



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:41 PM JST

PDB ID : 6JY3 / pdb_00006jy3
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

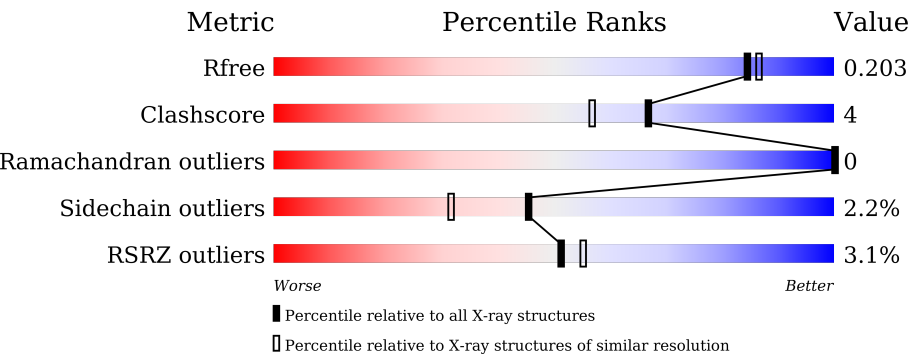
1 Overall quality at a glance i

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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	%93%6%
2	B	227	4%85%12%•
3	C	261	%90%8%•
4	D	147	3%86%7%7%
5	E	109	3%87%6%6%
6	F	98	5%82%7%••7%

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Mol	Chain	Length	Quality of chain
7	G	85	8% 73% 11% • 15%
8	H	85	4% 84% 5% 12%
9	I	73	7% 85% 10% • •
10	J	59	7% 88% 5% 7%
11	K	56	4% 80% 7% 12%
12	L	47	2% 79% 13% • 6%
13	M	46	80% • • 13%

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			

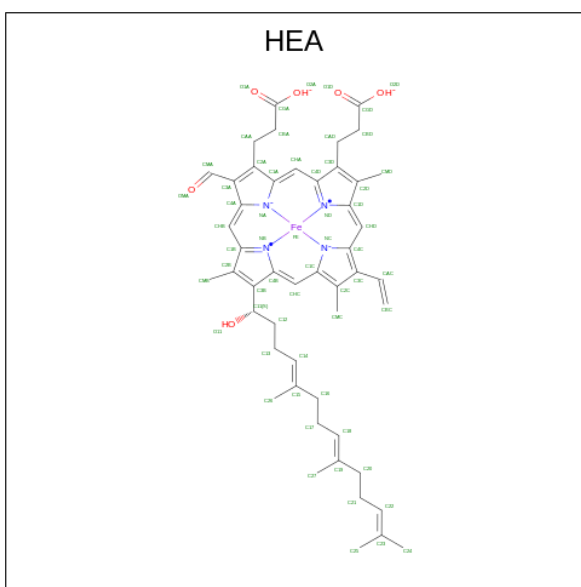
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 (CCD ID: 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 (CCD ID: CU) (formula: Cu).

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

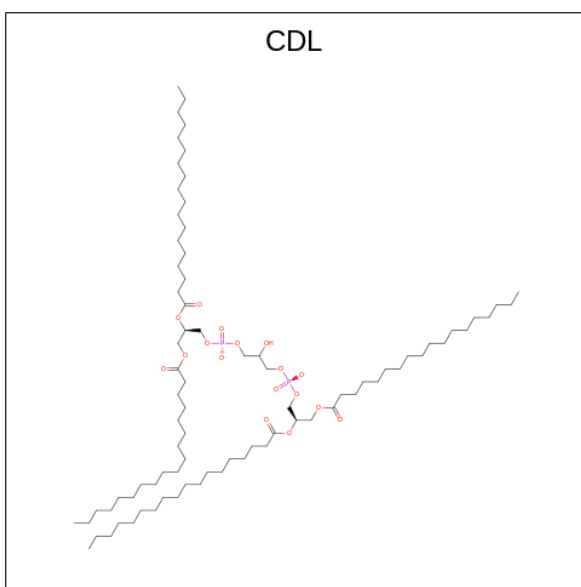
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

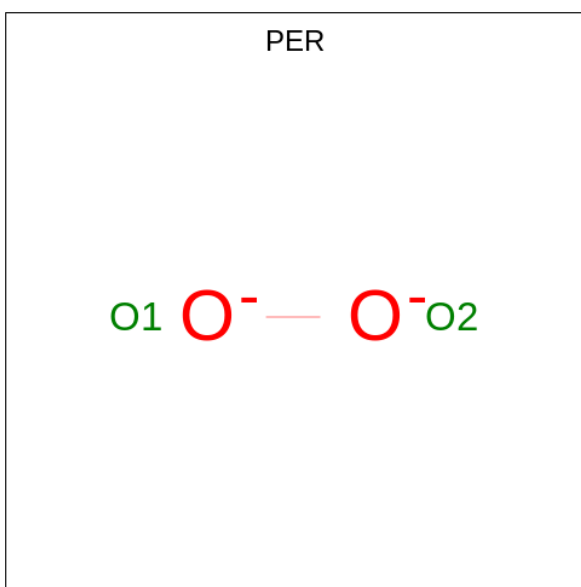
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



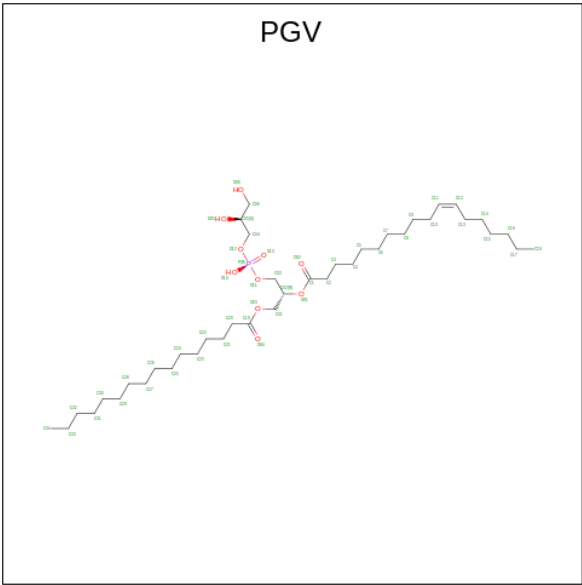
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			94	75	17	2		
18	B	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 19 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



