wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 03:33 am BST

PDB ID	:	4D6T / pdb_00004d6t
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 (i) 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 (i)) were used in the production of this report:

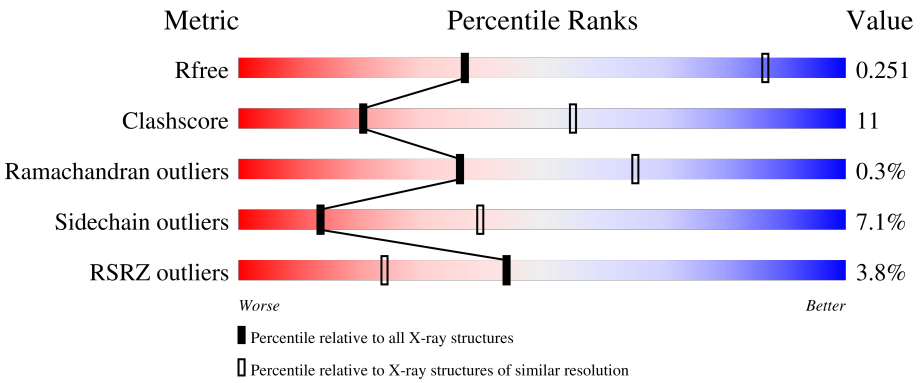
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (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 <=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	5% 74% 17% • • 8%
1	N	480	5% 75% 16% • 8%
2	B	453	3% 71% 19% • • 7%
3	C	379	2% 73% 21% • •
3	P	379	% 75% 19% • •

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Mol	Chain	Length	Quality of chain
4	D	265	2% 75% 13% 9%
4	Q	265	% 75% 13% 9%
5	E	274	% 20% 6% 73%
5	I	274	4% 92%
5	R	274	2% 54% 15% 28%
6	F	111	4% 66% 20% 12%
6	S	111	5% 63% 25% 11%
7	G	82	5% 71% 21% 5%
7	T	82	5% 65% 22% 10%
8	H	91	40% 23% 7% 29%
8	U	91	% 46% 19% 27%
9	J	64	75% 14% 9%
9	W	64	80% 9% 8%
10	O	453	4% 68% 21% 8%
11	V	274	4% 94%

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
15	PEE	C	505	X	-	-	-
15	PEE	D	506	X	-	-	-
15	PEE	P	505	X	-	-	-
15	PEE	Q	506	X	-	-	-
16	HEC	D	501	X	-	-	-
16	HEC	Q	501	X	-	-	-
18	FES	R	501	-	-	X	-

2 Entry composition (i)

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	3439	2148	607	664	20	0	0	0
1	N	444	3432	2142	607	663	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	3164	1988	561	608	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	2968	1993	463	494	18	0	0	0
3	P	370	2936	1973	456	489	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	1912	1222	329	346	15	0	0	0
4	Q	241	1918	1225	330	348	15	0	0	0

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

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

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	98	860	547	154	157	2	0	0	0
			Total	C	N	O	S			
6	S	99	869	553	156	158	2	0	0	0

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
			Total	C	N	O	S			
7	G	80	677	439	127	110	1	0	0	0
			Total	C	N	O	S			
7	T	74	624	408	117	98	1	0	0	0

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	65	529	321	96	107	5	0	0	0
			Total	C	N	O	S			
8	U	66	538	327	98	108	5	0	0	0

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

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

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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

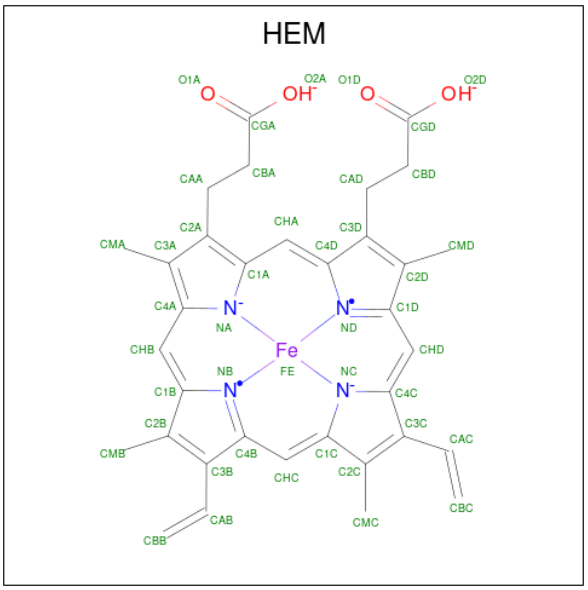
There is a discrepancy between the modelled and reference sequences:

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.

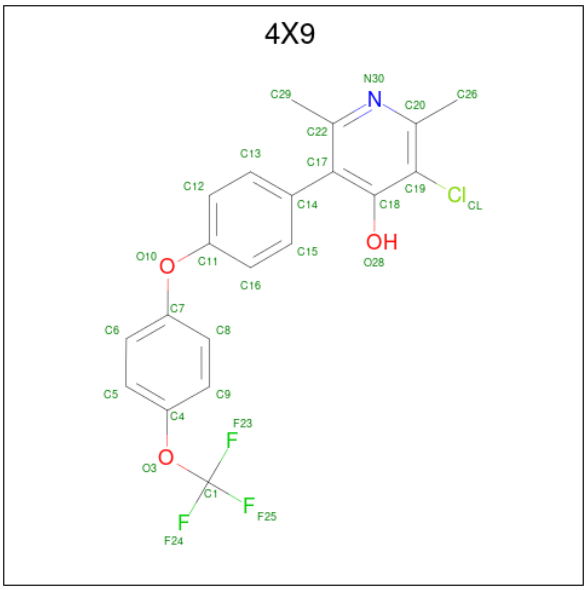
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	V	17	127	81	24	22	0	0	0

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



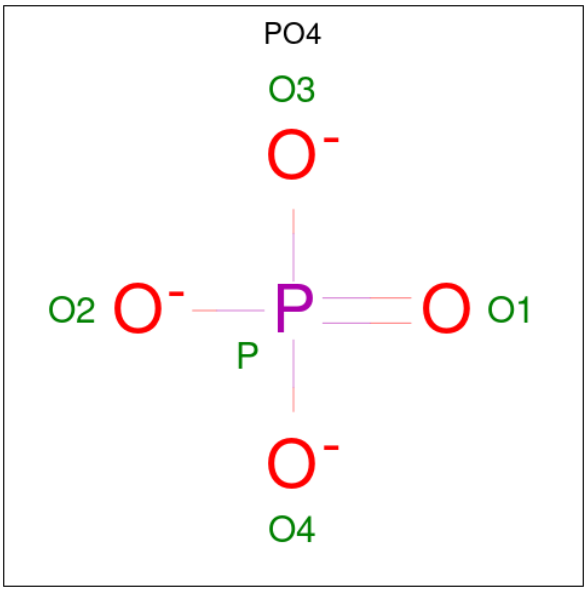
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0

- Molecule 13 is 3-chloro-2,6-dimethyl-5-{4-[4-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (CCD ID: 4X9) (formula: $C_{20}H_{15}ClF_3NO_3$).



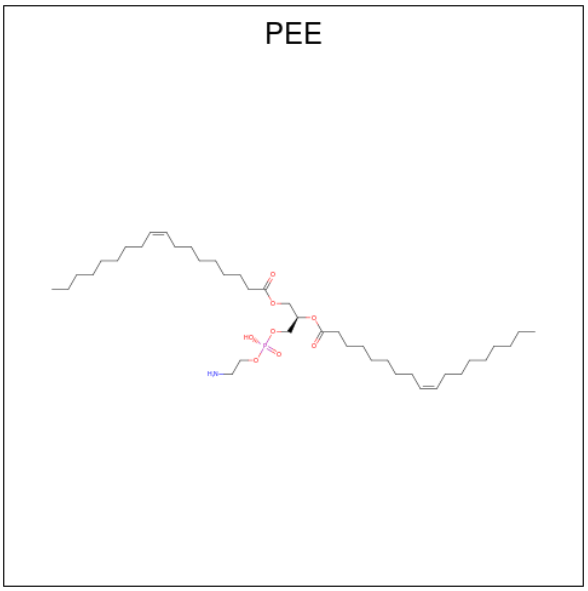
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
13	C	1	28	20	1	3	1	3	0	0
			Total	C	Cl	F	N	O		
13	P	1	28	20	1	3	1	3	0	0

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



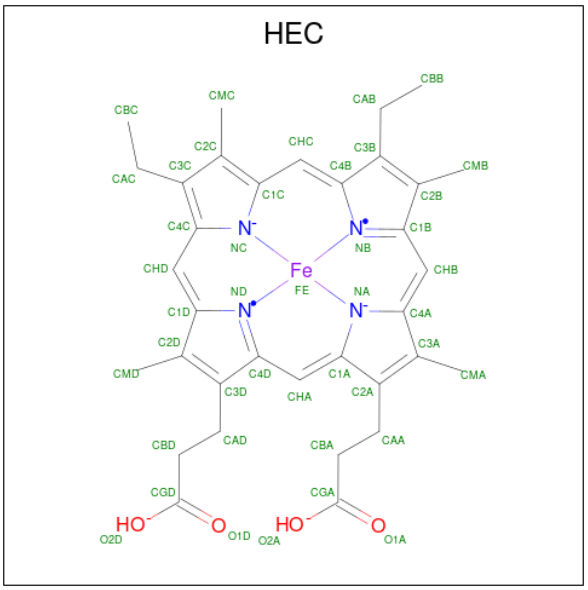
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
14	C	1	5	4	1		0	0
14	D	1	5	4	1		0	0
14	D	1	5	4	1		0	0
14	D	1	5	4	1		0	0
14	E	1	5	4	1		0	0
14	F	1	5	4	1		0	0
14	N	1	5	4	1		0	0
14	N	1	5	4	1		0	0
14	Q	1	5	4	1		0	0
14	Q	1	5	4	1		0	0
14	S	1	5	4	1		0	0

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



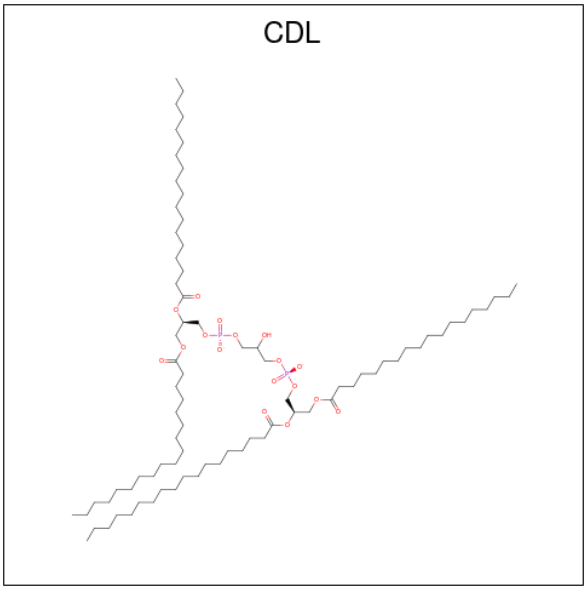
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
15	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
15	D	1	26	16	1	8	1	0	0
			Total	C	N	O	P		
15	P	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
15	Q	1	51	41	1	8	1	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



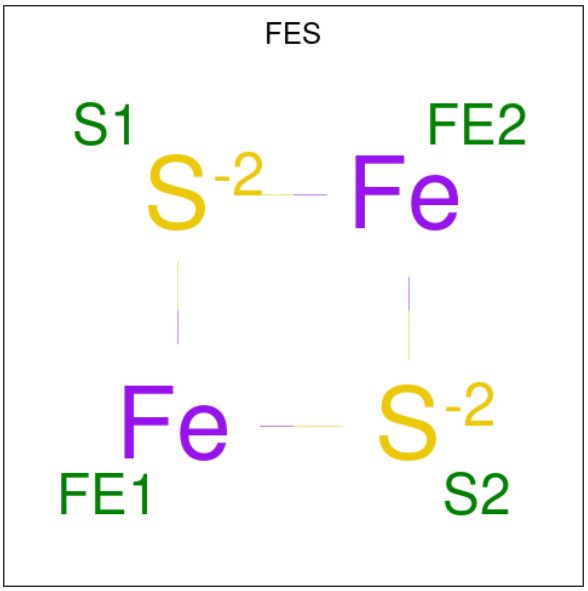
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
16	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
16	Q	1	43	34	1	4	4	0	0

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



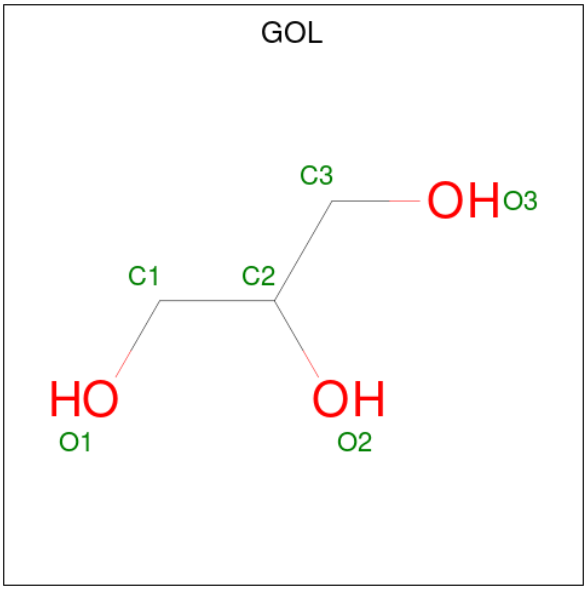
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
17	D	1	39	24	13	2	0	0
			Total	C	O	P		
17	G	1	44	25	17	2	0	0
			Total	C	O	P		
17	Q	1	39	24	13	2	0	0
			Total	C	O	P		
17	T	1	49	30	17	2	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



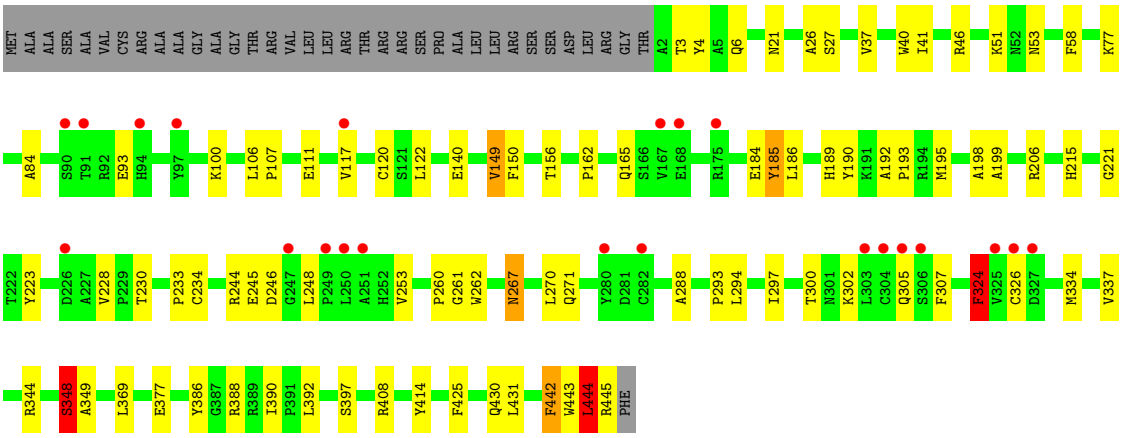
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	R	1	6	3	3	0	0

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.

