



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2026 – 05:11 am BST

PDB ID : 4D6U / pdb_00004d6u
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GSK932121
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 : 4.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

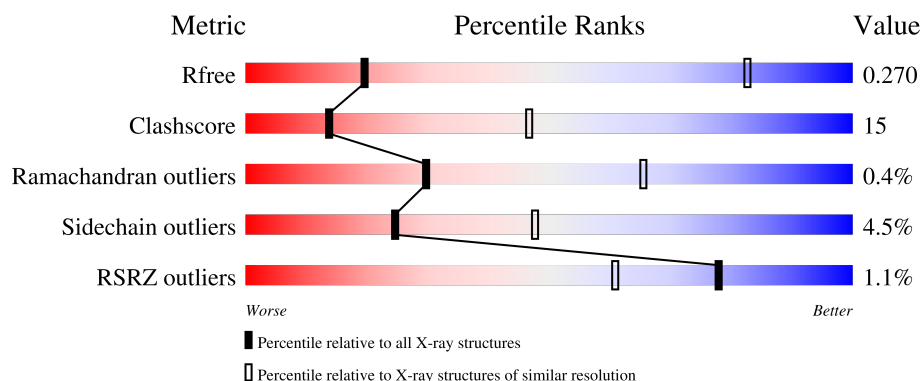
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



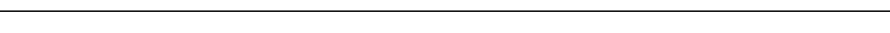
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	B	453	
3	C	379	
3	P	379	
4	D	325	

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Mol	Chain	Length	Quality of chain
4	Q	325	
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	N	480	
11	O	453	
12	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	G8U	C	503	-	-	X	-
14	G8U	P	503	-	-	X	-
16	PEE	C	505	X	-	-	-
16	PEE	D	506	X	-	-	-
16	PEE	P	505	X	-	-	-
16	PEE	Q	506	X	-	-	-
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 31080 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	444	Total	C	N	O	S	0	0	0
			3439	2148	607	664	20			

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

- 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
			1912	1222	329	346	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	27	Total	C	N	O	S	0	0	0
			196	121	38	36	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
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	444	Total	C	N	O	S	0	0	0
			3430	2142	605	663	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	445	LYS	ARG	conflict	UNP P31800

- Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

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

There is a discrepancy between the modelled and reference sequences:

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

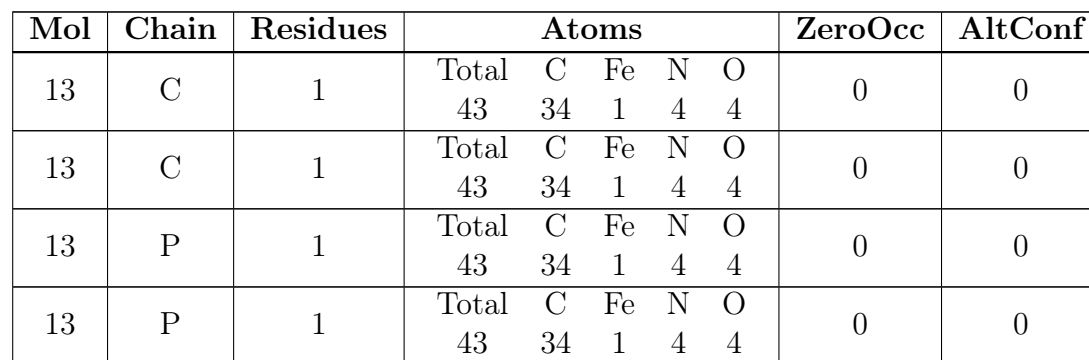
- Molecule 12 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

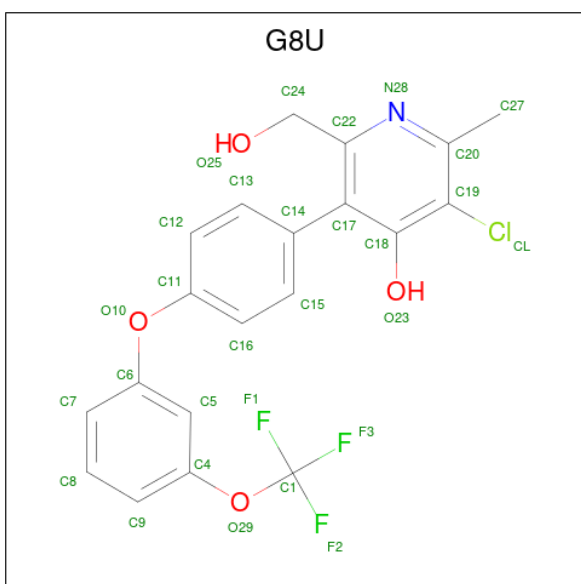
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	64	VAL	LEU	conflict	UNP P13272

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

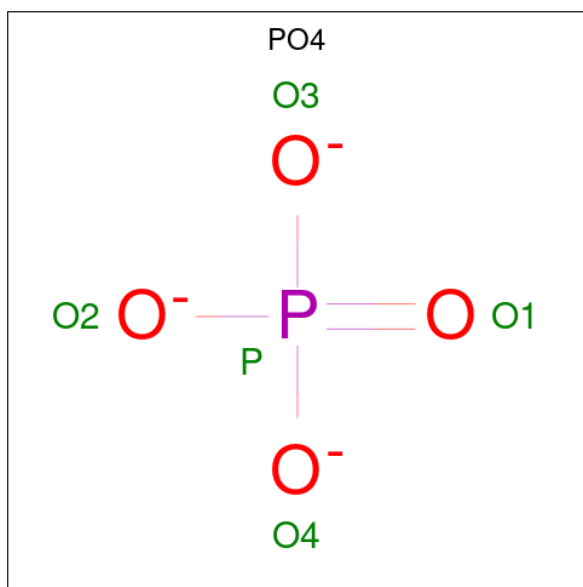


- Molecule 14 is 3-chloro-6-(hydroxymethyl)-2-methyl-5-{4-[3-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (CCD ID: G8U) (formula: $\text{C}_{20}\text{H}_{15}\text{ClF}_3\text{NO}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	Cl	F	N	O	0	0
			29	20	1	3	1	4		
14	P	1	Total	C	Cl	F	N	O	0	0
			29	20	1	3	1	4		

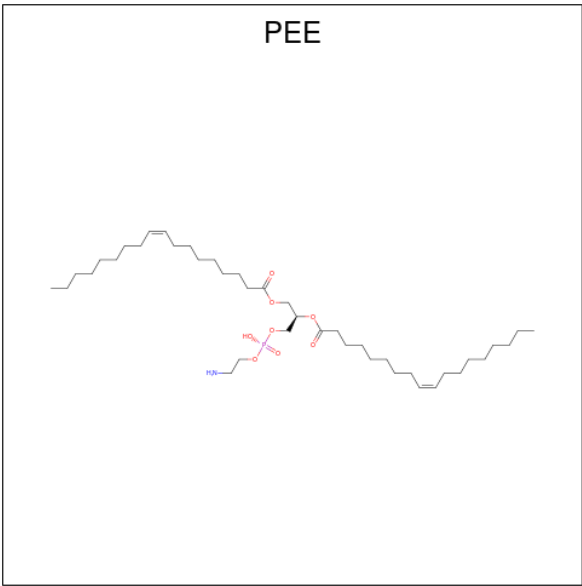
- Molecule 15 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

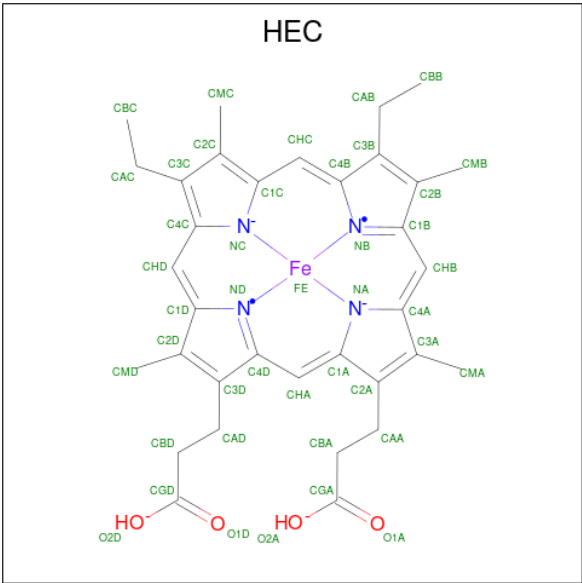
- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

C₄₁H₇₈NO₈P).



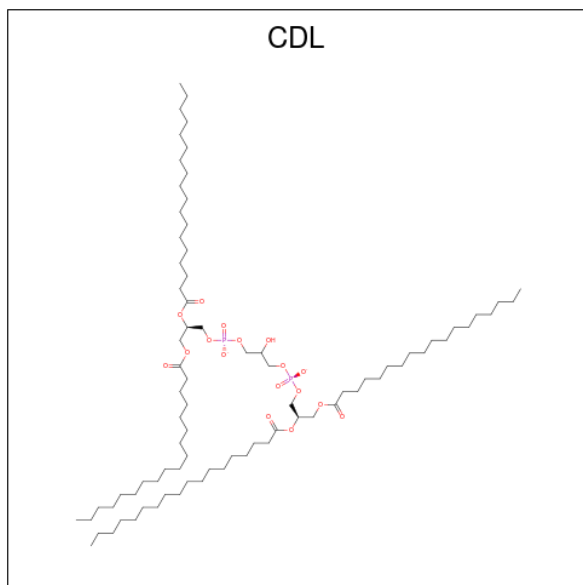
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
16	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



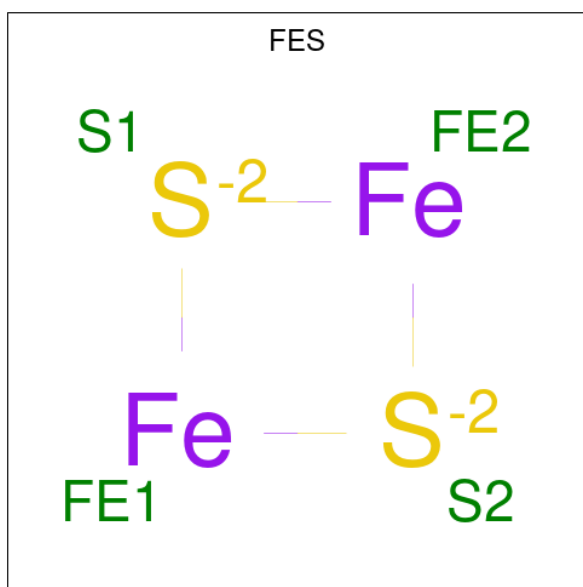
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



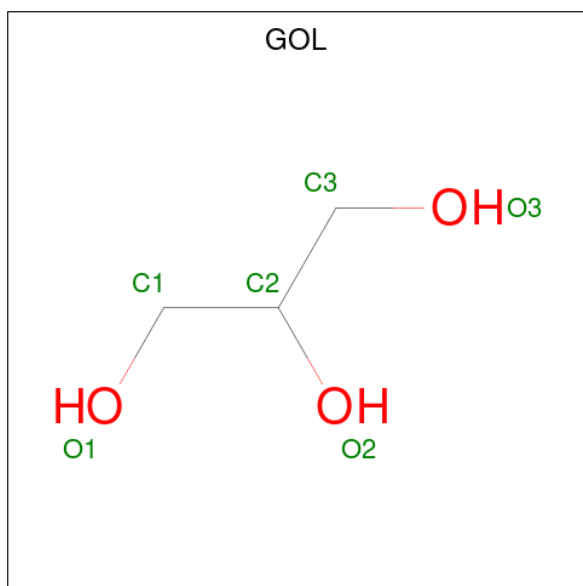
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			39	24	13	2		
18	G	1	Total	C	O	P	0	0
			44	25	17	2		
18	Q	1	Total	C	O	P	0	0
			39	24	13	2		
18	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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

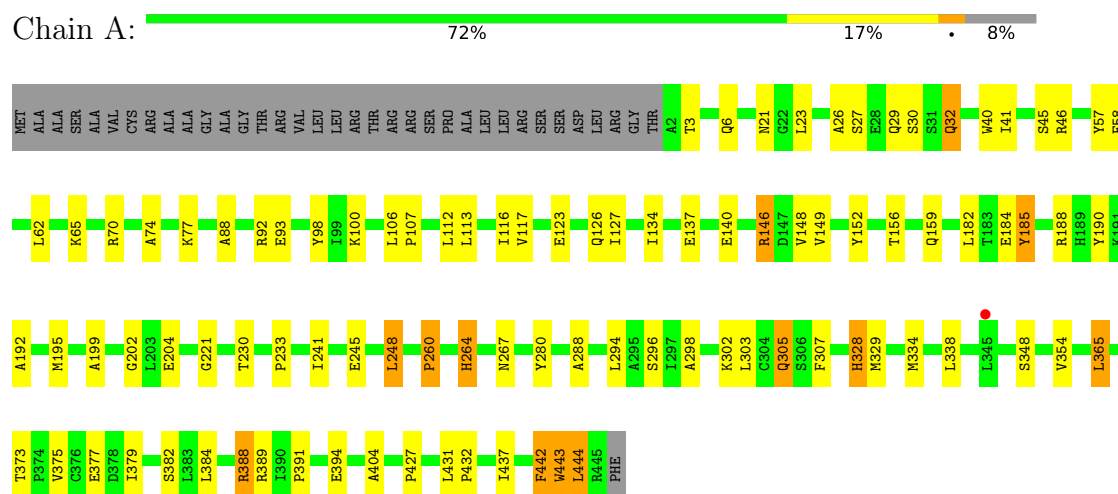


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	R	1	Total	C	O	0	0
			6	3	3		

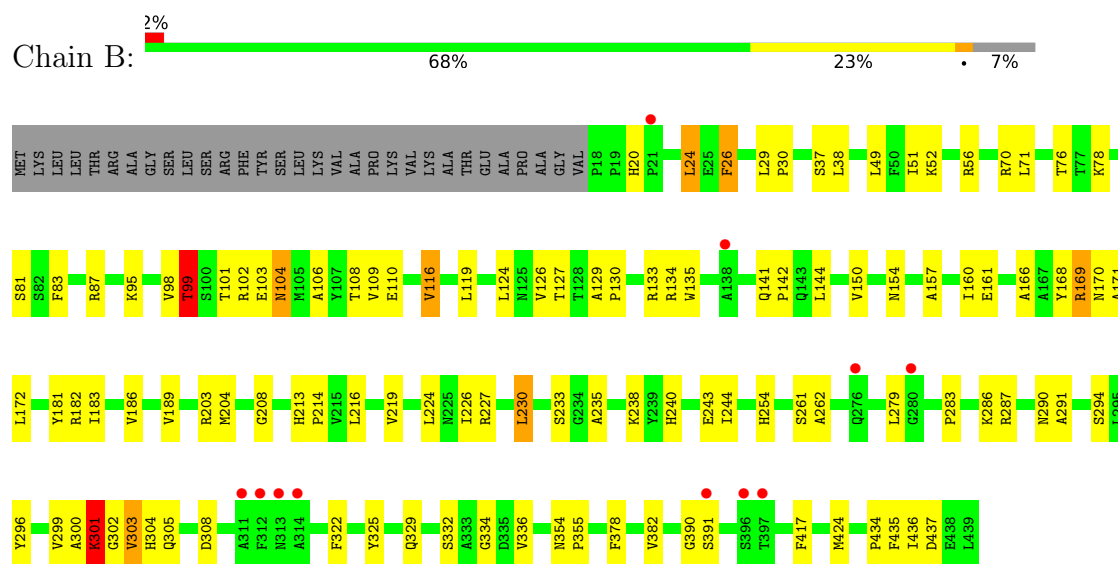
3 Residue-property plots

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

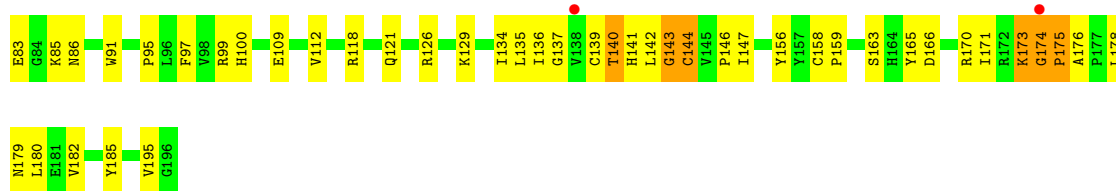


• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL



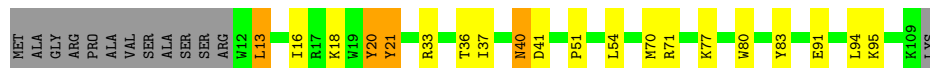
• Molecule 3: CYTOCHROME B





• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F: 70% 14% 12%



• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain S: 71% 15% 11%



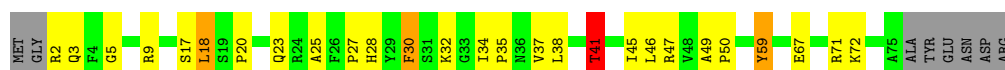
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain G: 55% 30% 10%



• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain T: 57% 28% 10%



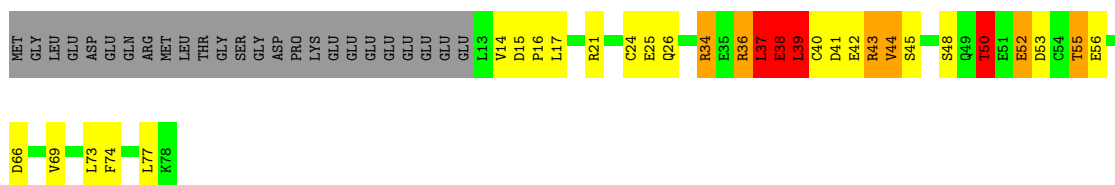
• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain H: 35% 30% 29%



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

Chain U: 40% 22% 7% 27%



• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J: 77% 11% 9%



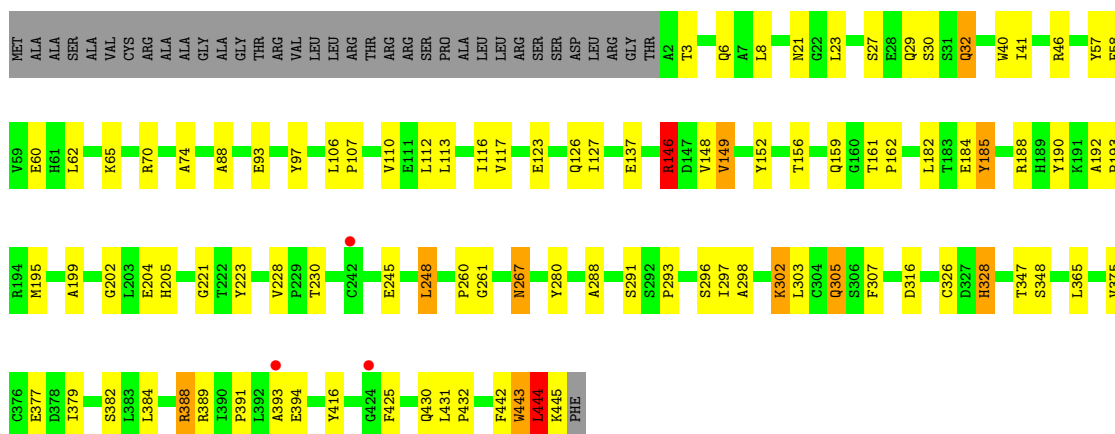
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain W: 67% 23% 8%



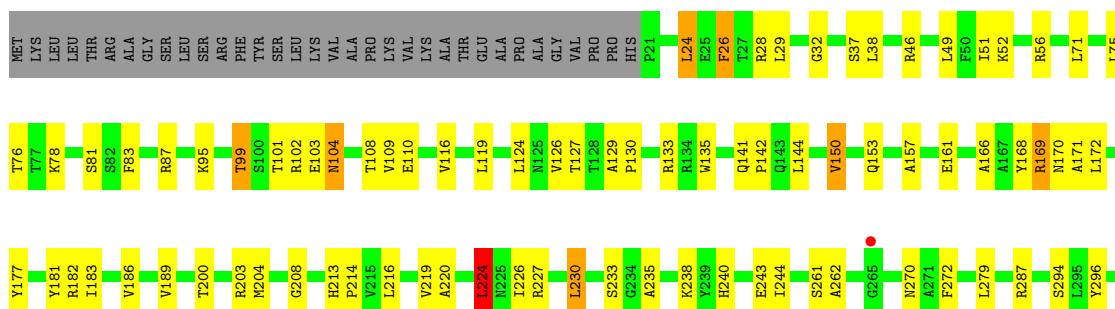
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

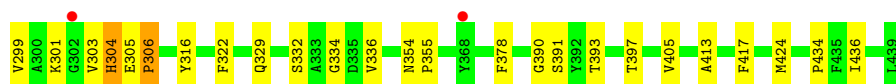
Chain N: 72% 18% 8%



• Molecule 11: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

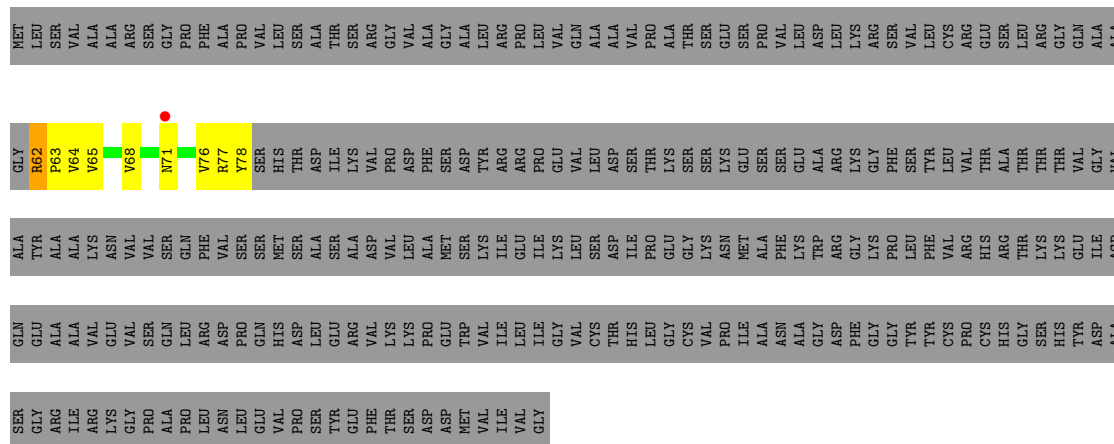
Chain O: 69% 22% 8%





● Molecule 12: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V: 94%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.49Å 129.49Å 719.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 4.09 50.00 – 4.09	Depositor EDS
% Data completeness (in resolution range)	80.6 (50.00-4.09) 80.6 (50.00-4.09)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.223 , 0.271 0.222 , 0.270	Depositor DCC
R_{free} test set	2147 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 156.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31080	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, HEC, G8U, HEM, PO4, GOL, PEE

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	0.62	3/3511 (0.1%)	0.93	10/4766 (0.2%)
2	B	0.78	12/3224 (0.4%)	1.00	16/4375 (0.4%)
3	C	0.70	6/3065 (0.2%)	0.92	4/4196 (0.1%)
3	P	0.67	5/3031 (0.2%)	0.91	5/4150 (0.1%)
4	D	0.66	5/1971 (0.3%)	0.90	3/2676 (0.1%)
4	Q	0.65	4/1977 (0.2%)	0.91	7/2684 (0.3%)
5	E	0.97	5/557 (0.9%)	0.96	2/752 (0.3%)
5	I	0.95	0/196	1.45	4/263 (1.5%)
5	R	0.71	5/1552 (0.3%)	1.07	11/2100 (0.5%)
6	F	0.73	4/879 (0.5%)	0.89	0/1180
6	S	0.71	3/888 (0.3%)	0.86	1/1191 (0.1%)
7	G	0.90	5/699 (0.7%)	1.75	10/946 (1.1%)
7	T	0.82	3/645 (0.5%)	0.93	2/873 (0.2%)
8	H	0.99	2/534 (0.4%)	1.45	9/718 (1.3%)
8	U	1.00	4/543 (0.7%)	1.38	8/729 (1.1%)
9	J	0.70	1/495 (0.2%)	0.83	0/667
9	W	0.64	0/500	0.86	2/675 (0.3%)
10	N	0.82	2/3501 (0.1%)	0.94	13/4752 (0.3%)
11	O	0.71	9/3197 (0.3%)	0.90	6/4336 (0.1%)
12	V	0.95	1/129 (0.8%)	1.37	3/177 (1.7%)
All	All	0.74	79/31094 (0.3%)	0.99	116/42206 (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	1
2	B	1	1
5	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	N	0	1
12	V	0	1
All	All	1	6

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	444	LEU	C-N	-32.90	0.87	1.33
2	B	169	ARG	CZ-NH1	14.43	1.52	1.32
4	D	93	LYS	CE-NZ	12.20	1.85	1.49
5	E	27	GLU	CD-OE1	11.86	1.47	1.25
3	P	194	MET	SD-CE	11.10	2.07	1.79

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	75	ALA	N-CA-C	31.03	145.86	112.97
7	G	75	ALA	CB-CA-C	-21.88	77.69	111.17
7	G	76	ALA	N-CA-CB	-16.55	85.61	110.60
2	B	300	ALA	CB-CA-C	-15.16	87.56	111.06
5	R	72	SER	N-CA-C	14.55	126.83	110.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	301	LYS	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ARG	Sidechain
2	B	301	LYS	Peptide
8	H	42	GLU	Sidechain
10	N	444	LEU	Mainchain
5	R	27	GLU	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3337	85	0
2	B	3164	0	3144	85	0
3	C	2968	0	3028	133	0
3	P	2936	0	2996	110	0
4	D	1912	0	1862	49	0
4	Q	1918	0	1870	55	0
5	E	549	0	547	20	0
5	I	196	0	204	32	0
5	R	1518	0	1504	60	0
6	F	860	0	849	25	0
6	S	869	0	862	23	0
7	G	677	0	673	57	0
7	T	624	0	630	19	0
8	H	529	0	511	38	0
8	U	538	0	524	30	0
9	J	482	0	483	6	0
9	W	487	0	487	13	0
10	N	3430	0	3329	83	0
11	O	3140	0	3121	75	0
12	V	127	0	135	10	0
13	C	86	0	60	8	0
13	P	86	0	60	12	0
14	C	29	0	13	13	0
14	P	29	0	13	9	0
15	C	5	0	0	0	0
15	D	15	0	0	0	0
15	E	5	0	0	0	0
15	F	5	0	0	0	0
15	N	5	0	0	0	0
15	P	5	0	0	0	0
15	S	5	0	0	0	0
16	C	49	0	72	0	0
16	D	26	0	26	2	0
16	P	49	0	72	4	0
16	Q	51	0	82	4	0
17	D	43	0	32	6	0
17	Q	43	0	32	5	0
18	D	39	0	39	0	0
18	G	44	0	32	0	0
18	Q	39	0	39	0	0
18	T	49	0	42	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	R	4	0	0	3	0
20	R	6	0	8	0	0
All	All	31080	0	30718	897	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 897 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:U:39:LEU:CD2	8:U:39:LEU:CG	1.74	1.56
2:B:301:LYS:CE	2:B:301:LYS:NZ	1.69	1.51
3:C:194:MET:SD	3:C:194:MET:CE	2.06	1.43
3:P:194:MET:SD	3:P:194:MET:CE	2.07	1.42
4:D:93:LYS:NZ	4:D:93:LYS:CE	1.85	1.39

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/480 (92%)	401 (91%)	38 (9%)	3 (1%)	18	55
2	B	420/453 (93%)	377 (90%)	43 (10%)	0	100	100
3	C	372/379 (98%)	334 (90%)	37 (10%)	1 (0%)	36	70
3	P	368/379 (97%)	331 (90%)	36 (10%)	1 (0%)	36	70
4	D	238/325 (73%)	219 (92%)	18 (8%)	1 (0%)	30	65
4	Q	239/325 (74%)	221 (92%)	16 (7%)	2 (1%)	16	52
5	E	71/274 (26%)	62 (87%)	8 (11%)	1 (1%)	9	39
5	I	23/274 (8%)	20 (87%)	3 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	194/274 (71%)	168 (87%)	25 (13%)	1 (0%)	24	61
6	F	96/111 (86%)	88 (92%)	8 (8%)	0	100	100
6	S	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
7	G	78/82 (95%)	71 (91%)	7 (9%)	0	100	100
7	T	72/82 (88%)	66 (92%)	6 (8%)	0	100	100
8	H	63/91 (69%)	53 (84%)	9 (14%)	1 (2%)	7	37
8	U	64/91 (70%)	54 (84%)	9 (14%)	1 (2%)	7	37
9	J	56/64 (88%)	47 (84%)	9 (16%)	0	100	100
9	W	57/64 (89%)	49 (86%)	8 (14%)	0	100	100
10	N	442/480 (92%)	402 (91%)	38 (9%)	2 (0%)	24	61
11	O	417/453 (92%)	378 (91%)	38 (9%)	1 (0%)	43	76
12	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3824/5066 (76%)	3443 (90%)	366 (10%)	15 (0%)	30	65

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	TRP
8	H	25	GLU
8	U	25	GLU
5	E	61	SER
1	A	267	ASN