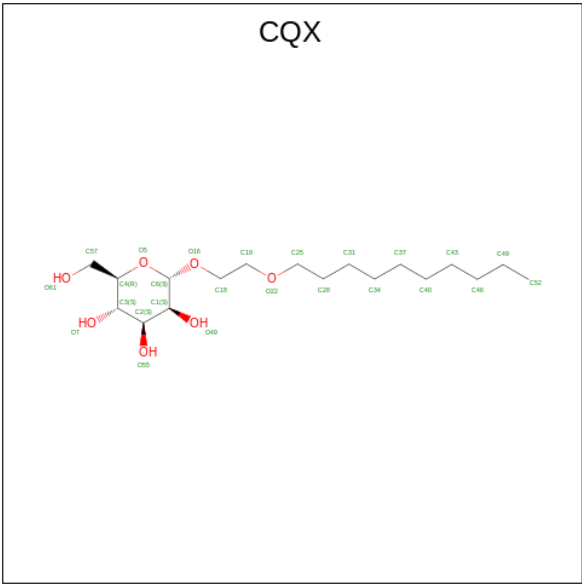
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		

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



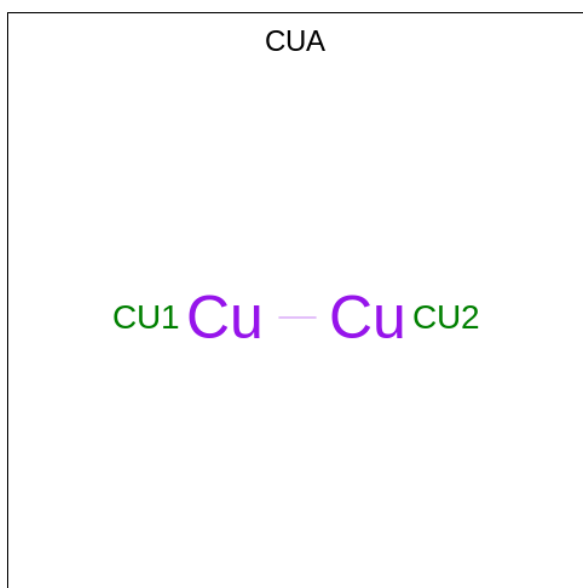
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			41	30	10	1		

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



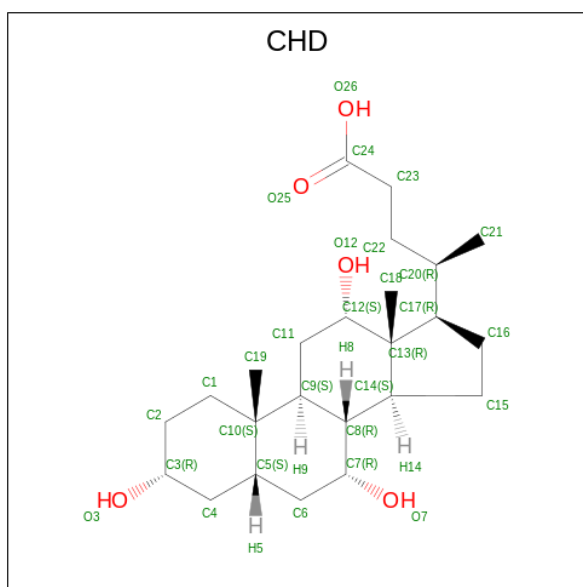
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 25 18 7	0	0
21	A	1	Total C O 25 18 7	0	0
21	A	1	Total C O 25 18 7	0	0
21	B	1	Total C O 25 18 7	0	0
21	B	1	Total C O 16 9 7	0	0
21	C	1	Total C O 25 18 7	0	0
21	C	1	Total C O 25 18 7	0	0
21	G	1	Total C O 25 18 7	0	0

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



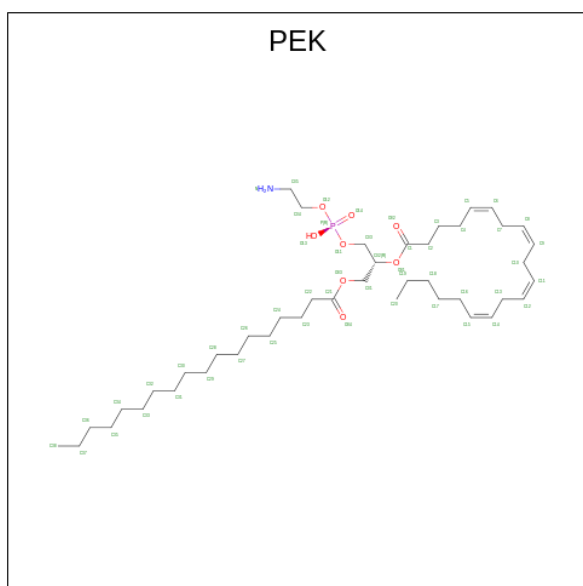
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

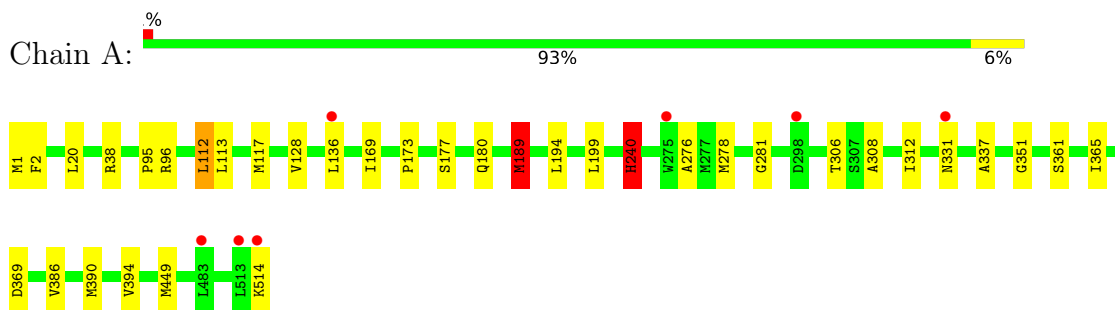
- Molecule 26 is water.

