



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 09:16 PM EDT

PDB ID : 2E75 / pdb_00002e75
Title : Crystal Structure of the Cytochrome b6f Complex with 2-nonyl-4-hydroxyquinoline N-oxide (NQNO) from *M. lamosus*
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
Resolution : 3.55 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 : 2022.3.0, CSD as543be (2022)
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

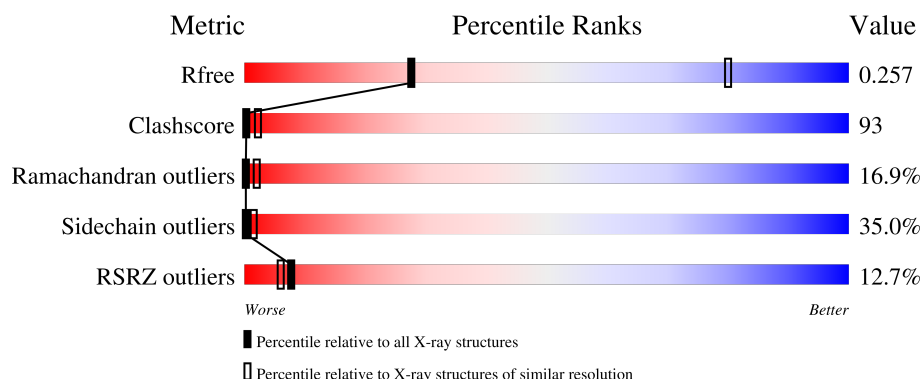
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	215	
2	B	160	
3	C	289	
4	D	179	
5	E	32	

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Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

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
10	HEM	A	301	-	-	X	-
10	HEM	A	302	-	-	X	-
10	HEM	C	301	-	-	X	-
11	HEC	A	303	X	-	-	-
12	OPC	A	1002	-	-	X	-
13	UMQ	A	1102	X	-	-	-
13	UMQ	A	1103	X	-	-	-
13	UMQ	A	1104	X	-	-	-
13	UMQ	C	1101	X	-	-	-
14	QNO	A	501	X	-	-	-
15	CLA	B	201	X	-	-	-
16	FES	D	200	-	-	X	-
17	SQD	D	201	X	X	-	-
18	BCR	G	101	-	X	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 8046 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1711	1140	272	288	11			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1249	841	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1260	805	218	230	7			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			242	165	35	40	2			

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | G | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 283 | 188 | 44 | 50 | 1 | | | |

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | H | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 230 | 156 | 36 | 36 | 2 | | | |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 9 | A | 1 | Total Cd
1 1 | 0 | 0 |
| 9 | B | 1 | Total Cd
1 1 | 0 | 0 |

-
- The diagram shows the chemical structure of the HEM molecule. The central iron atom (Fe) is coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with two hydroxyl groups (OH) and two carboxylate groups (COO). The atoms are labeled with their respective positions: O1A, O2A, O1D, O2D for the hydroxyl groups; CAA, CBA, CAD, CBD for the carboxylate groups; and CMA, CMB, CMC, CMD for the methyl groups. The nitrogen atoms are labeled NA, ND, NC, and NB. The iron atom is labeled FE. The bonds are shown with thermal ellipsoids at the 50% probability level.

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

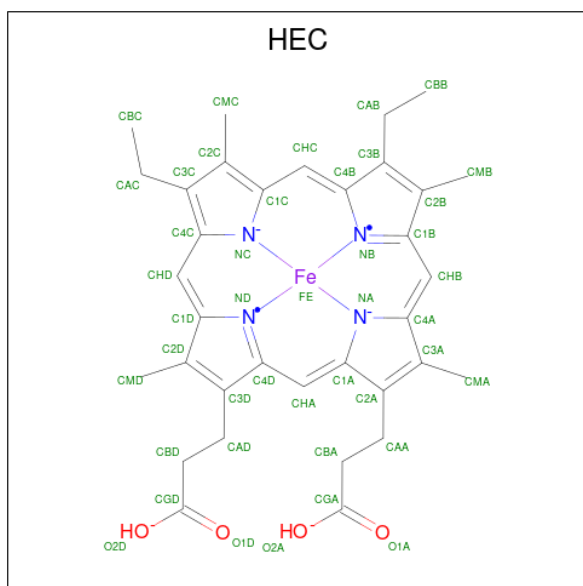


WORLD WIDE
PDB
PROTEIN DATA BANK

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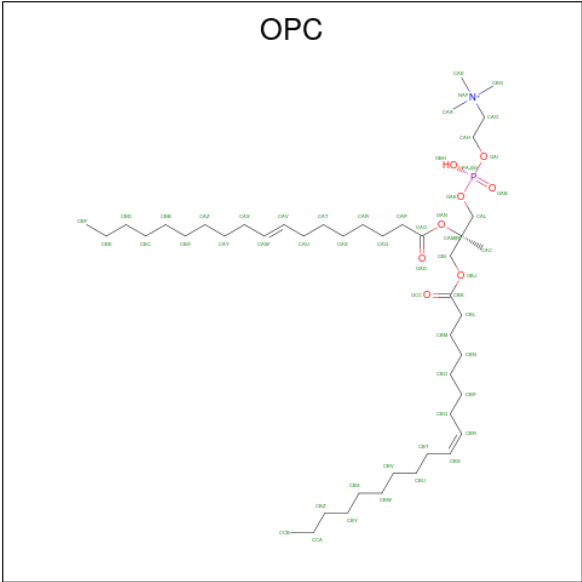
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



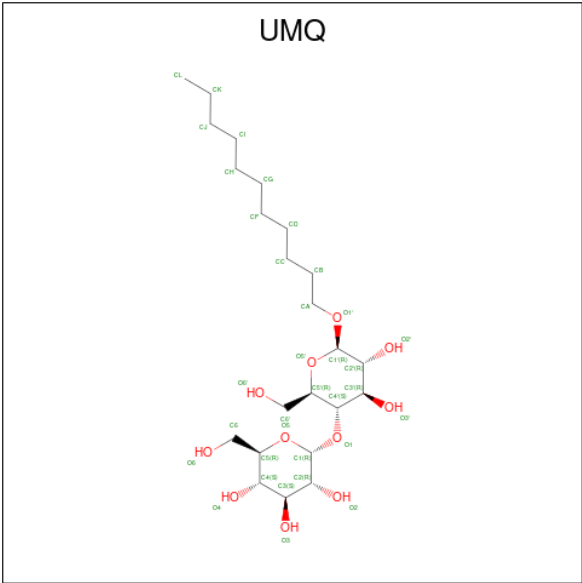
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 12 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: $C_{45}H_{87}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



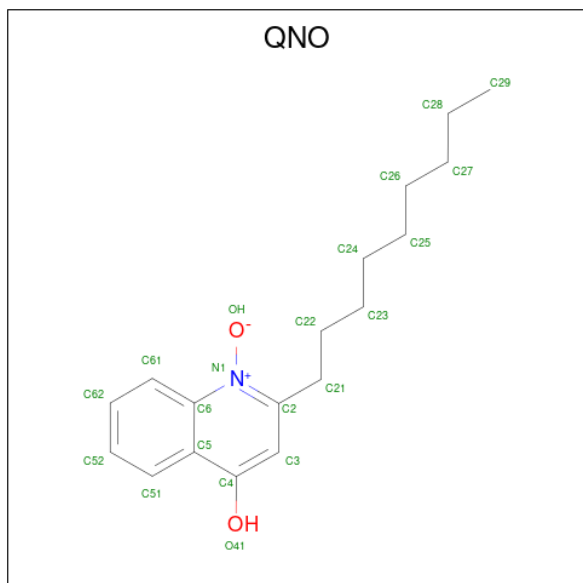
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		
13	A	1	Total	C	O	0	0
			34	23	11		

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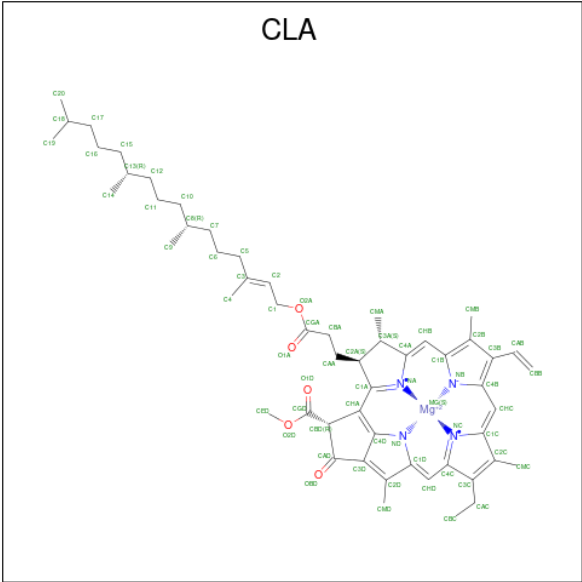
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		
13	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (CCD ID: QNO) (formula: $C_{18}H_{25}NO_2$).



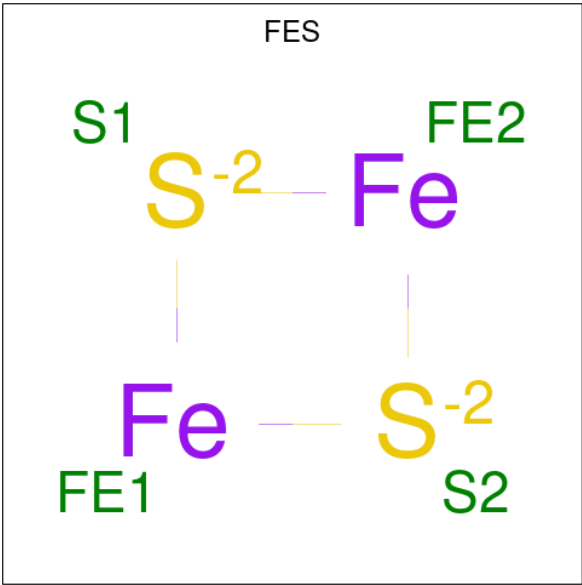
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



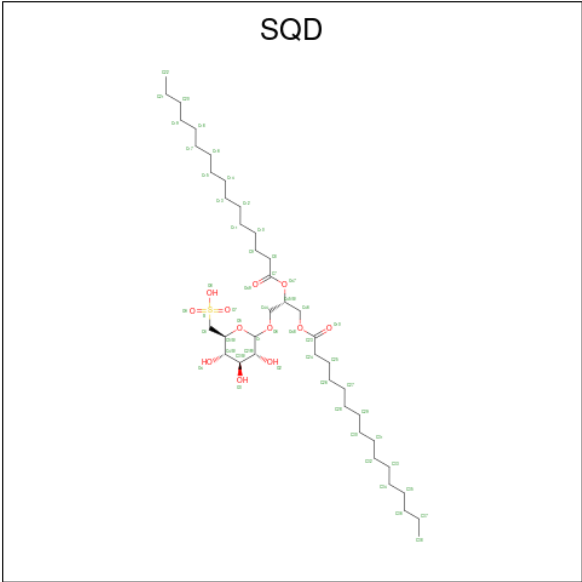
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



