%)
3	C	378/379 (99%)	-0.80	1 (0%)	90   82	28, 104, 140, 195	3 (0%)
4	D	240/325 (73%)	-0.69	0	100   100	91, 140, 171, 199	0
5	E	196/274 (71%)	-0.48	2 (1%)	79   60	88, 156, 199, 240	0
5	I	27/274 (9%)	0.16	2 (7%)	22   16	101, 143, 177, 188	0
6	F	98/111 (88%)	-0.72	0	100   100	82, 107, 149, 167	0
7	G	74/82 (90%)	-0.78	0	100   100	80, 115, 155, 176	0
8	H	65/109 (59%)	-0.52	0	100   100	126, 164, 182, 200	0
9	J	56/64 (87%)	-0.76	0	100   100	101, 121, 149, 167	0
10	K	39/56 (69%)	0.45	2 (5%)	34   24	152, 185, 233, 265	0
All	All	2027/2607 (77%)	-0.75	8 (0%)	89   79	28, 116, 177, 265	4 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	LEU	4.0
5	E	114	VAL	2.9
3	C	237	LEU	2.6
5	E	178	LEU	2.5
10	K	13	LEU	2.4

### 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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

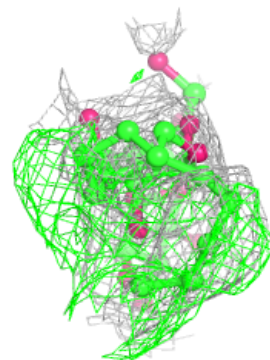
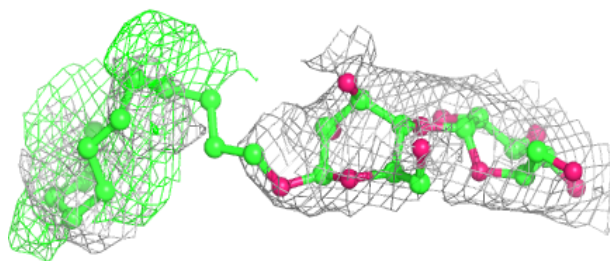
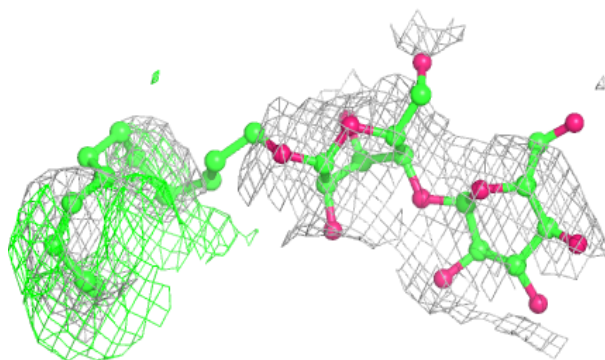
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
15	LMT	C	508	35/35	0.55	0.15	127,200,240,296	0
11	LOP	C	506	45/45	0.77	0.27	66,143,208,276	0
19	SO4	G	102	5/5	0.77	0.07	160,182,202,241	0
19	SO4	F	201	5/5	0.85	0.16	145,161,171,183	0
11	LOP	G	101	45/45	0.86	0.23	105,180,215,234	0
19	SO4	G	103	5/5	0.88	0.09	139,145,164,170	0
11	LOP	C	507	45/45	0.90	0.20	76,140,205,246	0
11	LOP	A	501	45/45	0.90	0.18	81,186,233,251	0
12	CDL	A	502	84/100	0.91	0.15	109,172,285,348	0
12	CDL	D	502	94/100	0.91	0.16	88,156,187,215	0
18	PSC	E	203	52/52	0.92	0.17	99,147,207,260	0
14	A1IKG	C	505	30/30	0.93	0.12	98,134,186,196	0
12	CDL	C	504	100/100	0.93	0.14	94,149,200,240	0
11	LOP	E	202	45/45	0.96	0.11	93,113,175,262	0
11	LOP	C	503	45/45	0.98	0.09	80,106,125,172	0
17	FES	E	201	4/4	0.98	0.06	220,233,252,274	0
16	HEC	D	501	43/43	0.99	0.07	116,138,150,162	0
13	HEM	C	501	43/43	0.99	0.05	86,94,105,128	0
13	HEM	C	502	43/43	0.99	0.06	62,96,111,124	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.