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

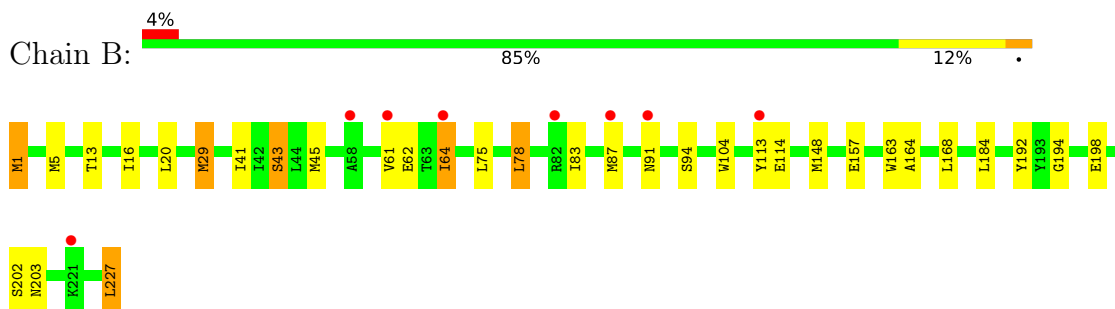
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

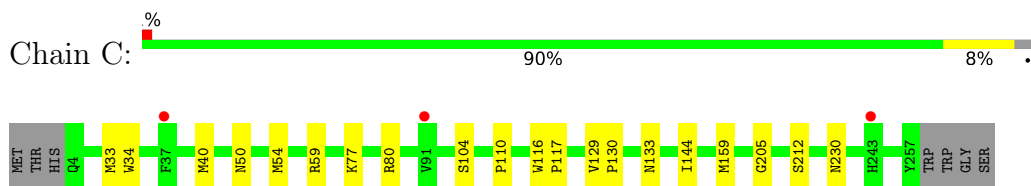
- Molecule 1: Cytochrome c oxidase subunit 1



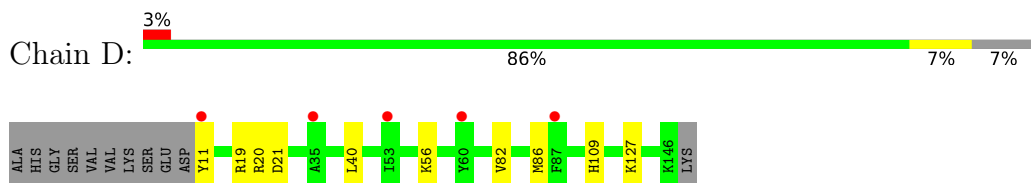
- Molecule 2: Cytochrome c oxidase subunit 2



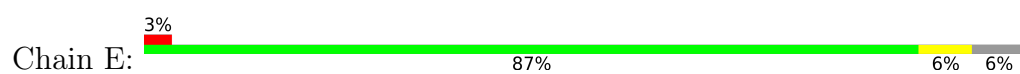
- Molecule 3: Cytochrome c oxidase subunit 3



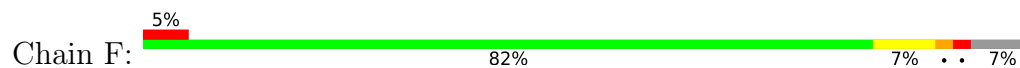
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



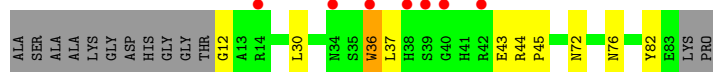
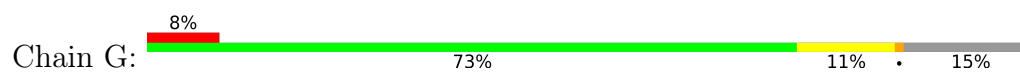
- Molecule 5: Cytochrome c oxidase subunit 5A



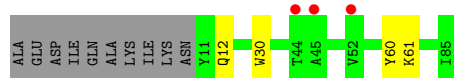
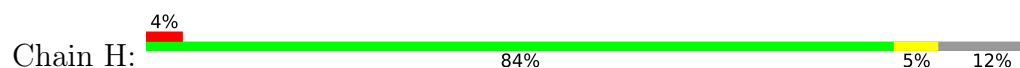
• Molecule 6: Cytochrome c oxidase subunit 5B



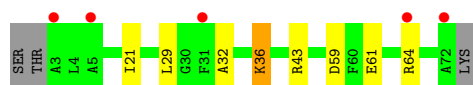
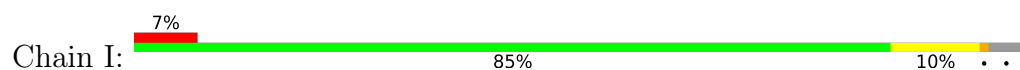
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



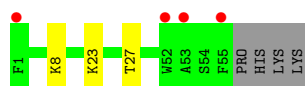
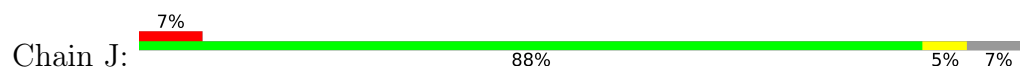
• Molecule 8: Cytochrome c oxidase subunit 6B1



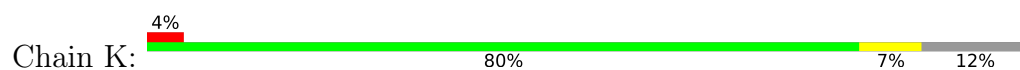
• Molecule 9: Cytochrome c oxidase subunit 6C



