wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 10:03 PM JST

PDB ID	:	6JY4
Title	:	Monomeric Form of Bovine Heart Cytochrome c Oxidase in the Fully Reduced State
Authors	:	Shinzawa-Itoh, K.; Muramoto, K.
Deposited on	:	2019-04-26
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

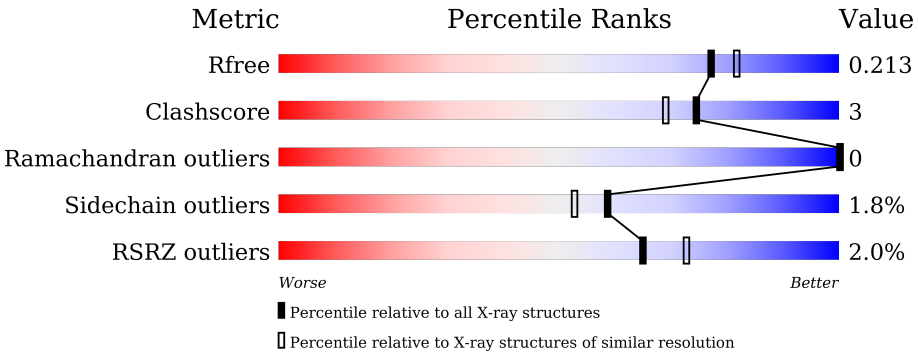
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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.



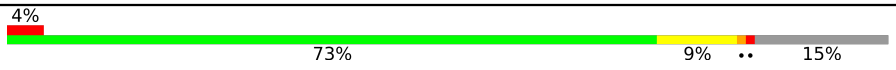
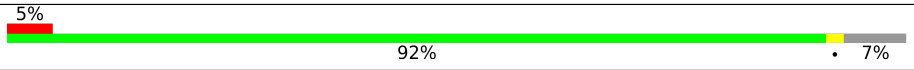
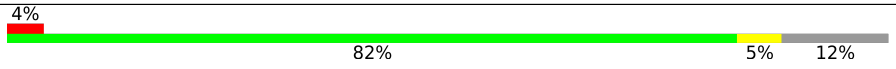
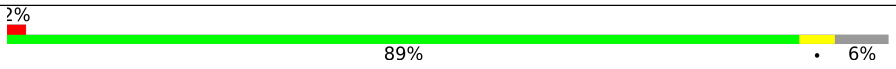
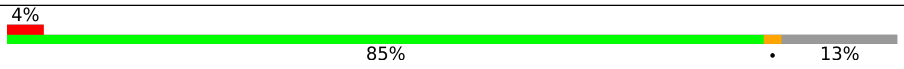
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	514	92% 8%
2	B	227	% 85% 12% •
3	C	261	94% • •
4	D	147	6% 88% • • 7%
5	E	109	3% 88% 6% 6%
6	F	98	4% 84% 8% • 7%

Continued on next page...

Continued from previous page...

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	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 15174 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			

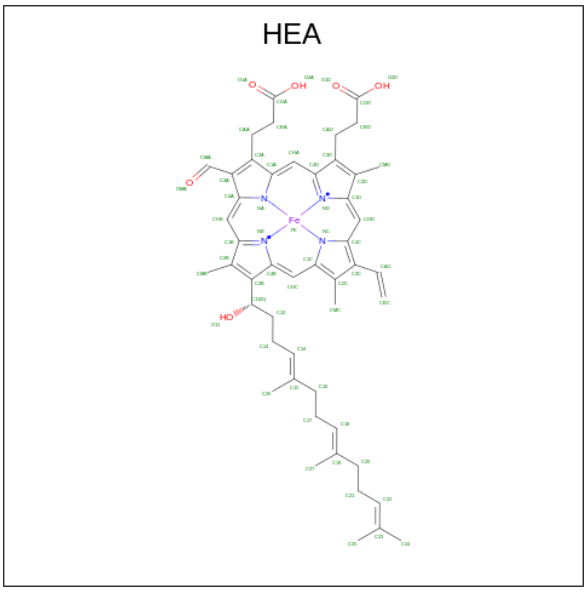
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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: $C_{49}H_{56}FeN_4O_6$).



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		

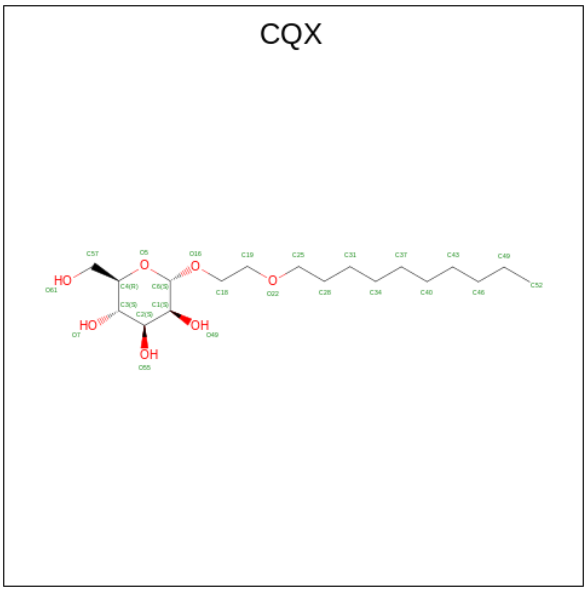
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

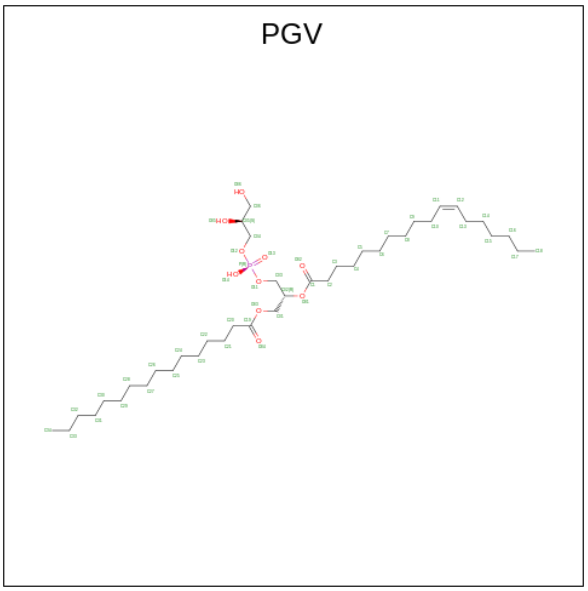
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		

- Molecule 18 is (2S,3S,4S,5S,6R)-2-(2-decoxyethoxy)-6-(hydroxymethyl)oxane-3,4,5-triol (three-letter code: CQX) (formula: $C_{18}H_{36}O_7$) (labeled as "Ligand of Interest" by depositor).



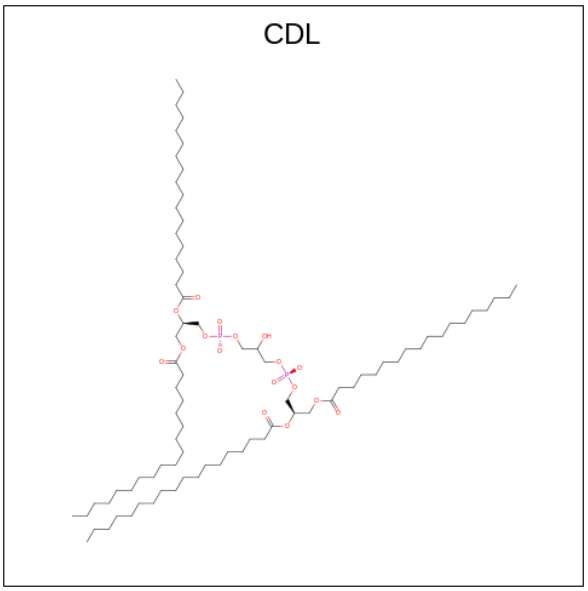
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 25 18 7	0	0
18	A	1	Total C O 25 18 7	0	0
18	A	1	Total C O 25 18 7	0	0
18	B	1	Total C O 16 9 7	0	0
18	C	1	Total C O 25 18 7	0	0
18	C	1	Total C O 25 18 7	0	0
18	G	1	Total C O 25 18 7	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



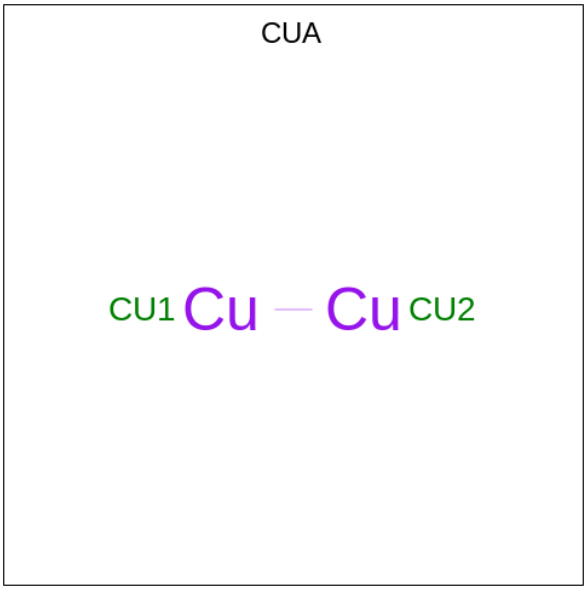
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	B	1	Total	C	O	P	0	0
			64	45	17	2		

Continued on next page...

Continued from previous page...

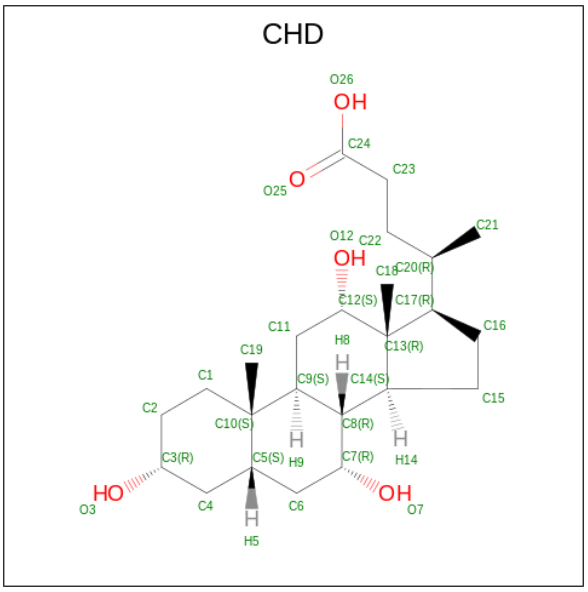
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			87	68	17	2		
20	L	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).

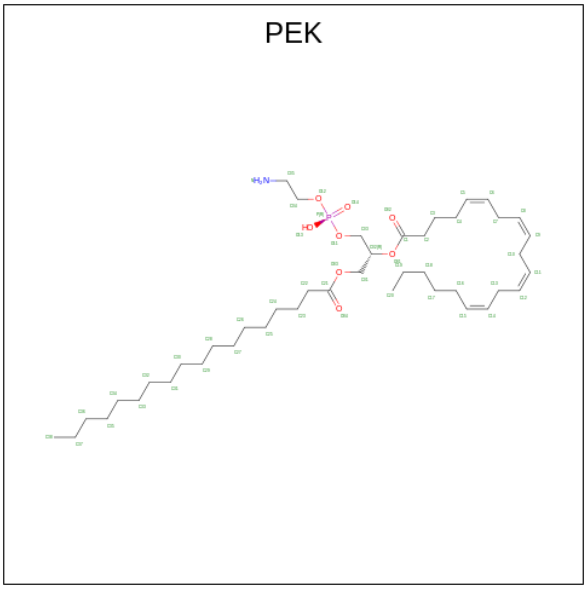


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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: $C_{43}H_{78}NO_8P$).



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

- Molecule 25 is water.

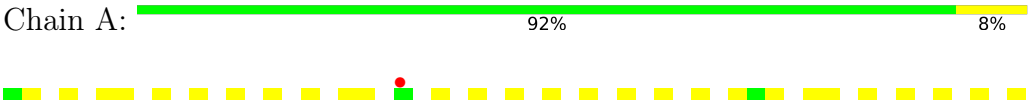
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	201	Total	O	0	1
			202	202		
25	B	107	Total	O	0	1
			108	108		
25	C	78	Total	O	0	0
			78	78		
25	D	37	Total	O	0	0
			37	37		
25	E	23	Total	O	0	0
			23	23		
25	F	43	Total	O	0	1
			44	44		
25	G	35	Total	O	0	0
			35	35		
25	H	33	Total	O	0	0
			33	33		
25	I	15	Total	O	0	0
			15	15		
25	J	8	Total	O	0	0
			8	8		
25	K	10	Total	O	0	0
			10	10		
25	L	11	Total	O	0	0
			11	11		
25	M	7	Total	O	0	0
			7	7		

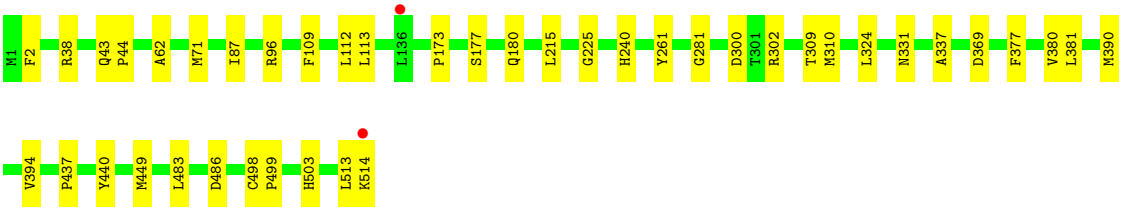
3 Residue-property plots (i)

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 c oxidase subunit 1

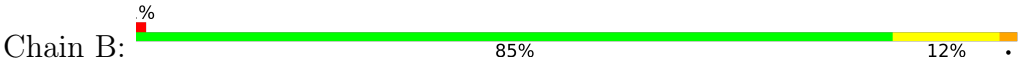
Chain A:

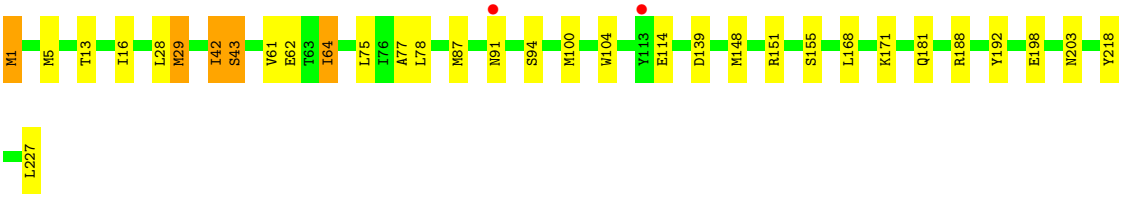




• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



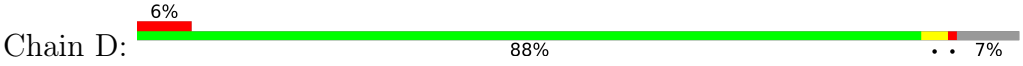


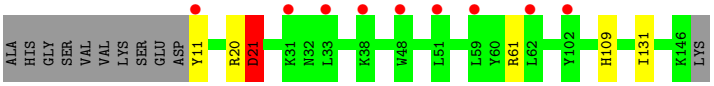
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