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	368/394 (93%)	354 (96%)	14 (4%)	29	51
2	B	331/355 (93%)	321 (97%)	10 (3%)	36	57
3	C	322/327 (98%)	313 (97%)	9 (3%)	38	59
3	P	318/327 (97%)	308 (97%)	10 (3%)	35	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	205/257 (80%)	197 (96%)	8 (4%)	28	51
4	Q	206/257 (80%)	198 (96%)	8 (4%)	28	51
5	E	63/228 (28%)	59 (94%)	4 (6%)	16	40
5	I	21/228 (9%)	19 (90%)	2 (10%)	8	27
5	R	168/228 (74%)	159 (95%)	9 (5%)	20	44
6	F	90/99 (91%)	85 (94%)	5 (6%)	19	43
6	S	91/99 (92%)	84 (92%)	7 (8%)	12	34
7	G	71/72 (99%)	62 (87%)	9 (13%)	4	19
7	T	66/72 (92%)	59 (89%)	7 (11%)	6	24
8	H	62/85 (73%)	55 (89%)	7 (11%)	5	22
8	U	63/85 (74%)	54 (86%)	9 (14%)	3	16
9	J	49/54 (91%)	47 (96%)	2 (4%)	27	50
9	W	49/54 (91%)	48 (98%)	1 (2%)	48	66
10	N	367/394 (93%)	355 (97%)	12 (3%)	33	55
11	O	328/355 (92%)	317 (97%)	11 (3%)	32	55
12	V	15/228 (7%)	14 (93%)	1 (7%)	15	39
All	All	3253/4198 (78%)	3108 (96%)	145 (4%)	24	48

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	76	ILE
12	V	71	ASN
5	R	182	VAL
7	T	18	LEU
6	F	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	225	HIS
5	R	141	HIS
10	N	118	GLN
5	R	57	GLN
3	P	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

27 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	PEE	C	505	-	48,48,50	1.26	4 (8%)	51,53,55	0.94	2 (3%)
19	FES	R	501	5	0,4,4	-	-	-		
15	PO4	S	501	-	4,4,4	0.88	0	6,6,6	0.36	0
18	CDL	G	501	-	43,43,99	1.50	4 (9%)	49,55,111	1.44	6 (12%)
14	G8U	P	503	3	31,31,31	2.16	6 (19%)	41,45,45	1.80	6 (14%)
15	PO4	D	502	-	4,4,4	0.83	0	6,6,6	0.44	0
15	PO4	C	504	-	4,4,4	1.01	0	6,6,6	0.21	0
13	HEM	P	501	3	50,50,50	1.62	9 (18%)	66,82,82	1.61	12 (18%)
15	PO4	E	501	-	4,4,4	0.81	0	6,6,6	0.70	0
17	HEC	Q	501	4	50,50,50	2.91	28 (56%)	68,82,82	2.27	25 (36%)
18	CDL	D	505	-	38,38,99	1.20	2 (5%)	43,47,111	1.08	4 (9%)
13	HEM	P	502	3	50,50,50	1.63	8 (16%)	66,82,82	1.83	14 (21%)
20	GOL	R	502	-	5,5,5	0.30	0	5,5,5	0.30	0
15	PO4	D	503	-	4,4,4	0.93	0	6,6,6	0.46	0
16	PEE	P	505	-	48,48,50	1.23	4 (8%)	51,53,55	0.98	2 (3%)
17	HEC	D	501	4	50,50,50	2.87	27 (54%)	68,82,82	2.49	28 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CDL	Q	505	-	38,38,99	1.19	2 (5%)	43,47,111	1.14	3 (6%)
16	PEE	D	506	-	25,25,50	1.42	2 (8%)	28,30,55	1.22	3 (10%)
15	PO4	D	504	-	4,4,4	0.92	0	6,6,6	0.41	0
15	PO4	F	501	-	4,4,4	0.92	0	6,6,6	0.51	0
13	HEM	C	502	3	50,50,50	1.72	11 (22%)	66,82,82	1.69	17 (25%)
15	PO4	P	504	-	4,4,4	0.86	0	6,6,6	0.68	0
15	PO4	N	501	-	4,4,4	0.93	0	6,6,6	0.39	0
13	HEM	C	501	3	50,50,50	1.62	7 (14%)	66,82,82	1.78	19 (28%)
16	PEE	Q	506	-	50,50,50	1.28	4 (8%)	53,55,55	0.98	3 (5%)
18	CDL	T	501	-	48,48,99	1.32	4 (8%)	54,60,111	1.25	4 (7%)
14	G8U	C	503	3	31,31,31	2.25	6 (19%)	41,45,45	1.66	8 (19%)

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
17	HEC	D	501	4	1/1/3/7	8/14/54/54	-
18	CDL	Q	505	-	-	13/43/43/110	-
20	GOL	R	502	-	-	3/4/4/4	-
16	PEE	D	506	-	1/1/4/8	13/29/29/54	-
16	PEE	C	505	-	1/1/4/8	26/52/52/54	-
14	G8U	C	503	3	-	5/15/15/15	0/3/3/3
13	HEM	P	501	3	-	8/14/54/54	-
14	G8U	P	503	3	-	4/15/15/15	0/3/3/3
13	HEM	C	502	3	-	4/14/54/54	-
19	FES	R	501	5	-	-	0/1/1/1
17	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
16	PEE	P	505	-	1/1/4/8	29/52/52/54	-
16	PEE	Q	506	-	1/1/4/8	28/54/54/54	-
13	HEM	C	501	3	-	6/14/54/54	-
18	CDL	T	501	-	-	29/57/57/110	-
18	CDL	D	505	-	-	24/43/43/110	-
18	CDL	G	501	-	-	32/52/52/110	-
13	HEM	P	502	3	-	6/14/54/54	-

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	503	G8U	C19-C20	7.20	1.48	1.38
14	P	503	G8U	C19-C20	6.55	1.47	1.38
14	C	503	G8U	C17-C18	5.56	1.47	1.40
13	C	501	HEM	FE-NB	5.50	2.11	1.94
13	P	502	HEM	FE-NB	5.45	2.11	1.94

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	C1B-C2B-C3B	-6.31	100.33	106.96
14	P	503	G8U	C27-C20-C19	-6.01	119.56	123.01
17	D	501	HEC	C2B-C1B-NB	5.89	116.94	109.88
14	P	503	G8U	C20-C19-C18	-5.71	119.16	122.79
18	G	501	CDL	OA6-CA5-C11	5.69	121.56	111.09

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	505	PEE	C2
16	D	506	PEE	C2
16	P	505	PEE	C2
16	Q	506	PEE	C2
17	D	501	HEC	NA

5 of 247 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	501	HEM	C3A-C2A-CAA-CBA
13	P	502	HEM	C2D-C3D-CAD-CBD
16	D	506	PEE	C4-O4P-P-O3P
16	D	506	PEE	C4-O4P-P-O1P
16	D	506	PEE	O4P-C4-C5-N

There are no ring outliers.

13 monomers are involved in 69 short contacts:

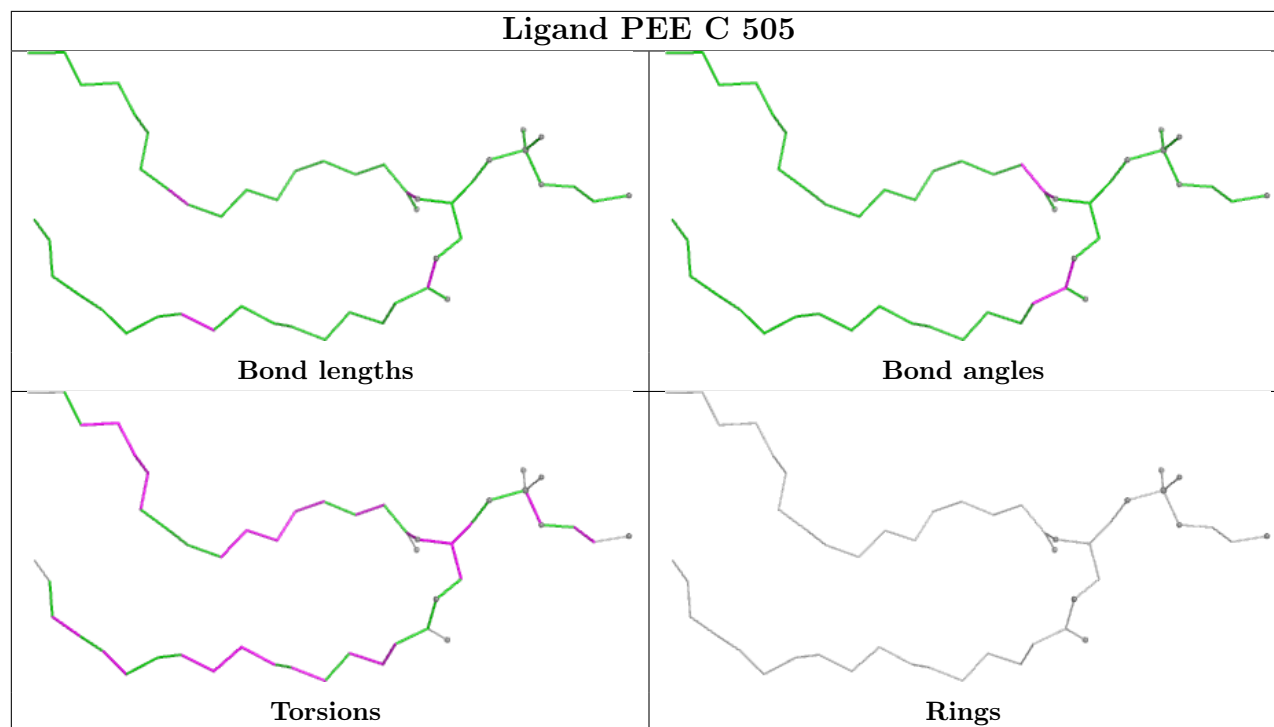
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	501	FES	3	0
14	P	503	G8U	9	0
13	P	501	HEM	10	0
17	Q	501	HEC	5	0

