



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:24 am BST

PDB ID : 6JY3
Title : Monomeric Form of Bovine Heart Cytochrome c Oxidase in the Fully Oxidized State
Authors : Shinzawa-Itoh, K.; Muramoto, K.
Deposited on : 2019-04-26
Resolution : 1.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

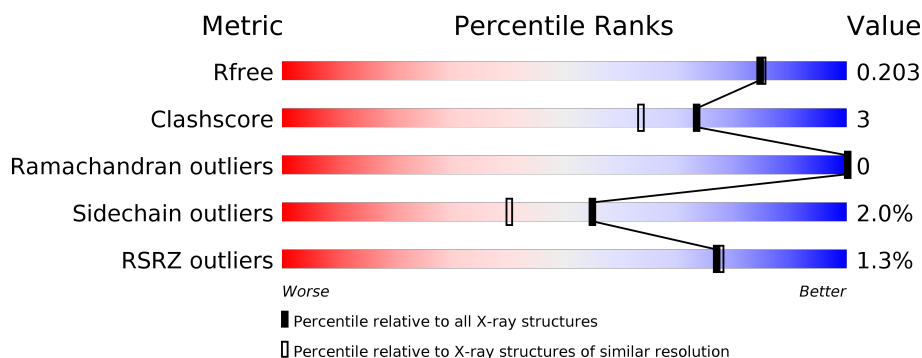
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	514	<div> <div style="width: 94%;"></div> <div style="width: 6%;"></div> </div>
2	B	227	<div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div>
3	C	261	<div> <div style="width: 92%;"></div> <div style="width: 5%;"></div> <div style="width: 3%;"></div> </div>
4	D	147	<div> <div style="width: 87%;"></div> <div style="width: 5%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div>
5	E	109	<div> <div style="width: 87%;"></div> <div style="width: 6%;"></div> <div style="width: 6%;"></div> </div>
6	F	98	<div> <div style="width: 82%;"></div> <div style="width: 8%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> </div>

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Mol	Chain	Length	Quality of chain
7	G	85	
8	H	85	
9	I	73	
10	J	59	
11	K	56	
12	L	47	
13	M	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 15245 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	254	Total	C	N	O	S	0	0	0
			2061	1379	327	343	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	136	Total	C	N	O	S	0	0	0
			1133	740	186	203	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	0	0
			694	432	122	135	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	72	Total	C	N	O	S	0	0	0
			595	387	113	94	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	55	Total	C	N	O	S	0	0	0
			434	280	72	79	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

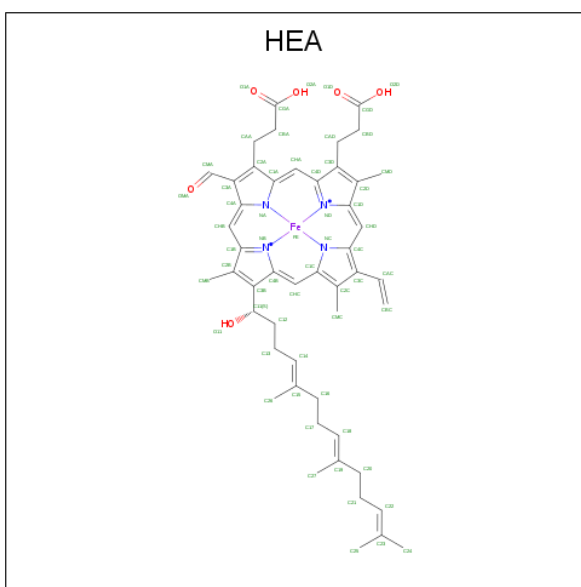
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	40	Total	C	N	O	0	0	0
			311	208	48	55			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		

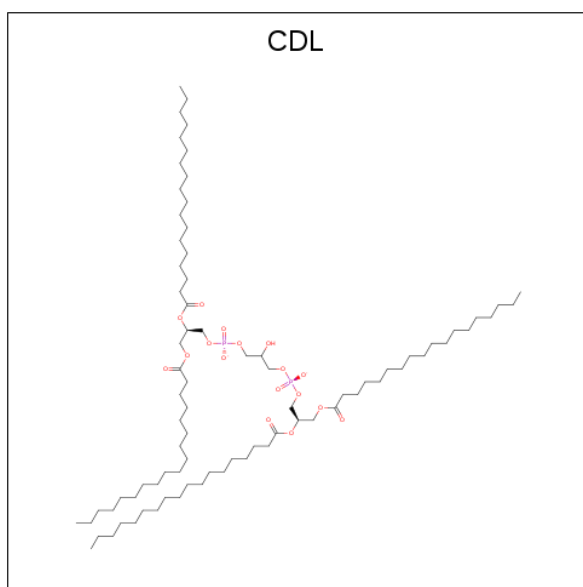
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

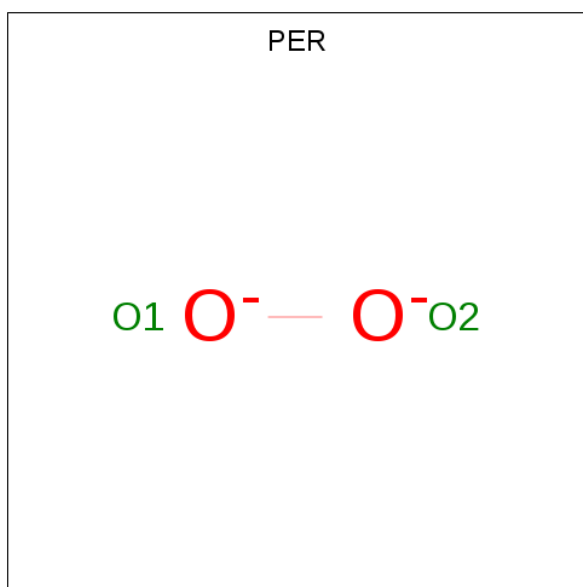
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by author).



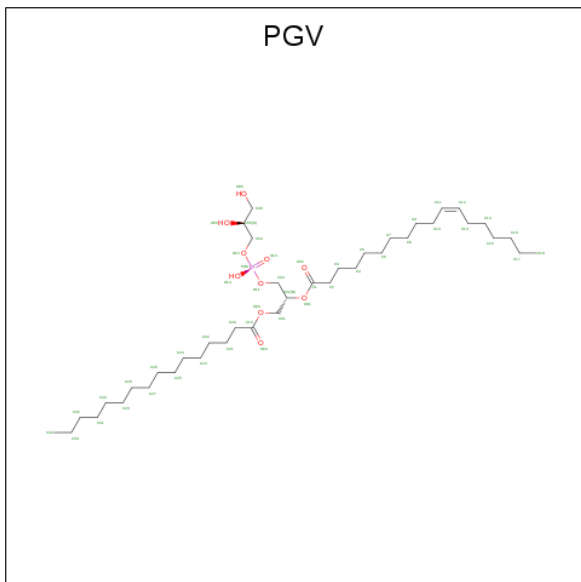
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			94	75	17	2		
18	B	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



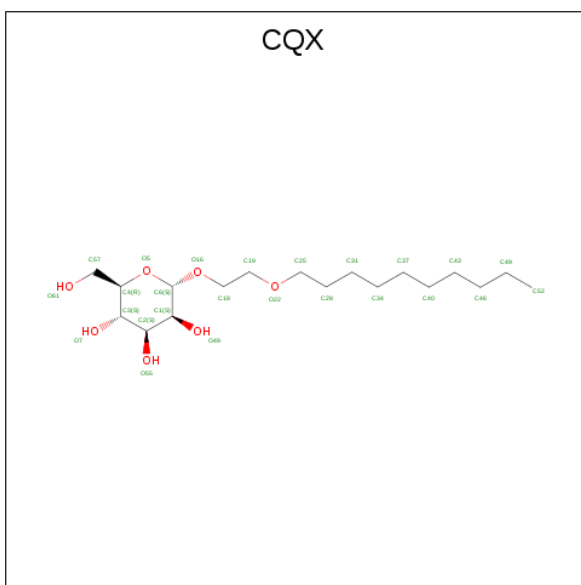
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



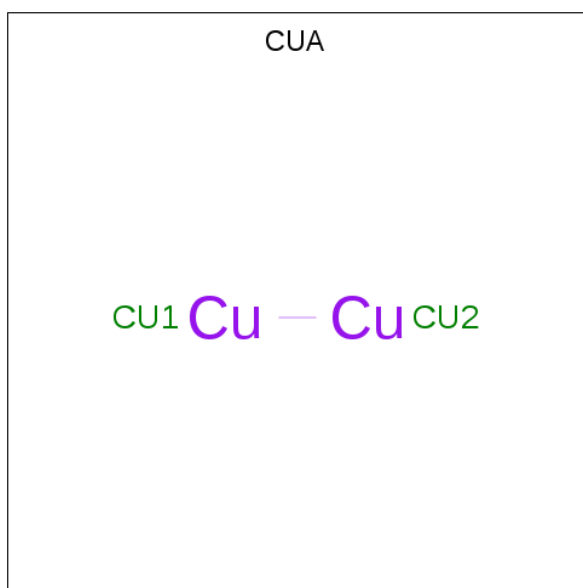
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			41	30	10	1		

- Molecule 21 is (2S,3S,4S,5S,6R)-2-(2-decoxyethoxy)-6-(hydroxymethyl)oxane-3,4,5-triol (three-letter code: CQX) (formula: C₁₈H₃₆O₇) (labeled as "Ligand of Interest" by author).



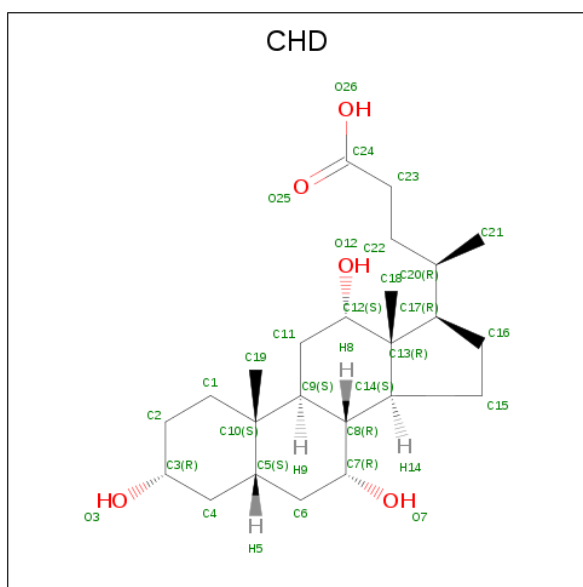
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			25	18	7		
21	A	1	Total	C	O	0	0
			25	18	7		
21	A	1	Total	C	O	0	0
			25	18	7		
21	B	1	Total	C	O	0	0
			25	18	7		
21	B	1	Total	C	O	0	0
			16	9	7		
21	C	1	Total	C	O	0	0
			25	18	7		
21	C	1	Total	C	O	0	0
			25	18	7		
21	G	1	Total	C	O	0	0
			25	18	7		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



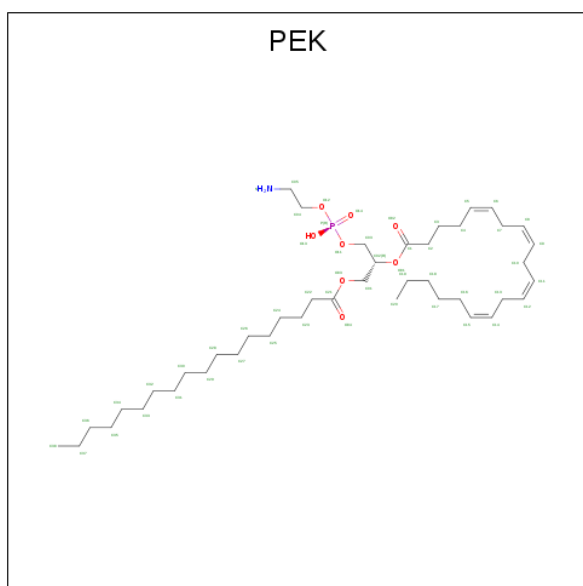
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Cu	0	0
			2	2		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	F	1	Total 1	Zn 1	0	0

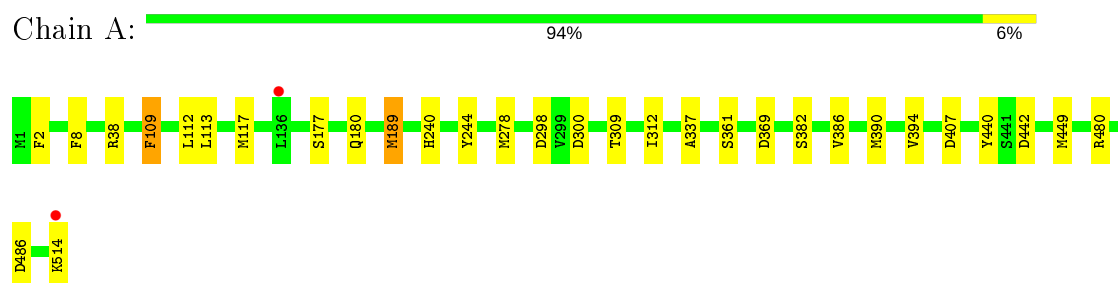
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	204	Total 205	O 205	0	1
26	B	124	Total 125	O 125	0	1
26	C	79	Total 79	O 79	0	0
26	D	41	Total 41	O 41	0	0
26	E	31	Total 31	O 31	0	0
26	F	46	Total 47	O 47	0	1
26	G	37	Total 37	O 37	0	0
26	H	40	Total 40	O 40	0	0
26	I	17	Total 17	O 17	0	0
26	J	9	Total 9	O 9	0	0
26	K	12	Total 12	O 12	0	0
26	L	13	Total 13	O 13	0	0
26	M	9	Total 9	O 9	0	0