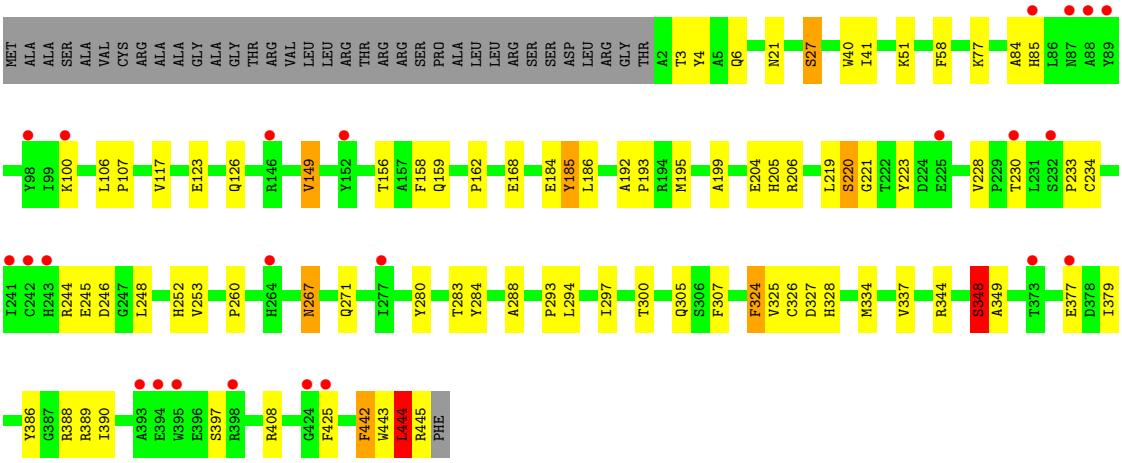
• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

Chain A:



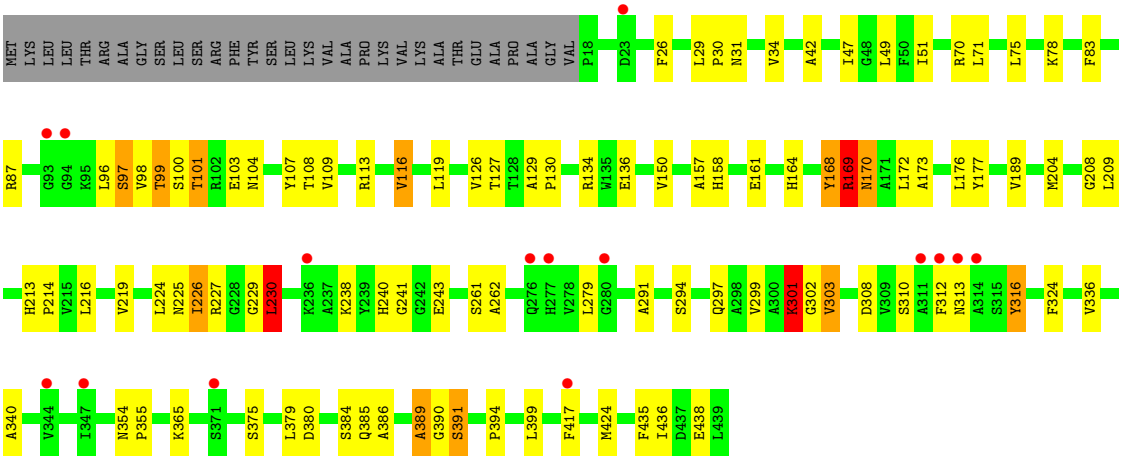
• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

Chain N:



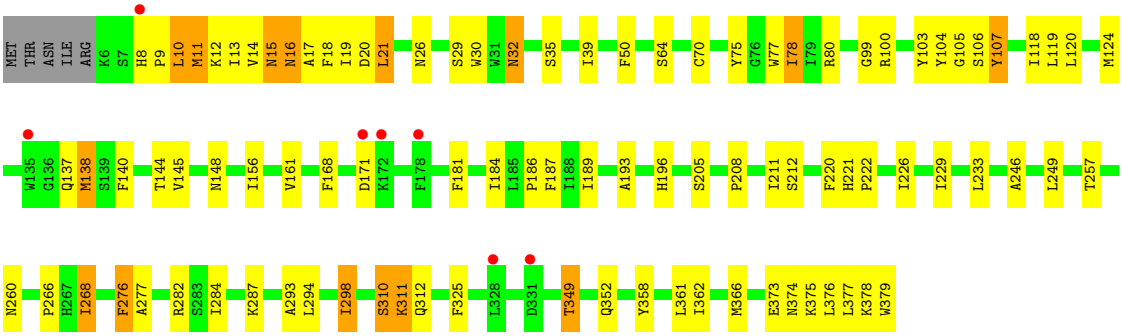
• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain B:



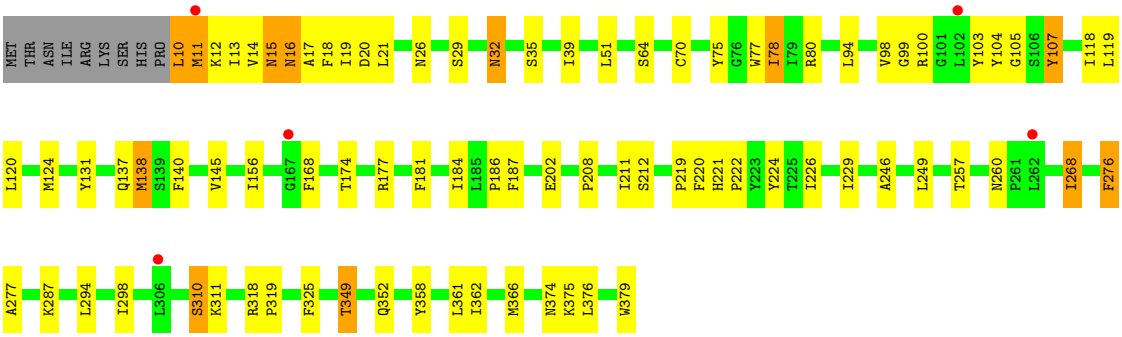
- Molecule 3: CYTOCHROME B

Chain C:



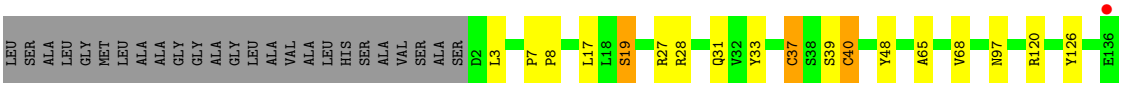
- Molecule 3: CYTOCHROME B

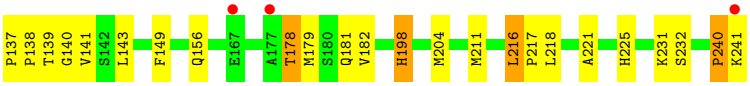
Chain P:



- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain D:



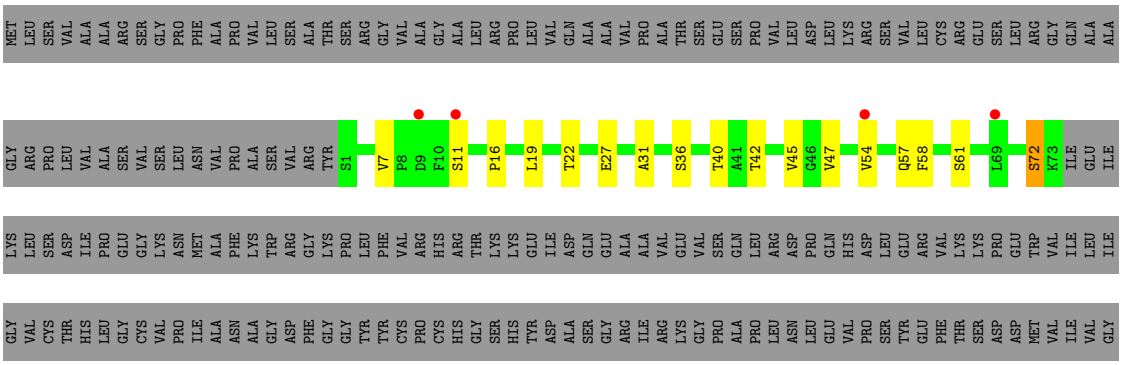


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain Q:

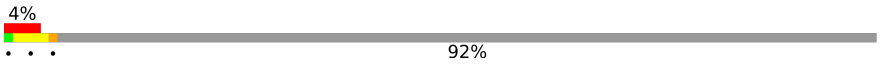
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

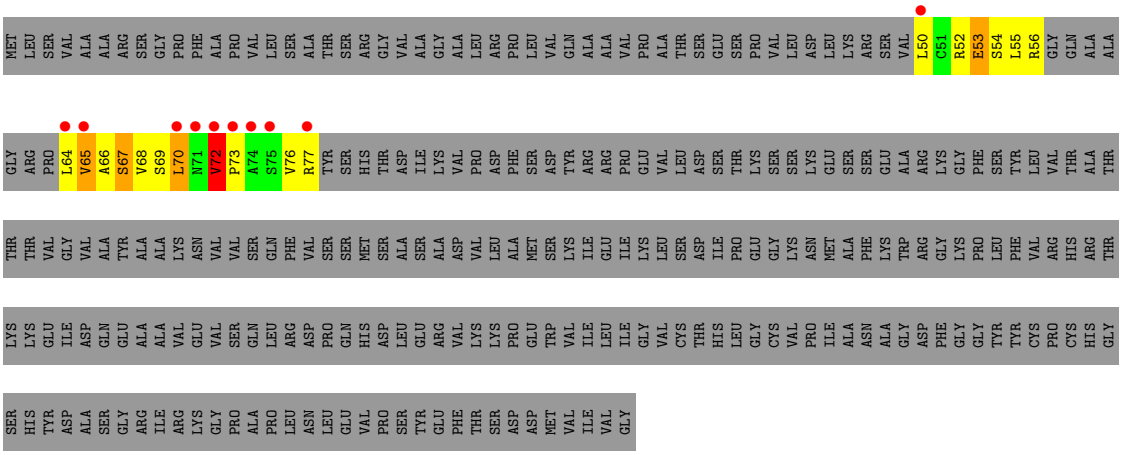
Chain E:



• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

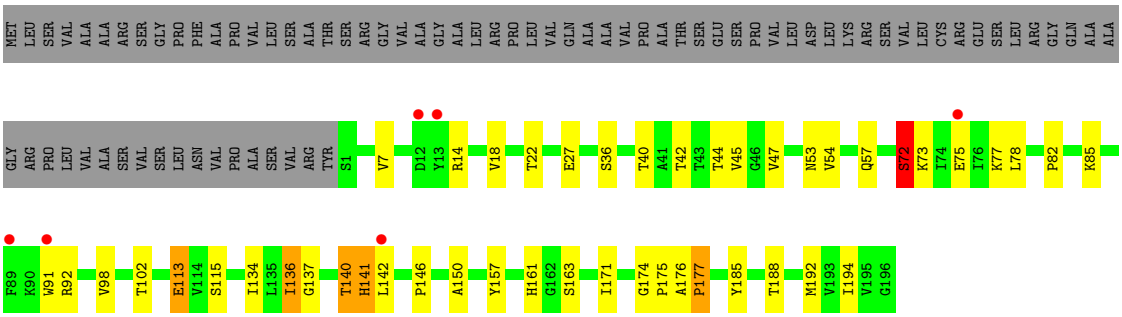
Chain I:





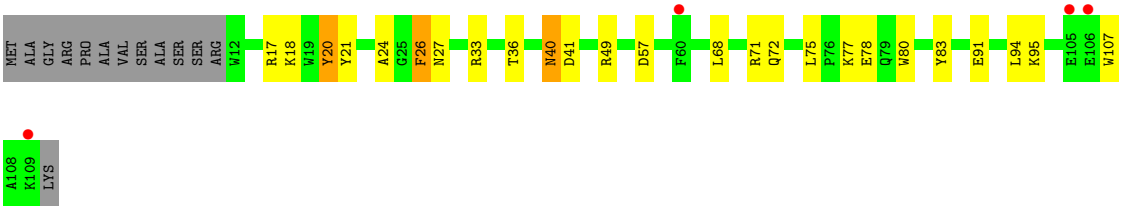
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain R:



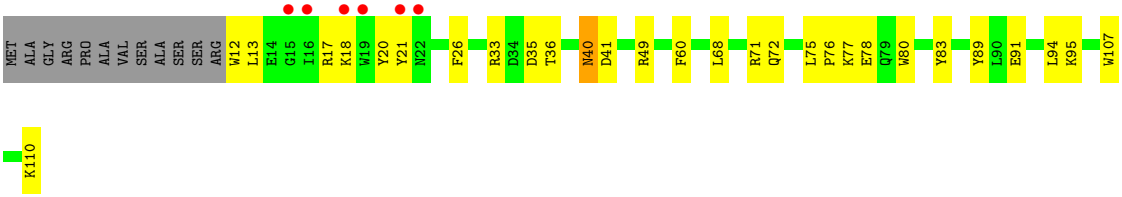
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F:



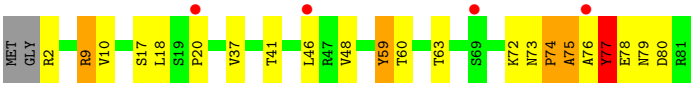
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain S:



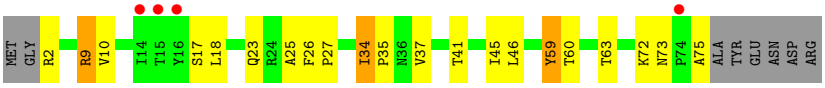
- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain G:



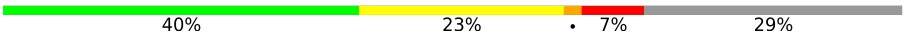
- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

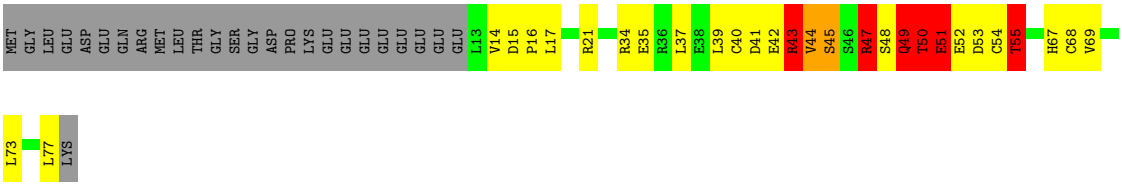
Chain T:



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

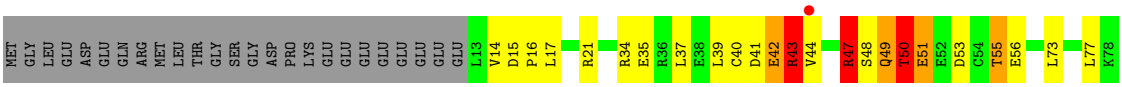
Chain H:





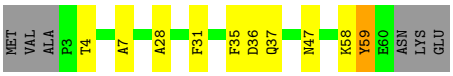
• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain U:



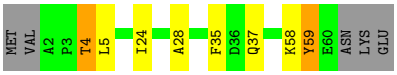
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J:



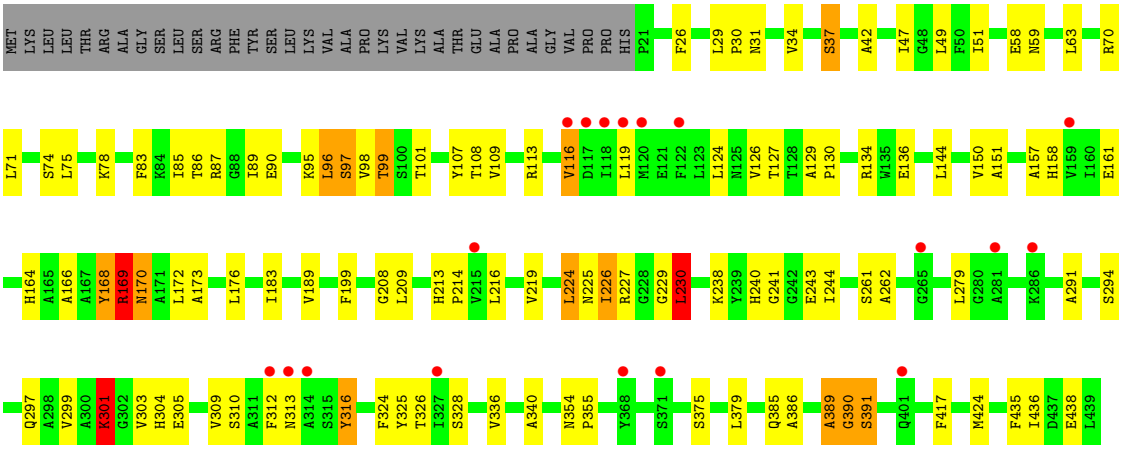
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain W:



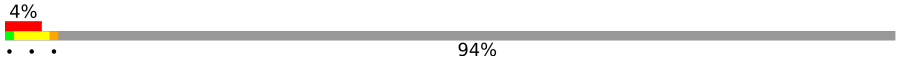
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