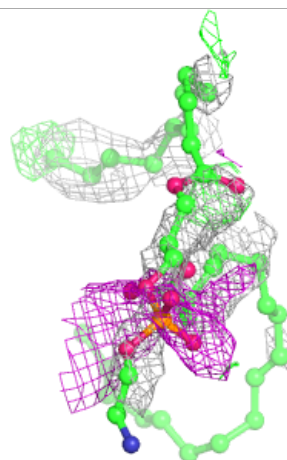
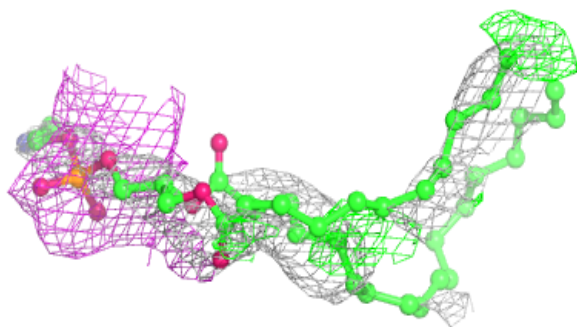
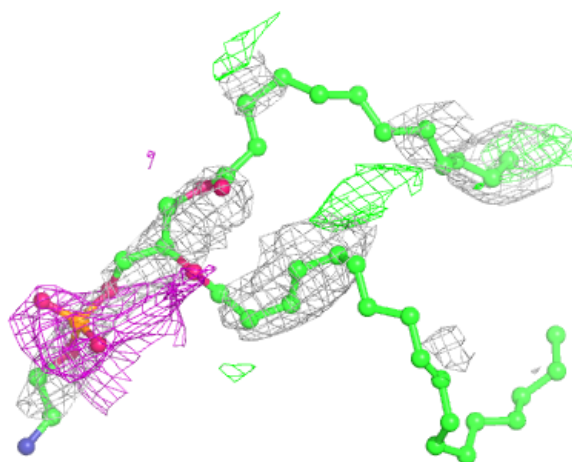
**Electron density around LMT C 508:**

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



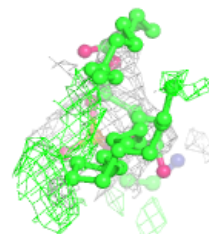
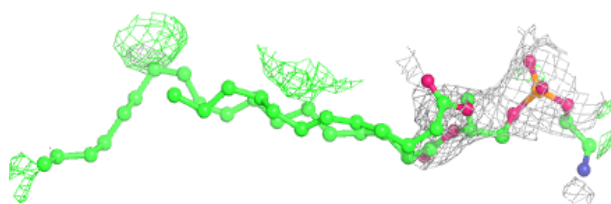
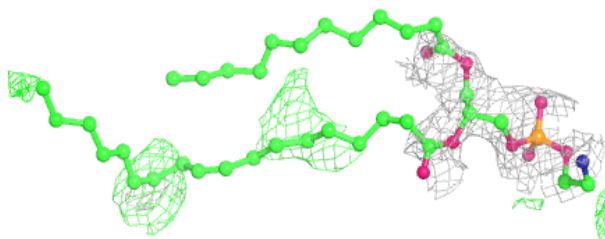
**Electron density around LOP C 506:**

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

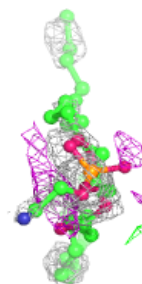
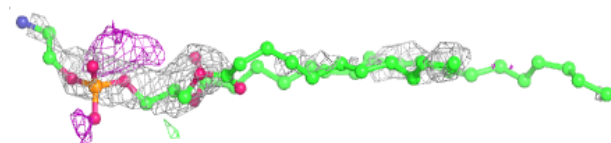
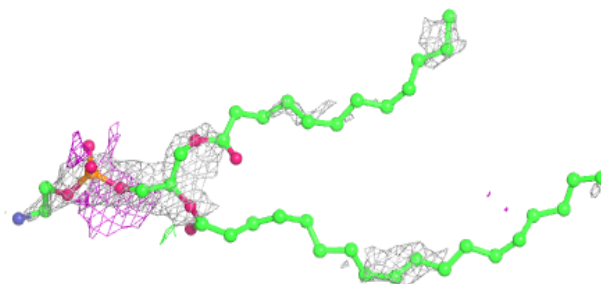