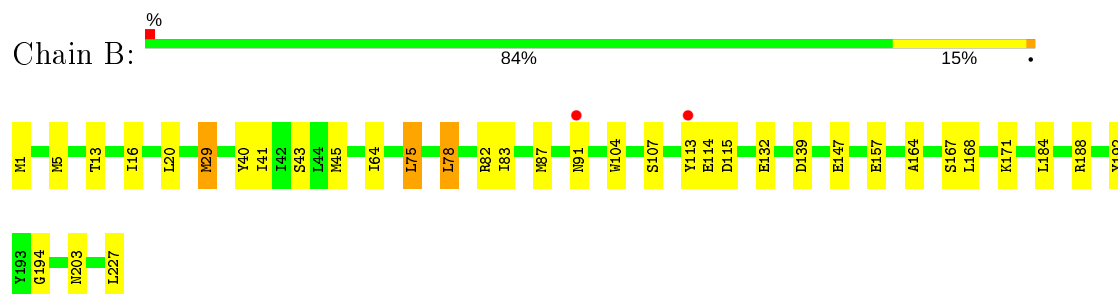
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

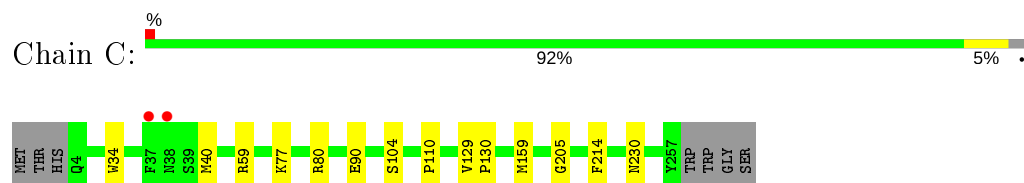
• Molecule 1: Cytochrome c oxidase subunit 1



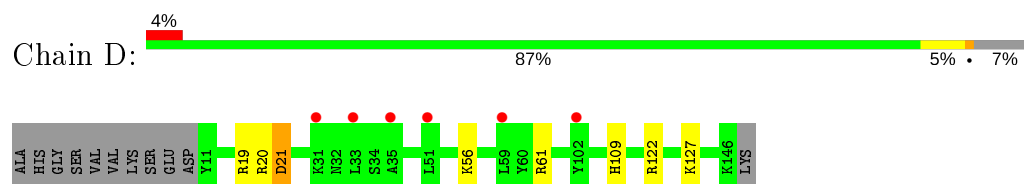
• Molecule 2: Cytochrome c oxidase subunit 2



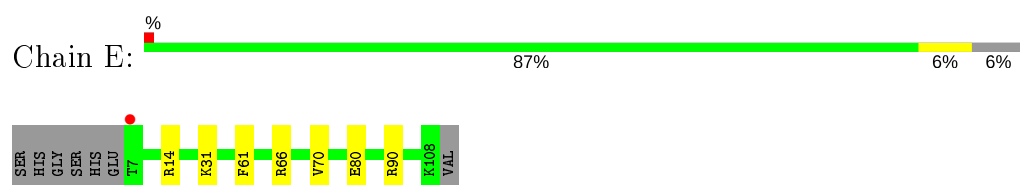
• Molecule 3: Cytochrome c oxidase subunit 3



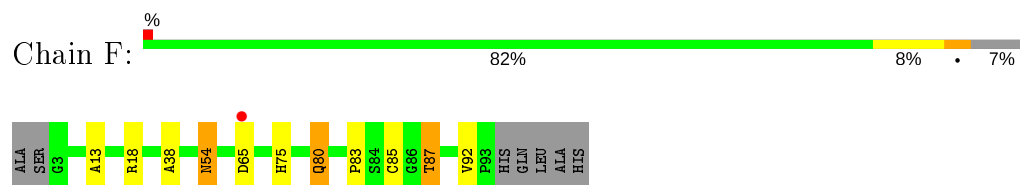
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



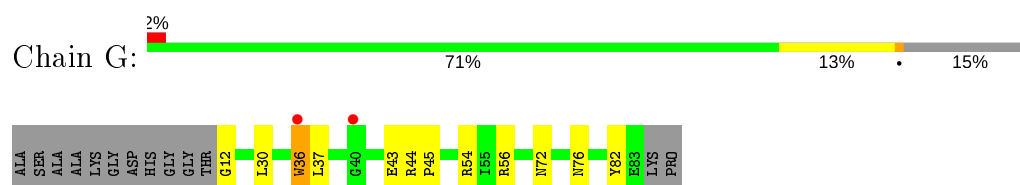
• Molecule 5: Cytochrome c oxidase subunit 5A



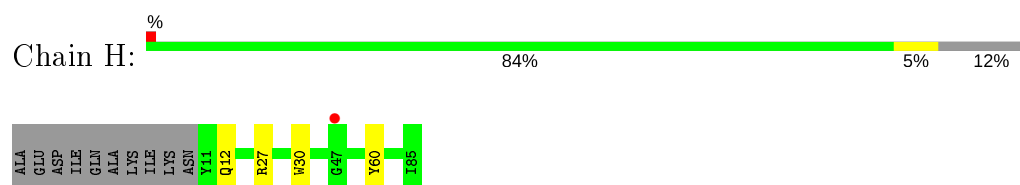
- Molecule 6: Cytochrome c oxidase subunit 5B



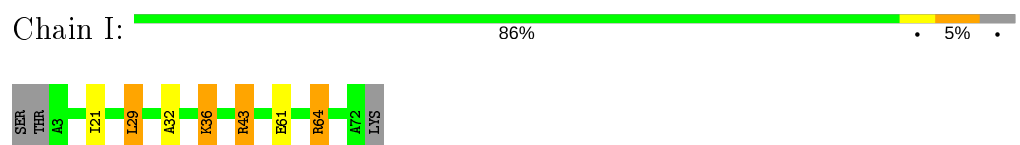
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



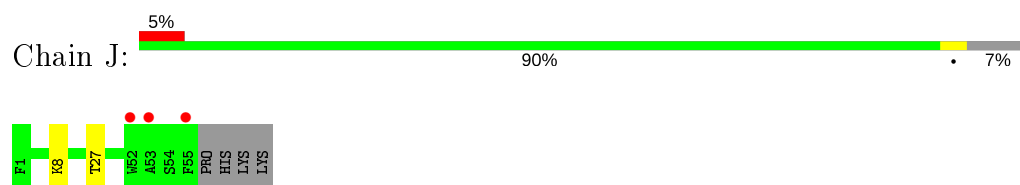
- Molecule 8: Cytochrome c oxidase subunit 6B1



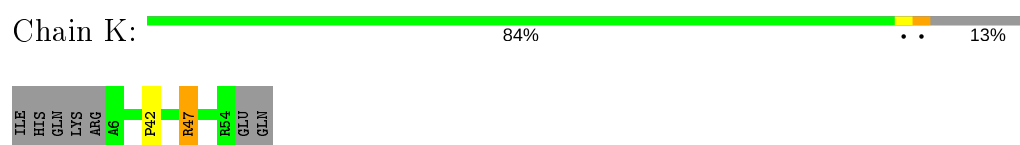
- Molecule 9: Cytochrome c oxidase subunit 6C



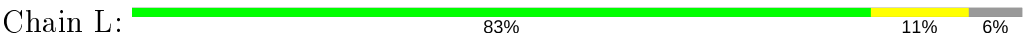
- Molecule 10: Cytochrome c oxidase subunit 7A1



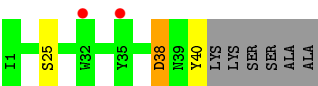
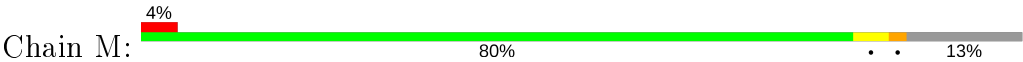
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.53Å 152.13Å 174.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 113.43 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-1.85) 98.9 (113.43-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.151 , 0.192 0.166 , 0.203	Depositor DCC
R_{free} test set	17846 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15245	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: ZN, CHD, CDL, NA, MG, PER, PGV, CQX, HEA, CUA, PEK, FME, CU

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	1.08	7/4156 (0.2%)	0.96	11/5678 (0.2%)
2	B	1.09	7/1860 (0.4%)	1.06	8/2534 (0.3%)
3	C	1.06	2/2143 (0.1%)	0.87	3/2931 (0.1%)
4	D	0.94	2/1167 (0.2%)	1.03	6/1577 (0.4%)
5	E	0.89	1/843 (0.1%)	0.85	3/1145 (0.3%)
6	F	0.90	0/709	0.87	0/963
7	G	1.21	1/621 (0.2%)	1.04	3/848 (0.4%)
8	H	0.98	0/648	0.89	1/877 (0.1%)
9	I	0.95	0/588	0.99	3/781 (0.4%)
10	J	0.91	0/443	0.87	0/598
11	K	0.93	0/398	0.95	1/546 (0.2%)
12	L	1.07	0/372	0.92	0/500
13	M	0.92	0/321	0.89	0/440
All	All	1.03	20/14269 (0.1%)	0.95	39/19418 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	F	0	1
All	All	0	2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	17.33	1.81	1.50
3	C	104	SER	CB-OG	13.02	1.59	1.42
3	C	104	SER	CA-CB	10.05	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	SER	CB-OG	-8.47	1.31	1.42
1	A	244	TYR	CE2-CZ	6.72	1.47	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	16.37	128.48	120.30
2	B	29	MET	CG-SD-CE	-11.55	81.71	100.20
4	D	21	ASP	CB-CG-OD1	10.61	127.84	118.30
4	D	21	ASP	CB-CG-OD2	-9.05	110.16	118.30
11	K	47	ARG	NE-CZ-NH1	9.03	124.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	65	ASP	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	4027	0	4001	23	0
2	B	1824	0	1833	17	0
3	C	2061	0	1992	7	0
4	D	1133	0	1119	3	0
5	E	825	0	823	2	0
6	F	694	0	677	8	0
7	G	595	0	569	11	0
8	H	628	0	580	1	0
9	I	575	0	584	5	0
10	J	434	0	432	4	0
11	K	384	0	366	1	0
12	L	360	0	360	4	0
13	M	311	0	321	4	0
14	A	120	0	108	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	1	0	0	0	0
16	A	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
18	A	94	0	141	10	0
18	B	64	0	72	0	0
18	C	87	0	124	9	0
19	A	2	0	0	1	0
20	A	51	0	76	1	0
20	C	41	0	55	0	0
21	A	75	0	0	2	0
21	B	41	0	0	0	0
21	C	50	0	0	1	0
21	G	25	0	0	0	0
22	B	2	0	0	0	0
23	C	29	0	39	1	0
24	C	43	0	58	2	0
25	F	1	0	0	0	0
26	A	205	0	0	5	0
26	B	125	0	0	2	0
26	C	79	0	0	0	0
26	D	41	0	0	1	0
26	E	31	0	0	0	0
26	F	47	0	0	0	0
26	G	37	0	0	3	0
26	H	40	0	0	0	0
26	I	17	0	0	1	0
26	J	9	0	0	1	0
26	K	12	0	0	0	0
26	L	13	0	0	0	0
26	M	9	0	0	2	0
All	All	15245	0	14330	94	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 3.

