



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 2E74 / pdb_00002e74
Title : Crystal Structure of the Cytochrome b6f Complex from M.laminosus
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
Resolution : 3.00 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:

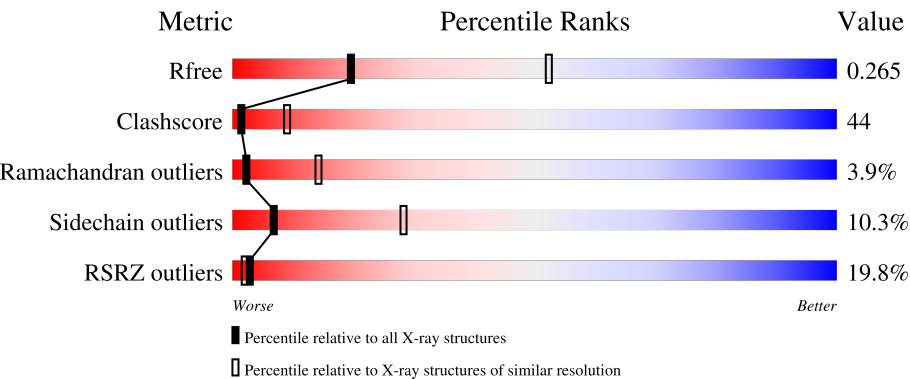
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	56%34%9%
2	B	160	40%48%11%
3	C	289	30%42%47%11%
4	D	179	48%37%49%6%7%
5	E	32	6%38%53%9%

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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
12	UMQ	A	1101	X	-	-	-
12	UMQ	A	1102	X	-	-	-
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
13	CLA	B	201	X	-	-	-
14	OPC	H	1002	-	-	X	-
15	FES	D	200	-	-	X	-
16	SQD	D	201	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 8025 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			

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

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

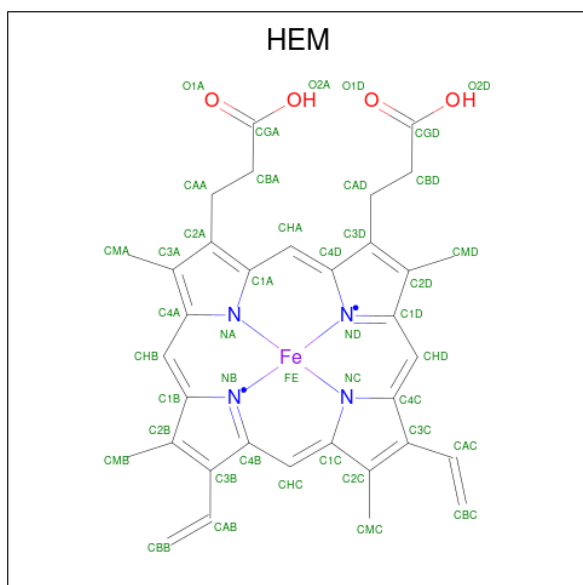
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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

- Molecule 9 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including two hydroxyethyl groups (O1A, OH, O2A, OH, O1D, OH, O2D) and several methyl and ethyl groups (CMA, C3A, C4A, C3B, C4B, C2B, C1B, C2C, C3C, C4C, C1C, C2D, C3D, C4D, C1D, C2E, C3E, C4E, C1E, C2F, C3F, C4F, C1F, C2G, C3G, C4G, C1G, C2H, C3H, C4H, C1H, C2I, C3I, C4I, C1I, C2J, C3J, C4J, C1J, C2K, C3K, C4K, C1K, C2L, C3L, C4L, C1L, C2M, C3M, C4M, C1M, C2N, C3N, C4N, C1N, C2O, C3O, C4O, C1O, C2P, C3P, C4P, C1P, C2Q, C3Q, C4Q, C1Q, C2R, C3R, C4R, C1R, C2S, C3S, C4S, C1S, C2T, C3T, C4T, C1T, C2U, C3U, C4U, C1U, C2V, C3V, C4V, C1V, C2W, C3W, C4W, C1W, C2X, C3X, C4X, C1X, C2Y, C3Y, C4Y, C1Y, C2Z, C3Z, C4Z, C1Z, C2AA, C3AA, C4AA, C1AA, C2AB, C3AB, C4AB, C1AB, C2AC, C3AC, C4AC, C1AC, C2AD, C3AD, C4AD, C1AD, C2AE, C3AE, C4AE, C1AE, C2AF, C3AF, C4AF, C1AF, C2AG, C3AG, C4AG, C1AG, C2AH, C3AH, C4AH, C1AH, C2AI, C3AI, C4AI, C1AI, C2AJ, C3AJ, C4AJ, C1AJ, C2AK, C3AK, C4AK, C1AK, C2AL, C3AL, C4AL, C1AL, C2AM, C3AM, C4AM, C1AM, C2AN, C3AN, C4AN, C1AN, C2AO, C3AO, C4AO, C1AO, C2AP, C3AP, C4AP, C1AP, C2AQ, C3AQ, C4AQ, C1AQ, C2AR, C3AR, C4AR, C1AR, C2AS, C3AS, C4AS, C1AS, C2AT, C3AT, C4AT, C1AT, C2AU, C3AU, C4AU, C1AU, C2AV, C3AV, C4AV, C1AV, C2AW, C3AW, C4AW, C1AW, C2AX, C3AX, C4AX, C1AX, C2AY, C3AY, C4AY, C1AY, C2AZ, C3AZ, C4AZ, C1AZ, C2BA, C3BA, C4BA, C1BA, C2BB, C3BB, C4BB, C1BB, C2BC, C3BC, C4BC, C1BC, C2BD, C3BD, C4BD, C1BD, C2BE, C3BE, C4BE, C1BE, C2BF, C3BF, C4BF, C1BF, C2BG, C3BG, C4BG, C1BG, C2BH, C3BH, C4BH, C1BH, C2BI, C3BI, C4BI, C1BI, C2BJ, C3BJ, C4BJ, C1BJ, C2BK, C3BK, C4BK, C1BK, C2BL, C3BL, C4BL, C1BL, C2BM, C3BM, C4BM, C1BM, C2BN, C3BN, C4BN, C1BN, C2BO, C3BO, C4BO, C1BO, C2BP, C3BP, C4BP, C1BP, C2BQ, C3BQ, C4BQ, C1BQ, C2BR, C3BR, C4BR, C1BR, C2BS, C3BS, C4BS, C1BS, C2BT, C3BT, C4BT, C1BT, C2BU, C3BU, C4BU, C1BU, C2BV, C3BV, C4BV, C1BV, C2BW, C3BW, C4BW, C1BW, C2BX, C3BX, C4BX, C1BX, C2BY, C3BY, C4BY, C1BY, C2BZ, C3BZ, C4BZ, C1BZ, C2CA, C3CA, C4CA, C1CA, C2CB, C3CB, C4CB, C1CB, C2CC, C3CC, C4CC, C1CC, C2CD, 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C1GX, C2GY, C3GY, C4GY, C1GY, C2GZ, C3GZ, C4GZ, C1GZ, C2HA, C3HA, C4HA, C1HA, C2HB, C3HB, C4HB, C1HB, C2HC, C3HC, C4HC, C1HC, C2HD, C3HD, C4HD, C1HD, C2HE, C3HE, C4HE, C1HE, C2HF, C3HF, C4HF, C1HF, C2HG, C3HG, C4HG, C1HG, C2HH, C3HH, C4HH, C1HH, C2HI, C3HI, C4HI, C1HI, C2HJ, C3HJ, C4HJ, C1HJ, C2HK, C3HK, C4HK, C1HK, C2HL, C3HL, C4HL, C1HL, C2HM, C3HM, C4HM, C1HM, C2HN, C3HN, C4HN, C1HN, C2HO, C3HO, C4HO, C1HO, C2HP, C3HP, C4HP, C1HP, C2HQ, C3HQ, C4HQ, C1HQ, C2HR, C3HR, C4HR, C1HR, C2HS, C3HS, C4HS, C1HS, C2HT, C3HT, C4HT, C1HT, C2HU, C3HU, C4HU, C1HU, C2HV, C3HV, C4HV, C1HV, C2HW, C3HW, C4HW, C1HW, C2HX, C3HX, C4HX, C1HX, C2HY, C3HY, C4HY, C1HY, C2HZ, C3HZ, C4HZ, C1HZ, C2IA, C3IA, C4IA, C1IA, C2IB, C3IB, C4IB, C1IB, C2IC, C3IC, C4IC, C1IC, C2ID, C3ID, C4ID, C1ID, C2IE, C3IE, C4IE, C1IE, C2IF, C3IF, C4IF, C1IF, C2IG, C3IG, C4IG, C1IG, C2IH, C3IH, C4IH, C1IH, C2II, C3II, C4II, C1II, C2IJ

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

-
- The chemical structure of UMQ (1-UMC) is shown. It features a long side chain (C1-C10) and a complex sugar moiety (C11-C20) with multiple hydroxyl groups (OH) and a methyl group (CH3). The side chain is labeled C1 through C10, and the sugar moiety is labeled C11 through C20. The structure is a complex molecule with multiple stereocenters and functional groups.

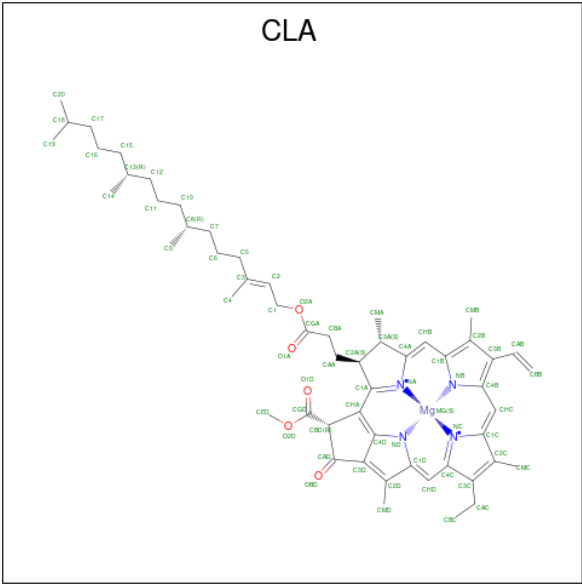
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		

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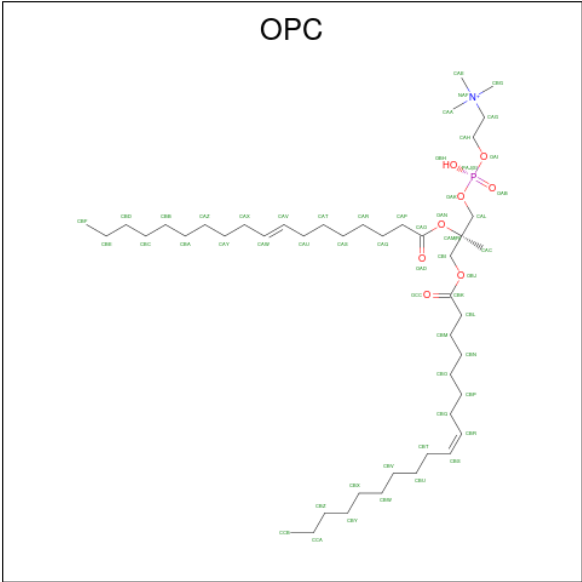
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



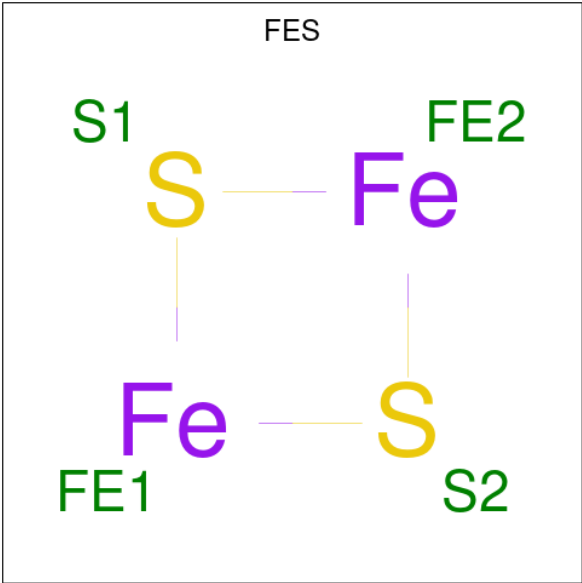
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 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: C₄₅H₈₇NO₈P).