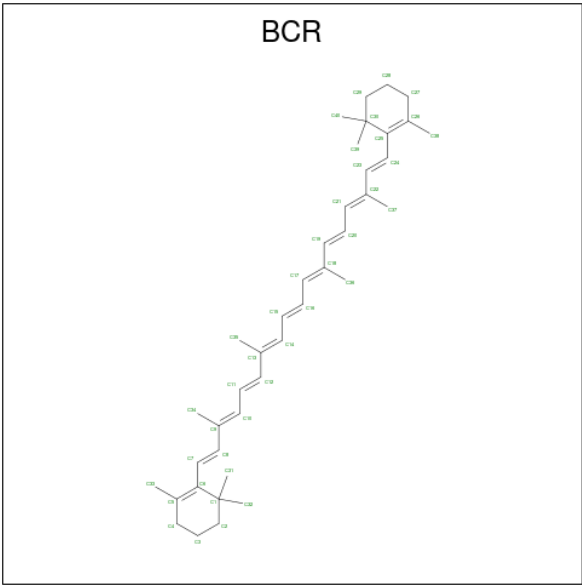
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	G	1	Total	C	0	0
			40	40		

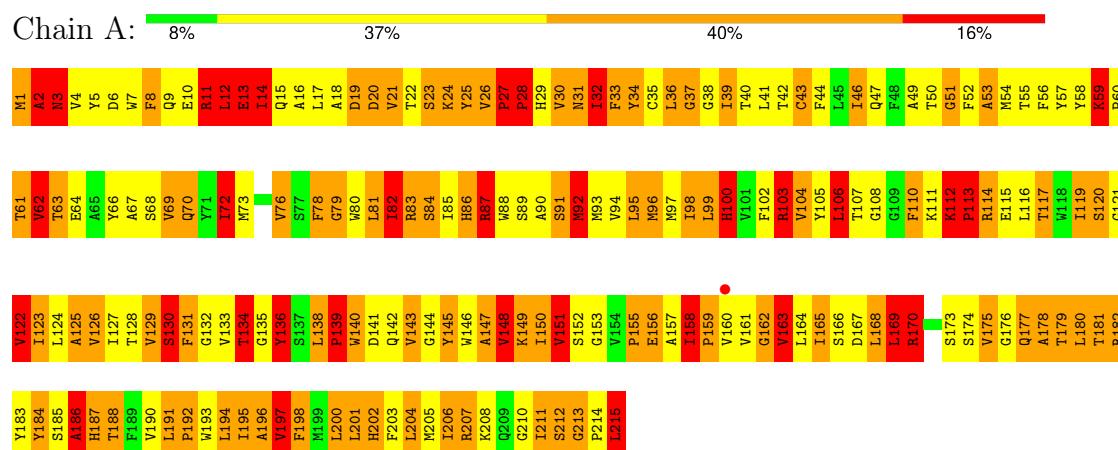
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	3	Total 3	O 3	0	0
19	B	2	Total 2	O 2	0	0

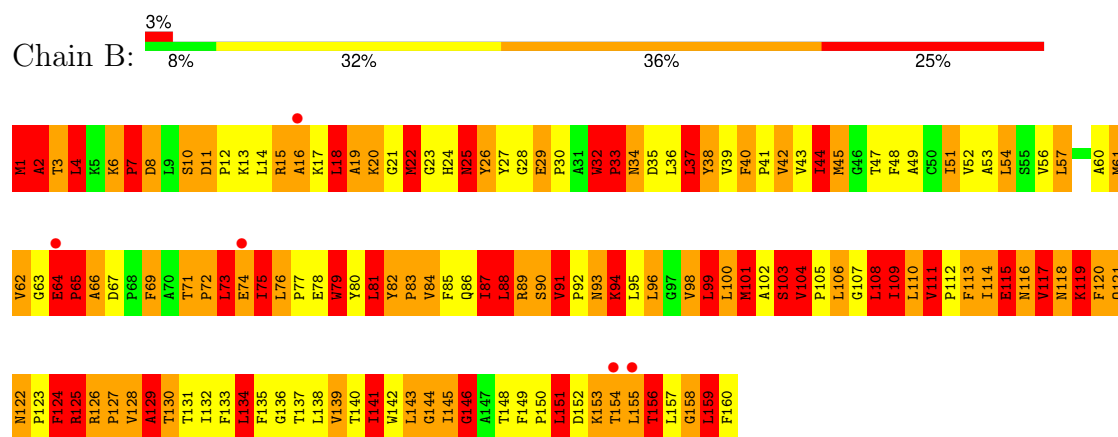
3 Residue-property plots

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.

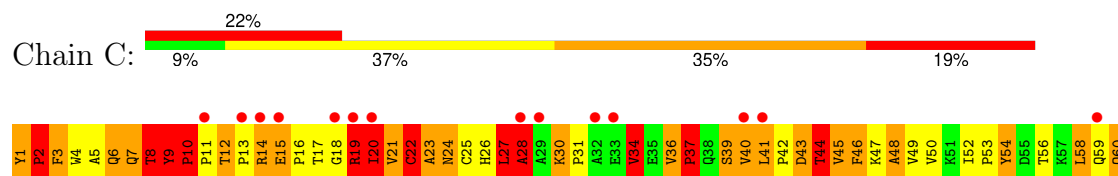
• Molecule 1: Cytochrome b6

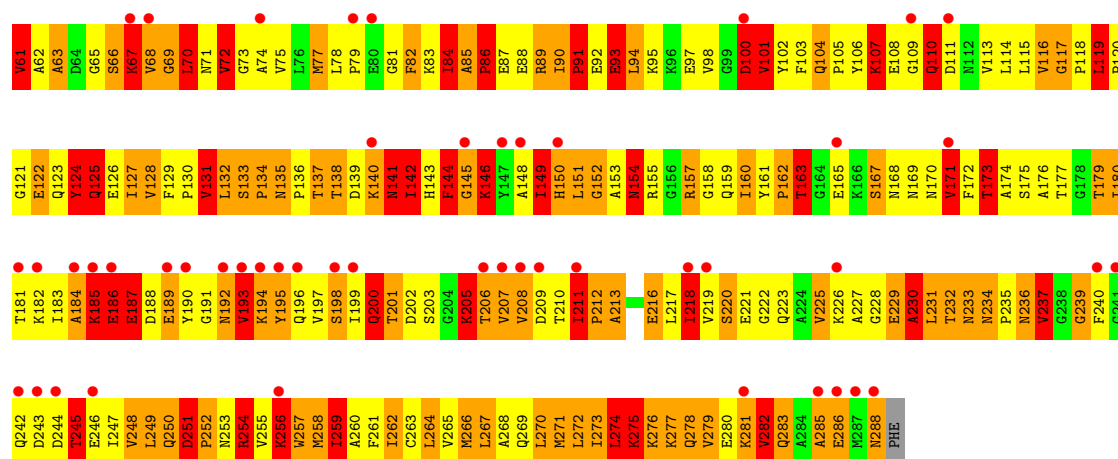


• Molecule 2: Cytochrome b6-f complex subunit 4

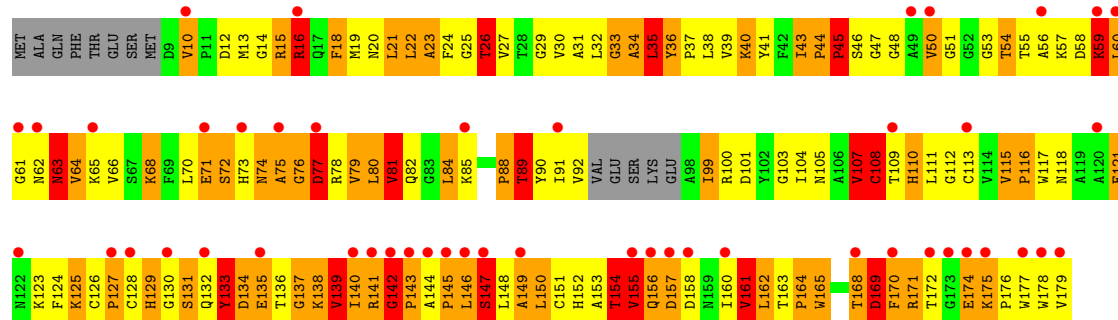


• Molecule 3: Apocytochrome f

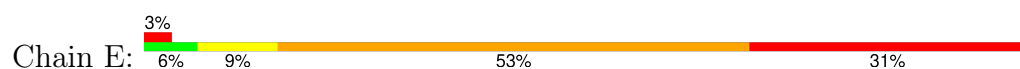




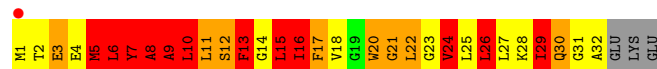
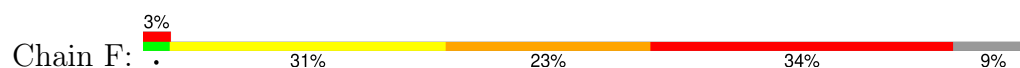
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 5: Cytochrome b6-f complex subunit 6



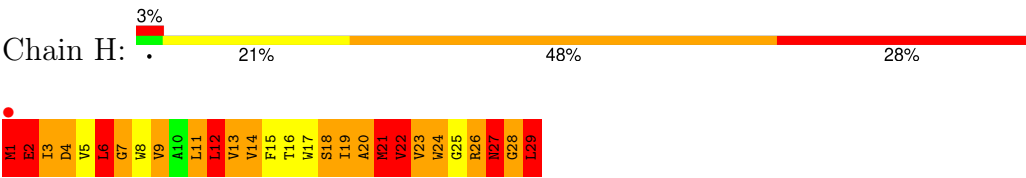
• Molecule 6: Cytochrome b6-f complex subunit 7



• Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.16Å 159.16Å 362.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 3.55 49.94 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.94-3.55) 99.7 (49.94-3.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.89 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.267 0.198 , 0.257	Depositor DCC
R_{free} test set	1703 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8046	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, SQD, OPC, BCR, HEM, HEC, CLA, CD, QNO, UMQ

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	2.41	81/1763 (4.6%)	2.56	145/2405 (6.0%)
2	B	2.17	45/1288 (3.5%)	2.47	90/1765 (5.1%)
3	C	1.93	62/2264 (2.7%)	2.22	124/3082 (4.0%)
4	D	1.67	17/1292 (1.3%)	1.86	43/1760 (2.4%)
5	E	2.26	11/253 (4.3%)	2.22	15/340 (4.4%)
6	F	2.58	17/246 (6.9%)	2.29	14/331 (4.2%)
7	G	2.03	6/289 (2.1%)	2.26	18/391 (4.6%)
8	H	2.35	15/236 (6.4%)	2.38	16/323 (5.0%)
All	All	2.10	254/7631 (3.3%)	2.30	465/10397 (4.5%)

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	6
2	B	0	7
3	C	0	8
5	E	0	4
6	F	0	1
7	G	0	4
8	H	0	2
All	All	0	32

The worst 5 of 254 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	CA-CB	-19.91	1.33	1.54
2	B	84	VAL	CA-CB	-12.42	1.39	1.54
1	A	49	ALA	CA-CB	-10.74	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	ARG	CZ-NH1	10.58	1.47	1.32
1	A	67	ALA	CA-CB	-10.53	1.36	1.53

The worst 5 of 465 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	CA-C-N	-19.77	95.13	119.84
1	A	112	LYS	C-N-CA	-19.77	95.13	119.84
3	C	9	TYR	CA-C-N	16.48	137.36	120.38
3	C	9	TYR	C-N-CA	16.48	137.36	120.38
3	C	85	ALA	CA-C-N	15.21	138.85	119.84

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	135	GLY	Peptide
1	A	158	ILE	Peptide
1	A	2	ALA	Peptide
1	A	27	PRO	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	1711	0	1736	361	0
2	B	1249	0	1308	330	0
3	C	2216	0	2232	425	0
4	D	1260	0	1243	195	0
5	E	248	0	284	81	0
6	F	242	0	260	74	0
7	G	283	0	289	63	0
8	H	230	0	239	80	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	86	0	60	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	23	0
11	A	43	0	31	10	0
12	A	54	0	79	26	0
12	B	54	0	83	11	0
13	A	102	0	123	13	0
13	C	34	0	42	10	0
14	A	21	0	24	7	0
15	B	65	0	72	14	0
16	D	4	0	0	3	0
17	D	54	0	53	11	0
18	G	40	0	52	13	0
19	A	3	0	0	0	0
19	B	2	0	0	0	0
All	All	8046	0	8240	1515	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 93.