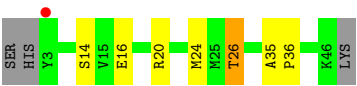
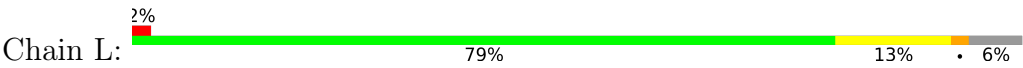
• Molecule 10: Cytochrome c oxidase subunit 7A1



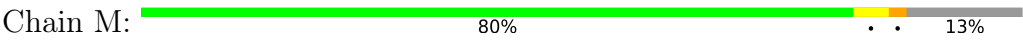
• Molecule 11: Cytochrome c oxidase subunit 7B



- 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 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-1.85) 99.0 (40.00-1.85)	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)	0.38 , 67.3	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	0.96	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, FME, CHD, HEA, PER, CQX, NA, MG, CDL, CUA, PEK, PGV, 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	1.38	20/4156 (0.5%)	1.10	4/5678 (0.1%)
2	B	1.36	4/1860 (0.2%)	1.16	5/2534 (0.2%)
3	C	1.27	5/2143 (0.2%)	1.03	1/2931 (0.0%)
4	D	1.14	1/1167 (0.1%)	1.11	2/1577 (0.1%)
5	E	1.13	1/843 (0.1%)	1.02	0/1145
6	F	1.11	0/709	1.09	2/963 (0.2%)
7	G	1.25	1/621 (0.2%)	1.14	1/848 (0.1%)
8	H	1.20	0/648	1.07	0/877
9	I	1.16	0/588	1.06	2/781 (0.3%)
10	J	1.16	0/443	1.00	1/598 (0.2%)
11	K	1.15	0/398	1.15	2/546 (0.4%)
12	L	1.35	1/372 (0.3%)	1.16	1/500 (0.2%)
13	M	1.20	0/321	1.05	0/440
All	All	1.28	33/14269 (0.2%)	1.09	21/19418 (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
1	A	0	1
6	F	0	1
All	All	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	MET	SD-CE	-13.69	1.45	1.79
7	G	36	TRP	CB-CG	10.06	1.81	1.50
3	C	104	SER	CA-CB	8.96	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	104	SER	CB-OG	8.51	1.59	1.42
1	A	189	MET	SD-CE	-7.95	1.59	1.79
1	A	173	PRO	CA-C	7.58	1.56	1.51
2	B	198	GLU	C-O	6.81	1.31	1.23
5	E	84	TYR	C-O	6.05	1.31	1.24
1	A	331	ASN	CA-CB	5.90	1.60	1.52
1	A	308	ALA	N-CA	-5.87	1.39	1.46
4	D	19	ARG	CZ-NH1	5.87	1.41	1.32
1	A	365	ILE	CB-CG1	5.86	1.65	1.53
1	A	189	MET	CG-SD	-5.85	1.66	1.80
2	B	198	GLU	CA-C	5.82	1.59	1.52
1	A	96	ARG	CA-CB	5.81	1.62	1.53
1	A	281	GLY	N-CA	5.78	1.53	1.45
1	A	351	GLY	N-CA	5.70	1.53	1.45
2	B	163	TRP	N-CA	-5.62	1.39	1.46
1	A	276	ALA	CA-C	5.60	1.59	1.52
1	A	199	LEU	C-O	-5.55	1.19	1.24
3	C	133	ASN	CG-OD1	-5.51	1.13	1.23
1	A	306	THR	N-CA	5.48	1.52	1.46
1	A	117	MET	N-CA	5.46	1.53	1.46
1	A	361	SER	CB-OG	-5.46	1.31	1.42
12	L	14	SER	C-O	-5.44	1.17	1.23
3	C	212	SER	N-CA	5.27	1.52	1.46
1	A	95	PRO	N-CA	5.23	1.54	1.47
1	A	194	LEU	CA-C	5.20	1.59	1.52
2	B	43	SER	CA-C	5.15	1.59	1.52
1	A	20	LEU	N-CA	5.13	1.52	1.46
1	A	240	HIS	CA-C	5.07	1.58	1.52
1	A	136	LEU	CA-C	5.04	1.59	1.53
3	C	33	MET	N-CA	5.03	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	10.31	128.48	119.20
2	B	29	MET	CG-SD-CE	-8.72	81.71	100.90
1	A	189	MET	CB-CG-SD	-8.03	88.61	112.70
7	G	36	TRP	CB-CA-C	7.43	124.94	110.67
11	K	49	THR	CA-C-N	-6.82	112.76	119.78
11	K	49	THR	C-N-CA	-6.82	112.76	119.78
1	A	240	HIS	N-CA-CB	6.77	118.41	110.42
6	F	87	THR	N-CA-CB	6.40	119.45	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	SER	N-CA-C	6.27	118.91	111.33
1	A	240	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	117	MET	CA-CB-CG	5.83	125.77	114.10
2	B	64	ILE	CB-CA-C	-5.61	103.17	112.26
4	D	20	ARG	NE-CZ-NH1	-5.60	115.90	121.50
10	J	23	LYS	CG-CD-CE	-5.54	98.56	111.30
9	I	59	ASP	N-CA-C	-5.42	105.28	111.07
6	F	65	ASP	N-CA-C	5.36	119.65	113.38
9	I	43	ARG	CG-CD-NE	5.29	123.63	112.00
12	L	26	THR	N-CA-CB	-5.24	102.41	110.12
3	C	80	ARG	CG-CD-NE	-5.22	100.51	112.00
2	B	157	GLU	CA-CB-CG	-5.17	103.76	114.10
2	B	113	TYR	CB-CA-C	-5.08	100.32	110.42

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	25	0
2	B	1824	0	1833	20	0
3	C	2061	0	1992	9	0
4	D	1133	0	1119	6	0
5	E	825	0	823	3	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	2	0
12	L	360	0	360	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	311	0	321	4	0
14	A	120	0	108	4	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	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	106	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 4.