The worst 5 of 94 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)
7:G:36:TRP:CG	7:G:36:TRP:CB	1.81	1.59
19:A:607:PER:O1	19:A:607:PER:O2	1.55	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HG	26:A:892:HOH:O	1.58	1.02
18:C:305:CDL:O1	10:J:8:LYS:HD2	1.65	0.95
1:A:312:ILE:HD12	26:A:837:HOH:O	1.65	0.94

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	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
2	B	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
3	C	252/261 (97%)	249 (99%)	3 (1%)	0	100	100
4	D	134/147 (91%)	128 (96%)	6 (4%)	0	100	100
5	E	100/109 (92%)	99 (99%)	1 (1%)	0	100	100
6	F	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
7	G	70/85 (82%)	66 (94%)	4 (6%)	0	100	100
8	H	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
9	I	68/73 (93%)	68 (100%)	0	0	100	100
10	J	53/59 (90%)	53 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
All	All	1703/1807 (94%)	1665 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	426/426 (100%)	422 (99%)	4 (1%)	78	72
2	B	210/210 (100%)	203 (97%)	7 (3%)	38	21
3	C	220/226 (97%)	218 (99%)	2 (1%)	78	72
4	D	120/129 (93%)	119 (99%)	1 (1%)	81	76
5	E	89/95 (94%)	87 (98%)	2 (2%)	52	36
6	F	76/81 (94%)	73 (96%)	3 (4%)	32	15
7	G	62/69 (90%)	59 (95%)	3 (5%)	25	10
8	H	67/75 (89%)	65 (97%)	2 (3%)	41	24
9	I	55/58 (95%)	52 (94%)	3 (6%)	21	7
10	J	46/50 (92%)	46 (100%)	0	100	100
11	K	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	36 (97%)	1 (3%)	44	29
13	M	34/38 (90%)	33 (97%)	1 (3%)	42	26
All	All	1481/1543 (96%)	1452 (98%)	29 (2%)	55	40

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	21	ASP
6	F	54	ASN
9	I	43	ARG
5	E	70	VAL
6	F	80	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	68	GLN
3	C	76	GLN

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Mol	Chain	Res	Type
6	F	80	GLN
3	C	50	ASN
7	G	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	FME	B	1	2	8,9,10	2.18	4 (50%)	7,9,11	6.04	4 (57%)
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	1.32	1 (14%)

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
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	5/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.54	1.12	1.22
2	B	1	FME	CN-N	3.52	1.45	1.33
2	B	1	FME	CG-SD	-2.19	1.69	1.81
2	B	1	FME	CA-N	2.14	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-12.03	104.31	122.82
2	B	1	FME	C-CA-N	8.75	125.52	109.73
2	B	1	FME	CG-CB-CA	-4.70	99.89	112.95
1	A	1	FME	CA-N-CN	-2.38	119.16	122.82
2	B	1	FME	O1-CN-N	-2.29	119.23	125.27

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 5 are monoatomic - leaving 19 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
24	PEK	C	303	-	42,42,52	0.80	2 (4%)	45,47,57	0.96	2 (4%)
21	CQX	C	307	-	25,25,25	0.57	0	30,30,30	0.82	1 (3%)
20	PGV	C	304	-	40,40,50	1.05	3 (7%)	43,46,56	1.35	4 (9%)
21	CQX	B	303	-	25,25,25	0.78	1 (4%)	30,30,30	1.99	11 (36%)
21	CQX	B	304	-	16,16,25	0.69	0	21,21,30	1.34	3 (14%)
22	CUA	B	302	2	0,1,1	0.00	-	-	-	-
21	CQX	C	306	-	25,25,25	1.22	2 (8%)	30,30,30	2.04	5 (16%)
20	PGV	A	608	-	50,50,50	0.92	3 (6%)	53,56,56	1.15	3 (5%)
19	PER	A	607	15,14	0,1,1	0.00	-	-	-	-
21	CQX	A	611	-	25,25,25	0.87	2 (8%)	30,30,30	1.65	7 (23%)
18	CDL	C	305	-	86,86,99	1.19	6 (6%)	92,98,111	1.38	13 (14%)
21	CQX	G	101	-	25,25,25	0.78	1 (4%)	30,30,30	0.89	0
21	CQX	A	610	-	25,25,25	1.06	2 (8%)	30,30,30	1.74	6 (20%)
14	HEA	A	601	1	44,67,67	1.34	7 (15%)	37,103,103	2.02	8 (21%)
18	CDL	B	301	-	63,63,99	1.53	5 (7%)	69,75,111	1.57	14 (20%)
21	CQX	A	609	-	25,25,25	0.88	1 (4%)	30,30,30	2.24	11 (36%)
23	CHD	C	301	-	29,32,32	0.83	1 (3%)	48,51,51	1.47	9 (18%)
18	CDL	A	606	-	93,93,99	0.98	4 (4%)	99,105,111	1.55	15 (15%)
14	HEA	A	602	1,19	44,67,67	1.18	3 (6%)	37,103,103	2.13	13 (35%)

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
24	PEK	C	303	-	-	8/46/46/56	-
21	CQX	C	307	-	-	7/16/36/36	0/1/1/1
20	PGV	C	304	-	-	9/45/45/55	-
21	CQX	B	303	-	-	7/16/36/36	0/1/1/1
21	CQX	B	304	-	-	0/7/27/36	0/1/1/1
20	PGV	A	608	-	-	7/55/55/55	-
21	CQX	C	306	-	-	7/16/36/36	0/1/1/1
21	CQX	A	611	-	-	4/16/36/36	0/1/1/1
18	CDL	C	305	-	-	51/97/97/110	-
21	CQX	G	101	-	-	1/16/36/36	0/1/1/1
21	CQX	A	610	-	-	2/16/36/36	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601	1	2/2/7/16	3/24/76/76	-
18	CDL	B	301	-	-	40/74/74/110	-
21	CQX	A	609	-	-	6/16/36/36	0/1/1/1
23	CHD	C	301	-	-	0/7/74/74	0/4/4/4
18	CDL	A	606	-	-	50/104/104/110	-
14	HEA	A	602	1,19	3/3/7/16	0/24/76/76	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	301	CDL	OA6-CA5	6.94	1.53	1.34
18	B	301	CDL	OB6-CB5	4.75	1.47	1.34
18	C	305	CDL	OB6-CB5	4.68	1.47	1.34
18	B	301	CDL	OB8-CB7	4.65	1.46	1.33
18	B	301	CDL	OA8-CA7	4.50	1.46	1.33

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C1B-C2B-C3B	-8.02	101.42	107.00
21	C	306	CQX	C18-O16-C6	6.78	125.09	113.84
18	A	606	CDL	CB4-OB6-CB5	-5.98	103.06	117.79
20	C	304	PGV	O03-C19-O04	-5.65	109.34	123.59
21	A	609	CQX	O16-C6-C1	-5.30	100.03	108.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA
14	A	602	HEA	NB

5 of 202 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	301	CDL	CA2-C1-CB2-OB2
18	B	301	CDL	CA3-OA5-PA1-OA2
18	B	301	CDL	CA3-OA5-PA1-OA3

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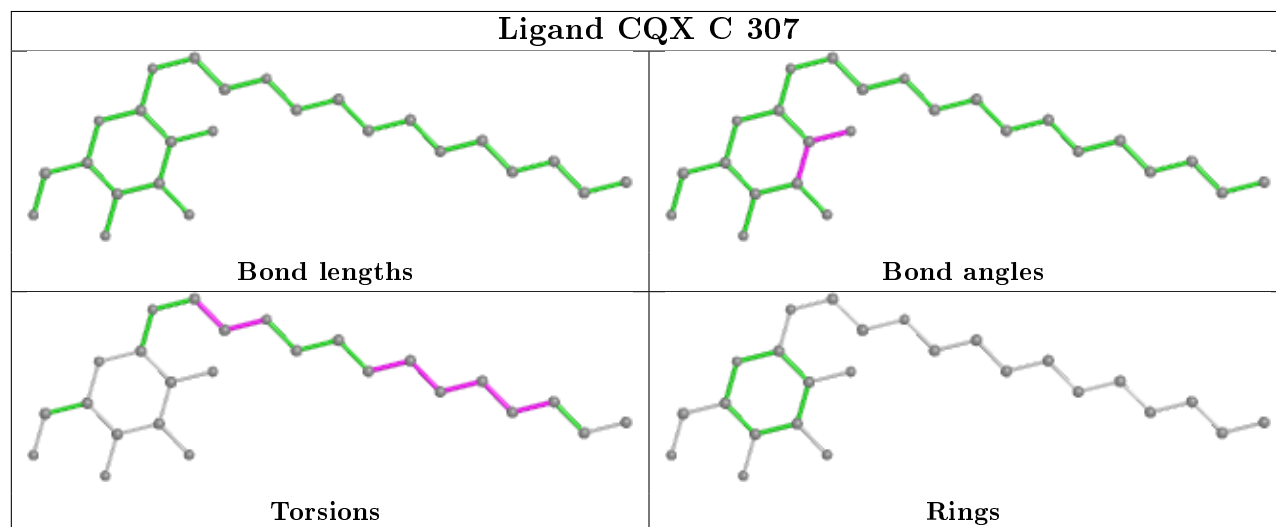
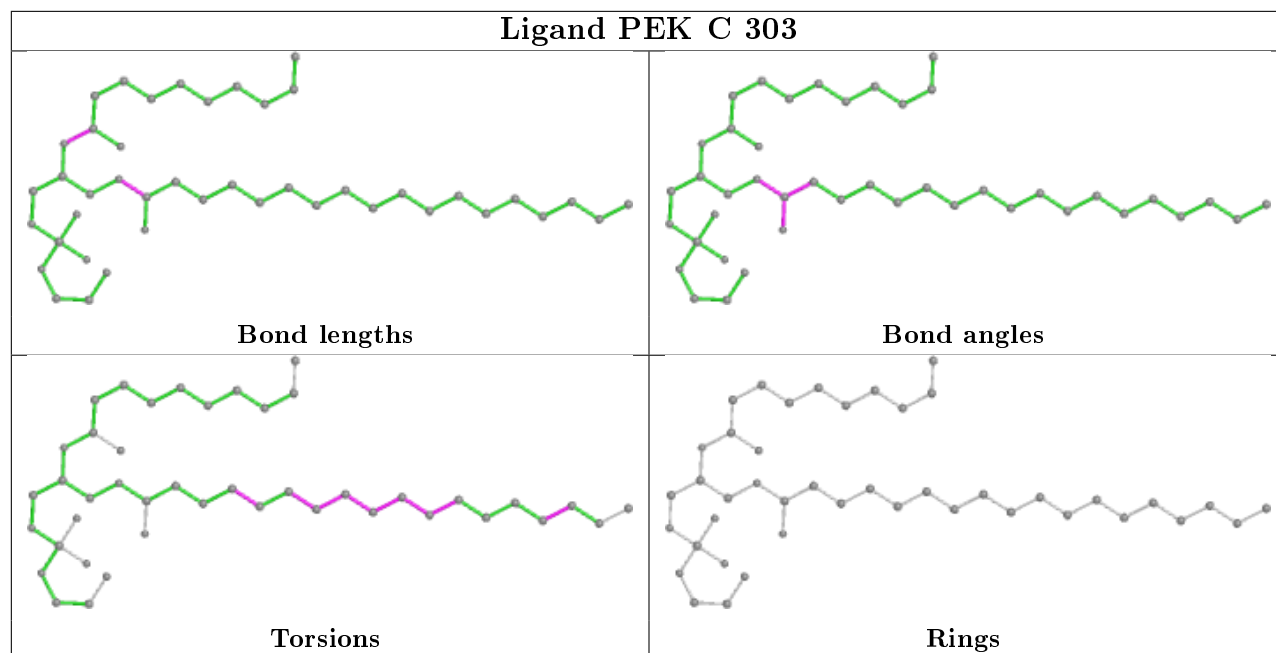
Mol	Chain	Res	Type	Atoms
18	B	301	CDL	CA3-OA5-PA1-OA4
18	B	301	CDL	C11-CA5-OA6-CA4

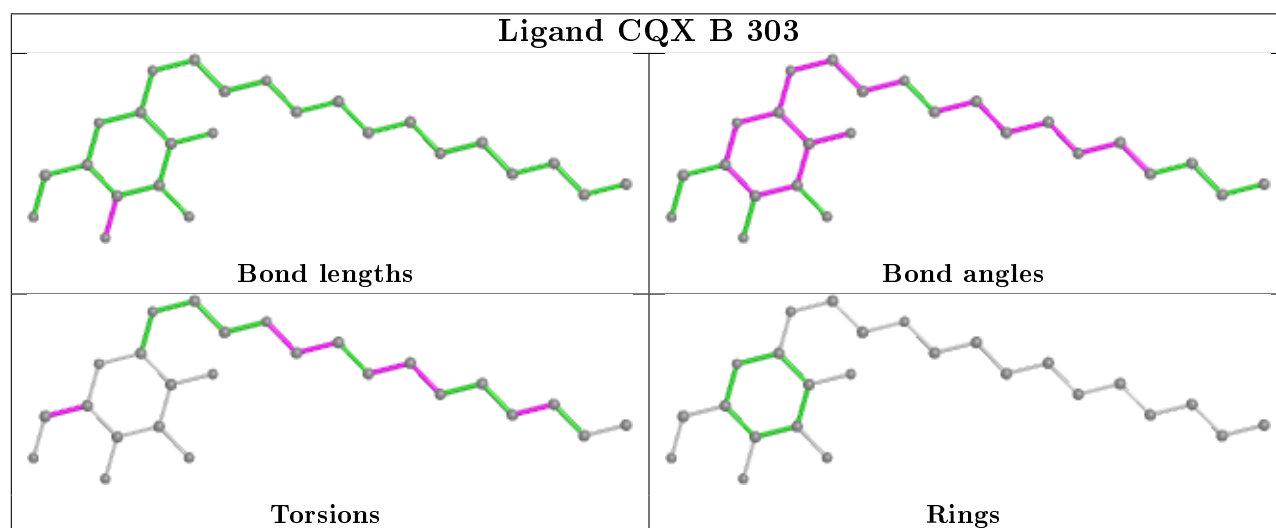
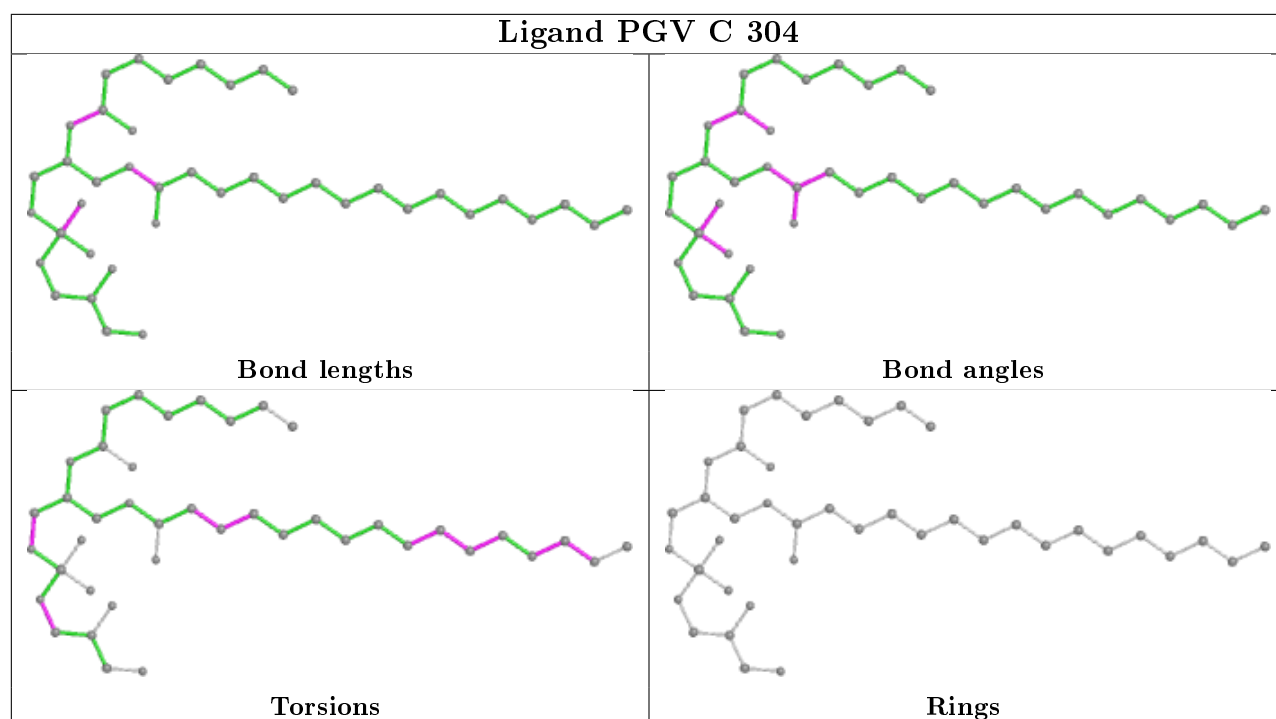
There are no ring outliers.