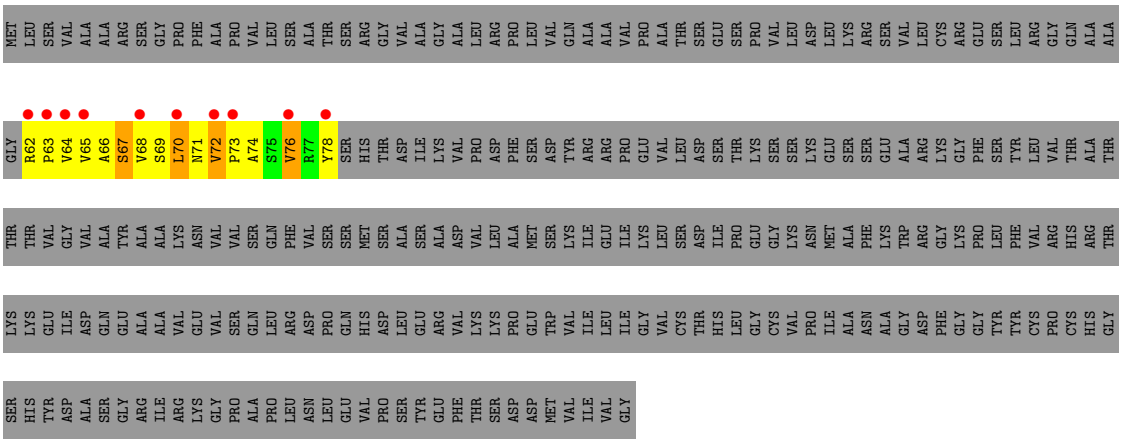
Chain O:



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

Chain V:




MET LEU SER VAL ALA ALA ARG SER GLY PRO PHE ALA PRO VAL LEU SER ALA THR SER ARG GLY VAL ALA GLY ALA LEU ARG PRO LEU VAL GLN ALA ALA VAL PRO ALA THR SER GLU SER PRO VAL LEU ASP LEU LYS ARG SER VAL LEU CYS ARG GLU SER LEU ARG GLY GLN ALA ALA
GLY R62 P63 V64 V65 A66 S67 V68 S69 L70 N71 V72 P73 A74 S75 V76 R77 Y78 SER HIS THR ASP ILE LYS VAL PRO ASP PHE SER ASP TYR ARG ARG PRO GLU VAL LEU ASP SER THR LYS SER SER LYS GLU SER SER GLU ALA ARG LYS GLY PHE SER TYR LEU VAL THR ALA THR
THR THR VAL GLY VAL ALA TYR ALA ALA LYS ASN VAL VAL SER GLN PHE VAL SER SER MET SER ALA SER ALA ASP VAL LEU ALA MET SER LYS ILE GLU ILE LYS LEU SER ASP ILE PRO GLU GLY LYS ASN MET ALA PHE LYS TRP ARG GLY LYS PRO LEU PHE VAL ARG HIS ARG THR
LYS LYS GLU ILE ASP GLN GLU ALA ALA VAL GLU VAL SER GLN LEU ARG ASP PRO GLN HIS ASP LEU GLU ARG VAL LYS LYS PRO GLU TRP VAL ILE LEU ILE GLY VAL CYS THR HIS LEU GLY CYS VAL PRO ILE ALA ASN ALA GLY ASP PHE GLY GLY TYR TYR CYS PRO CYS HIS GLY
SER HIS TYR ASP ALA SER GLY ARG ILE ARG LYS GLY PRO ALA PRO LEU ASN LEU GLU VAL PRO SER TYR GLU PHE THR SER ASP ASP MET VAL ILE VAL GLY

4 Data and refinement statistics (i)

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 50.00 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.57) 99.9 (50.00-3.57)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.252 0.207 , 0.251	Depositor DCC
R_{free} test set	3954 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	122.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, HEC, PEE, FES, PO4, CDL, GOL, 4X9

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	0.60	1/3511 (0.0%)	0.93	8/4766 (0.2%)
1	N	0.58	0/3503	0.94	9/4755 (0.2%)
2	B	0.80	3/3224 (0.1%)	1.20	15/4375 (0.3%)
3	C	0.68	0/3065	0.97	3/4196 (0.1%)
3	P	0.65	0/3031	0.99	4/4150 (0.1%)
4	D	0.58	0/1971	0.90	2/2676 (0.1%)
4	Q	0.60	0/1977	0.88	2/2684 (0.1%)
5	E	0.57	0/557	0.94	0/752
5	I	0.84	0/156	1.58	2/209 (1.0%)
5	R	0.64	0/1552	1.15	9/2100 (0.4%)
6	F	0.59	0/879	0.87	0/1180
6	S	0.59	0/888	0.86	0/1191
7	G	0.64	1/699 (0.1%)	1.77	13/946 (1.4%)
7	T	0.66	0/645	1.03	4/873 (0.5%)
8	H	2.23	6/534 (1.1%)	1.82	14/718 (1.9%)
8	U	1.56	5/543 (0.9%)	1.77	9/729 (1.2%)
9	J	0.60	0/495	0.85	0/667
9	W	0.61	0/500	0.86	0/675
10	O	0.67	2/3197 (0.1%)	1.30	16/4336 (0.4%)
11	V	0.85	0/129	1.24	0/177
All	All	0.73	18/31056 (0.1%)	1.09	110/42155 (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
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 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH2	28.09	1.70	1.33
8	H	43	ARG	NE-CZ	28.05	1.64	1.33
8	H	47	ARG	CZ-NH2	25.48	1.66	1.33
8	U	47	ARG	CZ-NH2	25.40	1.66	1.33
8	H	43	ARG	CZ-NH1	25.16	1.68	1.32

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	390	GLY	N-CA-C	31.63	151.42	112.83
10	O	390	GLY	N-CA-C	31.48	151.24	112.83
10	O	301	LYS	N-CA-C	25.58	144.84	113.38
2	B	301	LYS	N-CA-C	24.90	143.79	113.41
10	O	169	ARG	N-CA-C	24.53	138.26	111.03

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3337	49	0
1	N	3432	0	3330	48	0
2	B	3164	0	3144	81	0
3	C	2968	0	3028	88	0
3	P	2936	0	2996	79	0
4	D	1912	0	1861	47	0
4	Q	1918	0	1870	41	0
5	E	549	0	547	9	0
5	I	157	0	171	28	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	28	0
7	G	677	0	673	9	0
7	T	624	0	630	9	0
8	H	529	0	512	48	0
8	U	538	0	522	27	1
9	J	482	0	483	10	0
9	W	487	0	487	9	0
10	O	3140	0	3121	107	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	5	0
13	P	28	0	14	4	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	1	0
15	P	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	10	0
16	Q	43	0	32	6	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	30686	688	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 688 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%)	24	57
1	N	442/480 (92%)	407 (92%)	33 (8%)	2 (0%)	24	57
2	B	420/453 (93%)	375 (89%)	44 (10%)	1 (0%)	43	72
3	C	372/379 (98%)	347 (93%)	23 (6%)	2 (0%)	24	57
3	P	368/379 (97%)	337 (92%)	30 (8%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	238/265 (90%)	216 (91%)	21 (9%)	1 (0%)	30	60
4	Q	239/265 (90%)	218 (91%)	20 (8%)	1 (0%)	30	60
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%)	24	57
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%)	9	39
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%)	36	65

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%)	22	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	367/394 (93%)	349 (95%)	18 (5%)	22	49
2	B	331/355 (93%)	310 (94%)	21 (6%)	16	43
3	C	322/327 (98%)	301 (94%)	21 (6%)	15	42
3	P	318/327 (97%)	300 (94%)	18 (6%)	18	46
4	D	205/218 (94%)	195 (95%)	10 (5%)	22	49
4	Q	206/218 (94%)	196 (95%)	10 (5%)	22	49
5	E	63/228 (28%)	54 (86%)	9 (14%)	3	18
5	I	19/228 (8%)	13 (68%)	6 (32%)	0	2
5	R	168/228 (74%)	154 (92%)	14 (8%)	10	35
6	F	90/99 (91%)	83 (92%)	7 (8%)	11	37
6	S	91/99 (92%)	84 (92%)	7 (8%)	12	37
7	G	71/72 (99%)	60 (84%)	11 (16%)	2	16
7	T	66/72 (92%)	56 (85%)	10 (15%)	3	16
8	H	62/85 (73%)	51 (82%)	11 (18%)	2	11
8	U	63/85 (74%)	55 (87%)	8 (13%)	4	22
9	J	49/54 (91%)	46 (94%)	3 (6%)	17	44
9	W	49/54 (91%)	46 (94%)	3 (6%)	17	44
10	O	328/355 (92%)	306 (93%)	22 (7%)	15	42
11	V	15/228 (7%)	10 (67%)	5 (33%)	0	2
All	All	3251/4120 (79%)	3019 (93%)	232 (7%)	13	40

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	37	GLN
8	U	50	THR
10	O	158	HIS
8	U	47	ARG
6	S	26	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	57	HIS

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Mol	Chain	Res	Type
10	O	31	ASN
9	W	57	HIS
1	N	32	GLN
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 oligosaccharides 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	$\#\|Z\| > 2$
15	PEE	P	505	-	48,48,50	1.34	4 (8%)	51,53,55	0.93	1 (1%)
14	PO4	D	504	-	4,4,4	0.85	0	6,6,6	0.58	0
15	PEE	C	505	-	48,48,50	1.27	4 (8%)	51,53,55	1.03	4 (7%)
12	HEM	C	501	3	50,50,50	1.65	8 (16%)	66,82,82	1.65	13 (19%)
14	PO4	D	502	-	4,4,4	0.76	0	6,6,6	0.63	0
12	HEM	C	502	3	50,50,50	1.70	11 (22%)	66,82,82	1.54	11 (16%)
14	PO4	C	504	-	4,4,4	0.95	0	6,6,6	0.43	0
14	PO4	Q	1001	-	4,4,4	0.87	0	6,6,6	0.47	0
14	PO4	S	501	-	4,4,4	0.86	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	HEM	P	501	3	50,50,50	1.58	10 (20%)	66,82,82	1.70	16 (24%)
12	HEM	P	502	3	50,50,50	1.68	11 (22%)	66,82,82	1.85	18 (27%)
13	4X9	C	503	-	30,30,30	2.97	7 (23%)	43,44,44	1.43	3 (6%)
14	PO4	F	501	-	4,4,4	0.87	0	6,6,6	0.62	0
19	GOL	R	502	-	5,5,5	0.33	0	5,5,5	0.45	0
17	CDL	Q	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.19	5 (11%)
14	PO4	N	501	-	4,4,4	0.72	0	6,6,6	0.98	0
16	HEC	Q	501	4	50,50,50	2.86	26 (52%)	68,82,82	2.43	27 (39%)
17	CDL	T	501	-	48,48,99	1.39	4 (8%)	54,60,111	1.18	4 (7%)
15	PEE	Q	506	-	50,50,50	1.30	4 (8%)	53,55,55	1.29	6 (11%)
14	PO4	D	503	-	4,4,4	0.88	0	6,6,6	0.67	0
14	PO4	Q	1002	-	4,4,4	0.89	0	6,6,6	0.48	0
16	HEC	D	501	4	50,50,50	2.86	28 (56%)	68,82,82	2.68	33 (48%)
17	CDL	D	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.16	4 (9%)
13	4X9	P	503	-	30,30,30	2.79	6 (20%)	43,44,44	1.90	8 (18%)
14	PO4	N	1001	-	4,4,4	0.81	0	6,6,6	0.78	0
18	FES	R	501	5	0,4,4	-	-	-		
15	PEE	D	506	-	25,25,50	1.49	2 (8%)	28,30,55	1.46	4 (14%)
17	CDL	G	501	-	43,43,99	1.55	4 (9%)	49,55,111	1.57	8 (16%)
14	PO4	E	501	-	4,4,4	0.69	0	6,6,6	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GOL	R	502	-	-	2/4/4/4	-
13	4X9	P	503	-	-	3/13/13/13	0/3/3/3
17	CDL	Q	505	-	-	13/43/43/110	-
15	PEE	P	505	-	1/1/4/8	22/52/52/54	-
16	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
12	HEM	C	502	3	-	6/14/54/54	-
17	CDL	T	501	-	-	28/57/57/110	-
15	PEE	C	505	-	1/1/4/8	25/52/52/54	-
15	PEE	Q	506	-	1/1/4/8	24/54/54/54	-
18	FES	R	501	5	-	-	0/1/1/1
12	HEM	C	501	3	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEC	D	501	4	1/1/3/7	13/14/54/54	-
15	PEE	D	506	-	1/1/4/8	13/29/29/54	-
12	HEM	P	501	3	-	8/14/54/54	-
13	4X9	C	503	-	-	5/13/13/13	0/3/3/3
17	CDL	G	501	-	-	25/52/52/110	-
12	HEM	P	502	3	-	8/14/54/54	-
17	CDL	D	505	-	-	21/43/43/110	-

The worst 5 of 135 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
13	P	503	4X9	C17-C18	6.76	1.48	1.40

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	503	4X9	C20-C19-C18	-7.02	118.33	122.79
16	D	501	HEC	C1B-C2B-C3B	-5.73	100.93	106.96
16	Q	501	HEC	C1B-C2B-C3B	-5.50	101.18	106.96
16	D	501	HEC	CAD-C3D-C4D	5.39	134.07	124.66
16	Q	501	HEC	C2A-C1A-NA	5.24	115.42	110.32

5 of 6 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
16	D	501	HEC	NA

5 of 229 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

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Mol	Chain	Res	Type	Atoms
12	P	501	HEM	C1A-C2A-CAA-CBA
15	D	506	PEE	C1-O3P-P-O2P
15	D	506	PEE	C5-C4-O4P-P

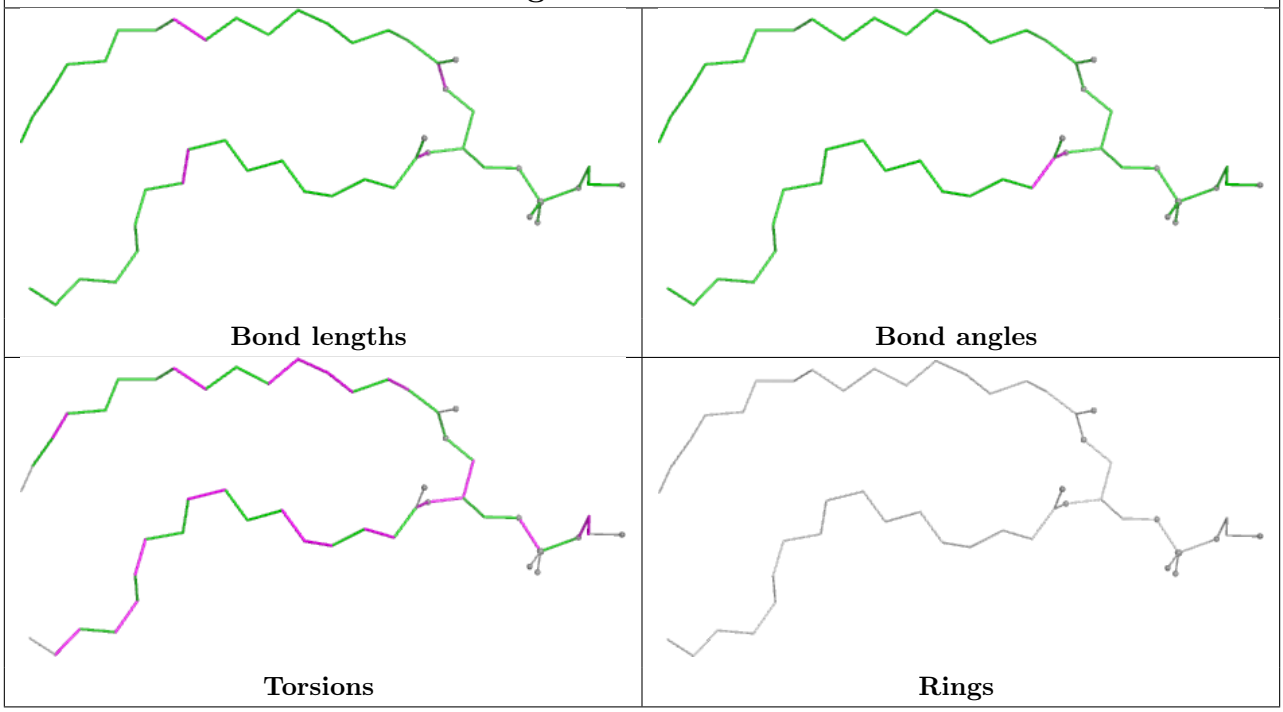
There are no ring outliers.