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

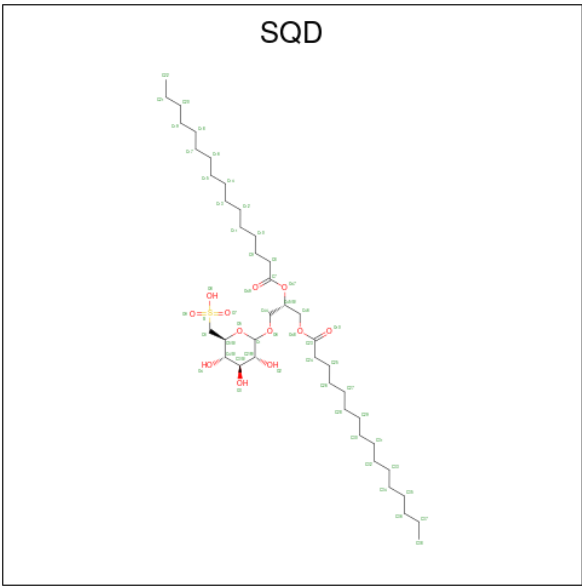
- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

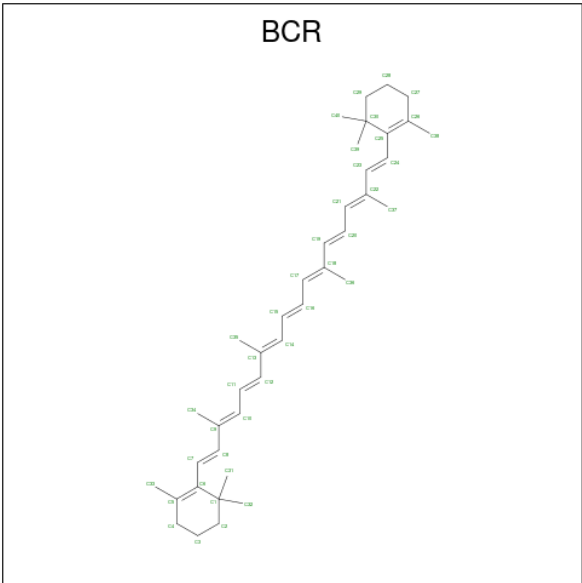
- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

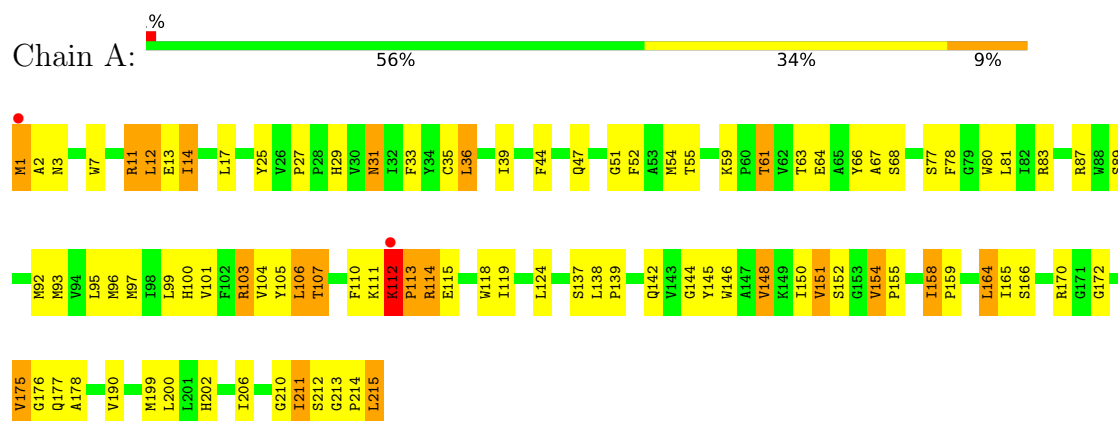
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	2	Total 2	O 2	0	0
18	B	2	Total 2	O 2	0	0
18	C	1	Total 1	O 1	0	0

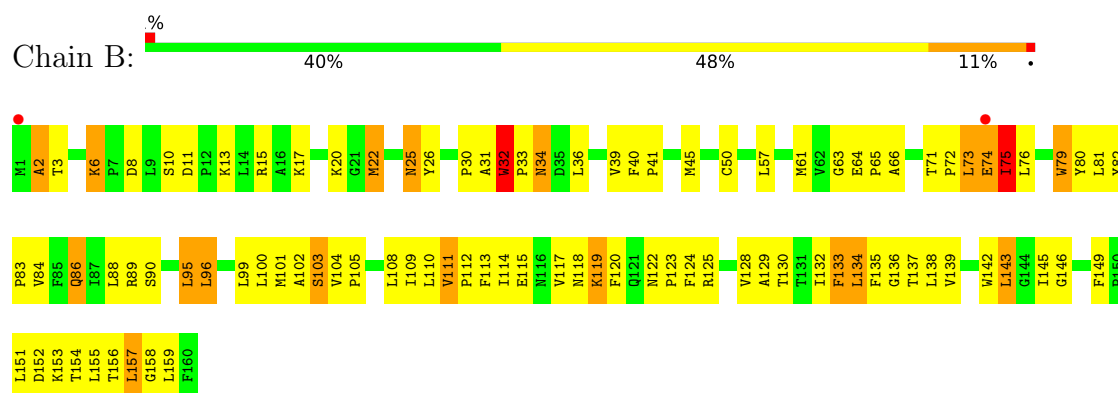
3 Residue-property plots [i](#)

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.

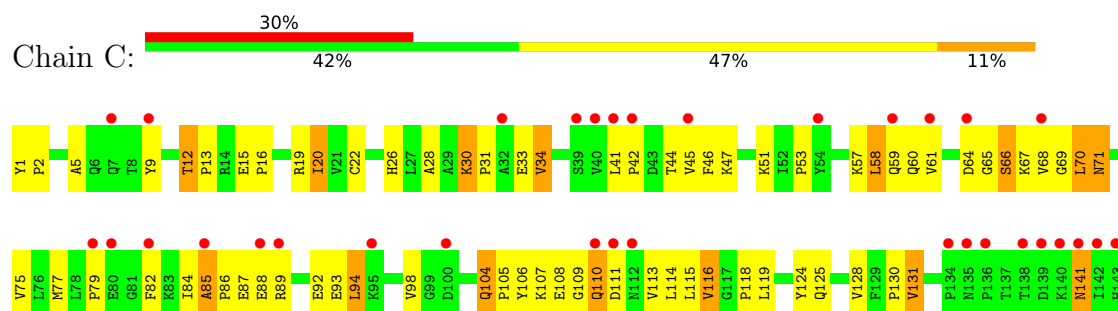
• Molecule 1: Cytochrome b6

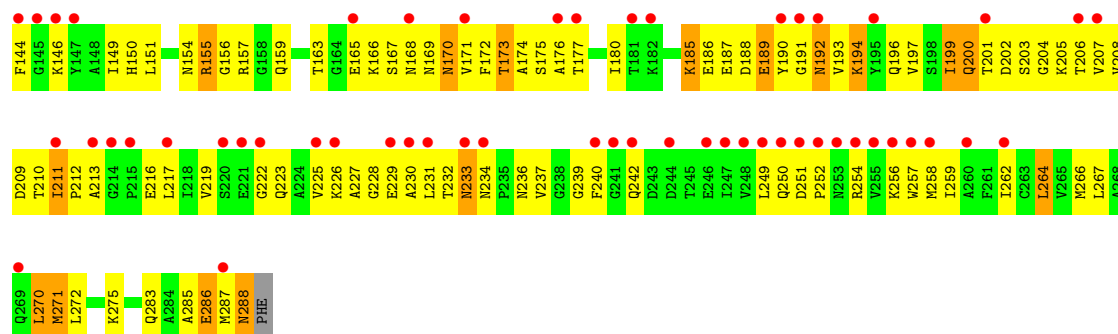


• Molecule 2: Cytochrome b6-f complex subunit 4

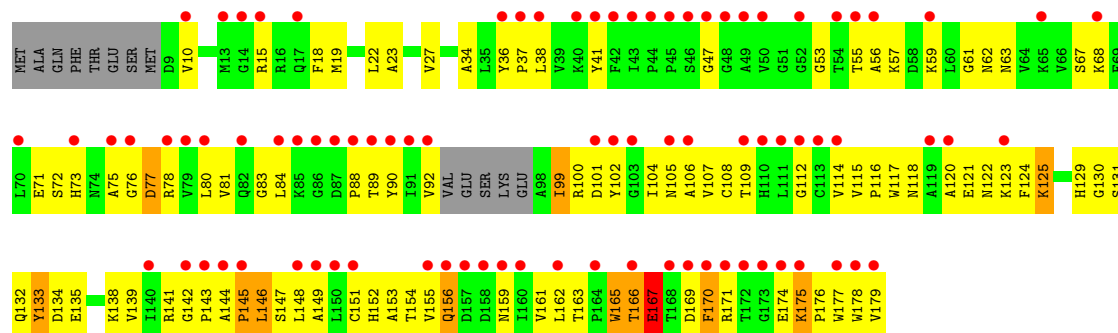


• Molecule 3: Apocytochrome f

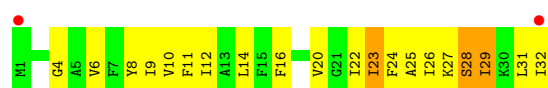




• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



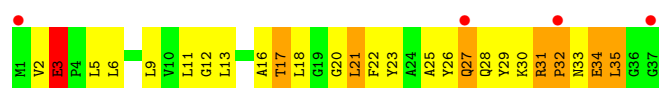
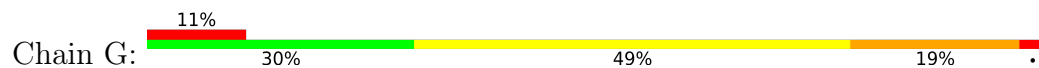
• Molecule 5: Cytochrome b6-f complex subunit 6



