



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:45 PM UTC

PDB ID : 4PD4 / pdb_00004pd4
Title : Structural analysis of atovaquone-inhibited cytochrome bc1 complex reveals the molecular basis of antimalarial drug action
Authors : Birth, D.; Kao, W.-C.; Hunte, C.
Deposited on : 2014-04-17
Resolution : 3.04 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)
Xtrriage (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

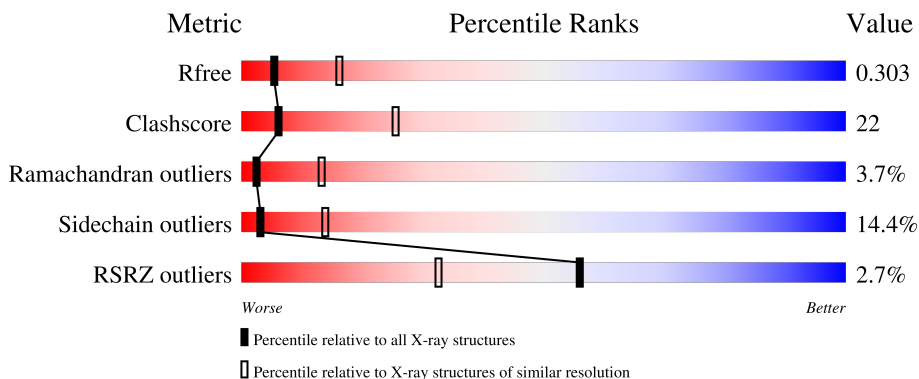
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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.






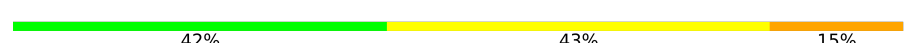
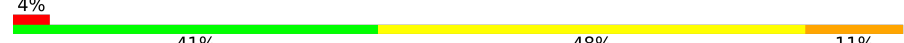
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	431	
2	B	352	
3	C	385	
4	D	248	
5	E	185	

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Mol	Chain	Length	Quality of chain
6	F	74	
7	G	126	
8	H	93	
9	I	57	
10	J	127	
11	K	107	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 17646 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	431	3344	2109	576	653	6	115	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

- 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	352	2735	1747	453	534	1	72	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	385	3090	2082	484	503	21	10	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	248	1961	1249	340	363	9	5	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	185	1411	893	242	266	10	27	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	74	624	391	108	123	2	0	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	126	1019	653	173	191	2	0	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	93	773	510	131	130	2	98	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	I	57	465	310	77	78	0	0	0

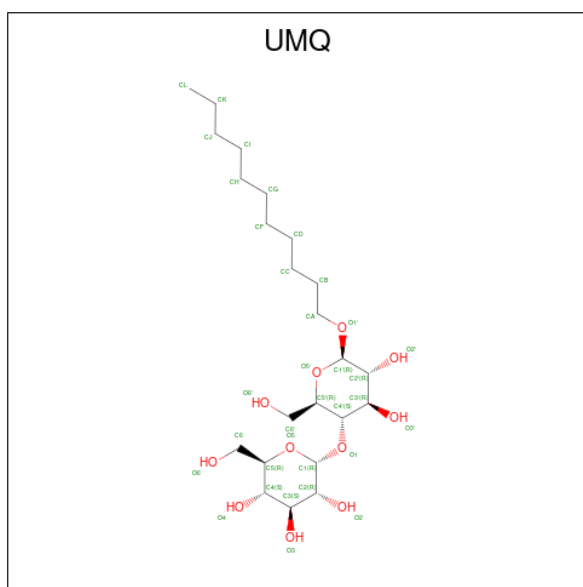
- Molecule 10 is a protein called Igh protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	127	1015	644	167	201	3	0	0	0

- Molecule 11 is a protein called Ig kappa chain V-V region HP 124E1.

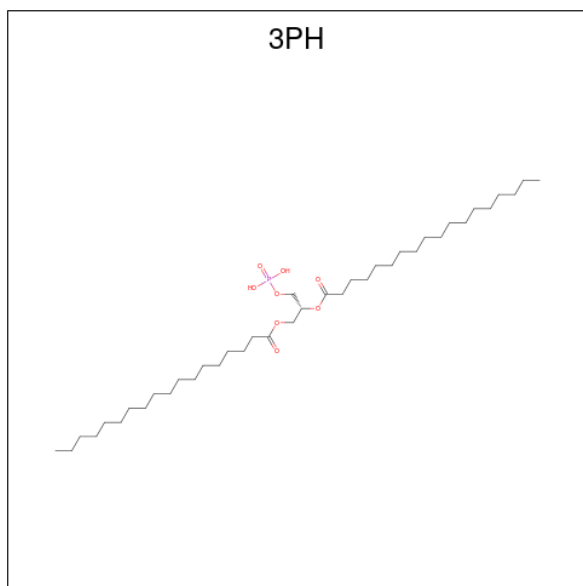
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	107	842	536	141	163	2	0	0	0

- Molecule 12 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



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

- Molecule 13 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



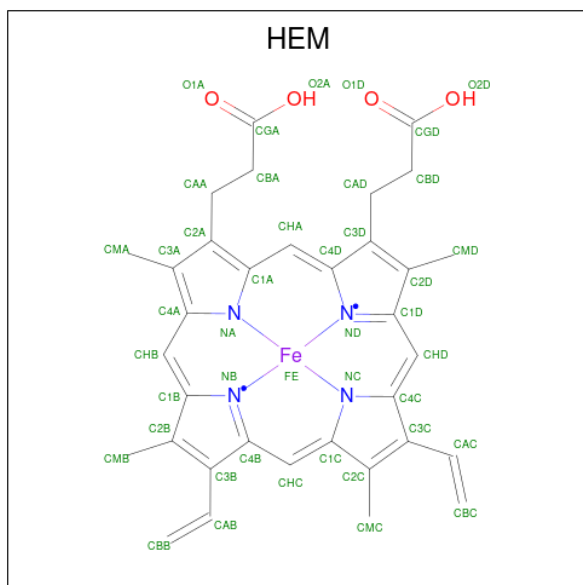
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			31	22	8	1		
13	C	1	Total	C	O	P	0	0
			35	26	8	1		

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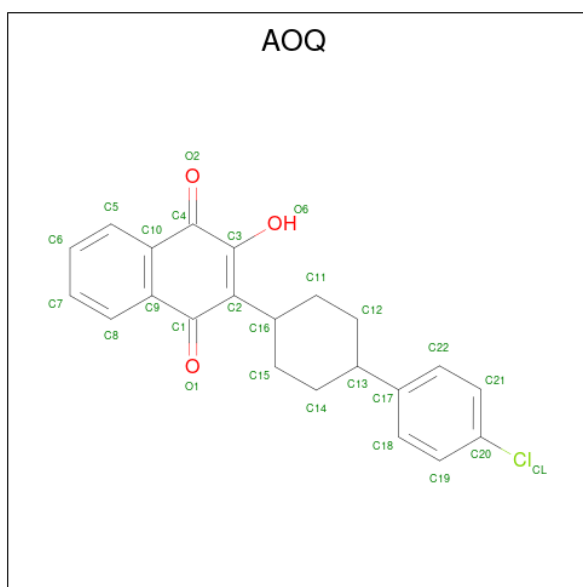
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	E	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



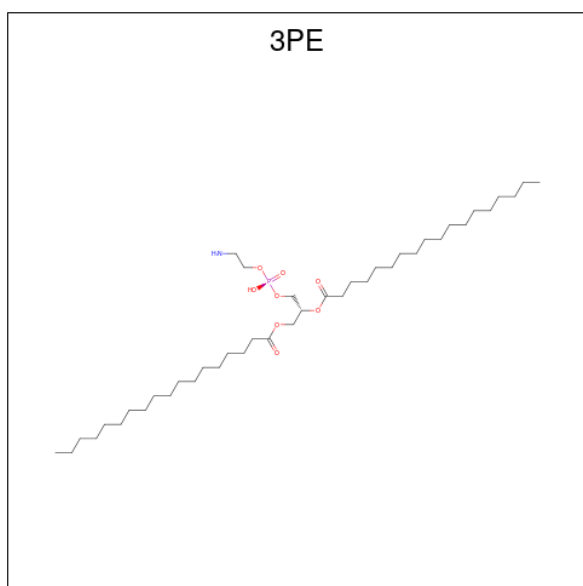
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (CCD ID: AOQ) (formula: $C_{22}H_{19}ClO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
15	C	1	26	22	1	3	0	0

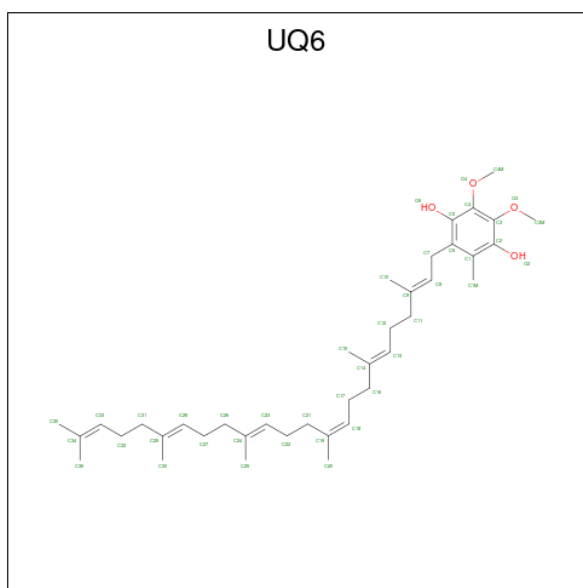
- Molecule 16 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	C	1	27	17	1	8	1	0	0

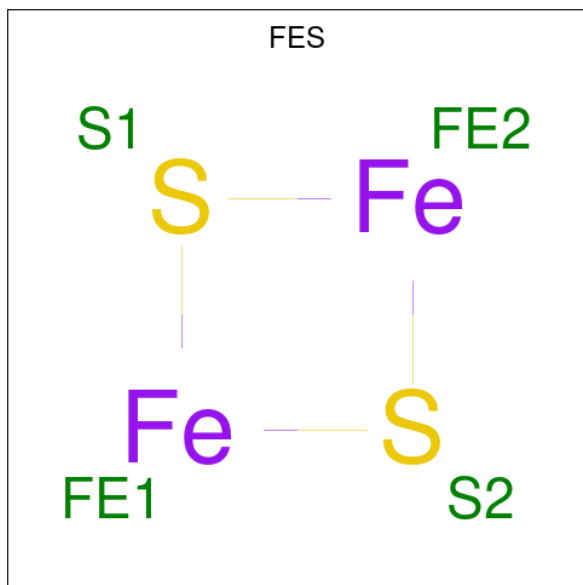
- Molecule 17 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{41}H_{82}O_4$).