**Electron density around LOP G 101:**

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

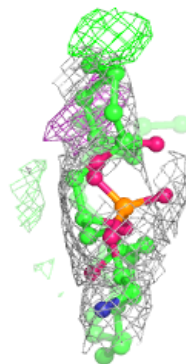
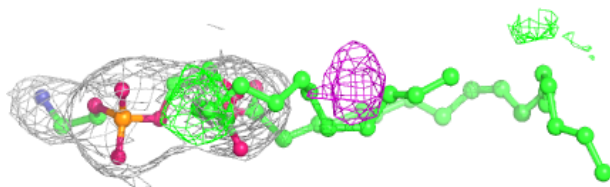
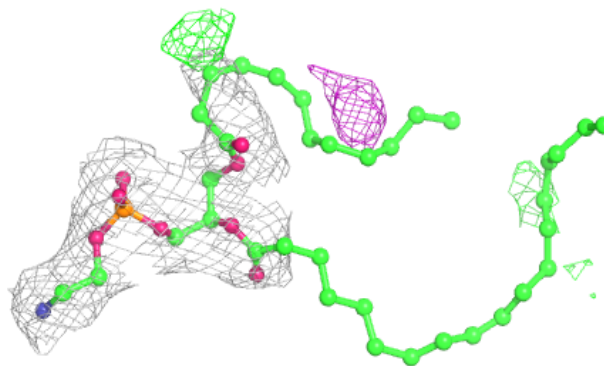
**Electron density around LOP C 507:**

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

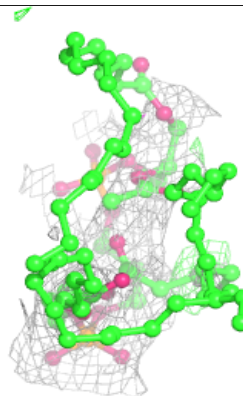
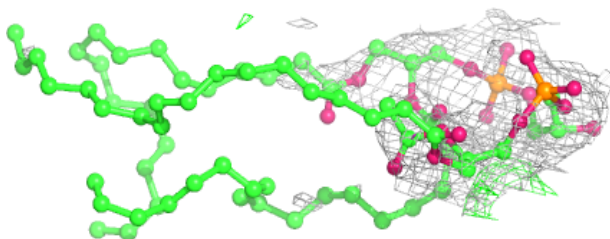
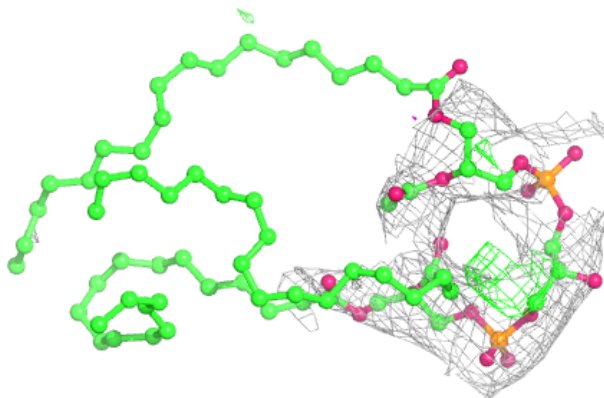