All (106) 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:CB	7:G:36:TRP:CG	1.81	1.59
19:A:607:PER:O1	19:A:607:PER:O2	1.55	1.22
2:B:16:ILE:HG23	2:B:87:MET:HE2	1.36	1.04
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
1:A:2:PHE:CZ	18:A:606:CDL:H712	2.05	0.91
6:F:85:CYS:SG	6:F:87:THR:HG23	2.15	0.87
1:A:113:LEU:CD1	18:A:606:CDL:H871	2.17	0.74
1:A:2:PHE:HZ	18:A:606:CDL:H712	1.49	0.74
18:C:305:CDL:O1	10:J:8:LYS:CD	2.36	0.74
7:G:72:ASN:H	7:G:76:ASN:HD22	1.33	0.73
6:F:75:HIS:H	6:F:80:GLN:HE22	1.35	0.73
10:J:27:THR:HG22	26:J:109:HOH:O	1.87	0.73
2:B:16:ILE:CG2	2:B:87:MET:HE2	2.19	0.72
6:F:54:ASN:H	6:F:54:ASN:HD22	1.39	0.70
1:A:2:PHE:CE2	18:A:606:CDL:H712	2.26	0.70
1:A:112:LEU:O	1:A:112:LEU:HD23	1.92	0.70
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.75	0.69
24:C:303:PEK:HN2	7:G:76:ASN:HD21	1.42	0.67
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.77	0.66
2:B:83:ILE:CG2	2:B:87:MET:HE3	2.25	0.65
7:G:36:TRP:CG	7:G:36:TRP:CA	2.77	0.64
2:B:13:THR:HB	2:B:168:LEU:HD23	1.79	0.63
18:C:305:CDL:O1	10:J:8:LYS:NZ	2.27	0.63
3:C:59:ARG:HG3	18:C:305:CDL:HA4	1.81	0.63
2:B:20:LEU:HD21	2:B:87:MET:HE1	1.81	0.62
1:A:177:SER:H	1:A:180:GLN:HE21	1.48	0.62
1:A:390:MET:HA	1:A:390:MET:HE3	1.82	0.60
3:C:205:GLY:HA3	21:C:306:CQX:C52	2.31	0.60
18:A:606:CDL:H822	18:A:606:CDL:H211	1.84	0.60
9:I:61:GLU:OE1	9:I:64:ARG:NH2	2.30	0.60
2:B:16:ILE:HD12	2:B:87:MET:HG2	1.83	0.59
26:A:775:HOH:O	3:C:77:LYS:HE3	2.03	0.58
12:L:20:ARG:HG3	12:L:20:ARG:HH11	1.68	0.58
1:A:113:LEU:HD12	18:A:606:CDL:H871	1.86	0.57
12:L:26:THR:HG23	13:M:25:SER:HB3	1.86	0.57
2:B:16:ILE:HG12	26:B:488:HOH:O	2.07	0.55
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.23	0.52
11:K:42:PRO:O	11:K:47:ARG:NH2	2.42	0.52
26:A:775:HOH:O	3:C:77:LYS:CE	2.57	0.52
1:A:113:LEU:CD1	18:A:606:CDL:C87	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:CD2	26:A:892:HOH:O	2.57	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
2:B:114:GLU:HB3	2:B:227:LEU:HD21	1.92	0.51
7:G:12:GLY:HA3	26:G:215:HOH:O	2.11	0.50
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.93	0.50
7:G:12:GLY:CA	26:G:215:HOH:O	2.60	0.49
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.49
7:G:36:TRP:HB3	26:G:234:HOH:O	2.12	0.48
7:G:45:PRO:O	7:G:82:TYR:OH	2.20	0.48
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.94	0.48
12:L:26:THR:HG23	13:M:25:SER:CB	2.44	0.48
18:C:305:CDL:OA8	18:C:305:CDL:H112	2.14	0.47
4:D:127:LYS:HD2	26:I:116:HOH:O	2.13	0.47
14:A:602:HEA:HBC1	14:A:602:HEA:HMC3	1.95	0.47
2:B:29:MET:HE3	9:I:32:ALA:HB1	1.96	0.47
1:A:112:LEU:HD23	1:A:112:LEU:C	2.40	0.47
2:B:29:MET:SD	9:I:36:LYS:HE2	2.54	0.47
1:A:112:LEU:CD2	1:A:112:LEU:C	2.87	0.47
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.97	0.46
1:A:386:VAL:HG11	14:A:601:HEA:H261	1.97	0.46
4:D:109:HIS:HD2	26:D:235:HOH:O	1.98	0.46
20:A:608:PGV:H183	24:C:303:PEK:H322	1.97	0.46
1:A:112:LEU:HD22	21:A:610:CQX:C49	2.45	0.46
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.51	0.46
23:C:301:CHD:H12	23:C:301:CHD:H212	1.98	0.46
1:A:2:PHE:CE2	18:A:606:CDL:C71	2.98	0.45
14:A:601:HEA:H122	14:A:601:HEA:HHC	1.98	0.45
2:B:61:VAL:O	2:B:62:GLU:C	2.57	0.45
5:E:31:LYS:HE2	6:F:83:PRO:O	2.17	0.45
3:C:129:VAL:N	3:C:130:PRO:CD	2.80	0.45
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.44
26:B:481:HOH:O	9:I:64:ARG:HD2	2.17	0.44
2:B:1:FME:O1	2:B:192:TYR:HA	2.16	0.44
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.44
7:G:72:ASN:H	7:G:76:ASN:ND2	2.09	0.44
12:L:20:ARG:NH1	12:L:24:MET:HE3	2.32	0.44
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.85	0.43
18:C:305:CDL:PA1	18:C:305:CDL:CB2	3.06	0.43
4:D:82:VAL:HG12	4:D:86:MET:HE2	2.01	0.43
6:F:13:ALA:O	6:F:18:ARG:HD2	2.19	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.54	0.43
9:I:21:ILE:HD12	9:I:21:ILE:HG23	1.81	0.43
2:B:29:MET:HE2	2:B:29:MET:C	2.44	0.42
6:F:92:VAL:HG23	6:F:92:VAL:O	2.19	0.42
7:G:43:GLU:OE2	7:G:43:GLU:HA	2.18	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.54	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.02	0.42
18:C:305:CDL:OA8	18:C:305:CDL:C11	2.67	0.42
5:E:23:ASP:O	5:E:24:ILE:C	2.61	0.42
18:C:305:CDL:OA8	18:C:305:CDL:CA5	2.67	0.41
4:D:56:LYS:HG2	5:E:61:PHE:CZ	2.55	0.41
18:A:606:CDL:C41	18:A:606:CDL:H842	2.50	0.41
13:M:40:TYR:O	26:M:101:HOH:O	2.22	0.41
18:C:305:CDL:C52	18:C:305:CDL:HB4	2.51	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.46	0.41
6:F:54:ASN:H	6:F:54:ASN:ND2	2.12	0.41
1:A:113:LEU:HD11	18:A:606:CDL:H871	2.01	0.41
4:D:11:TYR:CD1	4:D:11:TYR:C	2.99	0.41
1:A:113:LEU:HG	21:A:610:CQX:C52	2.51	0.40
7:G:37:LEU:HD23	7:G:37:LEU:HA	1.97	0.40
2:B:94:SER:HB2	2:B:148:MET:HE3	2.03	0.40
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.93	0.40
13:M:38:ASP:HB2	26:M:103:HOH:O	2.21	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	421 (99%)	5 (1%)	63	55
2	B	210/210 (100%)	203 (97%)	7 (3%)	33	18
3	C	220/226 (97%)	217 (99%)	3 (1%)	59	49
4	D	120/129 (93%)	118 (98%)	2 (2%)	53	42
5	E	89/95 (94%)	87 (98%)	2 (2%)	45	32
6	F	76/81 (94%)	72 (95%)	4 (5%)	20	7
7	G	62/69 (90%)	60 (97%)	2 (3%)	34	19
8	H	67/75 (89%)	64 (96%)	3 (4%)	24	10
9	I	55/58 (95%)	53 (96%)	2 (4%)	31	16
10	J	46/50 (92%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	36 (97%)	1 (3%)	39	24
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	22
All	All	1481/1543 (96%)	1449 (98%)	32 (2%)	45	32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	112	LEU
1	A	128	VAL
1	A	189	MET
1	A	369	ASP
2	B	43	SER
2	B	64	ILE
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	184	LEU
2	B	227	LEU
3	C	144	ILE
3	C	159	MET
3	C	230	ASN
4	D	21	ASP
4	D	40	LEU
5	E	70	VAL
5	E	90	ARG
6	F	54	ASN
6	F	65	ASP
6	F	80	GLN
6	F	87	THR
7	G	30	LEU
7	G	44	ARG
8	H	12	GLN
8	H	60	TYR
8	H	61	LYS
9	I	29	LEU
9	I	36	LYS
12	L	16	GLU
13	M	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	178	GLN
1	A	180	GLN
1	A	331	ASN
1	A	422	ASN
2	B	10	GLN
2	B	181	GLN
3	C	50	ASN
3	C	56	GLN
3	C	68	GLN
4	D	37	GLN
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	76	ASN
8	H	12	GLN
8	H	22	ASN
8	H	25	GLN
8	H	28	ASN
8	H	32	ASN
8	H	37	HIS
11	K	35	GLN