C₃₉H₆₀O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total	C O	0	0
			43	39 4		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

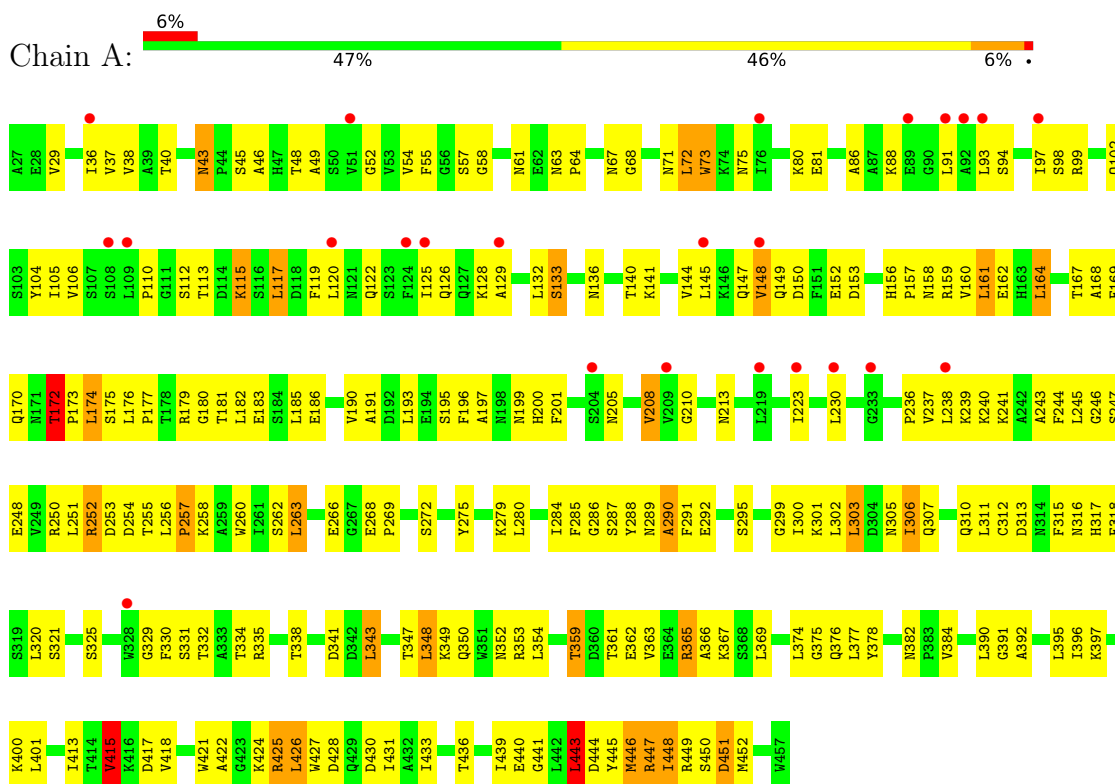


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	E	1	Total	Fe S	0	0
			4	2 2		

3 Residue-property plots [i](#)

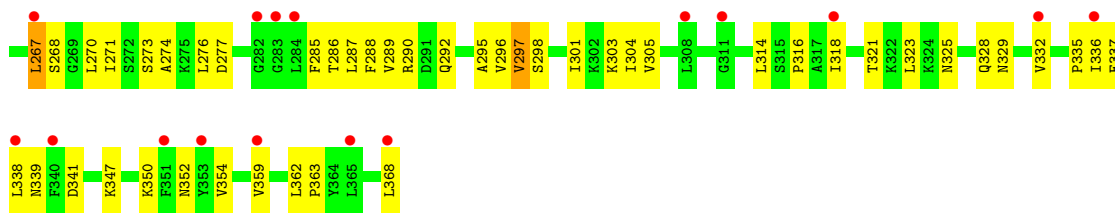
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



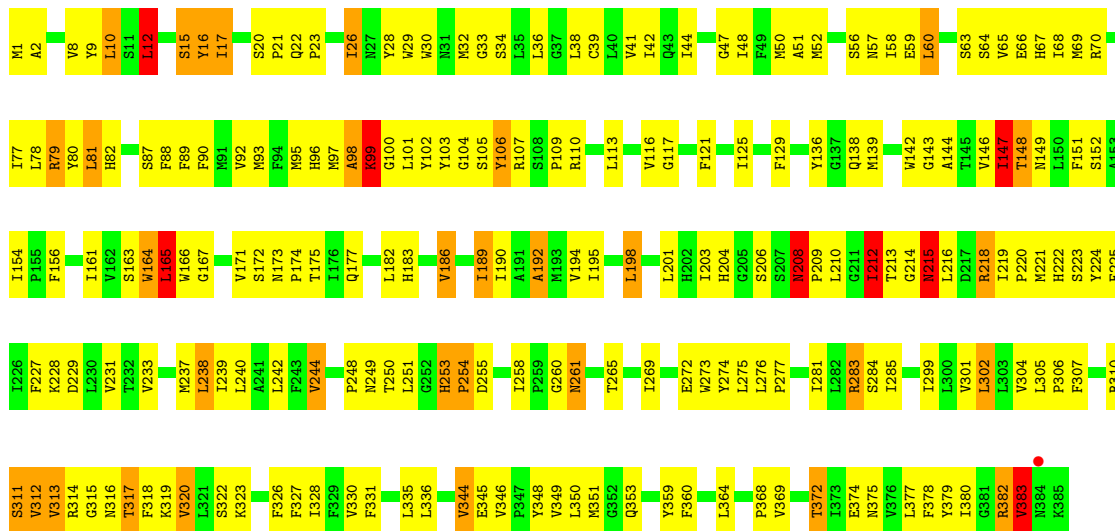
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





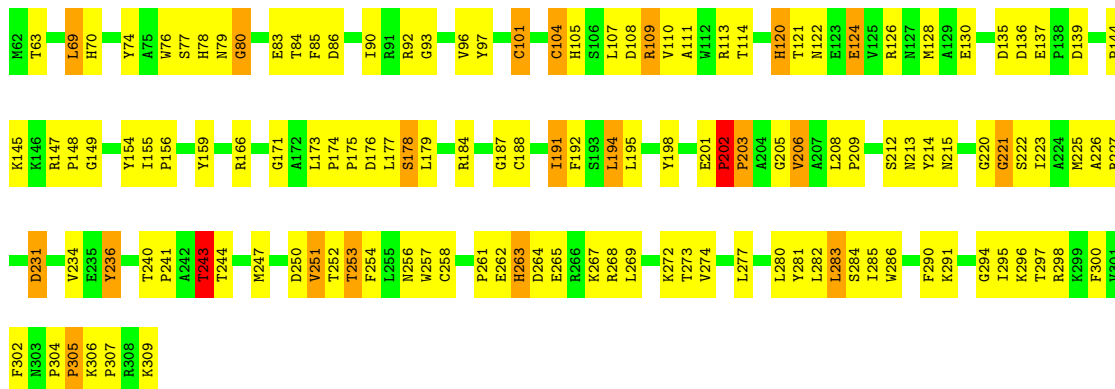
● Molecule 3: Cytochrome b

Chain C: 44% 45% 8%



● Molecule 4: Cytochrome c1, heme protein, mitochondrial

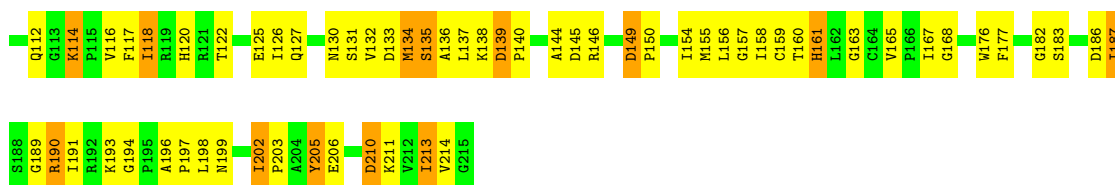
Chain D: 47% 44% 8%



● Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 45% 43% 12%

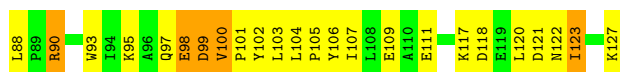
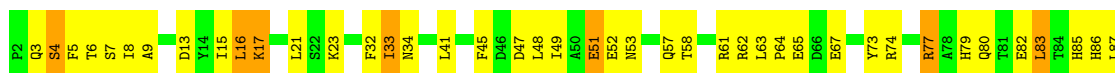




- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 7: Cytochrome b-c1 complex subunit 7



