



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 02:53 pm GMT

PDB ID : 4D6T
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GW844520
Authors : Capper, M.J.; O'Neill, P.M.; Fisher, N.; Strange, R.W.; Moss, D.; Ward, S.A.;
Berry, N.G.; Lawrenson, A.S.; Hasnain, S.S.; Biagini, G.A.; Antonyuk, S.V.
Deposited on : 2014-11-14
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

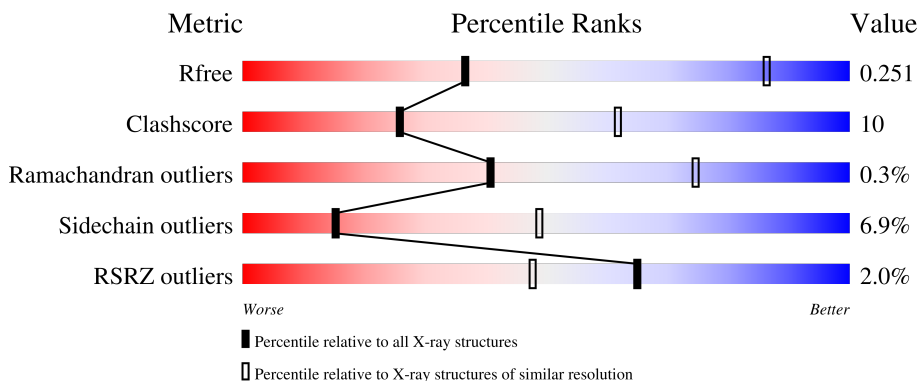
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	2% 75% 16% 8%
1	N	480	% 76% 15% 8%
2	B	453	6% 71% 19% 7%
3	C	379	75% 19% 8%
3	P	379	77% 17% 8%

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Mol	Chain	Length	Quality of chain
4	D	265	
4	Q	265	
5	E	274	
5	I	274	
5	R	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	J	64	
9	W	64	
10	O	453	
11	V	274	

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
14	PO4	F	501	-	-	-	X
14	PO4	N	501	-	-	-	X
14	PO4	S	501	-	-	-	X
15	PEE	C	505	X	-	-	-
15	PEE	D	506	X	-	-	-
15	PEE	P	505	X	-	-	-
15	PEE	Q	506	X	-	-	-
18	FES	R	501	-	-	X	-
19	GOL	R	502	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 31051 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
			Total	C	N	O	S			
1	A	444	Total 3439	C 2148	N 607	O 664	S 20	0	0	0
1	N	444	Total 3432	C 2142	N 607	O 663	S 20	0	0	0

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	422	Total 3164	C 1988	N 561	O 608	S 7	0	0	0

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	374	Total 2968	C 1993	N 463	O 494	S 18	0	0	0
3	P	370	Total 2936	C 1973	N 456	O 489	S 18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	240	Total 1912	C 1222	N 329	O 346	S 15	0	0	0
4	Q	241	Total 1918	C 1225	N 330	O 348	S 15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	73	Total	C	N	O	S	0	0	0
			549	341	92	114	2			
5	I	21	Total	C	N	O	S	0	0	0
			157	97	31	28	1			
5	R	196	Total	C	N	O	S	0	0	0
			1518	957	263	290	8			

- 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	154	157	2			
6	S	99	Total	C	N	O	S	0	0	0
			869	553	156	158	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
S	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			677	439	127	110	1			
7	T	74	Total	C	N	O	S	0	0	0
			624	408	117	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			
8	U	66	Total	C	N	O	S	0	0	0
			538	327	98	108	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	58	Total	C	N	O	0	0	0
			482	317	83	82			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	W	59	487	320	84	83	0	0	0

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	O	419	3140	1972	555	606	7	0	0	0

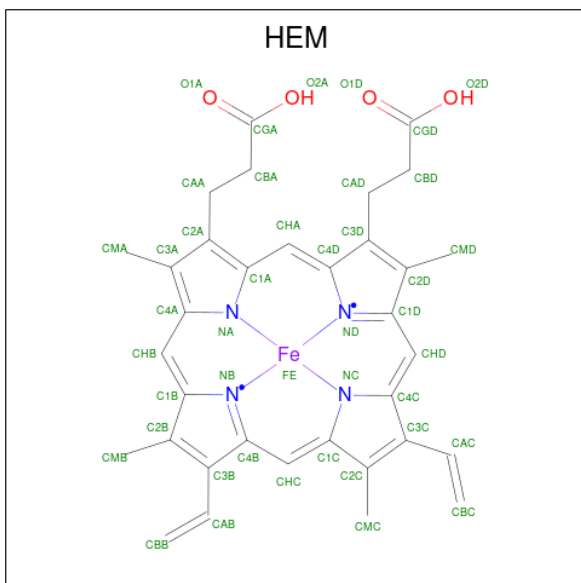
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	305	GLU	GLN	conflict	UNP P23004

- Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

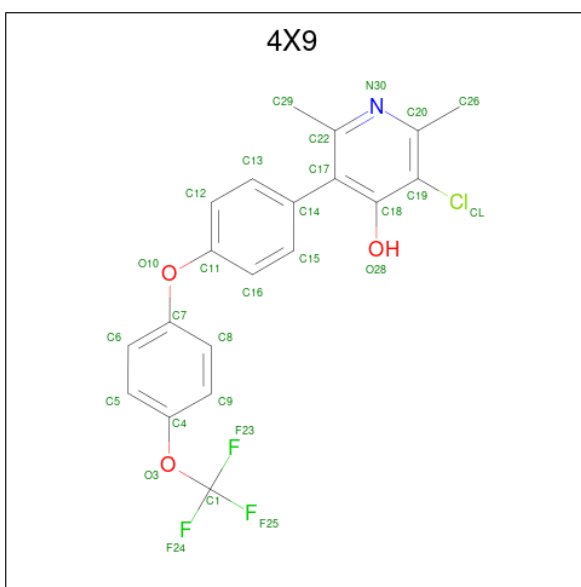
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	V	17	127	81	24	22	0	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 13 is 3-chloro-2,6-dimethyl-5-[4-[4-(trifluoromethoxy)phenoxy]phenyl]pyridin-4-ol (three-letter code: 4X9) (formula: C₂₀H₁₅ClF₃NO₃).



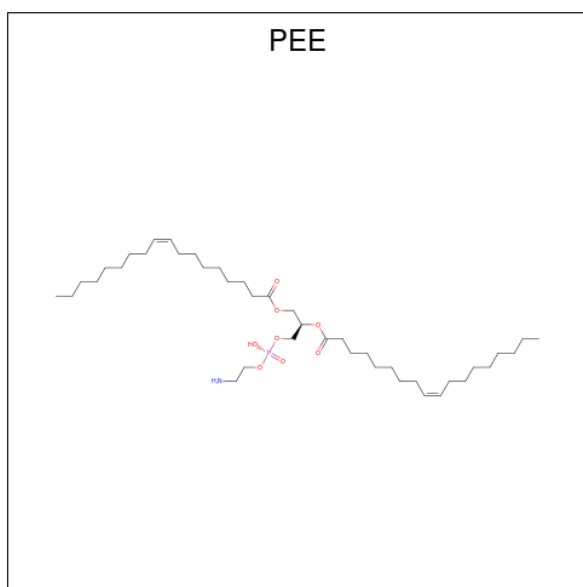
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
13	C	1	Total	C	Cl	F	N	O	0	0
			28	20	1	3	1	3		
13	P	1	Total	C	Cl	F	N	O	0	0
			28	20	1	3	1	3		

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



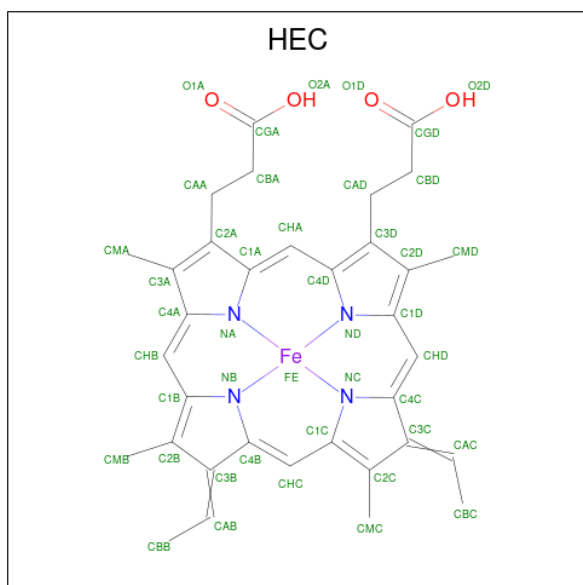
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total O P 5 4 1	0	0
14	D	1	Total O P 5 4 1	0	0
14	D	1	Total O P 5 4 1	0	0
14	D	1	Total O P 5 4 1	0	0
14	E	1	Total O P 5 4 1	0	0
14	F	1	Total O P 5 4 1	0	0
14	N	1	Total O P 5 4 1	0	0
14	N	1	Total O P 5 4 1	0	0
14	Q	1	Total O P 5 4 1	0	0
14	Q	1	Total O P 5 4 1	0	0
14	S	1	Total O P 5 4 1	0	0

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P).



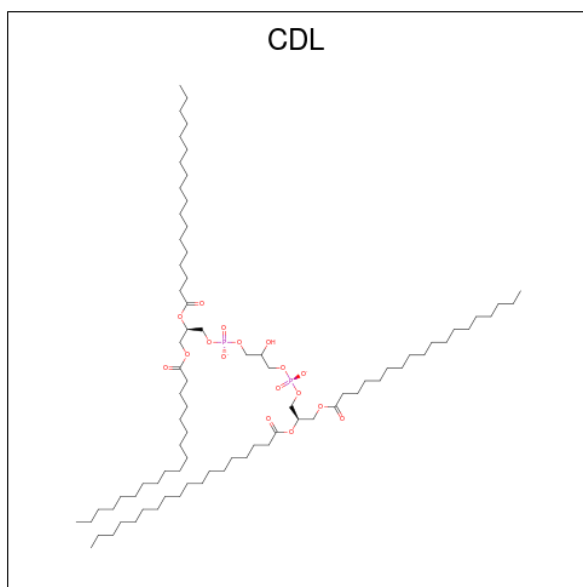
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
15	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	D	1	Total 26	C 16	N 1	O 8	P 1	0	0
15	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0

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



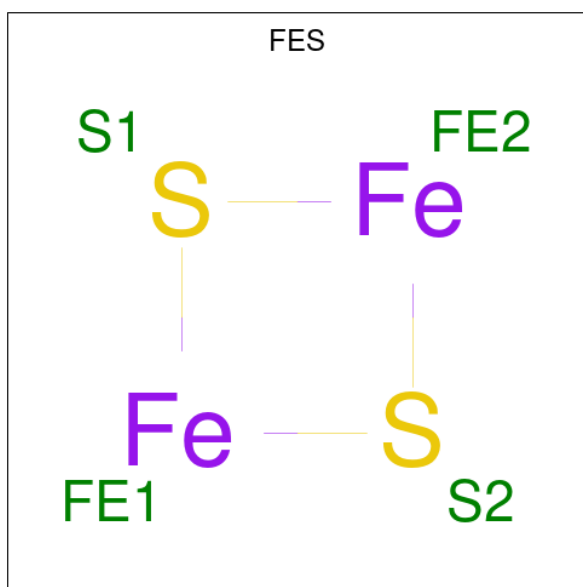
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
16	D	1	43	34	1	4	4	0	0
16	Q	1	43	34	1	4	4	0	0

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



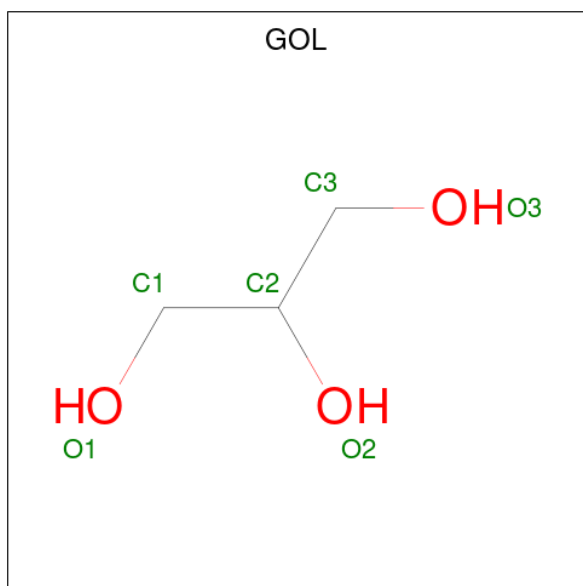
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
17	D	1	39	24	13	2	0	0
17	G	1	44	25	17	2	0	0
17	Q	1	39	24	13	2	0	0
17	T	1	49	30	17	2	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 19 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