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
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	1.32	1 (14%)
2	FME	B	1	2	8,9,10	2.18	4 (50%)	7,9,11	6.04	4 (57%)

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

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.

All (6) torsion outliers are listed below:

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

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 oligosaccharides 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
20	PGV	A	608	-	50,50,50	0.92	3 (6%)	53,56,56	1.15	3 (5%)
21	CQX	C	306	-	25,25,25	1.22	2 (8%)	30,30,30	2.04	5 (16%)
18	CDL	B	301	-	63,63,99	1.53	5 (7%)	69,75,111	1.57	14 (20%)
21	CQX	G	101	-	25,25,25	0.78	1 (4%)	30,30,30	0.89	0
20	PGV	C	304	-	40,40,50	1.05	3 (7%)	43,46,56	1.35	4 (9%)
21	CQX	B	304	-	16,16,25	0.69	0	21,21,30	1.34	3 (14%)
18	CDL	C	305	-	86,86,99	1.19	6 (6%)	92,98,111	1.38	13 (14%)
21	CQX	A	611	-	25,25,25	0.87	2 (8%)	30,30,30	1.65	7 (23%)
21	CQX	B	303	-	25,25,25	0.78	1 (4%)	30,30,30	1.99	11 (36%)
19	PER	A	607	14,15	1,1,1	1.26	0	-	-	-
23	CHD	C	301	-	32,32,32	0.95	2 (6%)	51,51,51	1.44	9 (17%)
24	PEK	C	303	-	42,42,52	0.80	2 (4%)	45,47,57	0.96	2 (4%)
14	HEA	A	601	1	66,67,67	1.97	17 (25%)	78,103,103	2.02	23 (29%)
21	CQX	A	609	-	25,25,25	0.88	1 (4%)	30,30,30	2.24	11 (36%)
14	HEA	A	602	19,1	66,67,67	1.78	16 (24%)	78,103,103	2.20	20 (25%)
21	CQX	A	610	-	25,25,25	1.06	2 (8%)	30,30,30	1.74	6 (20%)
22	CUA	B	302	2	0,1,1	-	-	-	-	-
21	CQX	C	307	-	25,25,25	0.57	0	30,30,30	0.82	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CDL	A	606	-	93,93,99	0.98	4 (4%)	99,105,111	1.55	15 (15%)

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
21	CQX	A	611	-	-	4/16/36/36	0/1/1/1
21	CQX	C	307	-	-	7/16/36/36	0/1/1/1
21	CQX	B	303	-	-	7/16/36/36	0/1/1/1
14	HEA	A	601	1	-	7/36/76/76	-
20	PGV	A	608	-	-	7/55/55/55	-
21	CQX	C	306	-	-	7/16/36/36	0/1/1/1
18	CDL	A	606	-	-	50/104/104/110	-
21	CQX	A	609	-	-	6/16/36/36	0/1/1/1
24	PEK	C	303	-	-	8/46/46/56	-
14	HEA	A	602	19,1	-	5/36/76/76	-
18	CDL	B	301	-	-	40/74/74/110	-
21	CQX	A	610	-	-	2/16/36/36	0/1/1/1
20	PGV	C	304	-	-	9/45/45/55	-
21	CQX	G	101	-	-	1/16/36/36	0/1/1/1
23	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	CQX	B	304	-	-	0/7/27/36	0/1/1/1
18	CDL	C	305	-	-	51/97/97/110	-