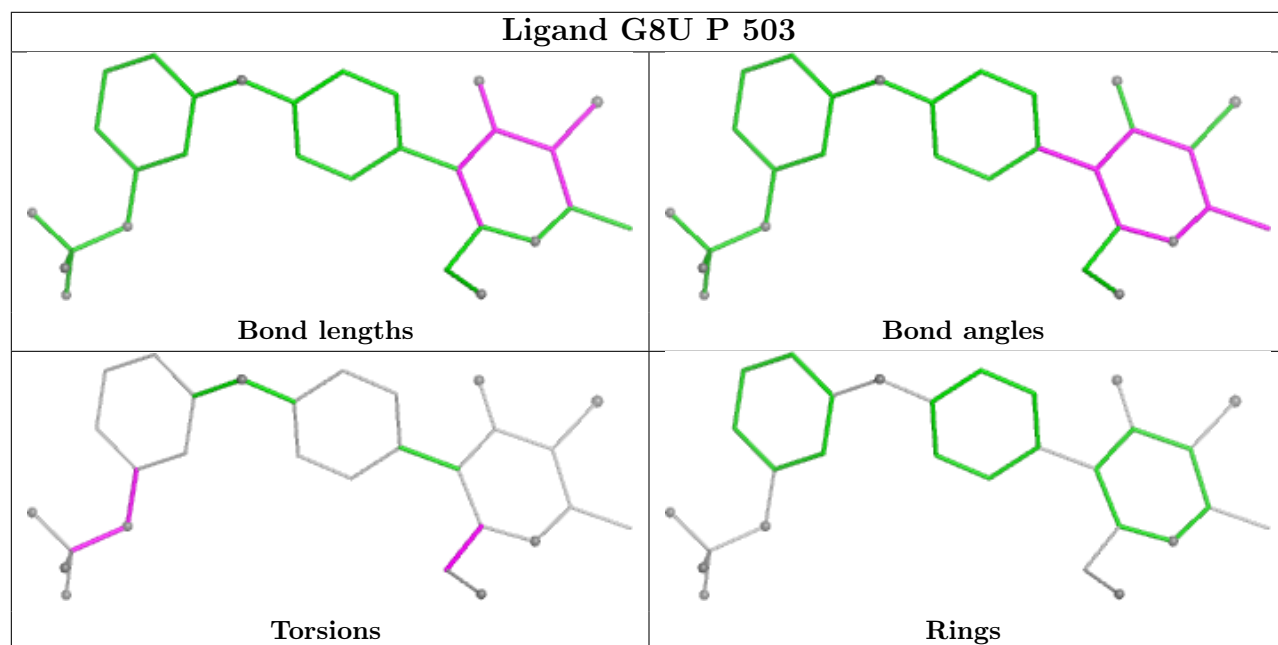
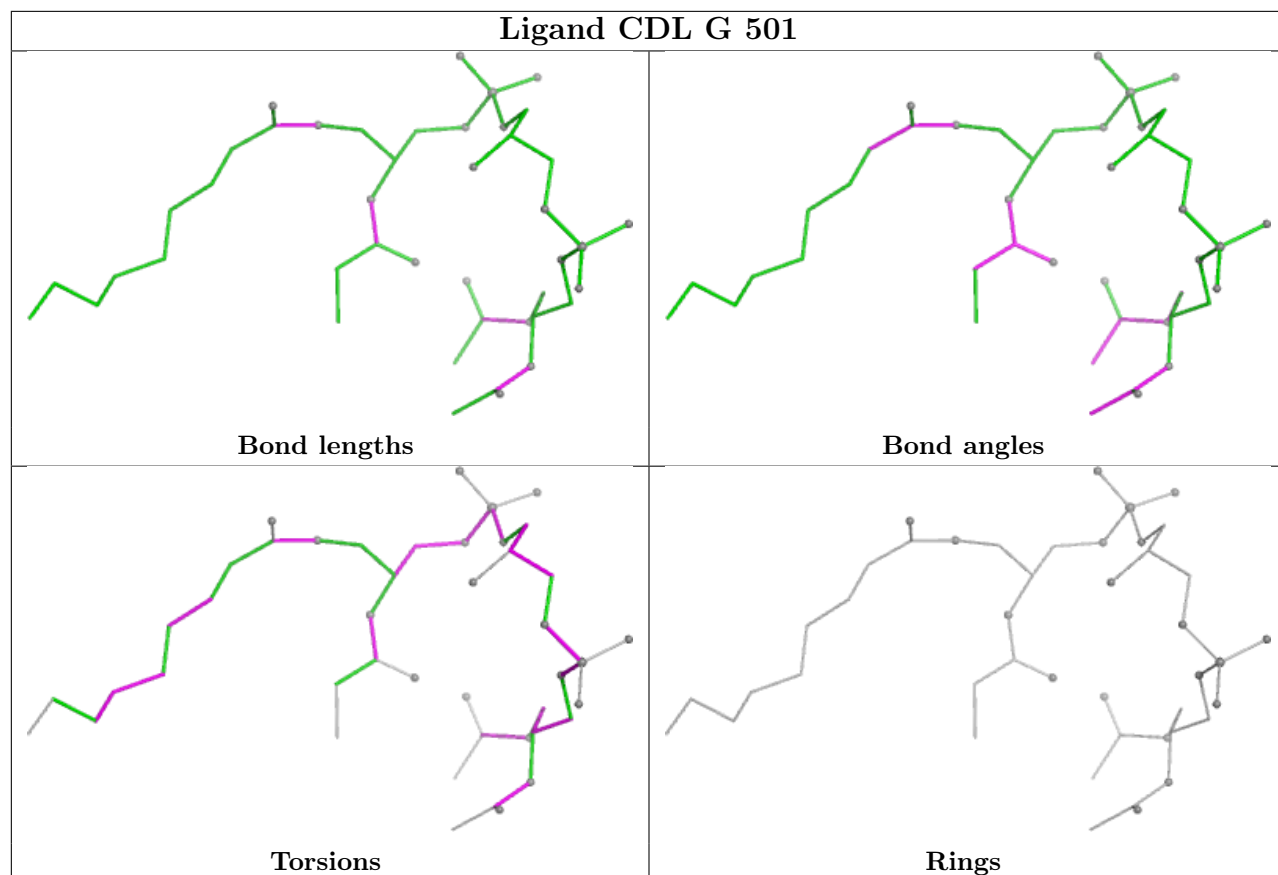
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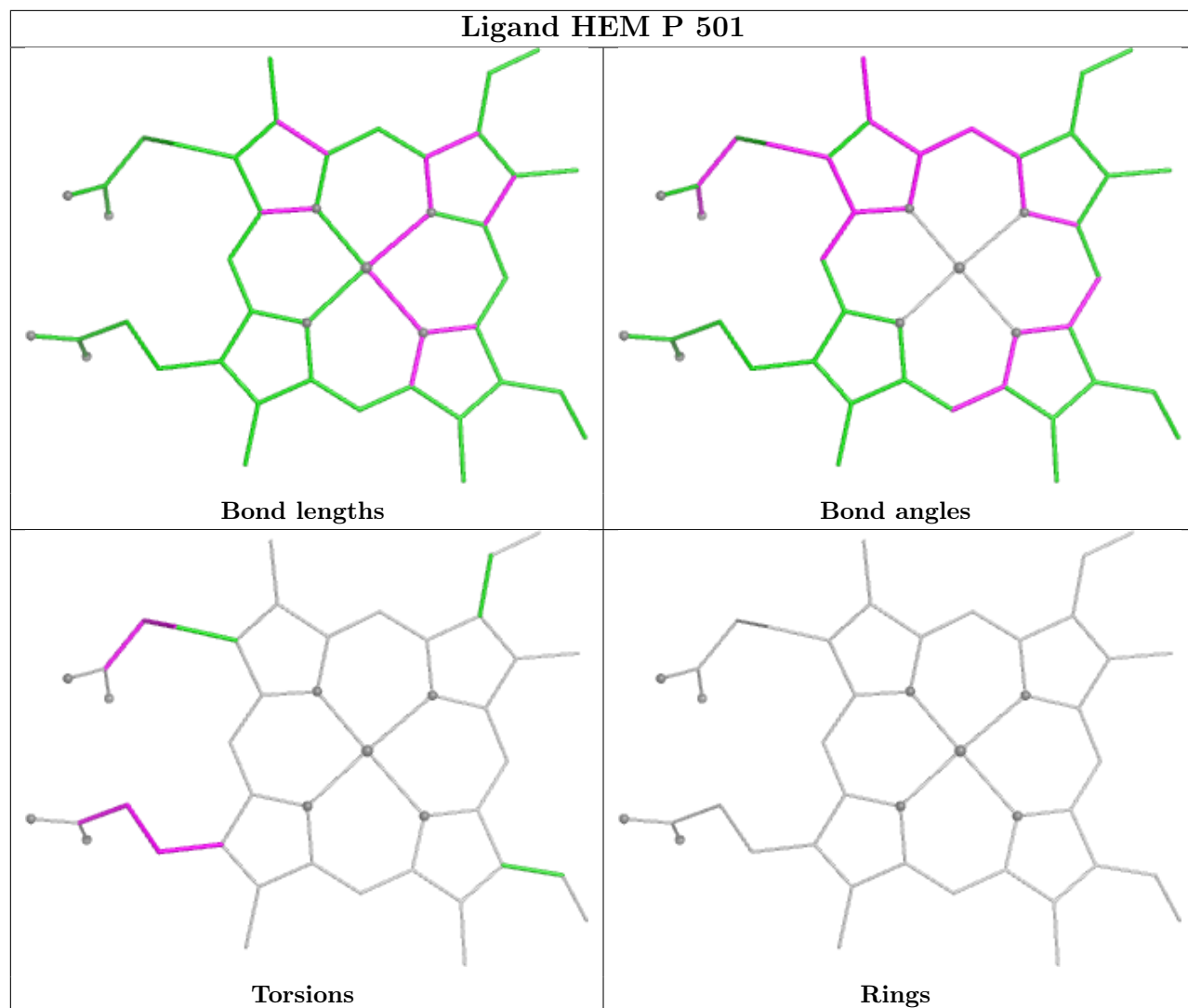
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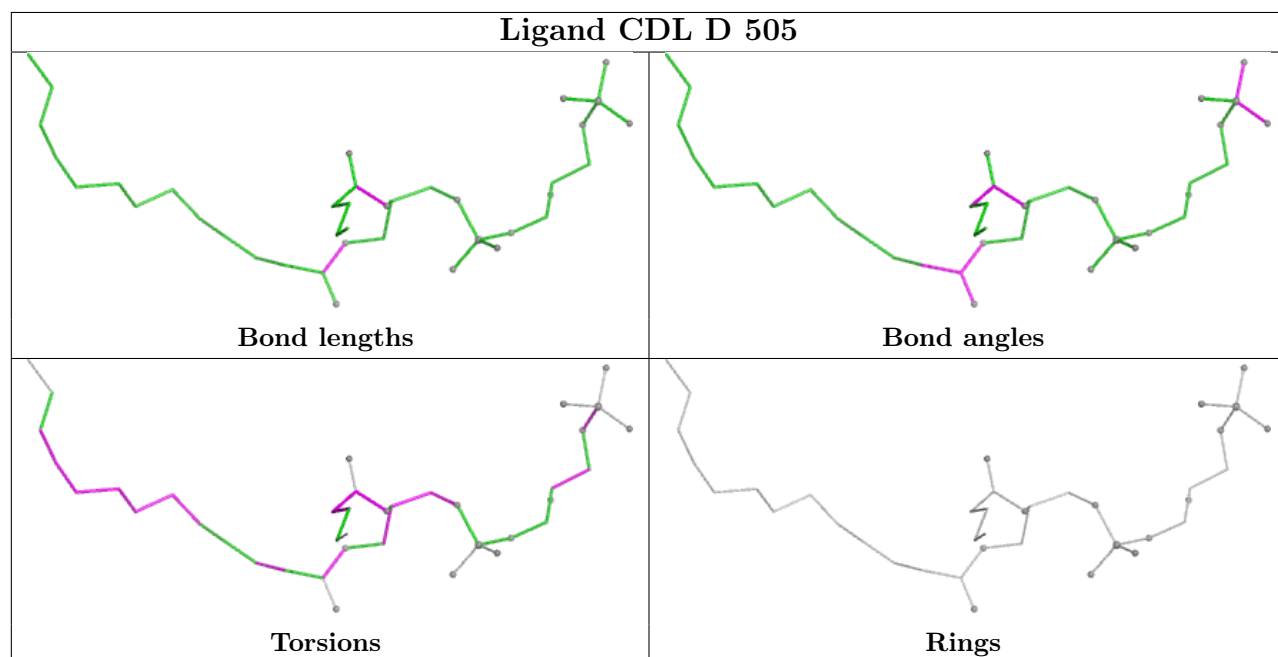
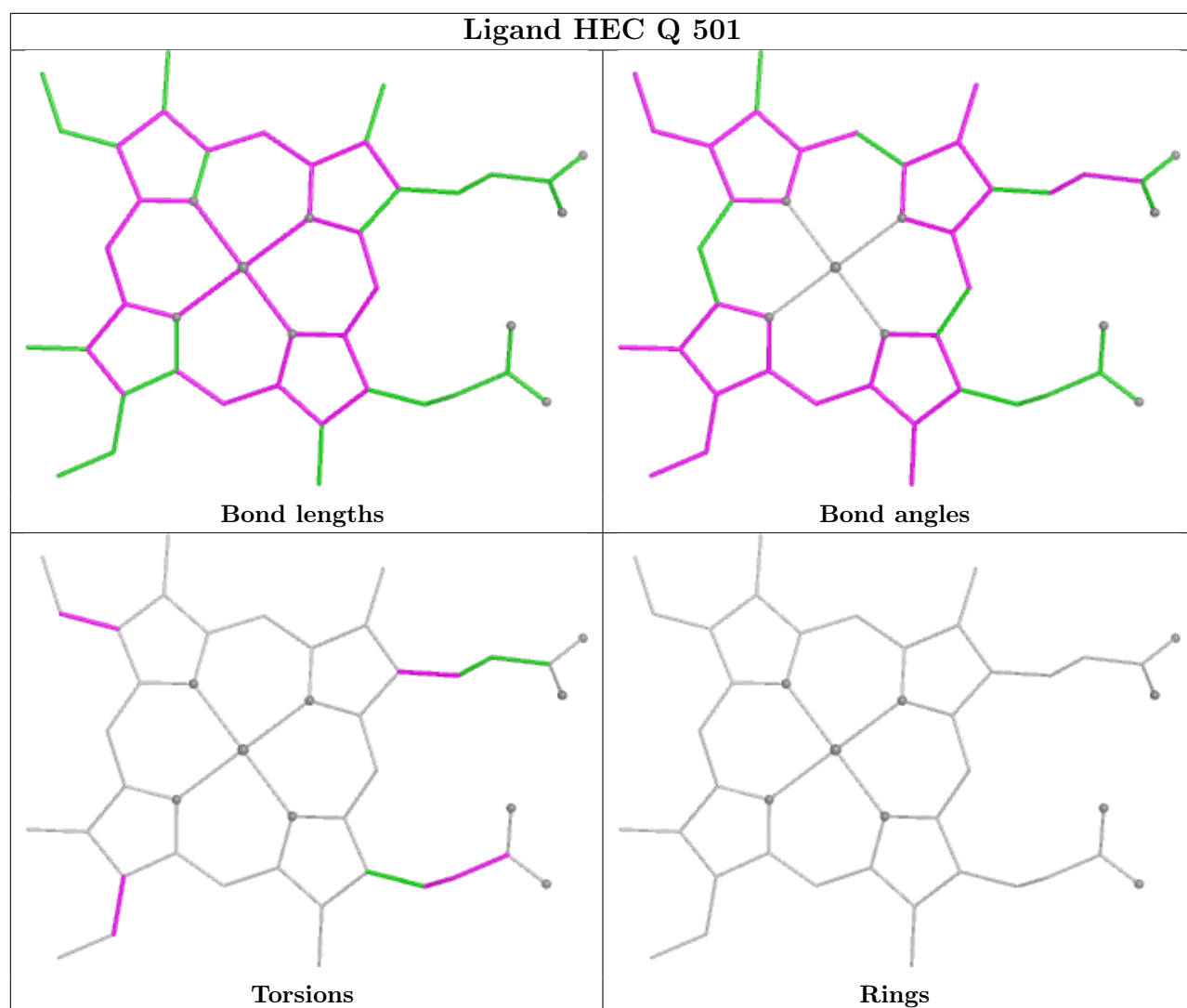
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	502	HEM	2	0
16	P	505	PEE	4	0
17	D	501	HEC	6	0
16	D	506	PEE	2	0
13	C	502	HEM	3	0
13	C	501	HEM	5	0
16	Q	506	PEE	4	0
18	T	501	CDL	5	0
14	C	503	G8U	13	0

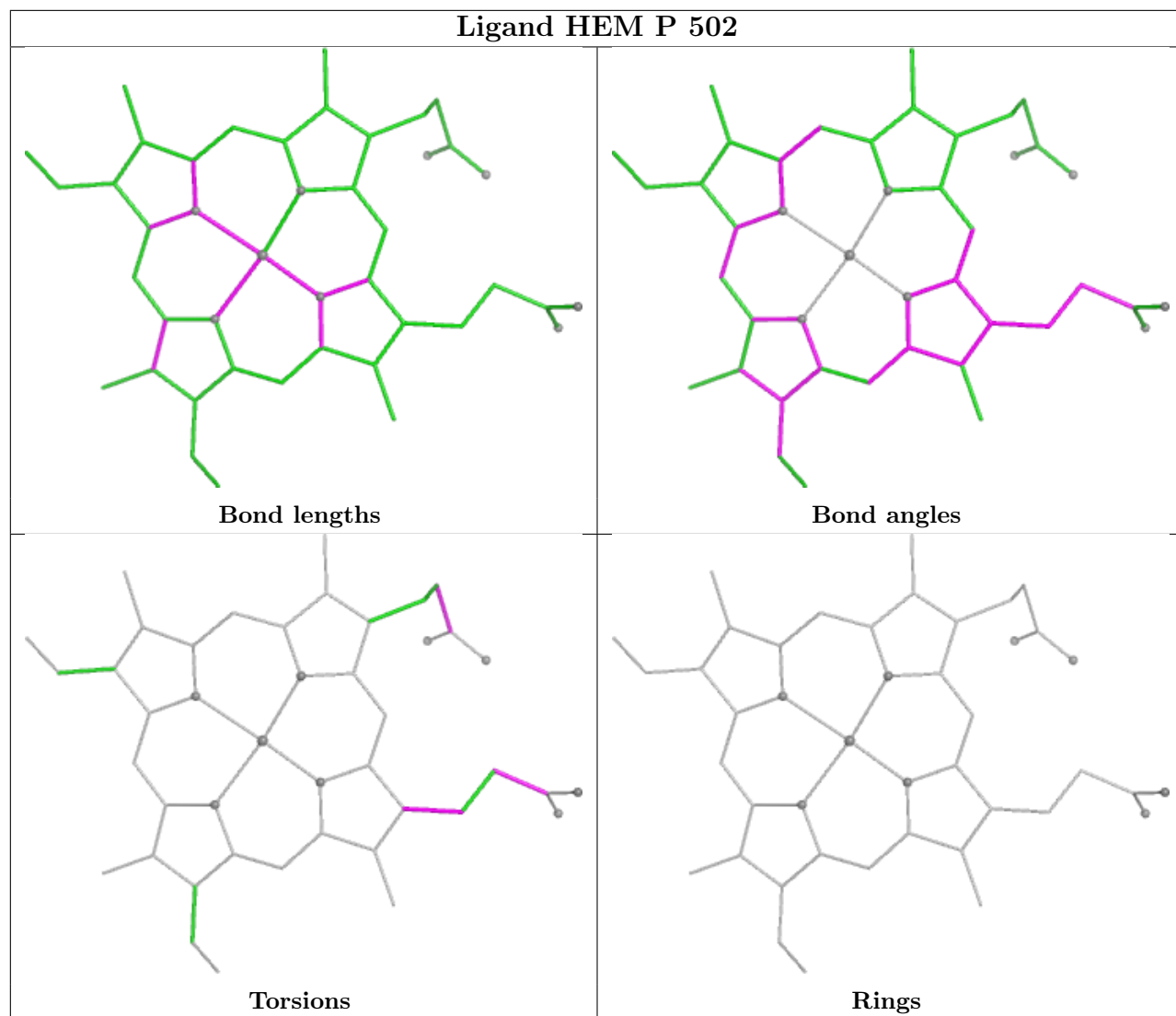
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