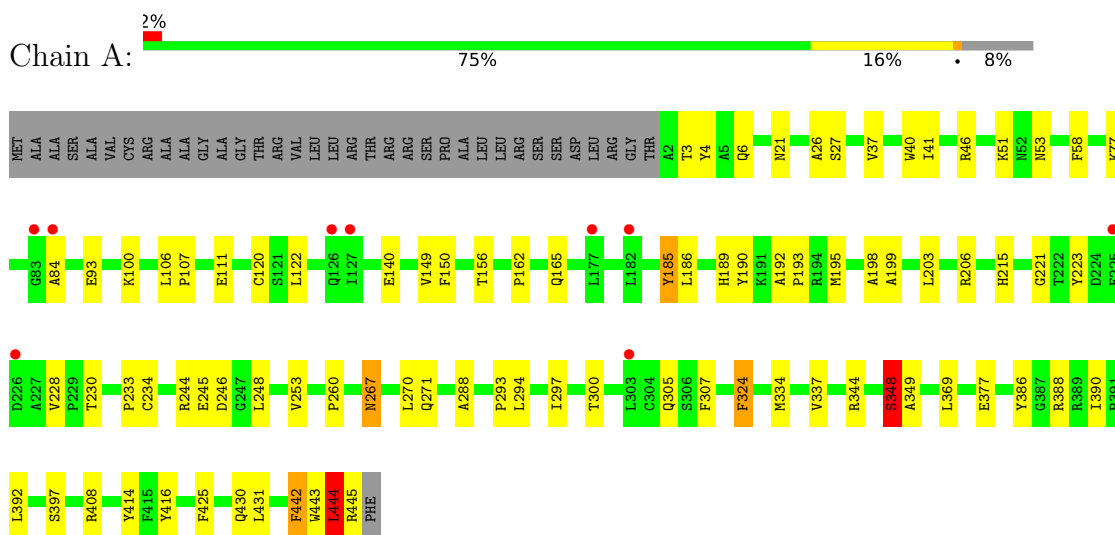


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	R	1	6	3	3	0	0

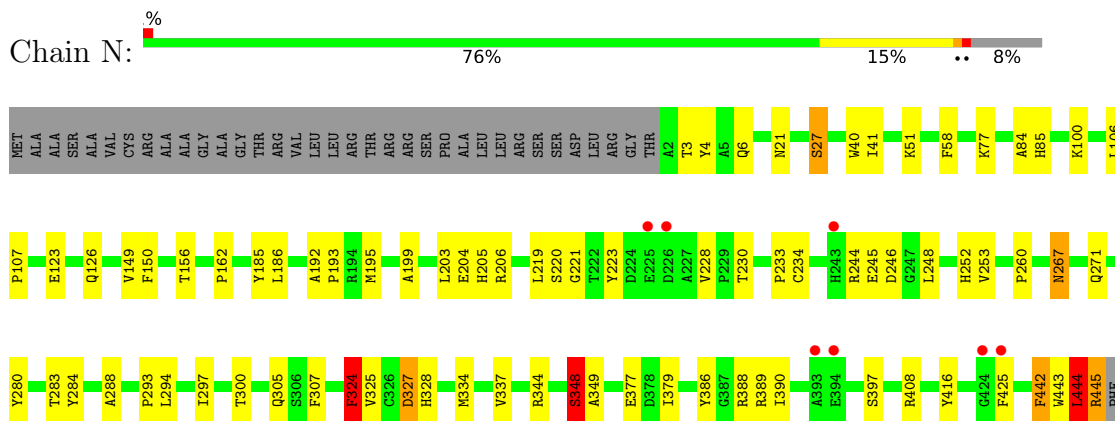
3 Residue-property plots [i](#)

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.

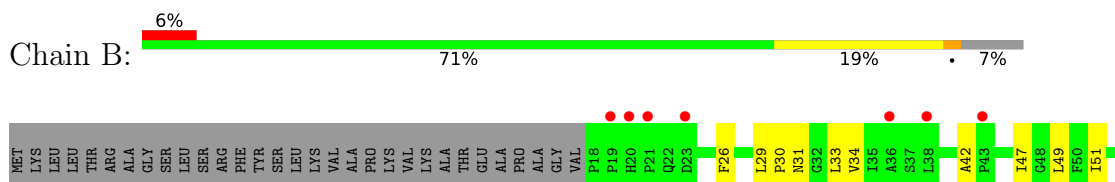
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

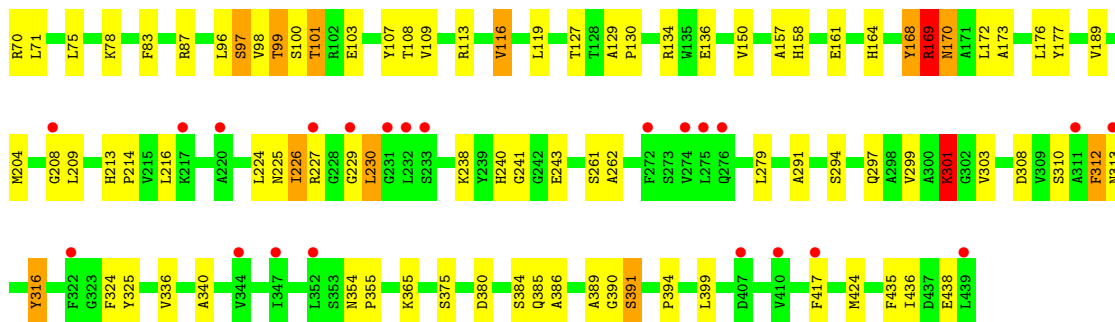


- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

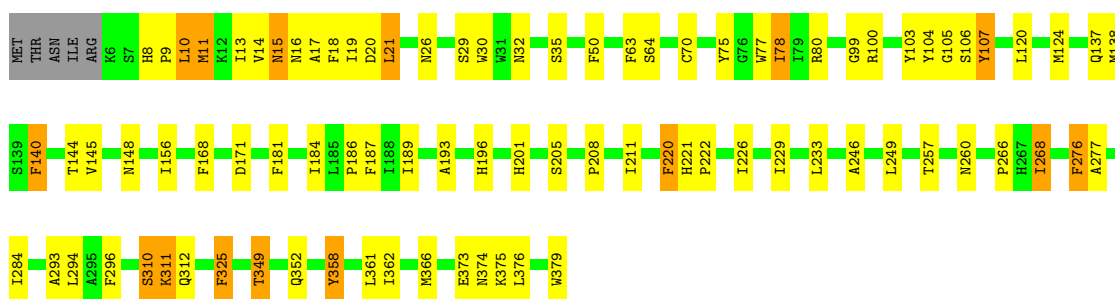
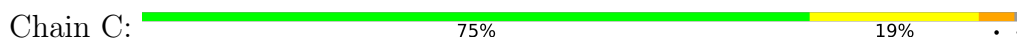


- Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

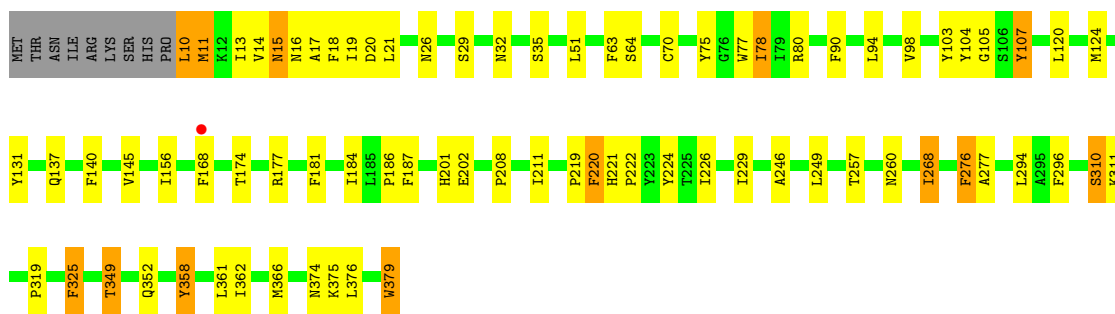
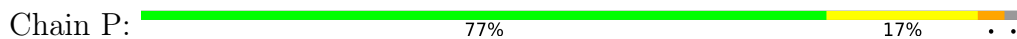




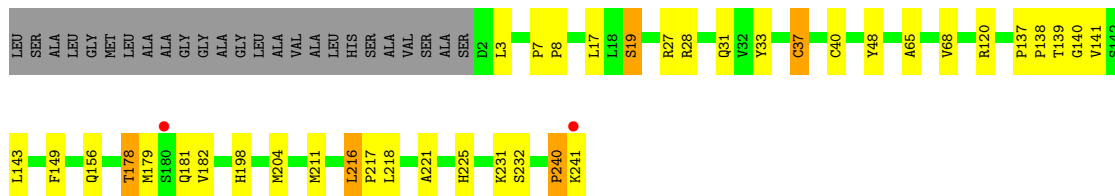
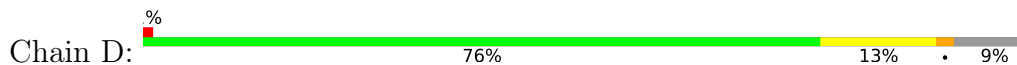
● Molecule 3: CYTOCHROME B



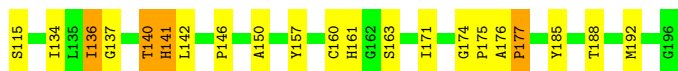
● Molecule 3: CYTOCHROME B



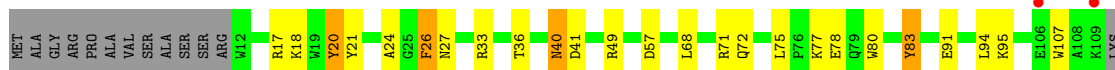
● Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



● Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



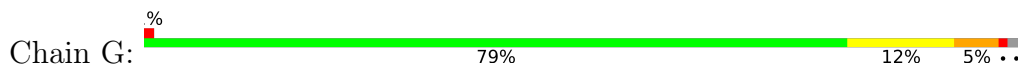
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



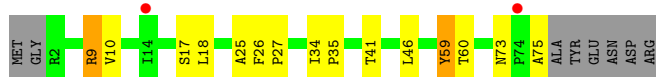
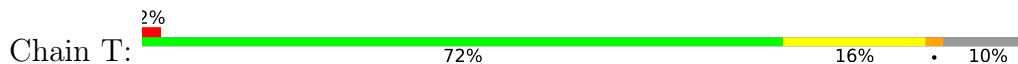
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



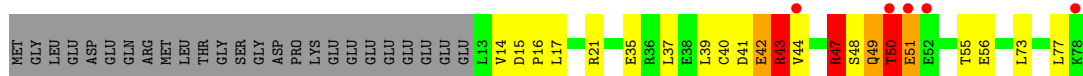
- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



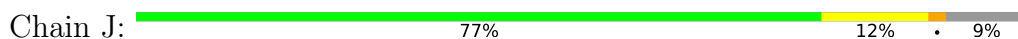
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.90Å 129.90Å 722.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.57 49.81 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.57) 99.9 (49.81-3.57)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.252 0.207 , 0.251	Depositor DCC
R_{free} test set	3953 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31051	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CDL, 4X9, HEC, PEE, HEM, FES, GOL

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	0.46	1/3511 (0.0%)	0.69	5/4766 (0.1%)
1	N	0.42	0/3503	0.70	7/4755 (0.1%)
2	B	0.69	3/3224 (0.1%)	0.80	10/4375 (0.2%)
3	C	0.50	0/3065	0.68	0/4196
3	P	0.48	1/3031 (0.0%)	0.67	0/4150
4	D	0.42	0/1971	0.62	0/2676
4	Q	0.42	0/1977	0.61	0/2684
5	E	0.41	0/557	0.62	0/752
5	I	0.57	0/156	1.24	2/209 (1.0%)
5	R	0.43	0/1552	0.78	7/2100 (0.3%)
6	F	0.46	0/879	0.68	0/1180
6	S	0.47	0/888	0.65	0/1191
7	G	0.52	1/699 (0.1%)	1.26	6/946 (0.6%)
7	T	0.49	0/645	0.74	0/873
8	H	2.11	7/534 (1.3%)	1.96	8/718 (1.1%)
8	U	1.48	6/543 (1.1%)	2.09	10/729 (1.4%)
9	J	0.42	0/495	0.59	0/667
9	W	0.43	0/500	0.60	0/675
10	O	0.50	2/3197 (0.1%)	0.95	12/4336 (0.3%)
11	V	0.58	0/129	0.86	0/177
All	All	0.59	21/31056 (0.1%)	0.82	67/42155 (0.2%)

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	1
1	N	0	1
2	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
8	U	0	3
10	O	0	2
All	All	0	11

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH2	28.39	1.70	1.33
8	H	43	ARG	CZ-NH1	26.86	1.68	1.33
8	H	47	ARG	CZ-NH2	25.79	1.66	1.33
8	U	47	ARG	CZ-NH2	25.71	1.66	1.33
8	H	43	ARG	NE-CZ	23.73	1.64	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	47	ARG	NE-CZ-NH2	-37.30	101.65	120.30
8	H	47	ARG	NE-CZ-NH2	33.38	136.99	120.30
7	G	75	ALA	N-CA-CB	-19.29	83.10	110.10
8	U	43	ARG	NH1-CZ-NH2	-18.82	98.69	119.40
10	O	169	ARG	NH1-CZ-NH2	-17.91	99.70	119.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	LEU	Peptide
2	B	169	ARG	Sidechain
2	B	301	LYS	Peptide
7	G	77	TYR	Peptide
8	H	50	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3337	45	0
1	N	3432	0	3330	42	0
2	B	3164	0	3144	80	0
3	C	2968	0	3028	82	0
3	P	2936	0	2996	71	0
4	D	1912	0	1861	42	0
4	Q	1918	0	1870	38	0
5	E	549	0	547	9	0
5	I	157	0	171	27	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	24	0
7	G	677	0	672	9	0
7	T	624	0	630	8	0
8	H	529	0	512	45	0
8	U	538	0	522	23	1
9	J	482	0	483	8	0
9	W	487	0	487	9	0
10	O	3140	0	3121	104	0
11	V	127	0	135	40	0
12	C	86	0	60	10	0
12	P	86	0	60	10	0
13	C	28	0	14	6	0
13	P	28	0	14	5	0
14	C	5	0	0	0	0
14	D	15	0	0	0	0
14	E	5	0	0	0	0
14	F	5	0	0	0	0
14	N	10	0	0	0	0
14	Q	10	0	0	0	0
14	S	5	0	0	0	0
15	C	49	0	72	1	0
15	D	26	0	26	0	0
15	P	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	12	0
16	Q	43	0	32	10	0
17	D	39	0	39	0	0
17	G	44	0	32	0	0
17	Q	39	0	39	1	0
17	T	49	0	42	1	0
18	R	4	0	0	3	0
19	R	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31051	0	30685	645	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 10.