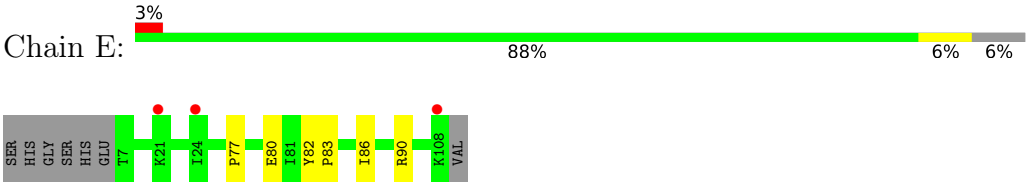
Chain D:





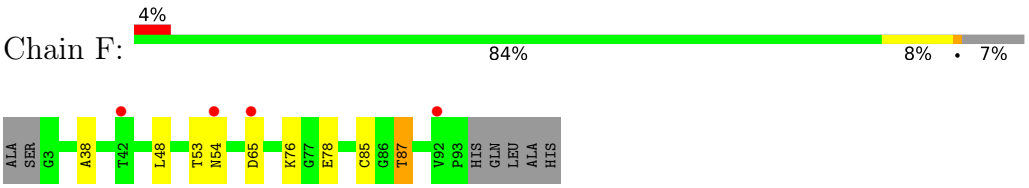
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



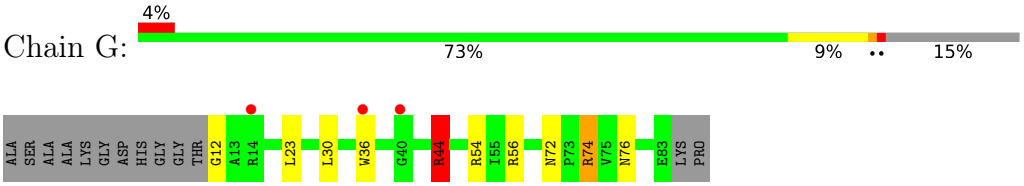
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



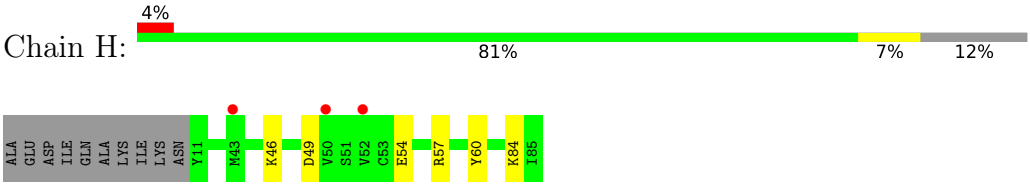
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



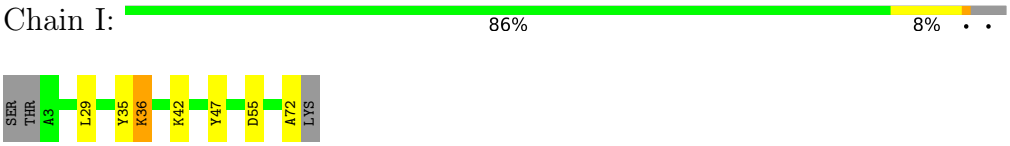
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



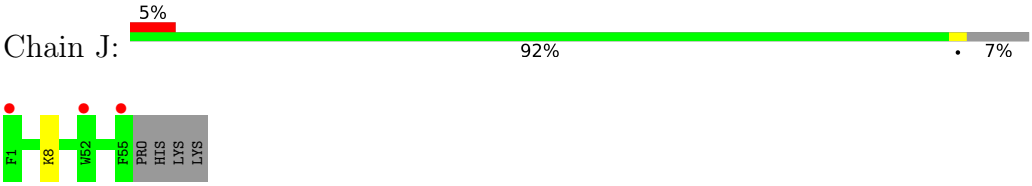
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



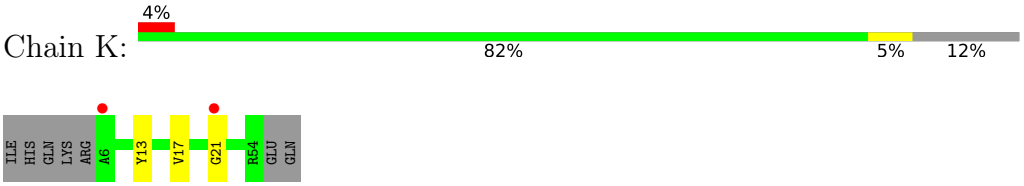
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



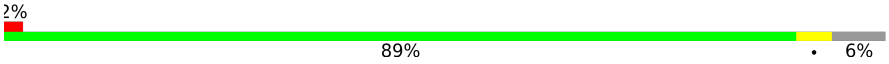
• Molecule 11: Cytochrome c oxidase subunit 7B

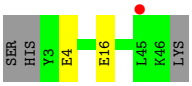
Chain K:



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

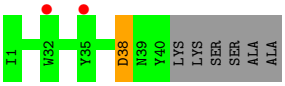
Chain L:





• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.40Å 152.40Å 174.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 113.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.2 (40.00-1.95) 89.3 (113.36-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.152 , 0.205 0.167 , 0.213	Depositor DCC
R_{free} test set	13861 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15174	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CQX, ZN, FME, MG, CU, PEK, CHD, NA, CUA, HEA, PGV, CDL

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	0.99	2/4156 (0.0%)	0.93	7/5678 (0.1%)
2	B	0.98	2/1860 (0.1%)	1.01	5/2534 (0.2%)
3	C	0.95	2/2143 (0.1%)	0.86	3/2931 (0.1%)
4	D	0.83	0/1167	0.93	4/1577 (0.3%)
5	E	0.86	0/843	0.84	0/1145
6	F	0.81	1/709 (0.1%)	0.81	0/963
7	G	1.01	2/621 (0.3%)	0.96	2/848 (0.2%)
8	H	0.92	0/648	0.90	3/877 (0.3%)
9	I	0.80	0/588	1.00	1/781 (0.1%)
10	J	0.83	0/443	0.83	0/598
11	K	0.84	1/398 (0.3%)	0.78	0/546
12	L	0.93	0/372	0.83	0/500
13	M	0.79	0/321	0.80	0/440
All	All	0.93	10/14269 (0.1%)	0.91	25/19418 (0.1%)

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
6	F	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	9.94	1.68	1.50
2	B	43	SER	CB-OG	-8.17	1.31	1.42
2	B	198	GLU	C-O	6.91	1.36	1.23
3	C	104	SER	CB-OG	6.77	1.51	1.42
1	A	281	GLY	N-CA	5.87	1.54	1.46

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	20	ARG	NE-CZ-NH2	-12.26	114.17	120.30
4	D	20	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	A	71	MET	CG-SD-CE	-9.37	85.21	100.20
4	D	21	ASP	CB-CG-OD1	7.67	125.21	118.30
8	H	49	ASP	CB-CG-OD2	7.26	124.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	65	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	33	0
2	B	1824	0	1833	22	0
3	C	2061	0	1992	4	0
4	D	1133	0	1119	4	0
5	E	825	0	823	3	0
6	F	694	0	677	5	0
7	G	595	0	569	6	0
8	H	628	0	580	1	0
9	I	575	0	584	6	0
10	J	434	0	432	6	0
11	K	384	0	366	1	0
12	L	360	0	360	1	0
13	M	311	0	321	1	0
14	A	120	0	108	6	0
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	75	0	0	0	0
18	B	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	50	0	0	2	0
18	G	25	0	0	0	0
19	A	51	0	76	1	0
19	C	51	0	76	0	0
20	B	64	0	72	2	0
20	C	87	0	124	9	0
20	L	94	0	141	8	0
21	B	2	0	0	0	0
22	C	29	0	39	0	0
23	F	1	0	0	0	0
24	G	43	0	58	3	0
25	A	202	0	0	4	0
25	B	108	0	0	3	0
25	C	78	0	0	0	0
25	D	37	0	0	4	0
25	E	23	0	0	0	0
25	F	44	0	0	0	0
25	G	35	0	0	2	0
25	H	33	0	0	0	0
25	I	15	0	0	0	0
25	J	8	0	0	0	0
25	K	10	0	0	0	0
25	L	11	0	0	1	0
25	M	7	0	0	1	0
All	All	15174	0	14351	93	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 93 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:HB2	25:D:232:HOH:O	1.76	0.85
6:F:85:CYS:SG	6:F:87:THR:HG23	2.18	0.84
1:A:2:PHE:CE1	20:L:101:CDL:H712	2.20	0.77
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.67	0.76
20:C:304:CDL:O1	10:J:8:LYS:CE	2.34	0.75

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%)	496 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
3	C	252/261 (97%)	249 (99%)	3 (1%)	0	100	100
4	D	134/147 (91%)	129 (96%)	5 (4%)	0	100	100
5	E	100/109 (92%)	98 (98%)	2 (2%)	0	100	100
6	F	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
7	G	70/85 (82%)	67 (96%)	3 (4%)	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%)	40 (95%)	2 (5%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
All	All	1703/1807 (94%)	1662 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	426/426 (100%)	423 (99%)	3 (1%)	84	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	210/210 (100%)	203 (97%)	7 (3%)	38 26
3	C	220/226 (97%)	218 (99%)	2 (1%)	78 77
4	D	120/129 (93%)	119 (99%)	1 (1%)	81 80
5	E	89/95 (94%)	88 (99%)	1 (1%)	73 71
6	F	76/81 (94%)	74 (97%)	2 (3%)	46 36
7	G	62/69 (90%)	58 (94%)	4 (6%)	17 6
8	H	67/75 (89%)	65 (97%)	2 (3%)	41 30
9	I	55/58 (95%)	53 (96%)	2 (4%)	35 23
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 34
13	M	34/38 (90%)	33 (97%)	1 (3%)	42 31
All	All	1481/1543 (96%)	1455 (98%)	26 (2%)	59 53

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	48	LEU
7	G	44	ARG
12	L	16	GLU
7	G	30	LEU
7	G	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	50	ASN
8	H	31	GLN
3	C	68	GLN
11	K	35	GLN
5	E	94	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	1.31	1 (12%)	7,9,11	4.49	3 (42%)
1	FME	A	1	1	8,9,10	0.42	0	7,9,11	1.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-2.65	1.14	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-9.46	108.28	122.82
2	B	1	FME	C-CA-N	6.38	121.24	109.73
2	B	1	FME	O1-CN-N	-2.54	118.59	125.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG

Continued on next page...

Continued from previous page...

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
18	CQX	A	608	-	25,25,25	0.73	0	30,30,30	1.62	6 (20%)
18	CQX	A	609	-	25,25,25	0.75	1 (4%)	30,30,30	1.24	4 (13%)
18	CQX	C	306	-	25,25,25	0.48	0	30,30,30	0.87	0
18	CQX	G	102	-	25,25,25	0.69	1 (4%)	30,30,30	0.99	3 (10%)
14	HEA	A	601	1	57,67,67	1.90	13 (22%)	61,103,103	2.23	17 (27%)
19	PGV	C	303	-	50,50,50	0.88	3 (6%)	53,56,56	1.00	3 (5%)
19	PGV	A	607	-	50,50,50	0.91	2 (4%)	53,56,56	1.12	3 (5%)
20	CDL	B	301	-	63,63,99	1.42	4 (6%)	69,75,111	1.60	13 (18%)
21	CUA	B	302	2	0,1,1	-	-	-		
22	CHD	C	301	-	32,32,32	0.93	2 (6%)	51,51,51	1.41	6 (11%)
24	PEK	G	101	-	42,42,52	0.91	3 (7%)	45,47,57	1.17	3 (6%)
14	HEA	A	602	1	57,67,67	1.53	9 (15%)	61,103,103	1.93	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CQX	A	606	-	25,25,25	0.78	1 (4%)	30,30,30	1.98	12 (40%)
18	CQX	C	305	-	25,25,25	0.95	2 (8%)	30,30,30	1.78	6 (20%)
20	CDL	C	304	-	86,86,99	1.09	4 (4%)	92,98,111	1.25	13 (14%)
18	CQX	B	303	-	16,16,25	1.23	1 (6%)	21,21,30	1.61	4 (19%)
20	CDL	L	101	-	93,93,99	0.95	5 (5%)	99,105,111	1.50	11 (11%)

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
18	CQX	A	608	-	-	5/16/36/36	0/1/1/1
18	CQX	A	609	-	-	5/16/36/36	0/1/1/1
18	CQX	C	306	-	-	7/16/36/36	0/1/1/1
18	CQX	G	102	-	-	0/16/36/36	0/1/1/1
14	HEA	A	601	1	-	6/32/76/76	-
19	PGV	C	303	-	-	11/55/55/55	-
19	PGV	A	607	-	-	4/55/55/55	-
20	CDL	B	301	-	-	42/74/74/110	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
24	PEK	G	101	-	-	6/46/46/56	-
14	HEA	A	602	1	-	5/32/76/76	-
18	CQX	A	606	-	-	6/16/36/36	0/1/1/1
18	CQX	C	305	-	-	7/16/36/36	0/1/1/1
20	CDL	C	304	-	-	54/97/97/110	-
18	CQX	B	303	-	-	3/7/27/36	0/1/1/1
20	CDL	L	101	-	-	43/104/104/110	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C4B-NB	-6.80	1.28	1.40
20	B	301	CDL	OA6-CA5	6.46	1.52	1.34
14	A	602	HEA	C4B-NB	-6.08	1.29	1.40
14	A	601	HEA	C1D-ND	-4.95	1.31	1.40
20	B	301	CDL	OB6-CB5	4.74	1.47	1.34

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601	HEA	C4A-CHB-C1B	7.73	132.76	122.56
14	A	601	HEA	C13-C12-C11	-6.95	103.92	114.35
20	B	301	CDL	CA4-OA6-CA5	6.03	132.63	117.79
20	L	101	CDL	OB6-CB5-C51	5.55	123.46	111.50
20	C	304	CDL	OB6-CB5-C51	5.11	122.52	111.50

There are no chirality outliers.

5 of 206 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602	HEA	C2D-C3D-CAD-CBD
20	B	301	CDL	CA2-C1-CB2-OB2
20	B	301	CDL	CA3-OA5-PA1-OA2
20	B	301	CDL	CA3-OA5-PA1-OA3
20	B	301	CDL	CA3-OA5-PA1-OA4

There are no ring outliers.