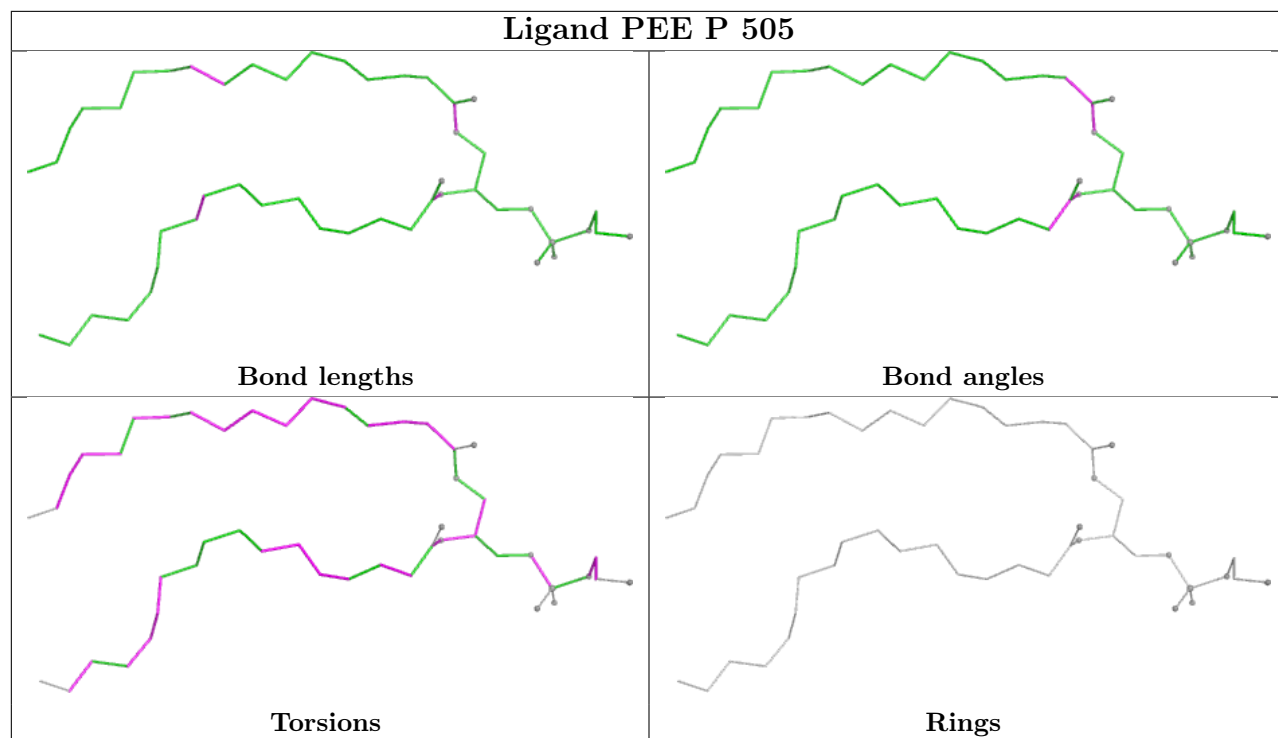


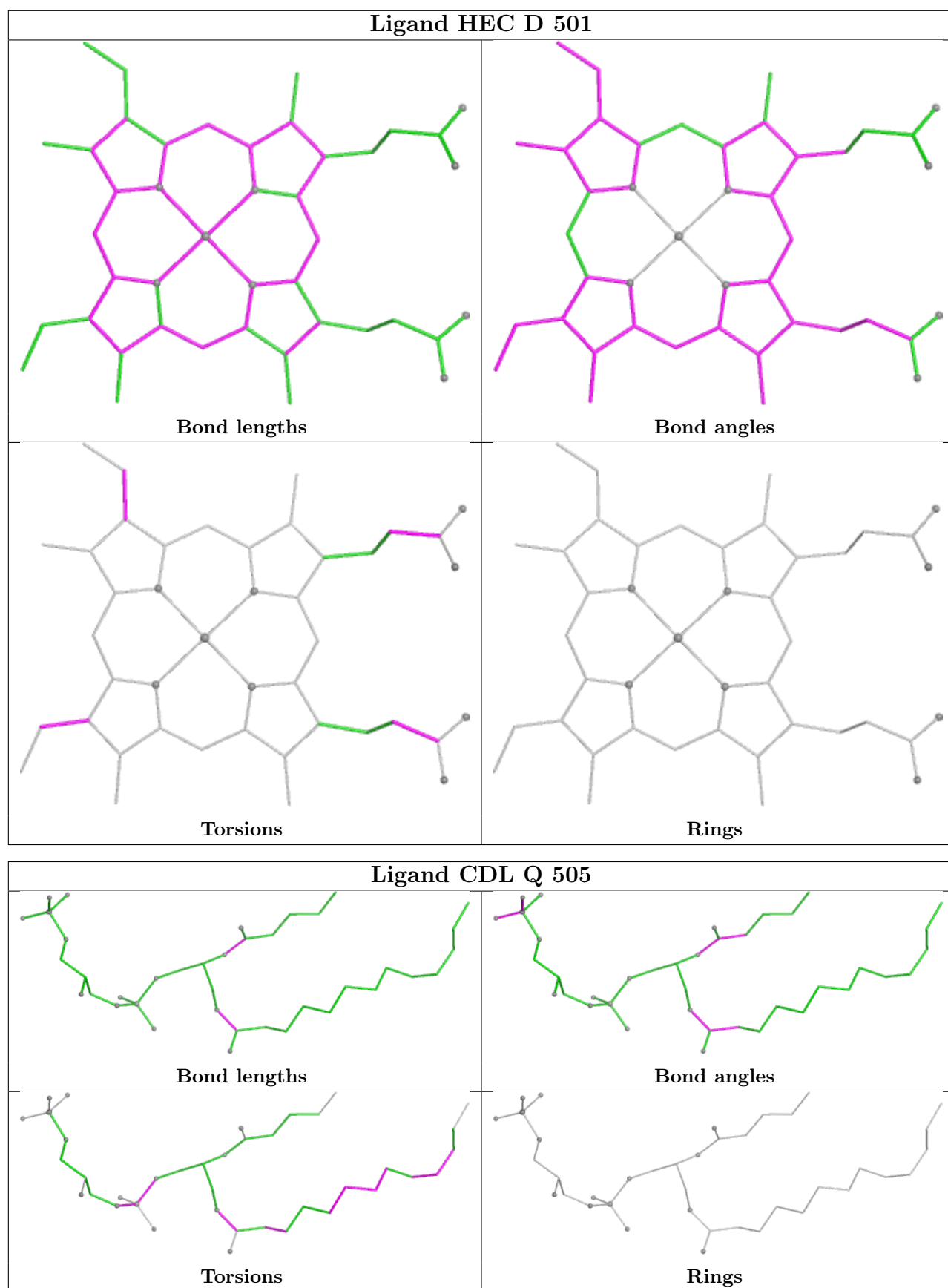


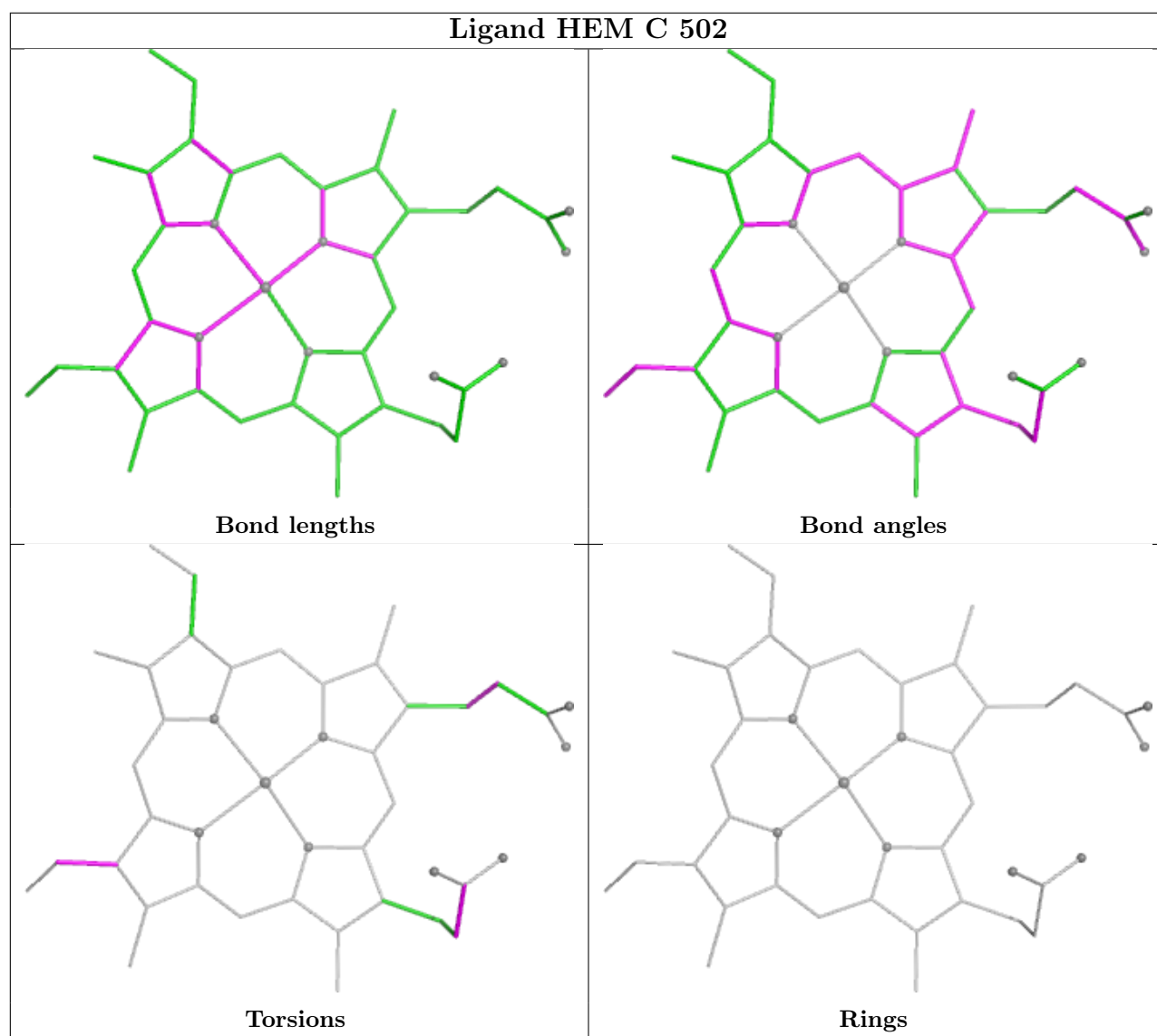
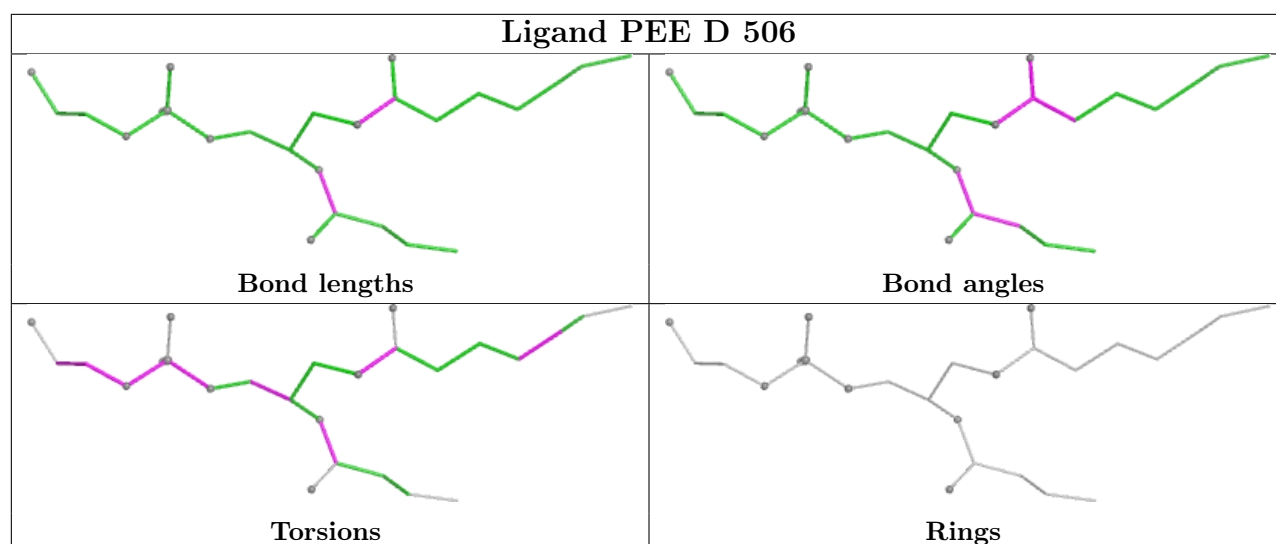