The worst 5 of 1515 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)
1:A:59:LYS:CE	1:A:59:LYS:CD	1.75	1.60
2:B:88:LEU:CG	2:B:88:LEU:CD1	1.75	1.59
6:F:6:LEU:CD2	6:F:6:LEU:CG	1.75	1.59
8:H:29:LEU:CD2	8:H:29:LEU:CG	1.78	1.58
5:E:12:ILE:CD1	5:E:12:ILE:CG1	1.79	1.58

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	213/215 (99%)	142 (67%)	53 (25%)	18 (8%)	0	7
2	B	158/160 (99%)	91 (58%)	36 (23%)	31 (20%)	0	1
3	C	286/289 (99%)	195 (68%)	50 (18%)	41 (14%)	0	3
4	D	162/179 (90%)	93 (57%)	39 (24%)	30 (18%)	0	1
5	E	30/32 (94%)	9 (30%)	10 (33%)	11 (37%)	0	0
6	F	30/35 (86%)	14 (47%)	8 (27%)	8 (27%)	0	0
7	G	35/37 (95%)	13 (37%)	9 (26%)	13 (37%)	0	0
8	H	27/29 (93%)	14 (52%)	6 (22%)	7 (26%)	0	0
All	All	941/976 (96%)	571 (61%)	211 (22%)	159 (17%)	0	2

5 of 159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	23	SER
1	A	28	PRO
1	A	112	LYS
1	A	136	TYR

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	184/184 (100%)	132 (72%)	52 (28%)	0	3
2	B	137/137 (100%)	90 (66%)	47 (34%)	0	2
3	C	242/243 (100%)	142 (59%)	100 (41%)	0	0
4	D	134/146 (92%)	93 (69%)	41 (31%)	0	2
5	E	25/25 (100%)	17 (68%)	8 (32%)	0	2
6	F	24/27 (89%)	12 (50%)	12 (50%)	0	0
7	G	28/28 (100%)	19 (68%)	9 (32%)	0	2
8	H	24/24 (100%)	14 (58%)	10 (42%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	798/814 (98%)	519 (65%)	279 (35%)	0 1

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	154	THR
4	D	174	GLU
7	G	1	MET
2	B	156	THR
2	B	152	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	242	GLN
4	D	62	ASN
3	C	288	ASN
4	D	82	GLN
3	C	110	GLN

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](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SQD	D	201	-	52,54,54	2.69	25 (48%)	62,65,65	4.75	35 (56%)
18	BCR	G	101	-	41,41,41	3.55	19 (46%)	56,56,56	6.93	36 (64%)
14	QNO	A	501	11	21,22,22	2.50	5 (23%)	22,28,28	2.20	6 (27%)
13	UMQ	A	1102	-	35,35,35	2.04	7 (20%)	46,46,46	3.07	20 (43%)
13	UMQ	C	1101	-	35,35,35	1.83	8 (22%)	46,46,46	3.42	20 (43%)
11	HEC	A	303	1,19,14	50,50,50	2.52	16 (32%)	68,82,82	2.80	24 (35%)
10	HEM	A	301	1	50,50,50	2.31	19 (38%)	67,82,82	3.02	31 (46%)
10	HEM	A	302	1	50,50,50	2.25	21 (42%)	67,82,82	3.08	27 (40%)
13	UMQ	A	1103	-	35,35,35	1.72	5 (14%)	46,46,46	2.96	16 (34%)
13	UMQ	A	1104	-	35,35,35	1.60	3 (8%)	46,46,46	2.82	12 (26%)
16	FES	D	200	4	0,4,4	-	-	-	-	-
12	OPC	A	1002	-	53,53,54	2.16	14 (26%)	59,61,64	2.84	27 (45%)
12	OPC	B	1001	-	53,53,54	2.20	19 (35%)	59,61,64	2.53	26 (44%)
15	CLA	B	201	19	69,73,73	1.98	17 (24%)	82,113,113	3.79	44 (53%)
10	HEM	C	301	3	50,50,50	2.27	22 (44%)	67,82,82	2.60	23 (34%)

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	SQD	D	201	-	3/3/9/9	25/49/69/69	0/1/1/1
18	BCR	G	101	-	-	10/29/63/63	0/2/2/2
14	QNO	A	501	11	1/1/0/0	4/9/9/9	0/2/2/2
13	UMQ	A	1102	-	2/2/10/10	12/20/60/60	0/2/2/2
13	UMQ	C	1101	-	2/2/10/10	9/20/60/60	0/2/2/2
11	HEC	A	303	1,19,14	1/1/3/7	13/14/54/54	-
10	HEM	A	301	1	-	3/14/54/54	-
13	UMQ	A	1103	-	2/2/10/10	12/20/60/60	0/2/2/2
13	UMQ	A	1104	-	2/2/10/10	16/20/60/60	0/2/2/2
10	HEM	A	302	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	FES	D	200	4	-	-	0/1/1/1
15	CLA	B	201	19	1/1/15/20	12/39/115/115	-
12	OPC	A	1002	-	-	23/57/57/60	-
12	OPC	B	1001	-	-	22/57/57/60	-
10	HEM	C	301	3	-	3/14/54/54	-

The worst 5 of 200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	101	BCR	C8-C9	-11.24	1.21	1.46
11	A	303	HEC	FE-ND	8.40	2.20	1.94
14	A	501	QNO	C2-N1	7.73	1.51	1.36
13	A	1102	UMQ	O1'-C1'	6.59	1.51	1.40
18	G	101	BCR	C23-C22	-6.55	1.31	1.46

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	101	BCR	C7-C8-C9	29.43	169.77	126.23
18	G	101	BCR	C24-C23-C22	26.06	164.79	126.23
18	G	101	BCR	C8-C7-C6	17.00	172.42	127.00
18	G	101	BCR	C23-C24-C25	15.39	168.11	127.00
15	B	201	CLA	CMB-C2B-C1B	13.36	145.75	125.42

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	303	HEC	NA
13	A	1102	UMQ	C1'
13	A	1102	UMQ	C2'
13	A	1103	UMQ	C1'
13	A	1103	UMQ	C2'

5 of 167 torsion outliers are listed below:

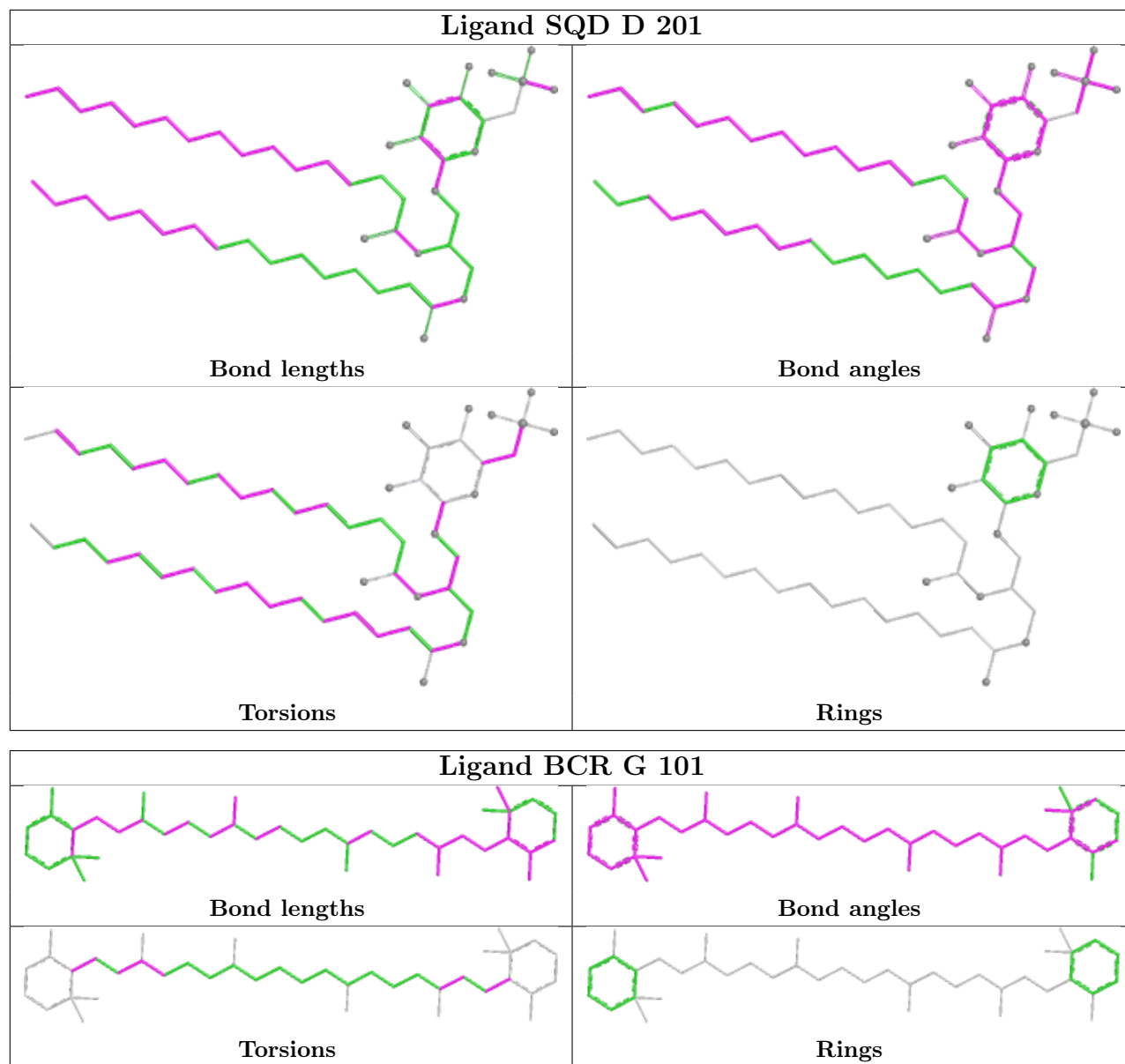
Mol	Chain	Res	Type	Atoms
12	A	1002	OPC	NAF-CAG-CAH-OAI
12	A	1002	OPC	CBO-CBP-CBQ-CBR
12	B	1001	OPC	CAH-OAI-PAJ-OAK
12	B	1001	OPC	CAH-OAI-PAJ-OBH
12	B	1001	OPC	CAH-OAI-PAJ-OAB