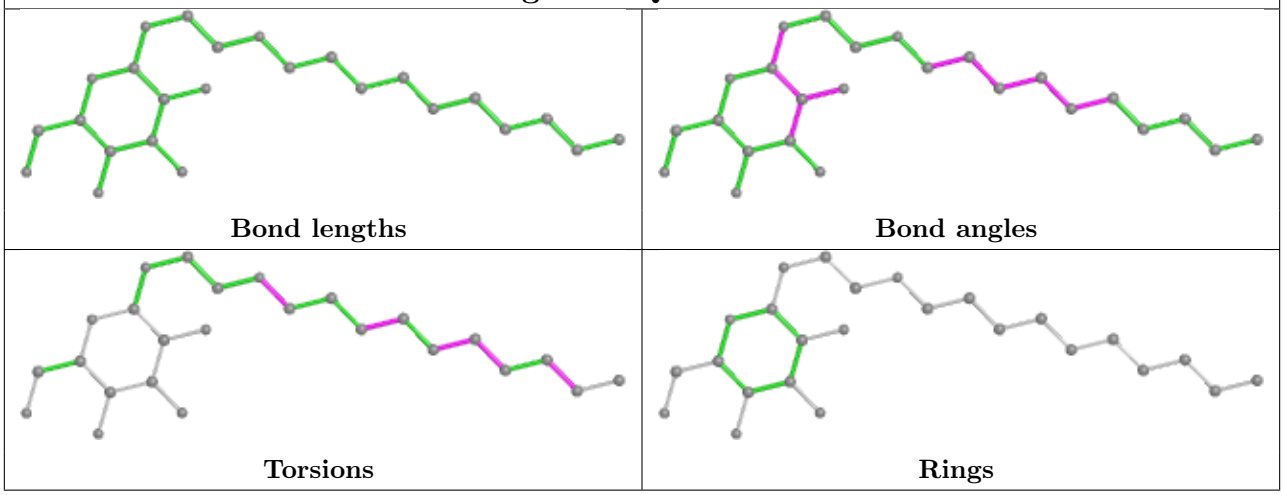
9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	2	0
19	A	607	PGV	1	0
20	B	301	CDL	2	0
24	G	101	PEK	3	0
14	A	602	HEA	4	0
18	C	305	CQX	2	0
20	C	304	CDL	9	0
18	B	303	CQX	1	0
20	L	101	CDL	8	0

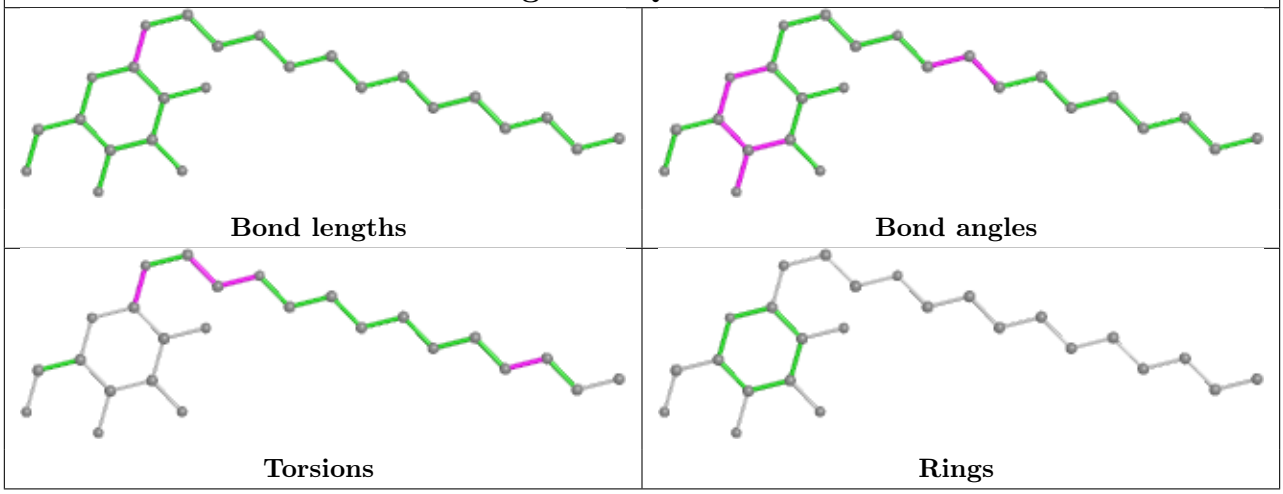
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