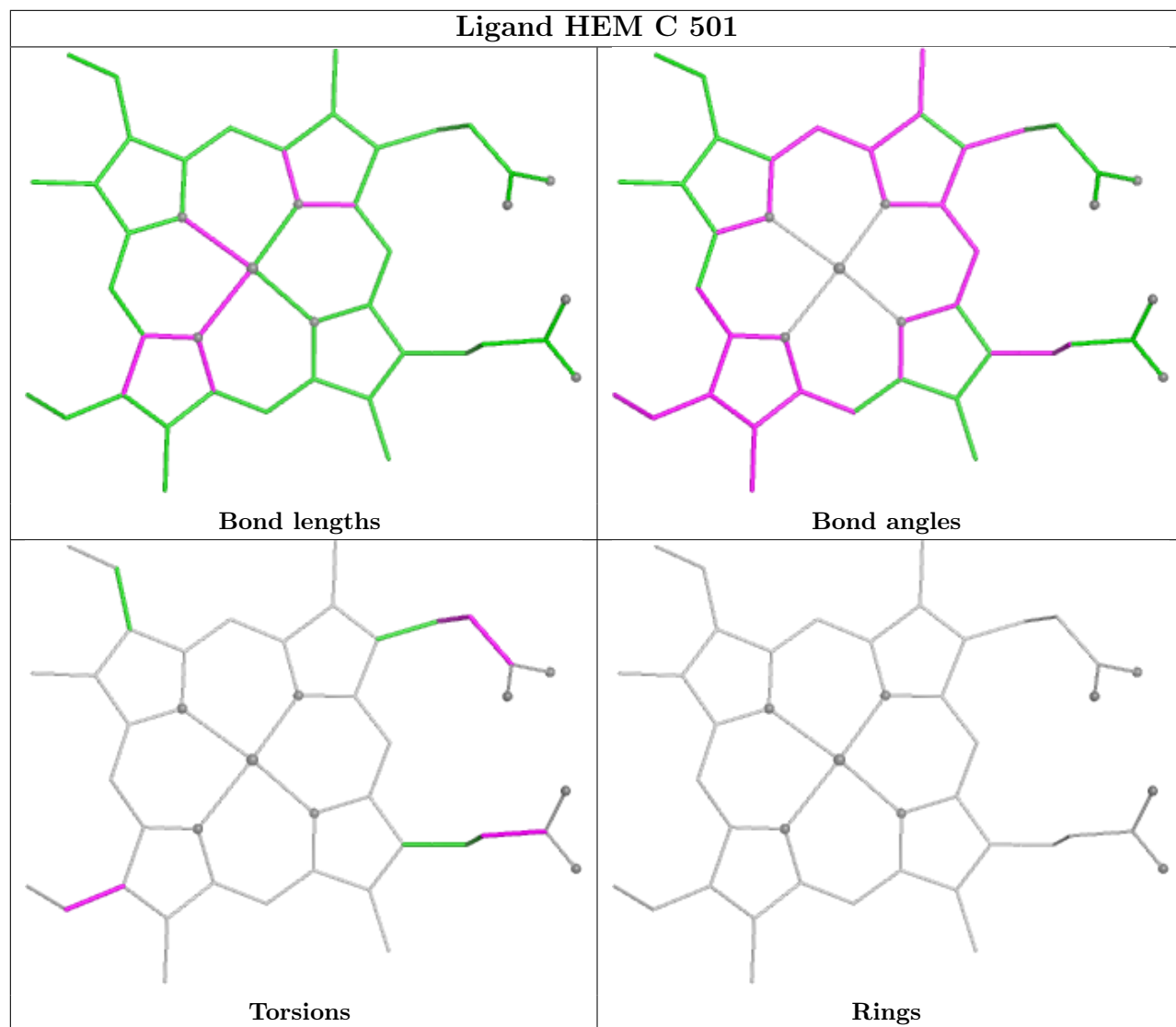


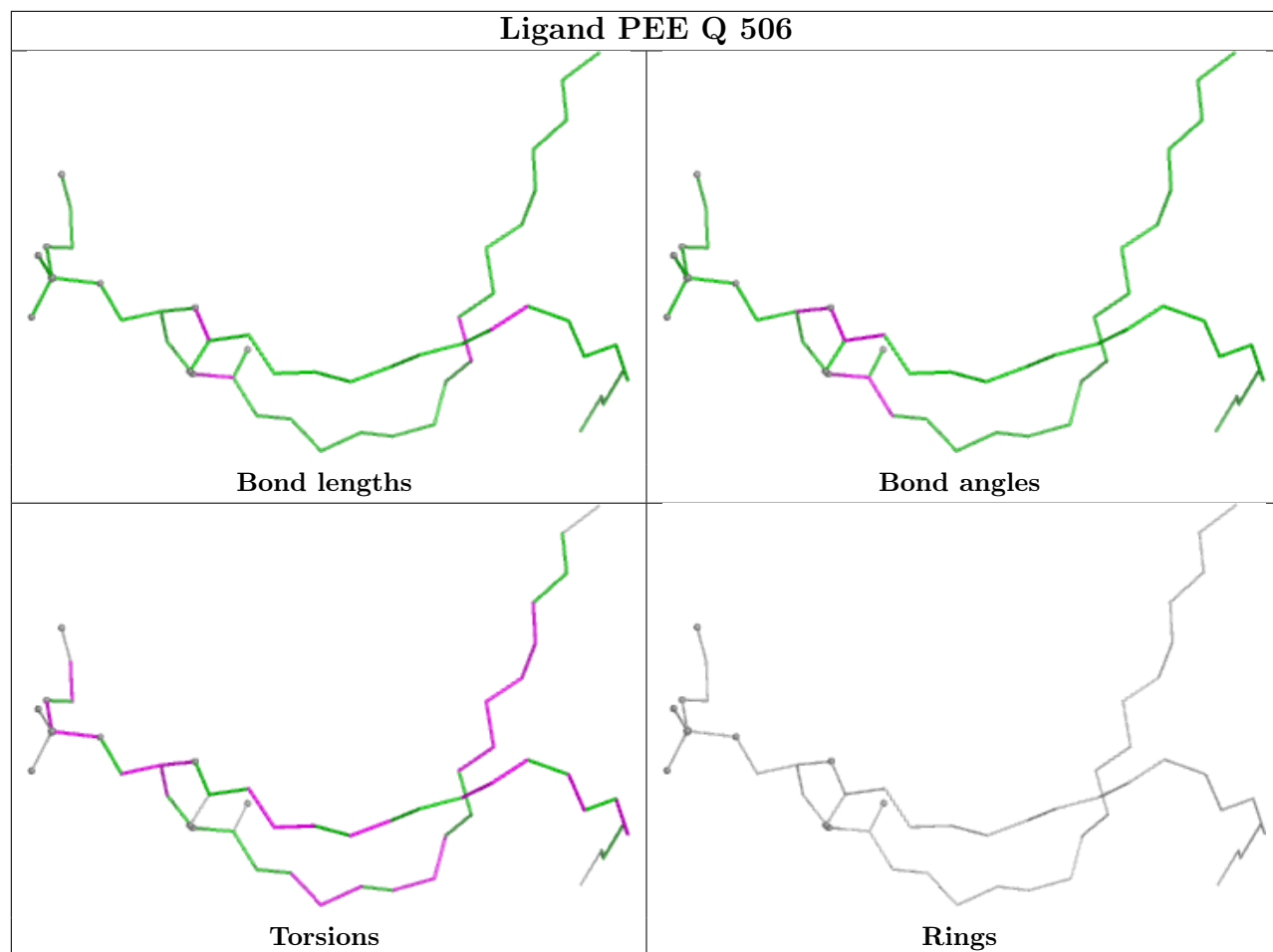




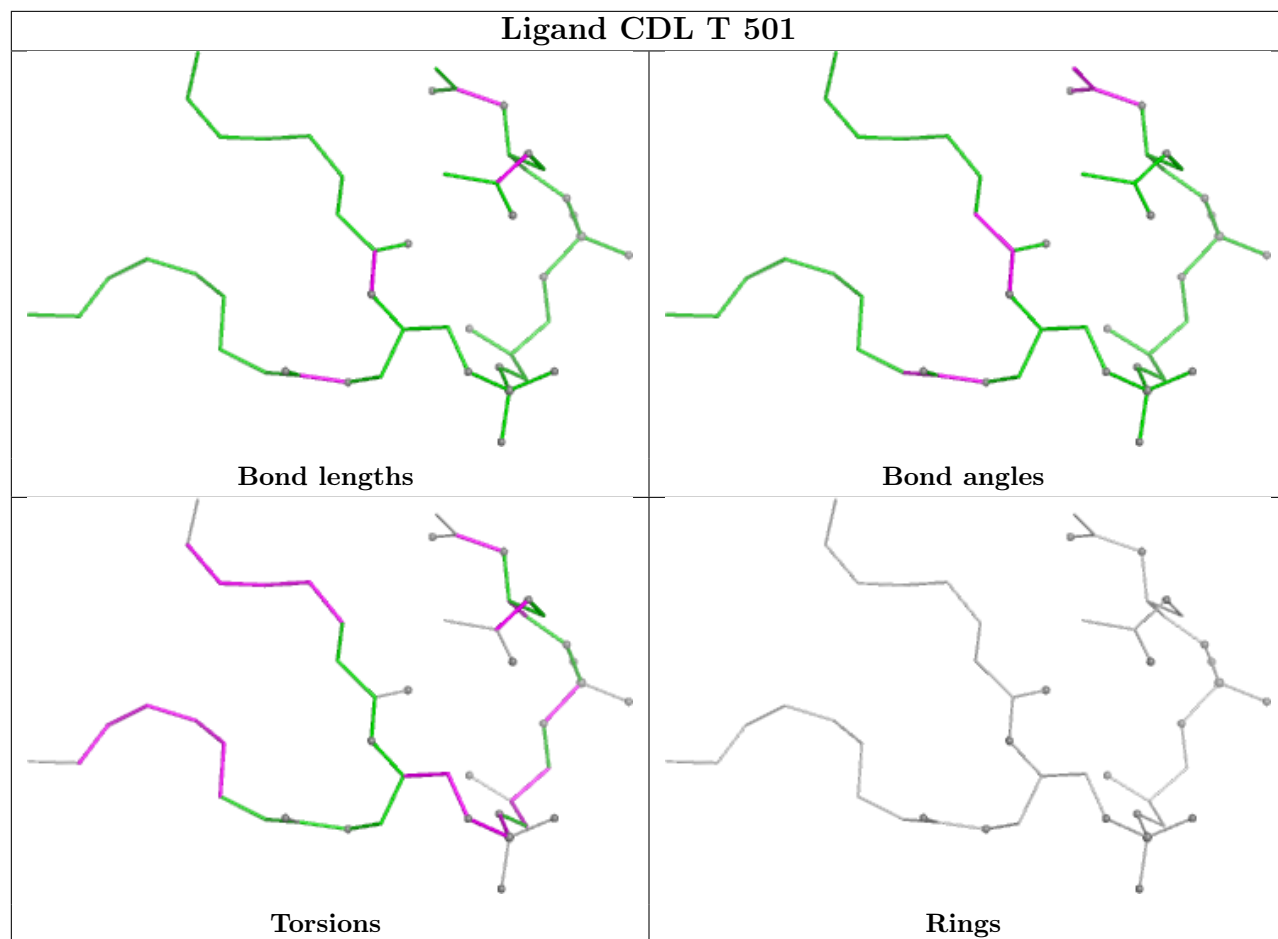




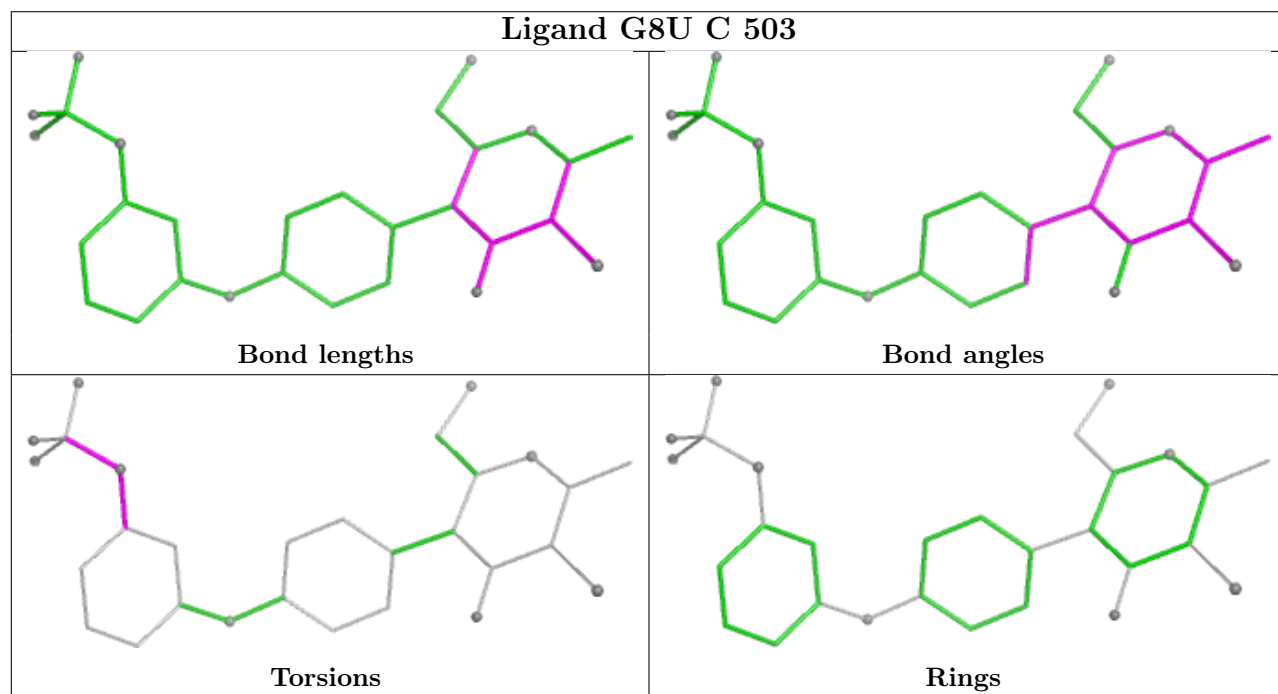




Ligand CDL T 501



Ligand G8U C 503



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	444:LEU	C	445:LYS	N	0.87

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, 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%)	-0.45	1 (0%) 91 82	24, 182, 228, 270	0
2	B	422/453 (93%)	-0.25	11 (2%) 57 42	126, 187, 223, 271	0
3	C	374/379 (98%)	-0.47	2 (0%) 87 74	23, 131, 164, 249	0
3	P	370/379 (97%)	-0.33	11 (2%) 52 39	99, 138, 177, 195	0
4	D	240/325 (73%)	-0.49	1 (0%) 88 76	119, 149, 186, 210	0
4	Q	241/325 (74%)	-0.46	1 (0%) 88 76	115, 162, 198, 232	0
5	E	73/274 (26%)	-0.30	0 100 100	123, 155, 194, 211	0
5	I	27/274 (9%)	0.23	2 (7%) 20 20	168, 214, 255, 306	0
5	R	196/274 (71%)	-0.39	3 (1%) 72 54	30, 190, 238, 288	0
6	F	98/111 (88%)	-0.37	0 100 100	121, 153, 190, 200	0
6	S	99/111 (89%)	-0.41	1 (1%) 79 62	117, 148, 182, 208	0
7	G	80/82 (97%)	-0.35	1 (1%) 75 58	30, 149, 204, 273	0
7	T	74/82 (90%)	-0.40	0 100 100	114, 156, 198, 212	0
8	H	65/91 (71%)	-0.35	1 (1%) 72 54	130, 160, 190, 202	0
8	U	66/91 (72%)	-0.58	0 100 100	161, 190, 238, 284	0
9	J	58/64 (90%)	-0.38	0 100 100	131, 158, 191, 222	0
9	W	59/64 (92%)	-0.72	0 100 100	115, 150, 186, 198	0
10	N	444/480 (92%)	-0.40	3 (0%) 84 69	24, 162, 208, 261	0
11	O	419/453 (92%)	-0.31	3 (0%) 84 69	30, 176, 212, 247	0
12	V	17/274 (6%)	-0.03	1 (5%) 28 25	174, 195, 225, 228	0
All	All	3866/5066 (76%)	-0.39	42 (1%) 78 61	23, 162, 216, 306	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	75	ALA	5.0
6	S	38	HIS	3.9
3	P	104	TYR	3.8
11	O	302	GLY	3.8
3	P	206	ASN	3.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	PO4	P	504	5/5	0.61	0.09	159,166,173,174	0
15	PO4	N	501	5/5	0.64	0.12	155,167,169,176	0
15	PO4	F	501	5/5	0.64	0.09	251,252,258,259	0
15	PO4	D	503	5/5	0.72	0.08	212,225,230,231	0
15	PO4	E	501	5/5	0.75	0.08	142,147,152,152	0
15	PO4	C	504	5/5	0.76	0.10	156,159,161,168	0
15	PO4	D	504	5/5	0.78	0.07	246,252,254,257	0
15	PO4	D	502	5/5	0.80	0.06	234,240,241,242	0
15	PO4	S	501	5/5	0.86	0.05	268,268,275,278	0
14	G8U	P	503	29/29	0.87	0.17	125,164,212,219	0
14	G8U	C	503	29/29	0.87	0.19	128,171,211,230	0
16	PEE	Q	506	51/51	0.93	0.16	125,148,166,171	0
18	CDL	D	505	39/100	0.94	0.09	112,152,165,174	0
18	CDL	Q	505	39/100	0.94	0.08	116,140,173,174	0
18	CDL	T	501	49/100	0.94	0.09	111,152,190,204	0
20	GOL	R	502	6/6	0.94	0.17	215,221,224,225	0
18	CDL	G	501	44/100	0.95	0.08	111,137,175,179	0
16	PEE	D	506	26/51	0.95	0.11	124,151,176,178	0
19	FES	R	501	4/4	0.97	0.03	200,213,218,224	0