• 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	158.34Å 158.34Å 361.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.30 – 3.00 39.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.30-3.00) 99.6 (39.30-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.268 0.219 , 0.265	Depositor DCC
R_{free} test set	2740 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8025	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: CD, SQD, BCR, FES, HEC, HEM, CLA, UMQ, OPC

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	1.01	3/1763 (0.2%)	1.21	11/2405 (0.5%)
2	B	0.90	0/1288	1.19	4/1765 (0.2%)
3	C	0.71	0/2264	1.05	12/3082 (0.4%)
4	D	0.60	0/1292	0.83	0/1760
5	E	0.73	0/253	1.15	2/340 (0.6%)
6	F	0.79	0/246	1.08	0/331
7	G	0.83	0/289	1.14	2/391 (0.5%)
8	H	0.98	0/236	1.11	1/323 (0.3%)
All	All	0.82	3/7631 (0.0%)	1.09	32/10397 (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
2	B	0	1
8	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	VAL	CA-CB	-6.17	1.48	1.54
1	A	67	ALA	CA-CB	-5.67	1.44	1.53
1	A	113	PRO	CB-CG	5.15	1.75	1.49

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	VAL	CA-C-N	-7.82	111.74	119.64
2	B	111	VAL	C-N-CA	-7.82	111.74	119.64
1	A	158	ILE	CA-C-N	7.81	129.60	119.84
1	A	158	ILE	C-N-CA	7.81	129.60	119.84
7	G	3	GLU	CA-C-N	7.20	126.73	119.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide
8	H	27	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1711	0	1736	145	1
2	B	1249	0	1308	143	0
3	C	2216	0	2232	203	2
4	D	1260	0	1243	125	0
5	E	248	0	284	30	0
6	F	242	0	260	27	0
7	G	283	0	289	45	1
8	H	230	0	239	21	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	86	0	60	19	0
11	A	43	0	31	6	0
11	C	43	0	31	6	0
12	A	136	0	164	13	0
13	B	65	0	72	4	0
14	B	54	0	83	2	0
14	H	54	0	83	23	0
15	D	4	0	0	2	0
16	D	54	0	57	11	0
17	G	40	0	52	11	0
18	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	2	0	0	0	0
18	C	1	0	0	0	0
All	All	8025	0	8224	717	2

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 44.

The worst 5 of 717 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)
16:D:201:SQD:C4	16:D:201:SQD:C3	1.85	1.54
1:A:113:PRO:CG	1:A:113:PRO:CB	1.75	1.41
16:D:201:SQD:C4	16:D:201:SQD:C2	2.11	1.27
2:B:151:LEU:O	2:B:154:THR:HG22	1.25	1.25
2:B:151:LEU:O	2:B:154:THR:CG2	1.86	1.23

All (2) 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)
3:C:108:GLU:OE1	7:G:33:ASN:CB[8_565]	1.89	0.31
1:A:112:LYS:CE	3:C:87:GLU:OE1[8_665]	2.14	0.06

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%)	185 (87%)	26 (12%)	2 (1%)	14	48
2	B	158/160 (99%)	126 (80%)	25 (16%)	7 (4%)	2	12
3	C	286/289 (99%)	244 (85%)	31 (11%)	11 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	162/179 (90%)	124 (76%)	28 (17%)	10 (6%)	1	6
5	E	30/32 (94%)	23 (77%)	6 (20%)	1 (3%)	3	17
6	F	30/35 (86%)	25 (83%)	5 (17%)	0	100	100
7	G	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	1
8	H	27/29 (93%)	24 (89%)	2 (7%)	1 (4%)	2	15
All	All	941/976 (96%)	767 (82%)	137 (15%)	37 (4%)	2	14

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
2	B	74	GLU
2	B	125	ARG
3	C	66	SER

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%)	167 (91%)	17 (9%)	8	33
2	B	137/137 (100%)	121 (88%)	16 (12%)	5	23
3	C	242/243 (100%)	219 (90%)	23 (10%)	8	31
4	D	134/146 (92%)	126 (94%)	8 (6%)	17	50
5	E	25/25 (100%)	23 (92%)	2 (8%)	11	38
6	F	24/27 (89%)	17 (71%)	7 (29%)	0	2
7	G	28/28 (100%)	24 (86%)	4 (14%)	3	16
8	H	24/24 (100%)	19 (79%)	5 (21%)	1	7
All	All	798/814 (98%)	716 (90%)	82 (10%)	7	28

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	72	SER
6	F	29	ILE
4	D	133	TYR
5	E	29	ILE
7	G	17	THR

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	82	GLN
3	C	288	ASN
4	D	118	ASN
3	C	59	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
12	UMQ	A	1102	-	35,35,35	1.61	4 (11%)	46,46,46	2.25	11 (23%)
14	OPC	H	1002	-	53,53,54	2.14	14 (26%)	59,61,64	2.30	16 (27%)
12	UMQ	A	1104	-	35,35,35	1.40	3 (8%)	46,46,46	2.08	8 (17%)
13	CLA	B	201	-	69,73,73	1.88	16 (23%)	82,113,113	2.56	27 (32%)
16	SQD	D	201	-	52,54,54	3.24	23 (44%)	62,65,65	4.54	23 (37%)
11	HEC	C	301	3	46,50,50	2.08	9 (19%)	58,82,82	1.56	13 (22%)
17	BCR	G	101	-	41,41,41	2.81	12 (29%)	56,56,56	7.05	17 (30%)
12	UMQ	A	1101	-	35,35,35	1.46	4 (11%)	46,46,46	2.16	9 (19%)
11	HEC	A	303	1	46,50,50	2.07	8 (17%)	58,82,82	1.57	7 (12%)
10	HEM	A	302	1	50,50,50	1.70	9 (18%)	67,82,82	1.24	7 (10%)
15	FES	D	200	4	0,4,4	-	-	-	-	-
14	OPC	B	202	-	53,53,54	2.07	14 (26%)	59,61,64	2.43	13 (22%)
10	HEM	A	301	1	50,50,50	1.81	8 (16%)	67,82,82	1.55	17 (25%)
12	UMQ	A	1103	-	35,35,35	1.50	4 (11%)	46,46,46	2.11	8 (17%)

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
12	UMQ	A	1102	-	2/2/10/10	11/20/60/60	0/2/2/2
14	OPC	H	1002	-	-	26/57/57/60	-
13	CLA	B	201	-	2/2/15/20	16/39/115/115	-
16	SQD	D	201	-	1/1/9/9	28/49/69/69	0/1/1/1
10	HEM	A	302	1	-	3/14/54/54	-
11	HEC	C	301	3	-	8/14/54/54	-
17	BCR	G	101	-	-	9/29/63/63	0/2/2/2
12	UMQ	A	1101	-	2/2/10/10	12/20/60/60	0/2/2/2
11	HEC	A	303	1	-	9/14/54/54	-
12	UMQ	A	1104	-	2/2/10/10	11/20/60/60	0/2/2/2
15	FES	D	200	4	-	-	0/1/1/1
14	OPC	B	202	-	-	22/57/57/60	-
10	HEM	A	301	1	-	5/14/54/54	-
12	UMQ	A	1103	-	2/2/10/10	5/20/60/60	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C4-C3	12.70	1.85	1.52
17	G	101	BCR	C8-C9	-8.96	1.26	1.46
17	G	101	BCR	C23-C22	-8.54	1.27	1.46
10	A	301	HEM	C3D-C2D	7.19	1.52	1.36
10	A	302	HEM	C3D-C2D	6.92	1.51	1.36

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C24-C23-C22	33.77	176.20	126.23
17	G	101	BCR	C7-C8-C9	29.62	170.05	126.23
16	D	201	SQD	C4-C3-C2	-19.42	76.74	110.83
17	G	101	BCR	C23-C24-C25	17.93	174.90	127.00
17	G	101	BCR	C8-C7-C6	17.39	173.47	127.00

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1101	UMQ	C1'
12	A	1101	UMQ	C2'
12	A	1102	UMQ	C1'
12	A	1102	UMQ	C2'
12	A	1103	UMQ	C1'

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	303	HEC	C2B-C3B-CAB-CBB
11	A	303	HEC	C4B-C3B-CAB-CBB
11	A	303	HEC	C4D-C3D-CAD-CBD
11	C	301	HEC	C2B-C3B-CAB-CBB
11	C	301	HEC	C4B-C3B-CAB-CBB

There are no ring outliers.

14 monomers are involved in 94 short contacts:

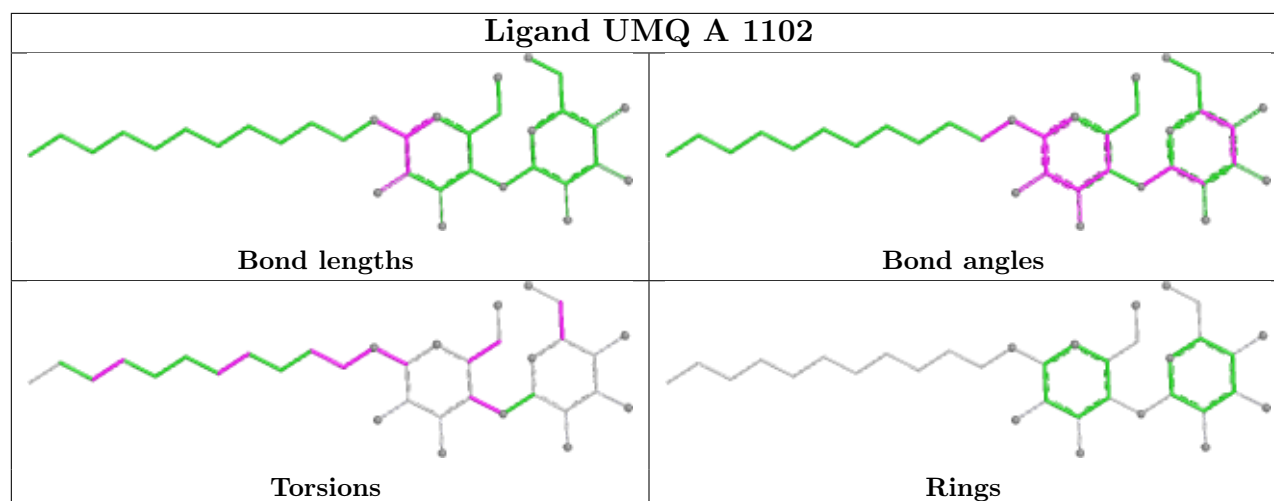
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1102	UMQ	2	0
14	H	1002	OPC	23	0
12	A	1104	UMQ	4	0
13	B	201	CLA	4	0
16	D	201	SQD	11	0