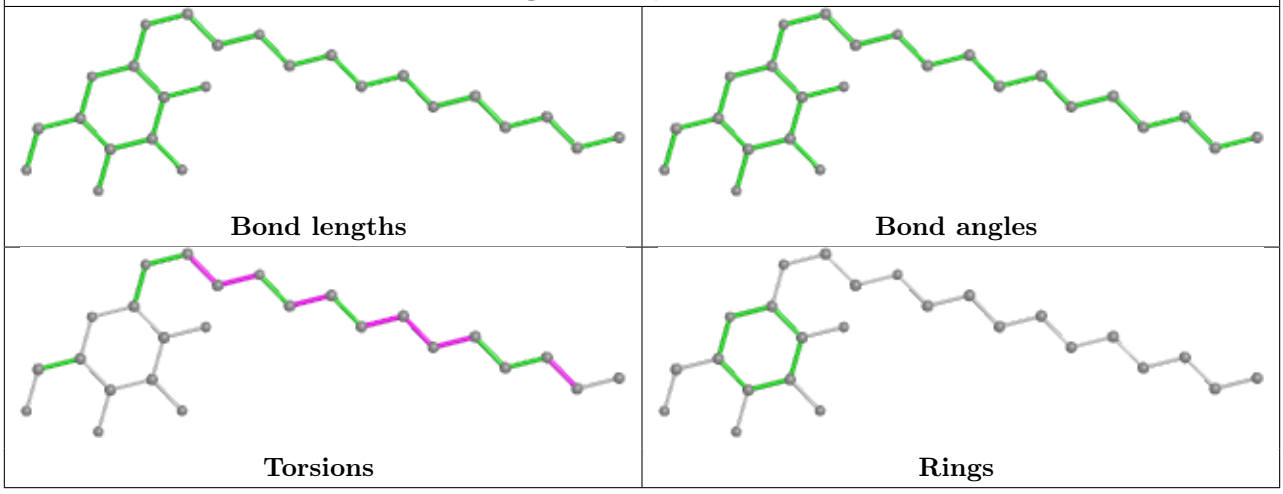
Ligand CQX A 608



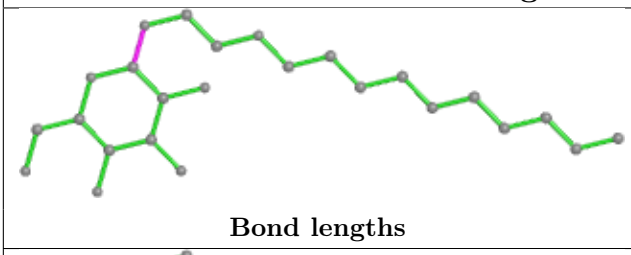
Ligand CQX A 609



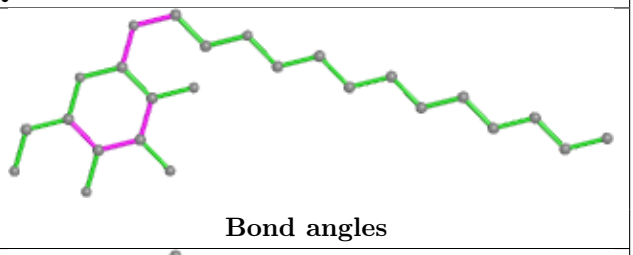
Ligand CQX C 306



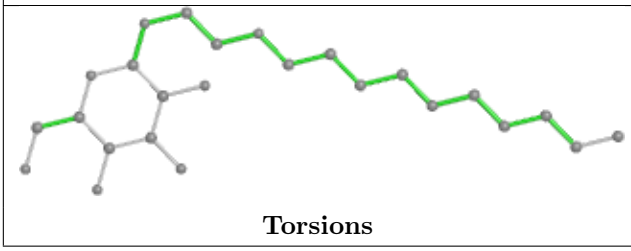
Ligand CQX G 102



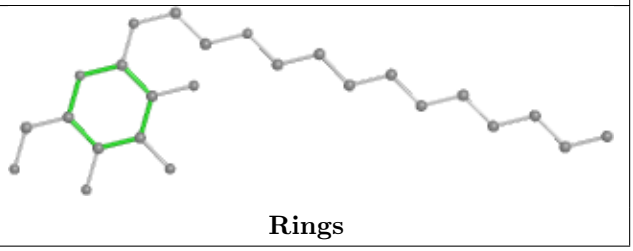
Bond lengths



Bond angles

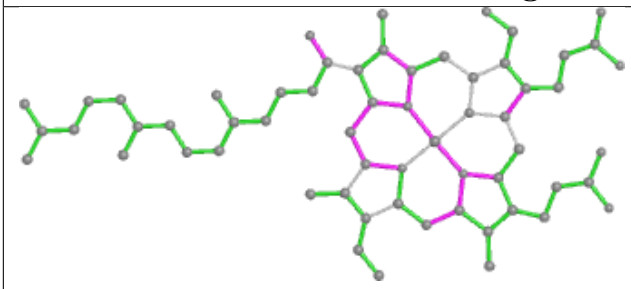


Torsions

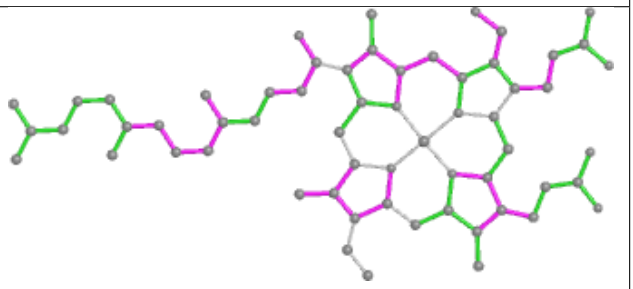


Rings

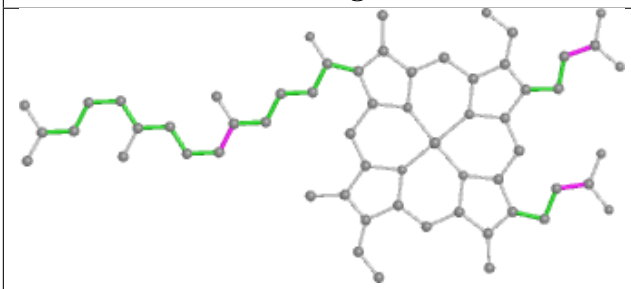
Ligand HEA A 601



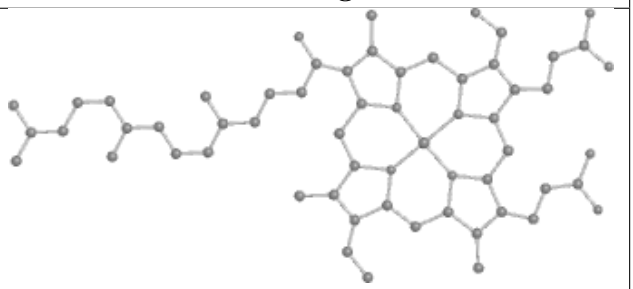
Bond lengths



Bond angles

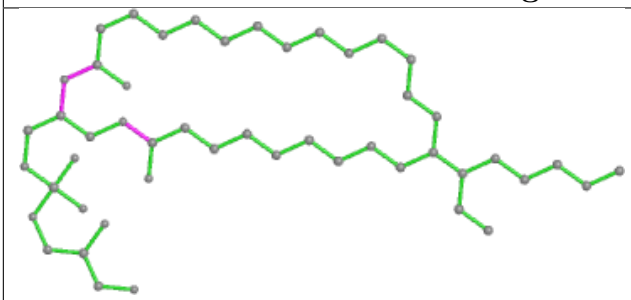


Torsions

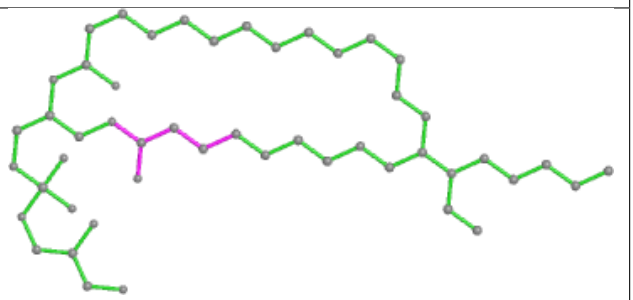


Rings

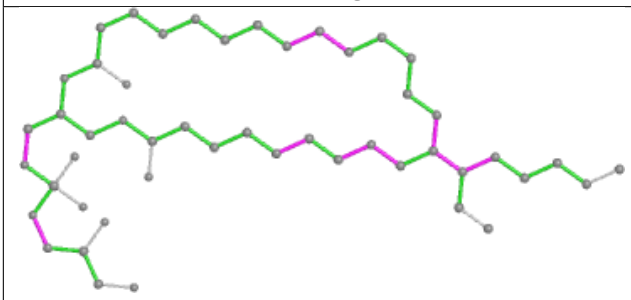
Ligand PGV C 303



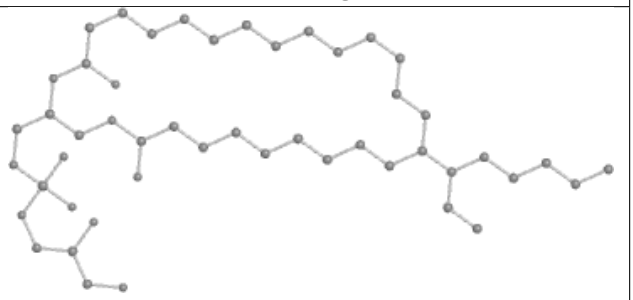
Bond lengths



Bond angles

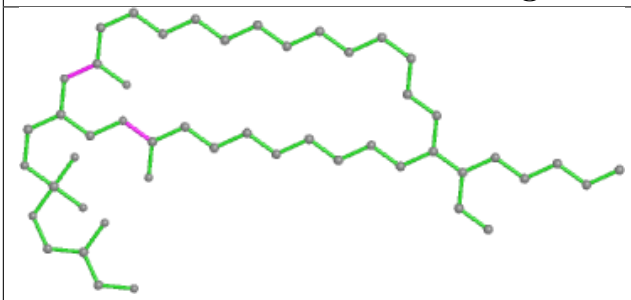


Torsions

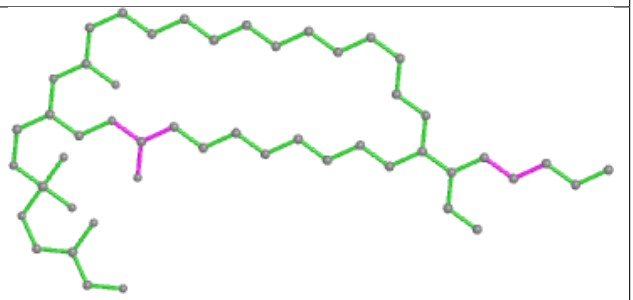


Rings

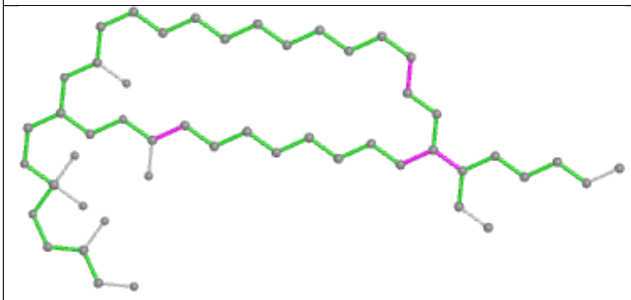
Ligand PGV A 607



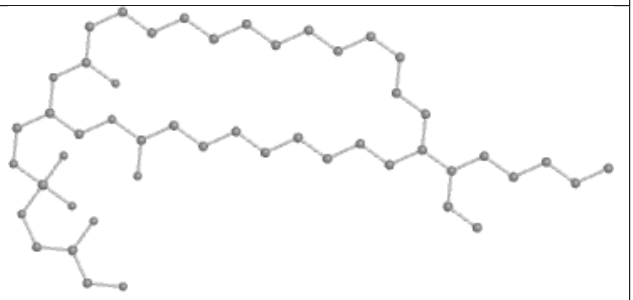
Bond lengths



Bond angles

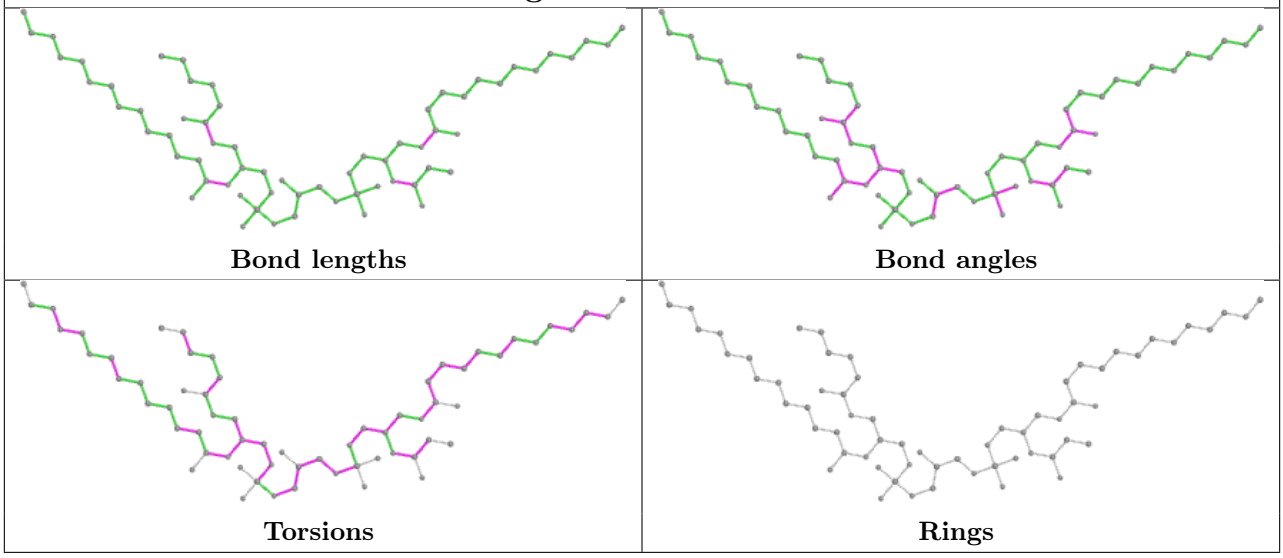


Torsions

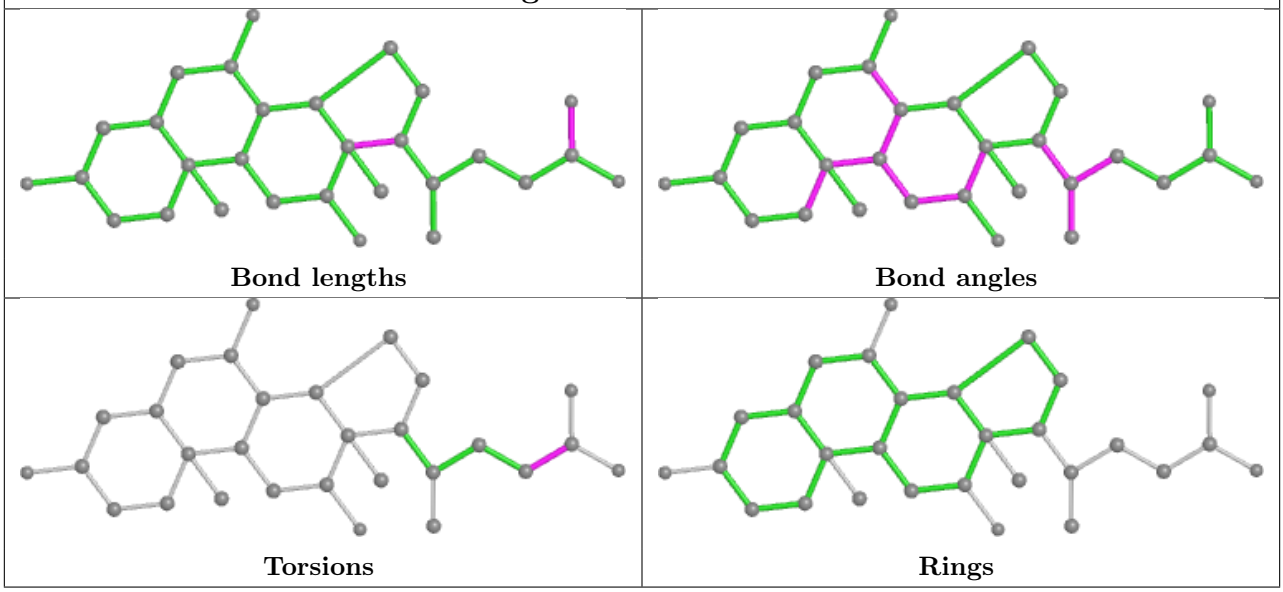


Rings

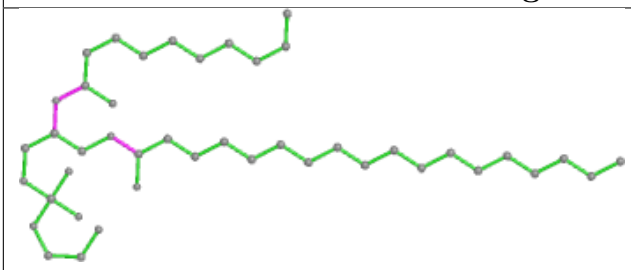
Ligand CDL B 301



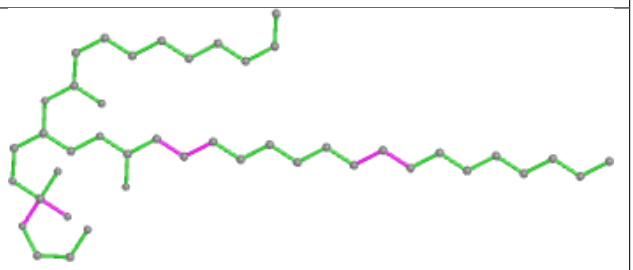
Ligand CHD C 301



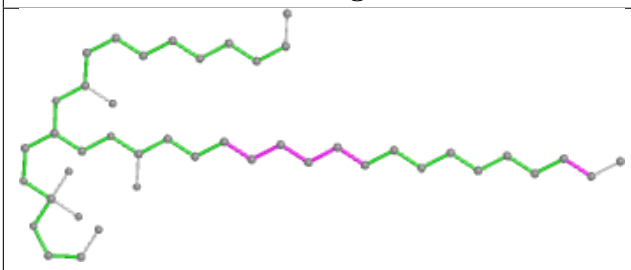
Ligand PEK G 101



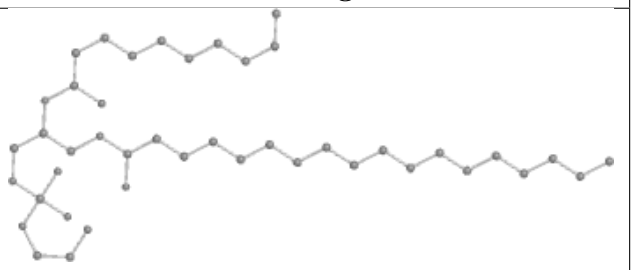
Bond lengths



Bond angles

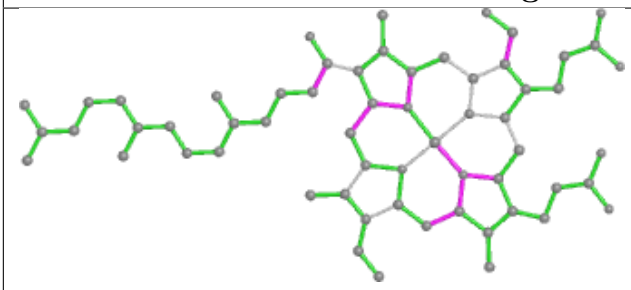


Torsions

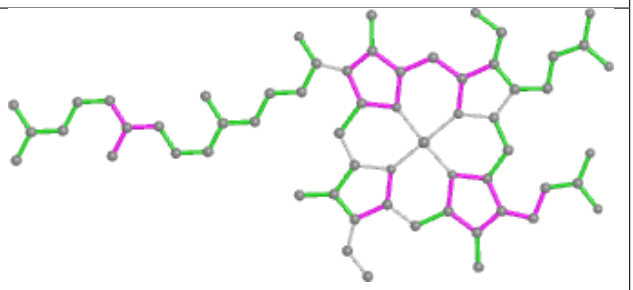


Rings

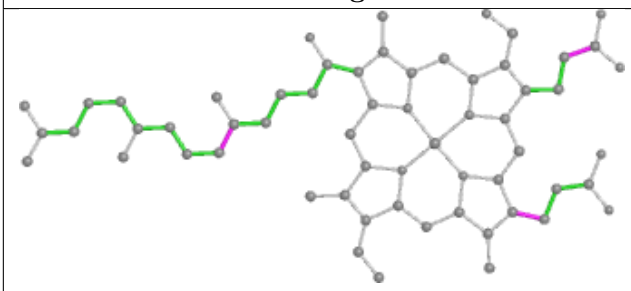
Ligand HEA A 602



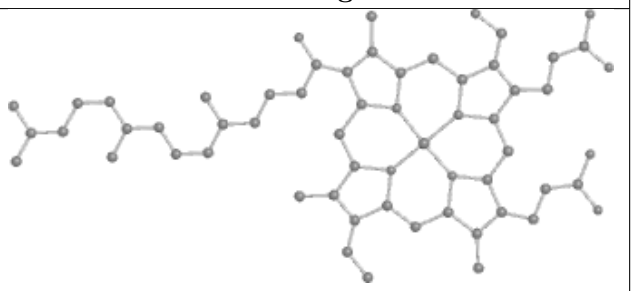
Bond lengths



Bond angles

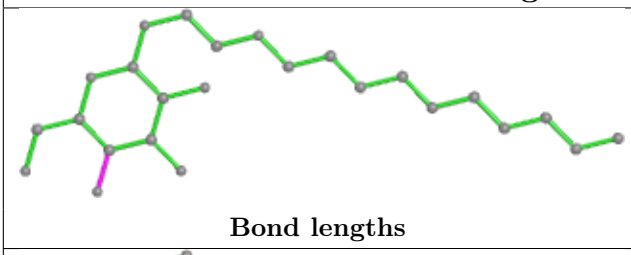


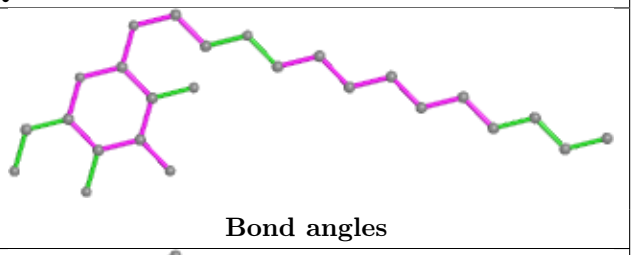
Torsions

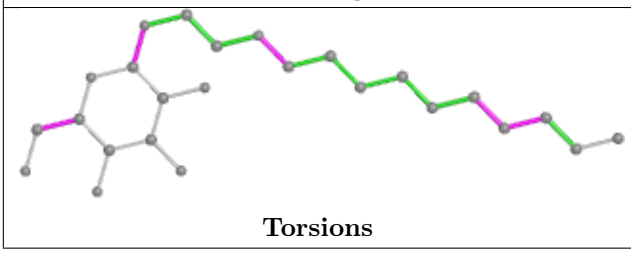


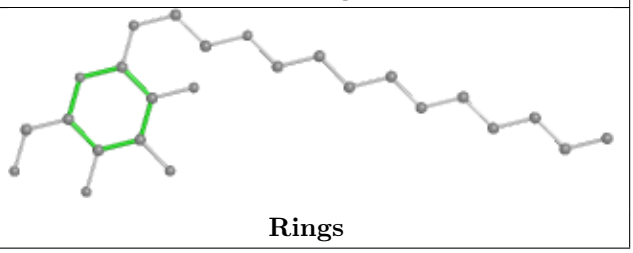
Rings

Ligand CQX A 606

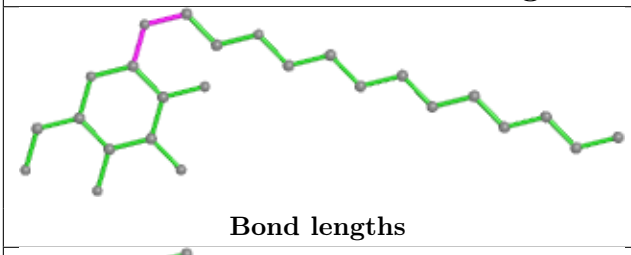

Bond lengths

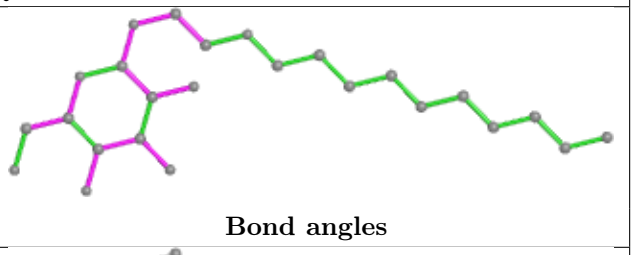

Bond angles

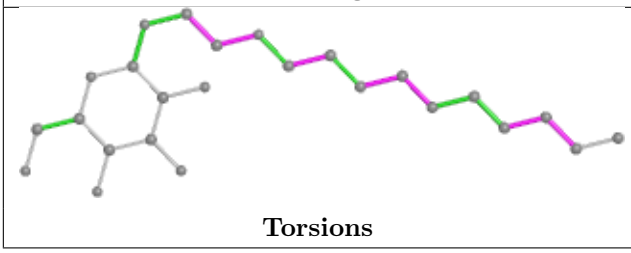

Torsions

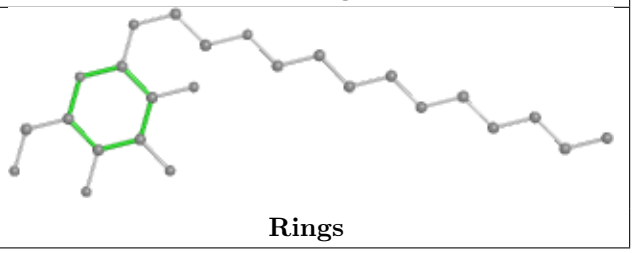

Rings

Ligand CQX C 305

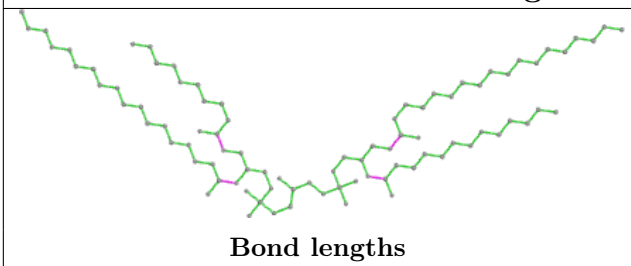

Bond lengths

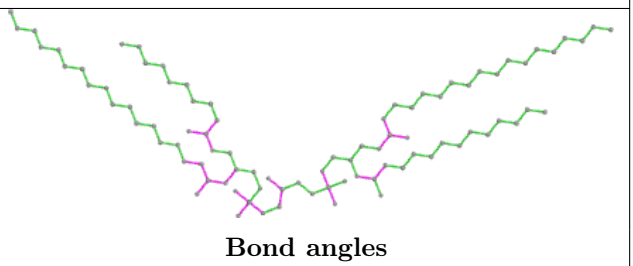

Bond angles

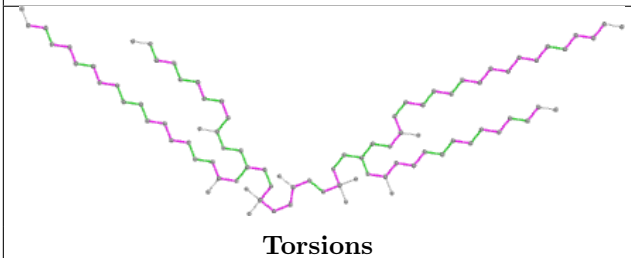

Torsions

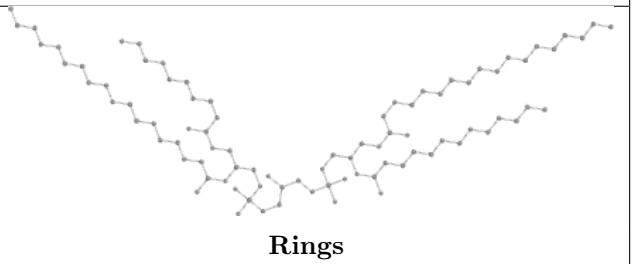

Rings

Ligand CDL C 304

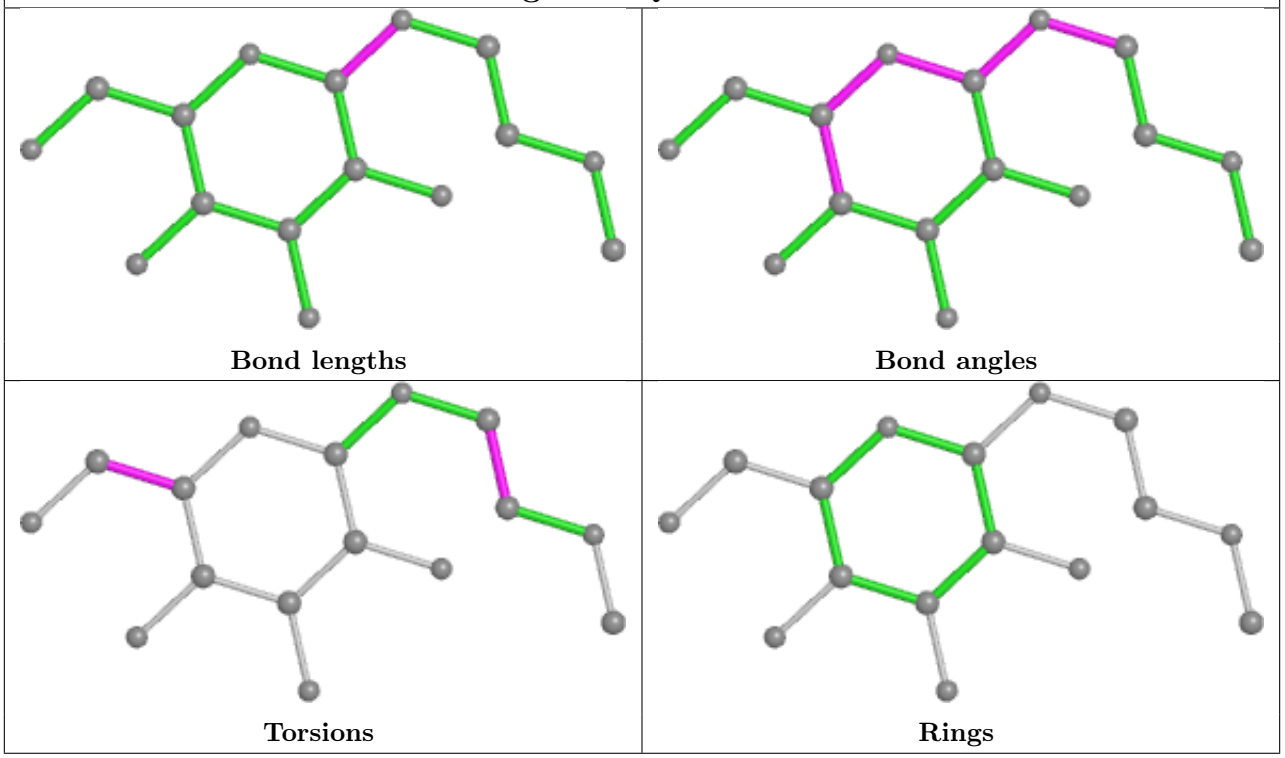

Bond lengths


Bond angles

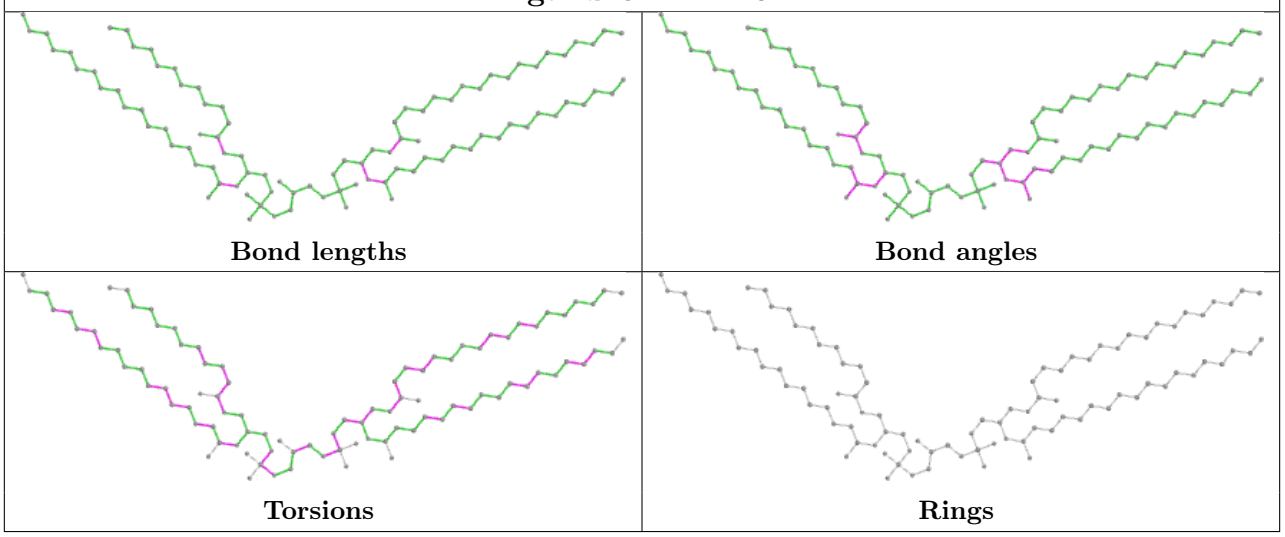