15 monomers are involved in 55 short contacts:

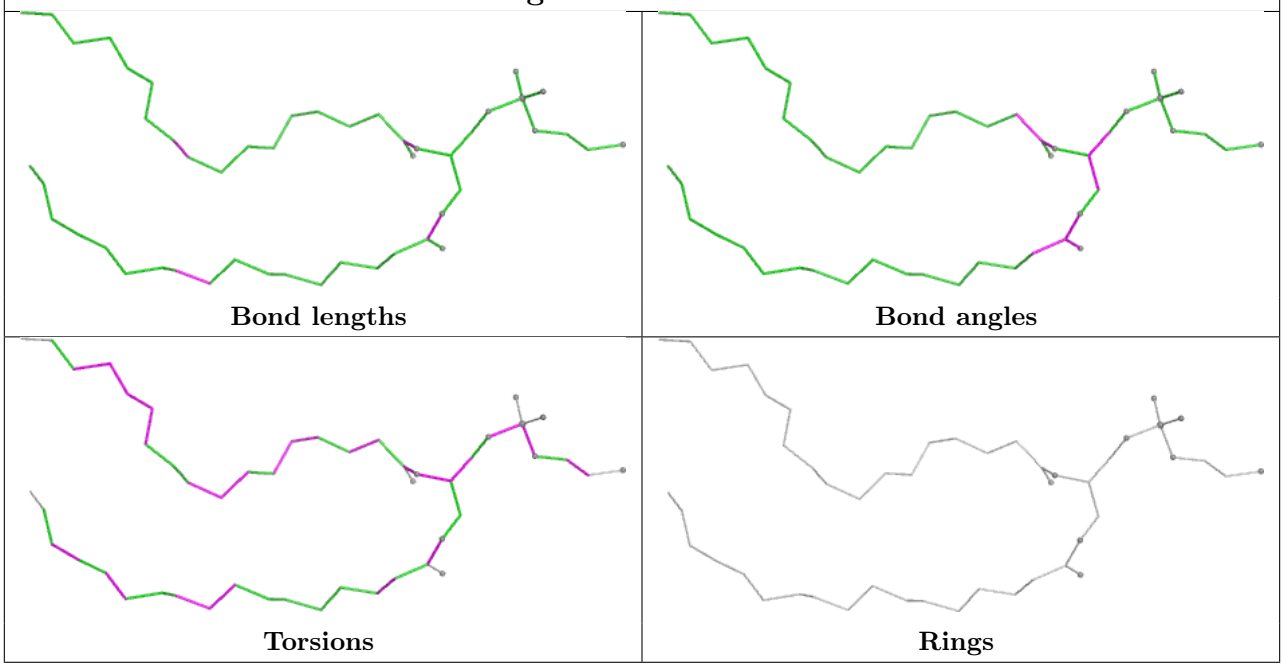
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	505	PEE	1	0
15	C	505	PEE	1	0
12	C	501	HEM	4	0
12	C	502	HEM	6	0
12	P	501	HEM	7	0
12	P	502	HEM	3	0
13	C	503	4X9	5	0
17	Q	505	CDL	1	0
16	Q	501	HEC	6	0
17	T	501	CDL	1	0
15	Q	506	PEE	3	0
16	D	501	HEC	10	0
13	P	503	4X9	4	0
18	R	501	FES	3	0
15	D	506	PEE	1	0