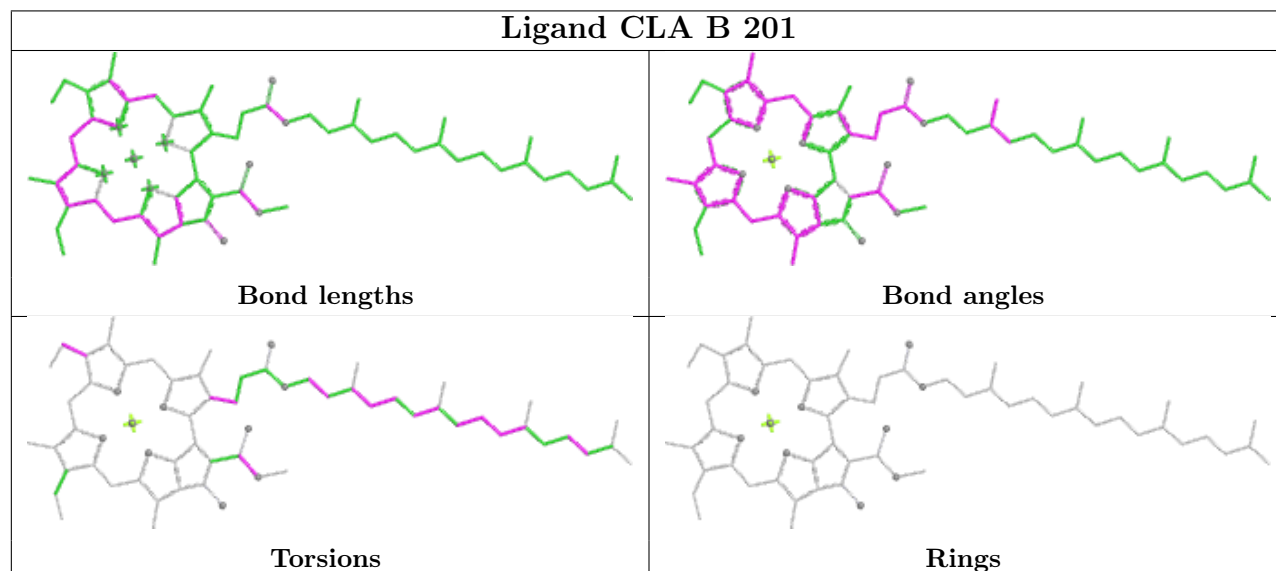
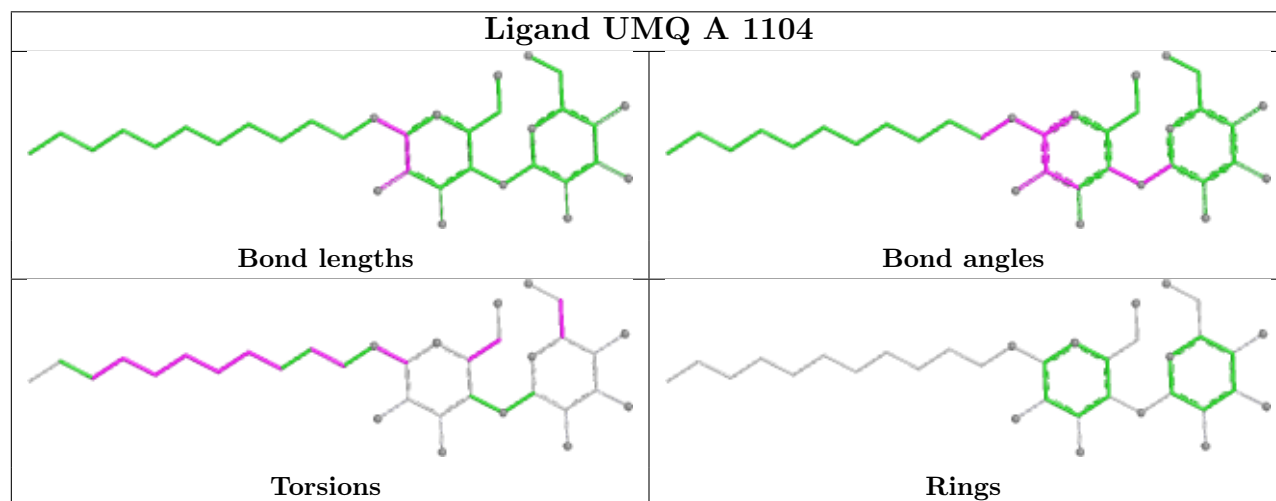
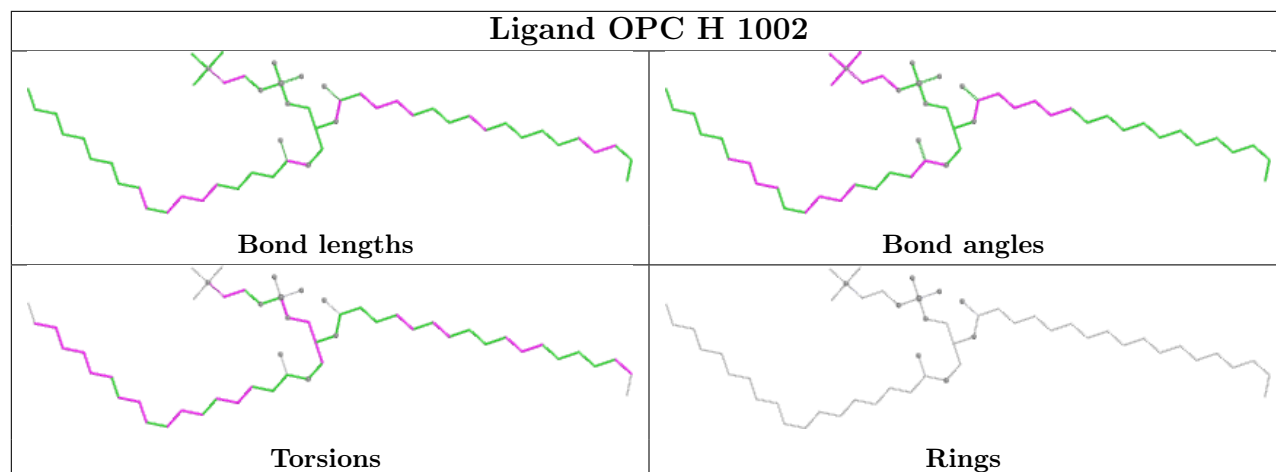
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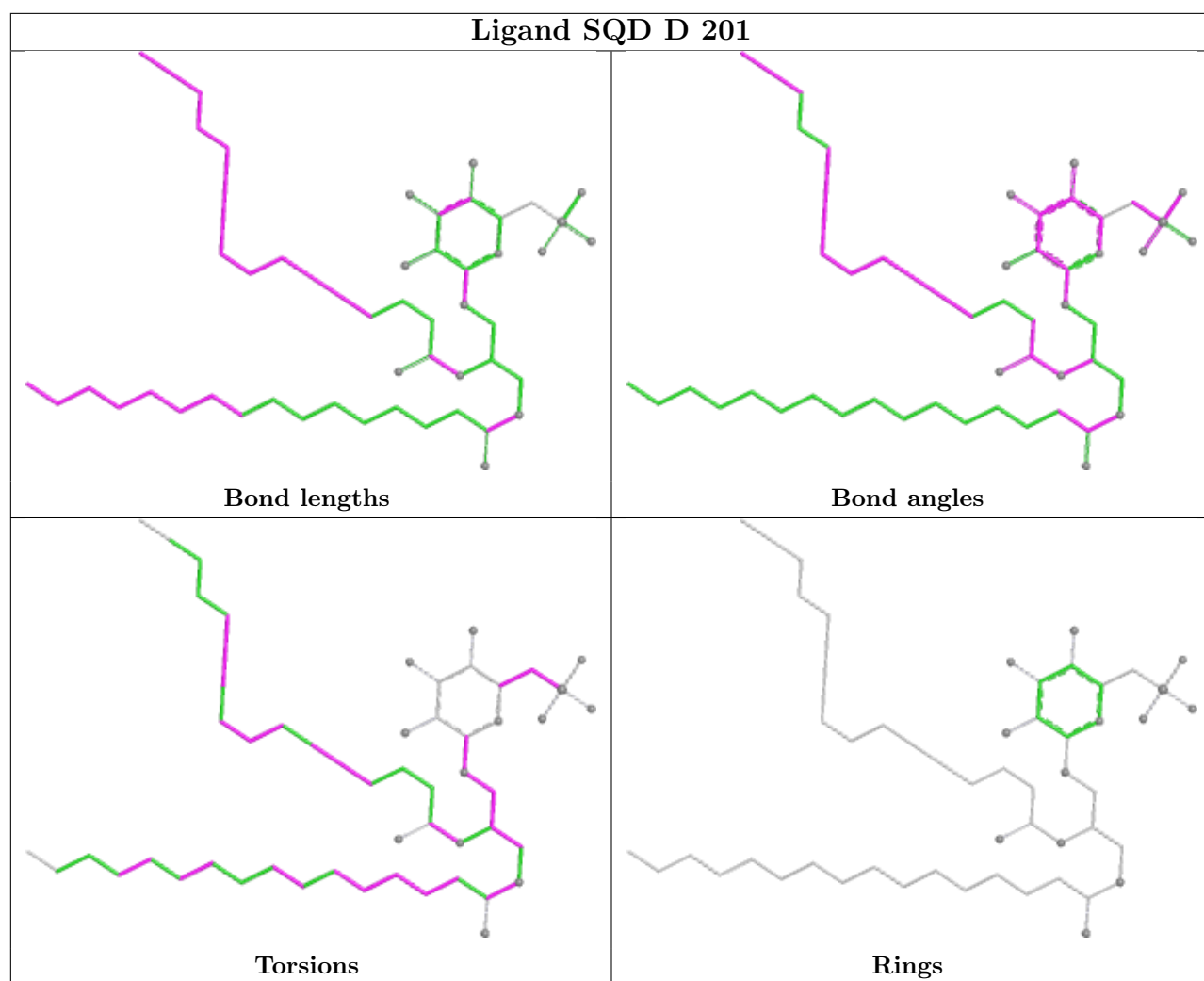
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	301	HEC	6	0
17	G	101	BCR	11	0
12	A	1101	UMQ	6	0
11	A	303	HEC	6	0
10	A	302	HEM	9	0
15	D	200	FES	2	0
14	B	202	OPC	2	0
10	A	301	HEM	10	0
12	A	1103	UMQ	1	0