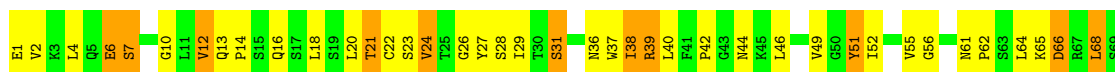
- Molecule 8: Cytochrome b-c1 complex subunit 8

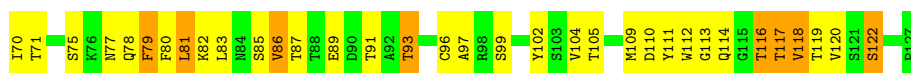


- Molecule 9: Cytochrome b-c1 complex subunit 9

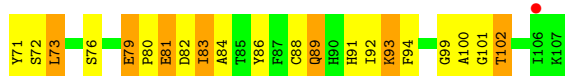
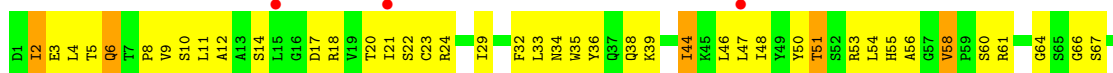


- Molecule 10: Igh protein





- Molecule 11: Ig kappa chain V-V region HP 124E1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.26Å 150.88Å 143.09Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	24.99 – 3.04 24.99 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.99-3.04) 98.4 (24.99-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.05Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.297 0.270 , 0.303	Depositor DCC
R_{free} test set	2008 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17646	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, UQ6, 3PE, FES, HEM, 3PH, AOQ

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	0.51	0/3405	0.96	8/4614 (0.2%)
2	B	0.50	0/2781	0.91	3/3764 (0.1%)
3	C	0.90	1/3192 (0.0%)	1.22	15/4354 (0.3%)
4	D	0.60	0/2022	1.11	9/2751 (0.3%)
5	E	0.71	1/1444 (0.1%)	1.20	8/1957 (0.4%)
6	F	0.46	0/638	0.94	0/858
7	G	0.73	0/1040	1.18	1/1408 (0.1%)
8	H	0.65	0/804	1.06	2/1088 (0.2%)
9	I	0.48	0/479	0.89	0/646
10	J	0.58	0/1043	1.01	2/1422 (0.1%)
11	K	0.51	0/863	0.87	0/1172
All	All	0.64	2/17711 (0.0%)	1.06	48/24034 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	147	ILE	CA-CB	-6.56	1.46	1.54
5	E	213	ILE	CA-CB	5.87	1.59	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	202	PRO	CA-C-N	9.37	131.55	119.84
4	D	202	PRO	C-N-CA	9.37	131.55	119.84
5	E	135	SER	N-CA-C	-8.72	103.76	114.75
3	C	261	ASN	CA-C-N	7.83	128.01	119.87
3	C	261	ASN	C-N-CA	7.83	128.01	119.87

There are no chirality outliers.

There are no planarity outliers.

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	3344	0	3321	159	0
2	B	2735	0	2774	109	0
3	C	3090	0	3129	173	0
4	D	1961	0	1890	104	0
5	E	1411	0	1386	70	0
6	F	624	0	581	23	0
7	G	1019	0	1034	54	0
8	H	773	0	736	39	0
9	I	465	0	459	19	0
10	J	1015	0	959	57	0
11	K	842	0	820	42	0
12	A	34	0	44	3	0
13	A	31	0	35	2	0
13	C	35	0	46	1	0
13	E	38	0	49	6	0
14	C	86	0	60	15	0
14	D	43	0	30	10	0
15	C	26	0	19	3	0
16	C	27	0	28	1	0
17	C	43	0	58	4	0
18	E	4	0	0	0	0
All	All	17646	0	17458	773	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 22.

The worst 5 of 773 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)
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.41	1.00
3:C:318:PHE:HD1	7:G:48:LEU:HD21	1.32	0.93
1:A:248:GLU:OE2	1:A:250:ARG:NH2	2.04	0.90
13:A:502:3PH:H321	13:A:502:3PH:H221	1.54	0.89
11:K:93:LYS:HD2	11:K:94:PHE:H	1.41	0.83

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	429/431 (100%)	349 (81%)	67 (16%)	13 (3%)	3	17
2	B	350/352 (99%)	284 (81%)	56 (16%)	10 (3%)	3	17
3	C	383/385 (100%)	318 (83%)	49 (13%)	16 (4%)	2	11
4	D	246/248 (99%)	199 (81%)	36 (15%)	11 (4%)	2	10
5	E	183/185 (99%)	142 (78%)	33 (18%)	8 (4%)	2	10
6	F	72/74 (97%)	60 (83%)	10 (14%)	2 (3%)	4	18
7	G	124/126 (98%)	102 (82%)	16 (13%)	6 (5%)	2	9
8	H	91/93 (98%)	61 (67%)	23 (25%)	7 (8%)	1	3
9	I	55/57 (96%)	41 (74%)	13 (24%)	1 (2%)	6	28
10	J	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	16	46
11	K	105/107 (98%)	76 (72%)	23 (22%)	6 (6%)	1	7
All	All	2163/2185 (99%)	1747 (81%)	335 (16%)	81 (4%)	2	13

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
2	B	153	LYS
3	C	99	LYS
3	C	164	TRP
3	C	165	LEU

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	370/370 (100%)	317 (86%)	53 (14%)	3	14
2	B	301/301 (100%)	267 (89%)	34 (11%)	5	22
3	C	338/338 (100%)	290 (86%)	48 (14%)	3	14
4	D	206/206 (100%)	177 (86%)	29 (14%)	3	14
5	E	151/151 (100%)	124 (82%)	27 (18%)	2	9
6	F	67/67 (100%)	61 (91%)	6 (9%)	9	31
7	G	110/110 (100%)	91 (83%)	19 (17%)	2	9
8	H	77/77 (100%)	67 (87%)	10 (13%)	4	17
9	I	47/47 (100%)	40 (85%)	7 (15%)	3	13
10	J	112/112 (100%)	90 (80%)	22 (20%)	1	7
11	K	93/93 (100%)	78 (84%)	15 (16%)	2	11
All	All	1872/1872 (100%)	1602 (86%)	270 (14%)	3	14

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	42	ASN
10	J	24	VAL
11	K	51	THR
3	C	79	ARG
3	C	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	79	HIS
8	H	34	GLN
11	K	90	HIS
7	G	97	GLN
8	H	47	ASN

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](#)

11 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
13	3PH	A	502	-	30,30,47	1.24	2 (6%)	33,35,52	1.16	3 (9%)
13	3PH	C	4006	-	34,34,47	1.17	2 (5%)	37,39,52	1.70	8 (21%)
13	3PH	E	302	-	37,37,47	1.10	2 (5%)	40,42,52	1.25	2 (5%)
14	HEM	C	4002	3	50,50,50	1.70	8 (16%)	67,82,82	1.63	12 (17%)
14	HEM	C	4001	3	50,50,50	2.00	9 (18%)	67,82,82	1.46	10 (14%)
18	FES	E	301	5	0,4,4	-	-	-	-	-
12	UMQ	A	501	-	35,35,35	0.47	0	46,46,46	1.20	7 (15%)
16	3PE	C	4004	-	26,26,50	1.37	2 (7%)	29,31,55	1.44	5 (17%)
17	UQ6	C	4005	-	43,43,43	1.20	3 (6%)	54,55,55	2.20	20 (37%)
14	HEM	D	401	4	50,50,50	2.02	9 (18%)	67,82,82	1.65	11 (16%)
15	AOQ	C	4003	-	29,29,29	1.73	7 (24%)	41,42,42	1.80	9 (21%)

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
13	3PH	A	502	-	-	14/32/32/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	3PH	C	4006	-	-	13/36/36/49	-
13	3PH	E	302	-	-	19/39/39/49	-
14	HEM	C	4002	3	-	4/14/54/54	-
14	HEM	C	4001	3	-	3/14/54/54	-
18	FES	E	301	5	-	-	0/1/1/1
12	UMQ	A	501	-	-	3/20/60/60	0/2/2/2
16	3PE	C	4004	-	-	14/30/30/54	-
17	UQ6	C	4005	-	-	14/39/39/39	0/1/1/1
14	HEM	D	401	4	-	4/14/54/54	-
15	AOQ	C	4003	-	-	5/8/38/38	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	C3D-C2D	8.21	1.54	1.36
14	C	4001	HEM	C3D-C2D	8.16	1.54	1.36
14	C	4002	HEM	C3D-C2D	7.23	1.52	1.36
14	C	4001	HEM	FE-NA	5.79	2.14	1.95
14	D	401	HEM	FE-NA	5.61	2.13	1.95

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	4002	HEM	C4D-ND-C1D	6.22	112.58	105.21
14	D	401	HEM	C4D-ND-C1D	5.99	112.30	105.21
15	C	4003	AOQ	C16-C2-C1	4.90	125.20	119.11
14	C	4001	HEM	C4D-ND-C1D	4.80	110.89	105.21
17	C	4005	UQ6	C10-C9-C11	4.62	123.25	115.23