**Electron density around LOP A 501:**

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

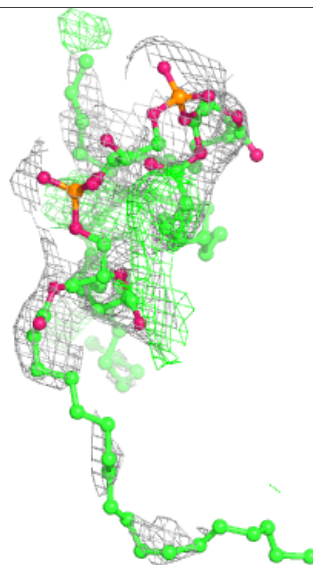
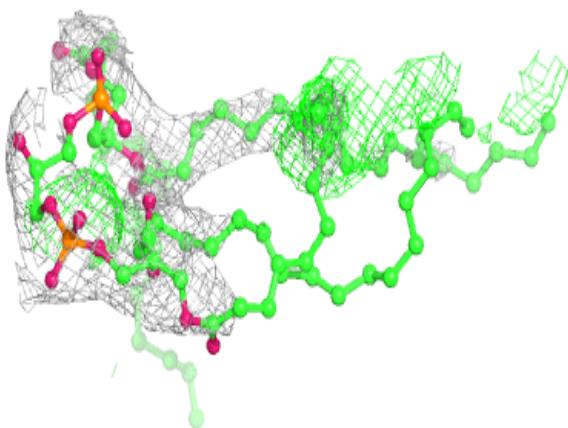
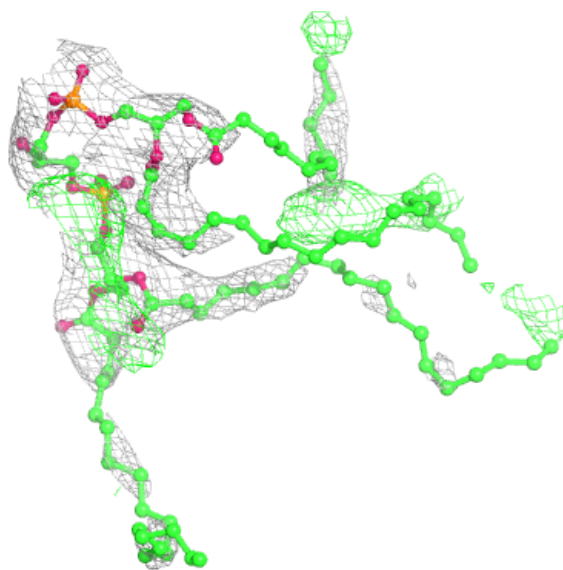
**Electron density around CDL A 502:**

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



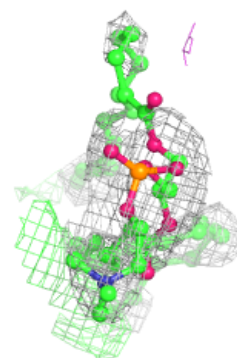
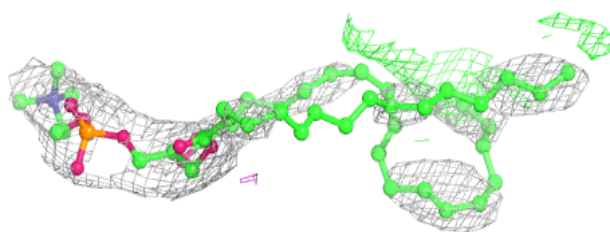
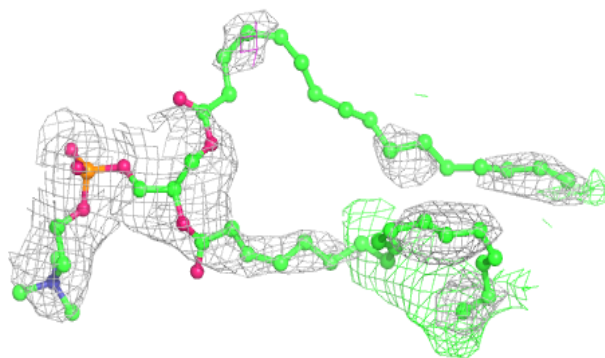
**Electron density around CDL D 502:**