The worst 5 of 645 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)
8:H:43:ARG:CZ	8:H:43:ARG:NH1	1.68	1.56
2:B:169:ARG:CZ	2:B:169:ARG:NH2	1.70	1.49
8:H:47:ARG:CD	8:H:50:THR:HG21	1.35	1.44
8:H:47:ARG:CD	8:H:50:THR:CG2	2.07	1.32
8:H:47:ARG:HD2	8:H:50:THR:CG2	1.62	1.28

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)
6:F:57:ASP:OD2	8:U:42:GLU:OE2[1_655]	1.73	0.47

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	442/480 (92%)	405 (92%)	35 (8%)	2 (0%)	29 67
1	N	442/480 (92%)	407 (92%)	33 (8%)	2 (0%)	29 67
2	B	420/453 (93%)	375 (89%)	44 (10%)	1 (0%)	47 80
3	C	372/379 (98%)	347 (93%)	23 (6%)	2 (0%)	29 67
3	P	368/379 (97%)	337 (92%)	30 (8%)	1 (0%)	41 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	238/265 (90%)	216 (91%)	21 (9%)	1 (0%)	34	71
4	Q	239/265 (90%)	218 (91%)	20 (8%)	1 (0%)	34	71
5	E	71/274 (26%)	64 (90%)	7 (10%)	0	100	100
5	I	17/274 (6%)	12 (71%)	5 (29%)	0	100	100
5	R	194/274 (71%)	174 (90%)	19 (10%)	1 (0%)	29	67
6	F	96/111 (86%)	87 (91%)	9 (9%)	0	100	100
6	S	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
7	G	78/82 (95%)	67 (86%)	10 (13%)	1 (1%)	12	49
7	T	72/82 (88%)	62 (86%)	10 (14%)	0	100	100
8	H	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
8	U	64/91 (70%)	61 (95%)	3 (5%)	0	100	100
9	J	56/64 (88%)	51 (91%)	5 (9%)	0	100	100
9	W	57/64 (89%)	51 (90%)	6 (10%)	0	100	100
10	O	417/453 (92%)	376 (90%)	41 (10%)	0	100	100
11	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3818/4946 (77%)	3470 (91%)	336 (9%)	12 (0%)	41	74

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	N	267	ASN
3	P	107	TYR
5	R	177	PRO
3	C	107	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/394 (93%)	350 (95%)	18 (5%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	367/394 (93%)	347 (95%)	20 (5%)	22	57
2	B	331/355 (93%)	309 (93%)	22 (7%)	16	51
3	C	322/327 (98%)	301 (94%)	21 (6%)	17	51
3	P	318/327 (97%)	297 (93%)	21 (7%)	16	51
4	D	205/218 (94%)	196 (96%)	9 (4%)	28	63
4	Q	206/218 (94%)	196 (95%)	10 (5%)	25	59
5	E	63/228 (28%)	57 (90%)	6 (10%)	8	37
5	I	19/228 (8%)	13 (68%)	6 (32%)	0	2
5	R	168/228 (74%)	158 (94%)	10 (6%)	19	54
6	F	90/99 (91%)	82 (91%)	8 (9%)	9	40
6	S	91/99 (92%)	84 (92%)	7 (8%)	13	44
7	G	71/72 (99%)	64 (90%)	7 (10%)	8	35
7	T	66/72 (92%)	59 (89%)	7 (11%)	6	33
8	H	62/85 (73%)	54 (87%)	8 (13%)	4	24
8	U	63/85 (74%)	56 (89%)	7 (11%)	6	31
9	J	49/54 (91%)	45 (92%)	4 (8%)	11	42
9	W	49/54 (91%)	44 (90%)	5 (10%)	7	34
10	O	328/355 (92%)	304 (93%)	24 (7%)	14	46
11	V	15/228 (7%)	12 (80%)	3 (20%)	1	8
All	All	3251/4120 (79%)	3028 (93%)	223 (7%)	15	49

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	186	LEU
9	W	37	GLN
10	O	230	LEU
9	W	13	LEU
6	S	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	225	HIS

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Mol	Chain	Res	Type
1	N	118	GLN
3	P	16	ASN
7	G	79	ASN
1	N	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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
19	GOL	R	502	-	5,5,5	0.33	0	5,5,5	0.45	0
12	HEM	C	501	3	41,50,50	1.43	6 (14%)	45,82,82	1.96	12 (26%)
15	PEE	C	505	-	48,48,50	1.27	4 (8%)	51,53,55	1.03	4 (7%)
16	HEC	D	501	4	32,50,50	2.21	12 (37%)	24,82,82	2.74	9 (37%)
16	HEC	Q	501	4	32,50,50	2.23	11 (34%)	24,82,82	2.29	6 (25%)
14	PO4	C	504	-	4,4,4	0.95	0	6,6,6	0.43	0
14	PO4	S	501	-	4,4,4	0.86	0	6,6,6	0.48	0
14	PO4	D	503	-	4,4,4	0.88	0	6,6,6	0.67	0
15	PEE	Q	506	-	50,50,50	1.30	4 (8%)	53,55,55	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CDL	G	501	-	43,43,99	1.55	4 (9%)	49,55,111	1.57	8 (16%)
12	HEM	P	502	3	41,50,50	1.45	7 (17%)	45,82,82	1.94	15 (33%)
12	HEM	P	501	3	41,50,50	1.38	6 (14%)	45,82,82	1.96	16 (35%)
14	PO4	Q	1002	-	4,4,4	0.89	0	6,6,6	0.48	0
12	HEM	C	502	3	41,50,50	1.49	7 (17%)	45,82,82	1.69	9 (20%)
17	CDL	D	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.16	4 (9%)
14	PO4	D	504	-	4,4,4	0.85	0	6,6,6	0.58	0
14	PO4	Q	1001	-	4,4,4	0.87	0	6,6,6	0.47	0
14	PO4	F	501	-	4,4,4	0.87	0	6,6,6	0.62	0
13	4X9	P	503	-	30,30,30	2.79	6 (20%)	43,44,44	1.90	8 (18%)
17	CDL	Q	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.19	5 (11%)
17	CDL	T	501	-	48,48,99	1.39	4 (8%)	54,60,111	1.18	4 (7%)
14	PO4	D	502	-	4,4,4	0.76	0	6,6,6	0.63	0
15	PEE	P	505	-	48,48,50	1.34	4 (8%)	51,53,55	0.93	1 (1%)
13	4X9	C	503	-	30,30,30	2.97	7 (23%)	43,44,44	1.43	3 (6%)
14	PO4	N	501	-	4,4,4	0.72	0	6,6,6	0.98	0
14	PO4	N	1001	-	4,4,4	0.81	0	6,6,6	0.78	0
18	FES	R	501	5	0,4,4	-	-	-	-	-
14	PO4	E	501	-	4,4,4	0.69	0	6,6,6	0.81	0
15	PEE	D	506	-	25,25,50	1.49	2 (8%)	28,30,55	1.46	4 (14%)

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
15	PEE	C	505	-	1/1/4/8	25/52/52/54	-
19	GOL	R	502	-	-	2/4/4/4	-
15	PEE	P	505	-	1/1/4/8	22/52/52/54	-
16	HEC	D	501	4	-	8/10/54/54	-
13	4X9	C	503	-	-	5/13/13/13	0/3/3/3
17	CDL	T	501	-	-	28/57/57/110	-
12	HEM	C	502	3	-	6/12/54/54	-
12	HEM	C	501	3	-	4/12/54/54	-
16	HEC	Q	501	4	-	5/10/54/54	-
17	CDL	D	505	-	-	21/43/43/110	-
15	PEE	Q	506	-	1/1/4/8	24/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CDL	G	501	-	-	25/52/52/110	-
18	FES	R	501	5	-	-	0/1/1/1
17	CDL	Q	505	-	-	13/43/43/110	-
13	4X9	P	503	-	-	3/13/13/13	0/3/3/3
12	HEM	P	502	3	-	7/12/54/54	-
12	HEM	P	501	3	-	8/12/54/54	-
15	PEE	D	506	-	1/1/4/8	13/29/29/54	-

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	503	4X9	C19-C20	8.52	1.50	1.38
13	C	503	4X9	C17-C18	8.10	1.50	1.40
13	C	503	4X9	C19-C20	7.70	1.49	1.38
13	C	503	4X9	C17-C22	7.65	1.49	1.40
16	D	501	HEC	C3C-C2C	6.89	1.47	1.40

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	503	4X9	C20-C19-C18	-7.02	118.33	122.79
16	Q	501	HEC	C1D-C2D-C3D	-6.86	102.23	107.00
16	D	501	HEC	CBA-CAA-C2A	6.42	123.43	112.60
16	D	501	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
16	D	501	HEC	CMC-C2C-C3C	5.18	131.91	125.82

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	505	PEE	C2
15	D	506	PEE	C2
15	P	505	PEE	C2
15	Q	506	PEE	C2

5 of 219 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	502	HEM	C2D-C3D-CAD-CBD
12	C	502	HEM	C4D-C3D-CAD-CBD
12	P	501	HEM	C1A-C2A-CAA-CBA

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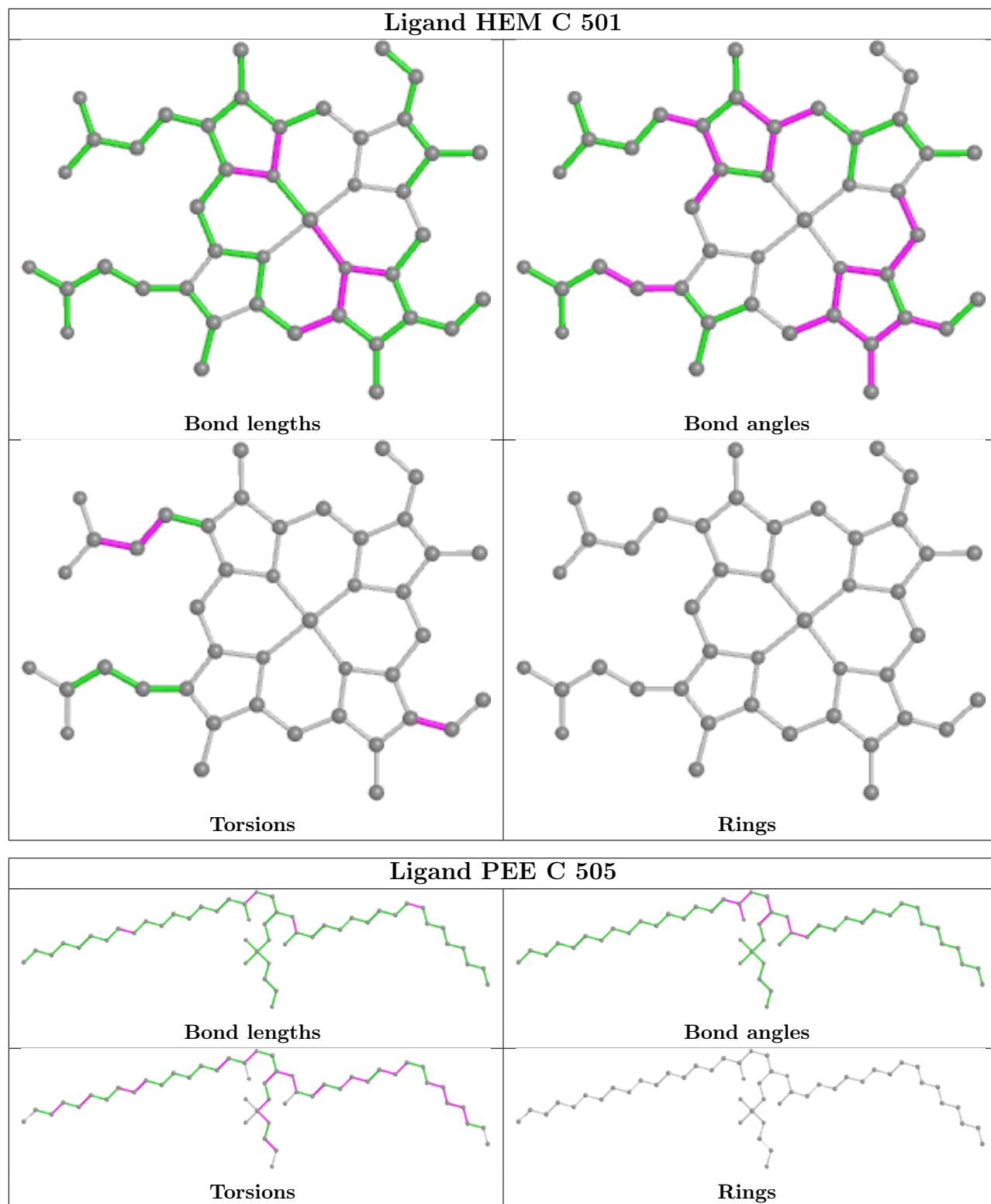
Mol	Chain	Res	Type	Atoms
12	P	501	HEM	C3A-C2A-CAA-CBA
15	D	506	PEE	C1-O3P-P-O2P