All (67) 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
14	A	601	HEA	C4B-NB	-6.36	1.29	1.40
18	B	301	CDL	OB6-CB5	4.75	1.47	1.34
14	A	602	HEA	C4B-NB	-4.71	1.32	1.40
18	C	305	CDL	OB6-CB5	4.68	1.47	1.34
18	B	301	CDL	OB8-CB7	4.65	1.46	1.33
14	A	601	HEA	C3A-C4A	-4.54	1.38	1.46
18	B	301	CDL	OA8-CA7	4.50	1.46	1.33
18	C	305	CDL	OB8-CB7	4.45	1.46	1.33
14	A	601	HEA	FE-ND	4.43	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	CDL	OB8-CB7	4.42	1.46	1.33
21	C	306	CQX	O16-C18	4.31	1.54	1.43
14	A	602	HEA	FE-ND	4.18	2.07	1.94
18	A	606	CDL	OA8-CA7	4.14	1.45	1.33
14	A	602	HEA	CHA-C1A	3.98	1.46	1.38
14	A	601	HEA	C1D-ND	-3.89	1.33	1.40
14	A	601	HEA	C1C-NC	-3.85	1.32	1.39
18	C	305	CDL	OA6-CA5	3.85	1.45	1.34
18	A	606	CDL	OA6-CA5	3.83	1.45	1.34
14	A	601	HEA	CHA-C1A	3.79	1.45	1.38
20	C	304	PGV	O03-C19	3.78	1.44	1.33
14	A	601	HEA	C1A-C2A	-3.72	1.38	1.45
18	C	305	CDL	OA8-CA7	3.68	1.44	1.33
14	A	601	HEA	FE-NB	3.66	2.06	1.94
18	C	305	CDL	PA1-OA3	3.62	1.63	1.50
14	A	601	HEA	C1B-NB	-3.55	1.31	1.38
14	A	602	HEA	CHB-C4A	3.48	1.45	1.38
20	A	608	PGV	O03-C19	3.35	1.43	1.33
14	A	602	HEA	C1A-C2A	-3.34	1.39	1.45
14	A	602	HEA	FE-NB	3.24	2.04	1.94
14	A	601	HEA	C3A-C2A	3.21	1.43	1.36
14	A	602	HEA	C1D-ND	-3.12	1.34	1.40
18	A	606	CDL	OB6-CB5	3.11	1.43	1.34
20	A	608	PGV	O01-C1	3.03	1.42	1.34
14	A	602	HEA	C4D-ND	-2.96	1.32	1.38
14	A	602	HEA	C3A-C4A	-2.88	1.41	1.46
21	A	611	CQX	O16-C6	2.83	1.45	1.40
14	A	602	HEA	CHC-C1C	2.80	1.45	1.39
14	A	602	HEA	CHD-C1D	2.78	1.44	1.38
14	A	602	HEA	C12-C11	2.75	1.57	1.52
14	A	602	HEA	C1B-NB	-2.73	1.33	1.38
14	A	601	HEA	O11-C11	2.72	1.48	1.42
21	A	610	CQX	O16-C6	2.71	1.44	1.40
14	A	601	HEA	C16-C17	-2.66	1.44	1.53
14	A	601	HEA	O1D-CGD	2.61	1.30	1.22
21	G	101	CQX	O16-C6	2.56	1.44	1.40
20	C	304	PGV	O01-C1	2.52	1.41	1.34
21	A	610	CQX	O55-C2	2.51	1.48	1.43
21	C	306	CQX	O16-C6	2.46	1.44	1.40
14	A	602	HEA	CHD-C4C	2.46	1.44	1.39
18	C	305	CDL	PB2-OB3	2.41	1.59	1.50
14	A	601	HEA	CHD-C1D	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	303	PEK	O03-C21	2.39	1.40	1.33
24	C	303	PEK	O01-C1	2.38	1.41	1.34
14	A	601	HEA	CHB-C4A	2.37	1.43	1.38
14	A	601	HEA	CHC-C1C	2.25	1.44	1.39
23	C	301	CHD	O26-C24	-2.20	1.23	1.30
18	B	301	CDL	OA7-CA5	2.20	1.29	1.22
14	A	602	HEA	CMA-C3A	2.20	1.49	1.45
21	B	303	CQX	O7-C3	2.15	1.48	1.43
14	A	601	HEA	CHD-C4C	2.15	1.44	1.39
20	A	608	PGV	C01-C02	2.08	1.57	1.50
14	A	602	HEA	C13-C14	2.07	1.57	1.50
21	A	609	CQX	C28-C25	-2.07	1.42	1.51
21	A	611	CQX	O49-C1	2.04	1.47	1.43
23	C	301	CHD	C20-C17	-2.04	1.50	1.54
20	C	304	PGV	P-O14	-2.03	1.45	1.55