Torsions


Rings

Ligand CQX B 303



Ligand CDL L 101



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, 95^{th} 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%)	0.25	2 (0%)	92	95	28, 35, 47, 94	0
2	B	226/227 (99%)	0.23	2 (0%)	84	89	31, 42, 69, 97	0
3	C	254/261 (97%)	0.21	1 (0%)	92	95	31, 40, 53, 82	0
4	D	136/147 (92%)	0.48	9 (6%)	18	26	41, 53, 76, 82	0
5	E	102/109 (93%)	0.31	3 (2%)	51	60	42, 55, 76, 89	0
6	F	91/98 (92%)	0.32	4 (4%)	34	44	38, 52, 75, 95	0
7	G	72/85 (84%)	0.33	3 (4%)	36	45	38, 48, 89, 105	0
8	H	75/85 (88%)	0.34	3 (4%)	38	48	37, 47, 77, 83	0
9	I	70/73 (95%)	0.14	0	100	100	37, 50, 70, 74	0
10	J	55/59 (93%)	0.51	3 (5%)	25	34	43, 51, 76, 87	0
11	K	49/56 (87%)	0.68	2 (4%)	37	46	47, 55, 69, 82	0
12	L	44/47 (93%)	0.24	1 (2%)	60	69	37, 46, 63, 68	0
13	M	40/46 (86%)	0.43	2 (5%)	28	39	44, 50, 69, 77	0
All	All	1727/1807 (95%)	0.30	35 (2%)	65	73	28, 43, 70, 105	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	36	TRP	5.3
2	B	113	TYR	4.6
13	M	32	TRP	4.5
10	J	52	TRP	4.4
10	J	55	PHE	4.4

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, 95^{th} 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	0.25	50,69,103,115	0
2	FME	B	1	10/11	0.98	0.11	35,46,57,59	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	0.54	0.36	42,42,42,42	1
20	CDL	C	304	87/100	0.86	0.26	50,96,139,153	0
20	CDL	B	301	64/100	0.90	0.18	54,89,130,135	0
18	CQX	A	609	25/25	0.90	0.26	55,70,87,108	0
20	CDL	L	101	94/100	0.90	0.25	48,83,125,140	0
18	CQX	B	303	16/25	0.92	0.13	53,74,86,92	0
18	CQX	A	608	25/25	0.94	0.19	49,65,75,92	0
18	CQX	A	606	25/25	0.94	0.14	41,55,68,81	0
18	CQX	G	102	25/25	0.96	0.10	46,54,61,67	0
18	CQX	C	306	25/25	0.97	0.16	43,63,101,108	0
18	CQX	C	305	25/25	0.97	0.13	44,54,91,100	0
19	PGV	C	303	51/51	0.97	0.16	35,45,107,132	0
24	PEK	G	101	43/53	0.97	0.13	34,46,65,86	0
22	CHD	C	301	29/29	0.98	0.13	31,37,42,57	0
19	PGV	A	607	51/51	0.98	0.14	30,43,75,83	0
17	NA	A	605	1/1	0.99	0.08	40,40,40,40	0
14	HEA	A	601	60/60	0.99	0.12	26,33,51,54	0
14	HEA	A	602	60/60	0.99	0.15	25,30,38,49	0
16	MG	A	604	1/1	0.99	0.11	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.20	29,29,29,29	0

Continued on next page...

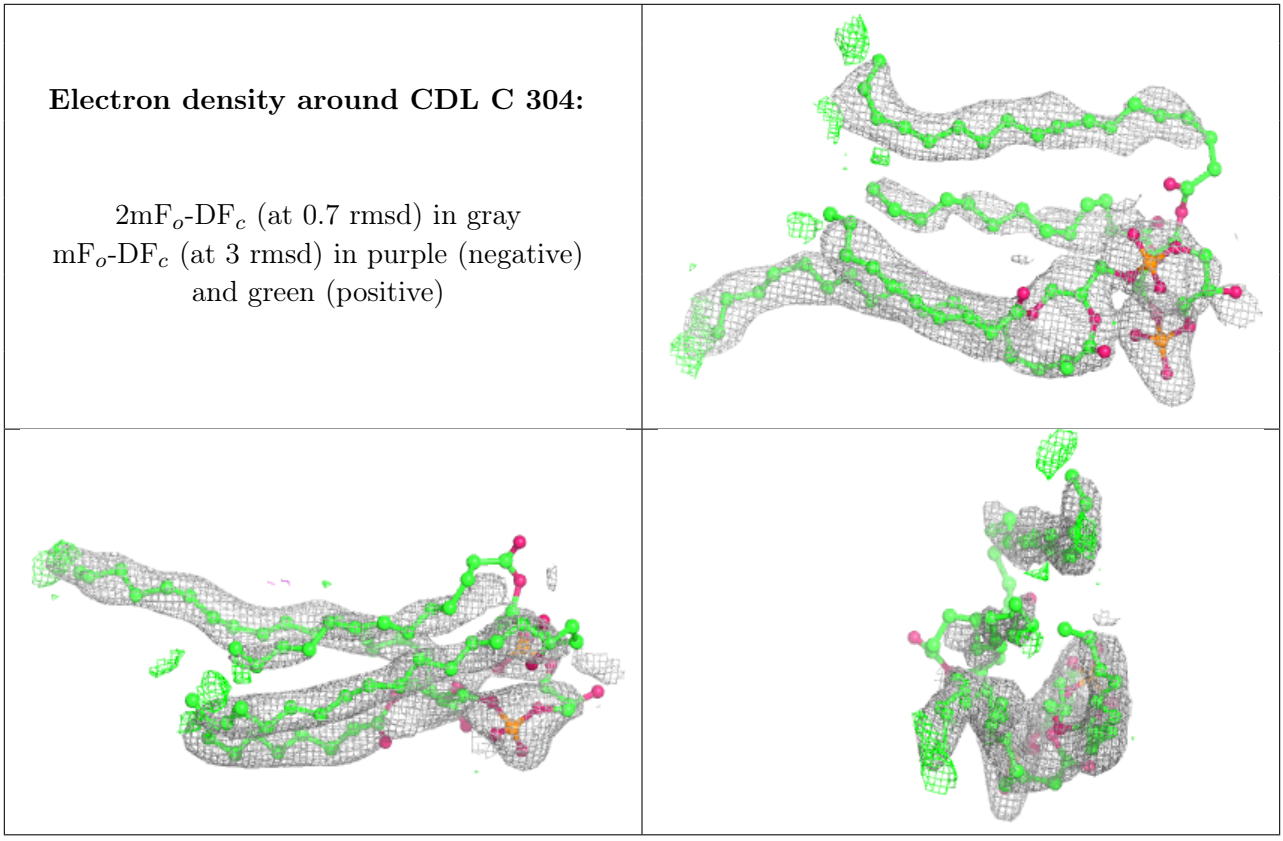
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	ZN	F	101	1/1	1.00	0.15	47,47,47,47	0
21	CUA	B	302	2/2	1.00	0.17	34,34,34,34	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.