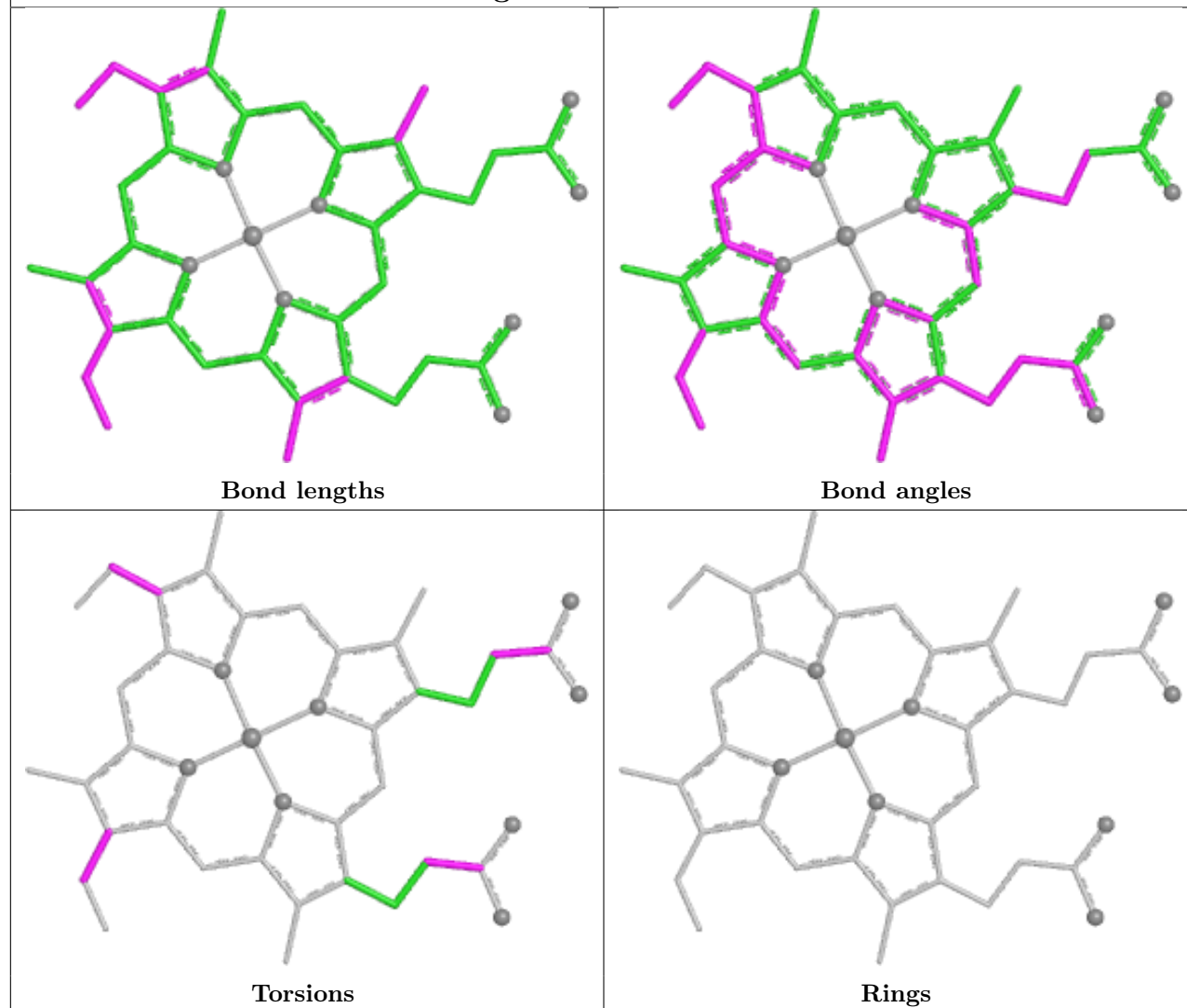
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