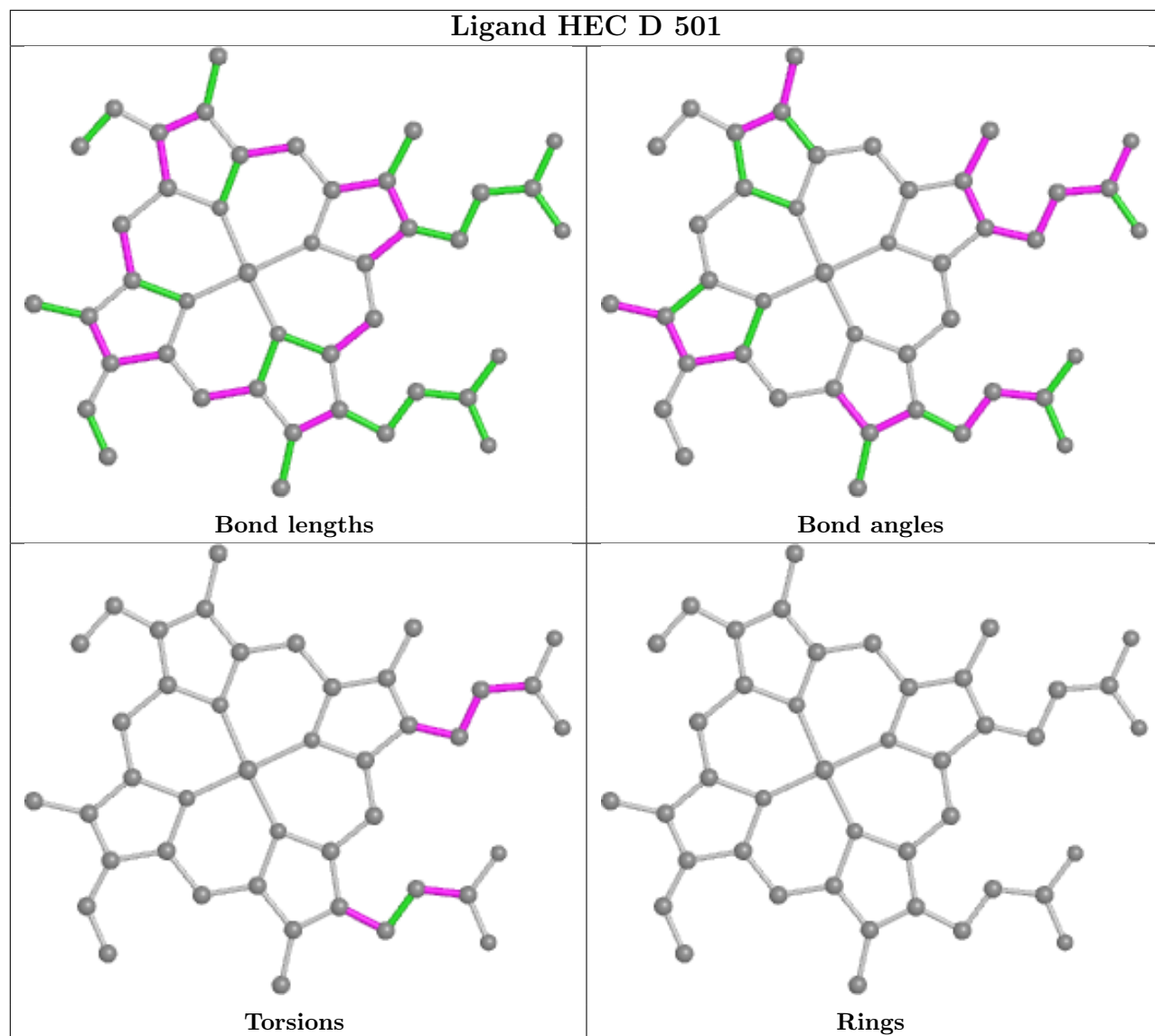
There are no ring outliers.

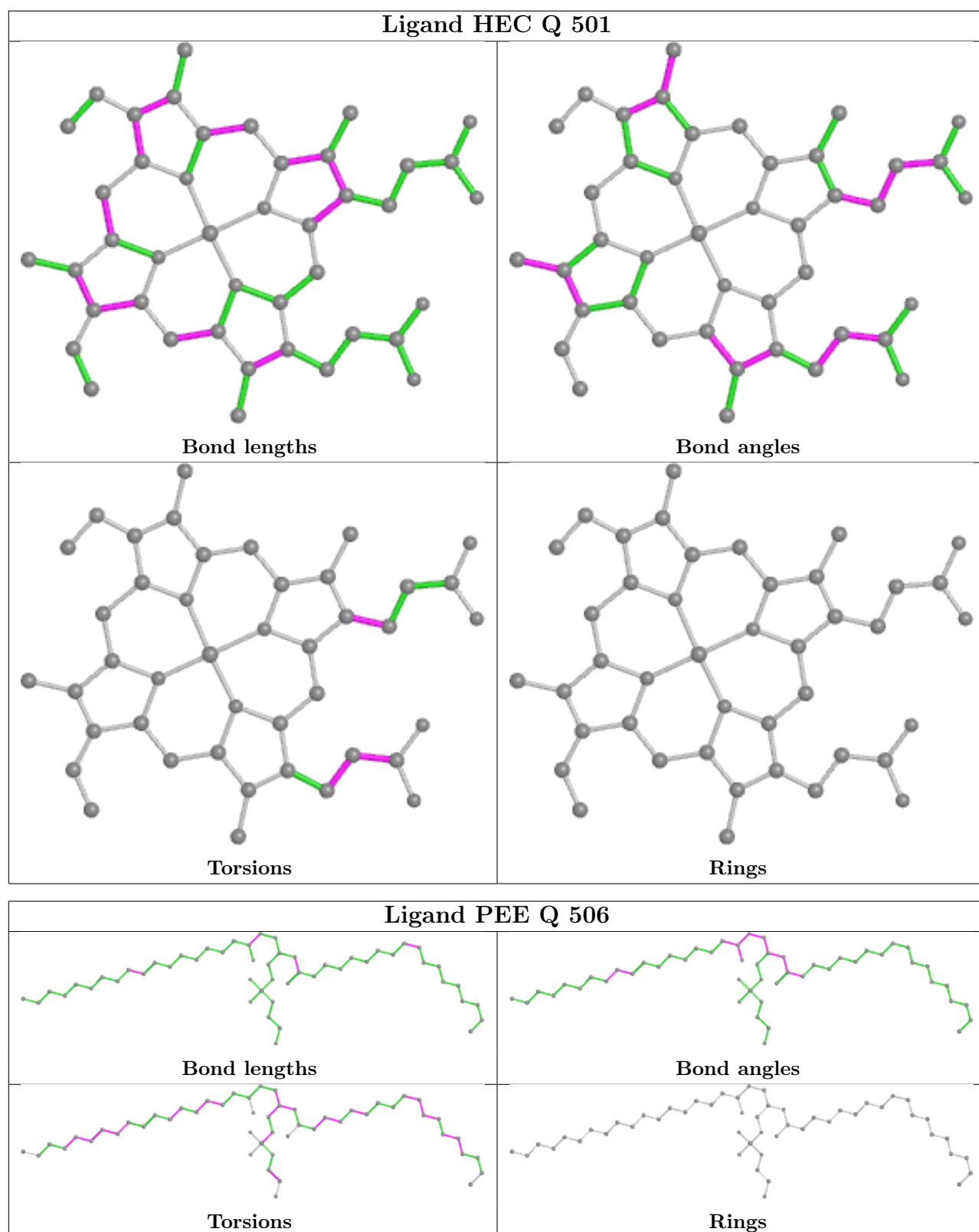
14 monomers are involved in 62 short contacts:

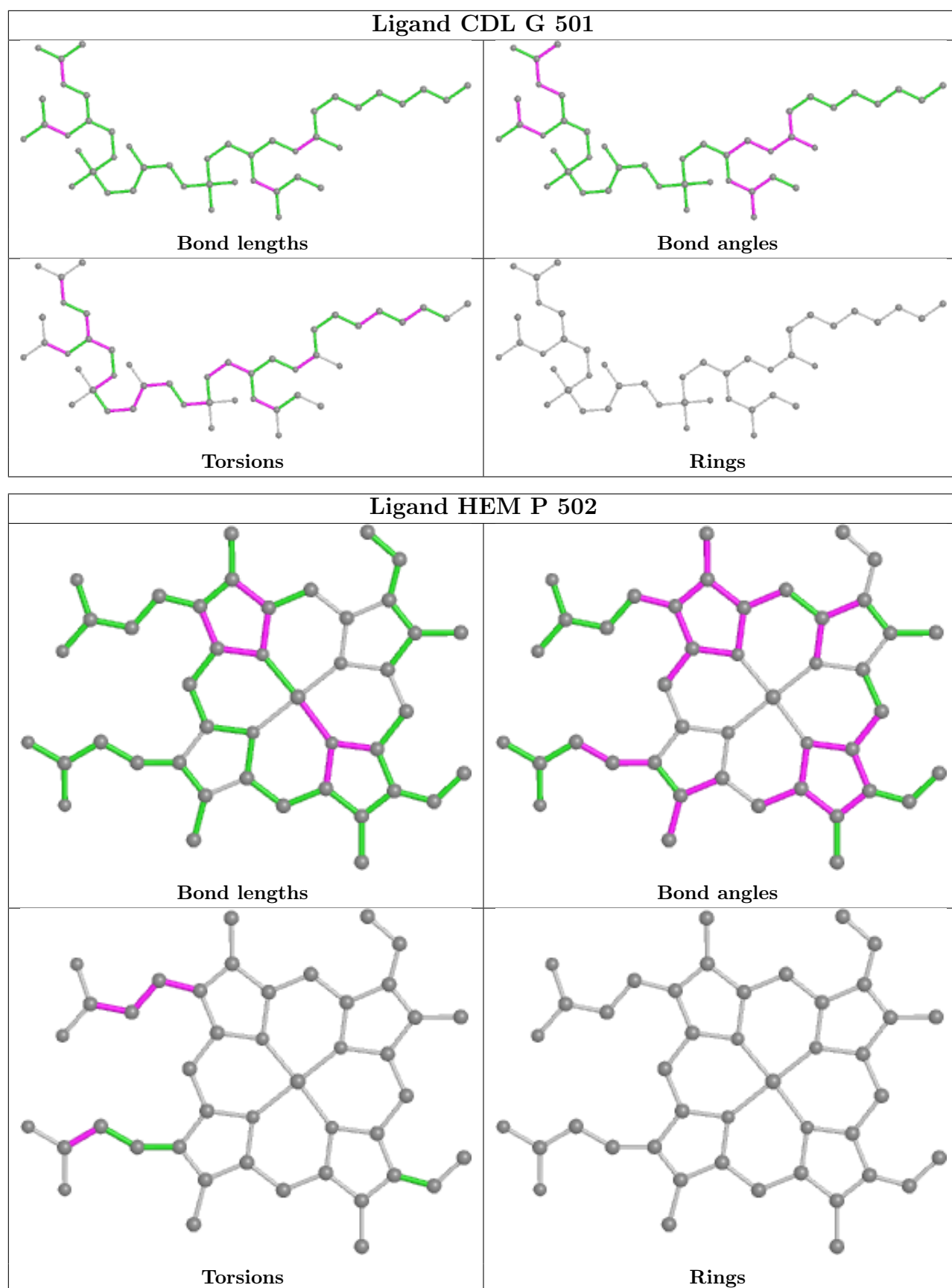
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	501	HEM	4	0
15	C	505	PEE	1	0
16	D	501	HEC	12	0
16	Q	501	HEC	10	0
15	Q	506	PEE	3	0
12	P	502	HEM	3	0
12	P	501	HEM	7	0
12	C	502	HEM	6	0
13	P	503	4X9	5	0
17	Q	505	CDL	1	0
17	T	501	CDL	1	0
15	P	505	PEE	1	0
13	C	503	4X9	6	0
18	R	501	FES	3	0

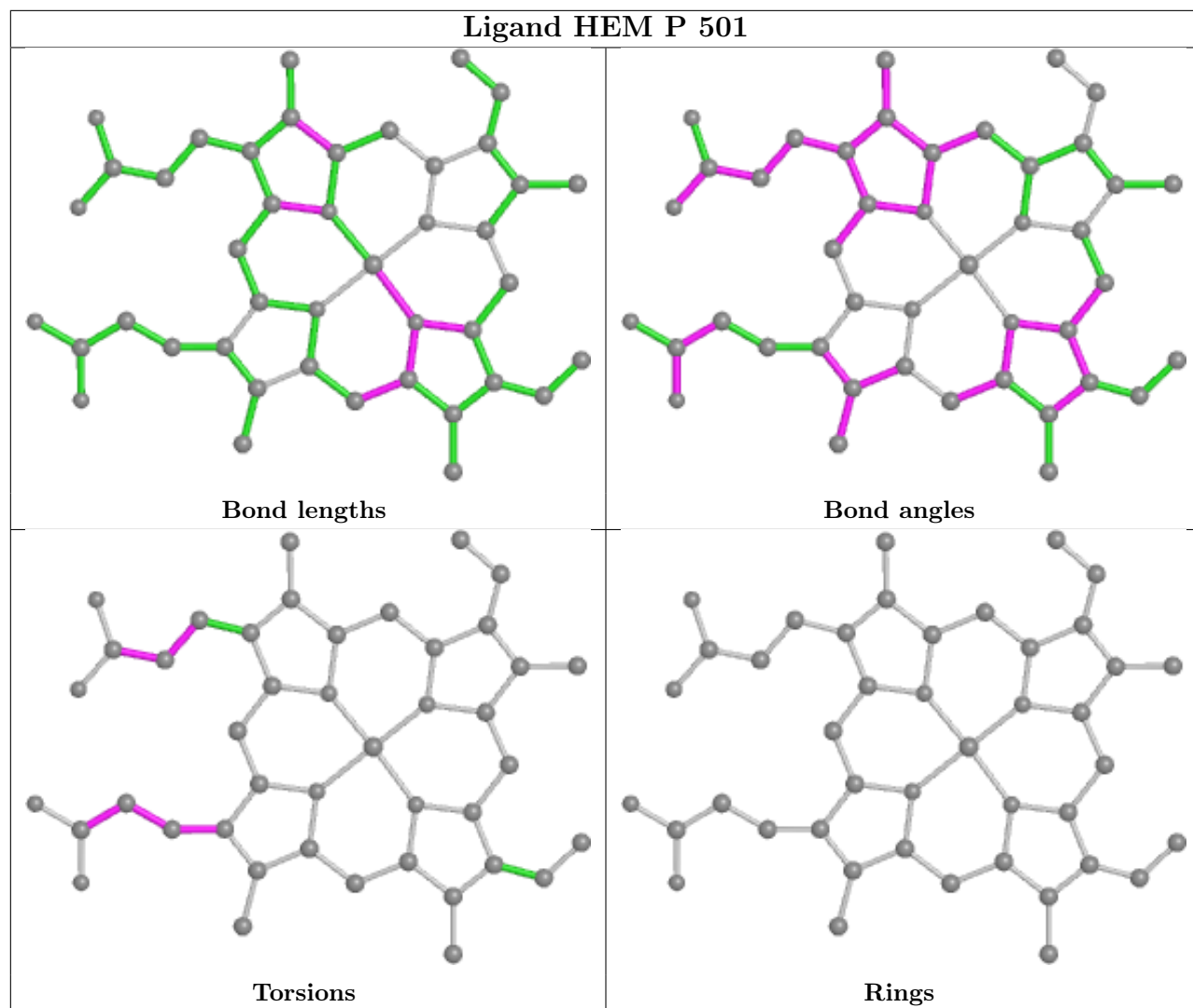
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