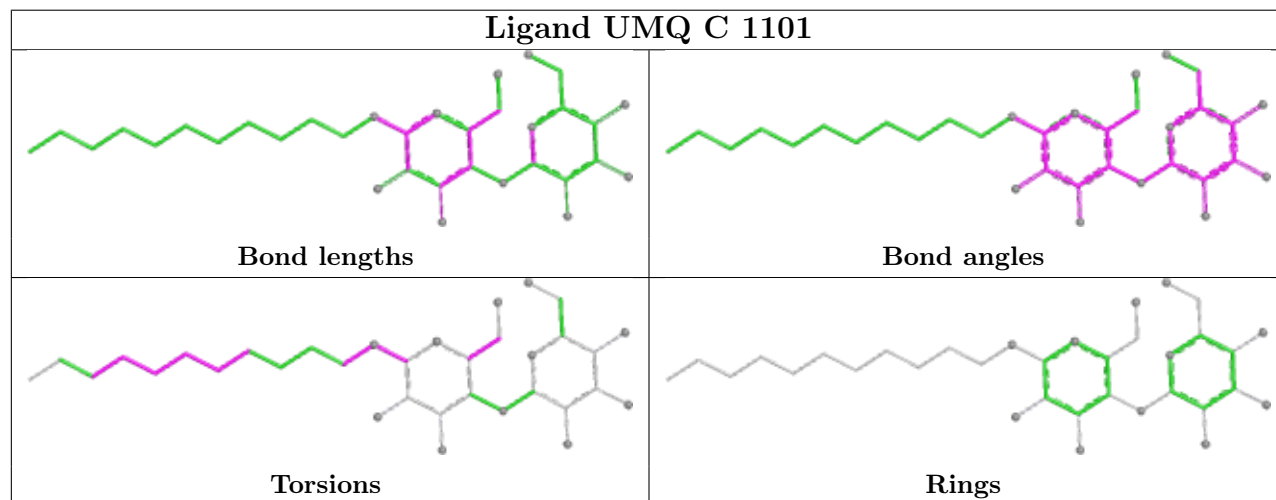
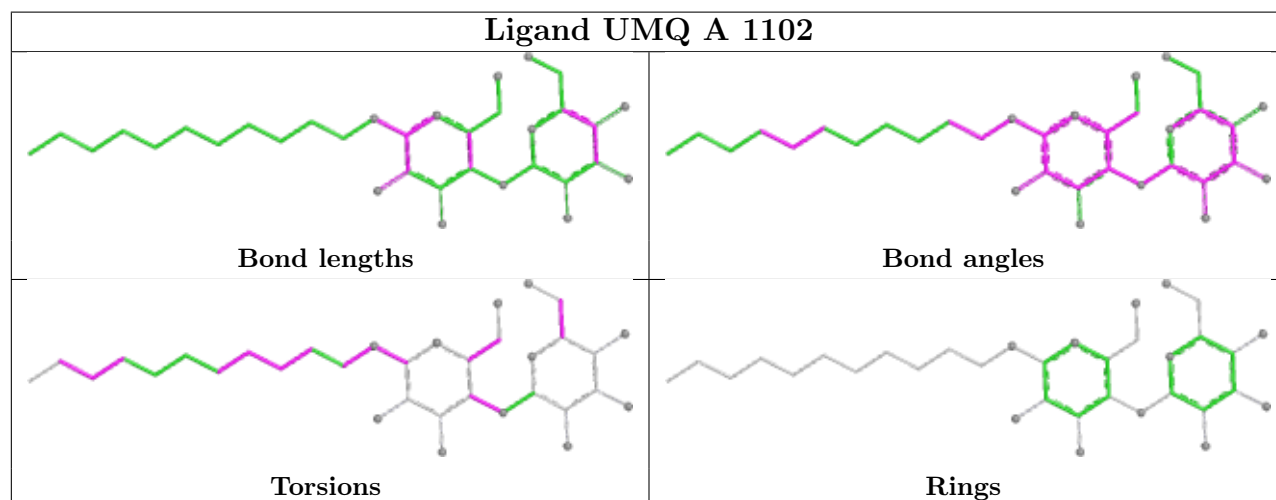
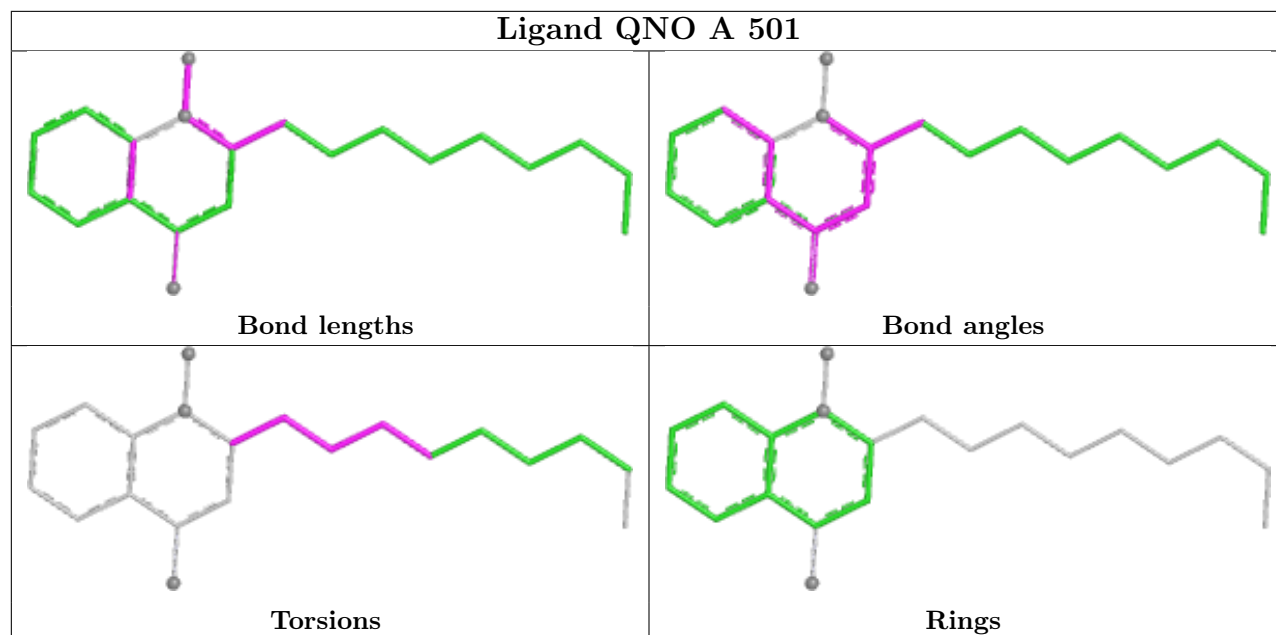
There are no ring outliers.

15 monomers are involved in 186 short contacts:

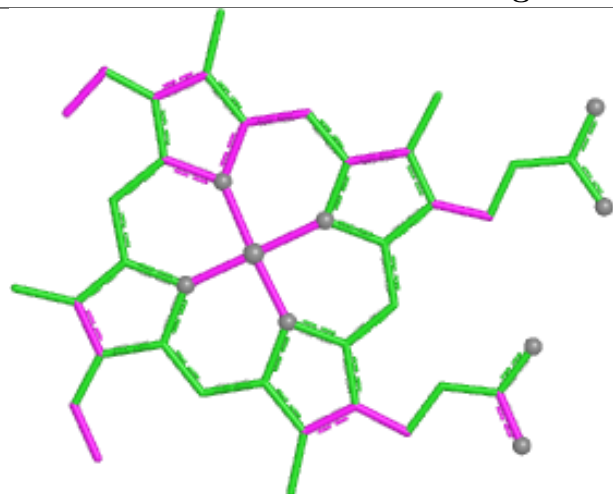
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	201	SQD	11	0
18	G	101	BCR	13	0
14	A	501	QNO	7	0
13	A	1102	UMQ	9	0
13	C	1101	UMQ	10	0
11	A	303	HEC	10	0
10	A	301	HEM	22	0
10	A	302	HEM	25	0
13	A	1103	UMQ	2	0
13	A	1104	UMQ	2	0
16	D	200	FES	3	0
12	A	1002	OPC	26	0
12	B	1001	OPC	11	0
15	B	201	CLA	14	0
10	C	301	HEM	23	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.