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

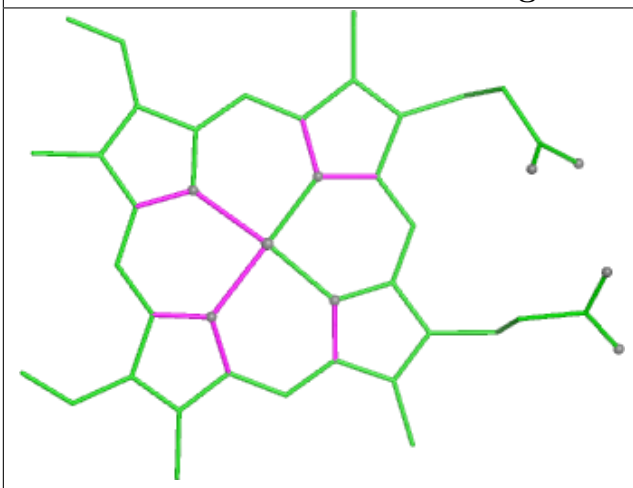
Ligand PEE P 505



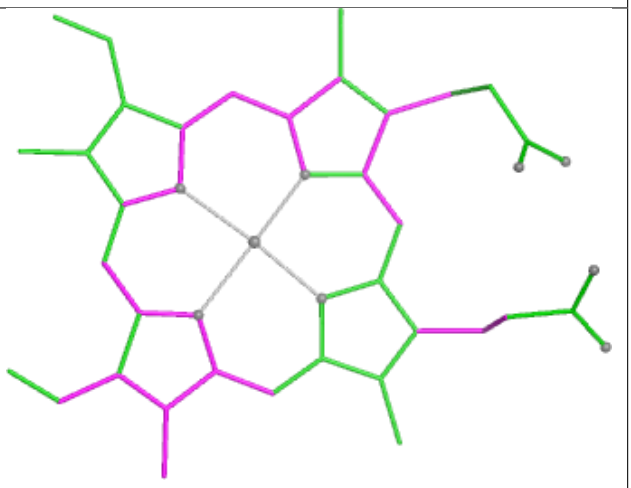
Ligand PEE C 505



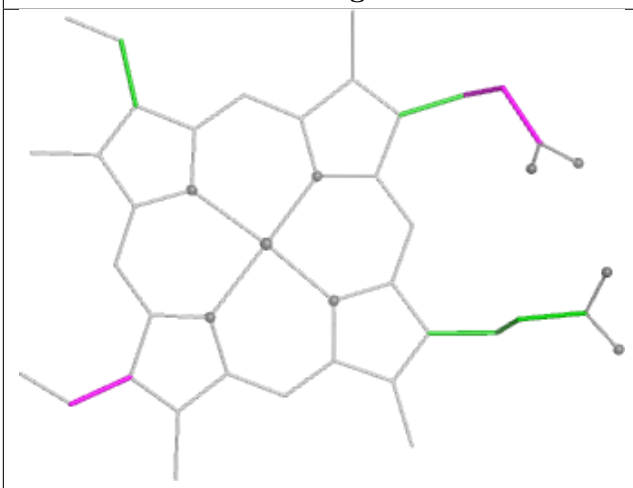
Ligand HEM C 501



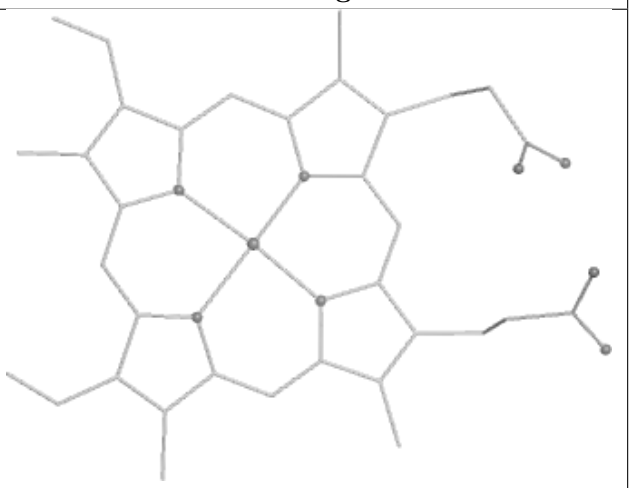
Bond lengths



Bond angles

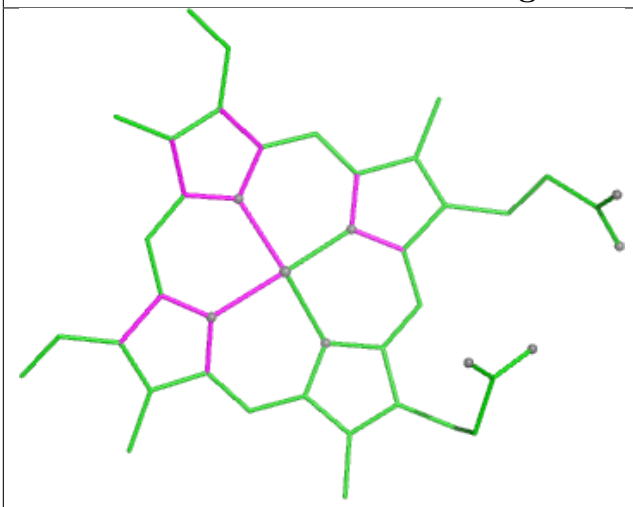


Torsions

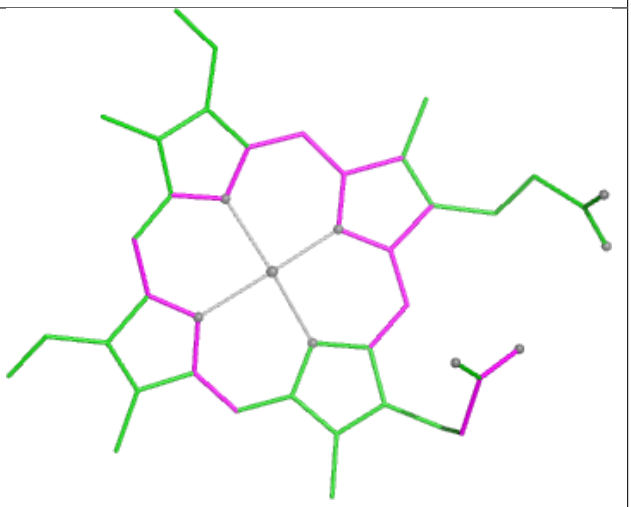


Rings

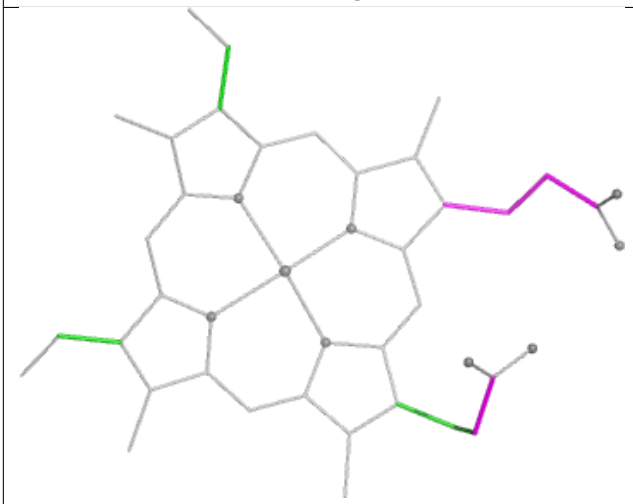
Ligand HEM C 502



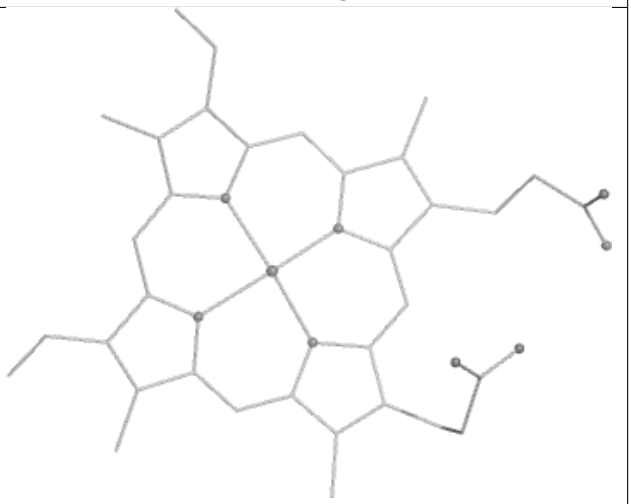
Bond lengths



Bond angles

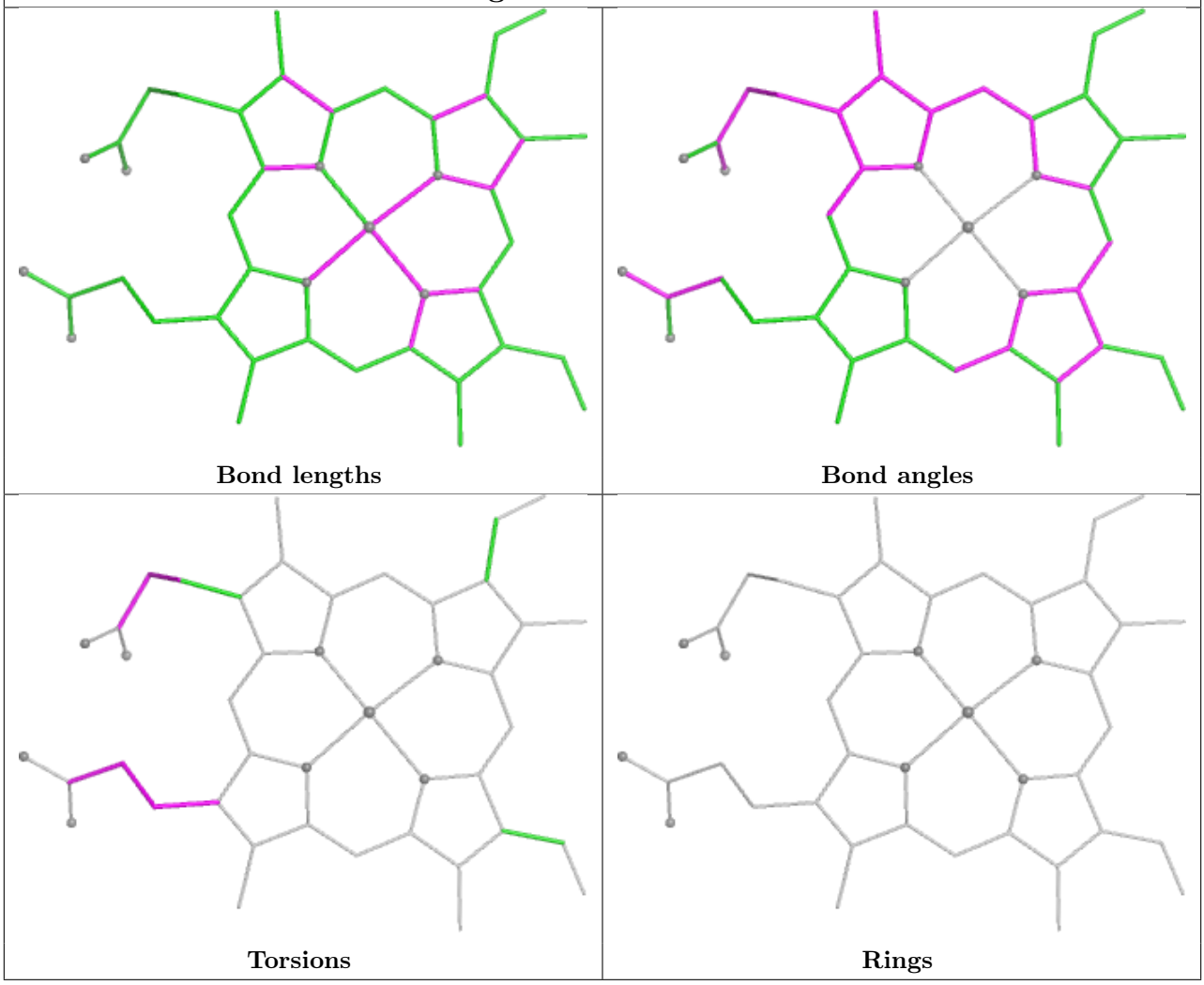


Torsions

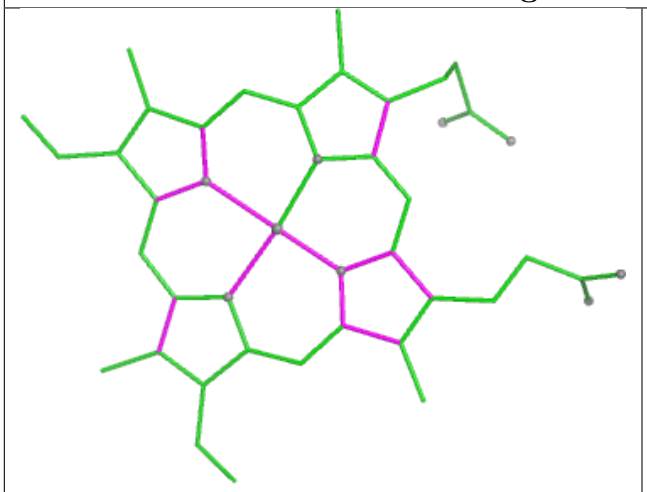


Rings

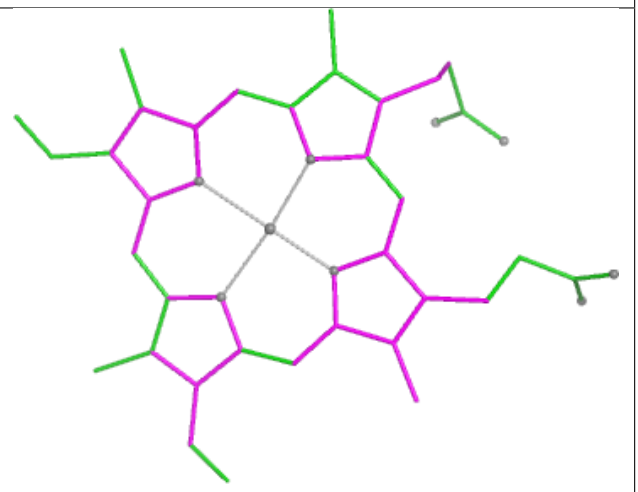
Ligand HEM P 501



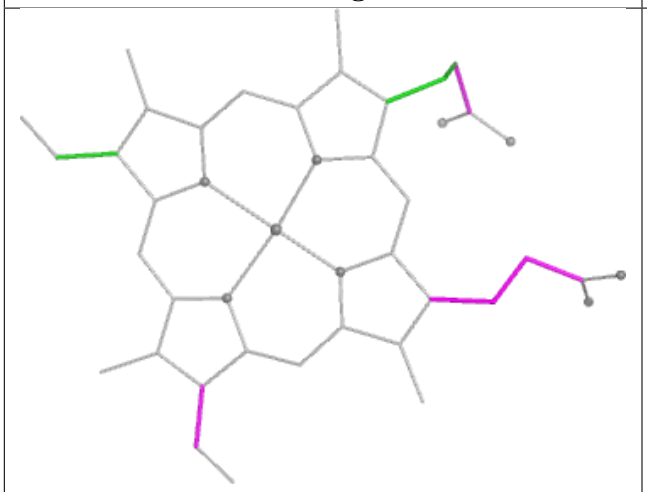
Ligand HEM P 502



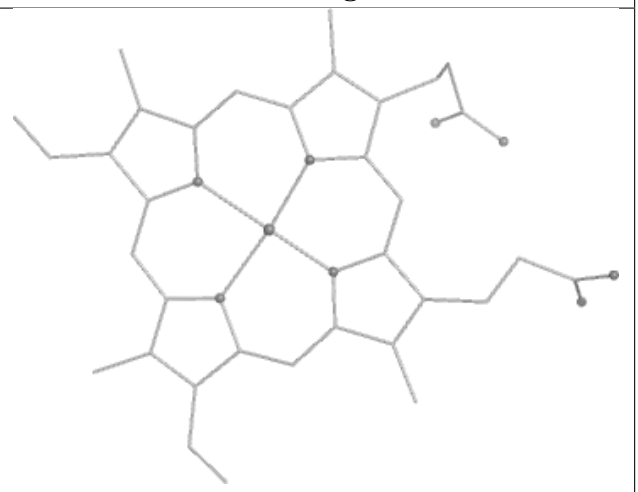
Bond lengths



Bond angles

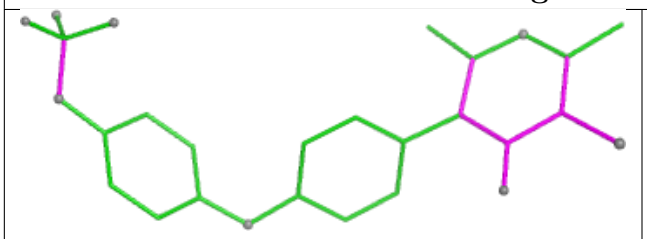


Torsions

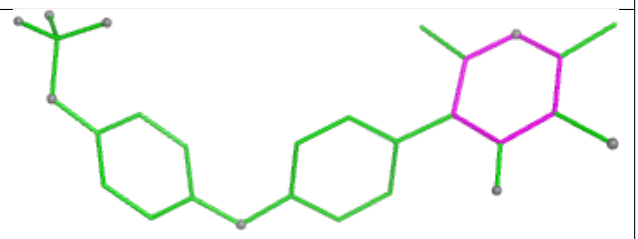


Rings

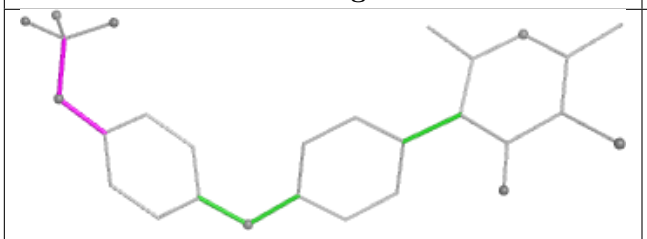
Ligand 4X9 C 503