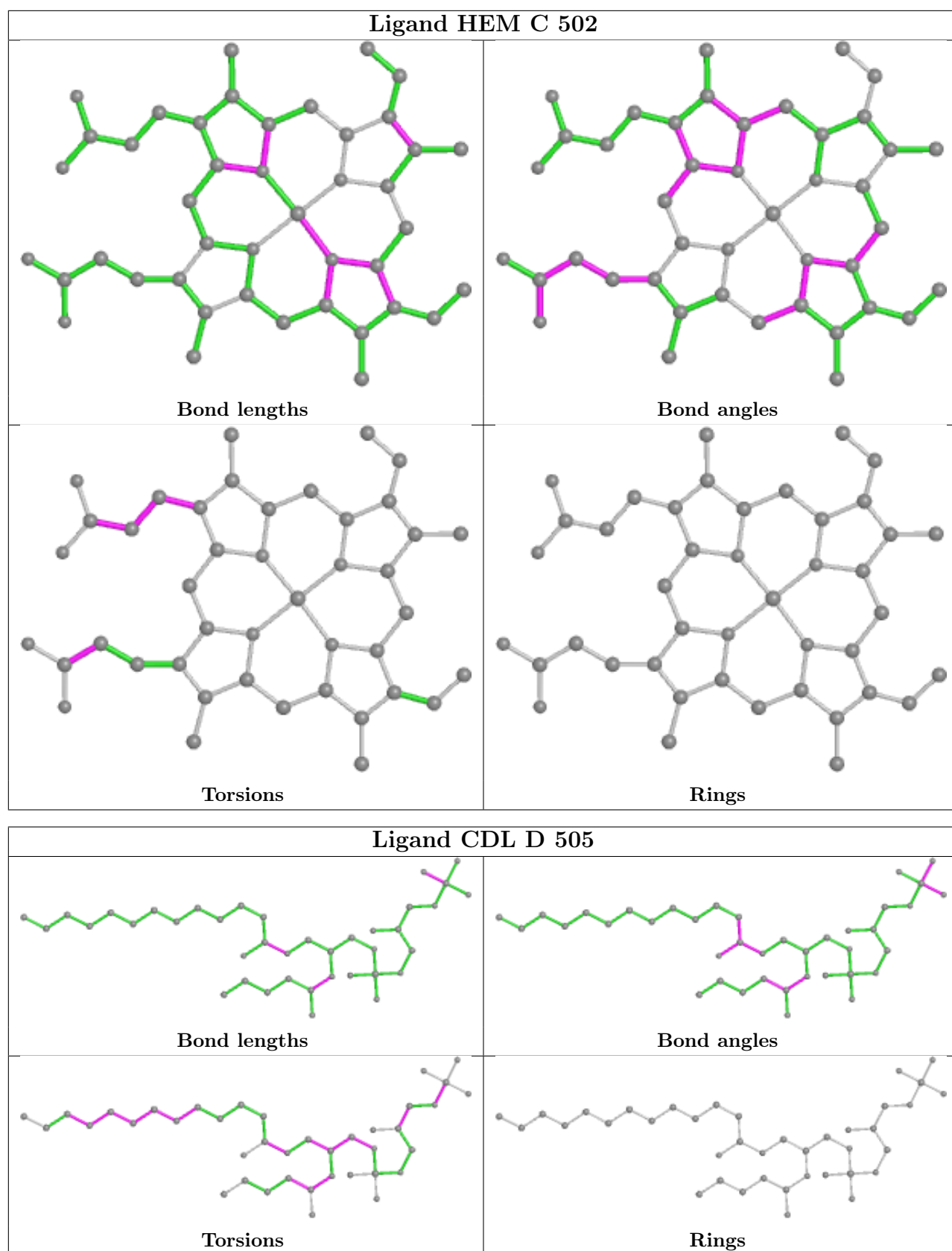


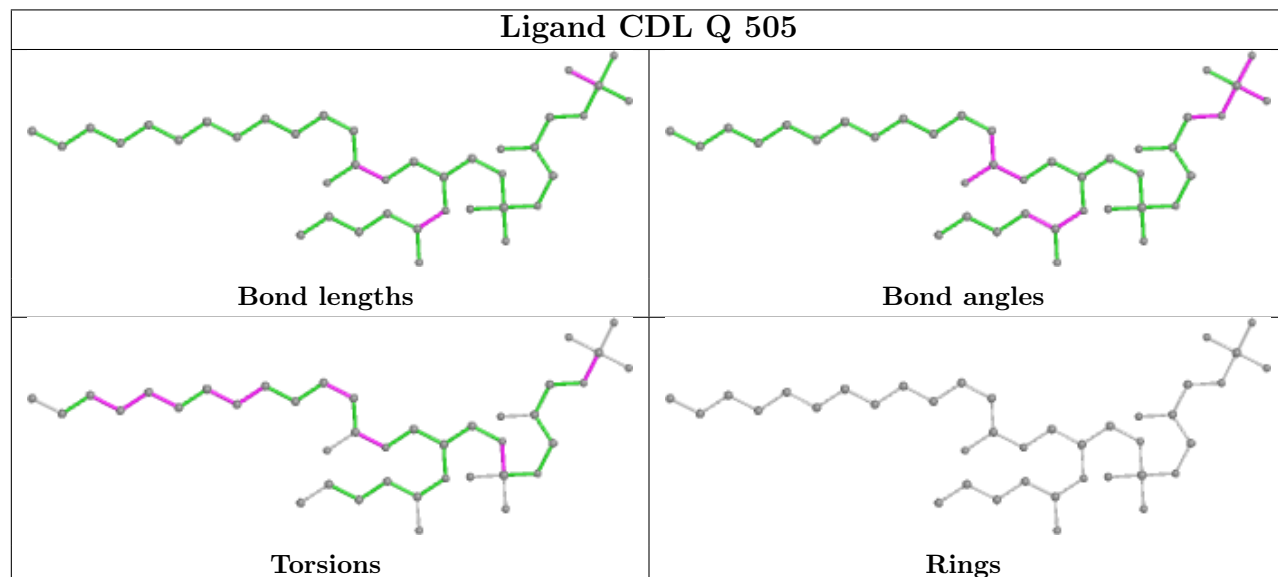
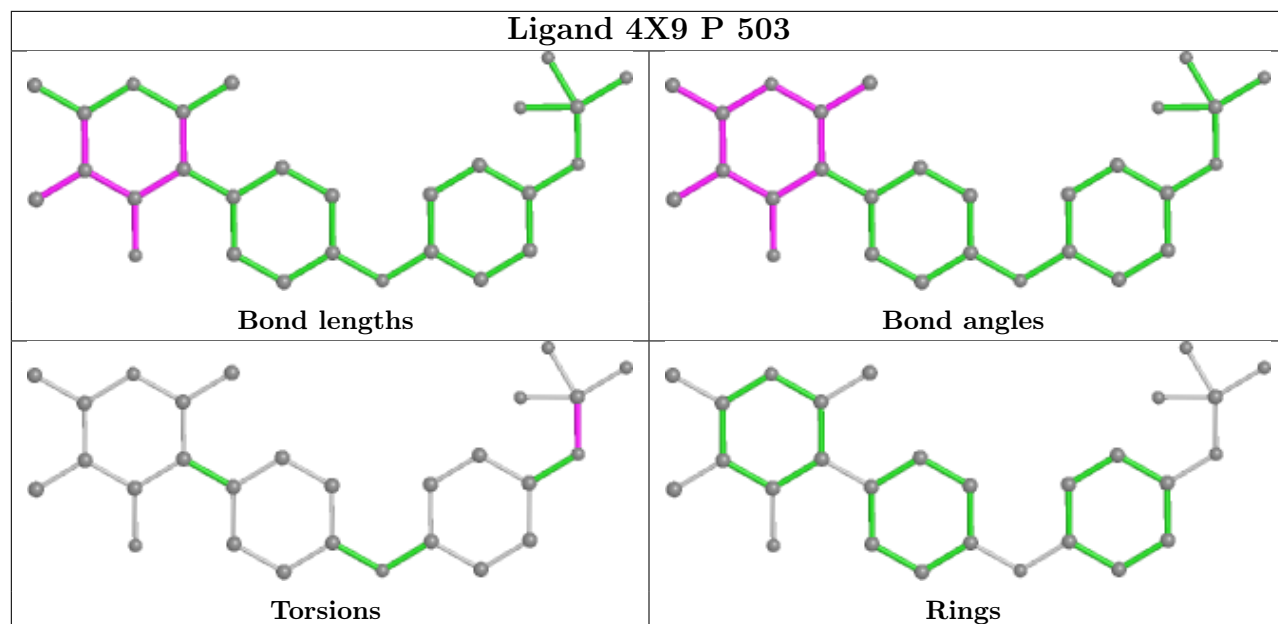