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

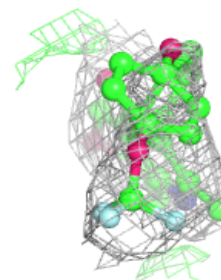
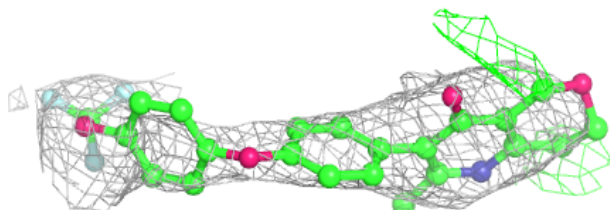
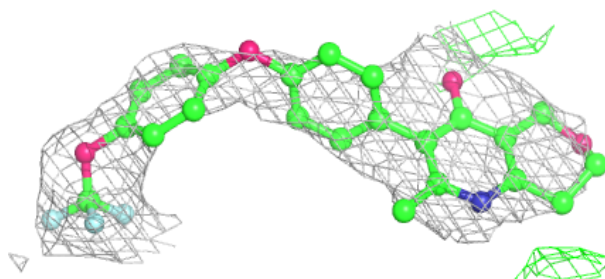


**Electron density around PSC E 203:**

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

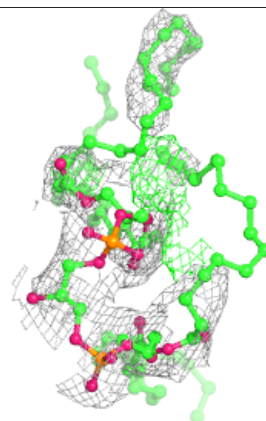
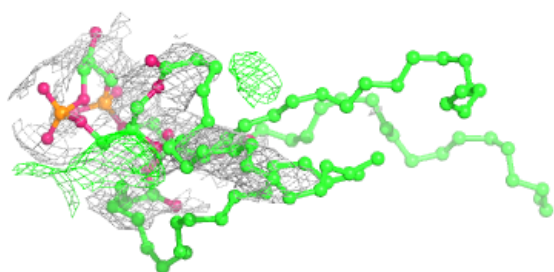
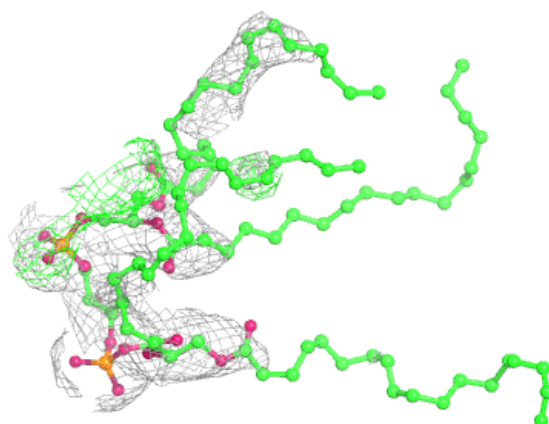
**Electron density around A1IKG C 505:**

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

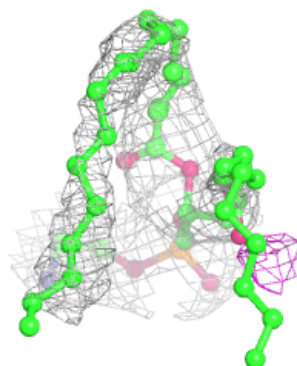
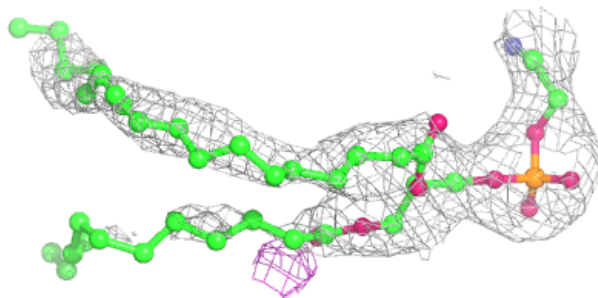
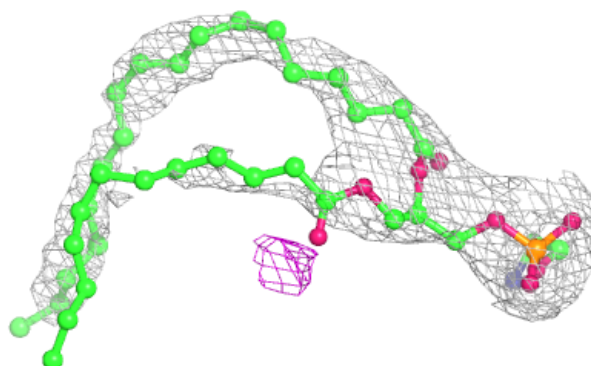