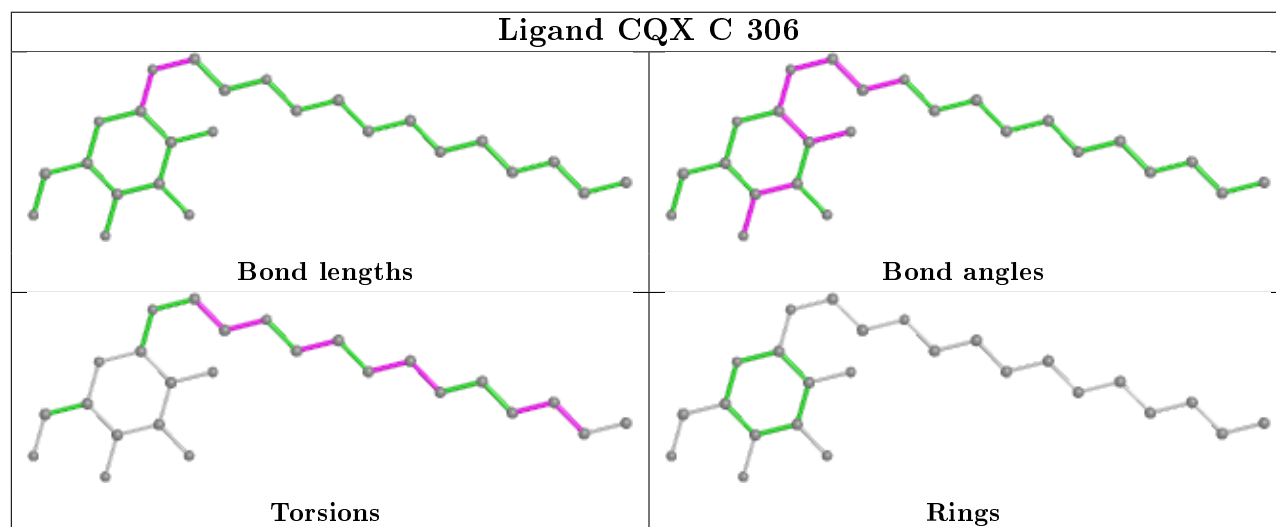
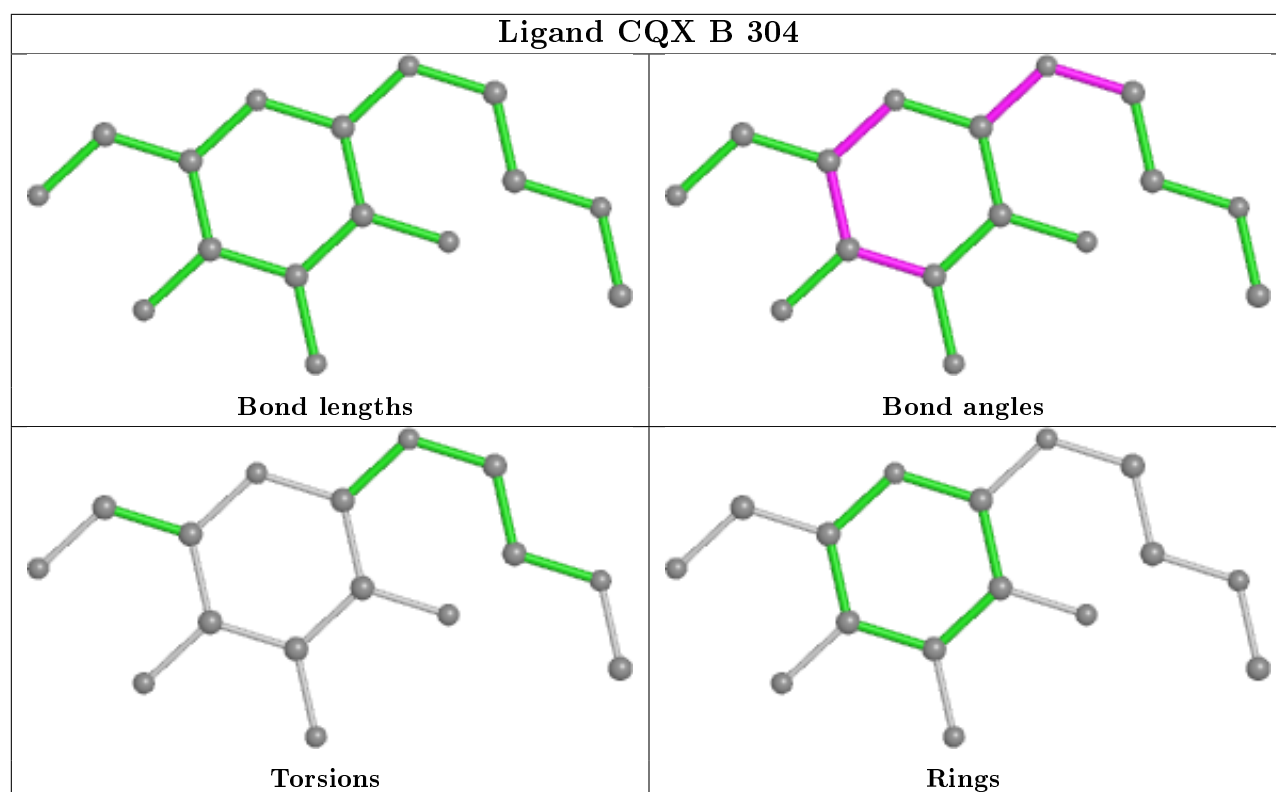
10 monomers are involved in 31 short contacts:

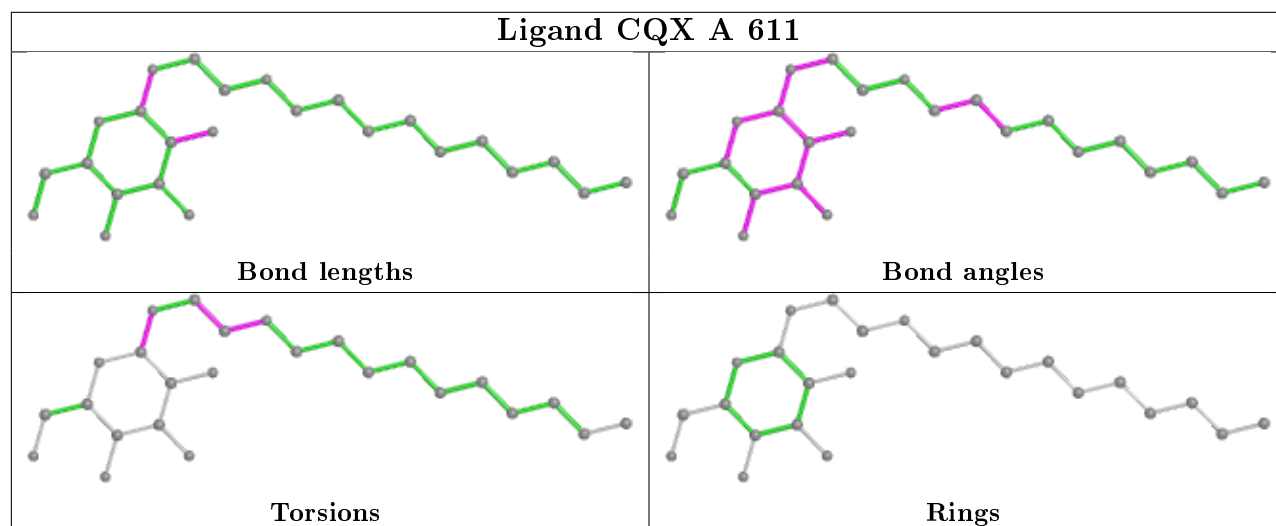
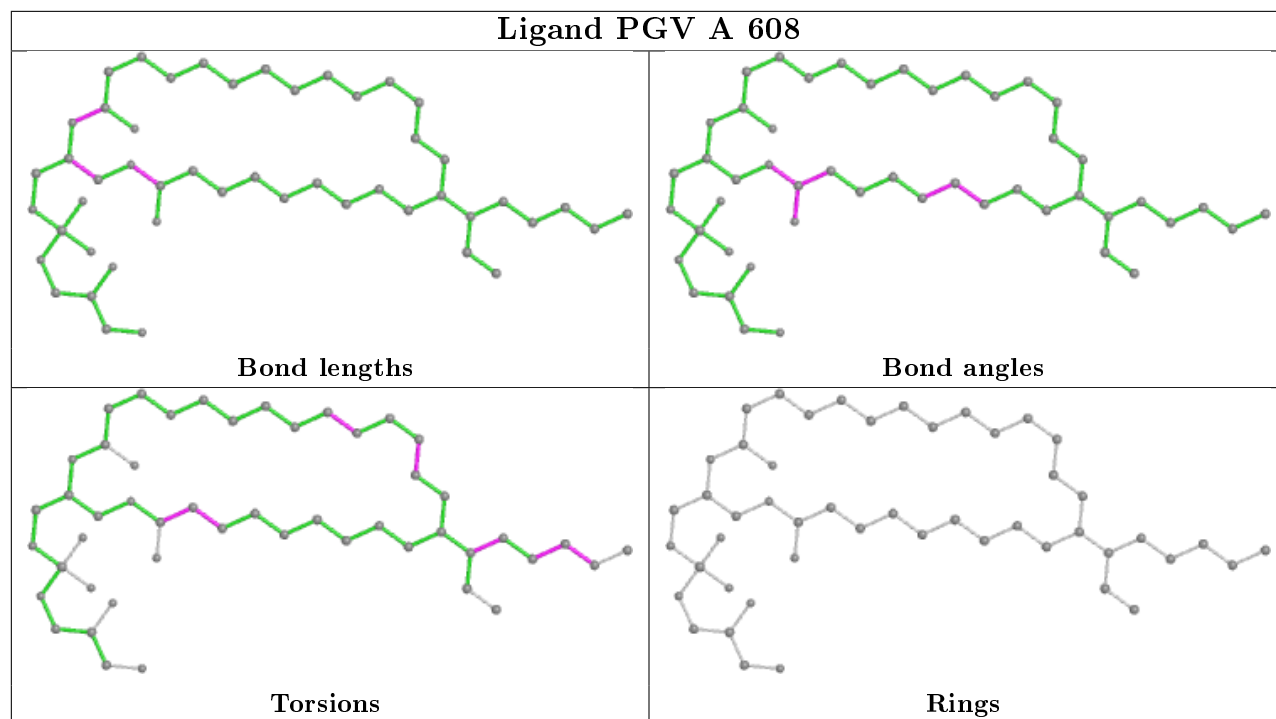
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	303	PEK	2	0
21	C	306	CQX	1	0
20	A	608	PGV	1	0
19	A	607	PER	1	0
18	C	305	CDL	9	0
21	A	610	CQX	2	0
14	A	601	HEA	3	0
23	C	301	CHD	1	0
18	A	606	CDL	10	0
14	A	602	HEA	2	0