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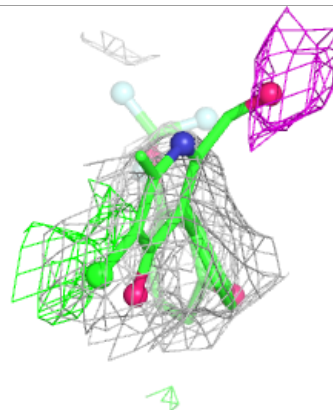
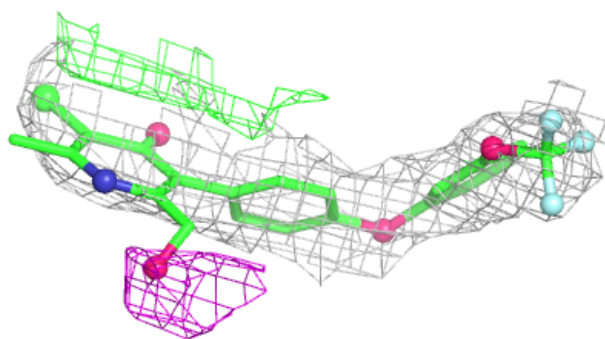
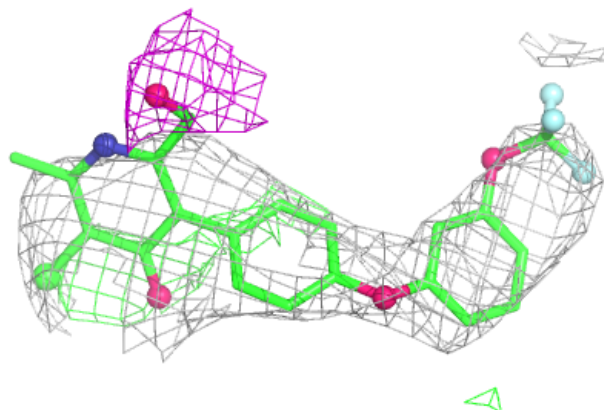
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	PEE	C	505	49/51	0.98	0.10	113,144,173,183	0
17	HEC	D	501	43/43	0.98	0.10	125,134,153,161	0
13	HEM	P	502	43/43	0.98	0.09	100,107,130,132	0
16	PEE	P	505	49/51	0.98	0.11	129,146,172,180	0
13	HEM	C	502	43/43	0.99	0.06	96,108,120,147	0
17	HEC	Q	501	43/43	0.99	0.06	119,145,161,164	0
13	HEM	P	501	43/43	0.99	0.07	113,130,145,151	0
13	HEM	C	501	43/43	0.99	0.09	110,118,132,142	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.

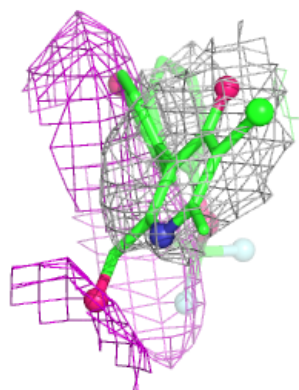
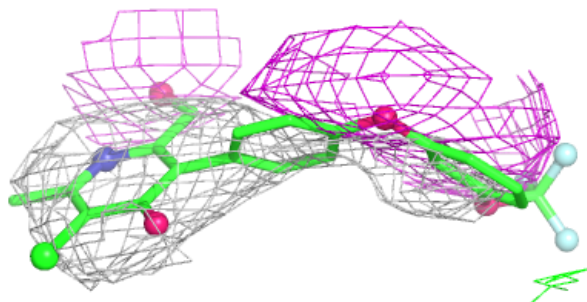
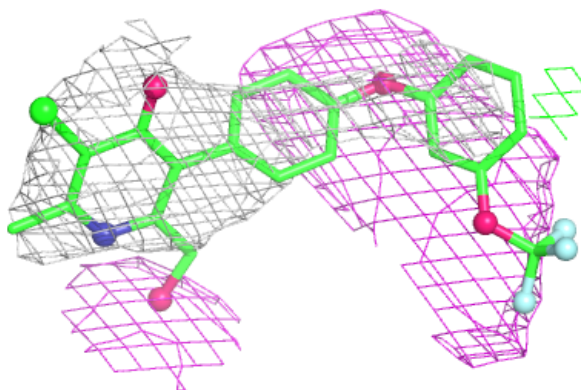
Electron density around G8U P 503:

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

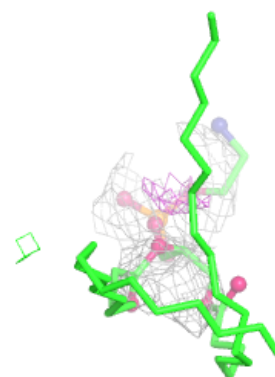
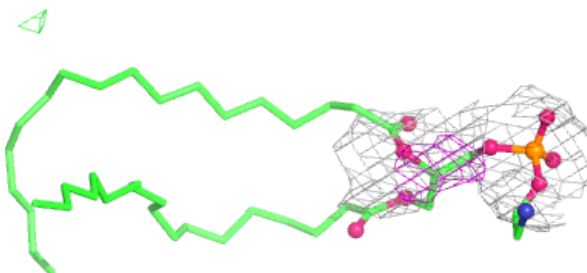
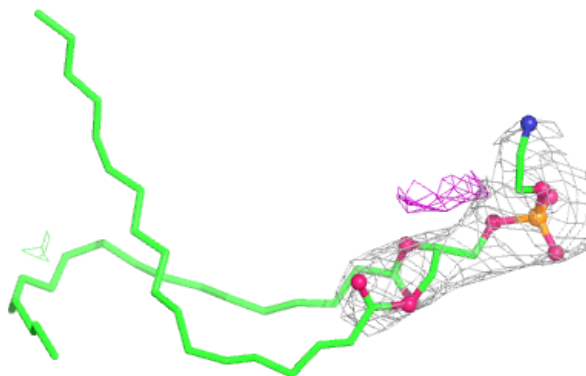


Electron density around G8U C 503:

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and green (positive)

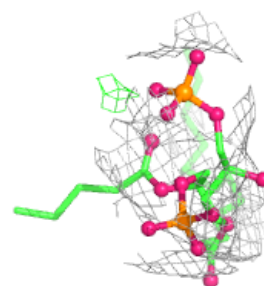
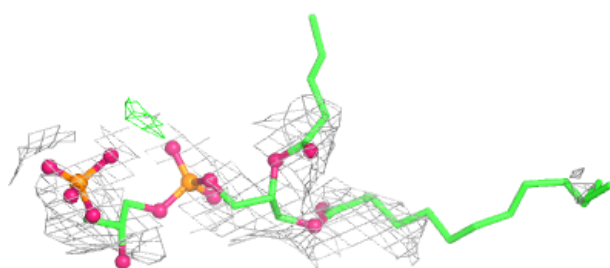
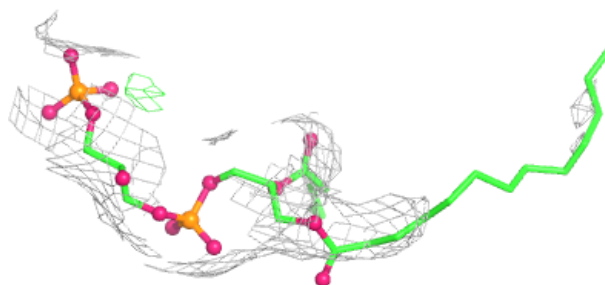
**Electron density around PEE Q 506:**

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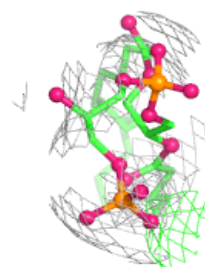
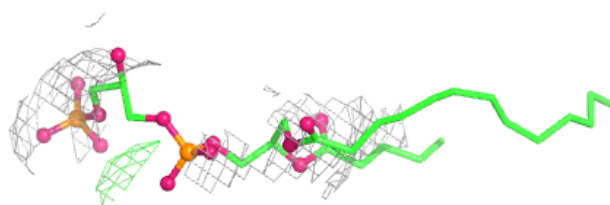
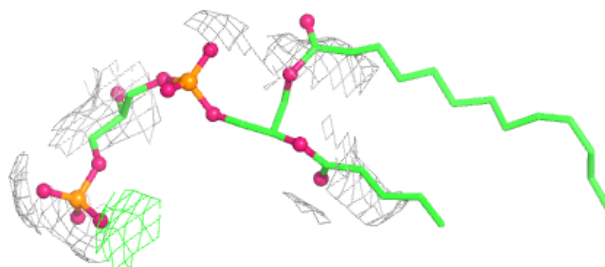


Electron density around CDL D 505:

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and green (positive)

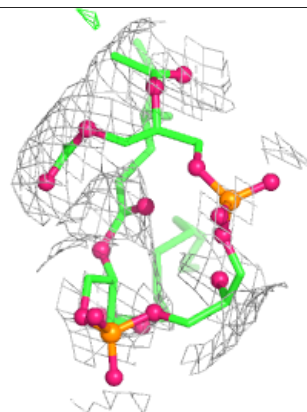
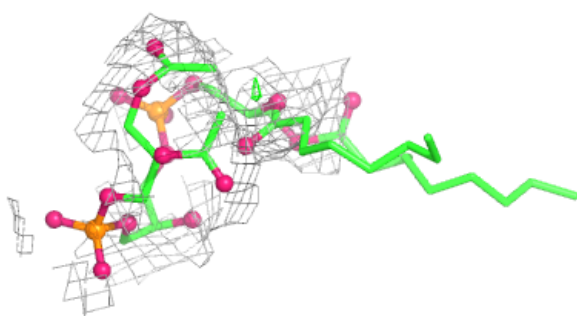
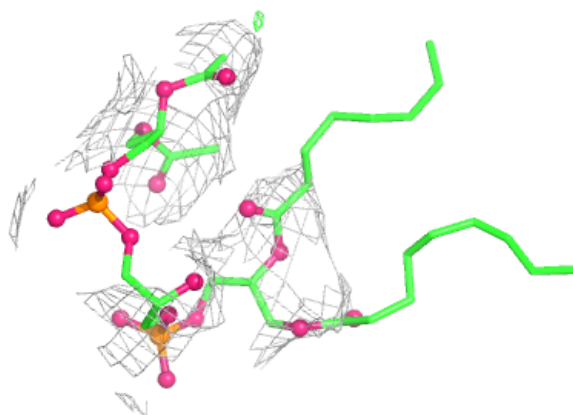
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and green (positive)

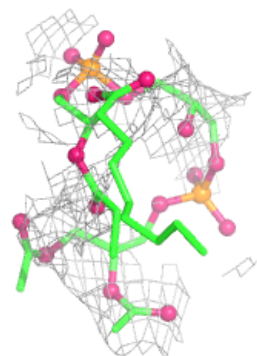
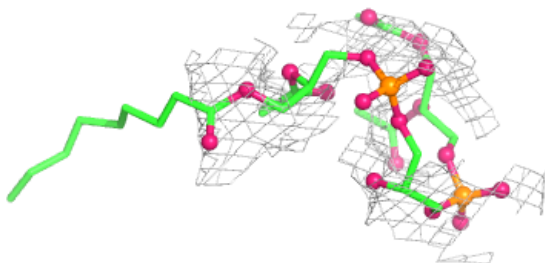
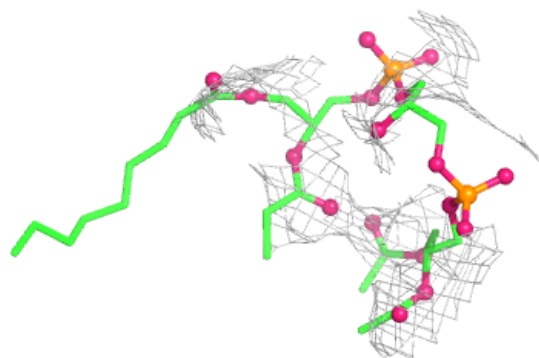


Electron density around CDL T 501:

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and green (positive)

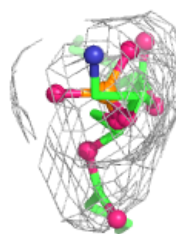
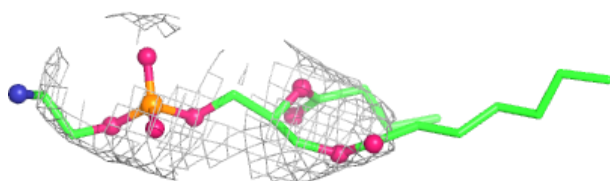
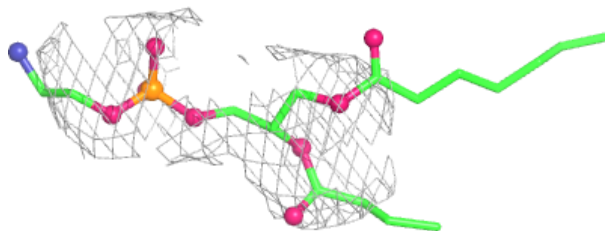
**Electron density around CDL G 501:**