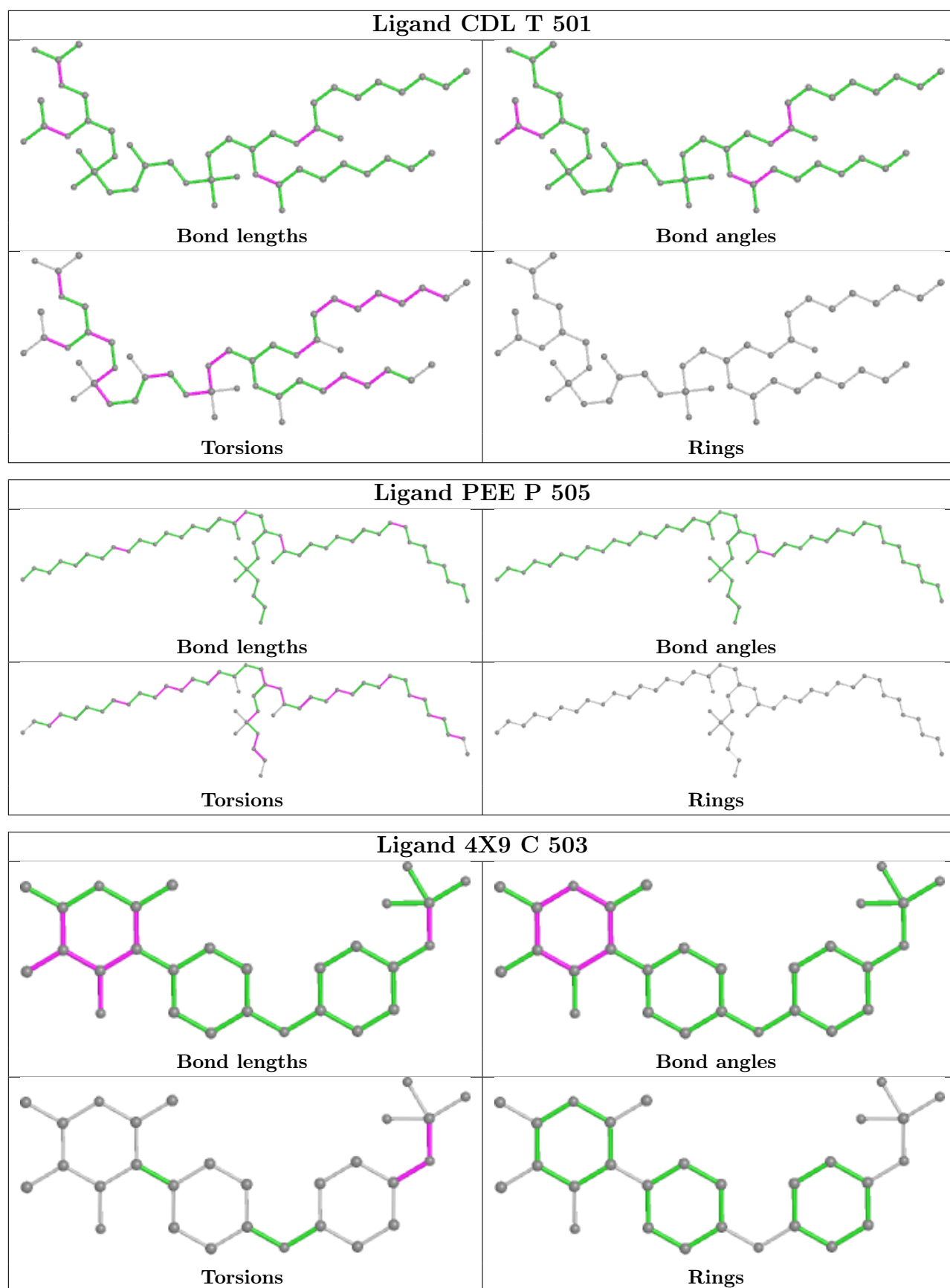


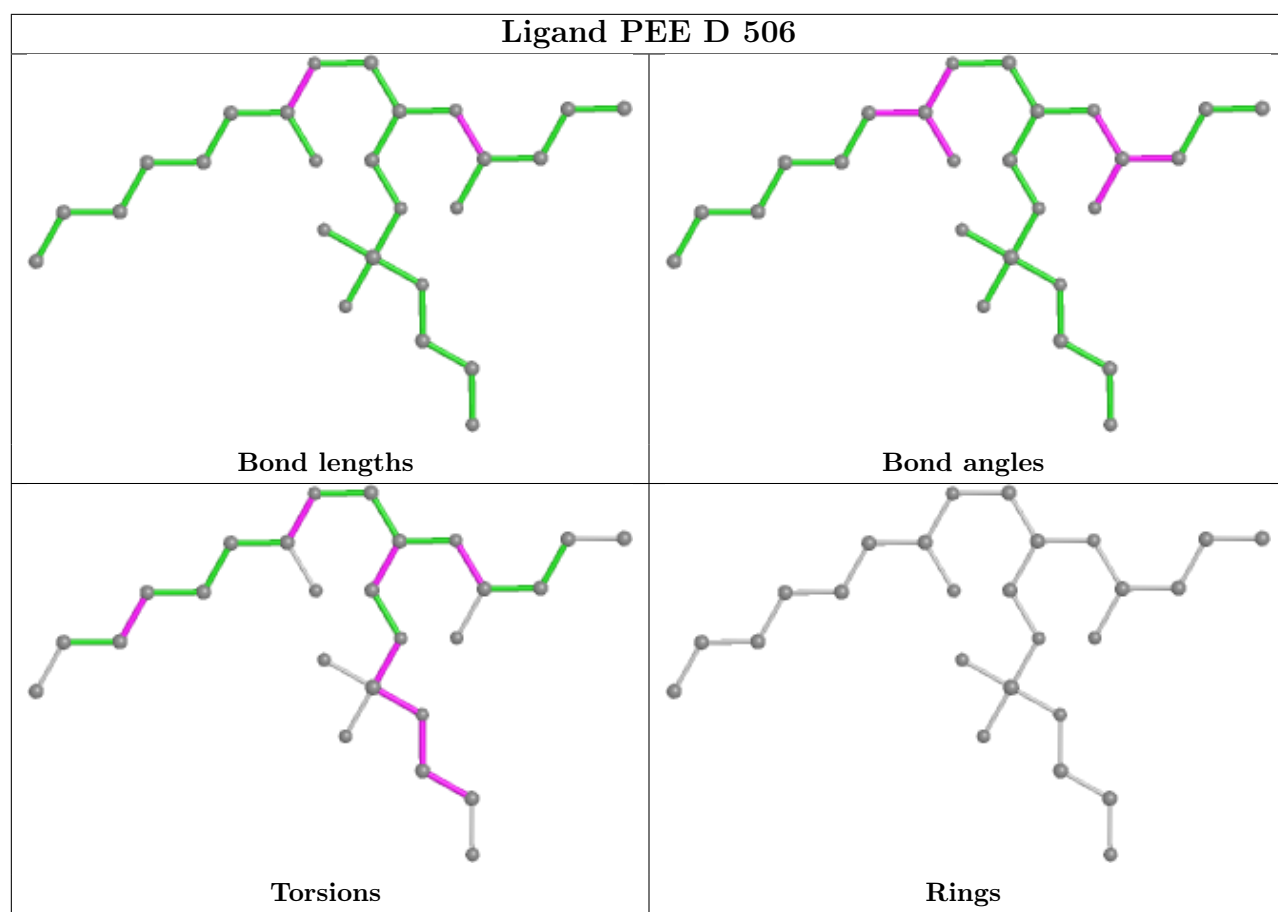












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/480 (92%)	-0.14	9 (2%) 65 48	92, 150, 191, 255	0
1	N	444/480 (92%)	-0.33	7 (1%) 72 55	87, 132, 176, 243	0
2	B	422/453 (93%)	0.13	29 (6%) 16 9	108, 157, 200, 247	0
3	C	374/379 (98%)	-0.50	0 100 100	77, 103, 137, 225	0
3	P	370/379 (97%)	-0.44	1 (0%) 94 88	79, 112, 148, 183	0
4	D	240/265 (90%)	-0.31	2 (0%) 86 73	92, 121, 153, 178	0
4	Q	241/265 (90%)	-0.10	6 (2%) 57 39	86, 131, 168, 211	0
5	E	73/274 (26%)	-0.36	1 (1%) 75 59	93, 130, 158, 170	0
5	I	21/274 (7%)	0.63	1 (4%) 30 18	146, 192, 220, 228	0
5	R	196/274 (71%)	-0.15	2 (1%) 82 69	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.44	2 (2%) 65 48	91, 124, 157, 171	0
6	S	99/111 (89%)	-0.44	0 100 100	85, 122, 168, 182	0
7	G	80/82 (97%)	-0.29	1 (1%) 77 61	88, 119, 189, 293	0
7	T	74/82 (90%)	-0.40	2 (2%) 54 36	83, 124, 181, 200	0
8	H	65/91 (71%)	-0.48	0 100 100	103, 136, 171, 223	0
8	U	66/91 (72%)	0.09	5 (7%) 13 7	132, 163, 213, 245	0
9	J	58/64 (90%)	-0.06	0 100 100	103, 137, 165, 175	0
9	W	59/64 (92%)	-0.19	1 (1%) 70 53	102, 121, 153, 162	0
10	O	419/453 (92%)	-0.21	7 (1%) 70 53	97, 146, 193, 250	0
11	V	17/274 (6%)	1.19	3 (17%) 1 0	176, 209, 228, 268	0
All	All	3860/4946 (78%)	-0.23	79 (2%) 65 48	77, 133, 189, 293	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.9
11	V	62	ARG	4.8
2	B	232	LEU	4.7
1	N	225	GLU	4.2
2	B	21	PRO	4.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

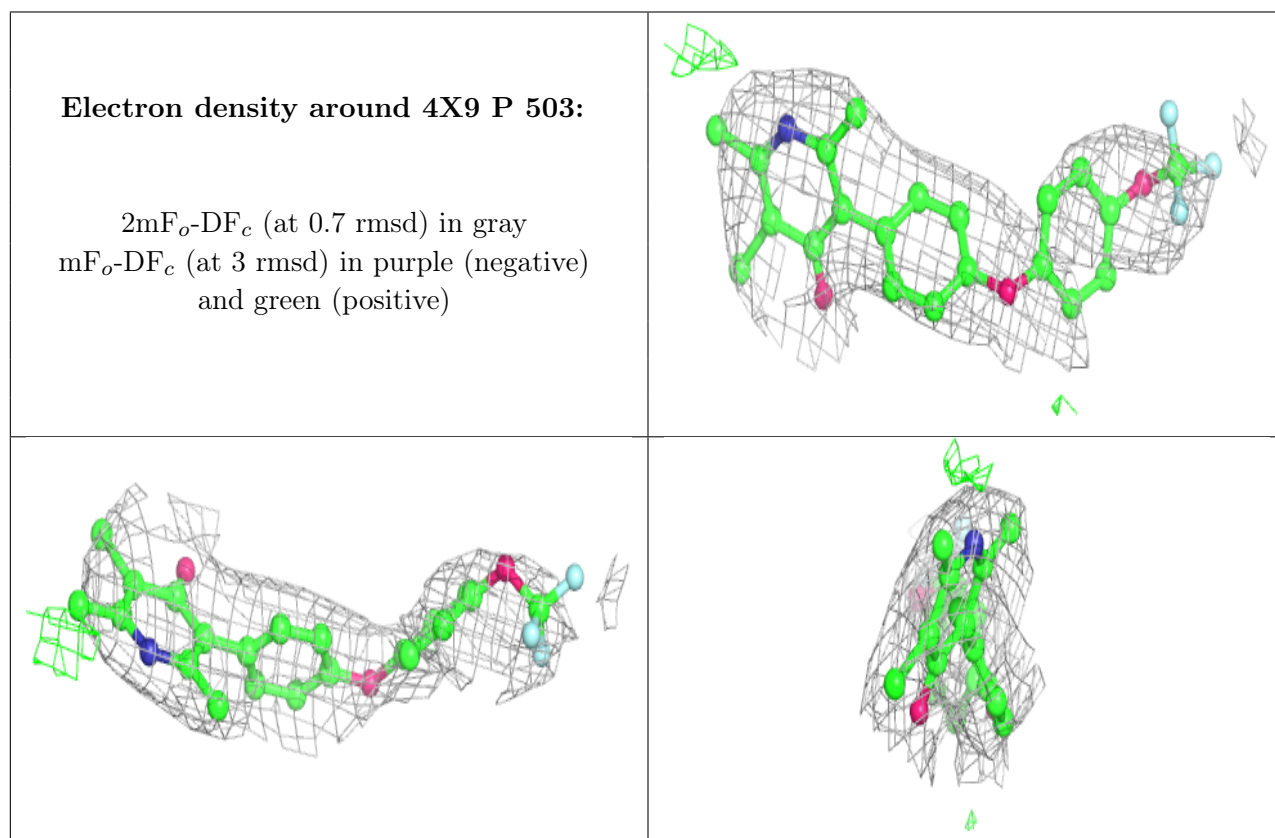
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	PO4	S	501	5/5	0.39	0.52	225,226,243,252	0
14	PO4	F	501	5/5	0.51	0.58	242,243,245,246	0
14	PO4	D	504	5/5	0.57	0.23	179,190,194,195	0
14	PO4	Q	1001	5/5	0.66	0.20	194,205,216,232	0
14	PO4	N	501	5/5	0.67	0.45	112,126,127,137	0
14	PO4	D	502	5/5	0.71	0.27	176,192,199,203	0
14	PO4	Q	1002	5/5	0.72	0.20	210,211,220,230	0
19	GOL	R	502	6/6	0.72	1.89	169,181,193,193	0
14	PO4	E	501	5/5	0.74	0.32	124,134,144,145	0
14	PO4	C	504	5/5	0.82	0.39	121,121,134,149	0
14	PO4	D	503	5/5	0.82	0.61	168,169,177,181	0
13	4X9	P	503	28/28	0.88	0.32	109,147,226,261	0
15	PEE	Q	506	51/51	0.90	0.40	100,134,171,187	0
13	4X9	C	503	28/28	0.90	0.39	116,143,206,215	0
17	CDL	D	505	39/100	0.91	0.27	85,124,146,148	0
15	PEE	C	505	49/51	0.91	0.49	94,116,135,137	0
17	CDL	T	501	49/100	0.92	0.31	93,129,160,167	0
17	CDL	G	501	44/100	0.92	0.28	95,115,153,168	0
15	PEE	P	505	49/51	0.93	0.33	100,122,154,156	0

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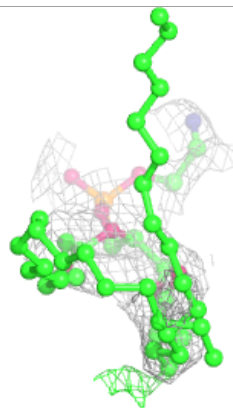
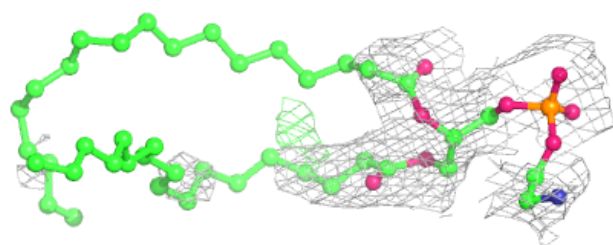
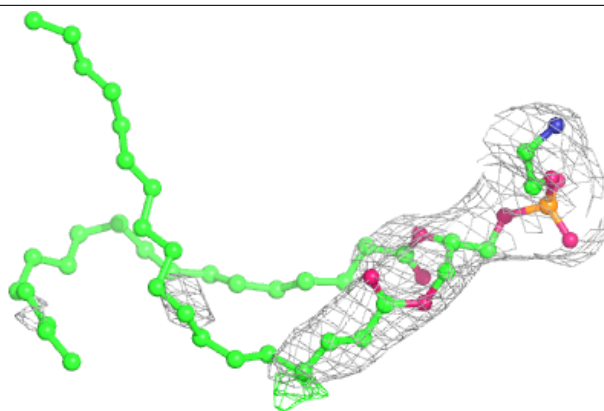
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CDL	Q	505	39/100	0.93	0.28	100,126,146,148	0
14	PO4	N	1001	5/5	0.93	0.42	120,127,135,137	0
15	PEE	D	506	26/51	0.93	0.26	107,127,169,176	0
18	FES	R	501	4/4	0.97	0.13	125,158,164,170	0
12	HEM	C	502	43/43	0.98	0.26	71,85,99,106	0
12	HEM	P	501	43/43	0.98	0.30	86,101,116,124	0
12	HEM	P	502	43/43	0.98	0.23	74,89,104,106	0
12	HEM	C	501	43/43	0.98	0.27	89,99,107,115	0
16	HEC	D	501	43/43	0.98	0.24	80,111,127,138	0
16	HEC	Q	501	43/43	0.98	0.28	106,117,136,143	0

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

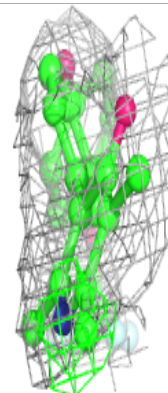
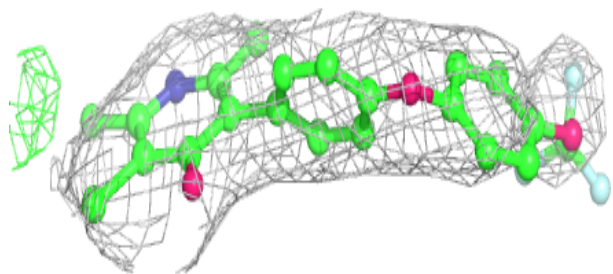
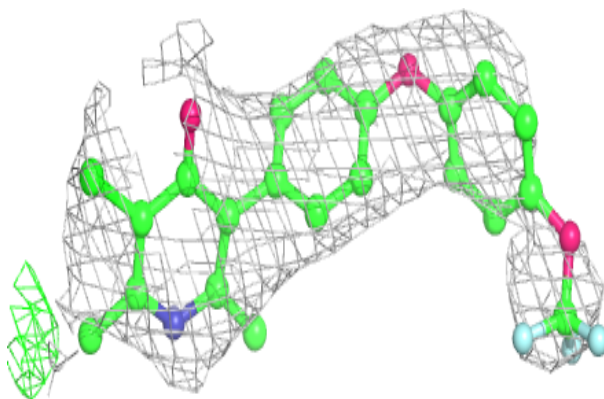