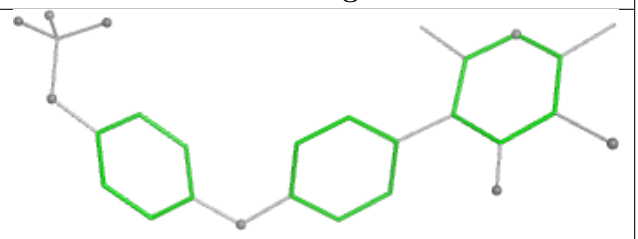
Bond lengths



Bond angles

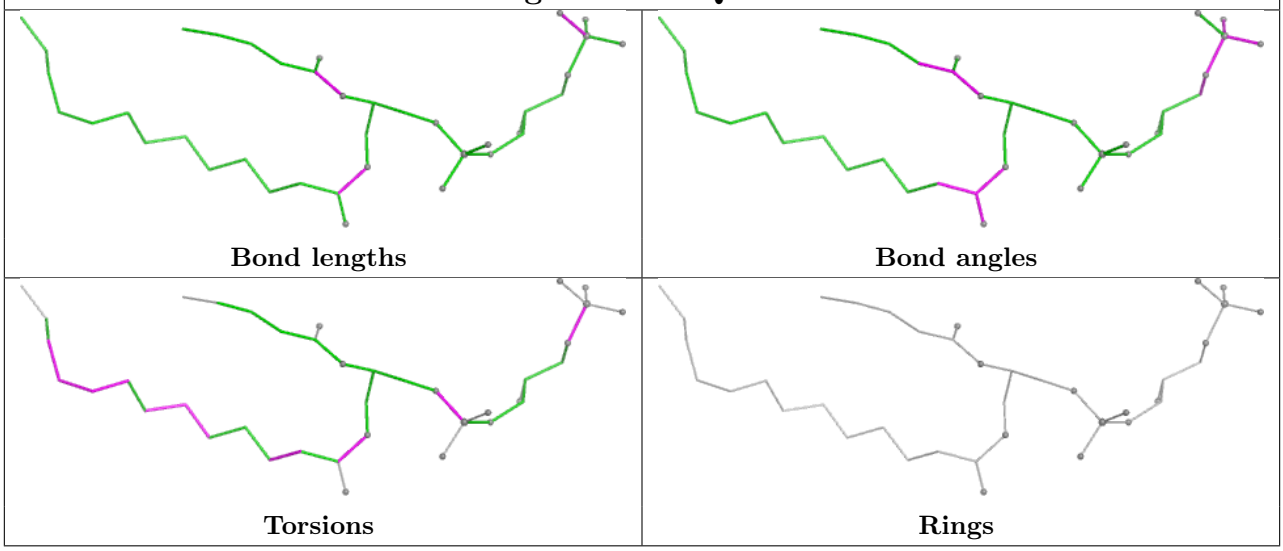


Torsions

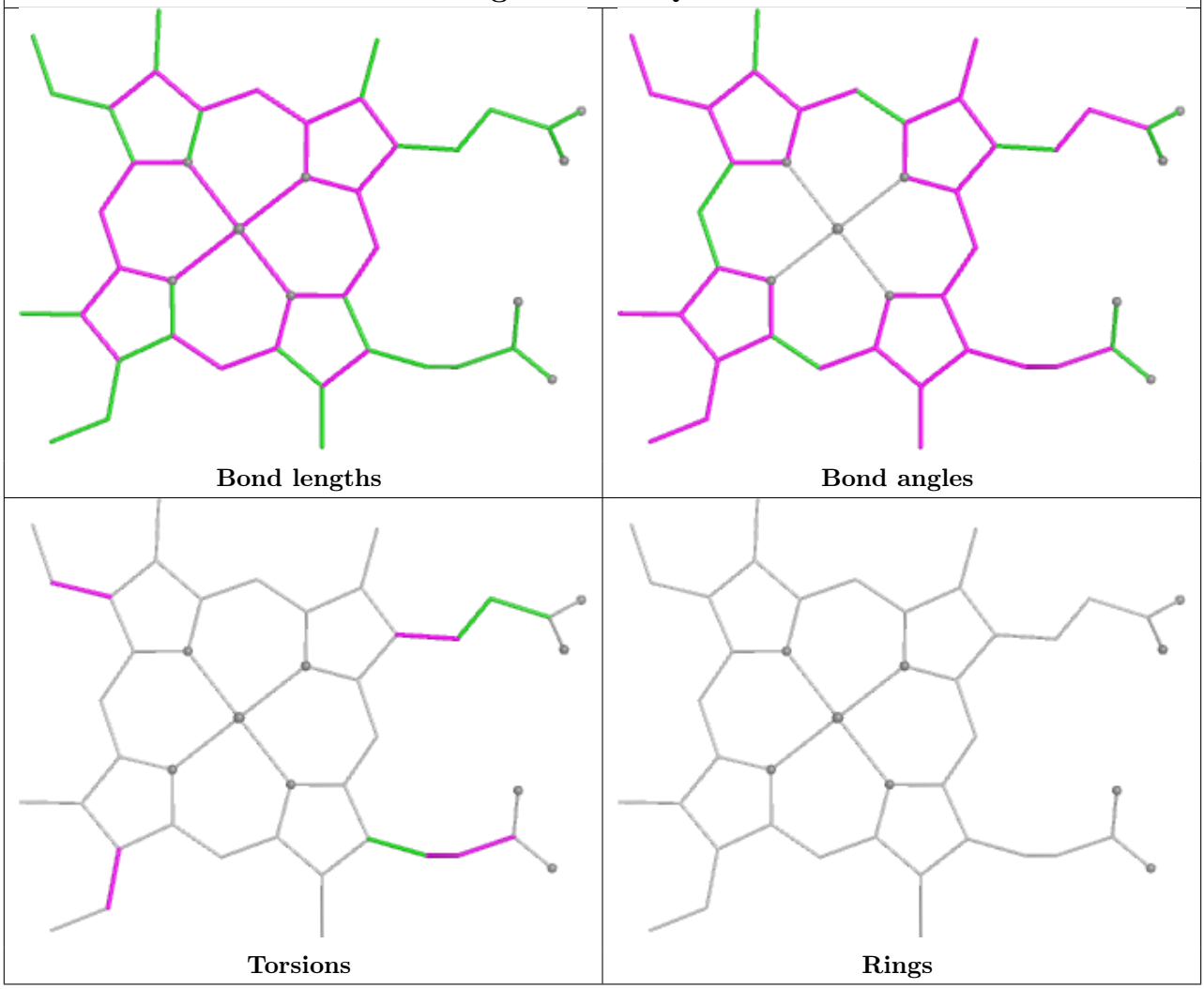


Rings

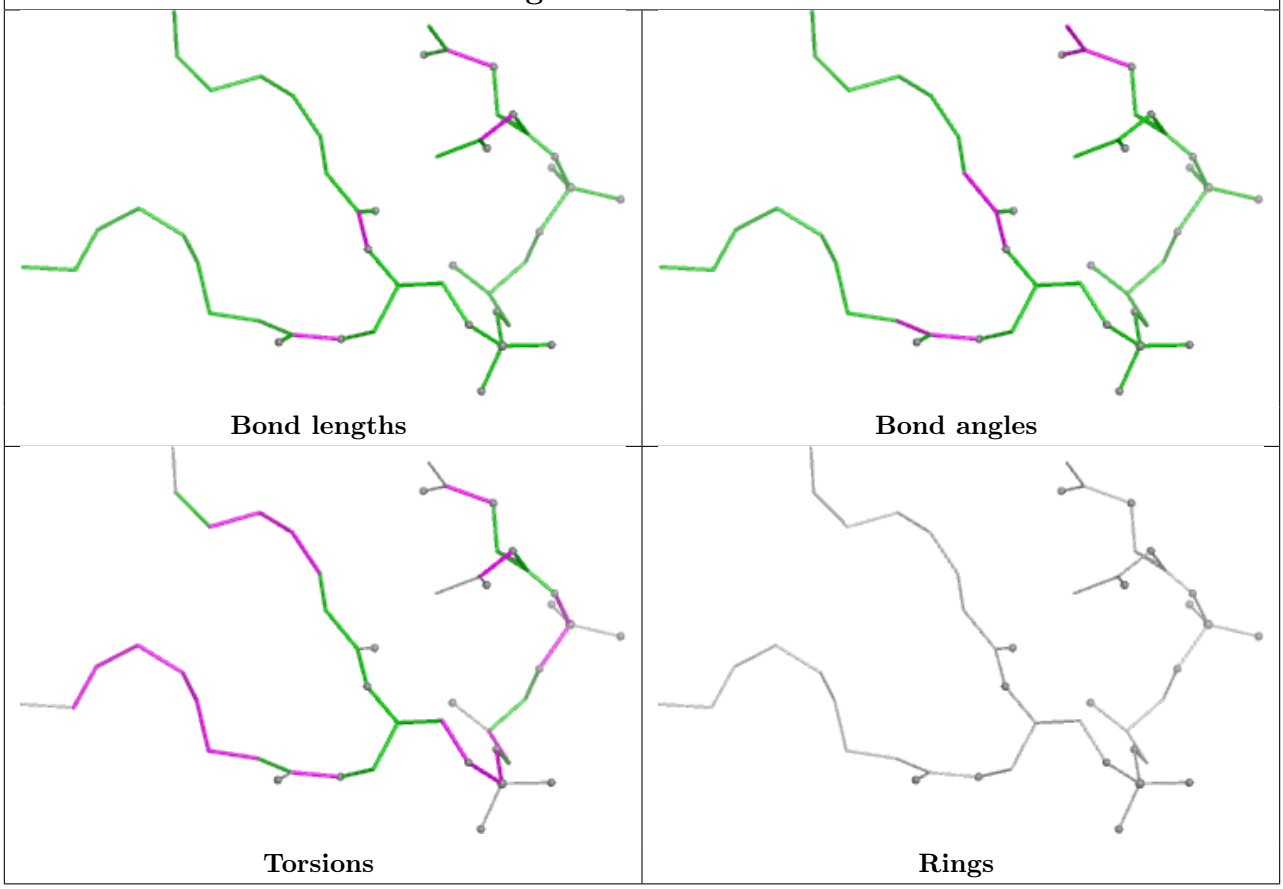
Ligand CDL Q 505



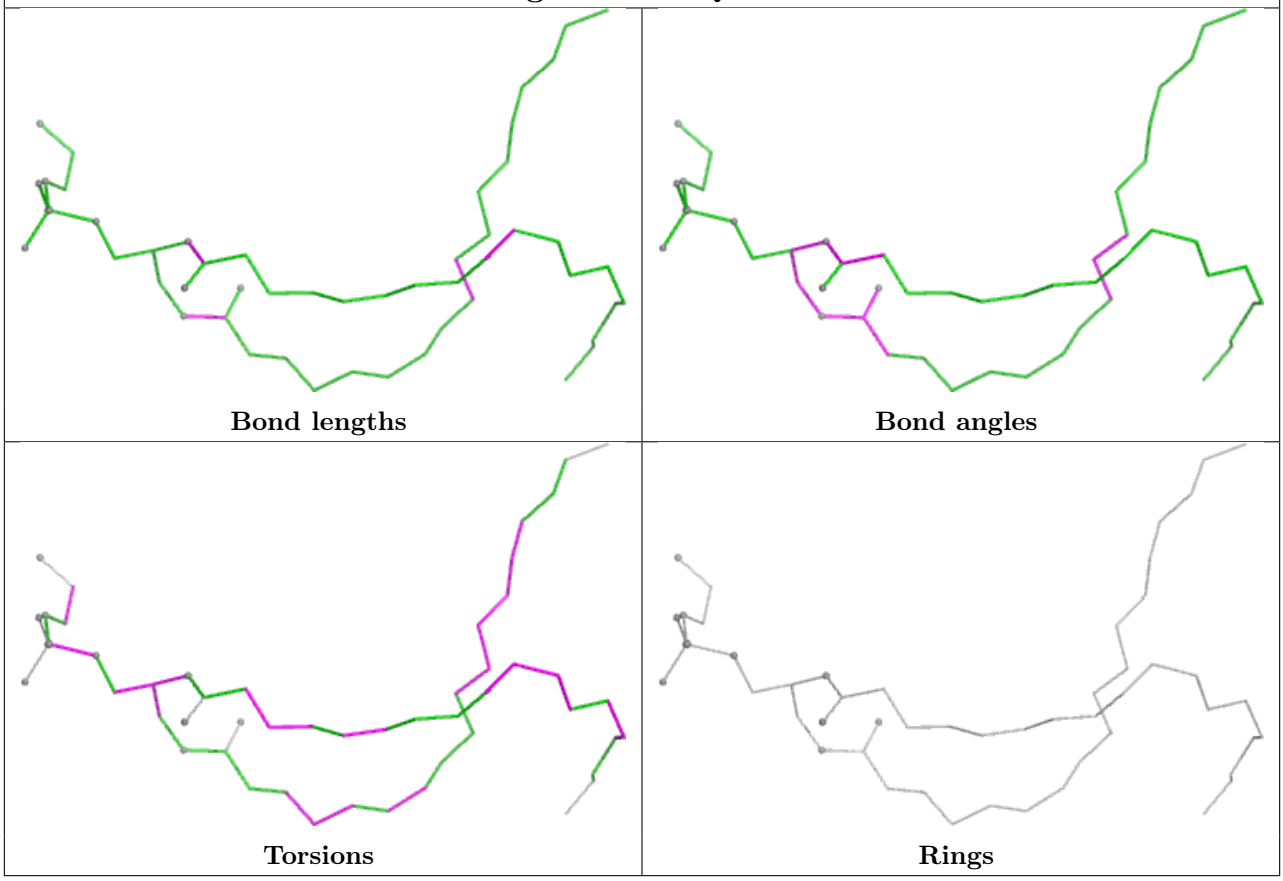
Ligand HEC Q 501



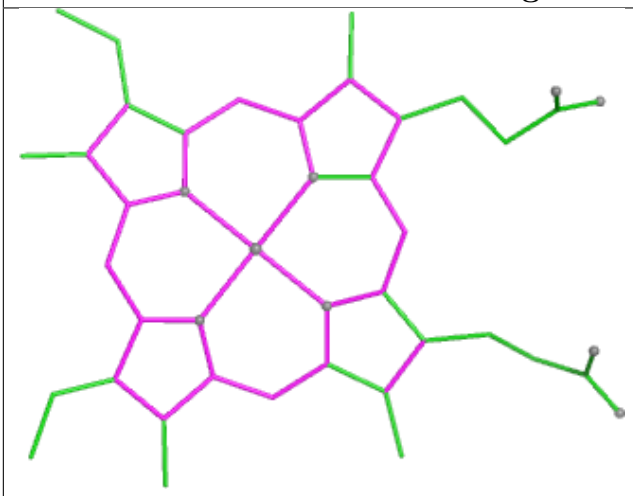
Ligand CDL T 501



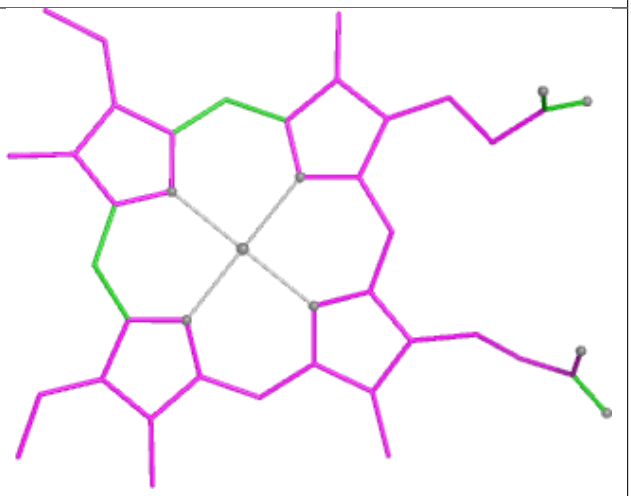
Ligand PEE Q 506



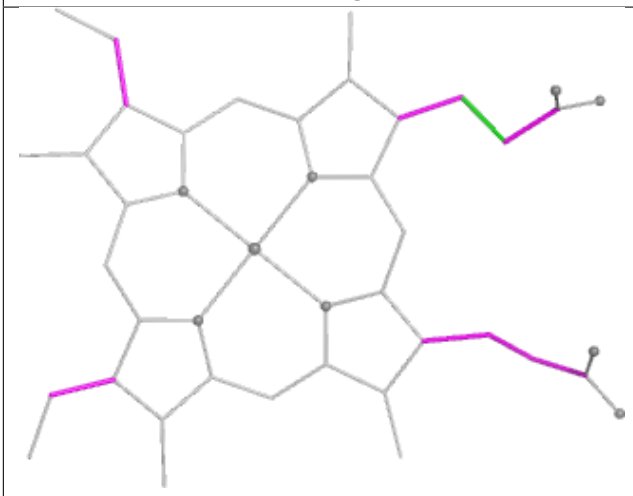
Ligand HEC D 501



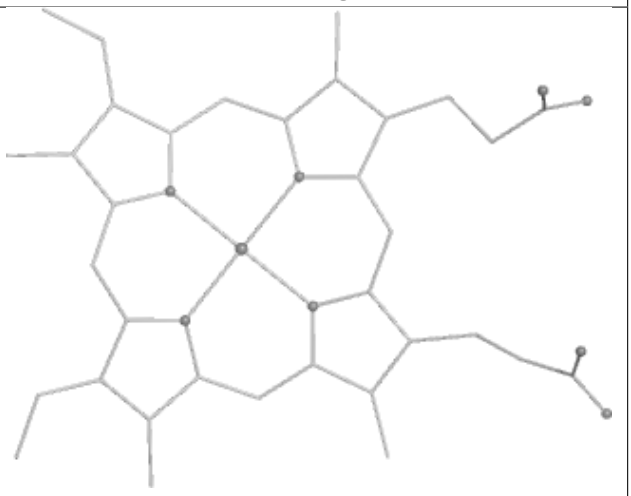
Bond lengths



Bond angles

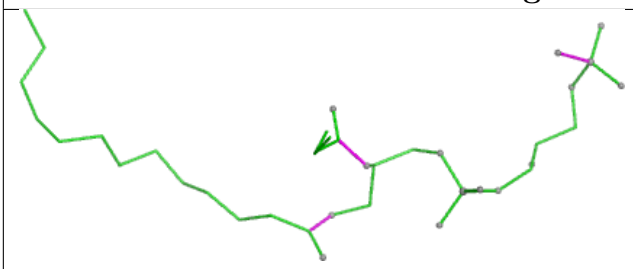


Torsions



Rings

Ligand CDL D 505



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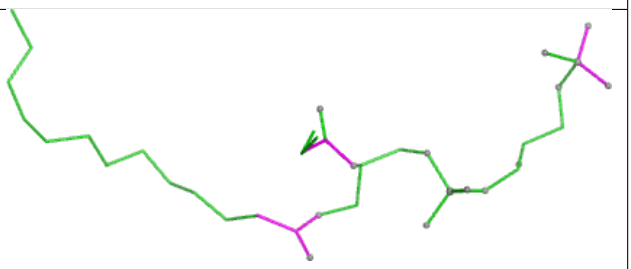
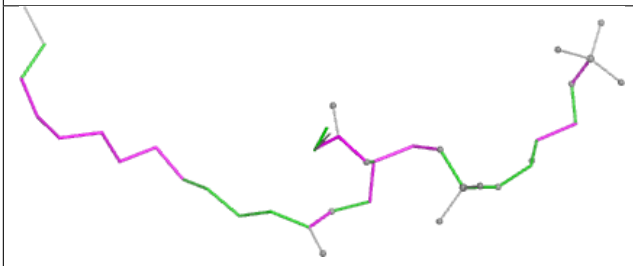
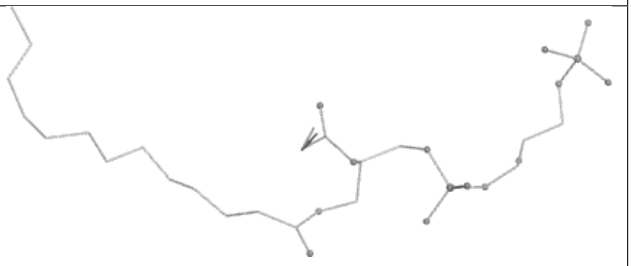


Bond angles

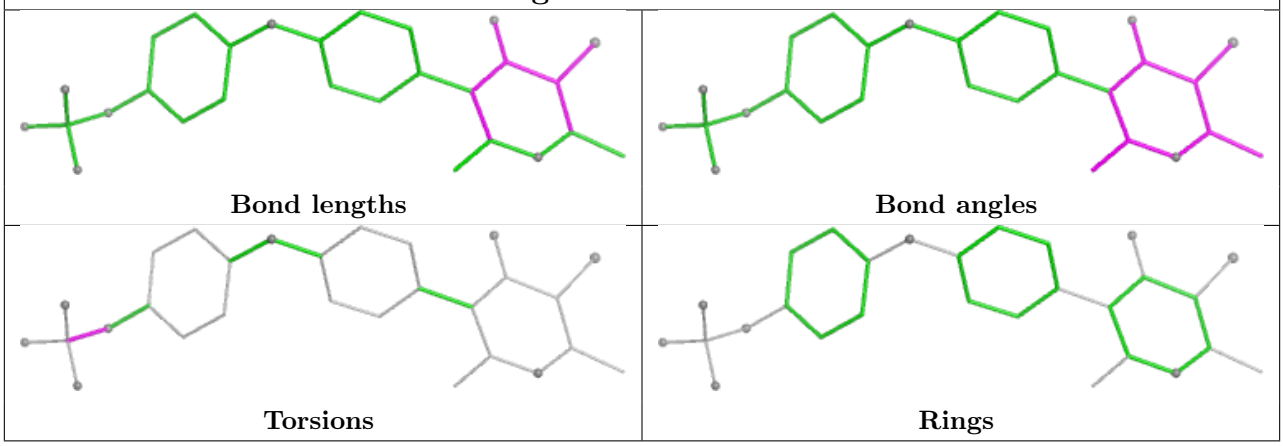


Torsions



Rings

Ligand 4X9 P 503



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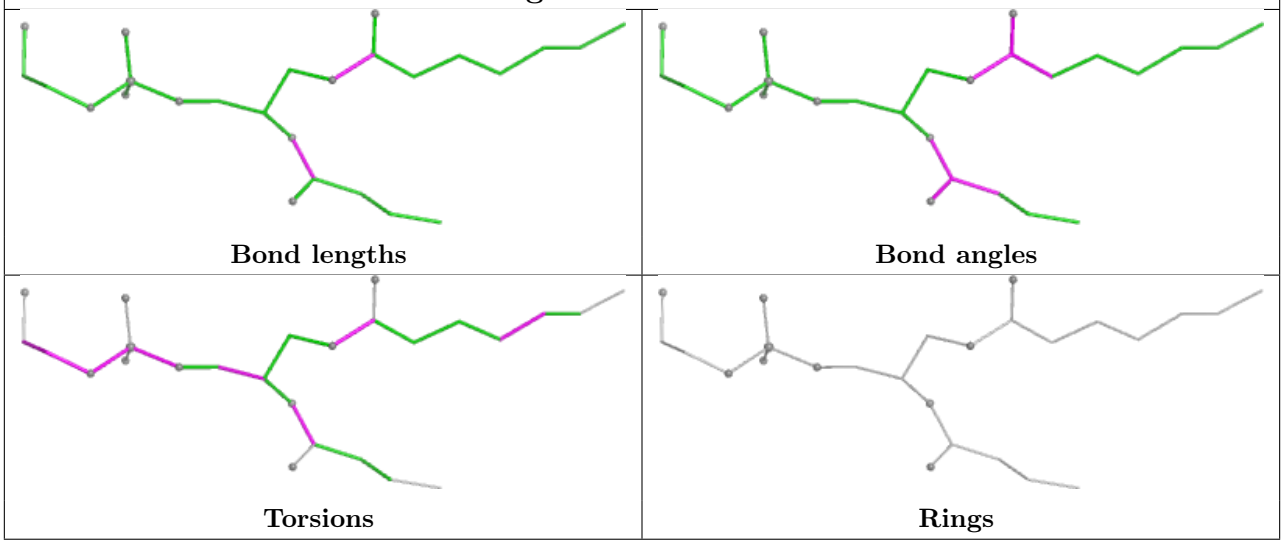