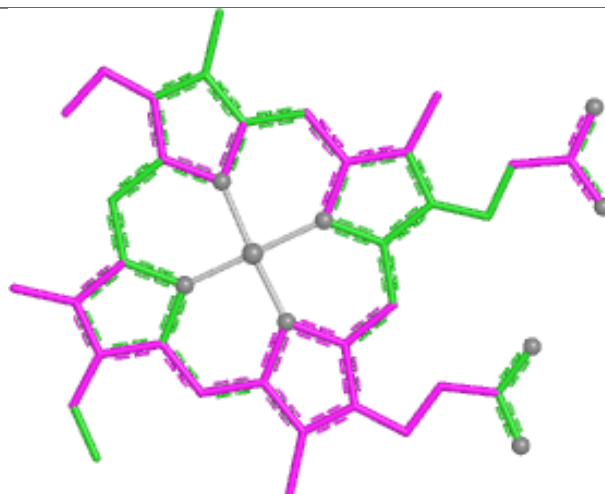




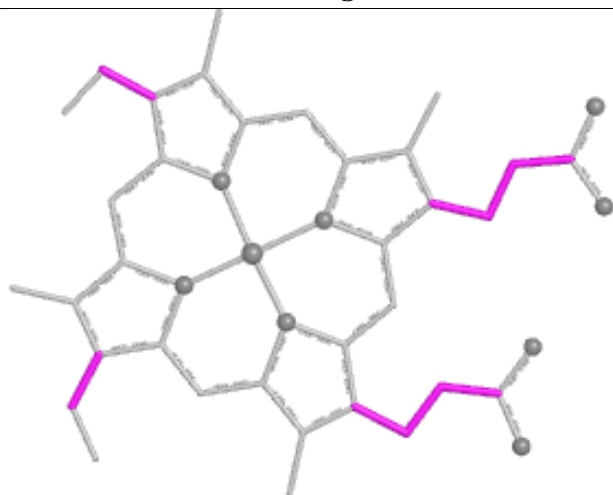
Ligand HEC A 303



Bond lengths



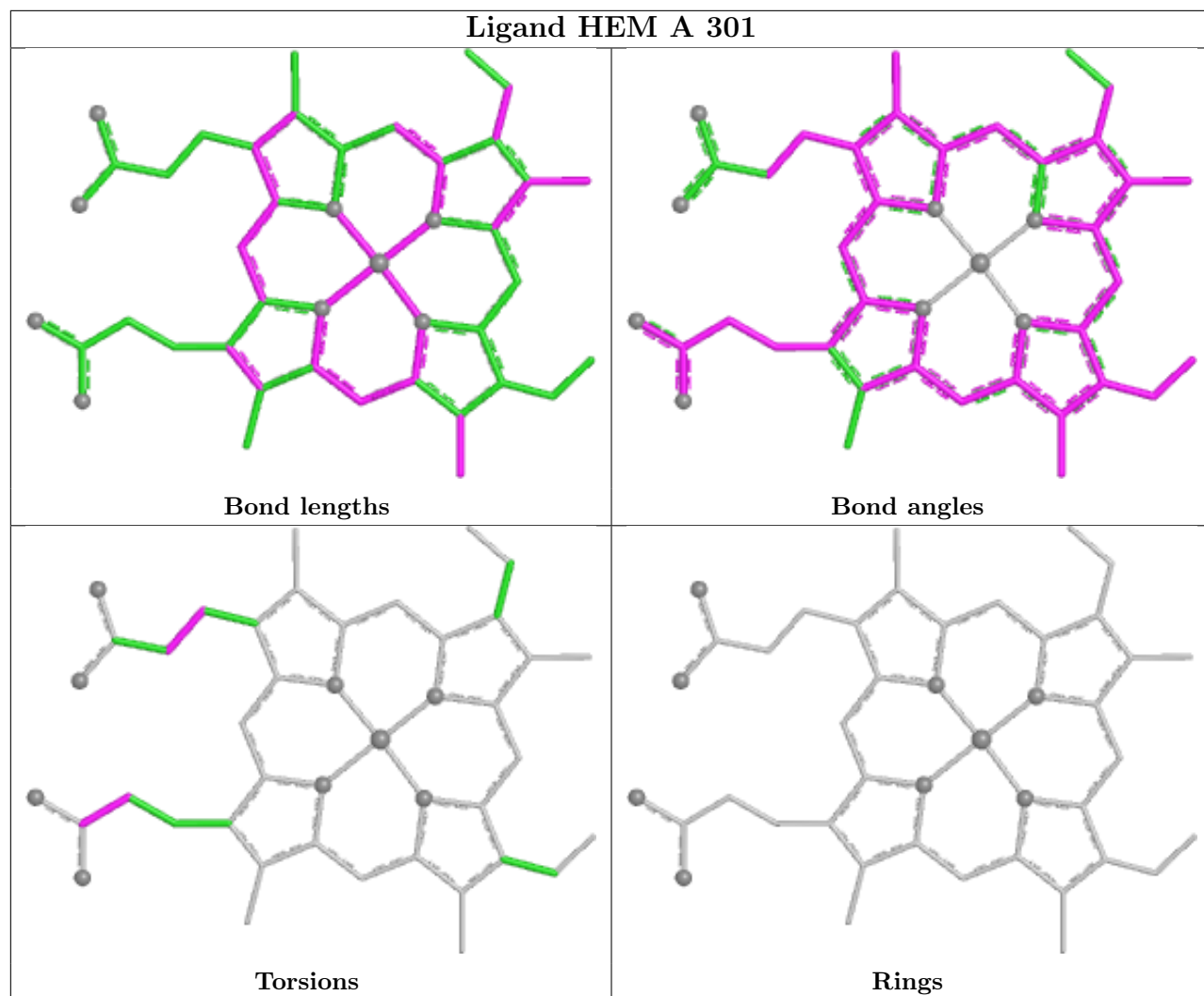
Bond angles

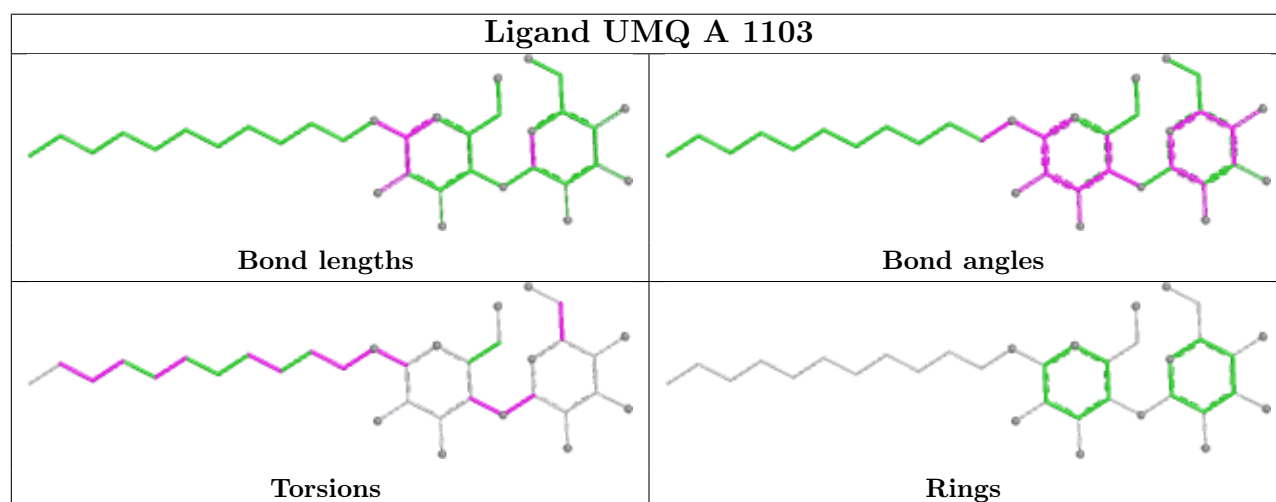
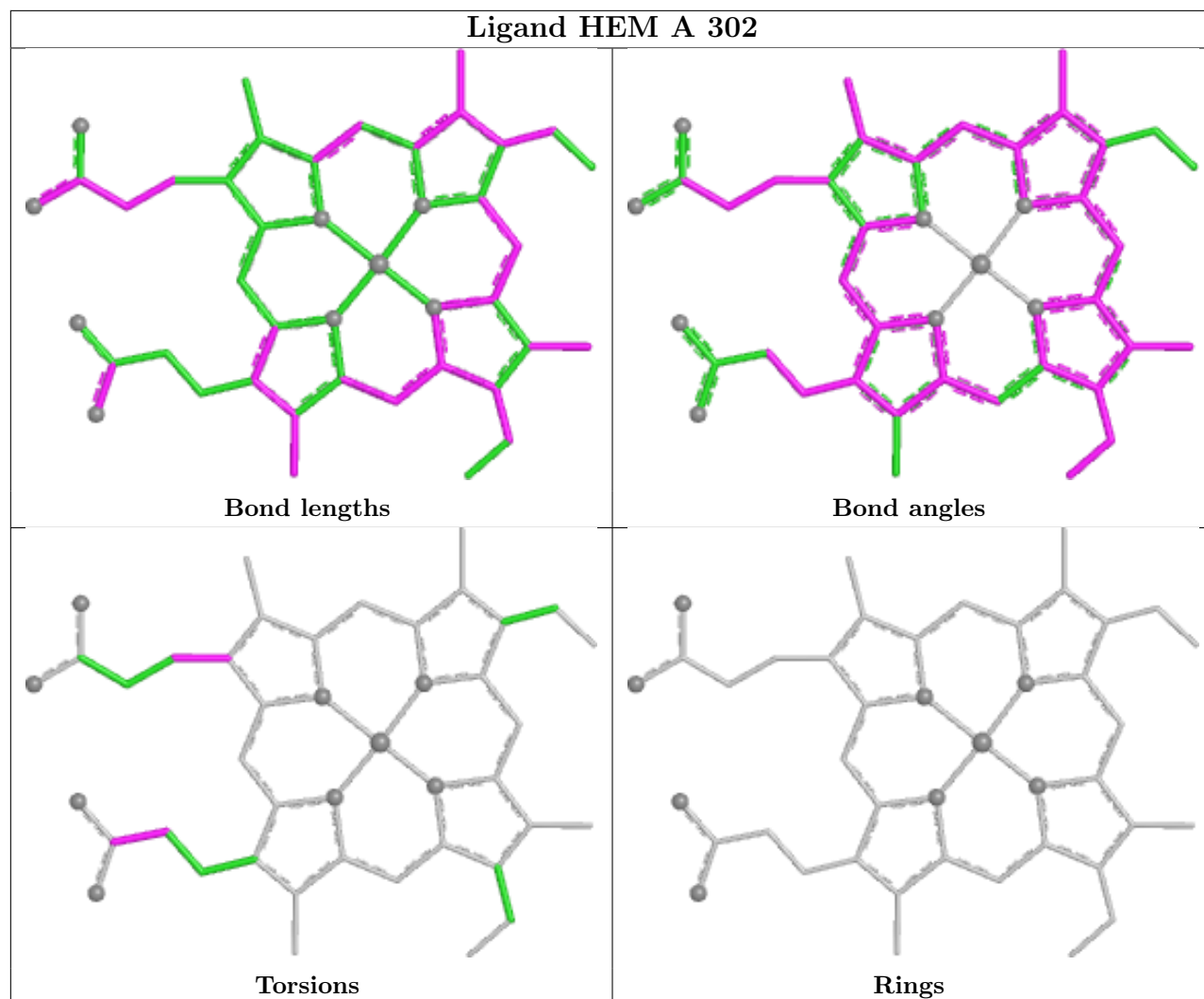