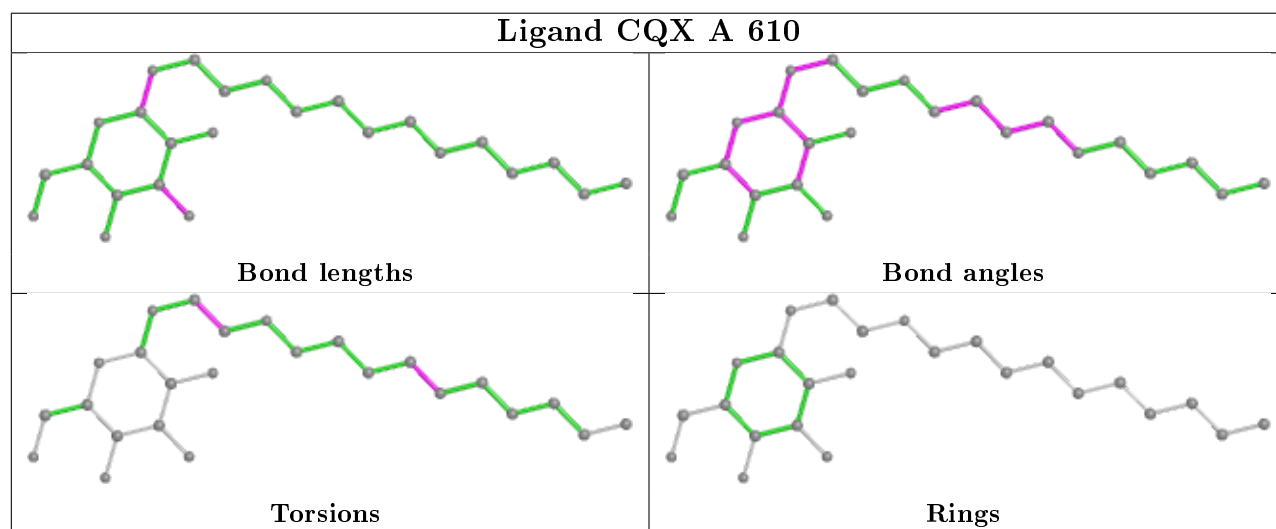
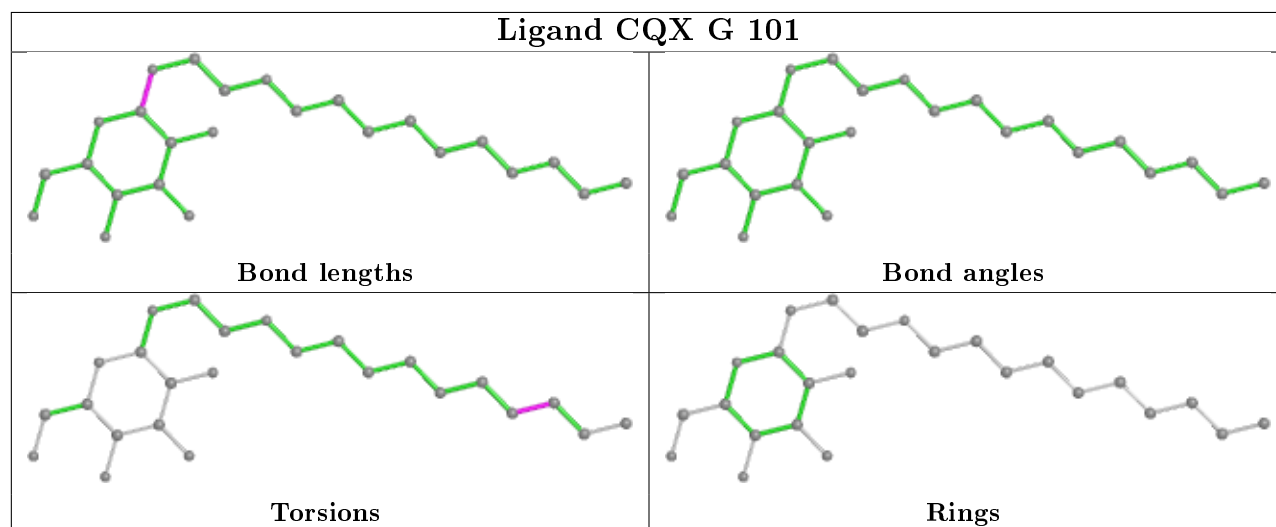
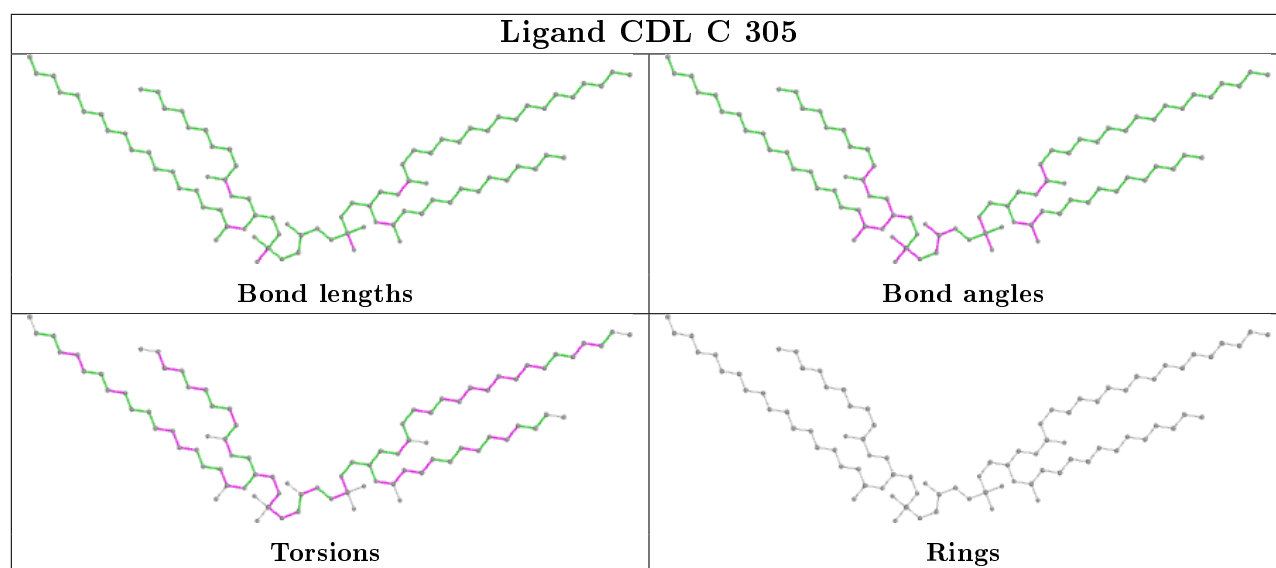
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

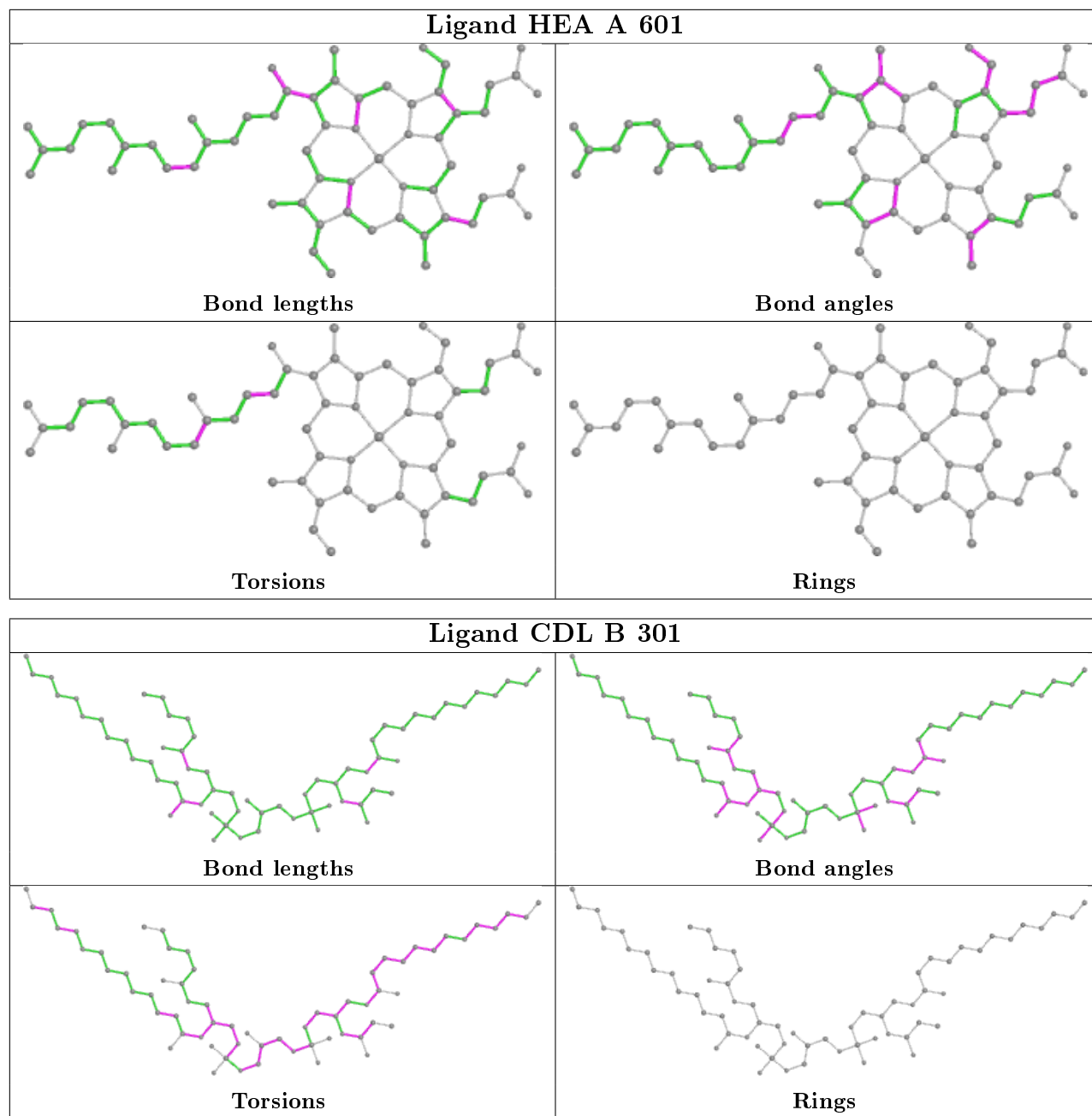


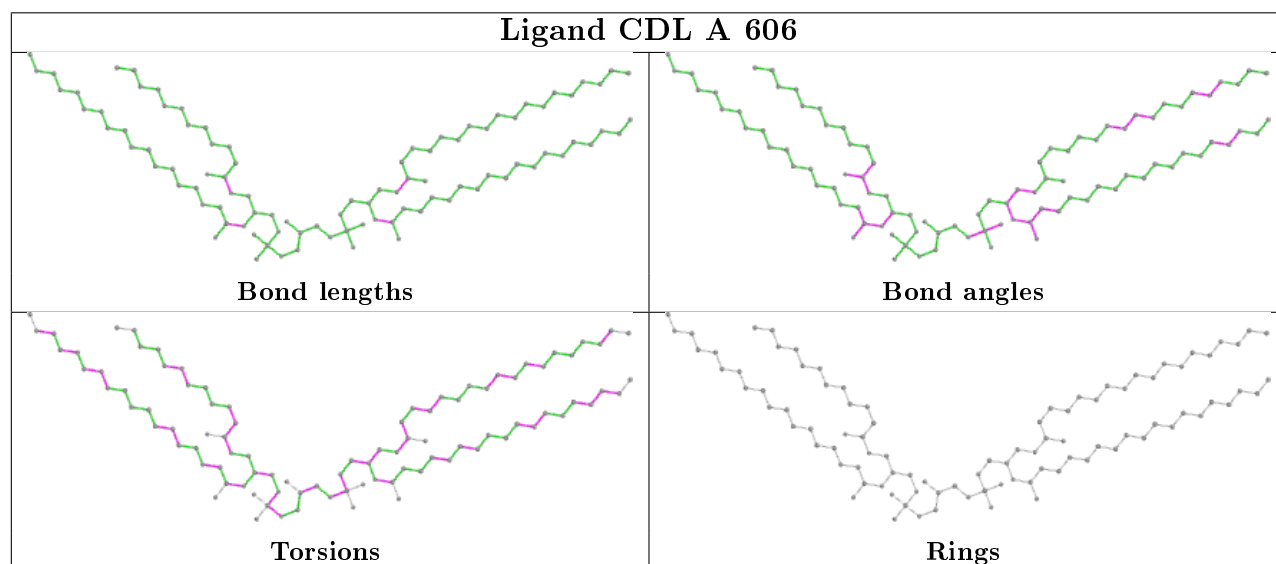
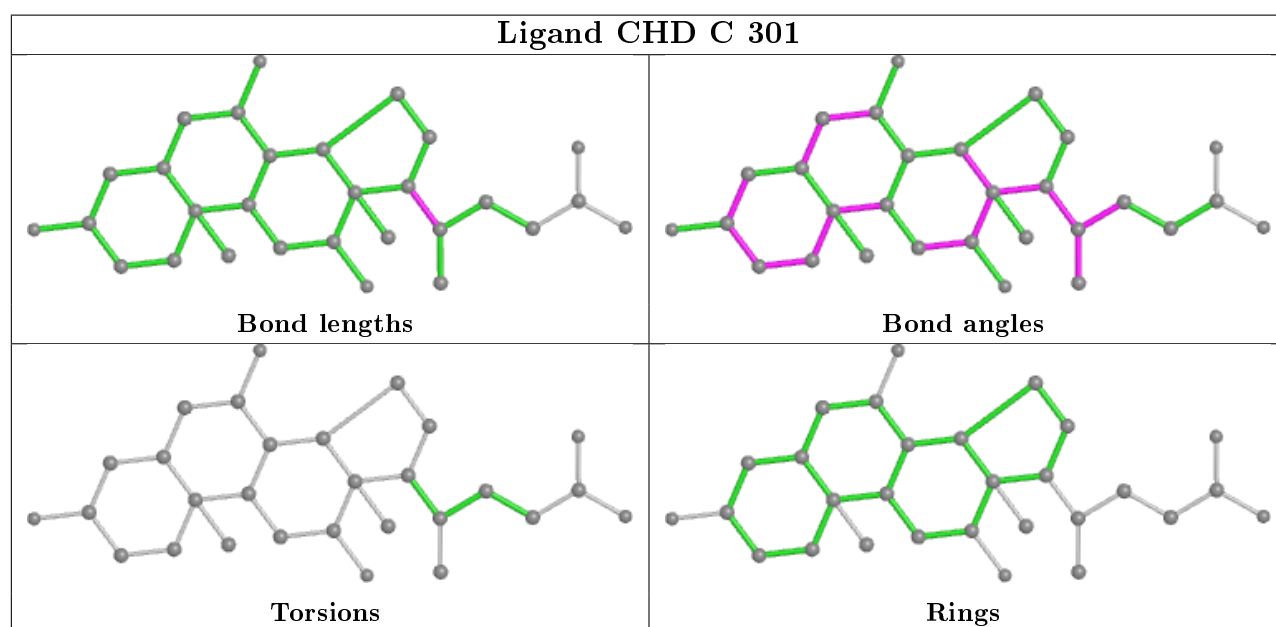
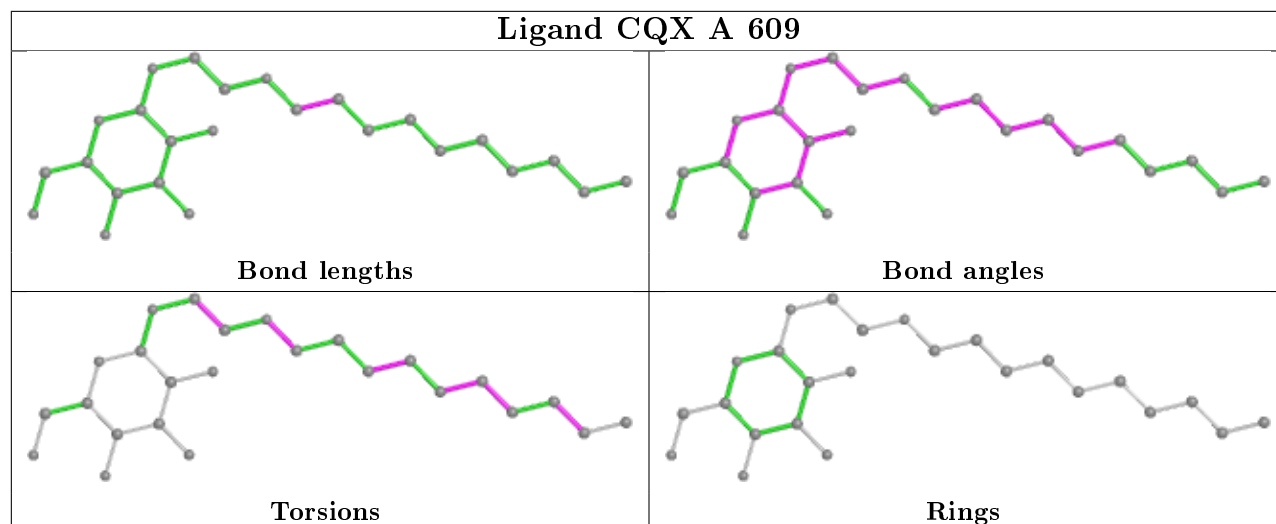