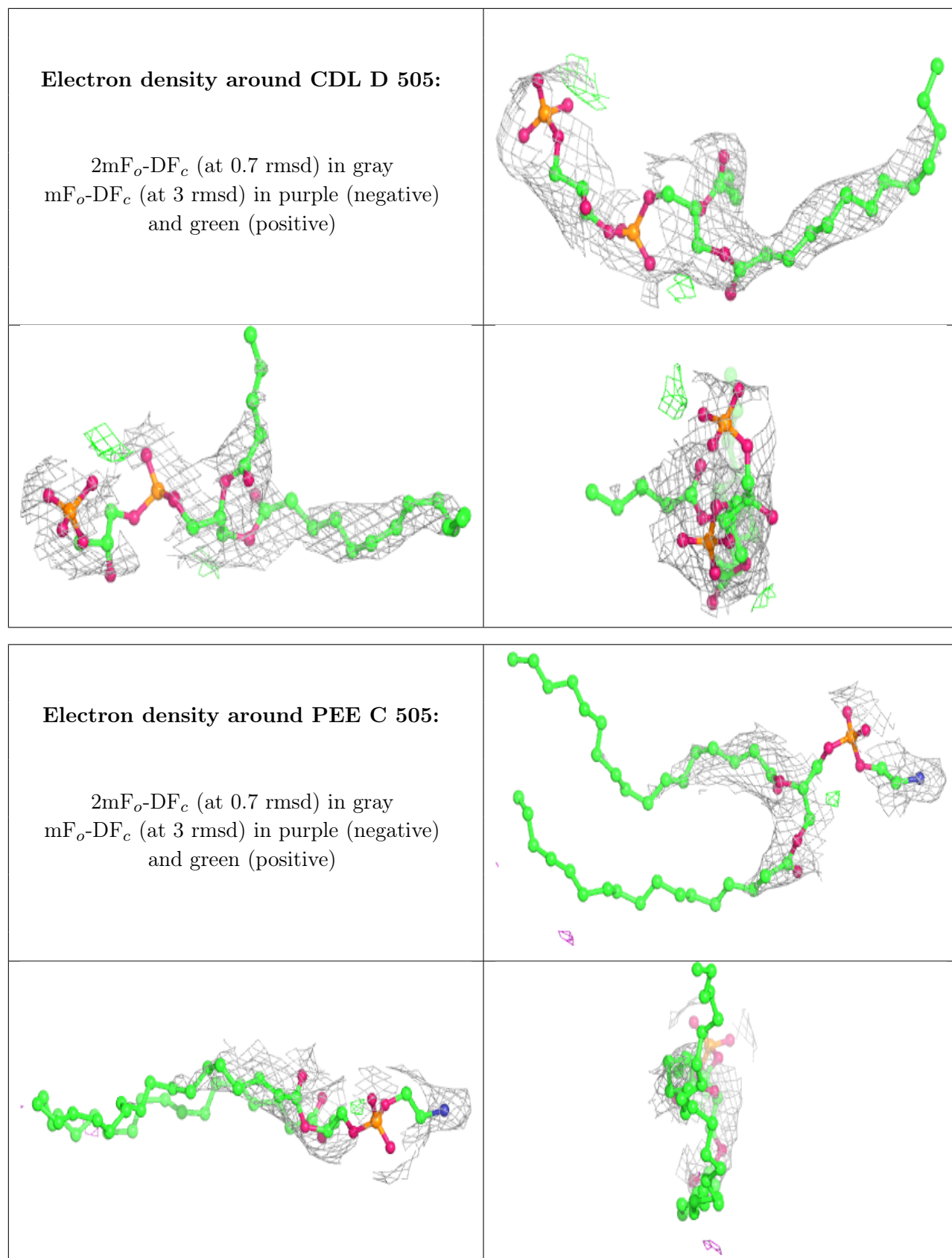
Electron density around PEE Q 506:

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

**Electron density around 4X9 C 503:**

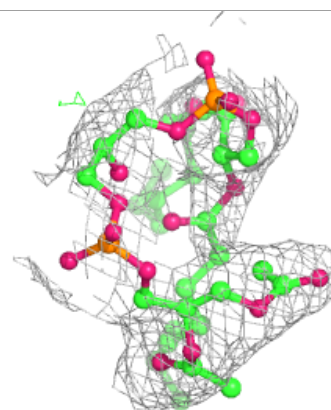
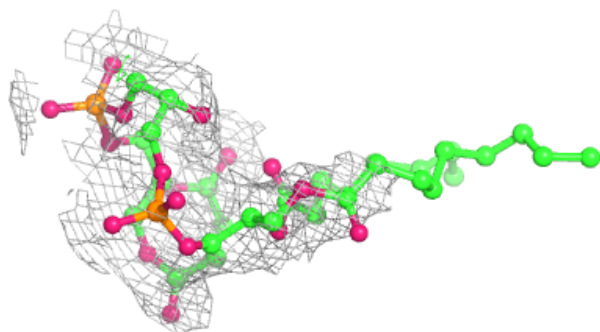
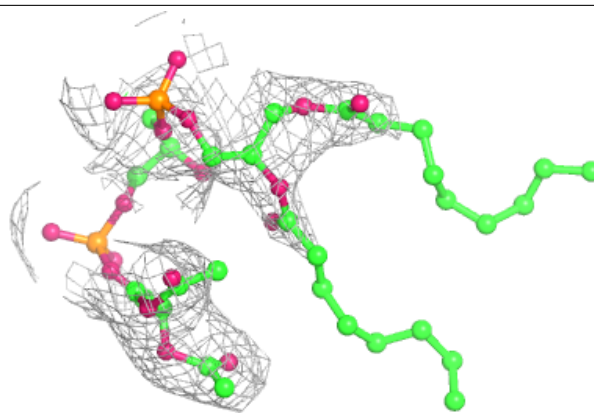
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



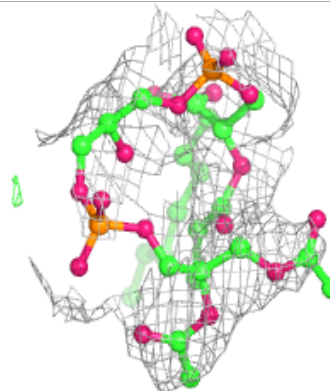
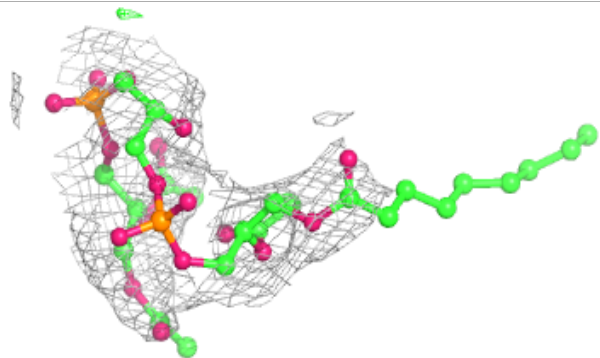
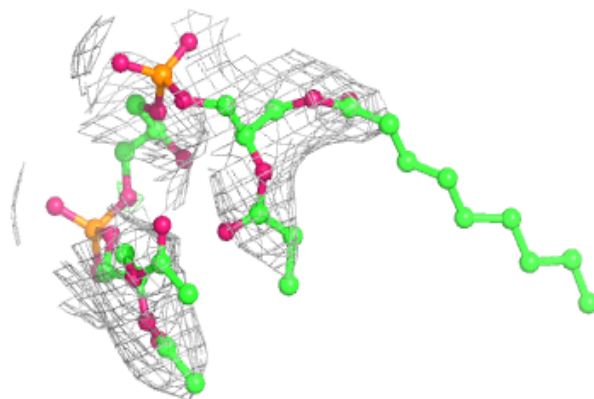


Electron density around CDL T 501:

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

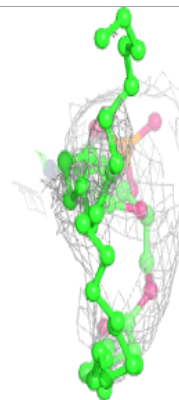
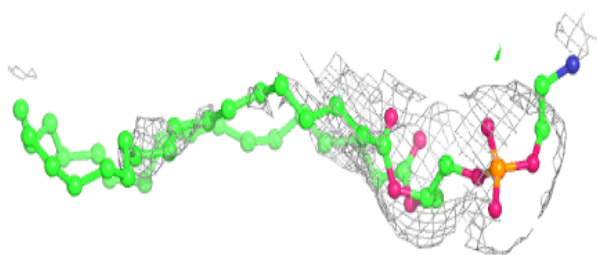
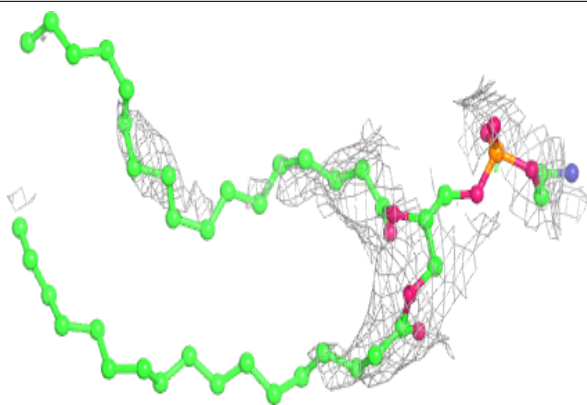
**Electron density around CDL G 501:**

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and green (positive)

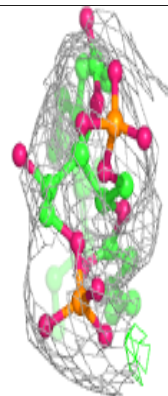
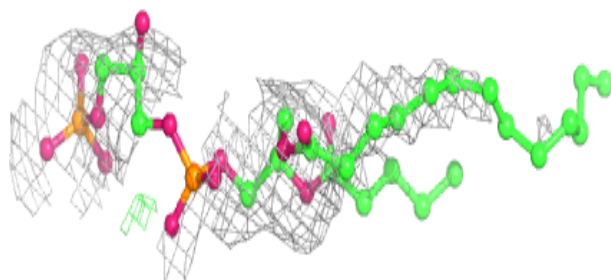
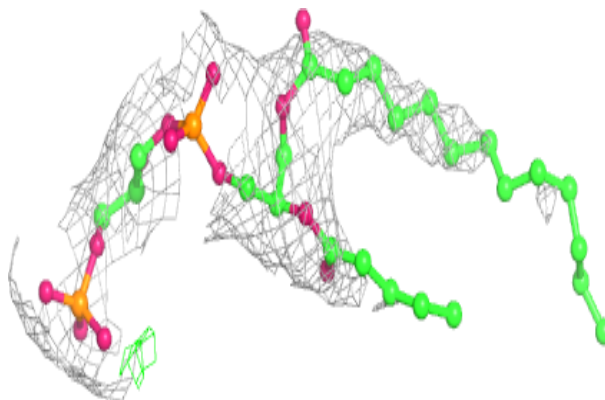


Electron density around PEE P 505:

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

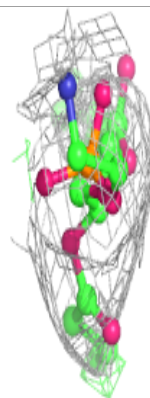
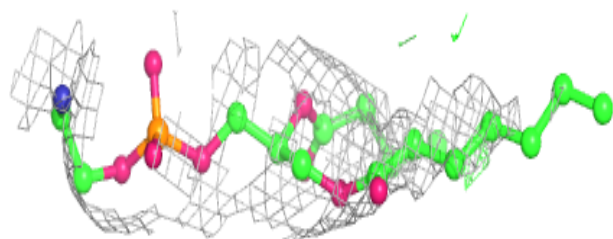
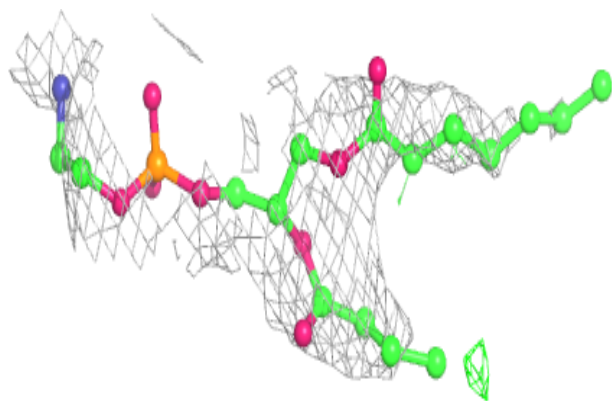
**Electron density around CDL Q 505:**

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



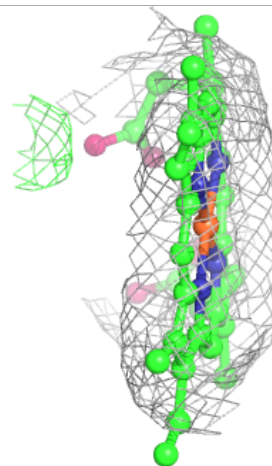
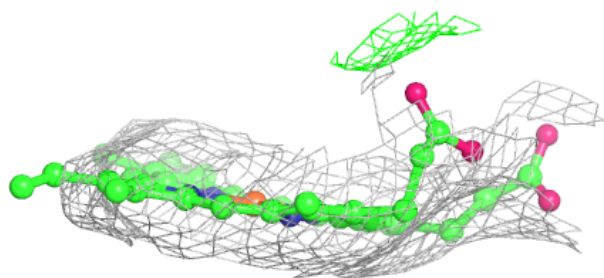
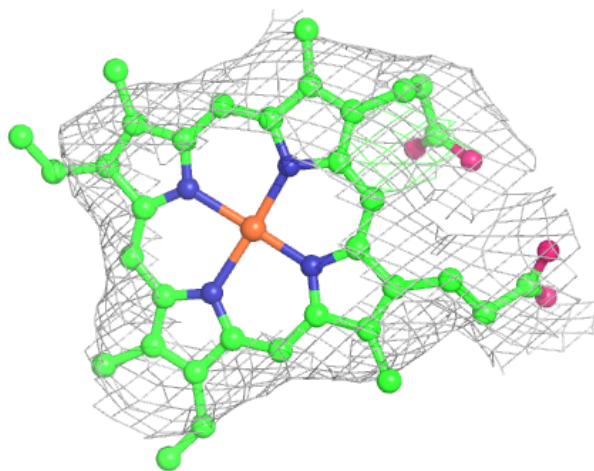
Electron density around PEE D 506:

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



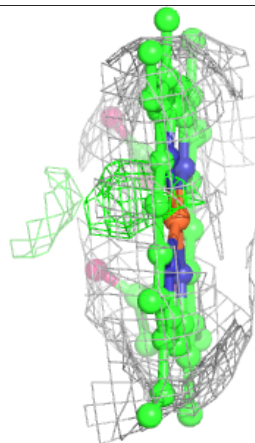
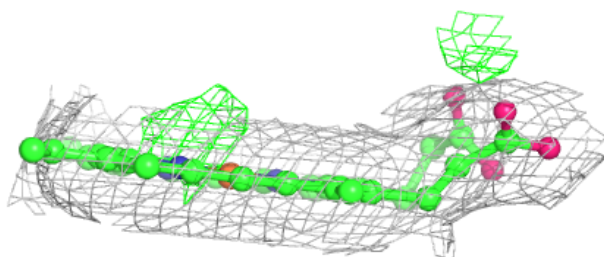
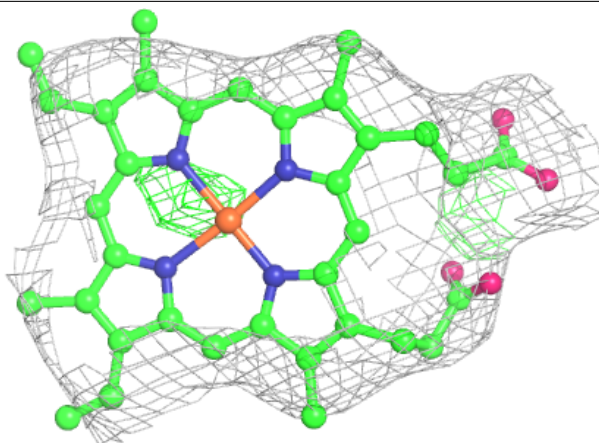
Electron density around HEM C 502:

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



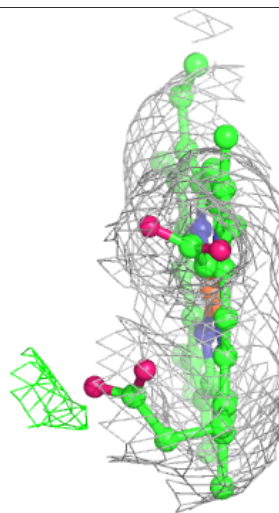
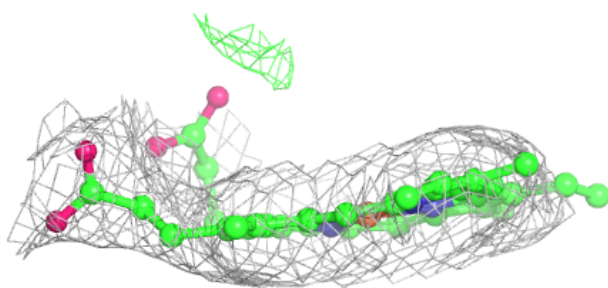
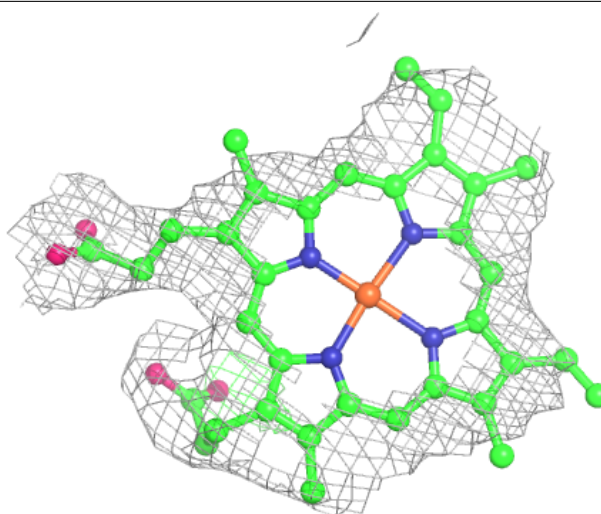
Electron density around HEM P 501:

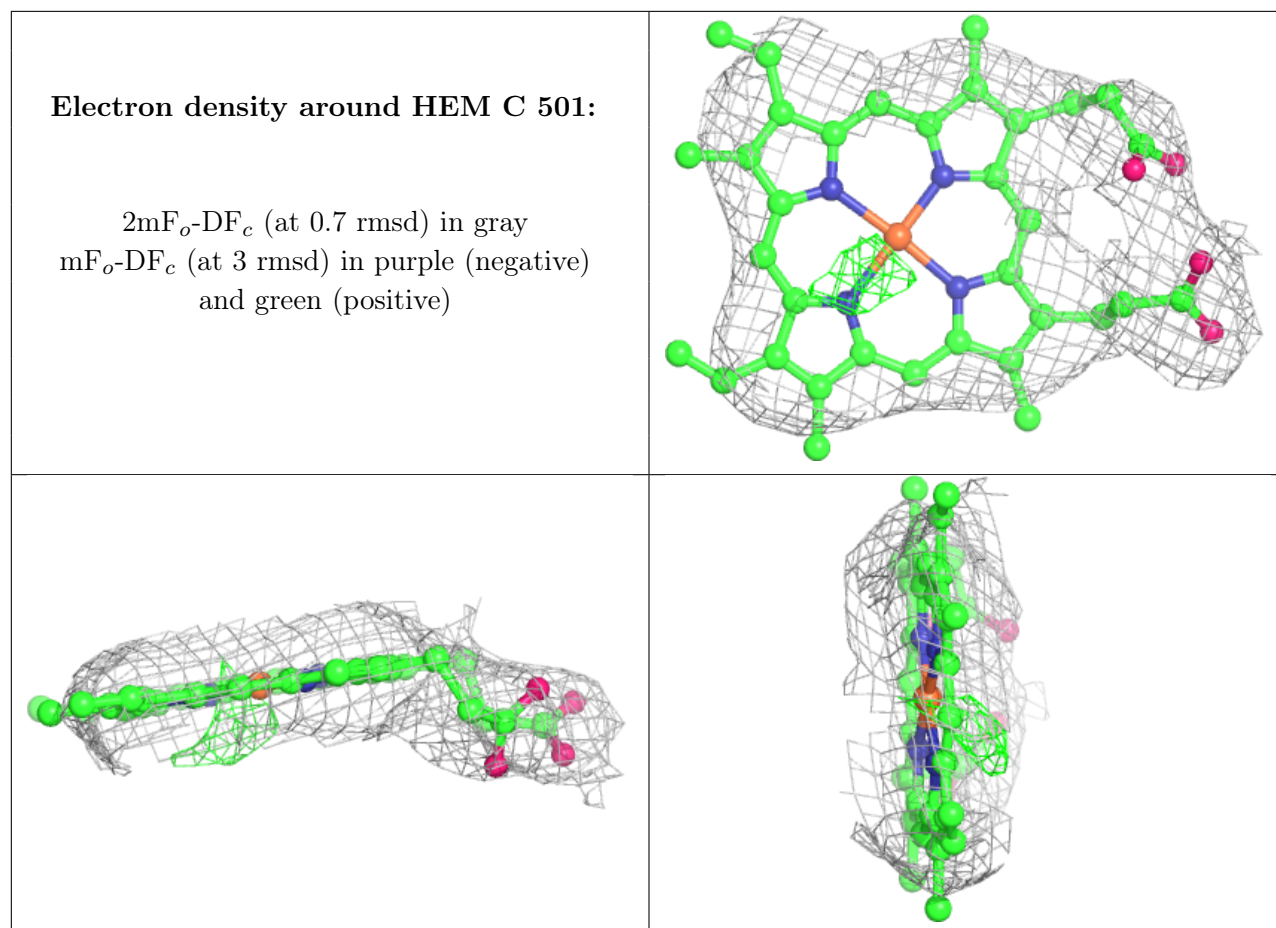
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM P 502:

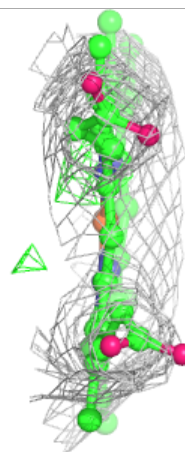
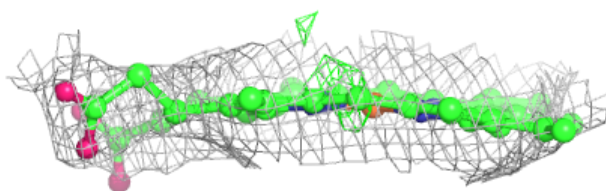
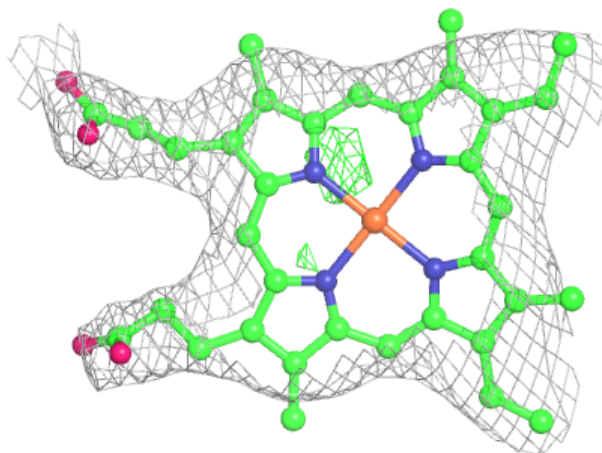
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and green (positive)

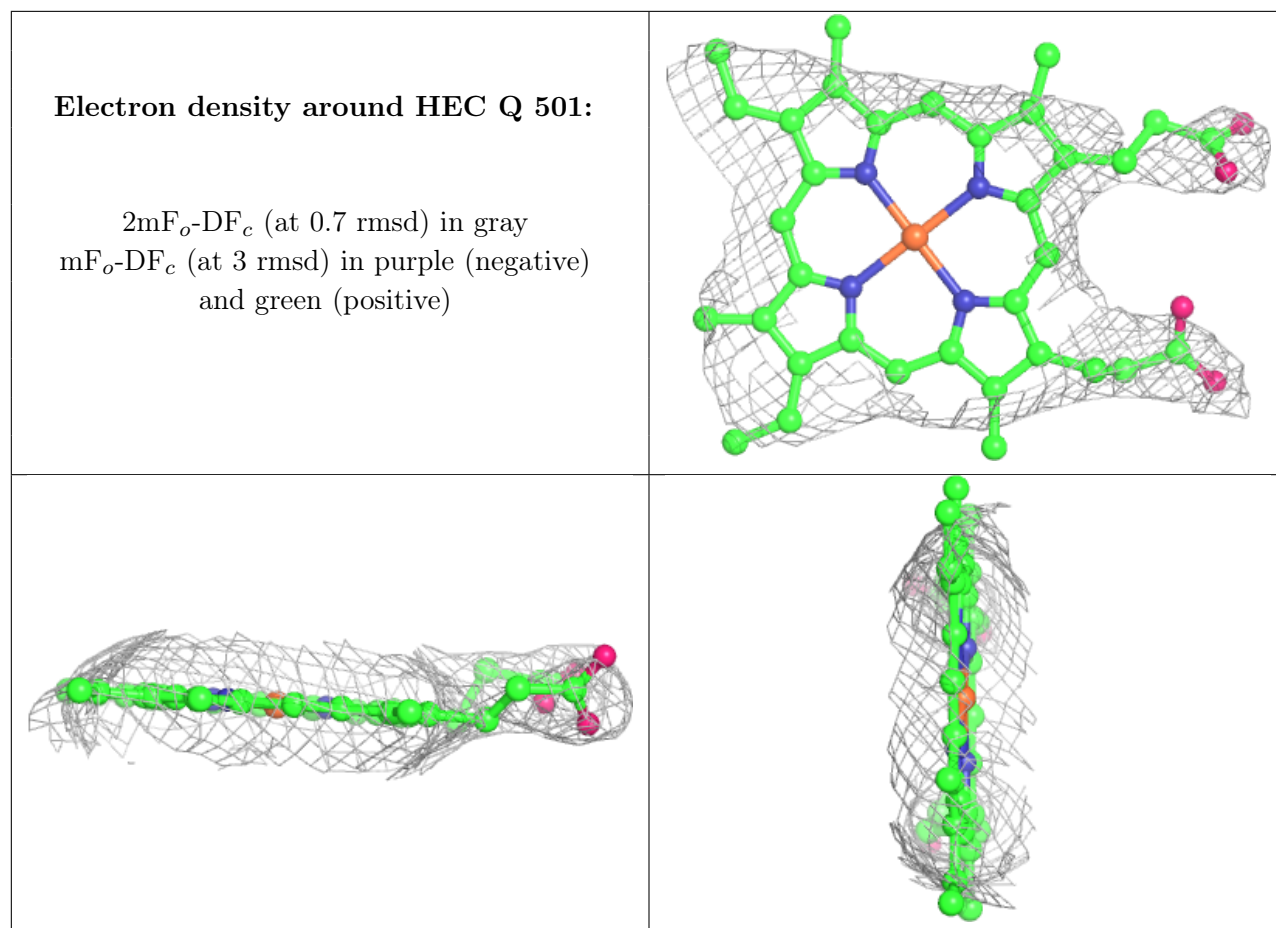




Electron density around HEC D 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.