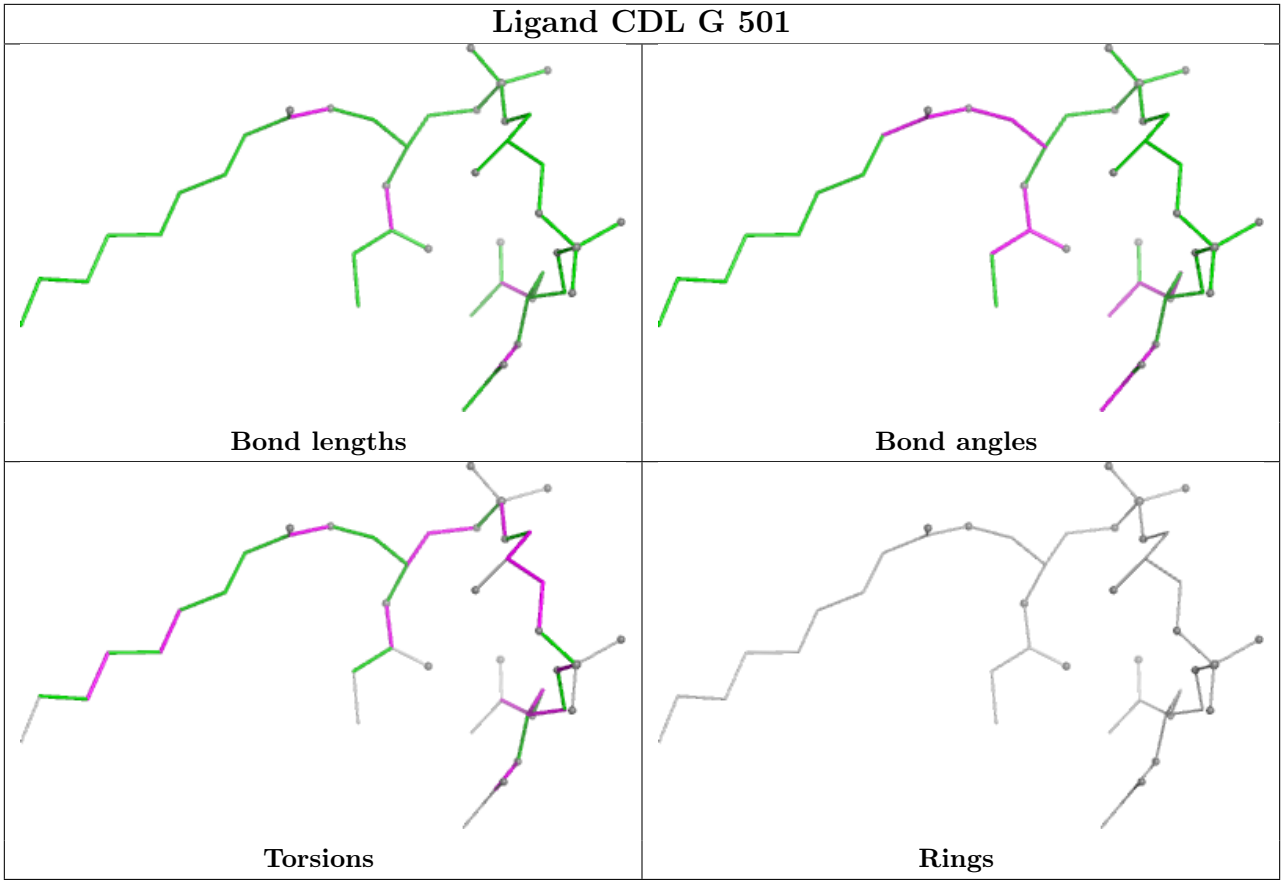

5.7 Other polymers (i)

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%)	0.12	22 (4%)	34	19	92, 150, 191, 255	0
1	N	444/480 (92%)	-0.05	24 (5%)	31	17	87, 132, 176, 243	0
2	B	422/453 (93%)	0.03	15 (3%)	46	25	108, 157, 200, 247	0
3	C	374/379 (98%)	-0.21	7 (1%)	66	38	77, 103, 137, 225	0
3	P	370/379 (97%)	-0.23	5 (1%)	73	45	79, 112, 148, 183	0
4	D	240/265 (90%)	-0.26	4 (1%)	69	40	92, 121, 153, 178	0
4	Q	241/265 (90%)	-0.26	3 (1%)	76	49	86, 131, 168, 211	0
5	E	73/274 (26%)	-0.02	4 (5%)	30	17	93, 130, 158, 170	0
5	I	21/274 (7%)	1.68	10 (47%)	0	1	146, 192, 220, 228	0
5	R	196/274 (71%)	-0.19	6 (3%)	51	28	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.17	4 (4%)	41	22	91, 124, 157, 171	0
6	S	99/111 (89%)	0.06	6 (6%)	27	15	85, 122, 168, 182	0
7	G	80/82 (97%)	-0.04	4 (5%)	34	19	88, 119, 189, 293	0
7	T	74/82 (90%)	-0.24	4 (5%)	31	17	83, 124, 181, 200	0
8	H	65/91 (71%)	0.16	0	100	100	103, 136, 171, 223	0
8	U	66/91 (72%)	-0.16	1 (1%)	72	44	132, 163, 213, 245	0
9	J	58/64 (90%)	-0.58	0	100	100	103, 137, 165, 175	0
9	W	59/64 (92%)	-0.34	0	100	100	102, 121, 153, 162	0
10	O	419/453 (92%)	-0.02	18 (4%)	40	21	97, 146, 193, 250	0
11	V	17/274 (6%)	2.44	10 (58%)	0	0	176, 209, 228, 268	0
All	All	3860/4946 (78%)	-0.08	147 (3%)	44	24	77, 133, 189, 293	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	V	78	TYR	8.5
10	O	117	ASP	7.7
6	F	106	GLU	7.4
10	O	313	ASN	5.9
2	B	313	ASN	5.7

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	PO4	Q	1001	5/5	0.41	0.10	194,205,216,232	0
14	PO4	D	502	5/5	0.52	0.08	176,192,199,203	0
14	PO4	F	501	5/5	0.58	0.10	242,243,245,246	0
14	PO4	D	503	5/5	0.58	0.08	168,169,177,181	0
14	PO4	S	501	5/5	0.64	0.08	225,226,243,252	0
14	PO4	D	504	5/5	0.65	0.08	179,190,194,195	0
14	PO4	N	501	5/5	0.73	0.11	112,126,127,137	0
14	PO4	C	504	5/5	0.78	0.08	121,121,134,149	0
14	PO4	Q	1002	5/5	0.83	0.06	210,211,220,230	0
14	PO4	E	501	5/5	0.88	0.07	124,134,144,145	0
19	GOL	R	502	6/6	0.88	0.11	169,181,193,193	0
14	PO4	N	1001	5/5	0.90	0.06	120,127,135,137	0
15	PEE	Q	506	51/51	0.93	0.21	100,134,171,187	0
13	4X9	P	503	28/28	0.93	0.16	109,147,226,261	0
13	4X9	C	503	28/28	0.94	0.12	116,143,206,215	0
17	CDL	D	505	39/100	0.95	0.11	85,124,146,148	0
15	PEE	D	506	26/51	0.96	0.12	107,127,169,176	0
17	CDL	G	501	44/100	0.96	0.11	95,115,153,168	0
15	PEE	C	505	49/51	0.96	0.15	94,116,135,137	0

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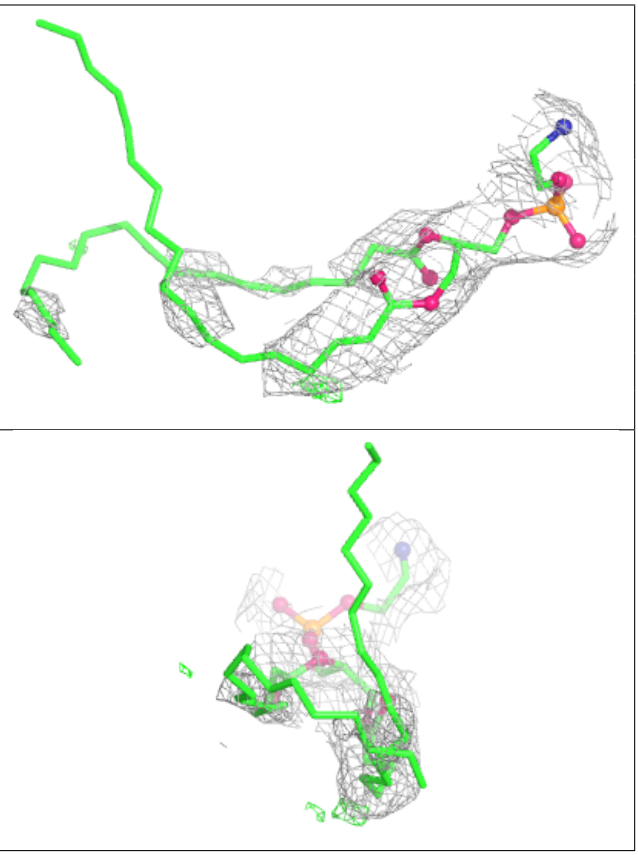
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CDL	T	501	49/100	0.97	0.09	93,129,160,167	0
17	CDL	Q	505	39/100	0.97	0.10	100,126,146,148	0
12	HEM	C	502	43/43	0.98	0.07	71,85,99,106	0
15	PEE	P	505	49/51	0.98	0.12	100,122,154,156	0
12	HEM	P	502	43/43	0.98	0.07	74,89,104,106	0
16	HEC	D	501	43/43	0.98	0.09	80,111,127,138	0
18	FES	R	501	4/4	0.98	0.03	125,158,164,170	0
16	HEC	Q	501	43/43	0.98	0.07	106,117,136,143	0
12	HEM	C	501	43/43	0.99	0.07	89,99,107,115	0
12	HEM	P	501	43/43	0.99	0.07	86,101,116,124	0

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

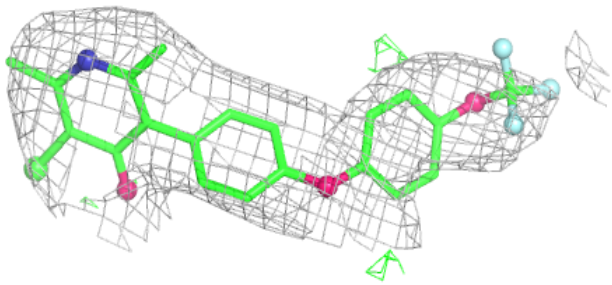
Electron density around PEE Q 506:

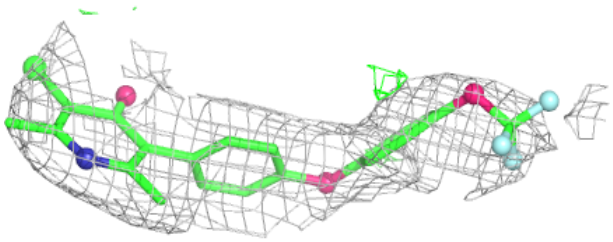
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

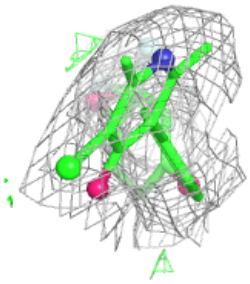


Electron density around 4X9 P 503:

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

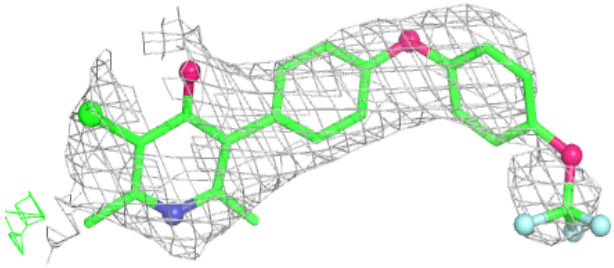


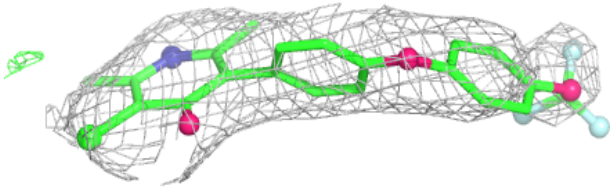


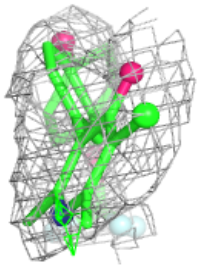


Electron density around 4X9 C 503:

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

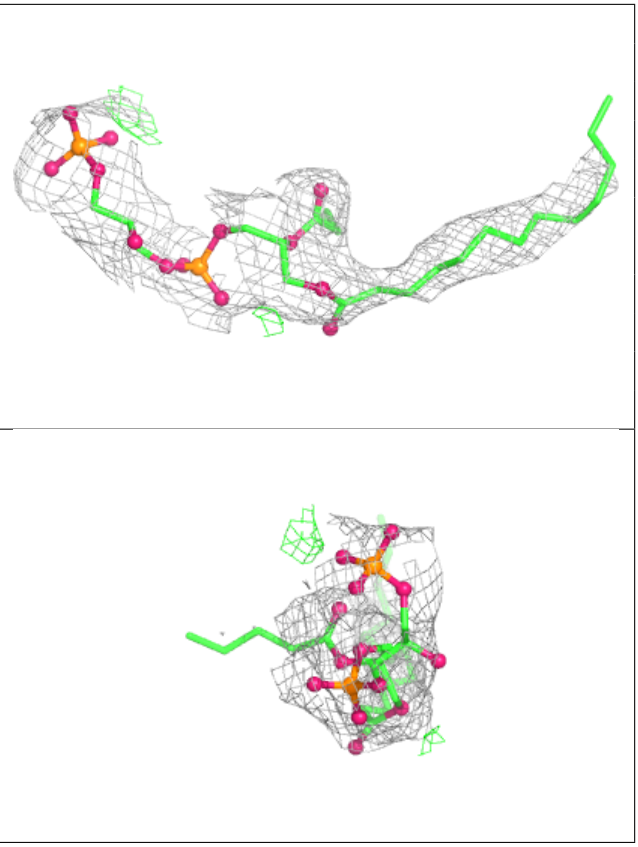






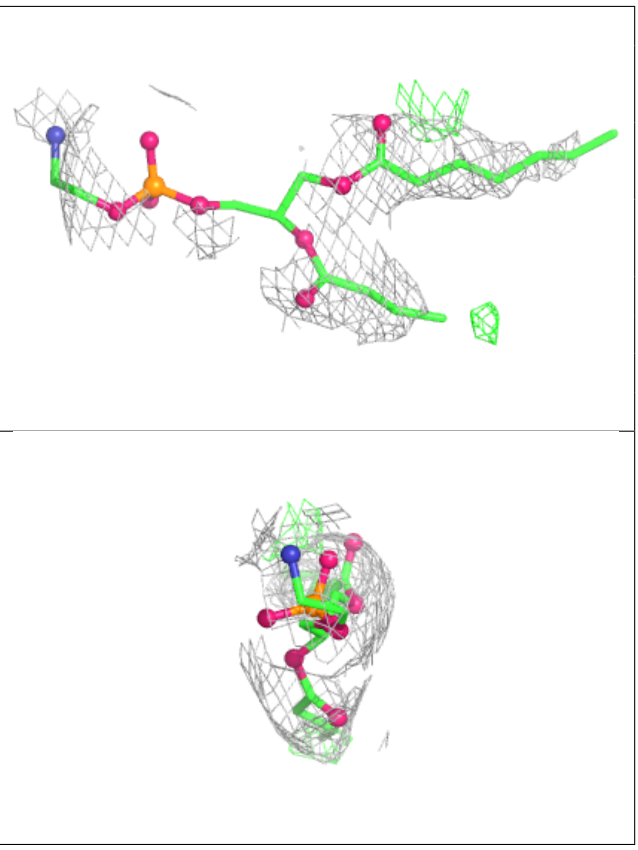
Electron density around CDL D 505:

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



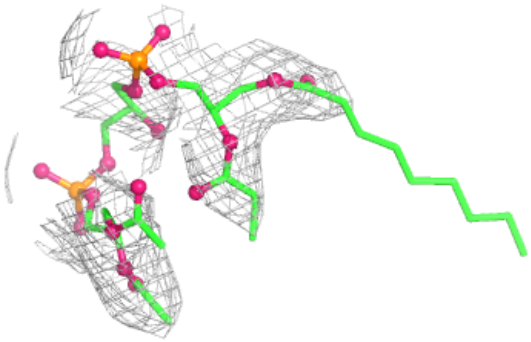
Electron density around PEE D 506:

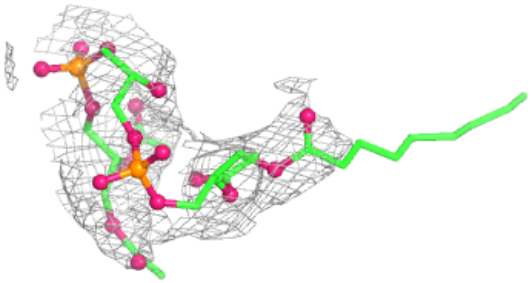
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CDL G 501:

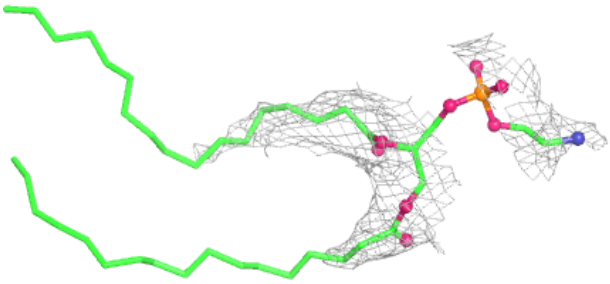
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

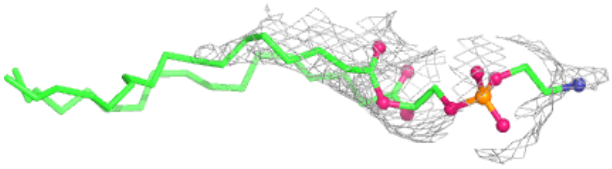




Electron density around PEE C 505:

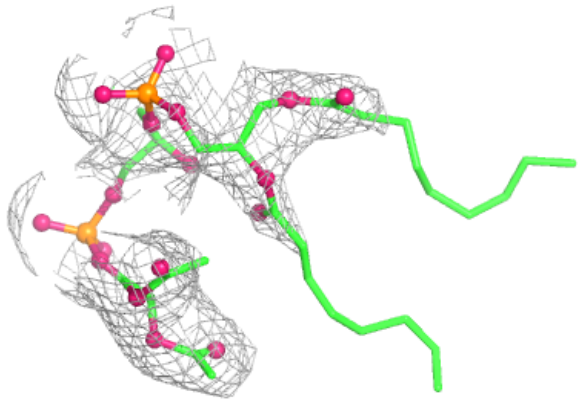
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