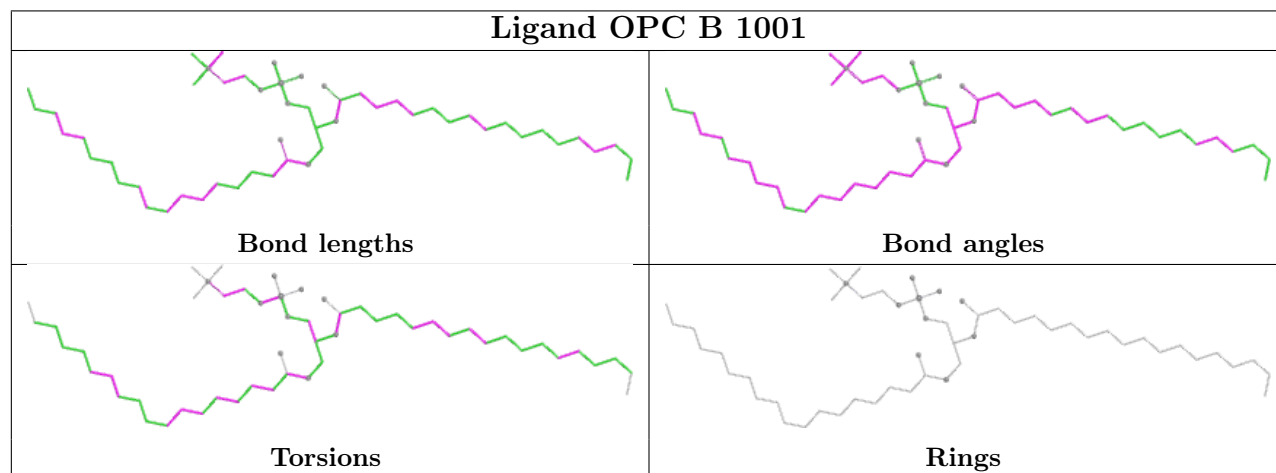
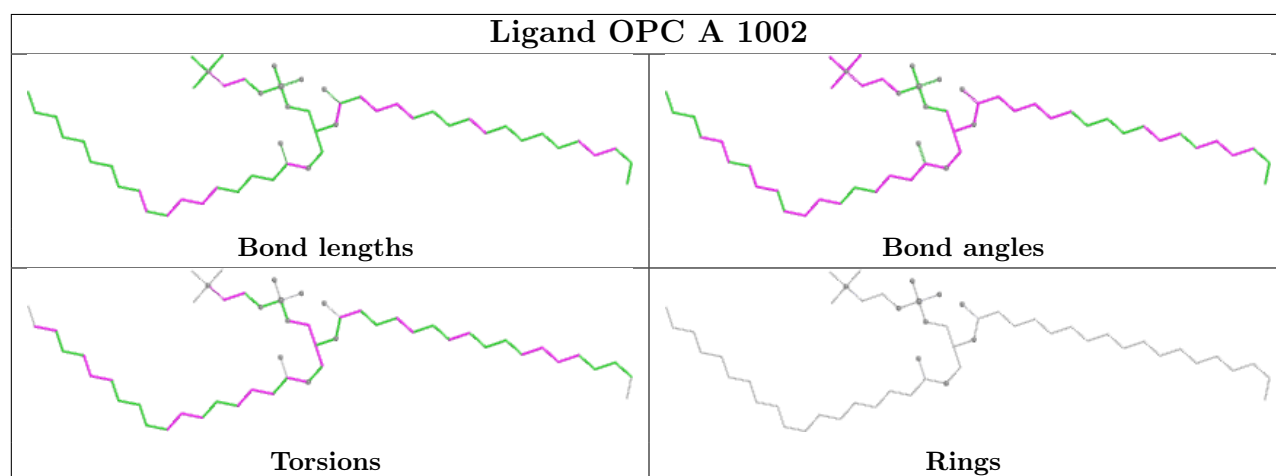
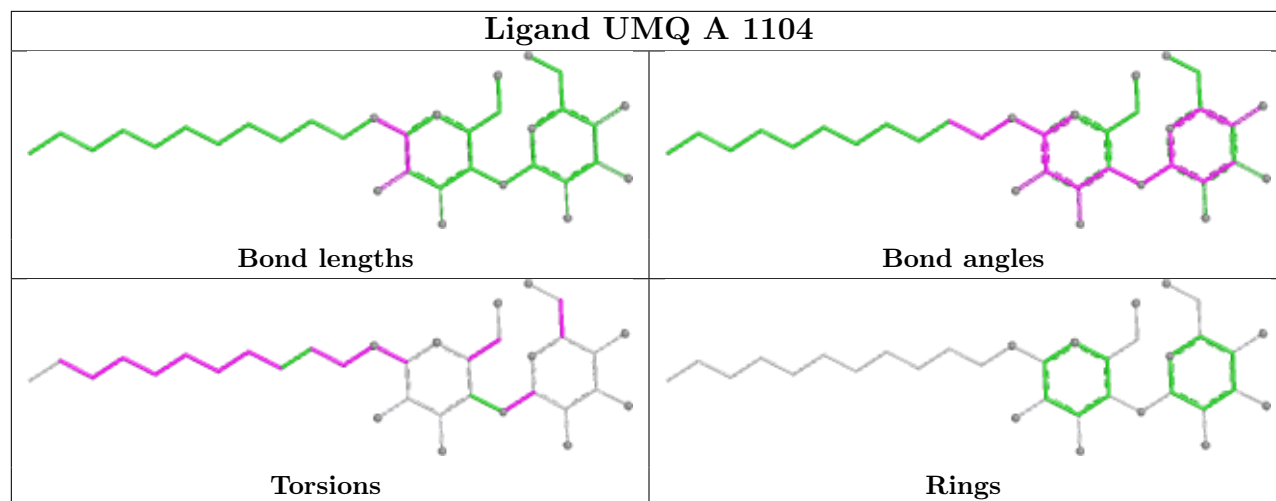
Torsions



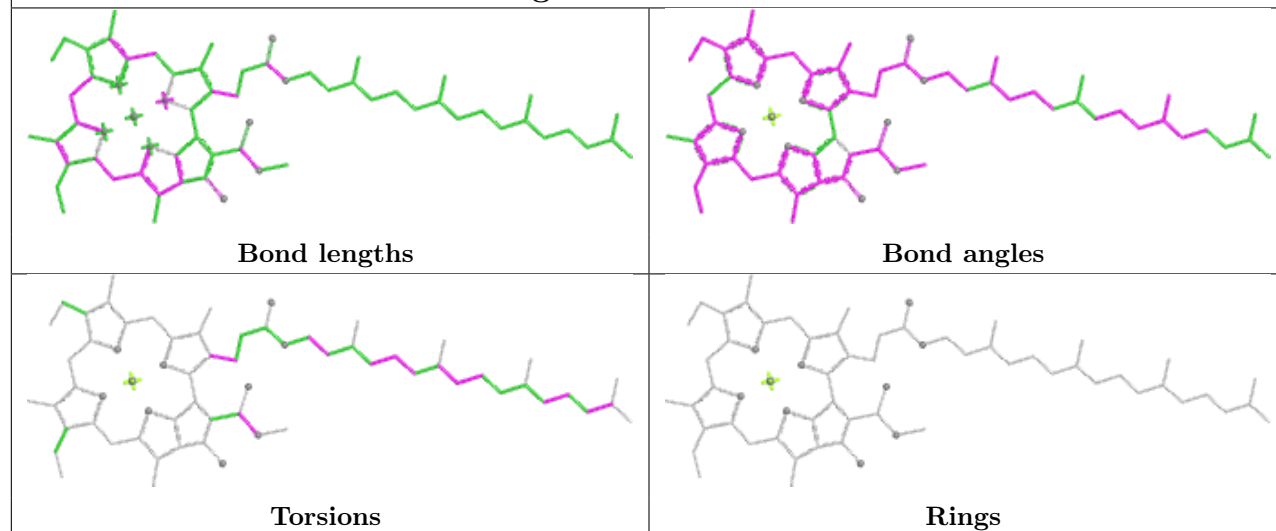
Rings



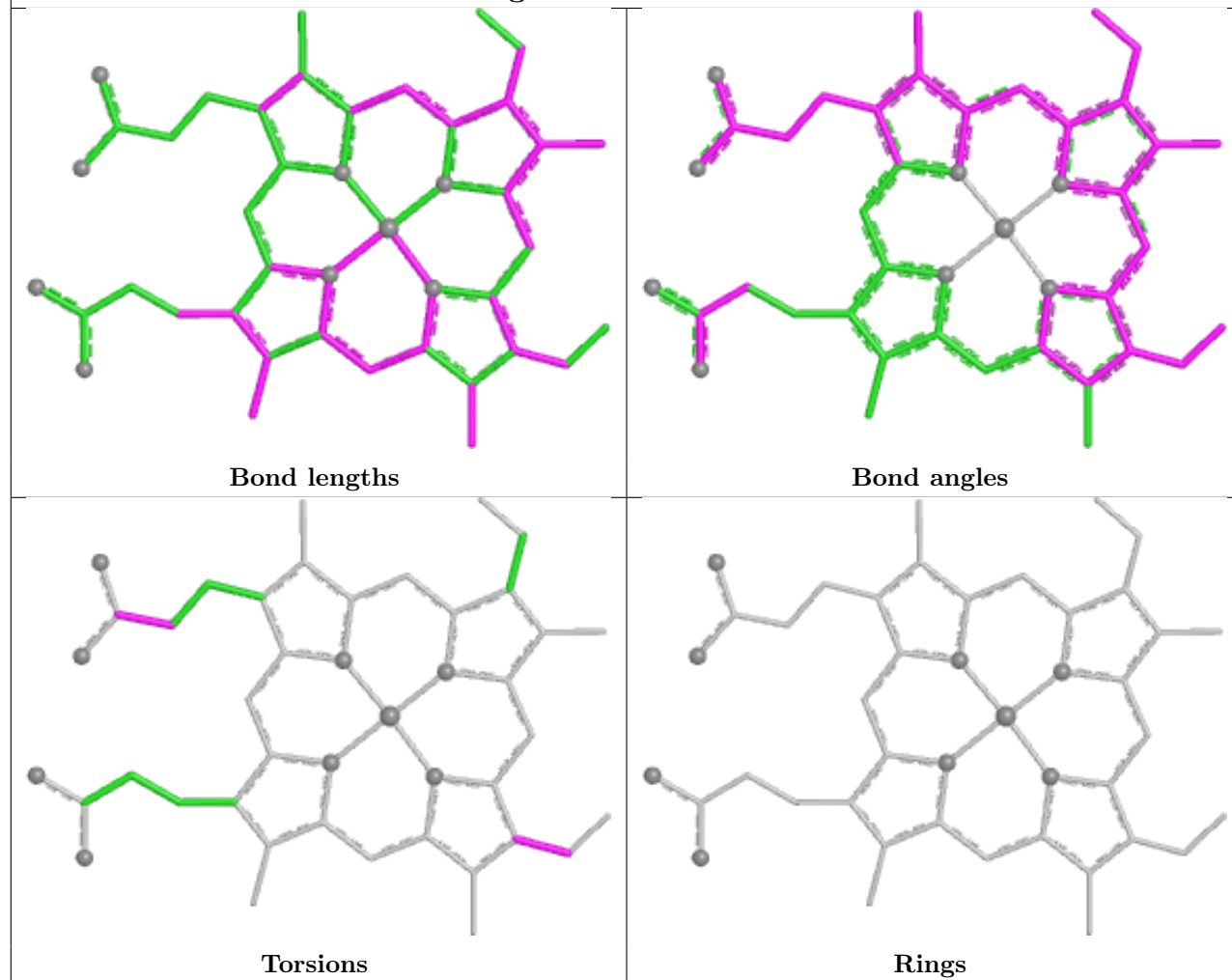




Ligand CLA B 201



Ligand HEM C 301



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	215/215 (100%)	-0.54	1 (0%) 87 66	4, 22, 60, 162	0
2	B	160/160 (100%)	-0.12	5 (3%) 51 28	9, 41, 93, 133	0
3	C	288/289 (99%)	1.06	63 (21%) 2 2	2, 47, 145, 170	1 (0%)
4	D	166/179 (92%)	1.70	48 (28%) 1 1	8, 101, 150, 182	0
5	E	32/32 (100%)	-0.25	1 (3%) 51 28	22, 52, 98, 119	0
6	F	32/35 (91%)	0.10	1 (3%) 51 28	10, 41, 112, 123	0
7	G	37/37 (100%)	-0.06	2 (5%) 31 18	13, 33, 115, 123	0
8	H	29/29 (100%)	-0.40	1 (3%) 48 26	15, 28, 50, 97	0
All	All	959/976 (98%)	0.45	122 (12%) 8 6	2, 42, 139, 182	1 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	145	PRO	13.5
4	D	144	ALA	13.4
4	D	179	VAL	11.9
4	D	177	TRP	9.5
4	D	143	PRO	8.7