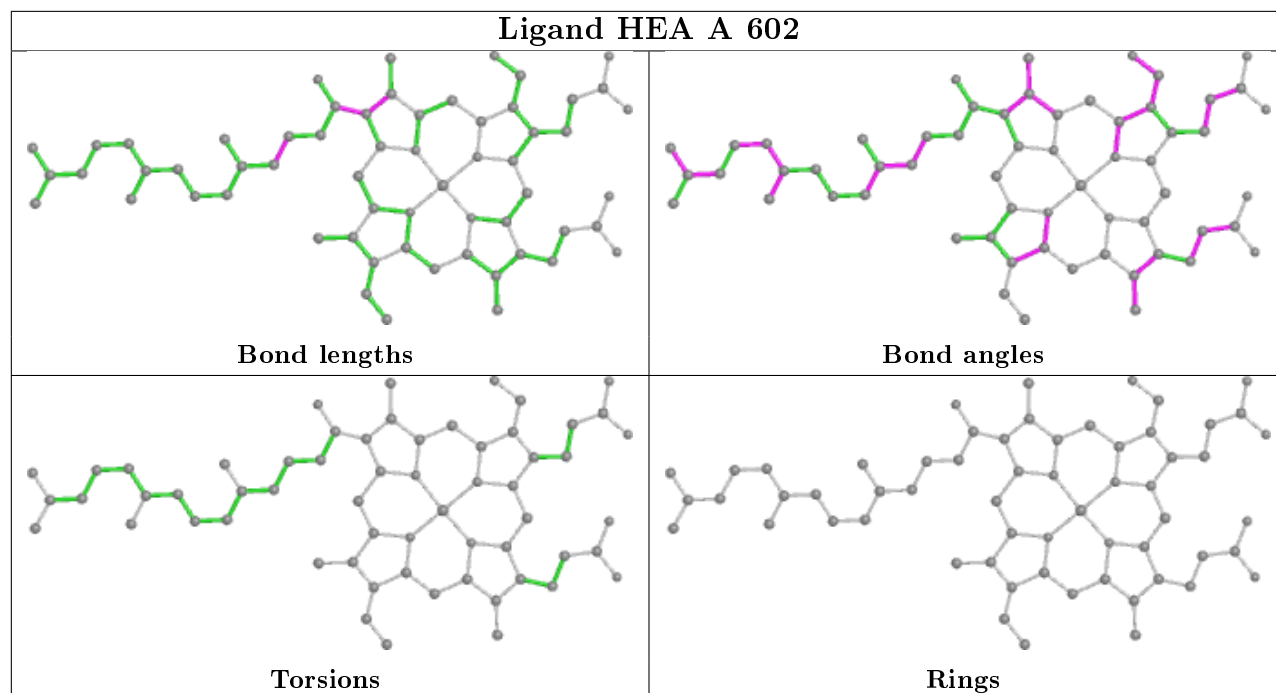












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.10	2 (0%) 92 92	25, 32, 42, 96	0
2	B	226/227 (99%)	-0.11	2 (0%) 84 84	29, 38, 63, 95	0
3	C	254/261 (97%)	-0.13	2 (0%) 86 86	28, 37, 51, 80	0
4	D	136/147 (92%)	0.19	6 (4%) 34 33	37, 50, 77, 84	0
5	E	102/109 (93%)	-0.02	1 (0%) 82 82	39, 52, 71, 86	0
6	F	91/98 (92%)	-0.03	1 (1%) 80 81	34, 49, 72, 93	0
7	G	72/85 (84%)	0.03	2 (2%) 53 52	35, 45, 89, 102	0
8	H	75/85 (88%)	-0.13	1 (1%) 77 78	33, 43, 76, 84	0
9	I	70/73 (95%)	-0.18	0 100 100	36, 46, 68, 81	0
10	J	55/59 (93%)	0.19	3 (5%) 25 24	38, 48, 77, 86	0
11	K	49/56 (87%)	0.19	0 100 100	42, 52, 69, 83	0
12	L	44/47 (93%)	-0.22	0 100 100	34, 41, 58, 67	0
13	M	40/46 (86%)	-0.06	2 (5%) 28 27	39, 47, 62, 71	0
All	All	1727/1807 (95%)	-0.06	22 (1%) 77 78	25, 39, 68, 102	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	55	PHE	5.9
10	J	52	TRP	4.9
7	G	36	TRP	4.8
2	B	113	TYR	4.6
3	C	37	PHE	4.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.95	0.27	47,60,99,117	0
2	FME	B	1	10/11	0.98	0.11	28,42,55,64	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	NA	C	302	1/1	0.44	0.19	64,64,64,64	0
18	CDL	C	305	87/100	0.82	0.27	44,87,139,152	0
21	CQX	A	611	25/25	0.85	0.21	49,63,92,102	0
18	CDL	A	606	94/100	0.90	0.22	46,79,133,139	0
18	CDL	B	301	64/100	0.91	0.16	52,88,124,138	0
21	CQX	B	303	25/25	0.93	0.11	40,53,73,75	0
21	CQX	B	304	16/25	0.93	0.10	46,54,81,83	0
21	CQX	A	610	25/25	0.95	0.17	47,57,72,80	0
21	CQX	A	609	25/25	0.95	0.16	40,60,74,99	0
21	CQX	G	101	25/25	0.95	0.09	43,49,59,61	0
20	PGV	C	304	41/51	0.96	0.12	32,39,68,84	0
21	CQX	C	306	25/25	0.96	0.11	38,49,93,95	0
23	CHD	C	301	29/29	0.97	0.12	29,34,39,48	0
21	CQX	C	307	25/25	0.97	0.13	40,57,89,98	0
19	PER	A	607	2/2	0.97	0.10	25,25,25,33	0
24	PEK	C	303	43/53	0.97	0.13	31,42,69,97	0
20	PGV	A	608	51/51	0.97	0.12	28,38,78,102	0
14	HEA	A	602	60/60	0.98	0.12	21,26,34,45	0
14	HEA	A	601	60/60	0.99	0.11	24,29,49,60	0
16	MG	A	604	1/1	0.99	0.12	31,31,31,31	0

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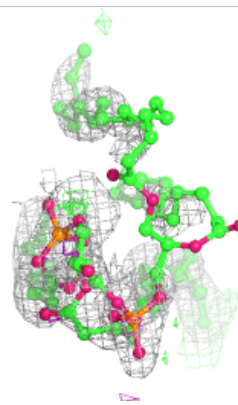
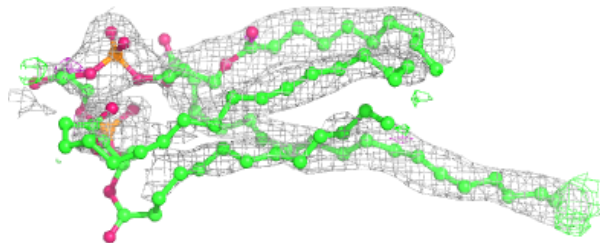
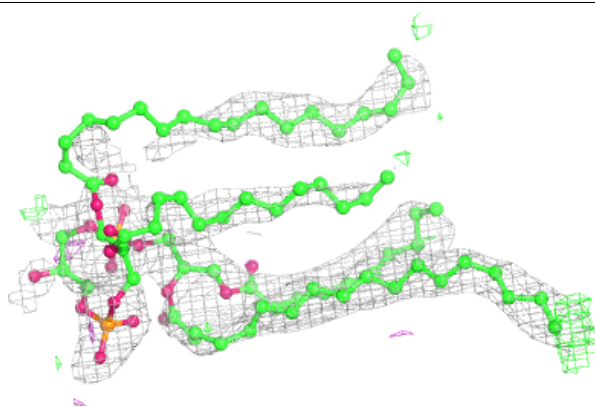
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CUA	B	302	2/2	1.00	0.15	30,30,30,31	0
17	NA	A	605	1/1	1.00	0.06	35,35,35,35	0
15	CU	A	603	1/1	1.00	0.18	26,26,26,26	0
25	ZN	F	101	1/1	1.00	0.12	43,43,43,43	0

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.

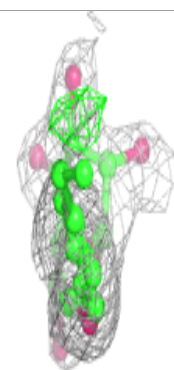
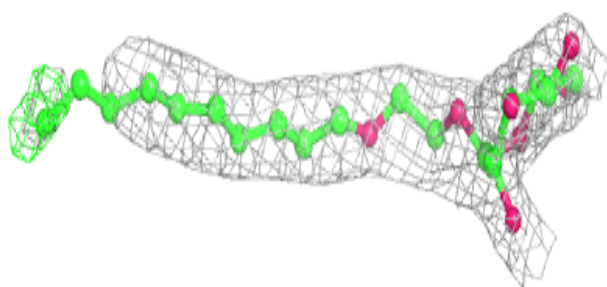
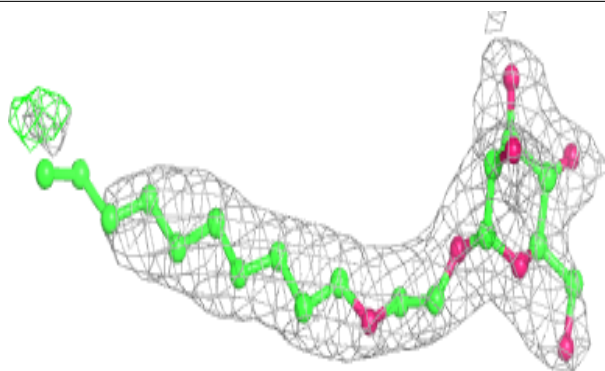
Electron density around CDL C 305:

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



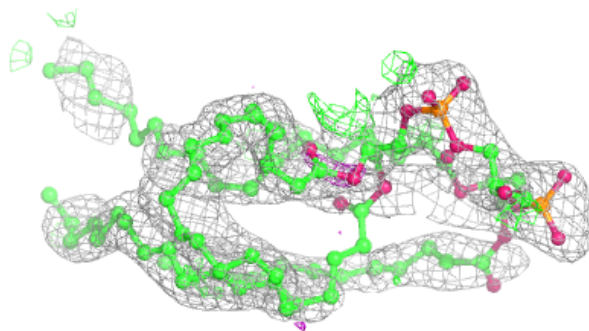
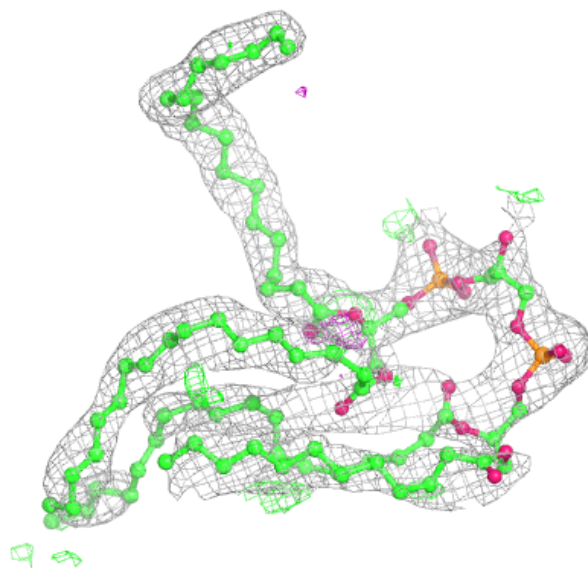
Electron density around CQX A 611:

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



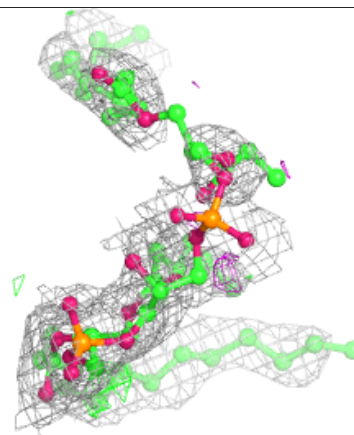
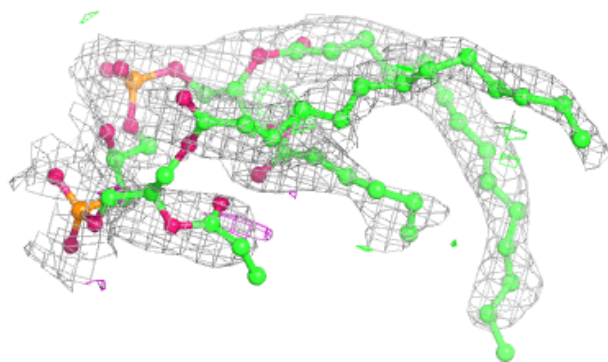
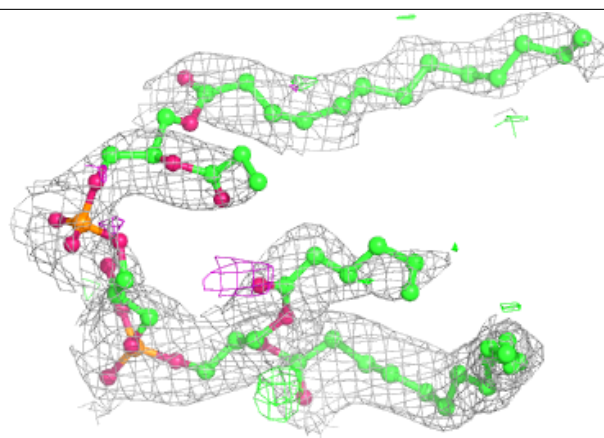
Electron density around CDL A 606:

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and green (positive)

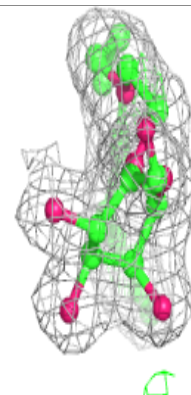
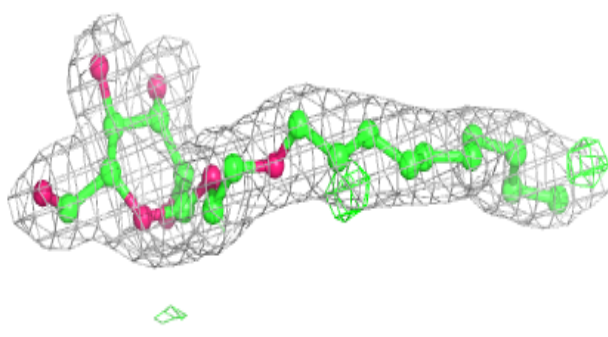
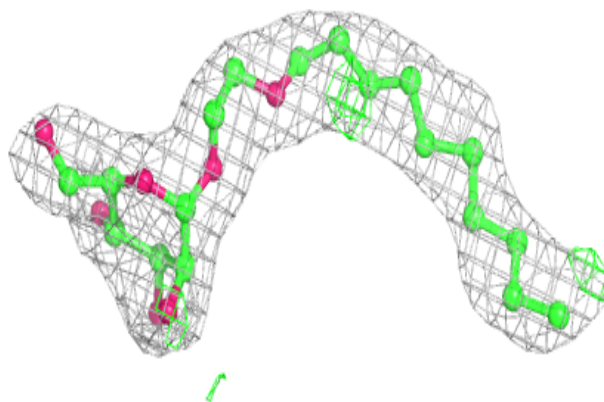


Electron density around CDL B 301:

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

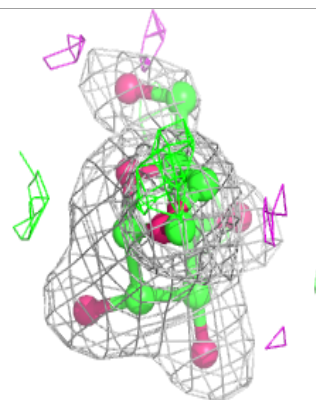
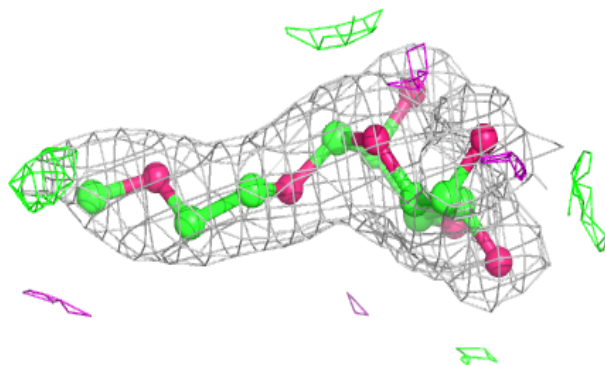
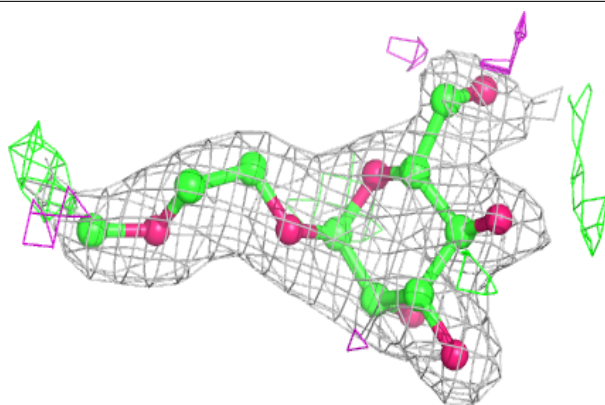
**Electron density around CQX B 303:**

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

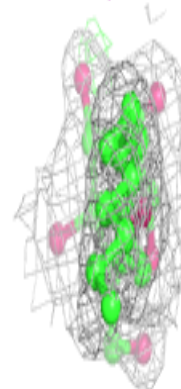
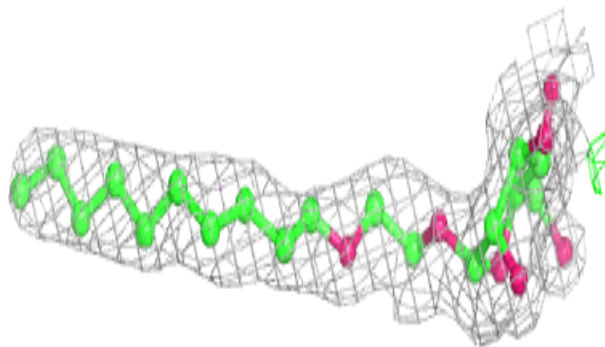
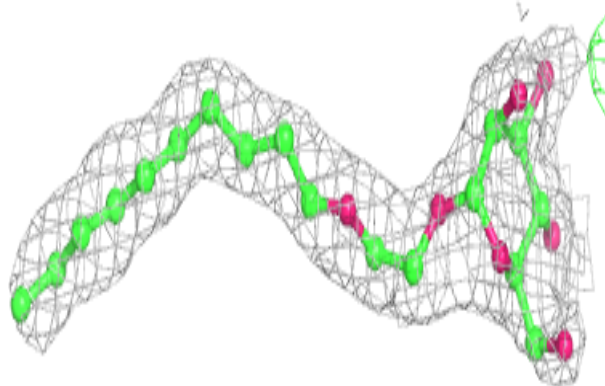


Electron density around CQX B 304:

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

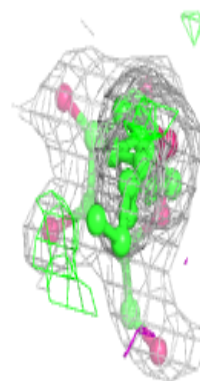
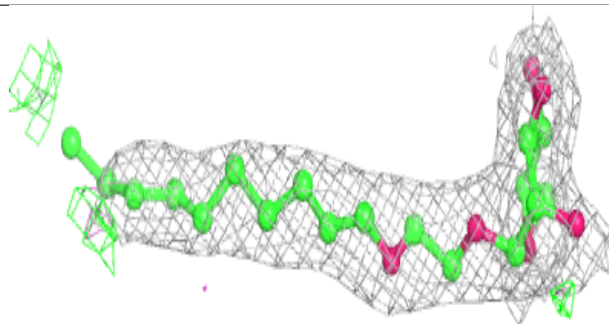
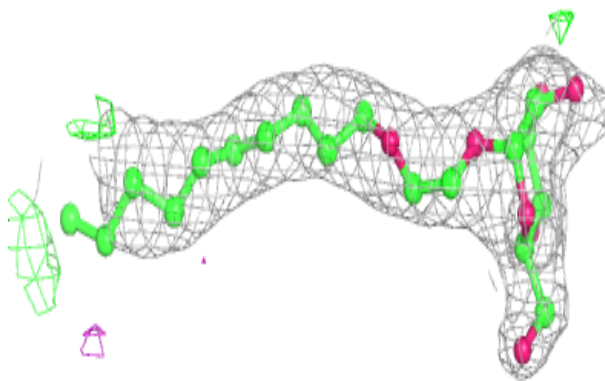
**Electron density around CQX A 610:**

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

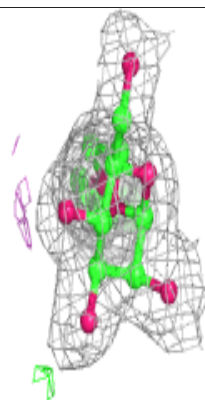
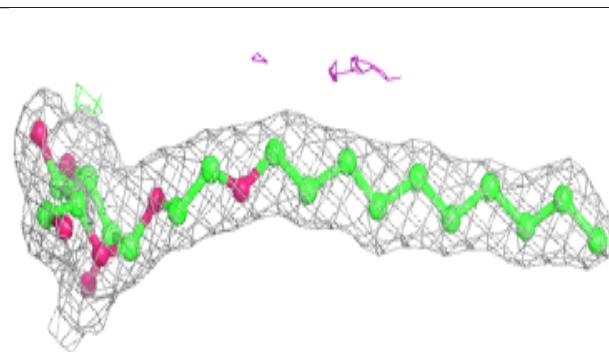
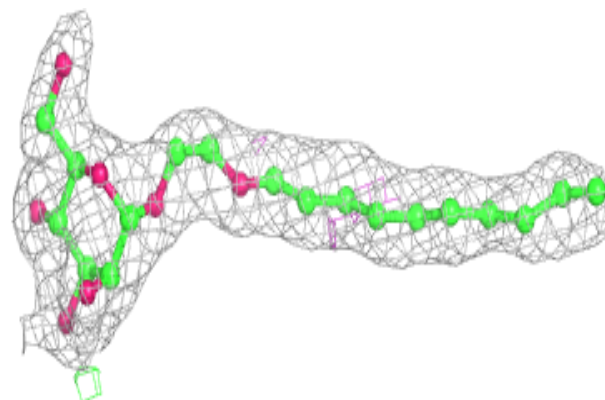


Electron density around CQX A 609:

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

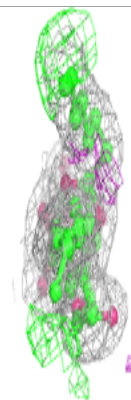
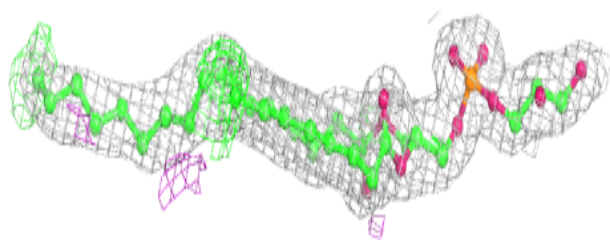
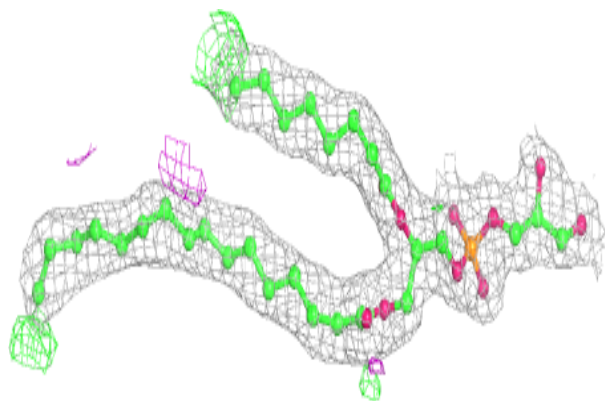
**Electron density around CQX G 101:**

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

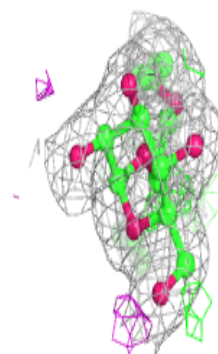
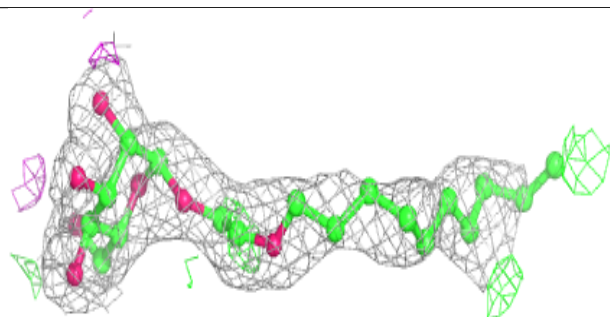
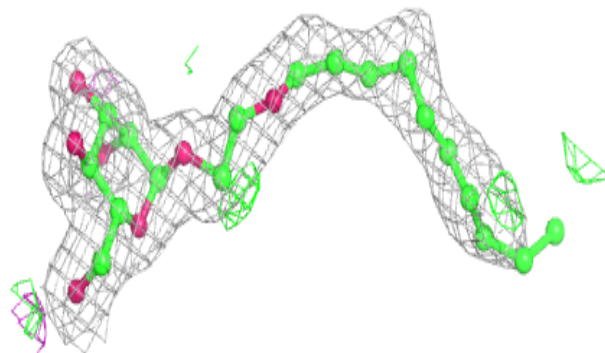


Electron density around PGV C 304:

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

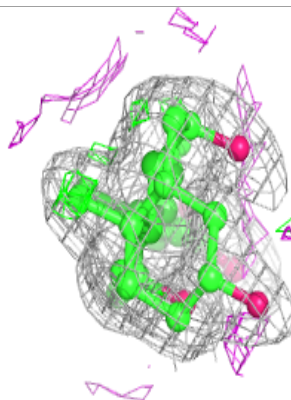
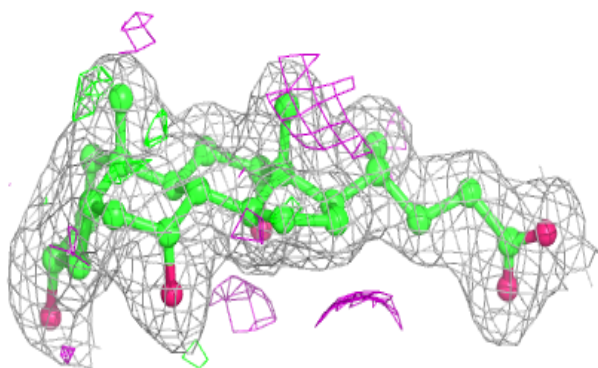
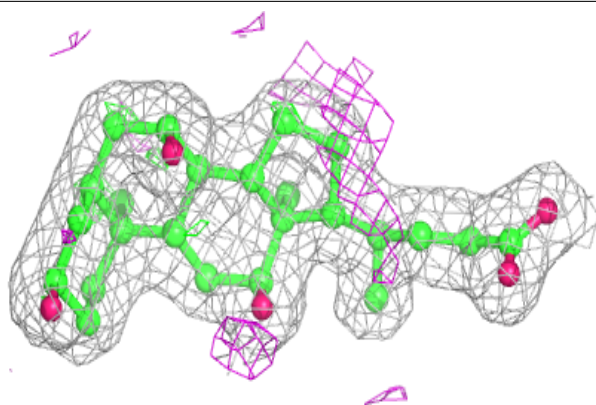
**Electron density around CQX C 306:**

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

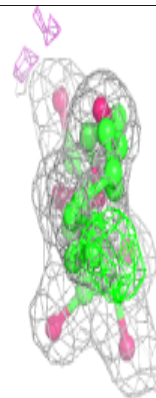
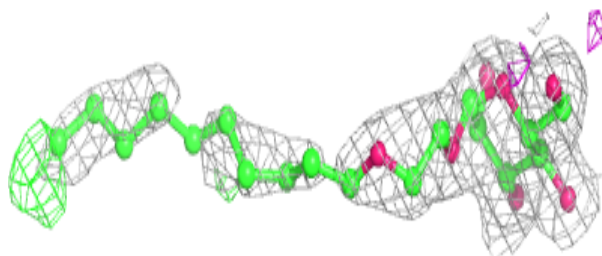
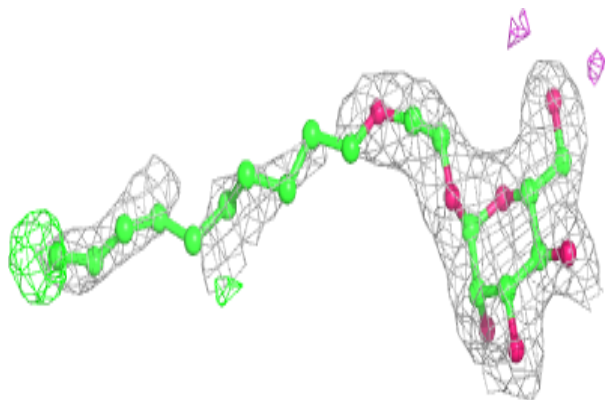


Electron density around CHD C 301:

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

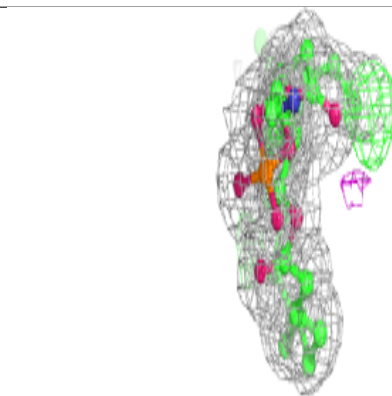
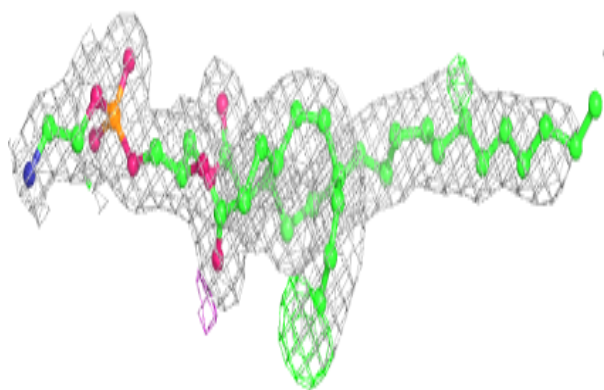
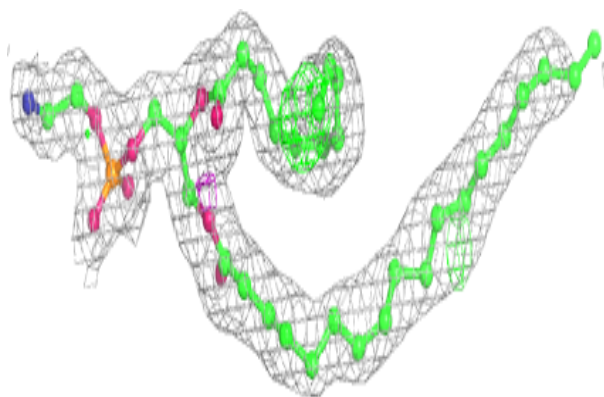
**Electron density around CQX C 307:**

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

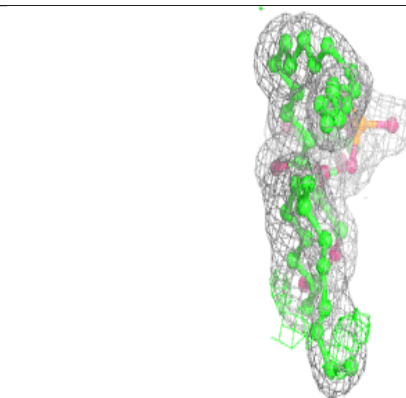
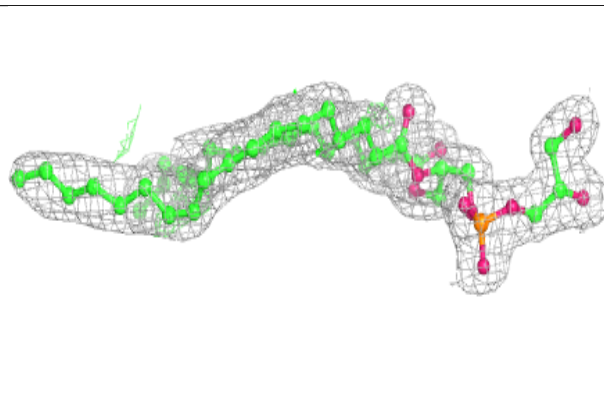
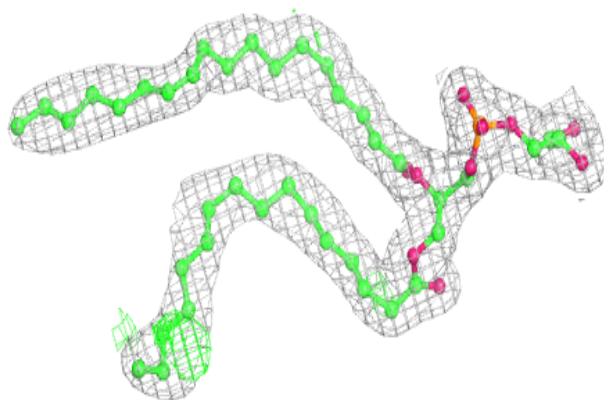


Electron density around PEK C 303:

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

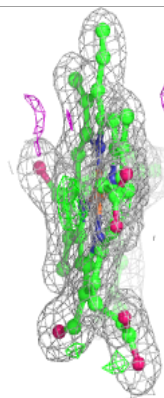
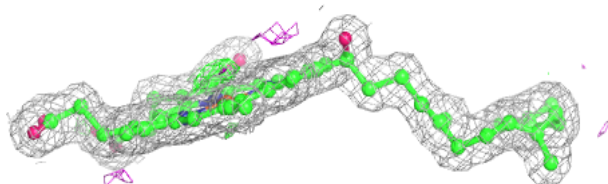
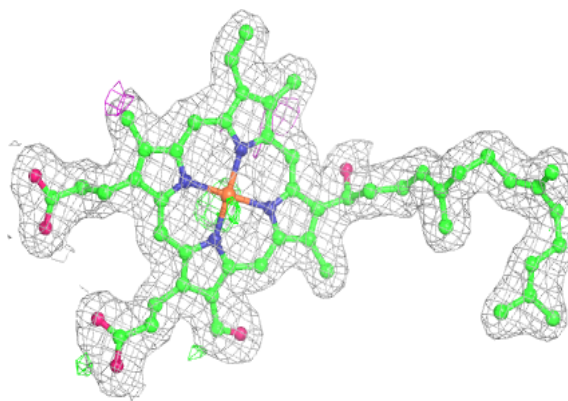
**Electron density around PGV A 608:**

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

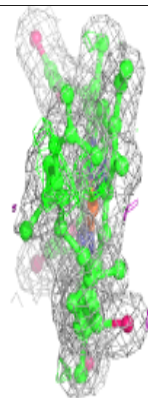
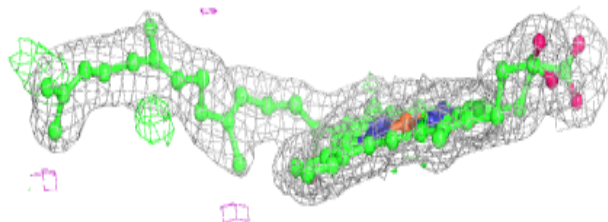
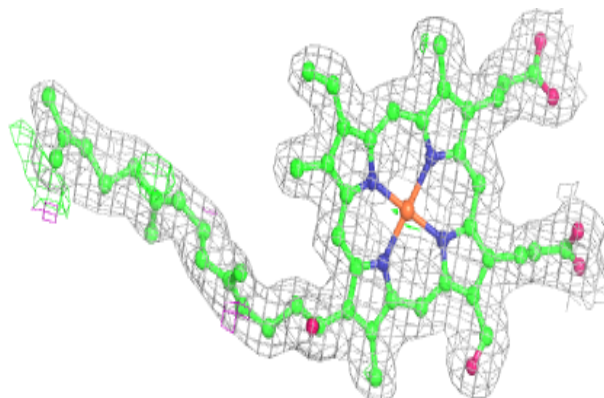


Electron density around HEA A 602:

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

**Electron density around HEA A 601:**

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 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.