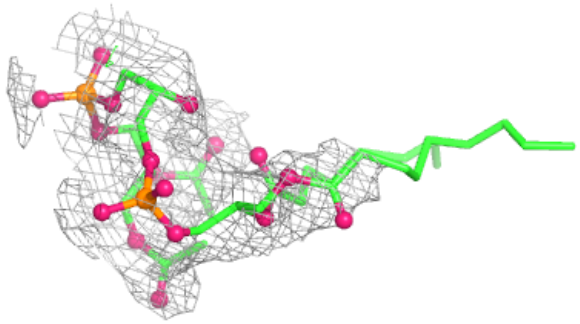


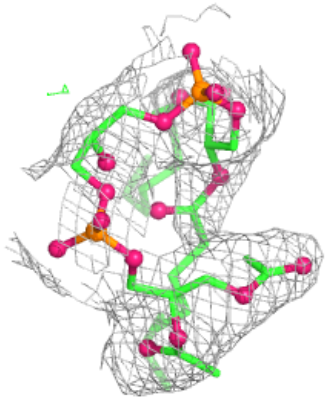


Electron density around CDL T 501:

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

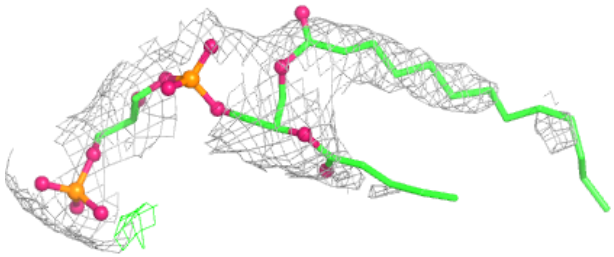


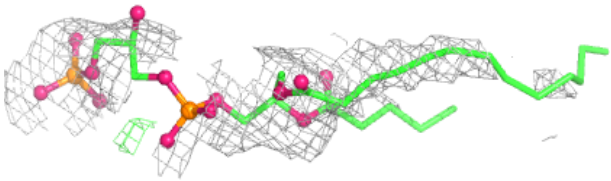


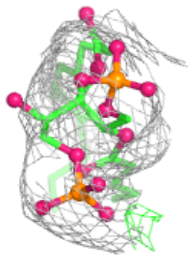


Electron density around CDL Q 505:

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

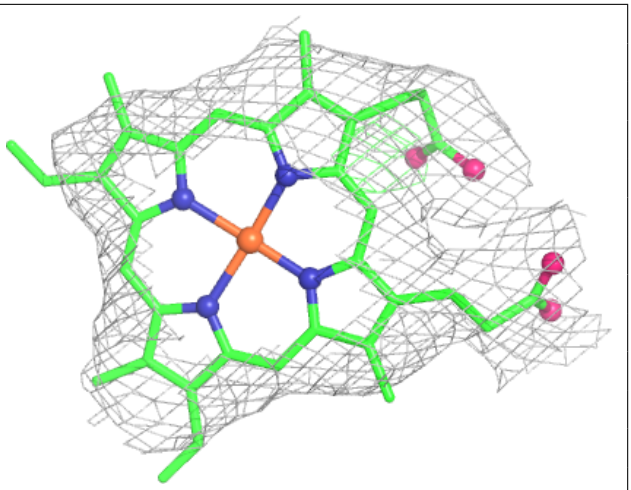


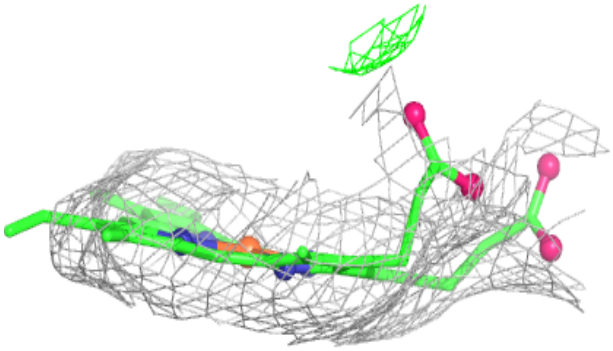


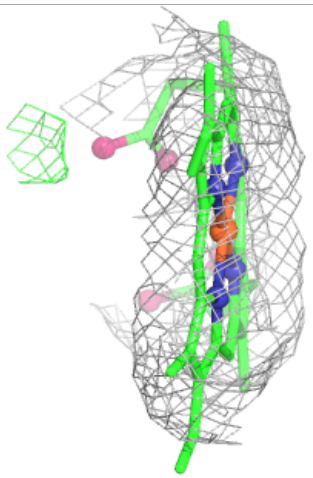


Electron density around HEM C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

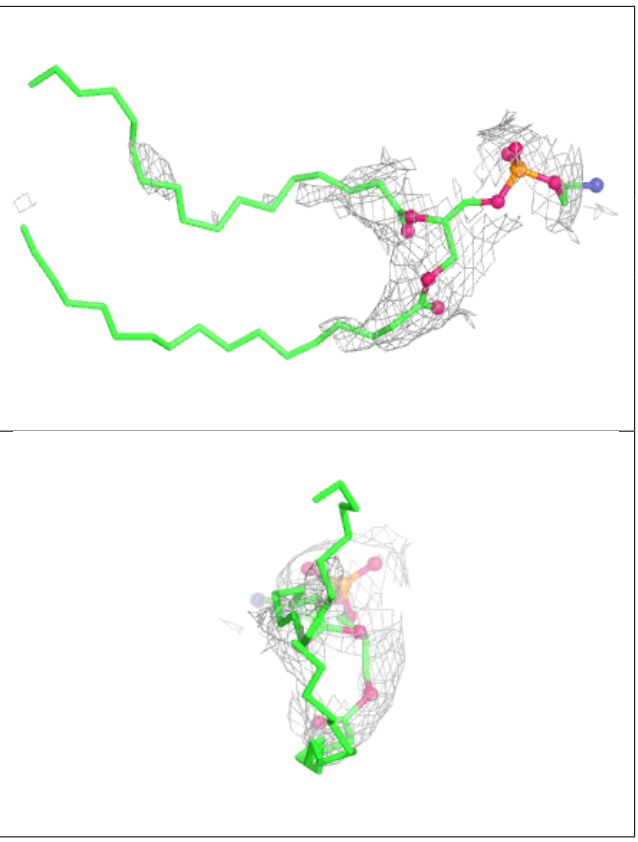






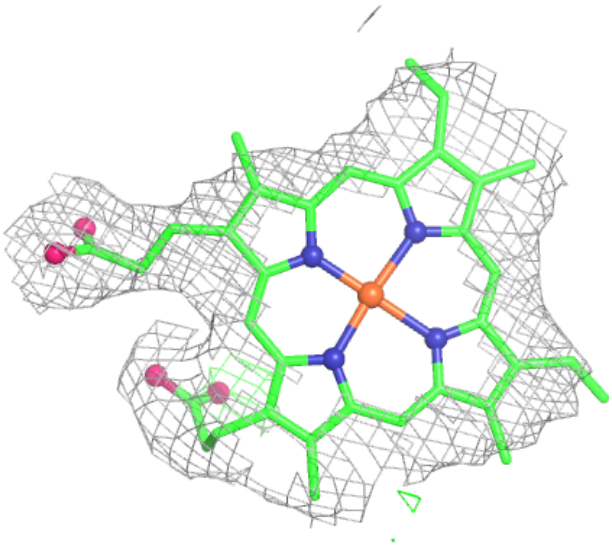
Electron density around PEE P 505:

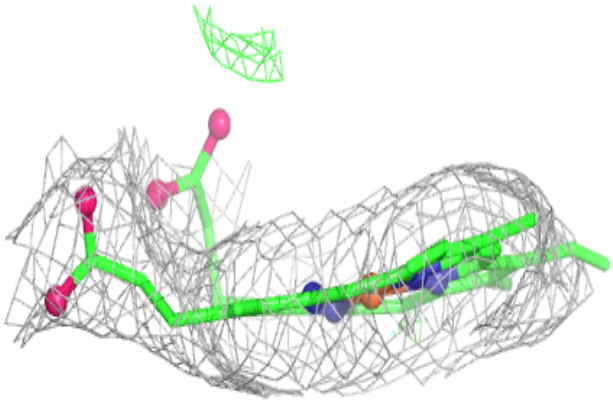
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

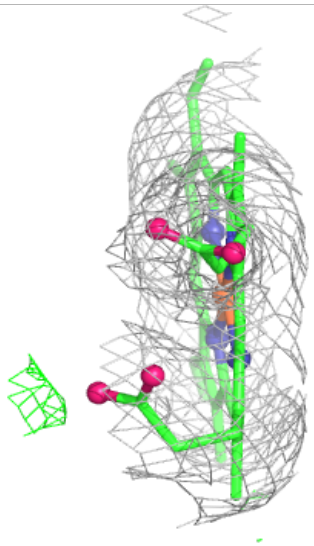


Electron density around HEM P 502:

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

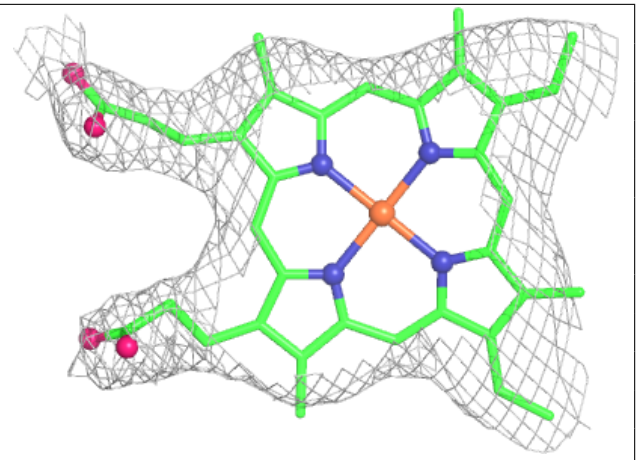


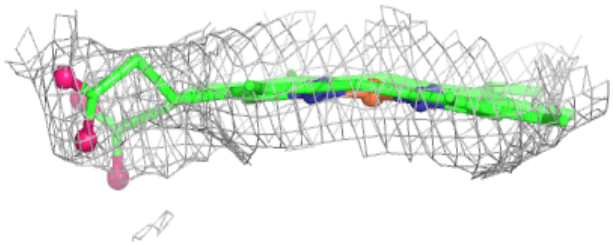


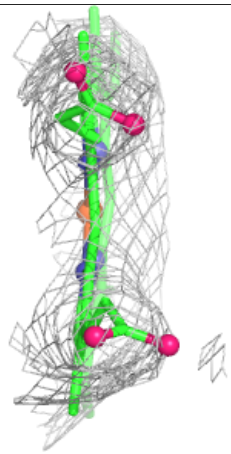


Electron density around HEC D 501:

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

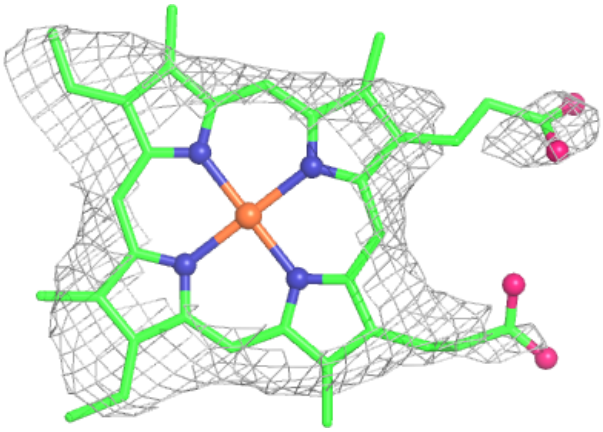


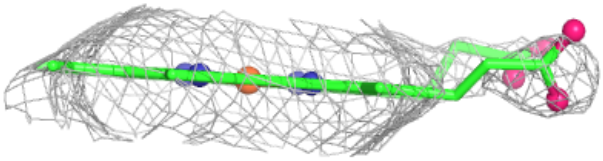


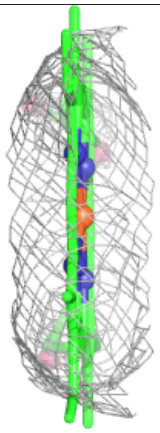


Electron density around HEC Q 501:

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

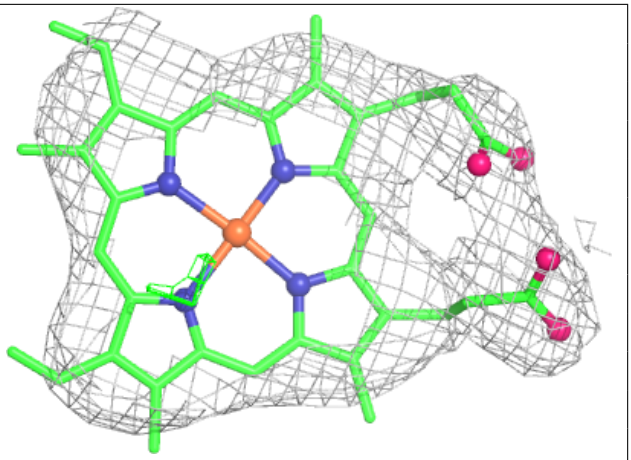


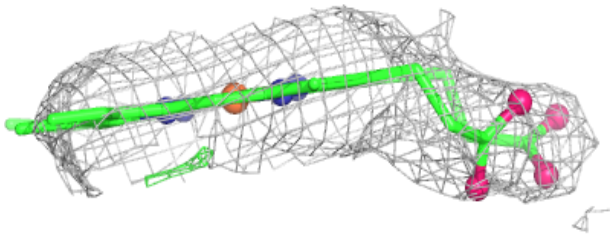


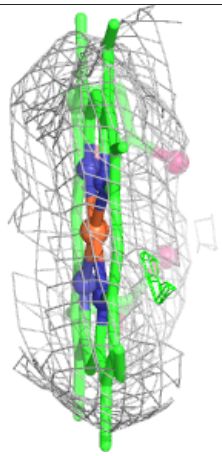


Electron density around HEM C 501:

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

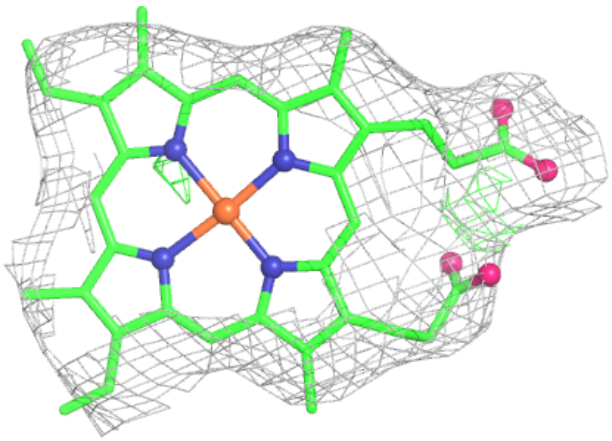


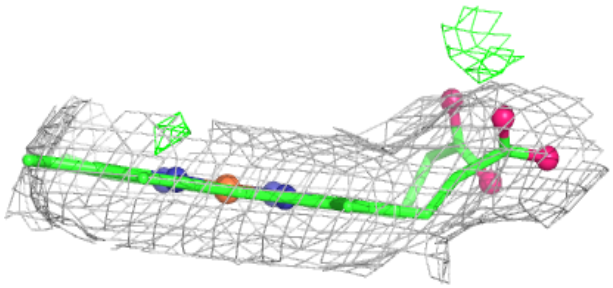


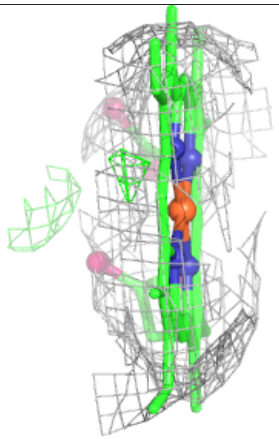


Electron density around HEM P 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.