**Electron density around CDL C 504:**

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

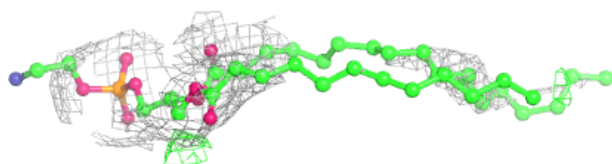
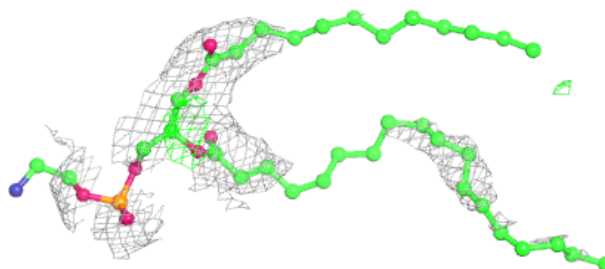
**Electron density around LOP E 202:**

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

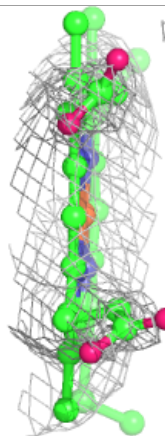
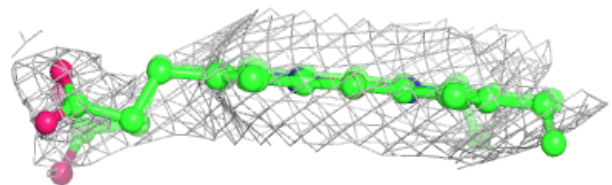
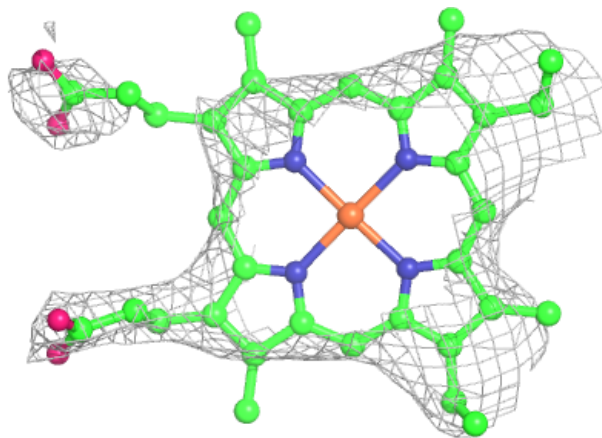


**Electron density around LOP C 503:**

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

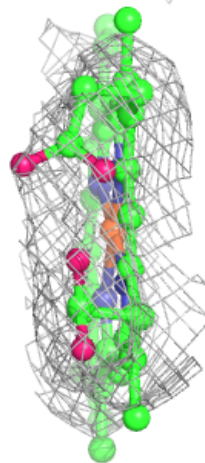
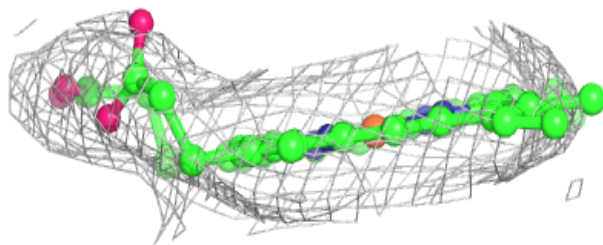
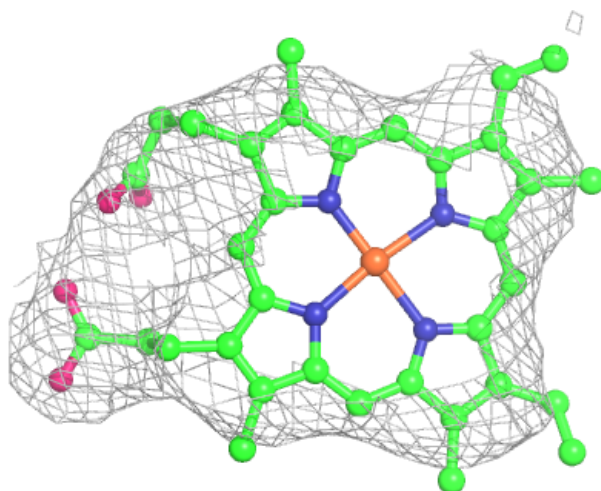
**Electron density around HEC D 501:**