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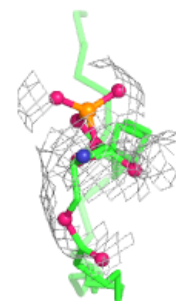
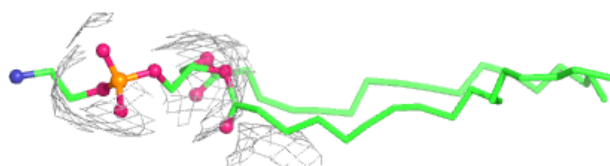
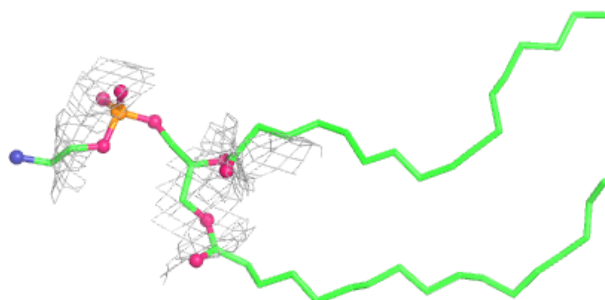


Electron density around PEE D 506:

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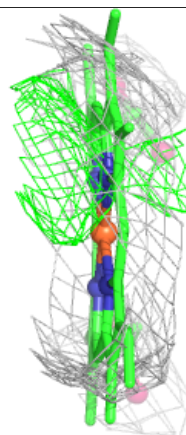
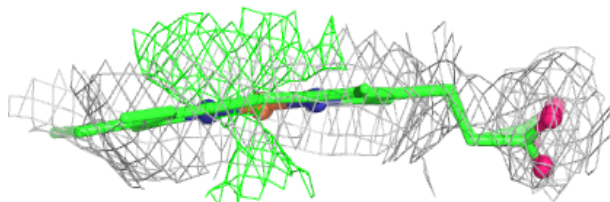
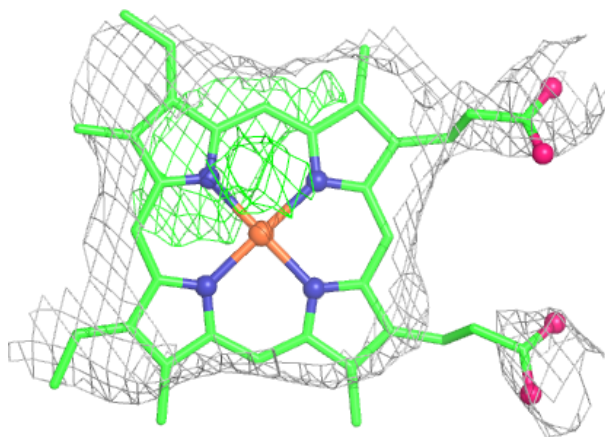
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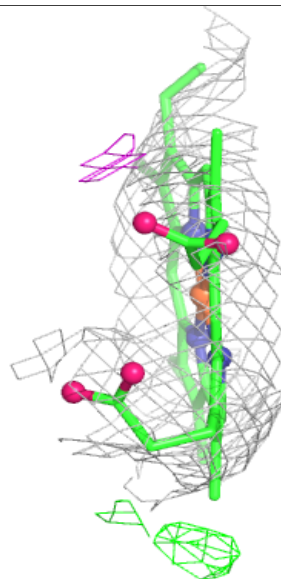
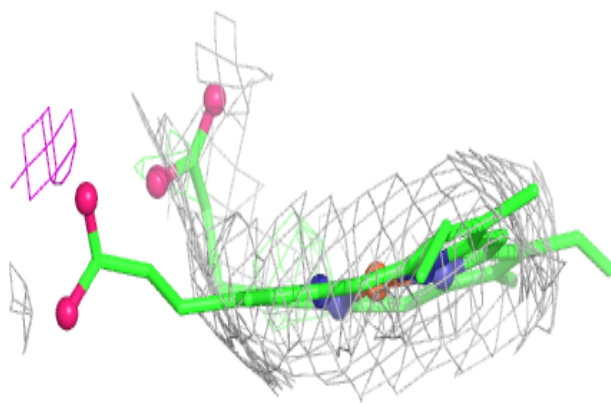
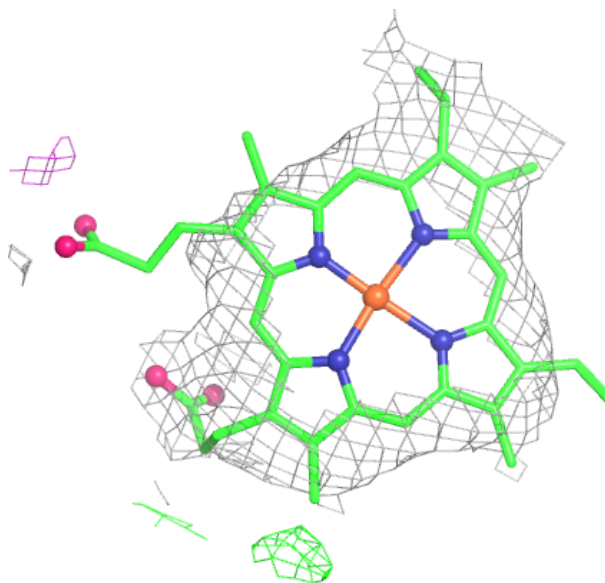
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and green (positive)



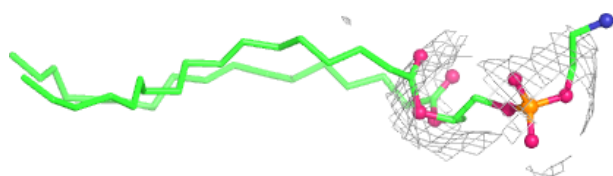
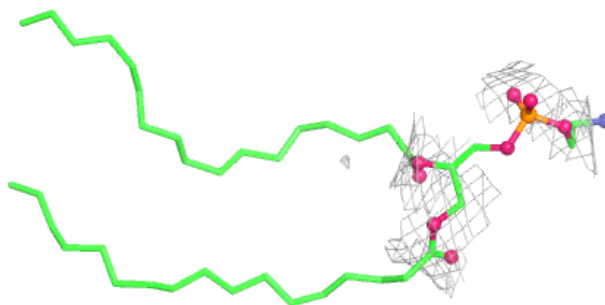
Electron density around HEM P 502:

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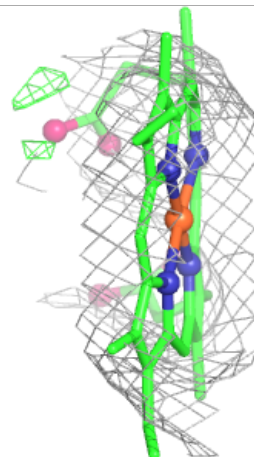
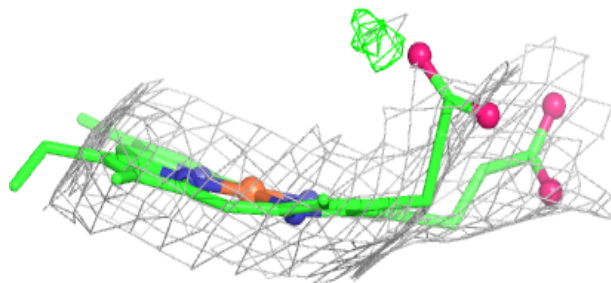
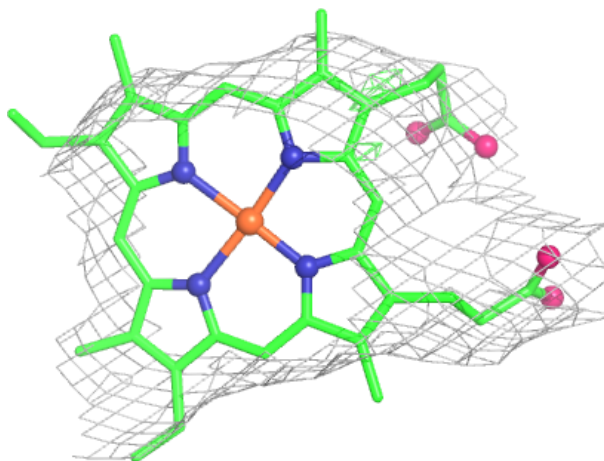
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and green (positive)



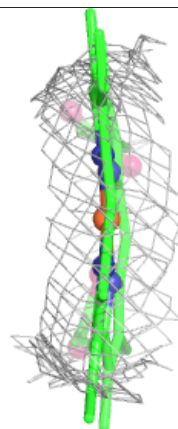
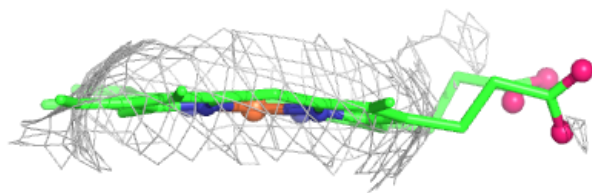
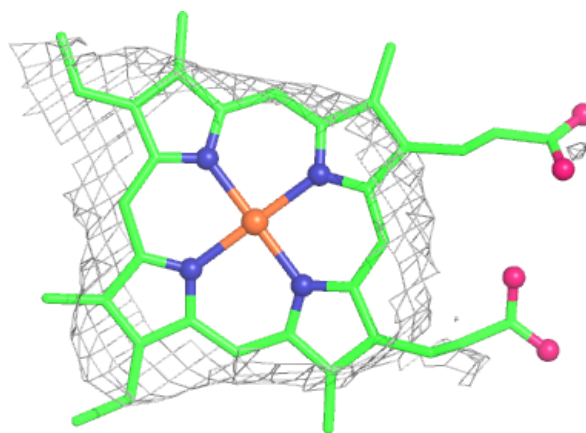
Electron density around HEM C 502:

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and green (positive)



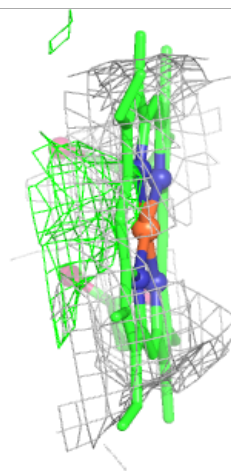
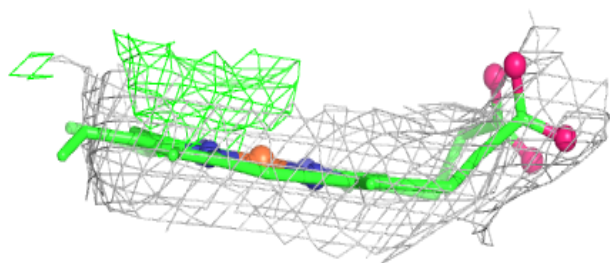
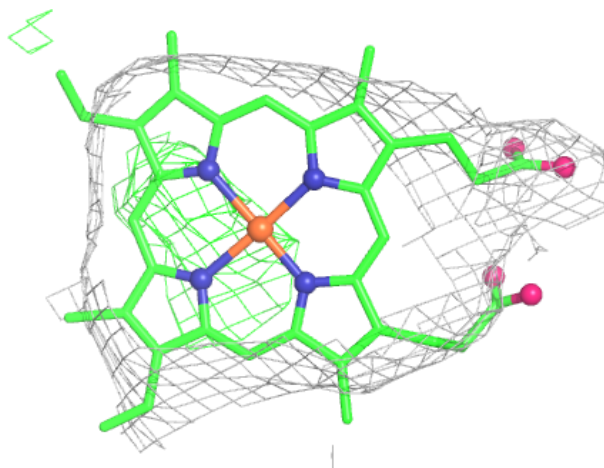
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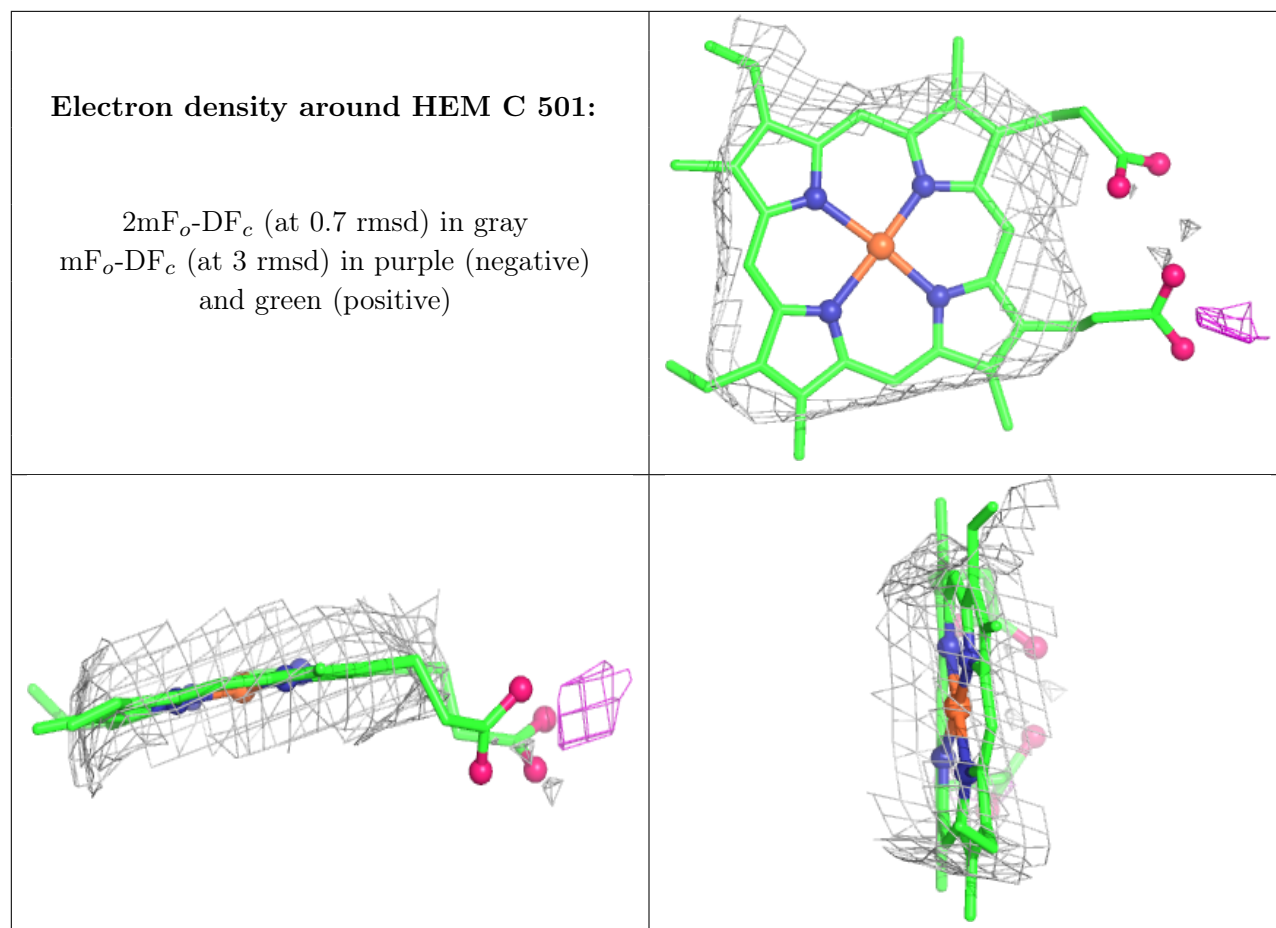
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and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.