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

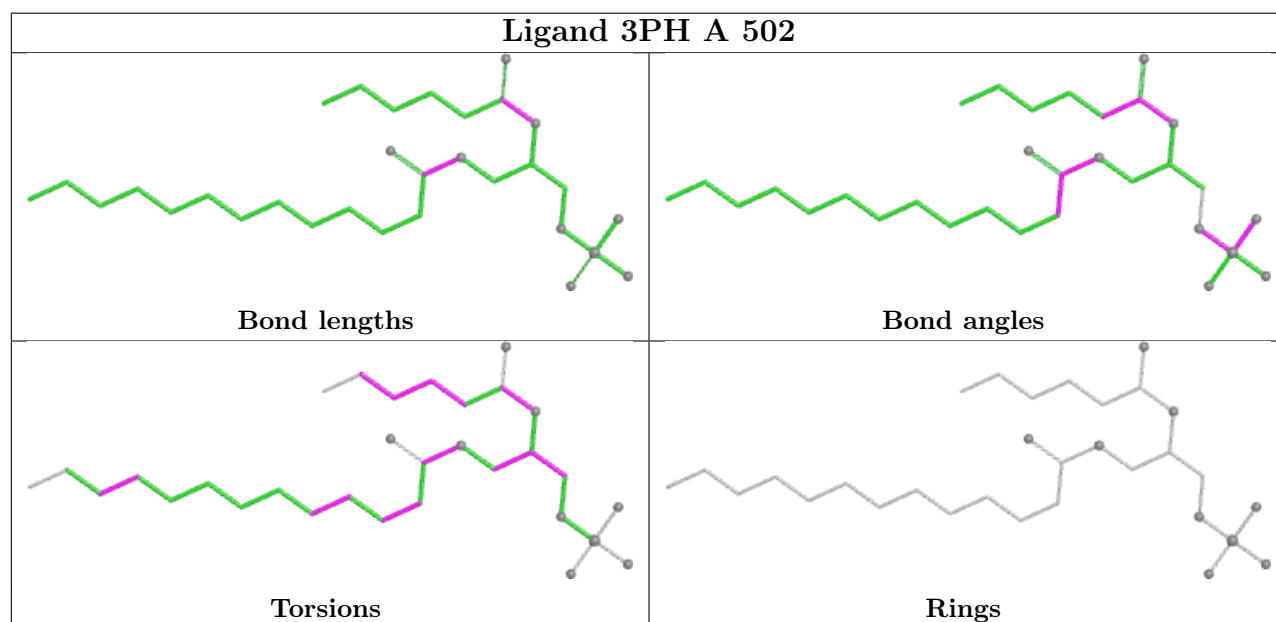
Mol	Chain	Res	Type	Atoms
13	A	502	3PH	C22-C21-O21-C2
13	E	302	3PH	C1-O11-P-O13
13	E	302	3PH	C1-O11-P-O14
13	E	302	3PH	C1-O11-P-O12
15	C	4003	AOQ	C11-C16-C2-C1

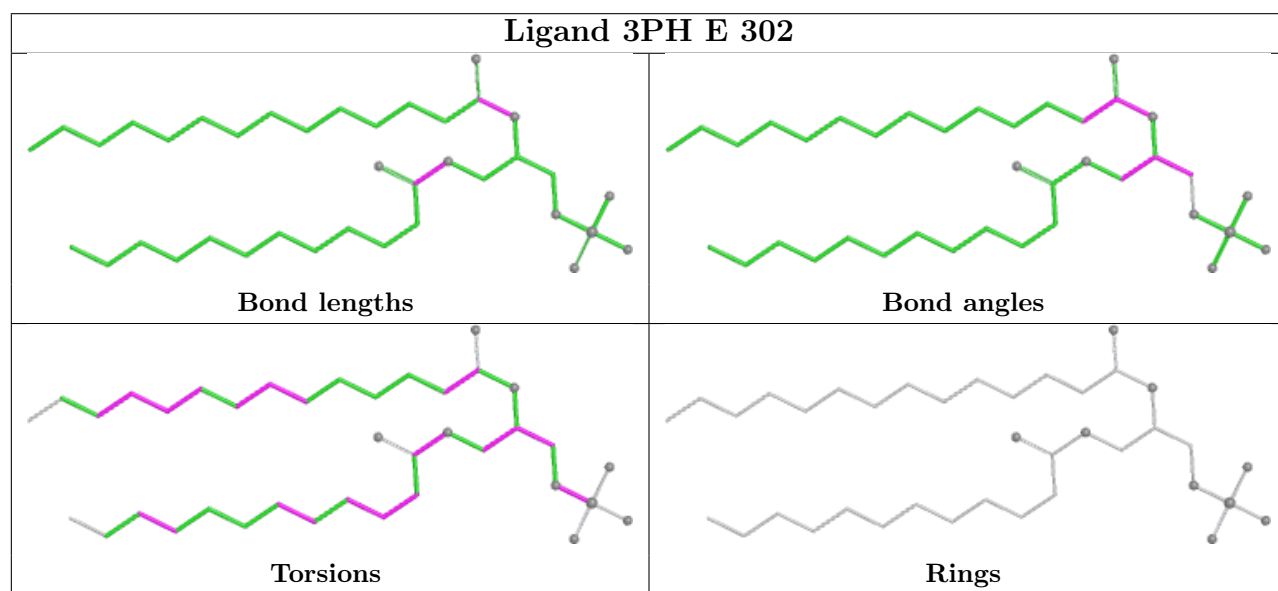
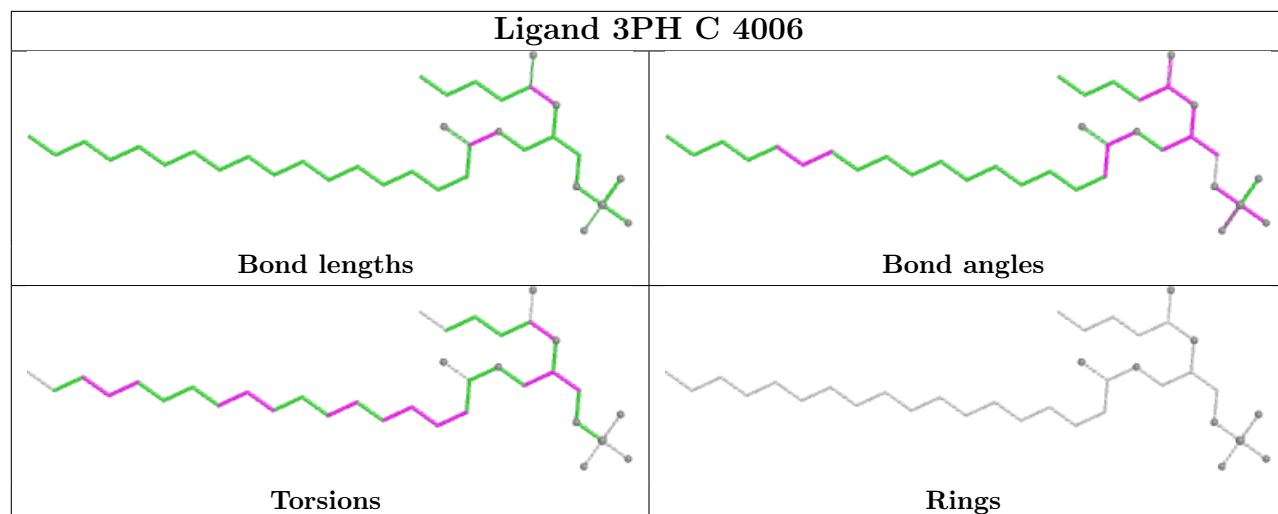
There are no ring outliers.

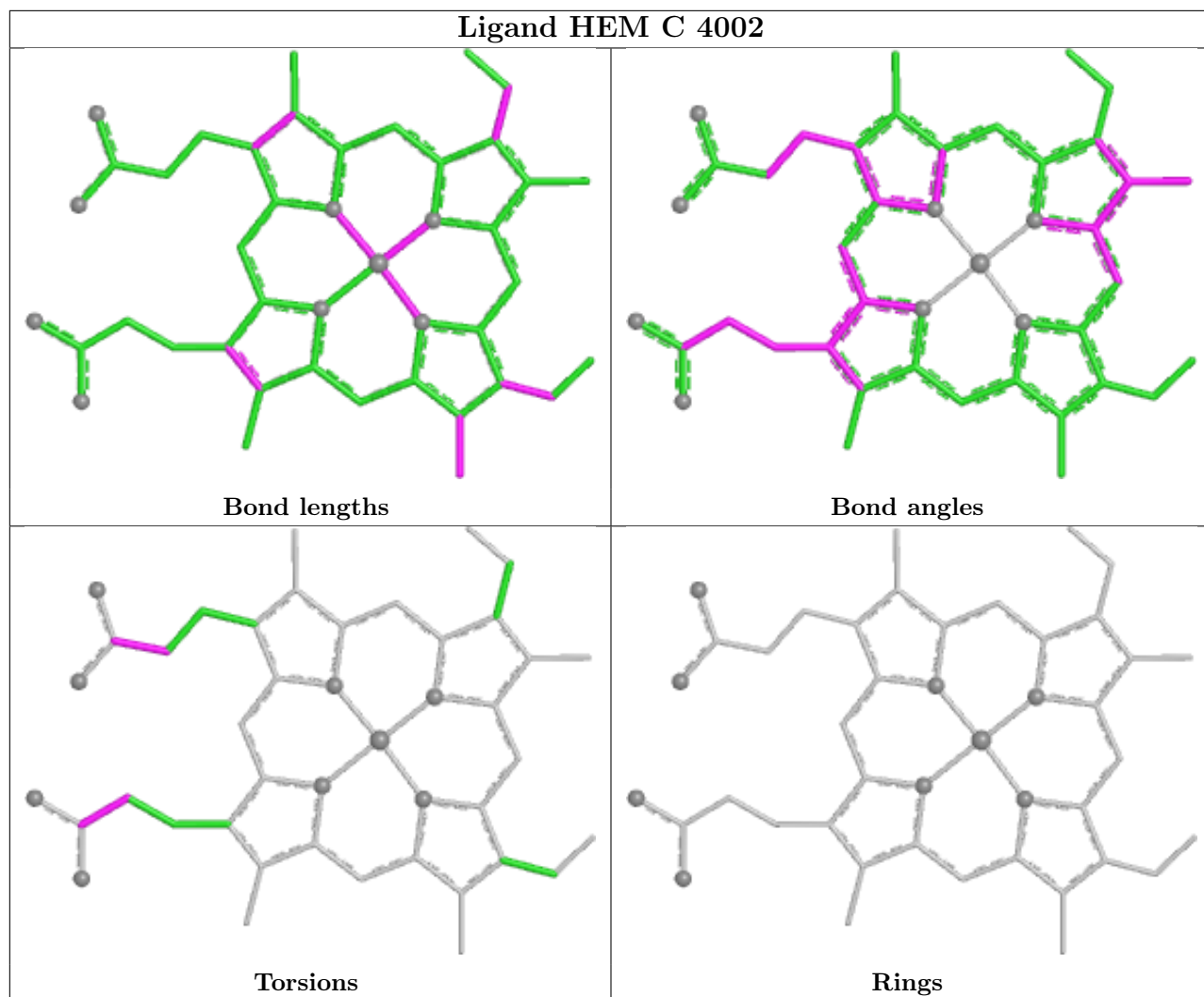
10 monomers are involved in 45 short contacts:

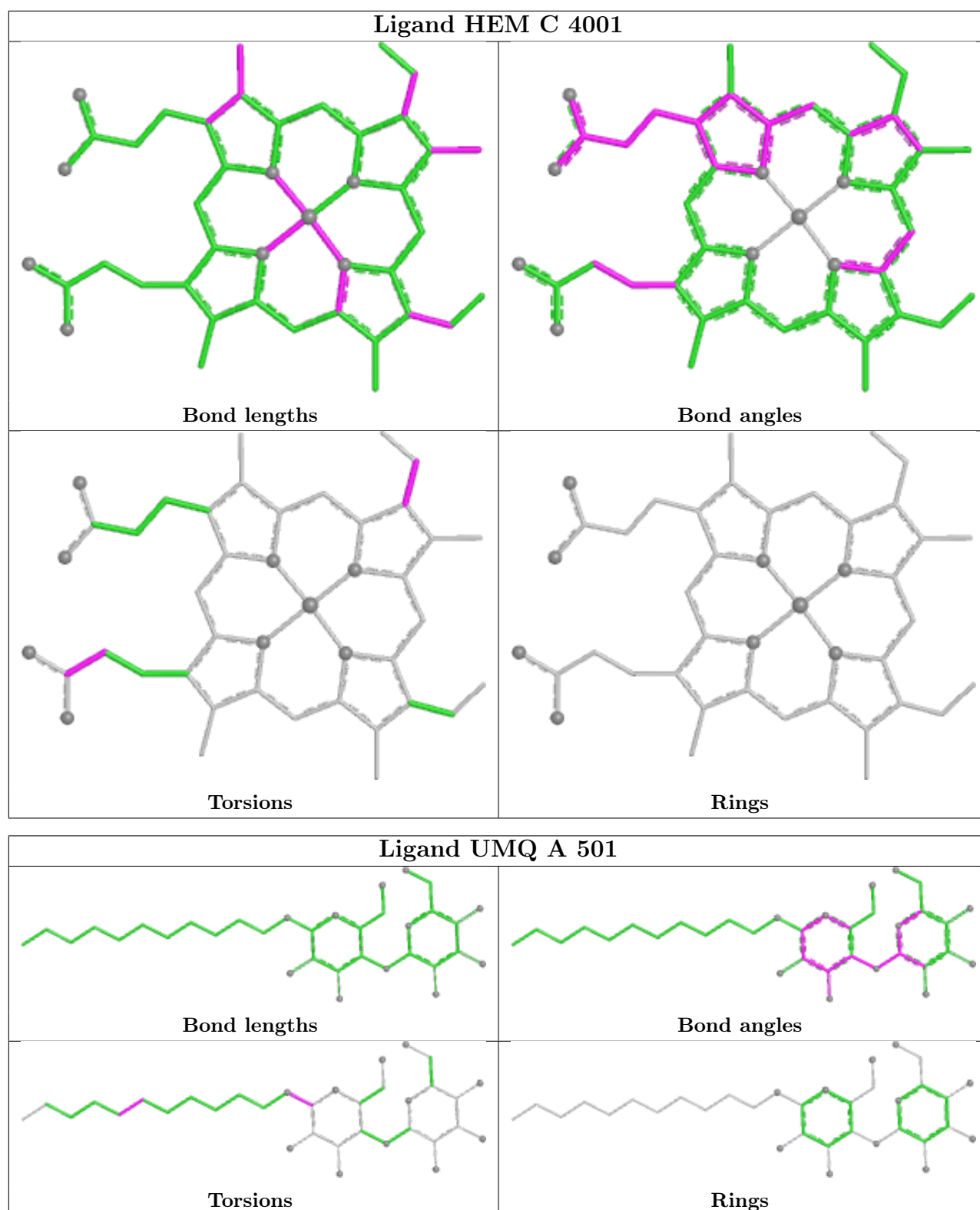
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	502	3PH	2	0
13	C	4006	3PH	1	0
13	E	302	3PH	6	0
14	C	4002	HEM	8	0
14	C	4001	HEM	7	0
12	A	501	UMQ	3	0
16	C	4004	3PE	1	0
17	C	4005	UQ6	4	0
14	D	401	HEM	10	0
15	C	4003	AOQ	3	0

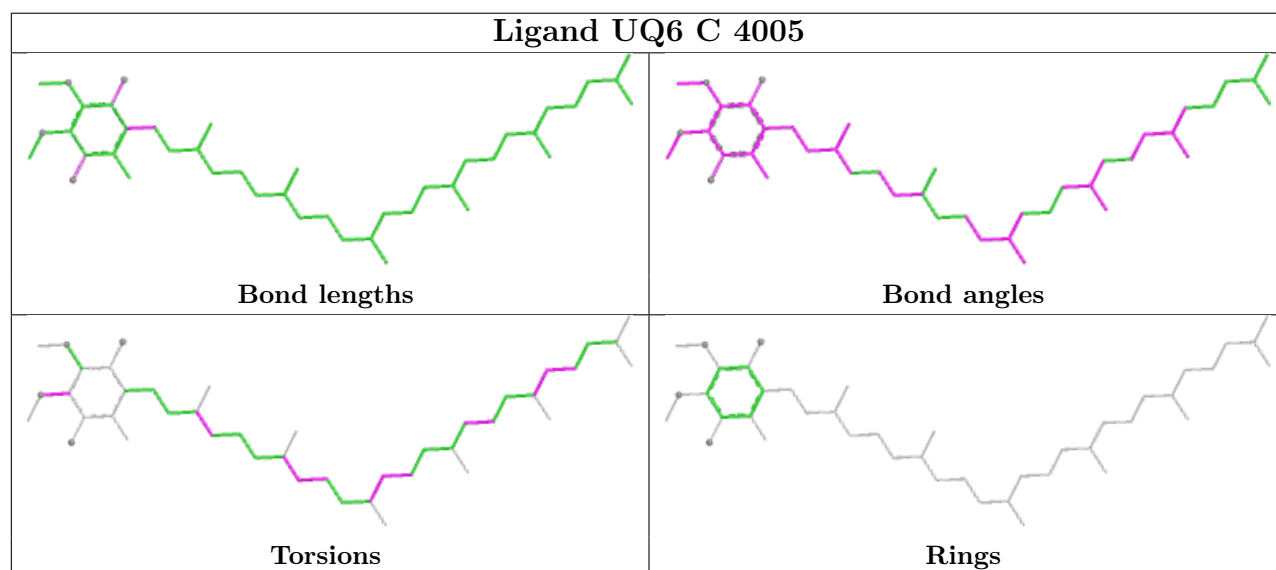
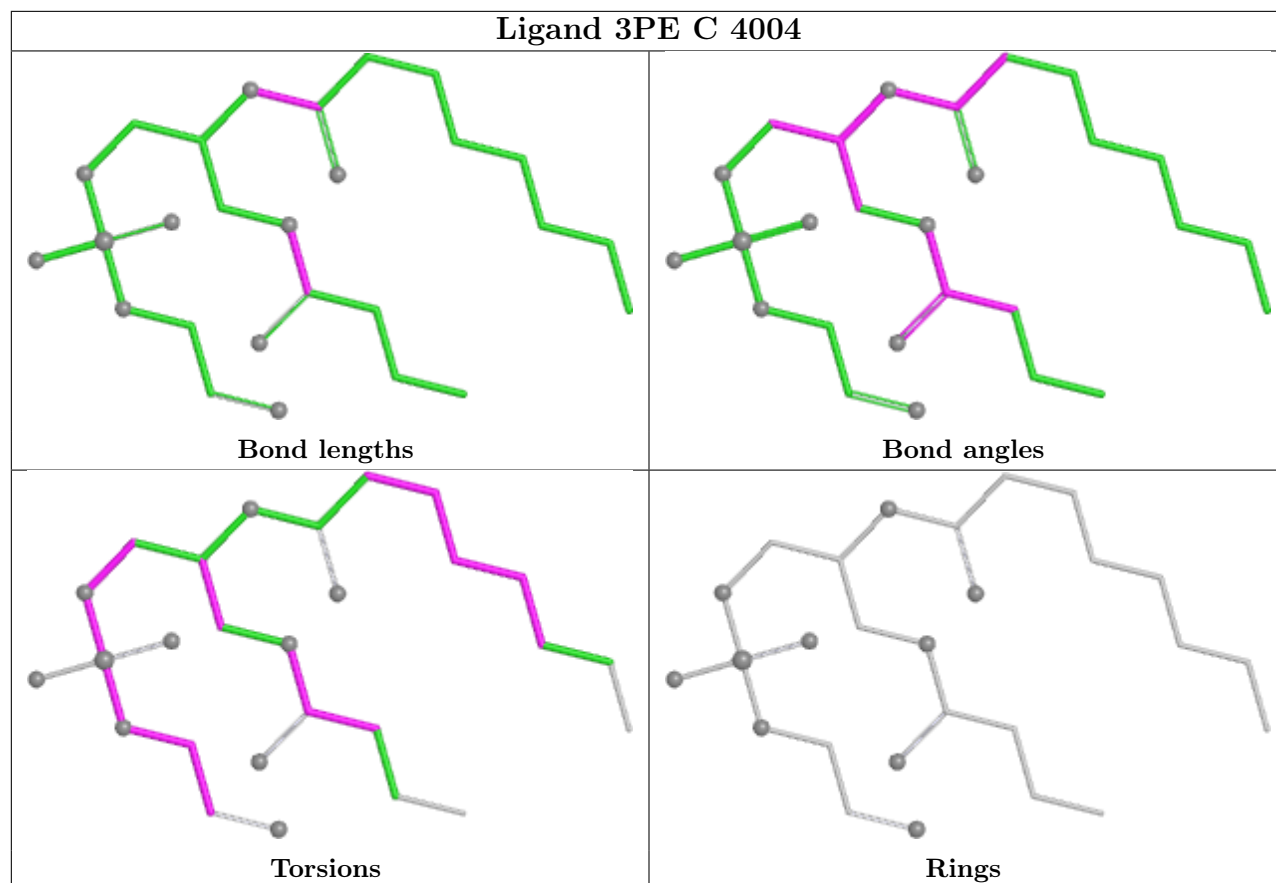
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