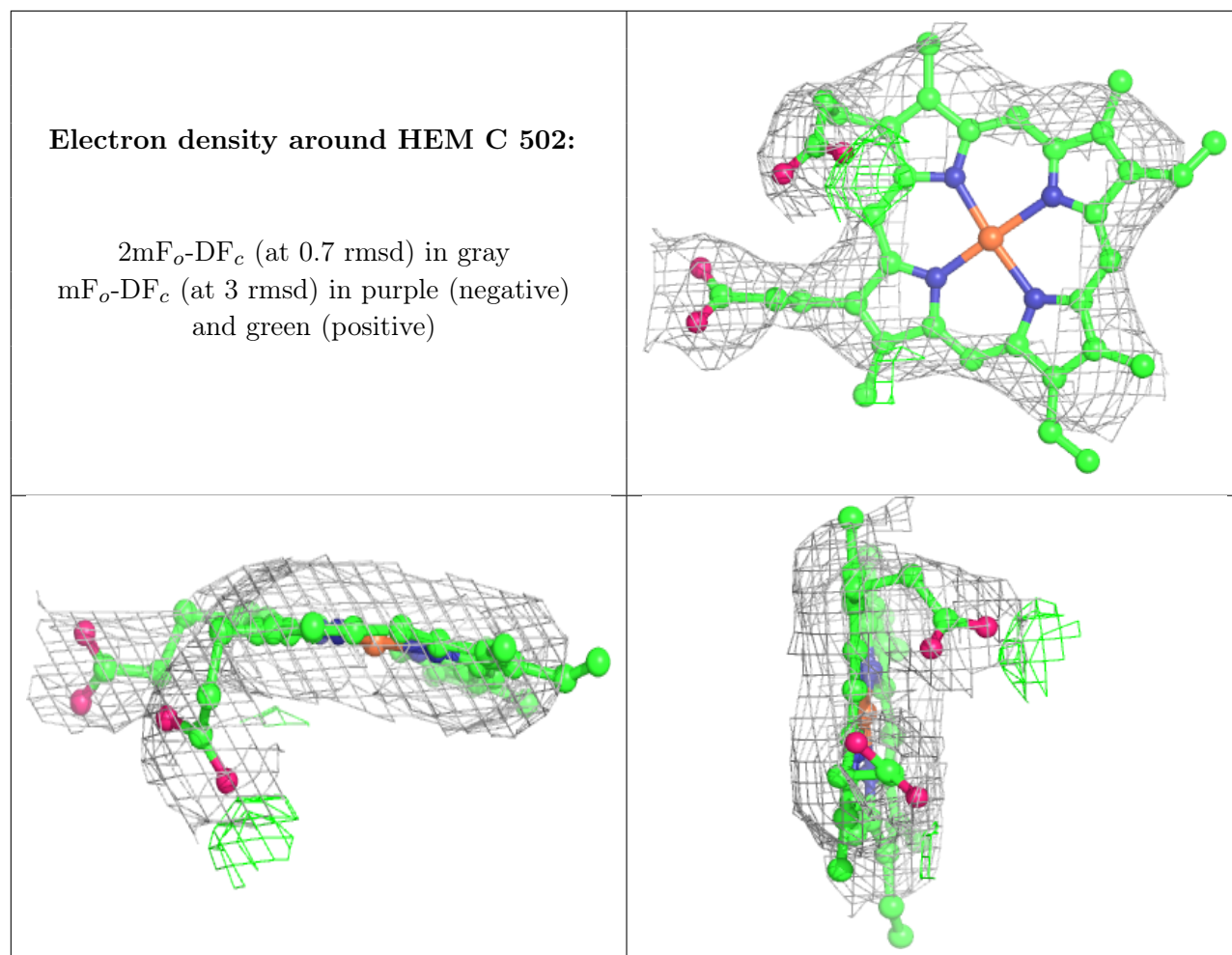
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.