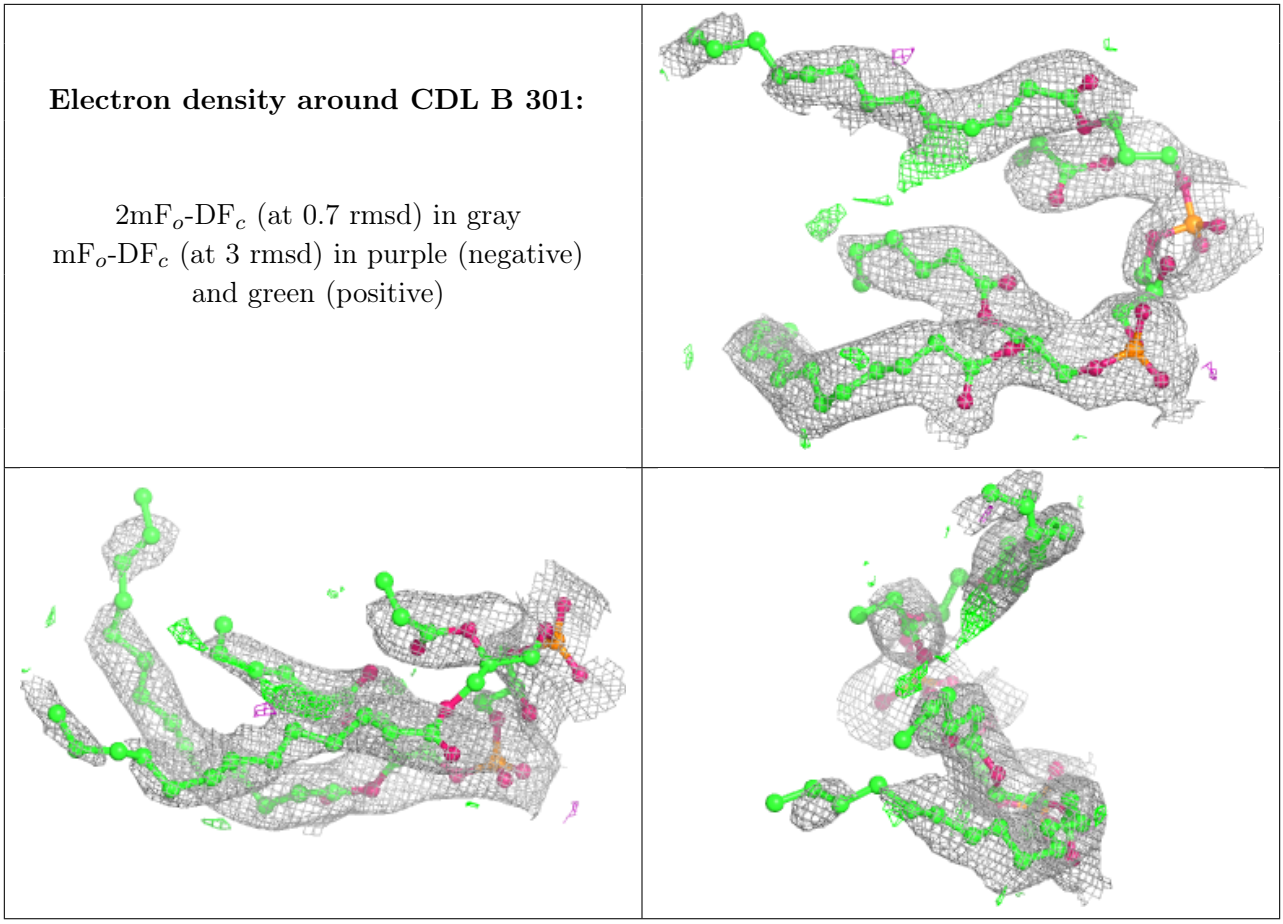
Electron density around CDL C 304:

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



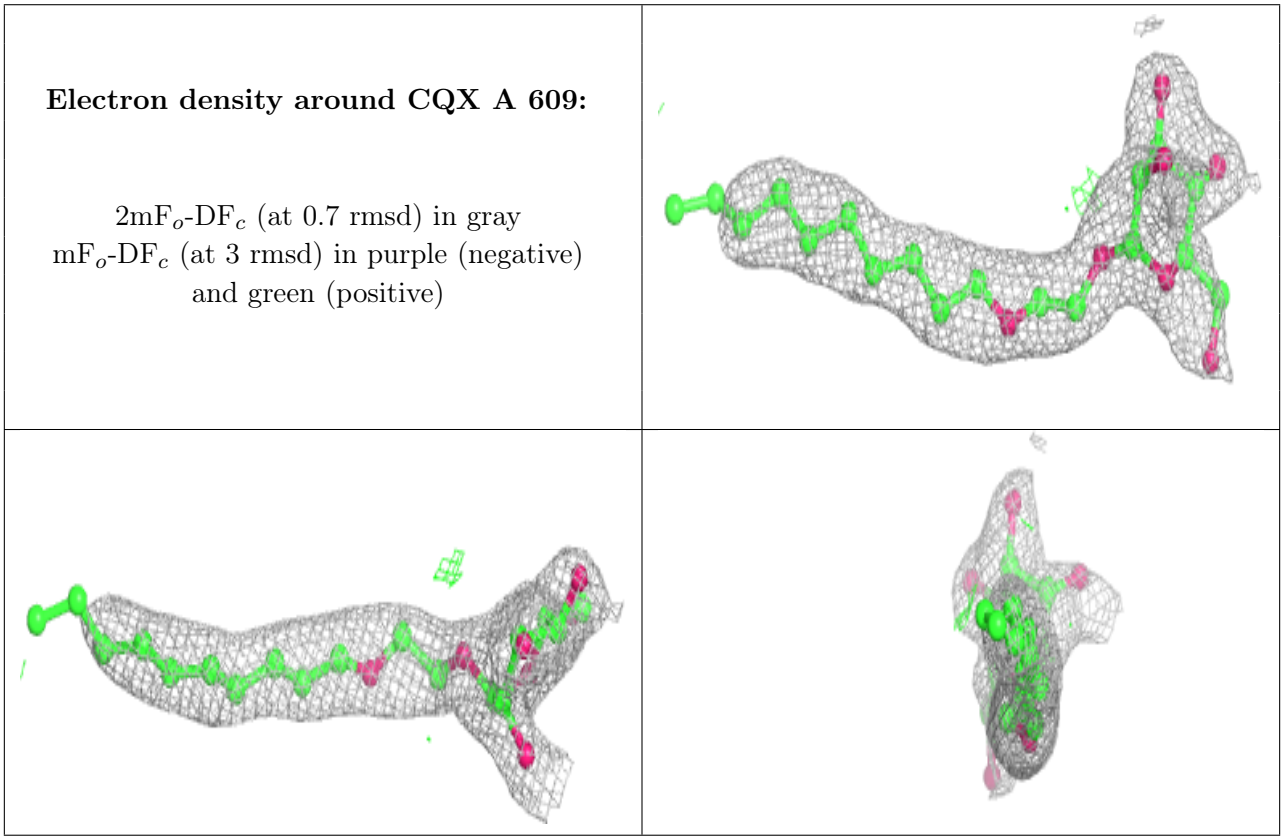
Electron density around CDL B 301:

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



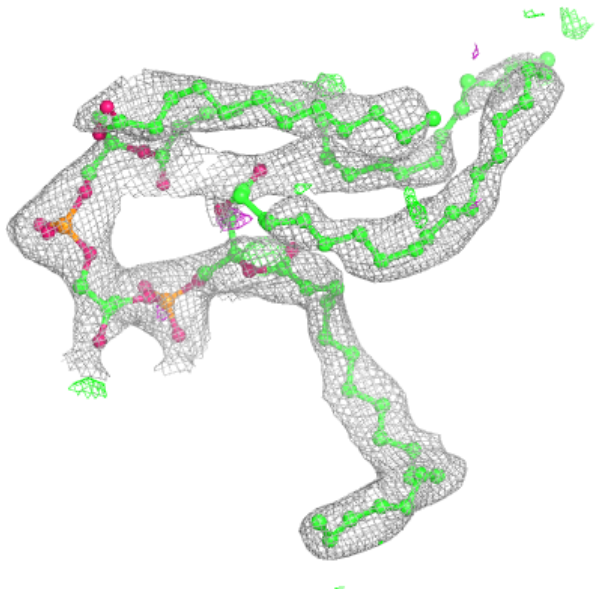
Electron density around CQX A 609:

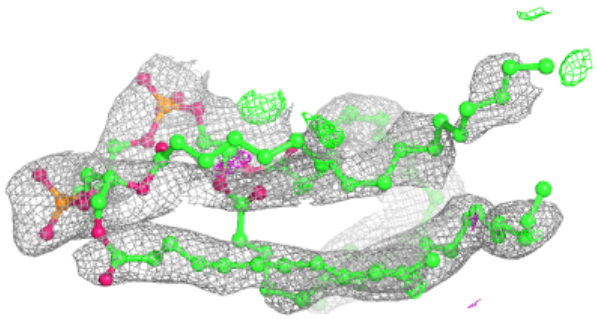
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

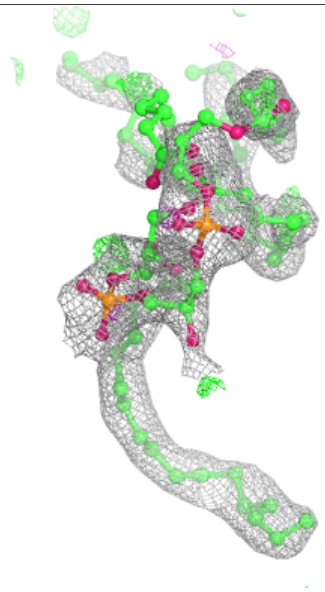


Electron density around CDL L 101:

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

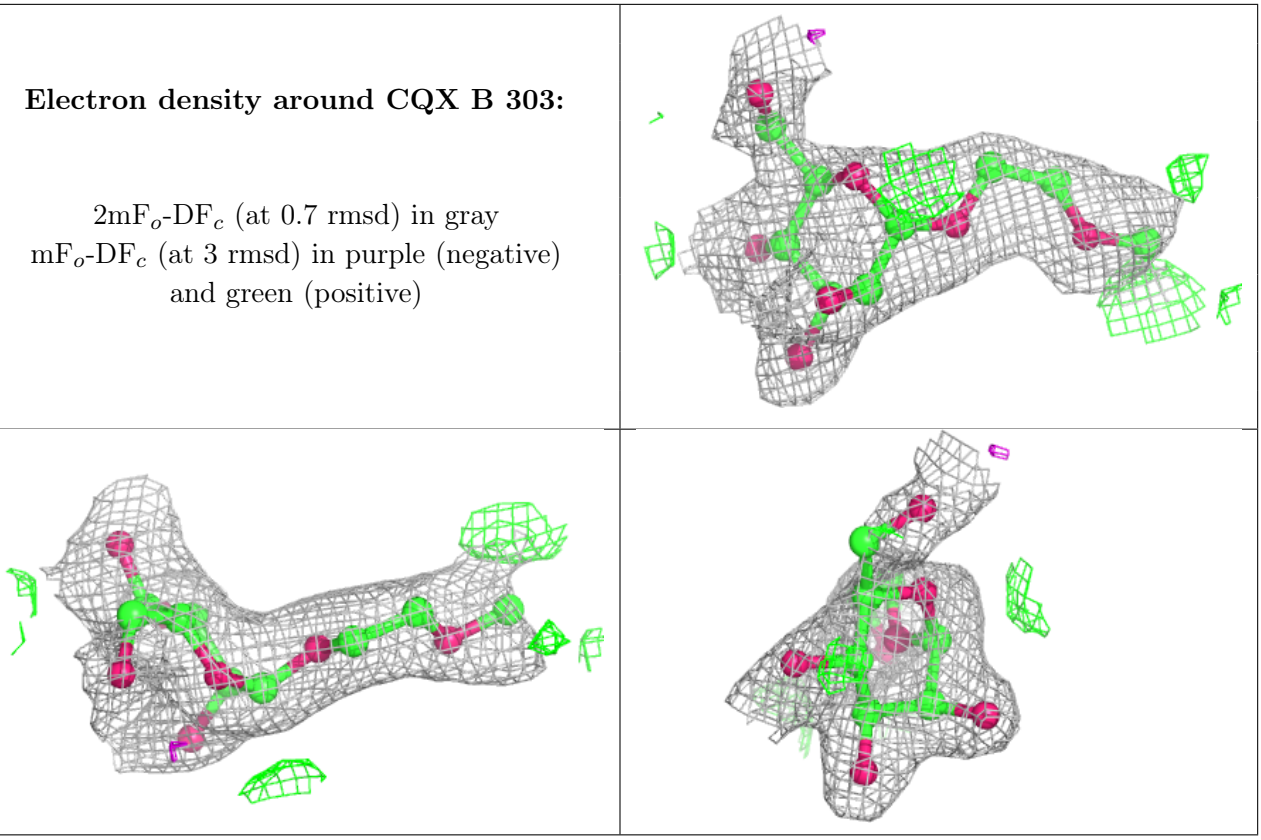






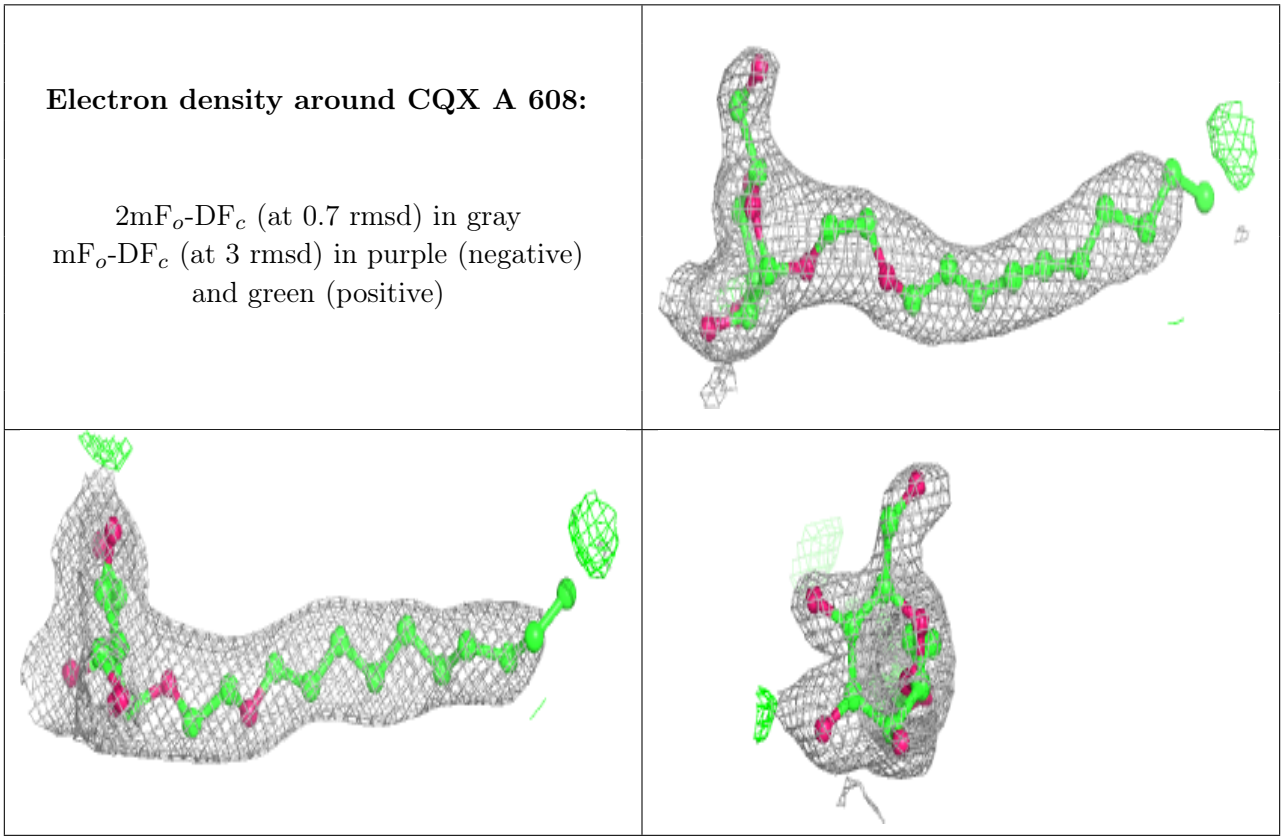
Electron density around CQX B 303:

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



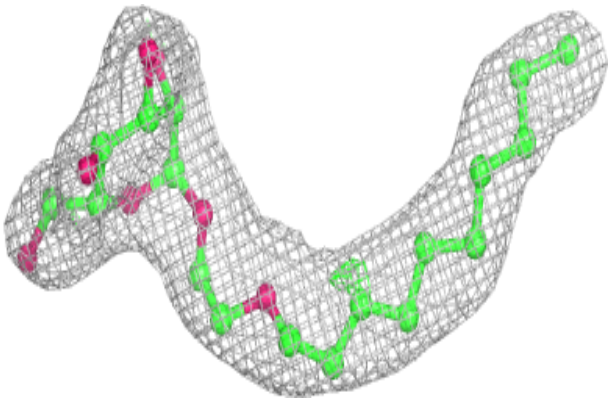
Electron density around CQX A 608:

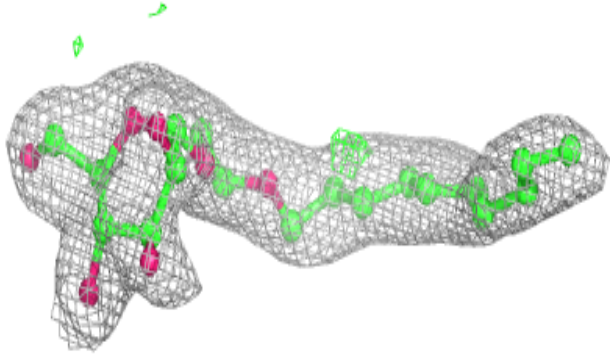
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

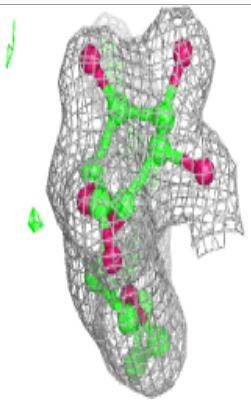


Electron density around CQX A 606:

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

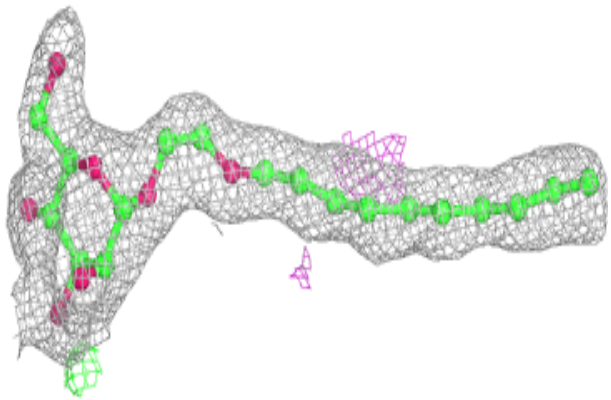


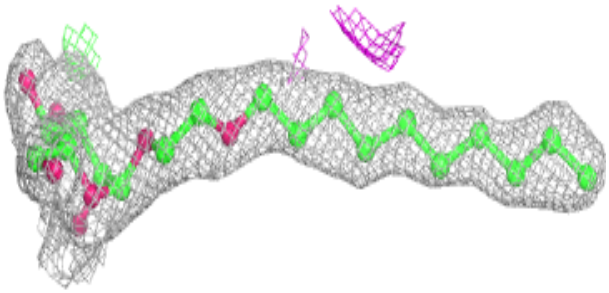


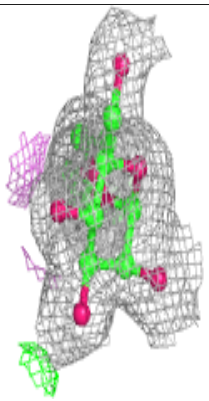


Electron density around CQX G 102:

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

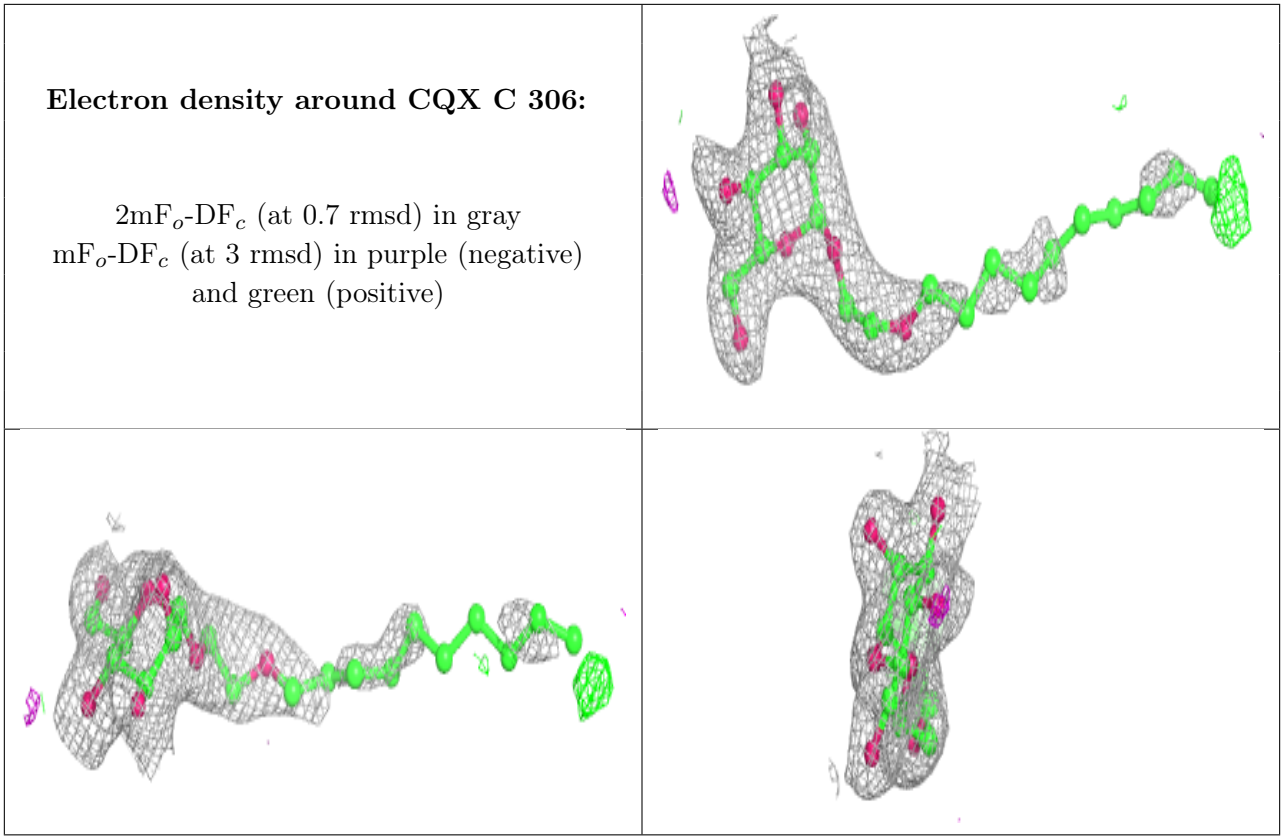






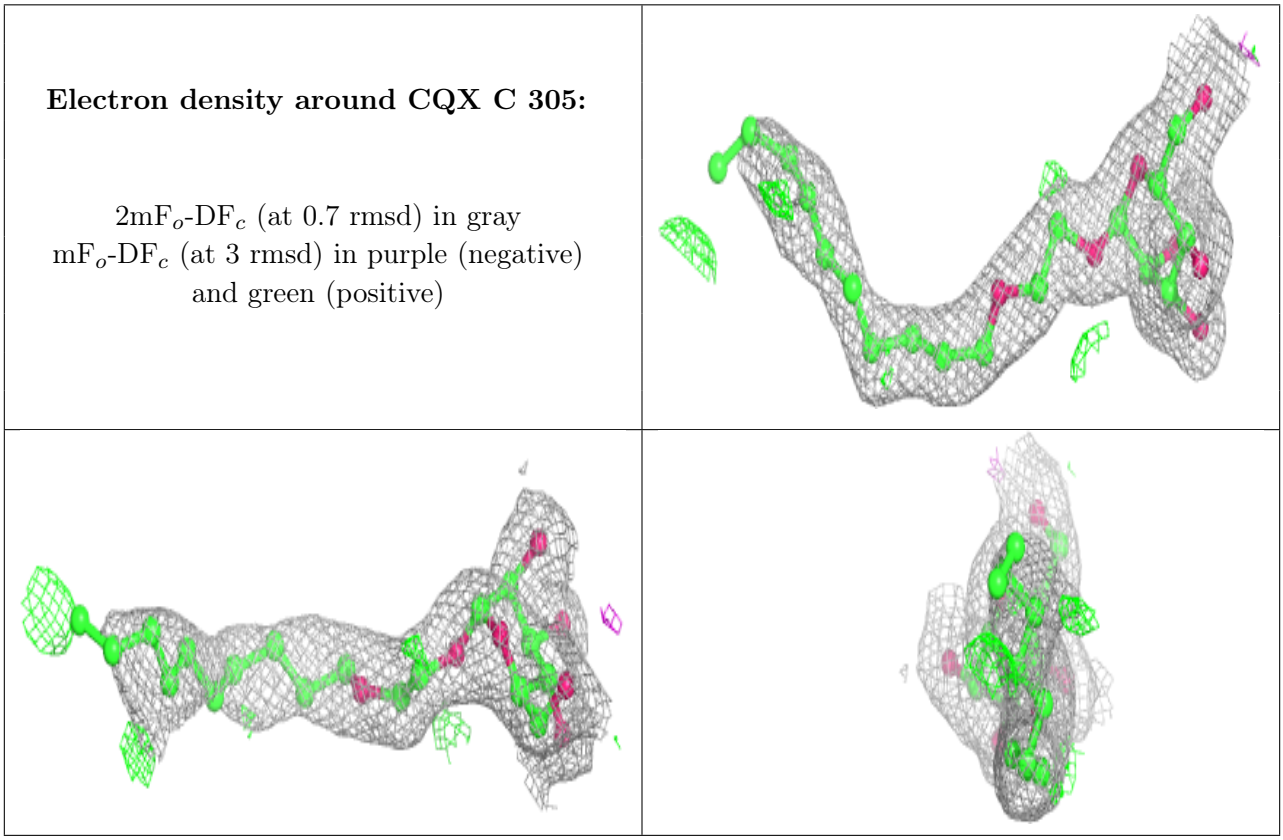
Electron density around CQX C 306:

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



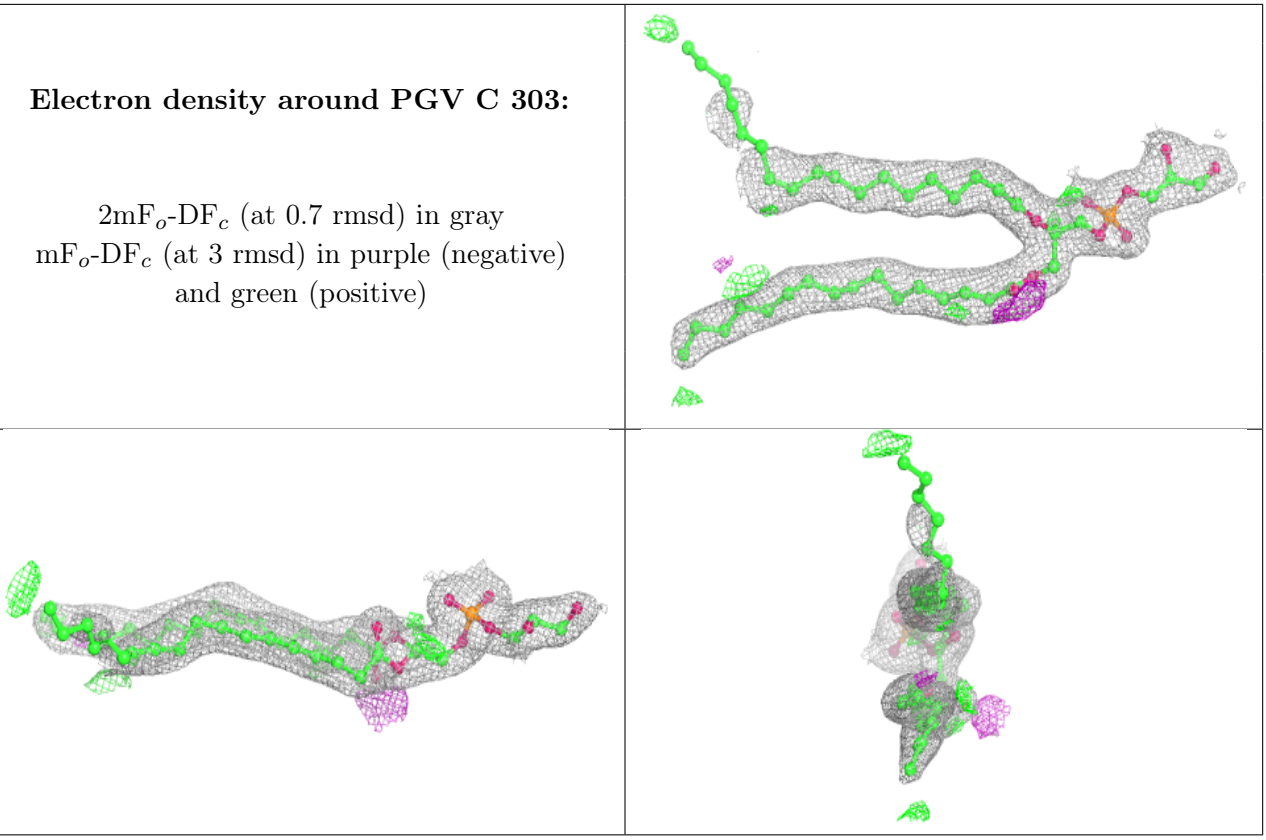
Electron density around CQX C 305:

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



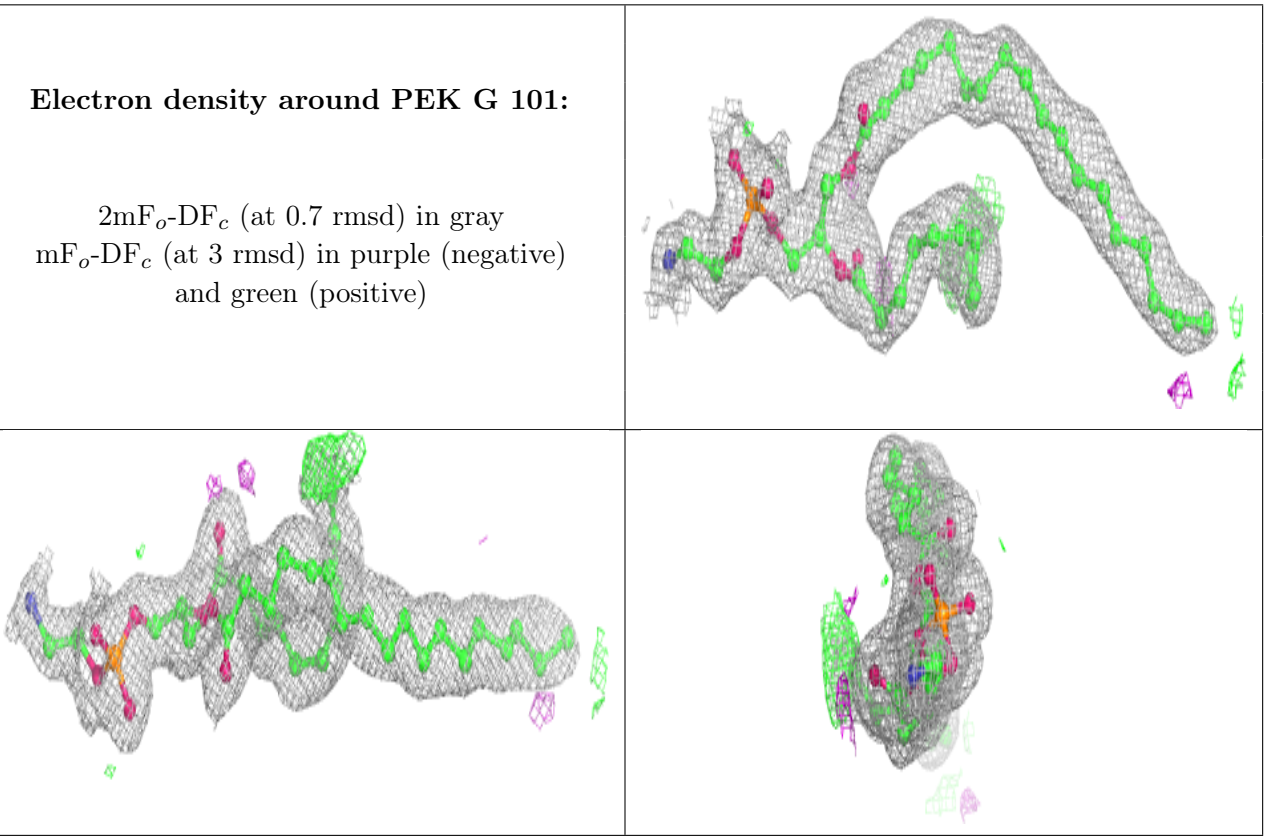
Electron density around PGV C 303:

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



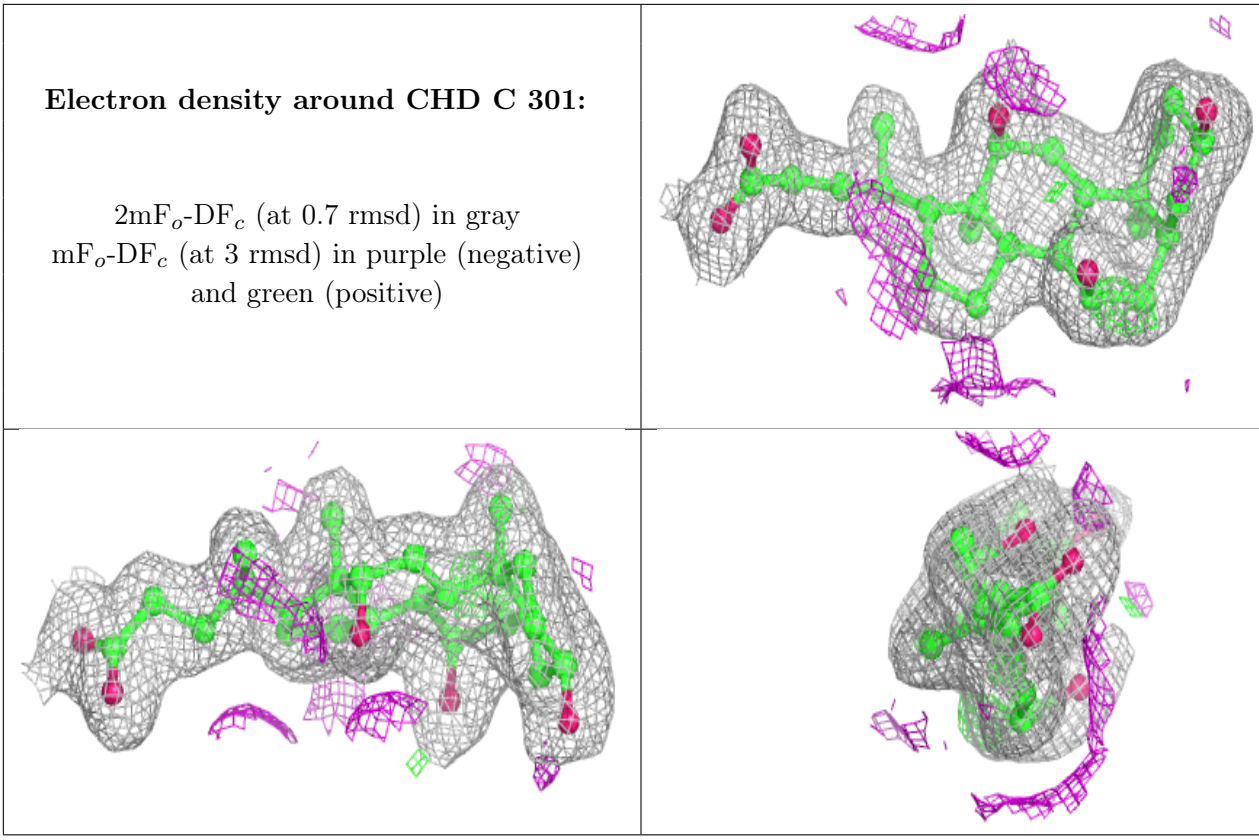
Electron density around PEK G 101:

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



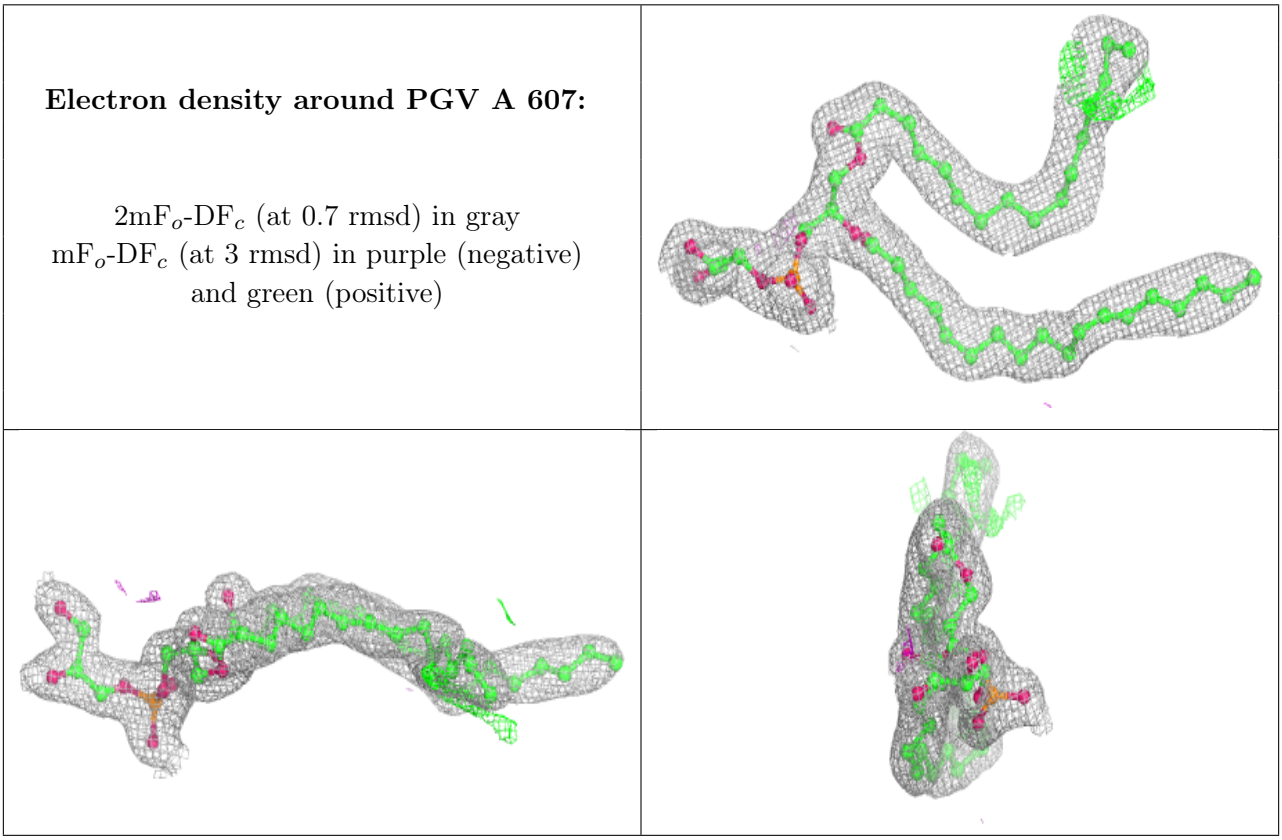
Electron density around CHD C 301:

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



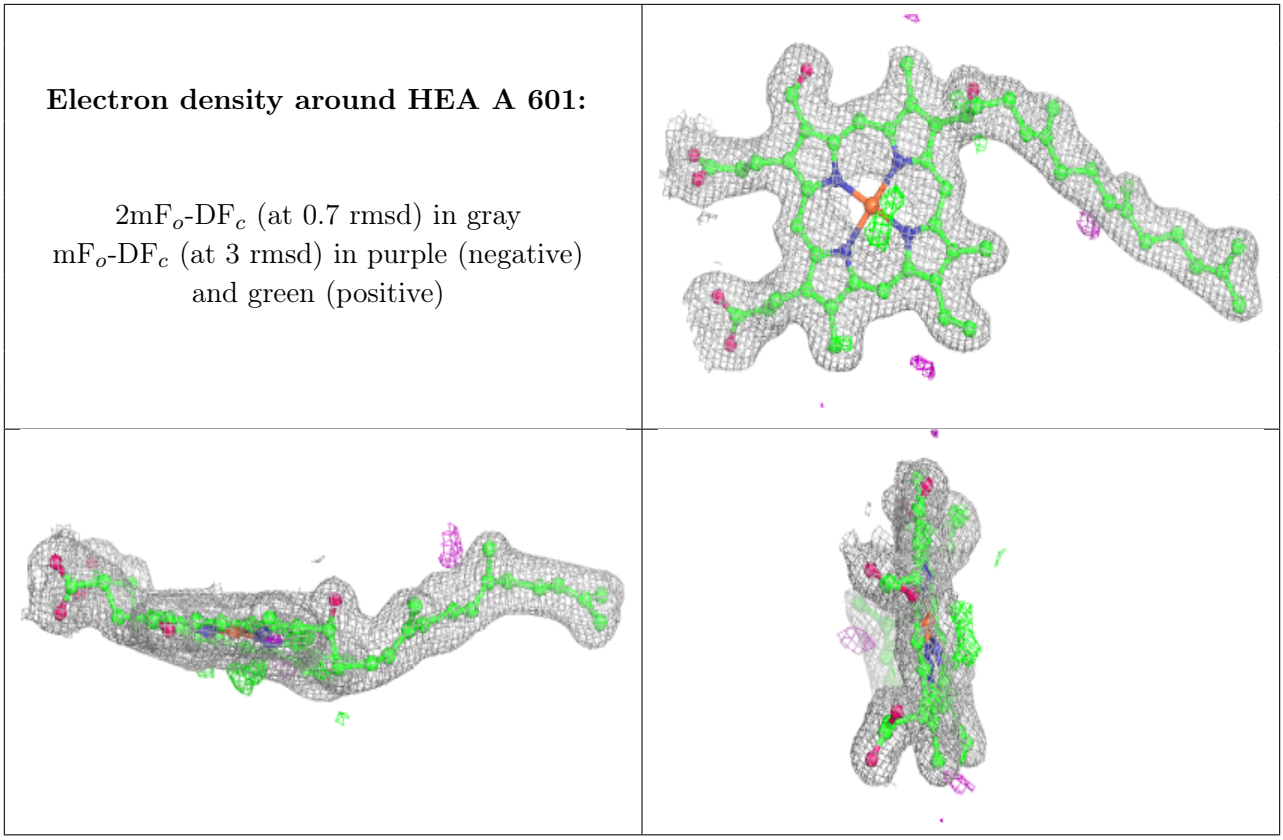
Electron density around PGV A 607:

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



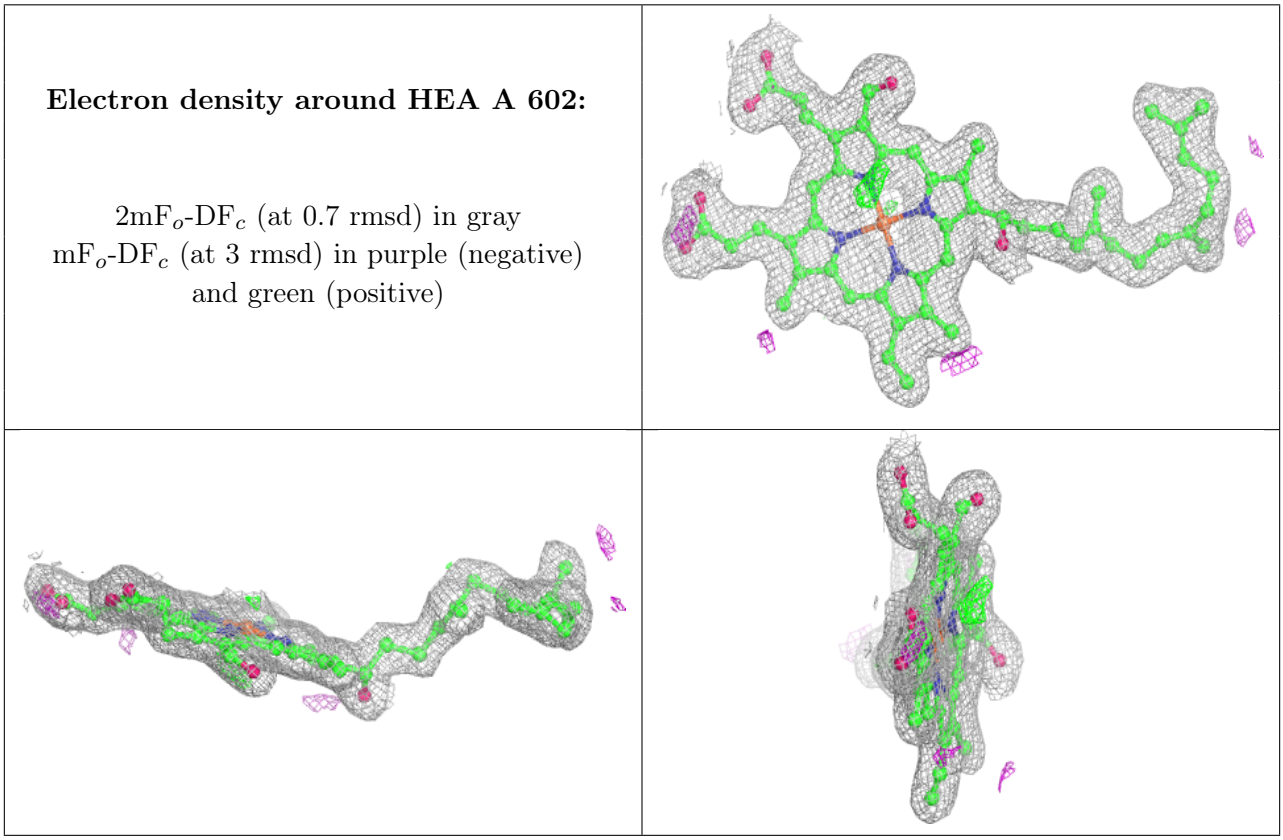
Electron density around HEA A 601:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.