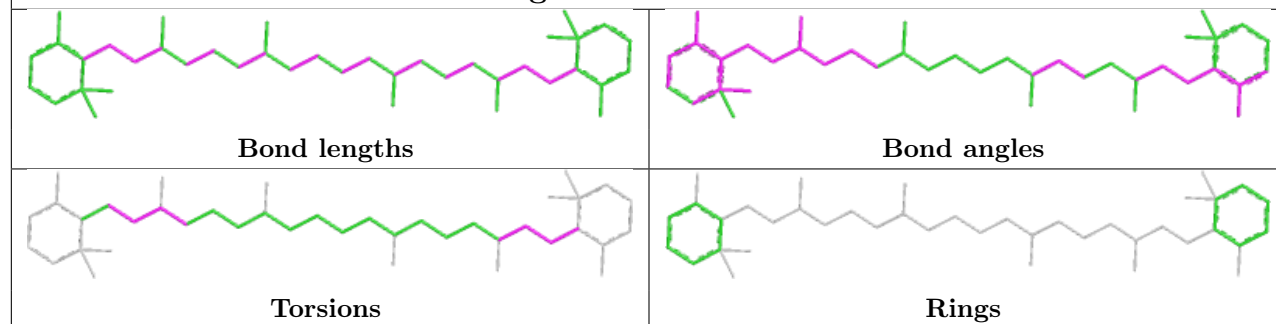




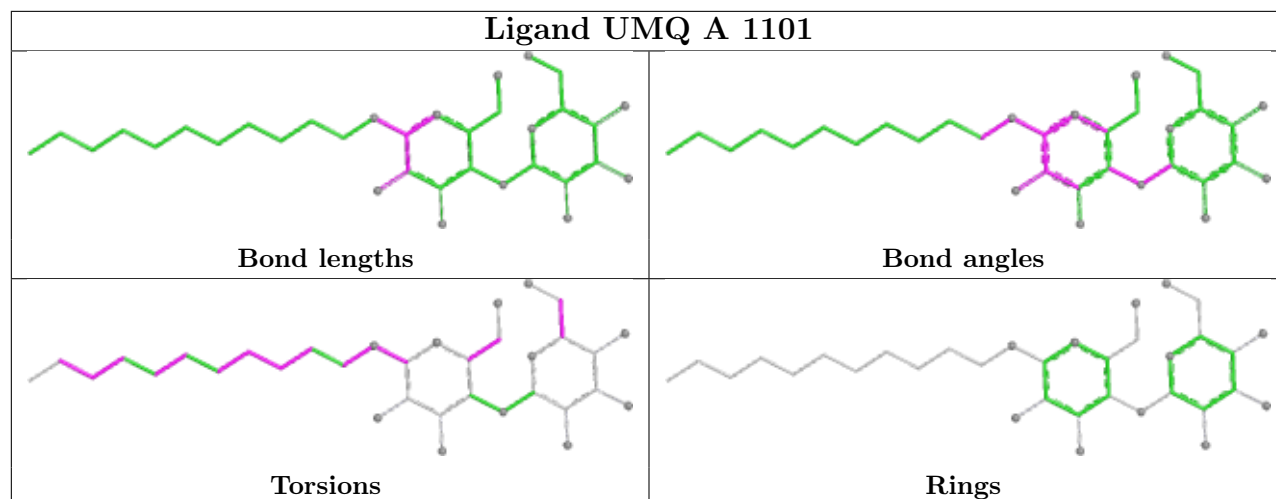
Ligand HEC C 301



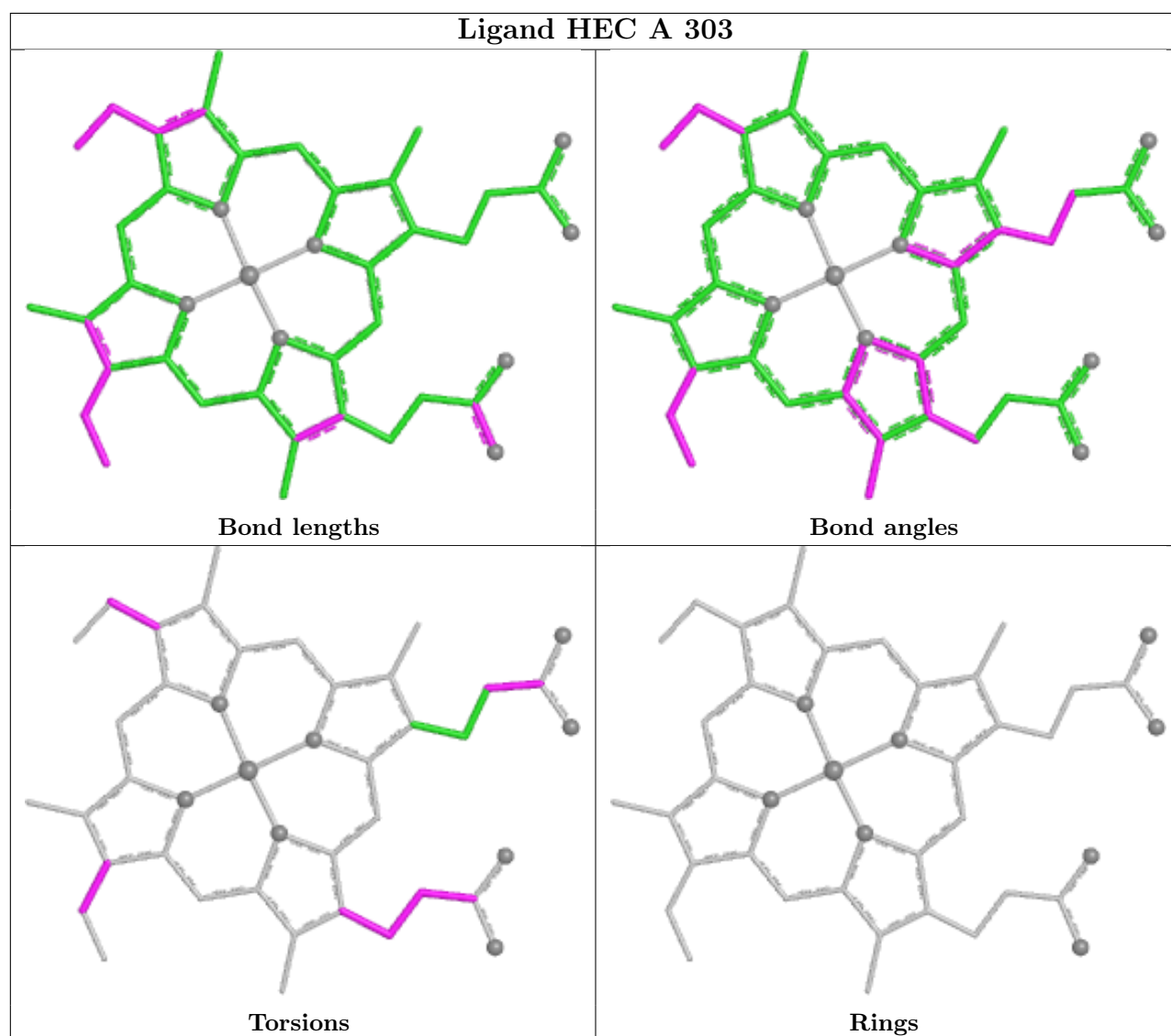
Ligand BCR G 101

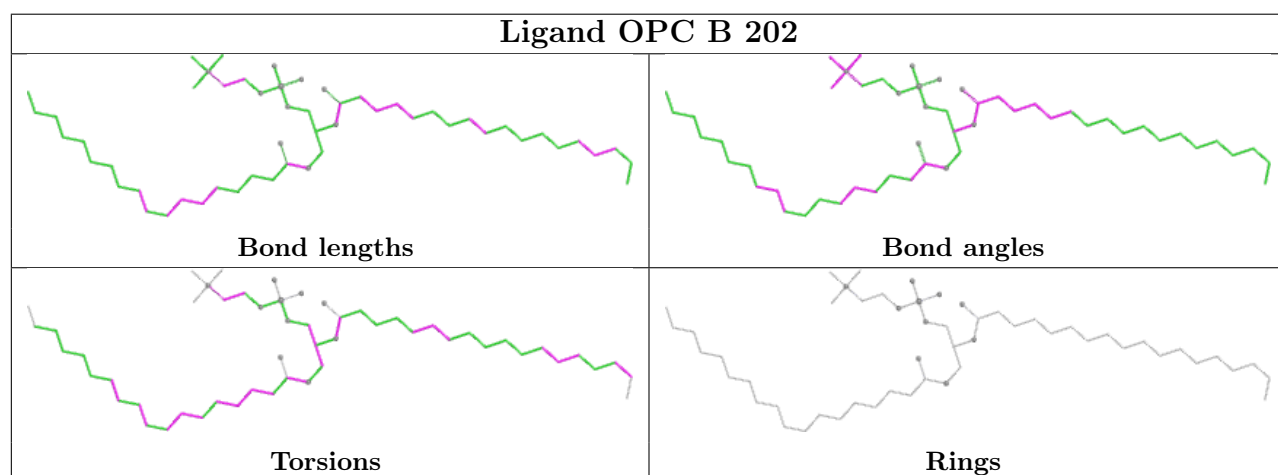
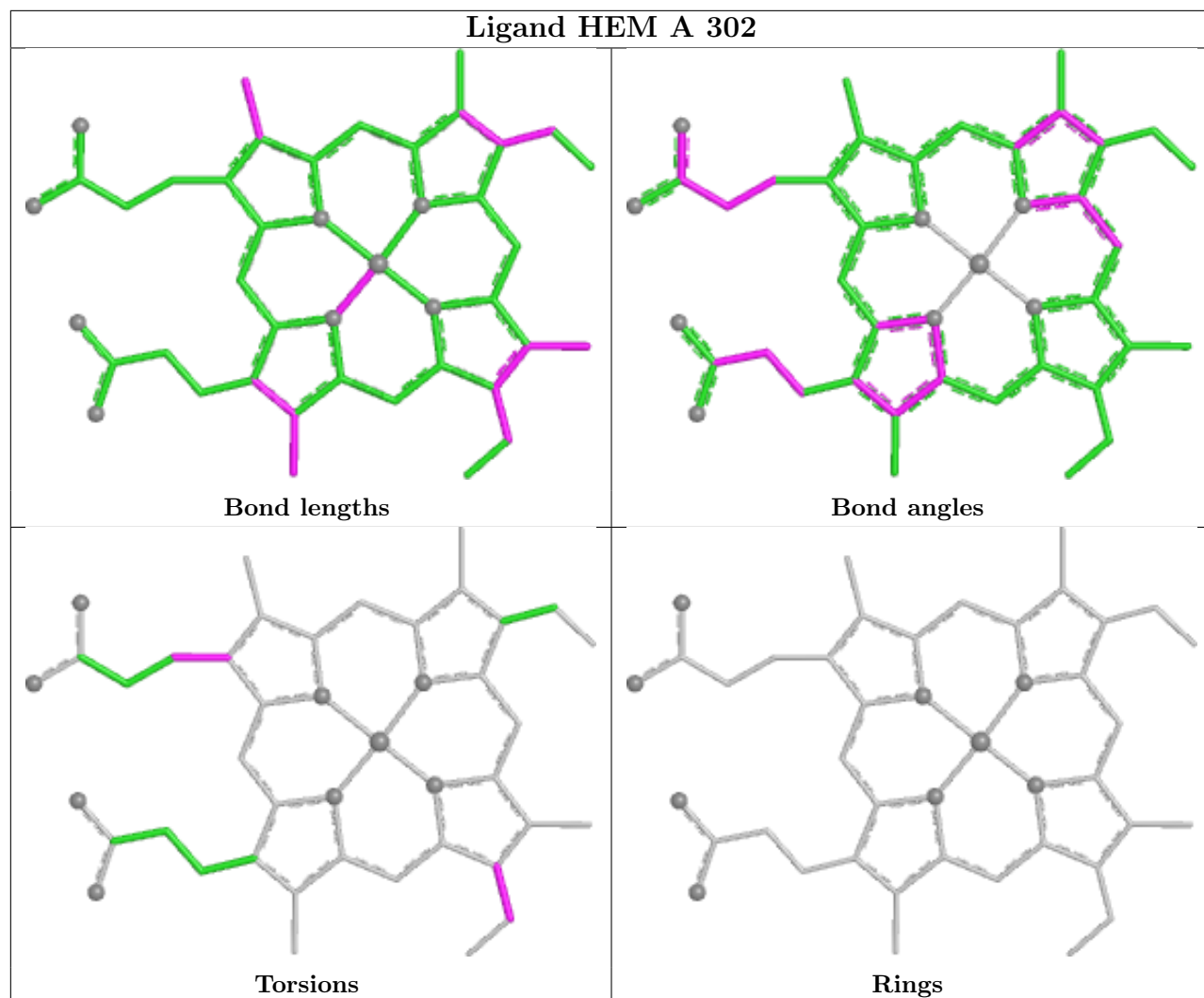


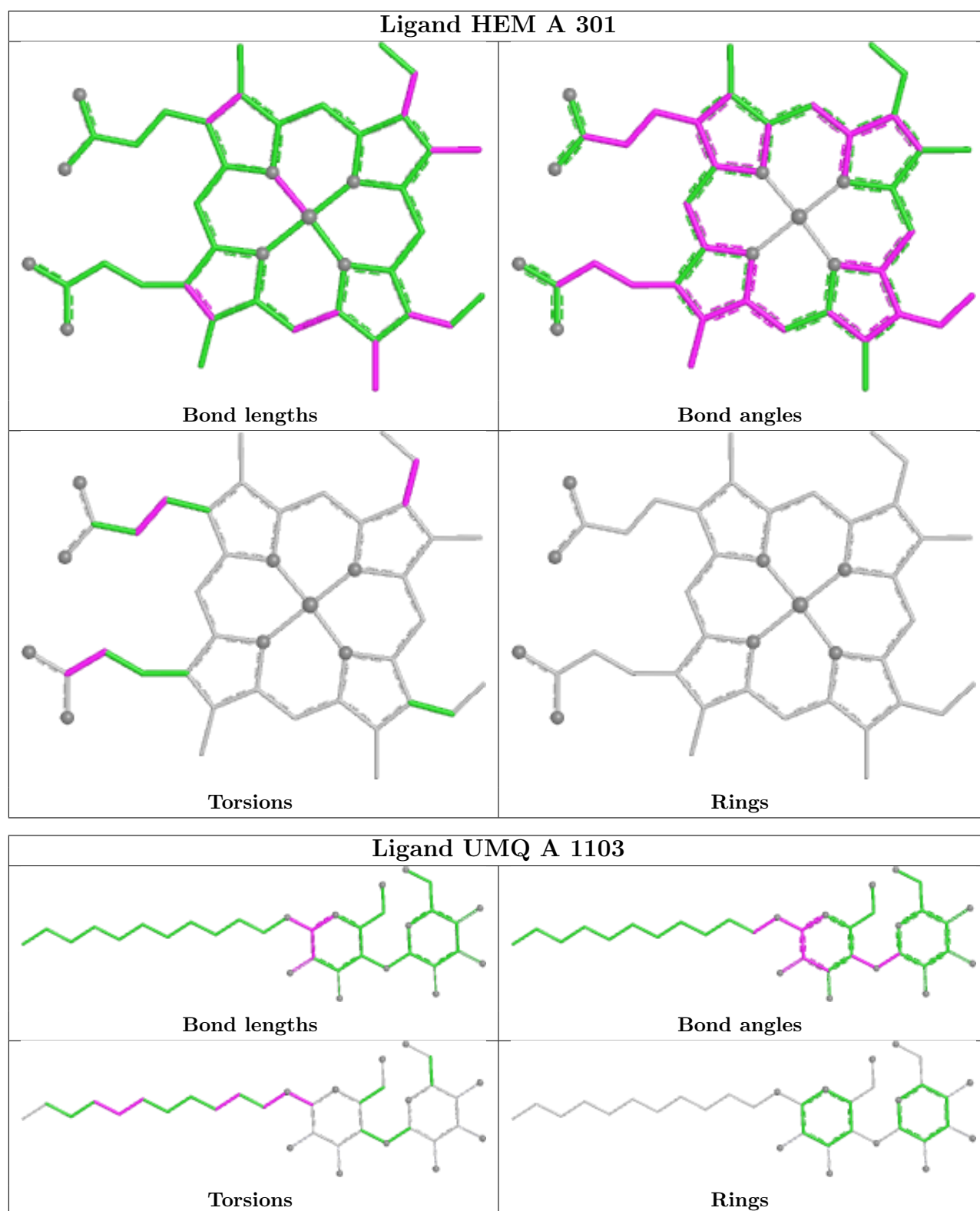
Ligand UMQ A 1101



Ligand HEC A 303







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.39	2 (0%) 81 61	21, 41, 72, 160	0
2	B	160/160 (100%)	0.09	2 (1%) 75 53	32, 57, 103, 135	0
3	C	288/289 (99%)	1.64	87 (30%) 1 1	10, 54, 114, 130	1 (0%)
4	D	166/179 (92%)	2.20	86 (51%) 0 0	38, 91, 125, 171	0
5	E	32/32 (100%)	0.46	2 (6%) 26 13	60, 75, 106, 122	0
6	F	32/35 (91%)	0.50	5 (15%) 5 3	47, 69, 124, 139	0
7	G	37/37 (100%)	0.25	4 (10%) 11 6	42, 57, 123, 131	0
8	H	29/29 (100%)	0.12	2 (6%) 23 12	40, 52, 76, 118	0
All	All	959/976 (98%)	0.85	190 (19%) 3 2	10, 57, 115, 171	1 (0%)

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	40	VAL	10.7
4	D	149	ALA	8.6
4	D	173	GLY	7.6
4	D	50	VAL	6.0
6	F	1	MET	5.9

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

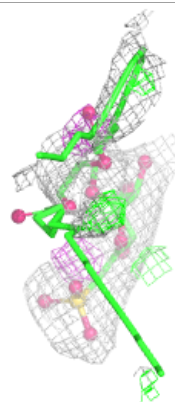
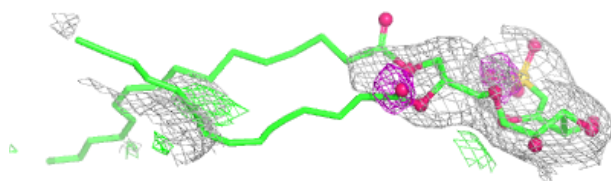
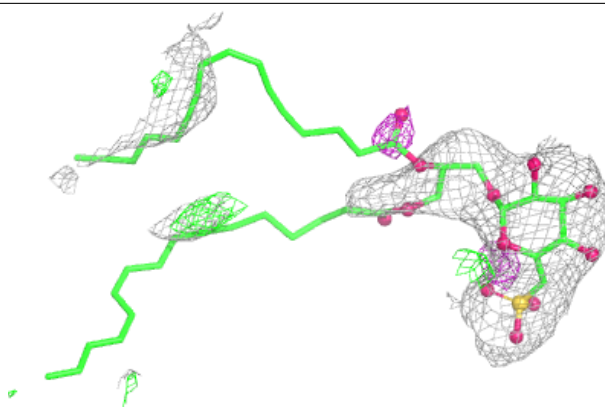
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	SQD	D	201	54/54	0.76	0.31	67,164,194,196	0
12	UMQ	A	1101	34/34	0.77	0.22	35,109,146,149	0
12	UMQ	A	1104	34/34	0.80	0.21	86,134,171,175	0
17	BCR	G	101	40/40	0.83	0.24	33,70,131,136	0
12	UMQ	A	1102	34/34	0.84	0.18	62,119,148,149	0
14	OPC	H	1002	54/55	0.85	0.23	41,93,187,196	0
14	OPC	B	202	54/55	0.88	0.20	48,82,157,162	0
12	UMQ	A	1103	34/34	0.88	0.17	76,112,134,135	0
13	CLA	B	201	65/65	0.95	0.11	41,60,91,99	0
15	FES	D	200	4/4	0.95	0.10	96,101,102,113	0
9	CD	B	161	1/1	0.96	0.06	166,166,166,166	0
10	HEM	A	302	43/43	0.97	0.09	9,34,57,74	0
11	HEC	C	301	43/43	0.97	0.10	29,54,89,97	0
11	HEC	A	303	43/43	0.98	0.07	26,59,68,76	0
10	HEM	A	301	43/43	0.98	0.08	9,32,51,75	0
9	CD	A	1001	1/1	0.99	0.04	65,65,65,65	0