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 ⓘ

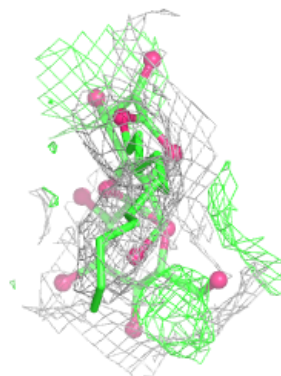
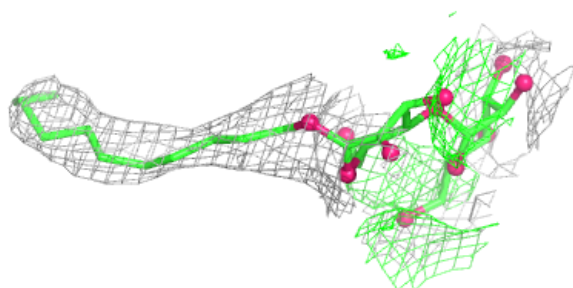
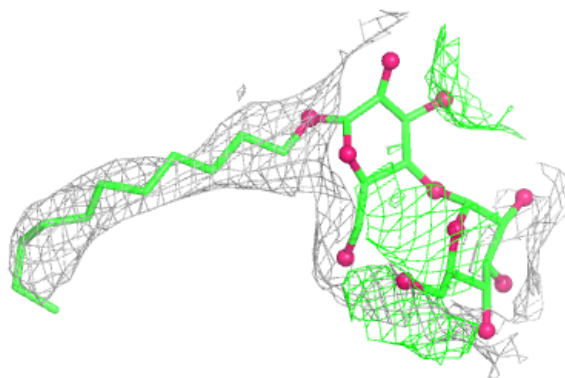
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	UMQ	C	1101	34/34	0.79	0.22	4,86,151,160	0
13	UMQ	A	1104	34/34	0.86	0.19	23,131,208,216	0
17	SQD	D	201	54/54	0.86	0.26	39,165,201,204	0
12	OPC	A	1002	54/55	0.87	0.22	2,64,206,220	0
18	BCR	G	101	40/40	0.89	0.20	2,49,145,149	0
13	UMQ	A	1102	34/34	0.91	0.18	31,112,145,149	0
14	QNO	A	501	21/21	0.92	0.18	45,63,95,120	0
12	OPC	B	1001	54/55	0.93	0.18	8,70,138,157	0
13	UMQ	A	1103	34/34	0.94	0.11	40,101,144,155	0
15	CLA	B	201	65/65	0.97	0.10	12,42,72,111	0
16	FES	D	200	4/4	0.97	0.09	89,90,95,104	0
11	HEC	A	303	43/43	0.98	0.07	2,35,56,61	0
9	CD	B	161	1/1	0.98	0.10	161,161,161,161	0
10	HEM	A	302	43/43	0.98	0.07	2,8,43,49	0
10	HEM	C	301	43/43	0.98	0.07	2,33,74,95	0
10	HEM	A	301	43/43	0.99	0.07	2,13,37,60	0
9	CD	A	216	1/1	1.00	0.03	47,47,47,47	0

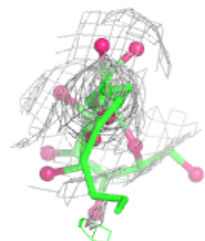
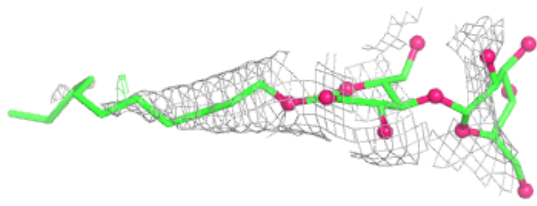
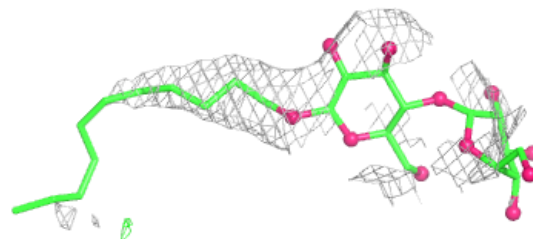
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMQ C 1101:

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

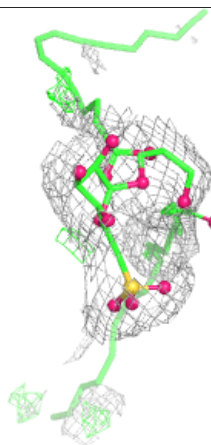
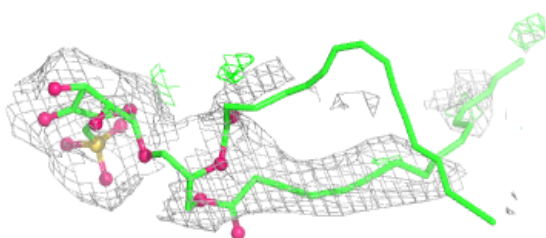
**Electron density around UMQ A 1104:**

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



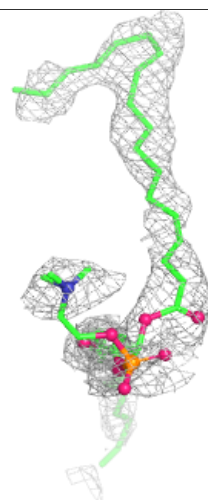
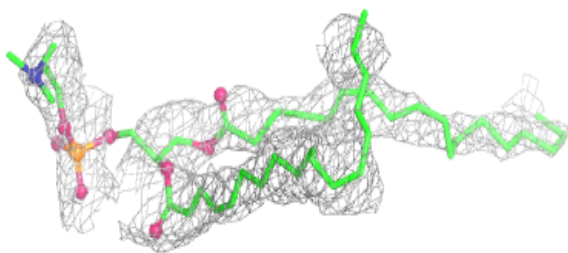
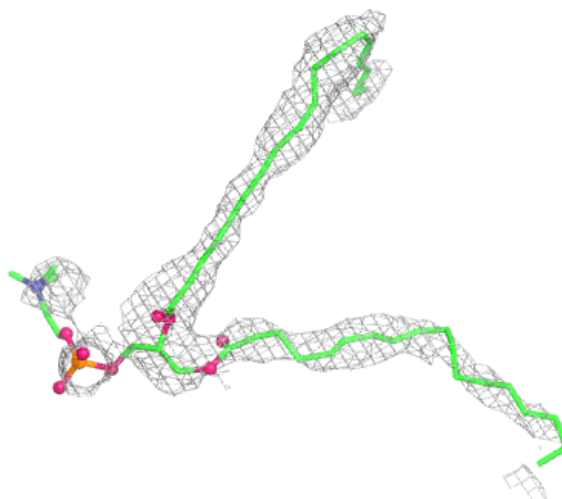
Electron density around SQD D 201:

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



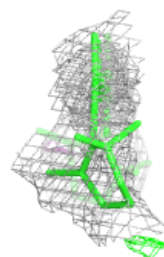
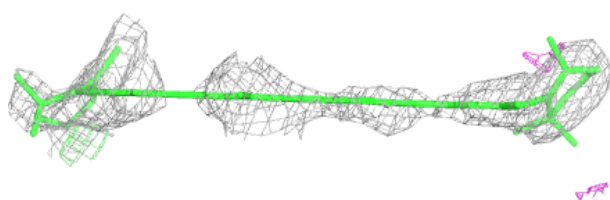
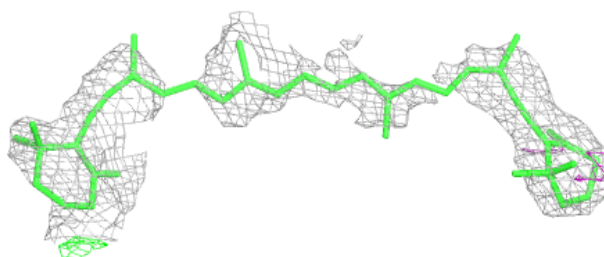
Electron density around OPC A 1002:

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

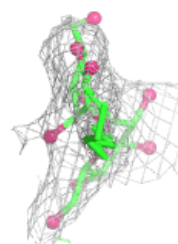
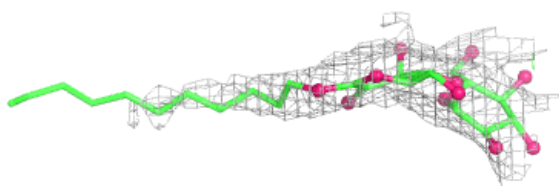
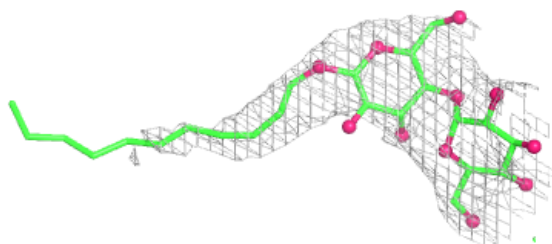


Electron density around BCR G 101:

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and green (positive)

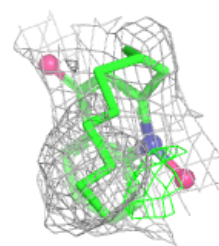
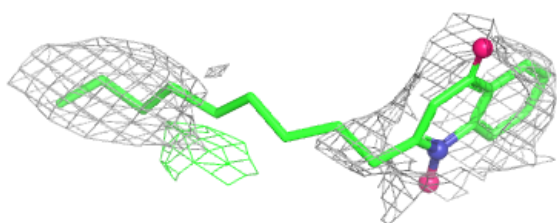
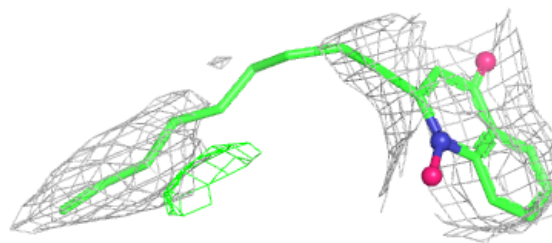
**Electron density around UMQ A 1102:**

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

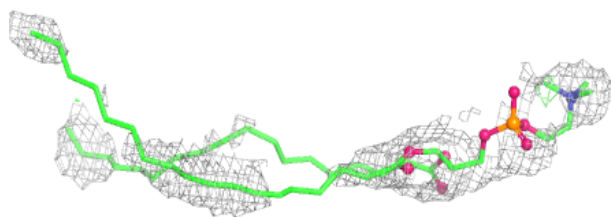
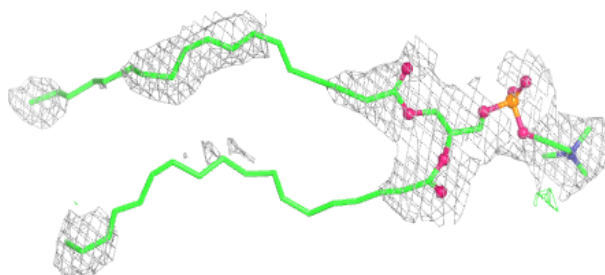


Electron density around QNO A 501:

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

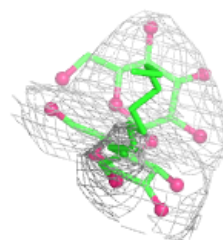
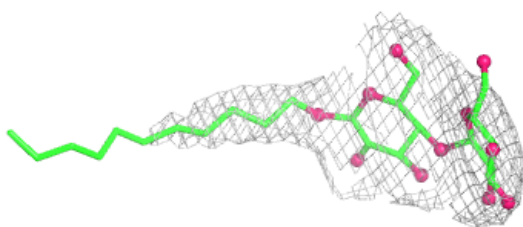
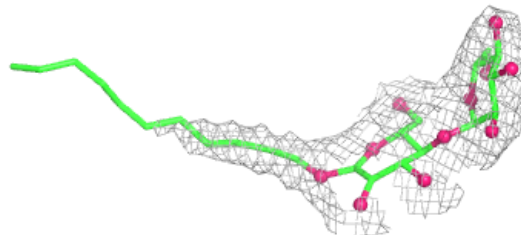
**Electron density around OPC B 1001:**