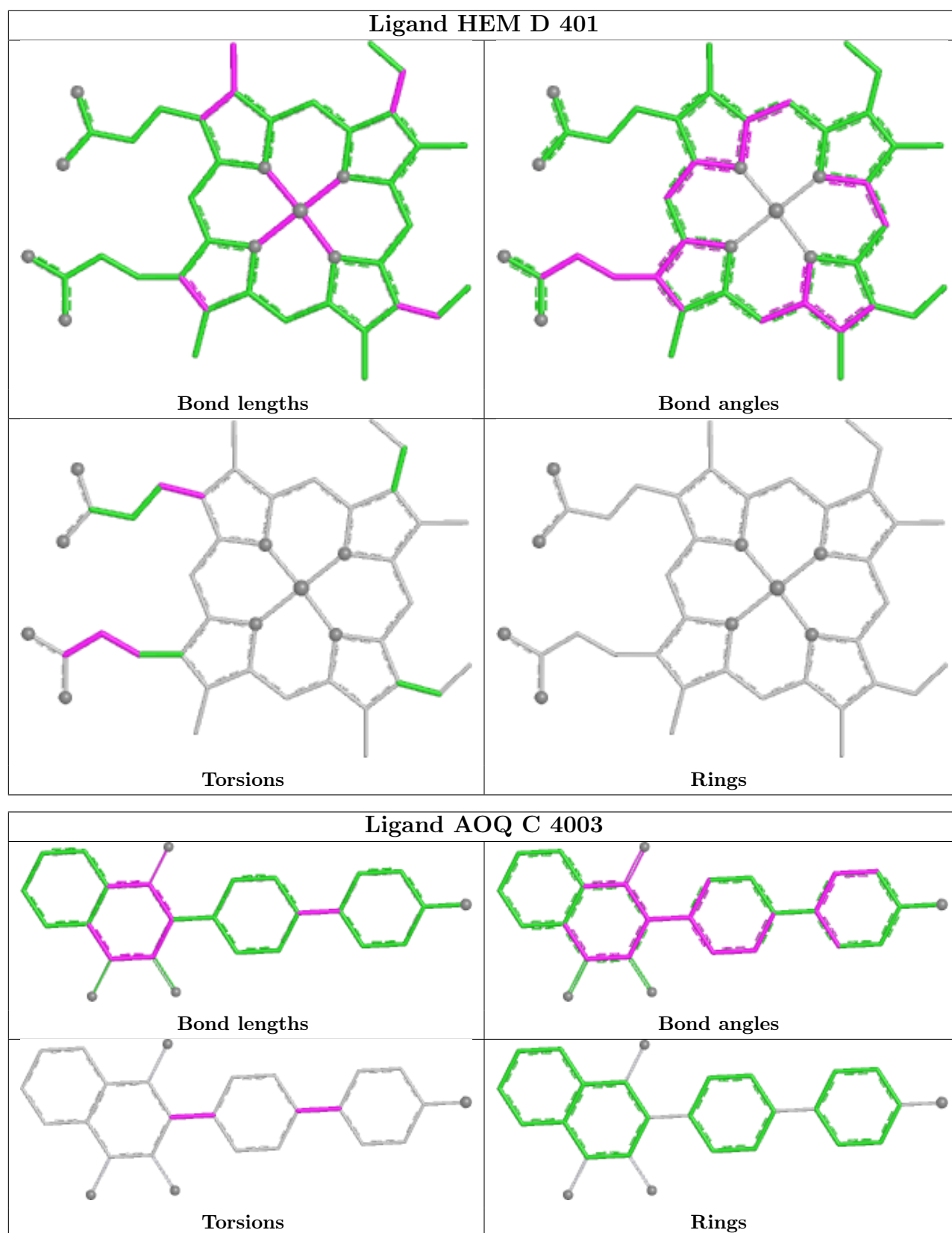












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/431 (96%)	0.42	24 (5%) 29 14	17, 69, 116, 122	0
2	B	344/352 (97%)	0.52	22 (6%) 25 13	29, 71, 104, 127	0
3	C	384/385 (99%)	-0.40	1 (0%) 90 79	0, 7, 18, 69	0
4	D	248/248 (100%)	-0.00	0 100 100	16, 40, 63, 83	1 (0%)
5	E	182/185 (98%)	-0.20	2 (1%) 78 56	4, 26, 70, 112	0
6	F	74/74 (100%)	0.30	1 (1%) 73 50	38, 61, 92, 94	0
7	G	126/126 (100%)	-0.39	0 100 100	6, 27, 48, 67	0
8	H	82/93 (88%)	-0.00	3 (3%) 45 25	7, 29, 67, 88	1 (1%)
9	I	57/57 (100%)	0.04	1 (1%) 67 43	24, 45, 78, 102	0
10	J	127/127 (100%)	-0.05	0 100 100	27, 44, 63, 68	0
11	K	107/107 (100%)	0.32	4 (3%) 45 25	36, 67, 105, 116	0
All	All	2148/2185 (98%)	0.08	58 (2%) 56 32	0, 42, 102, 127	2 (0%)

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	4.7
3	C	384	ASN	4.5
8	H	45	VAL	4.2
2	B	230	ARG	4.2
11	K	15	LEU	4.1

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](#)

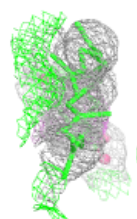
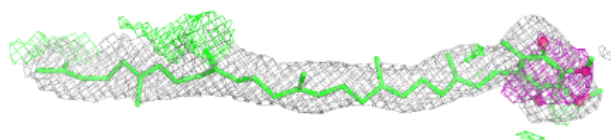
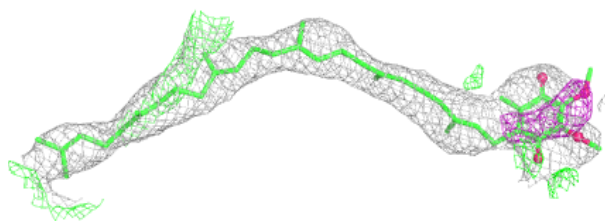
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	UQ6	C	4005	43/43	0.76	0.16	6,12,21,24	0
13	3PH	C	4006	35/48	0.88	0.12	3,17,29,39	0
12	UMQ	A	501	34/34	0.89	0.10	13,31,43,48	0
13	3PH	A	502	31/48	0.90	0.10	13,20,33,38	0
13	3PH	E	302	38/48	0.92	0.11	7,15,21,23	0
15	AOQ	C	4003	26/26	0.94	0.08	7,12,16,22	0
16	3PE	C	4004	27/51	0.95	0.07	4,8,12,14	0
14	HEM	D	401	43/43	0.95	0.10	22,31,37,43	0
14	HEM	C	4001	43/43	0.98	0.10	0,2,7,20	0
14	HEM	C	4002	43/43	0.98	0.09	2,5,10,11	0
18	FES	E	301	4/4	0.99	0.03	6,7,7,13	0

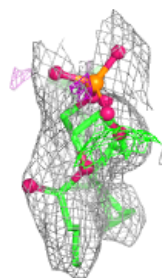
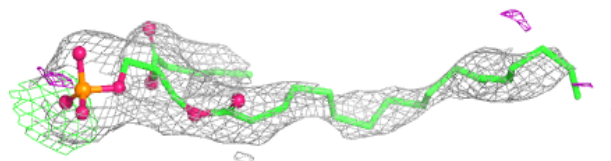
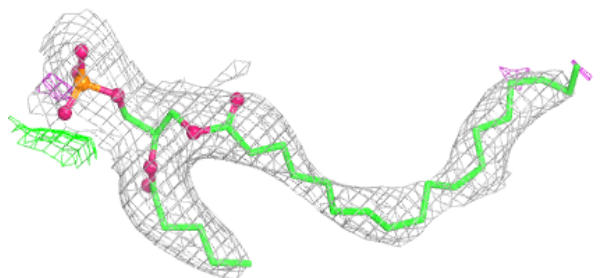
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ6 C 4005:

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

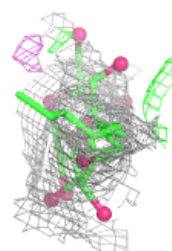
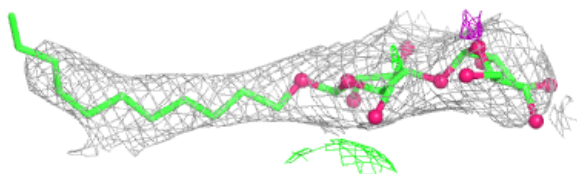
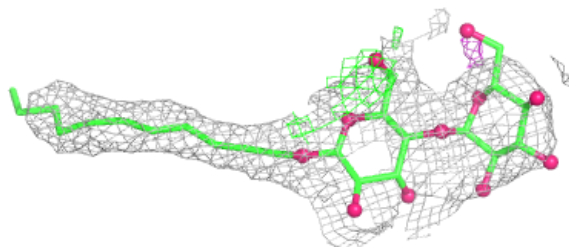
**Electron density around 3PH C 4006:**

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

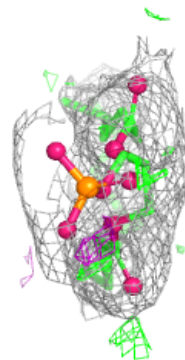
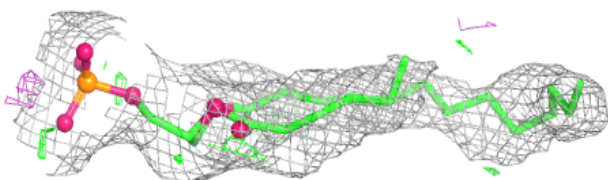
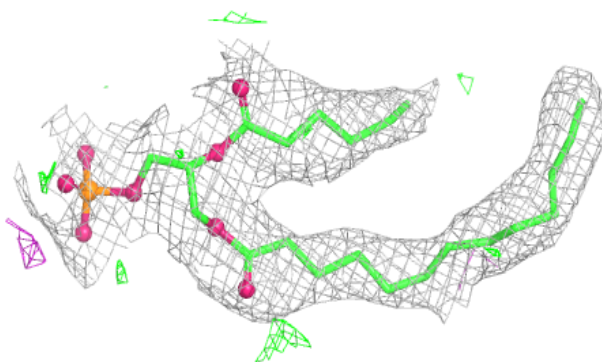


Electron density around UMQ A 501:

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

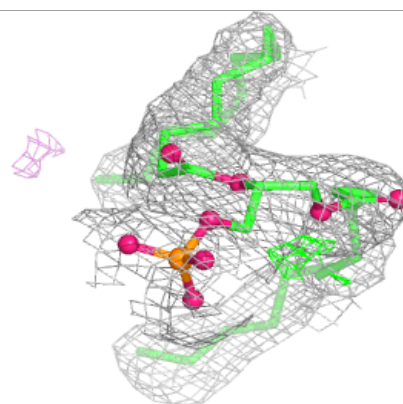
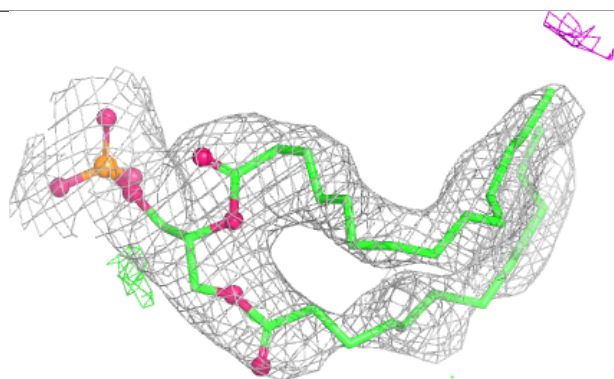
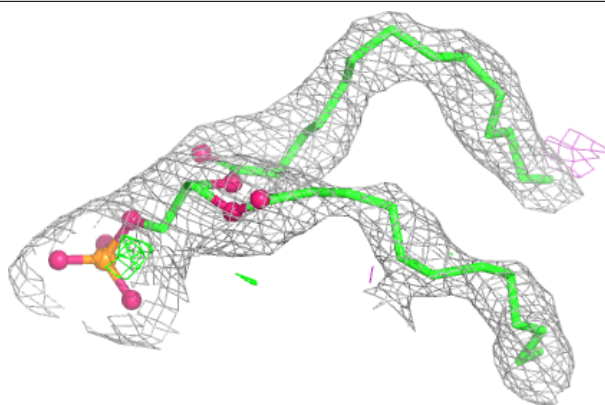
**Electron density around 3PH A 502:**

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

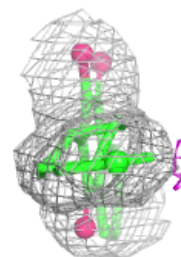
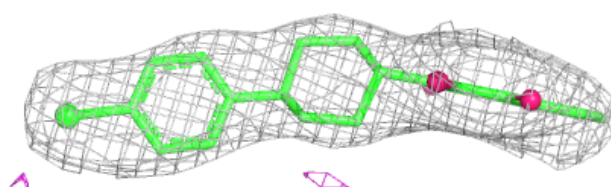
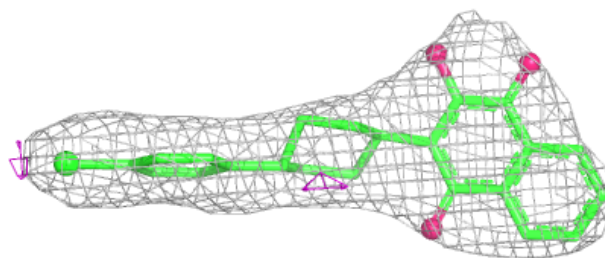


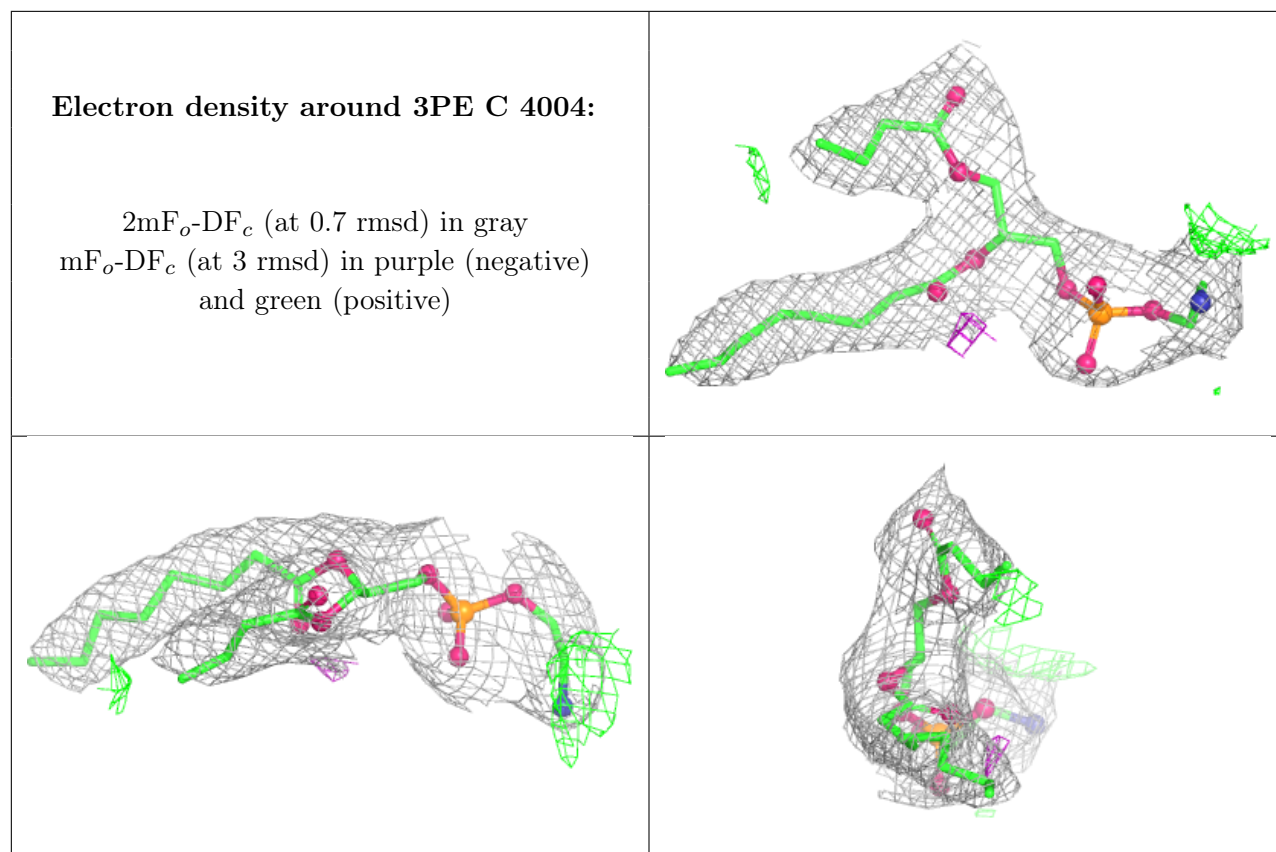
Electron density around 3PH E 302:

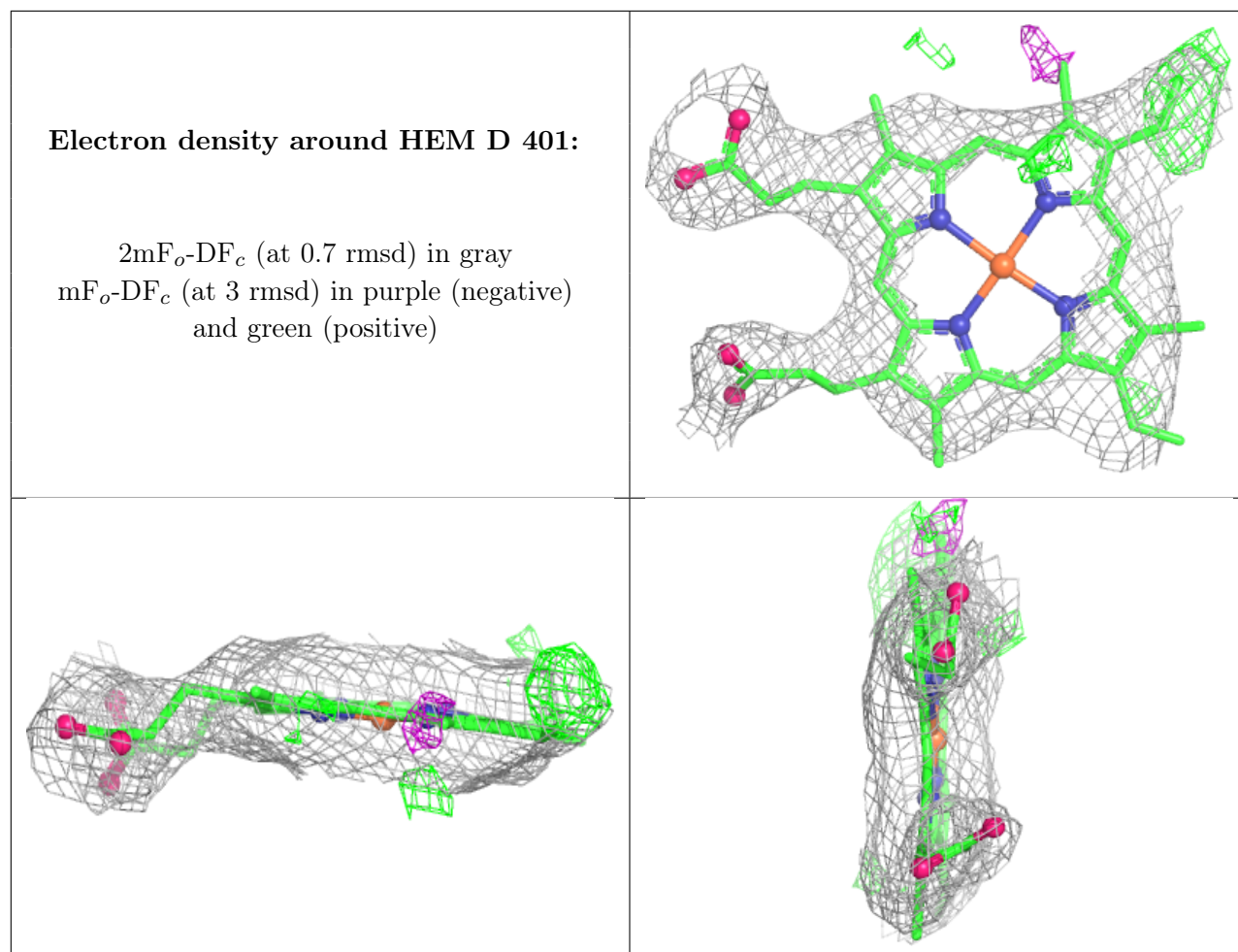
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AOQ C 4003:**

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

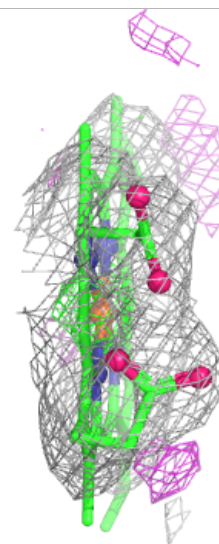
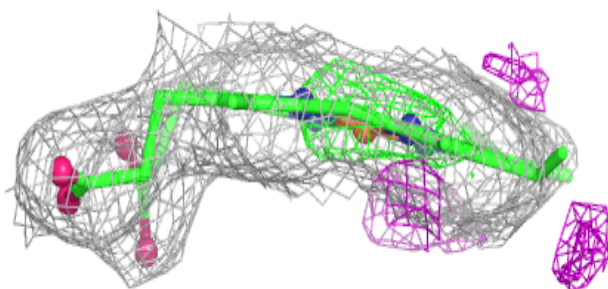
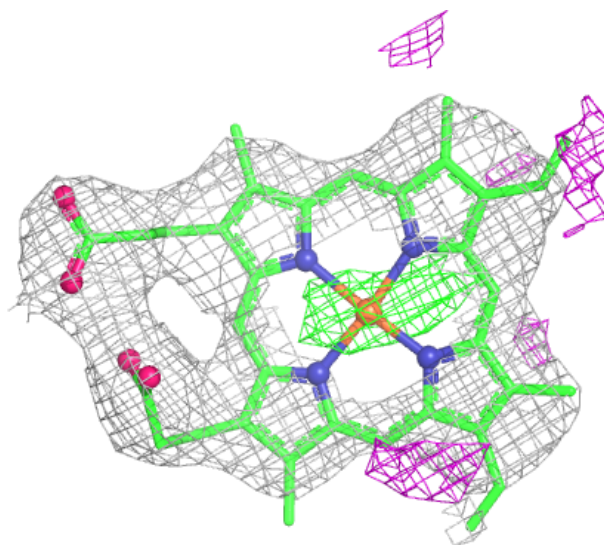


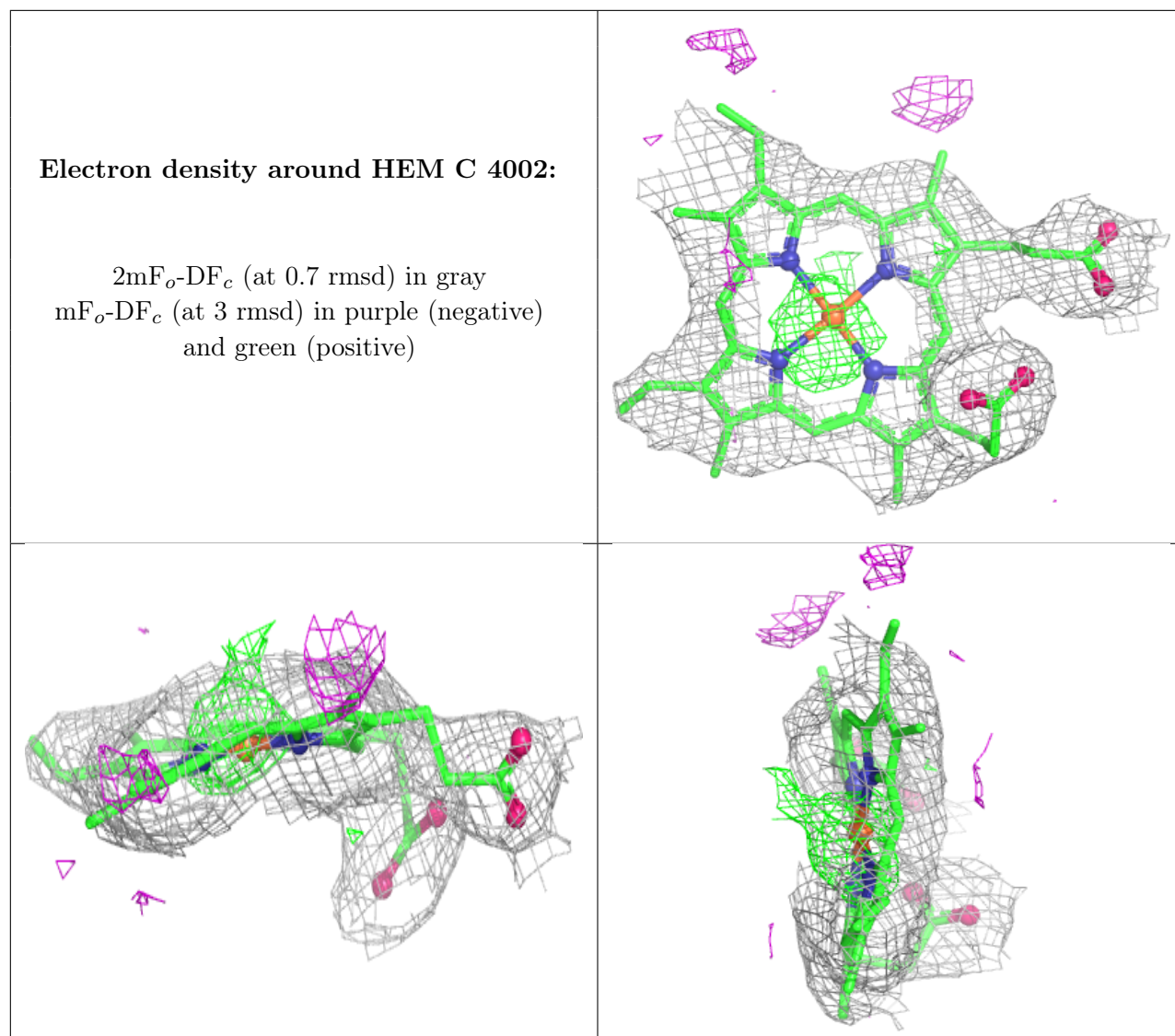




Electron density around HEM C 4001:

$2mF_o-DF_c$ (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.