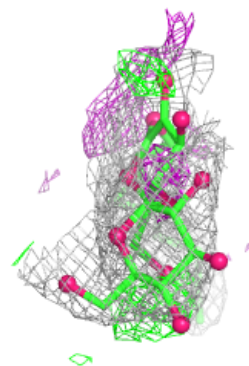
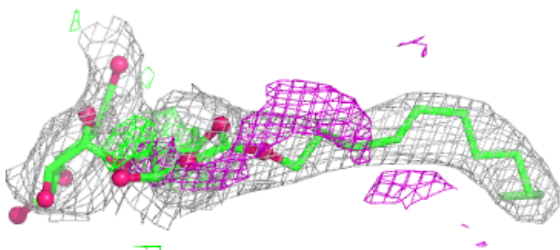
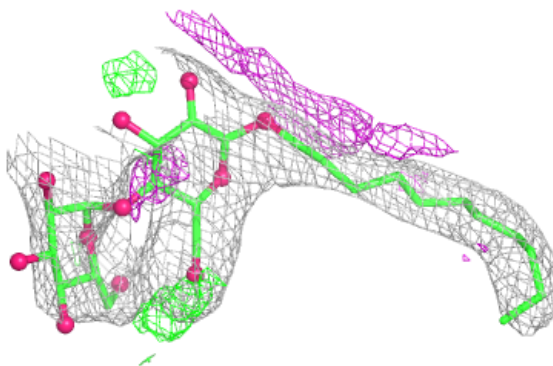
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

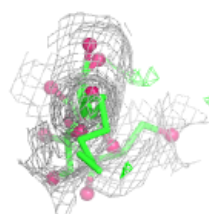
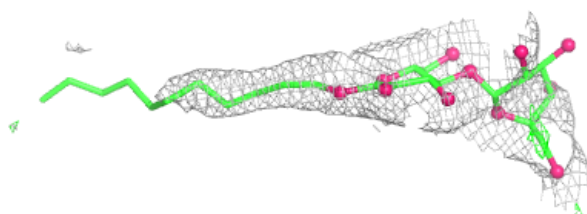
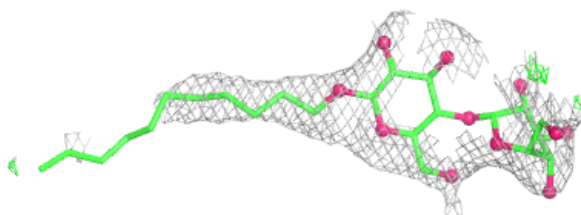
**Electron density around UMQ A 1101:**

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

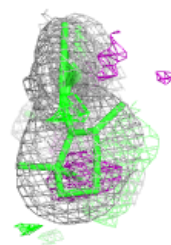
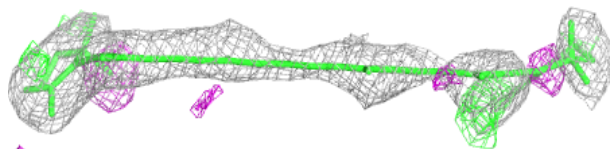
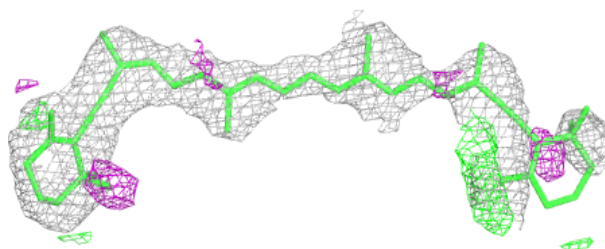


Electron density around UMQ A 1104:

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

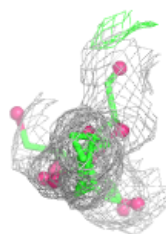
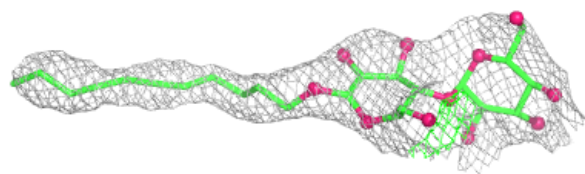
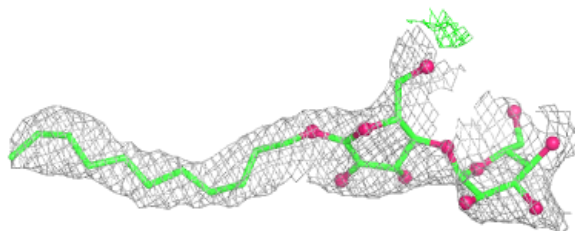
**Electron density around BCR G 101:**

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

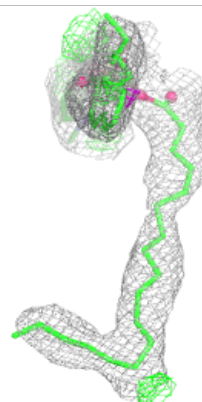
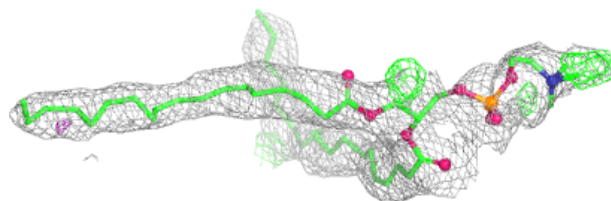
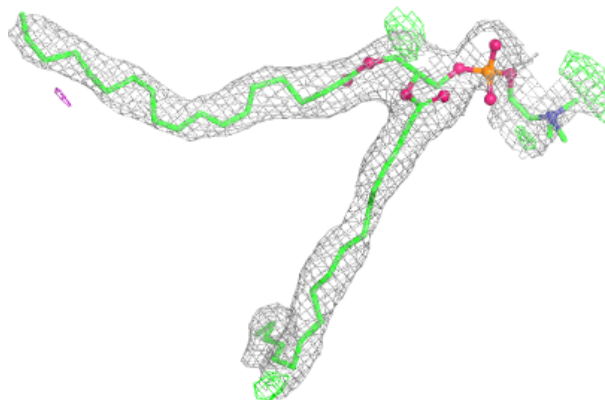


Electron density around UMQ A 1102:

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

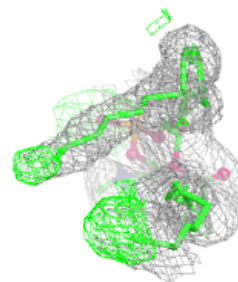
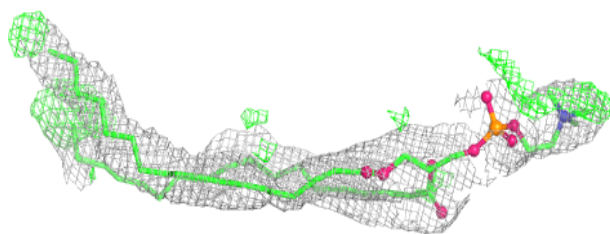
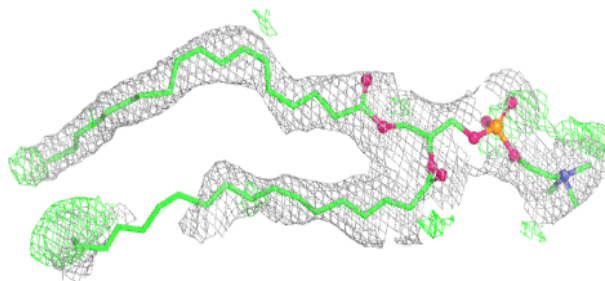
**Electron density around OPC H 1002:**

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

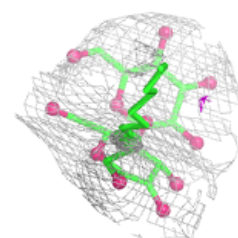
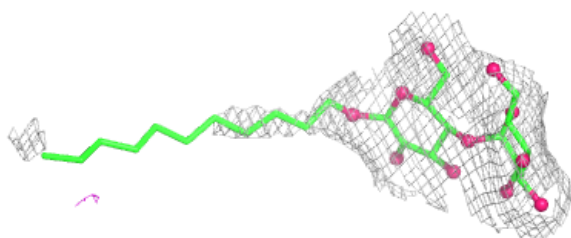
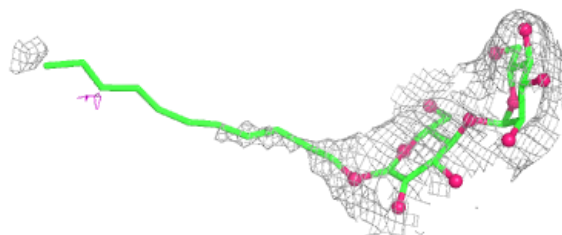


Electron density around OPC B 202:

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

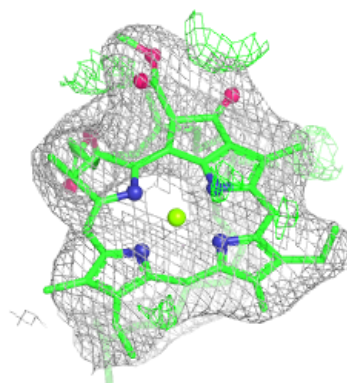
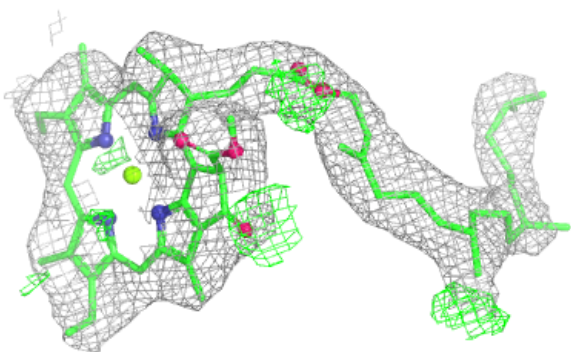
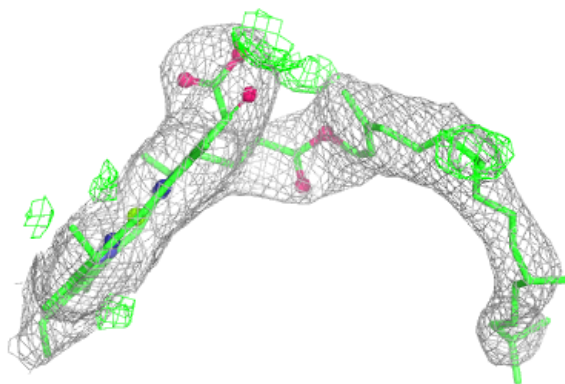
**Electron density around UMQ A 1103:**