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

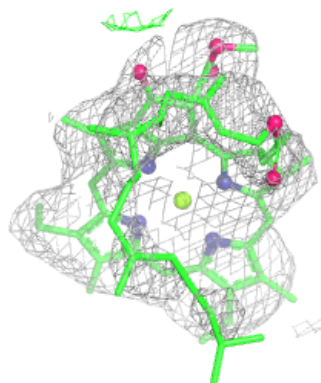
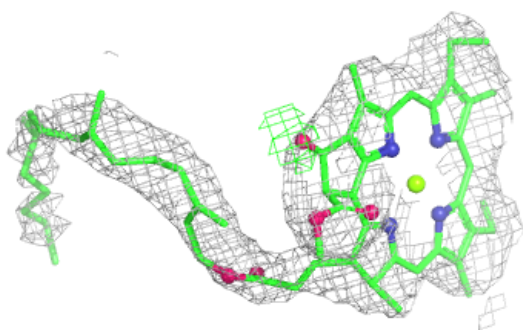
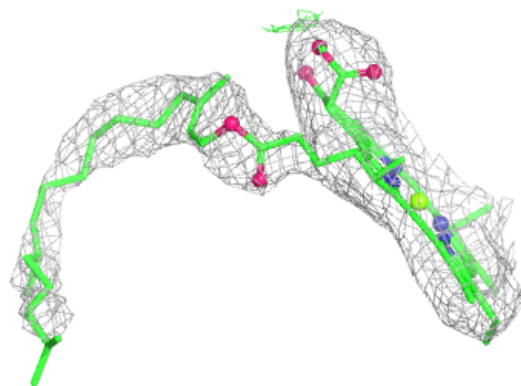


Electron density around UMQ A 1103:

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

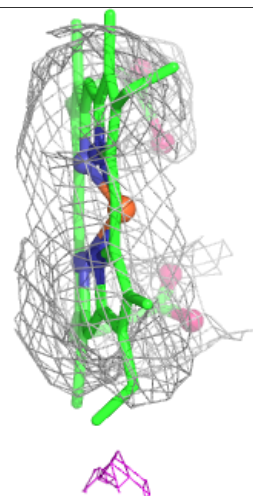
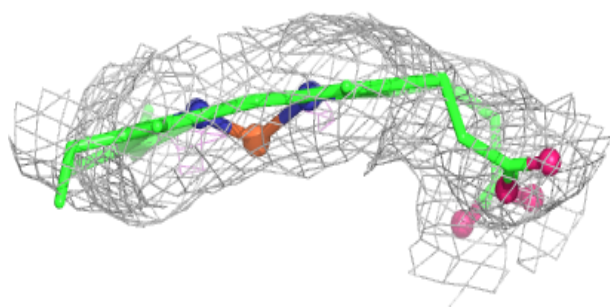
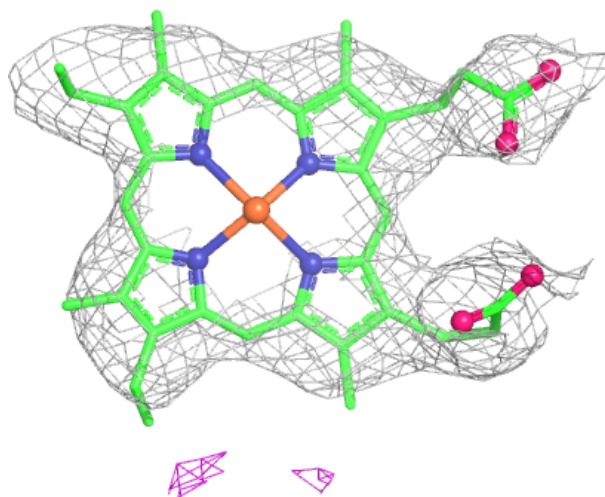
**Electron density around CLA B 201:**

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



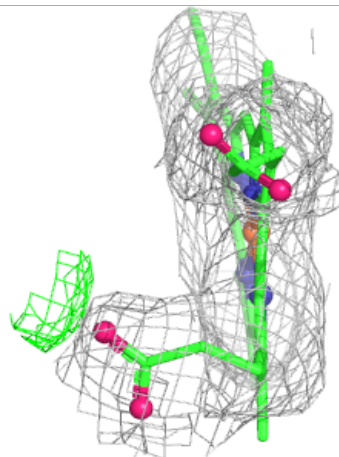
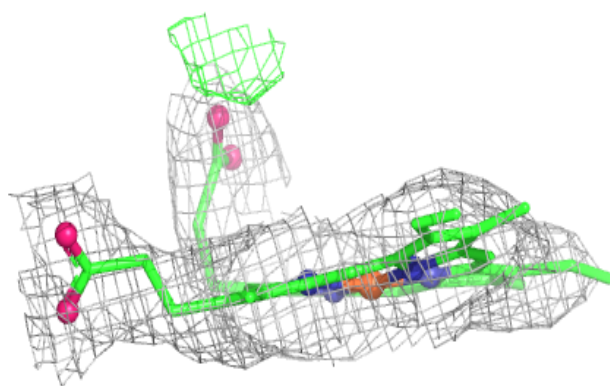
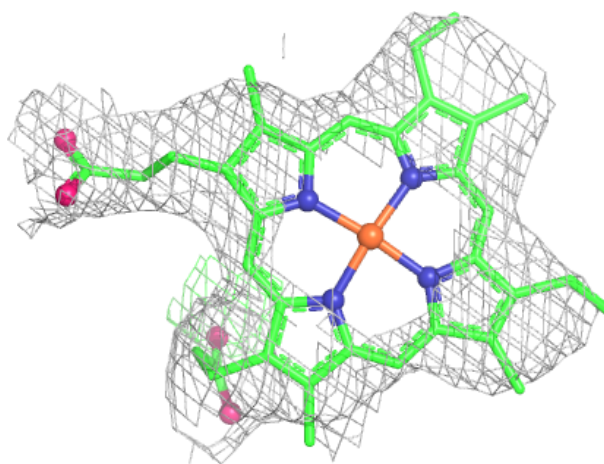
Electron density around HEC A 303:

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



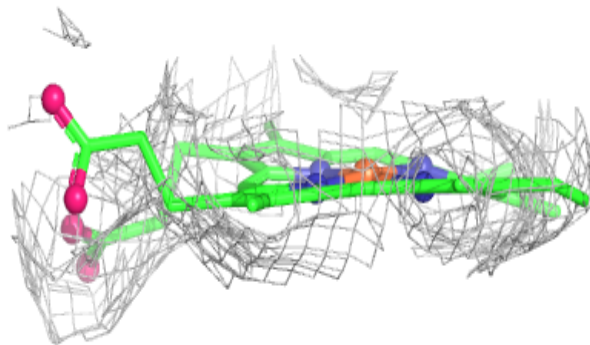
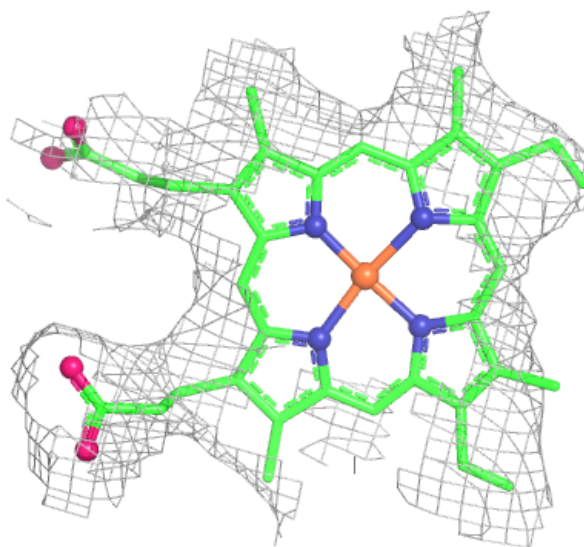
Electron density around HEM A 302:

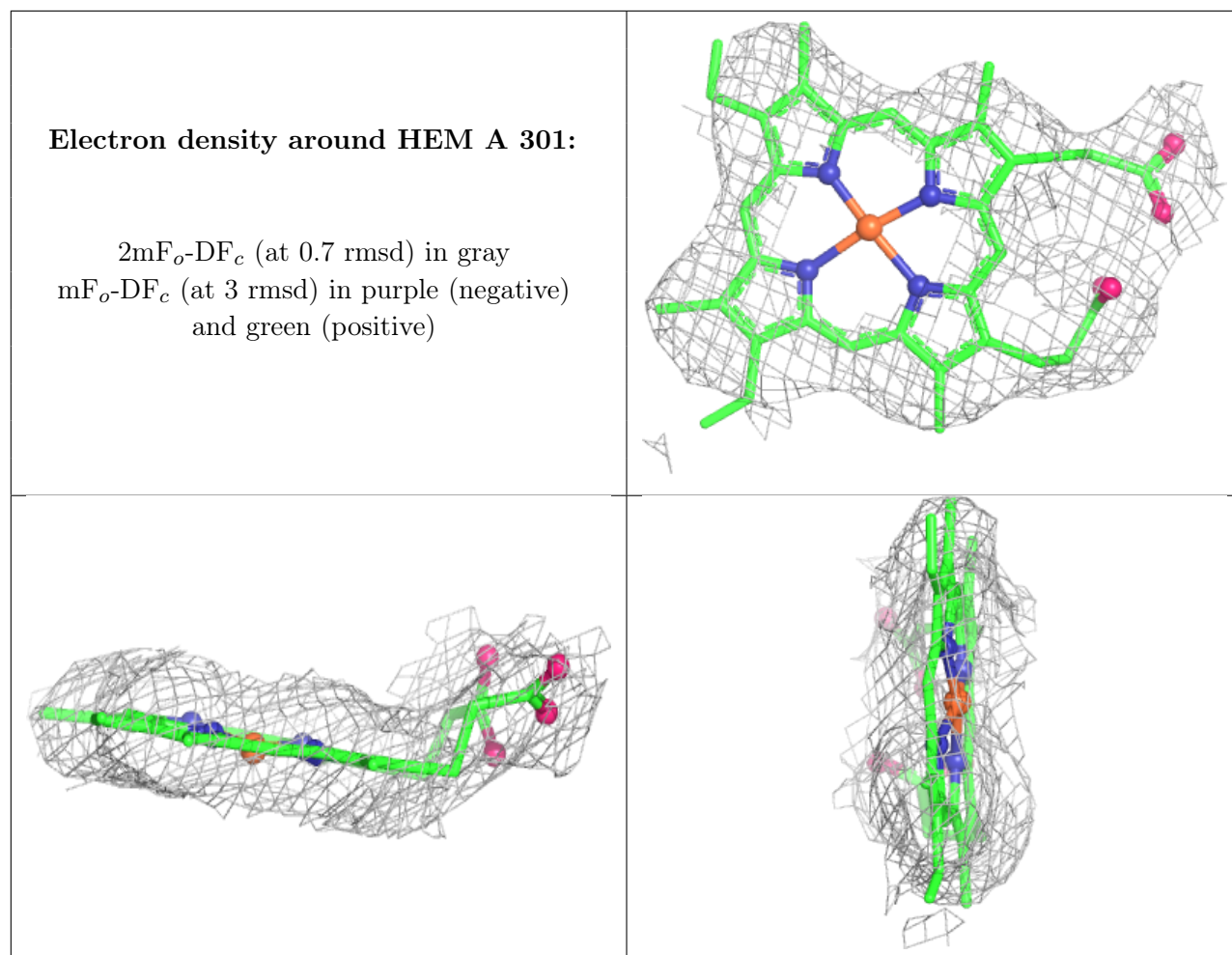
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 301:

$2mF_o-DF_c$ (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.