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



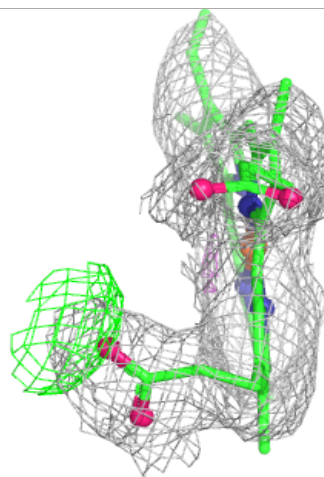
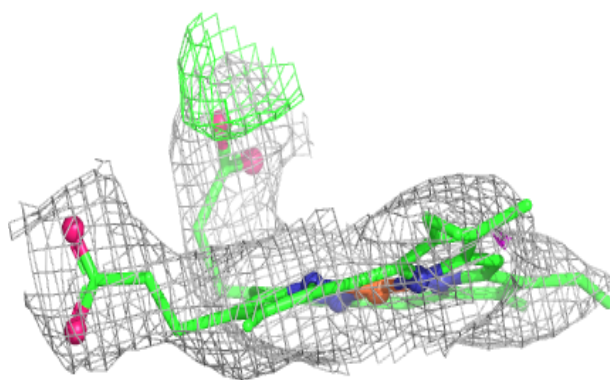
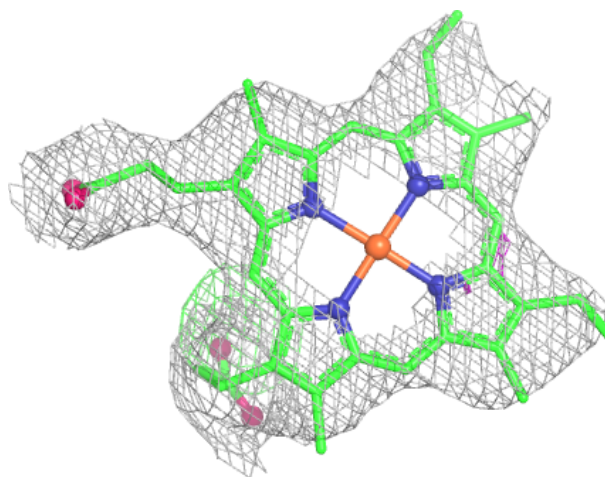
Electron density around CLA B 201:

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



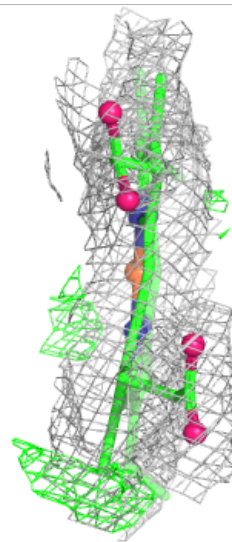
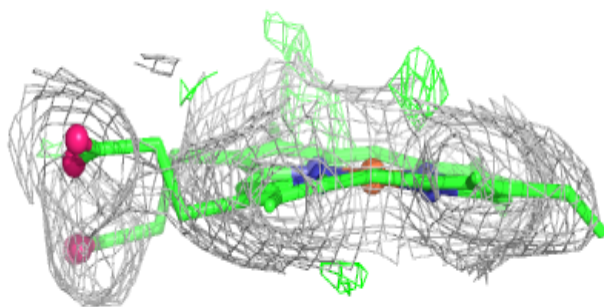
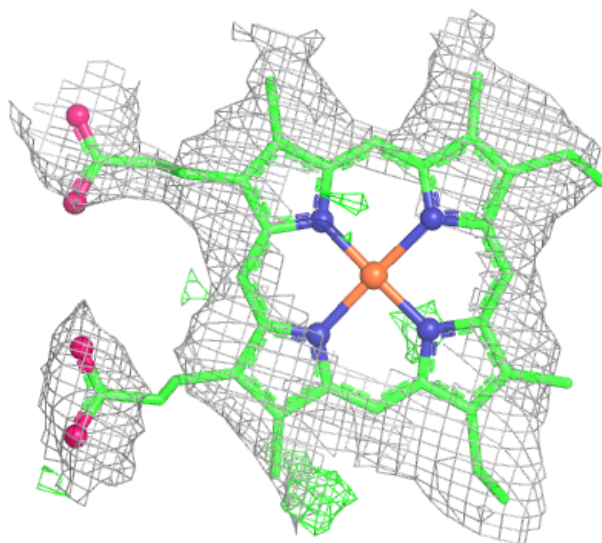
Electron density around HEM A 302:

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



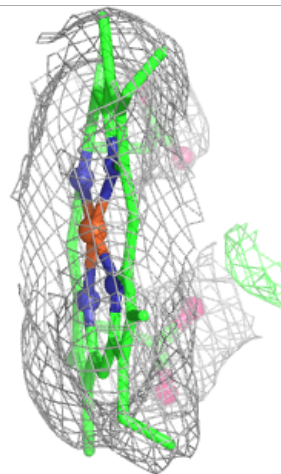
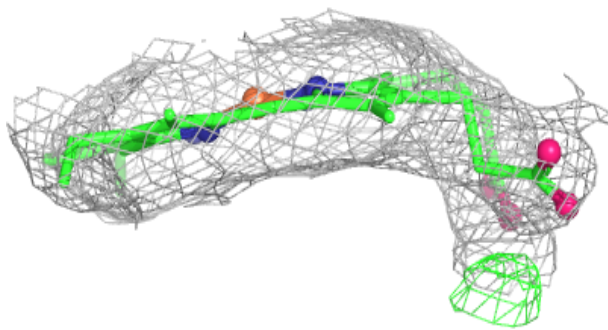
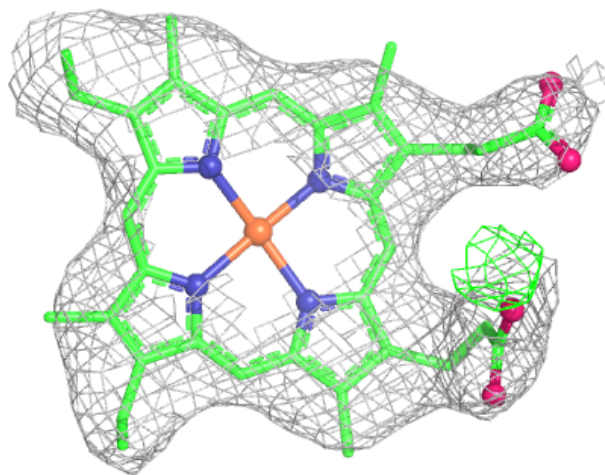
Electron density around HEC C 301:

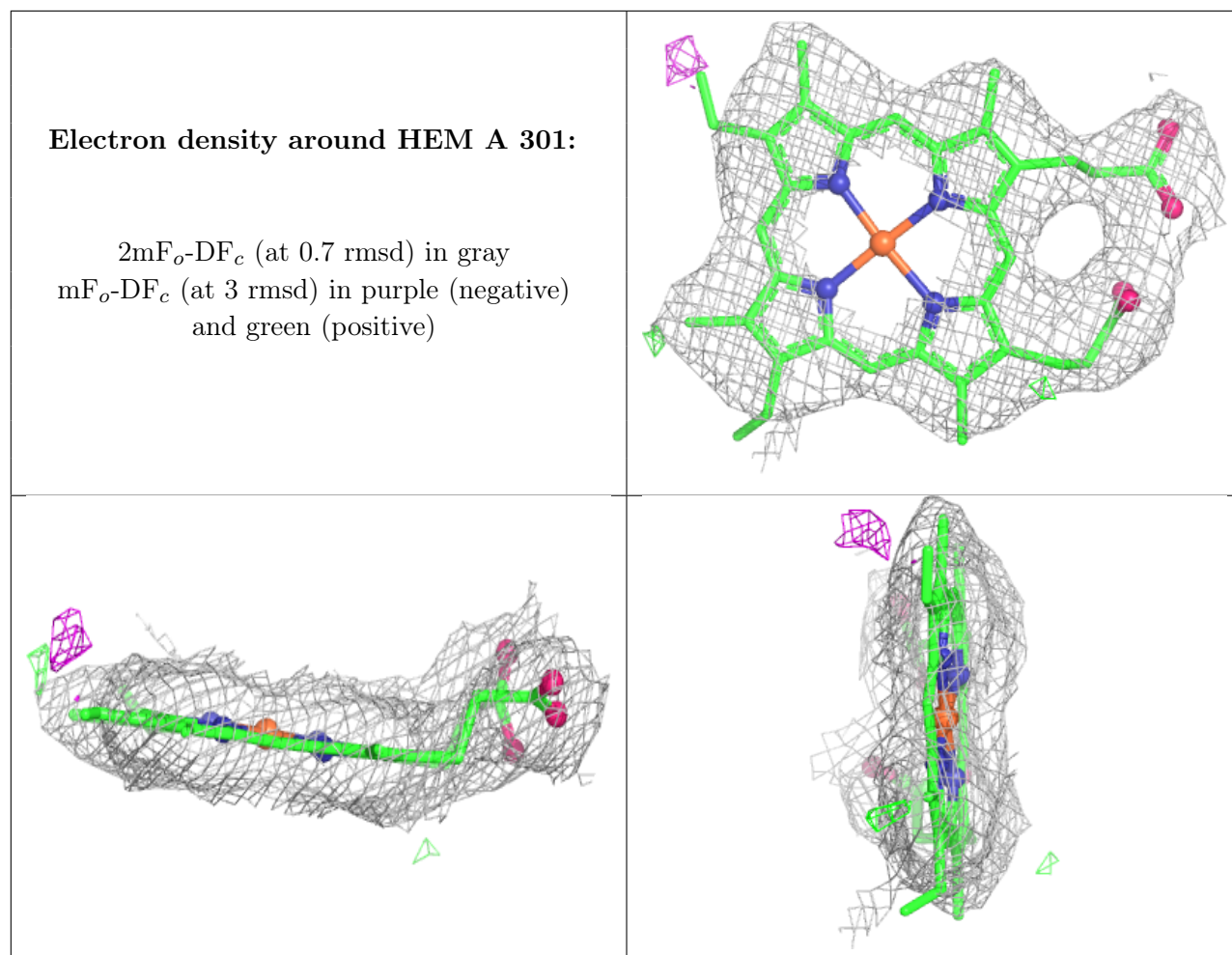
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.