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	306	CQX	C18-O16-C6	6.78	125.09	113.84
14	A	602	HEA	C4A-NA-C1A	-6.61	98.88	105.35
14	A	602	HEA	C4C-NC-C1C	-6.21	99.27	105.35
14	A	602	HEA	CHB-C4A-NA	-6.11	117.83	124.44
14	A	601	HEA	C3C-C4C-NC	6.02	113.95	110.25
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
14	A	602	HEA	C3C-C4C-NC	5.65	113.72	110.25
21	A	609	CQX	O16-C6-C1	-5.30	100.03	108.30
14	A	601	HEA	C2B-C1B-NB	5.11	116.01	109.88
21	C	306	CQX	O16-C18-C19	-4.97	92.47	109.72
18	C	305	CDL	OB6-CB5-C51	4.96	122.19	111.50
18	A	606	CDL	OA6-CA5-C11	4.96	122.19	111.50
18	A	606	CDL	OB6-CB5-C51	4.84	121.94	111.50
21	C	306	CQX	O22-C19-C18	4.78	131.93	110.39
21	A	610	CQX	C6-C1-C2	4.67	119.72	110.00
14	A	602	HEA	C4A-C3A-C2A	-4.63	102.95	106.75
14	A	602	HEA	CAD-CBD-CGD	-4.56	103.79	113.60
21	A	609	CQX	C34-C31-C28	-4.55	91.33	114.42
21	A	610	CQX	C18-O16-C6	4.54	121.37	113.84
14	A	601	HEA	C1B-C2B-C3B	-4.50	101.42	106.80
14	A	601	HEA	CHB-C4A-NA	-4.47	119.60	124.44
20	A	608	PGV	O03-C19-O04	-4.42	112.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	303	CQX	C6-O5-C4	4.41	122.34	113.69
14	A	602	HEA	C2A-C1A-NA	4.37	114.58	110.32
21	A	609	CQX	O49-C1-C2	4.37	120.44	110.35
18	A	606	CDL	CA4-OA6-CA5	-4.26	107.30	117.79
18	B	301	CDL	CA4-OA6-CA5	4.25	128.26	117.79
14	A	602	HEA	C2C-C1C-NC	4.08	116.28	110.08
14	A	601	HEA	C4C-NC-C1C	-4.00	101.43	105.35
18	B	301	CDL	OA8-CA7-C31	3.94	124.27	111.91
21	A	611	CQX	O7-C3-C2	3.90	119.37	110.35
21	B	304	CQX	C2-C3-C4	-3.89	103.30	110.24
18	C	305	CDL	OA2-PA1-OA3	3.83	124.03	109.07
14	A	602	HEA	CMC-C2C-C1C	3.73	131.05	125.37
18	B	301	CDL	OB6-CB5-C51	3.72	121.16	110.80
21	B	303	CQX	C18-O16-C6	-3.69	107.71	113.84
21	A	609	CQX	C6-C1-C2	-3.58	102.55	110.00
18	B	301	CDL	CA6-CA4-CA3	-3.57	103.34	111.79
18	C	305	CDL	CA4-OA6-CA5	-3.57	109.01	117.79
21	B	303	CQX	C31-C28-C25	-3.55	97.75	113.49
21	A	609	CQX	C31-C28-C25	-3.55	97.77	113.49
23	C	301	CHD	C17-C13-C12	-3.54	114.43	117.67
14	A	601	HEA	C4A-C3A-C2A	-3.52	103.86	106.75
14	A	601	HEA	C2C-C1C-NC	3.52	115.44	110.08
18	A	606	CDL	OA8-CA7-C31	3.51	122.91	111.91
14	A	602	HEA	OMA-CMA-C3A	-3.50	117.78	125.69
14	A	601	HEA	C4A-CHB-C1B	3.46	133.51	126.06
18	B	301	CDL	OA6-CA5-C11	3.39	118.80	111.50
23	C	301	CHD	C1-C10-C9	3.36	116.63	111.35
18	A	606	CDL	OA6-CA5-OA7	-3.34	115.64	123.70
14	A	601	HEA	OMA-CMA-C3A	-3.31	118.20	125.69
21	A	611	CQX	O55-C2-C3	3.30	117.97	110.35
18	C	305	CDL	OA4-PA1-OA2	-3.24	92.69	107.75
18	B	301	CDL	OA8-CA7-OA9	-3.24	115.42	123.59
18	C	305	CDL	OB5-PB2-OB3	3.22	121.65	109.07
21	A	610	CQX	O5-C4-C3	3.19	115.50	109.69
14	A	601	HEA	O2A-CGA-CBA	3.18	124.23	114.03
20	A	608	PGV	O03-C19-C20	3.17	121.87	111.91
21	A	609	CQX	C40-C37-C34	-3.17	98.33	114.42
21	A	609	CQX	C18-O16-C6	-3.12	108.66	113.84
21	A	611	CQX	C31-C28-C25	-3.12	99.65	113.49
14	A	602	HEA	C2B-C1B-NB	3.12	113.62	109.88
20	C	304	PGV	O03-C19-C20	3.11	121.68	111.91
18	B	301	CDL	OA6-CA4-CA6	3.09	119.60	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	303	CQX	C37-C34-C31	-3.09	98.72	114.42
21	B	303	CQX	O5-C4-C3	3.01	115.17	109.69
21	B	303	CQX	C43-C40-C37	-3.01	99.13	114.42
23	C	301	CHD	C14-C13-C12	3.01	110.20	107.40
14	A	601	HEA	CHB-C1B-NB	-2.98	121.17	124.42
14	A	602	HEA	C3C-C2C-C1C	-2.98	103.56	107.16
18	A	606	CDL	OB6-CB5-OB7	-2.96	116.55	123.70
18	C	305	CDL	O1-C1-CA2	-2.94	99.24	109.56
18	B	301	CDL	OB8-CB7-C71	2.92	121.08	111.91
21	A	611	CQX	O16-C6-C1	2.92	112.86	108.30
14	A	601	HEA	C12-C13-C14	2.85	119.76	112.23
18	B	301	CDL	OA7-CA5-C11	-2.84	112.64	123.73
18	C	305	CDL	OB8-CB7-C71	2.83	120.80	111.91
21	A	610	CQX	C6-O5-C4	-2.75	108.29	113.69
24	C	303	PEK	O03-C21-O04	-2.75	116.65	123.59
14	A	602	HEA	CHD-C4C-NC	-2.75	118.79	123.85
24	C	303	PEK	O04-C21-C22	2.73	134.37	123.73
18	C	305	CDL	OA8-CA7-C31	2.72	120.44	111.91
21	A	609	CQX	O5-C6-C1	2.70	116.06	110.35
21	B	303	CQX	C2-C3-C4	2.69	115.04	110.24
21	C	306	CQX	O49-C1-C6	2.66	116.50	110.05
14	A	602	HEA	C1B-C2B-C3B	-2.65	103.63	106.80
18	B	301	CDL	OA5-PA1-OA3	2.65	119.42	109.07
14	A	602	HEA	C24-C23-C22	2.64	130.28	122.65
23	C	301	CHD	C21-C20-C22	-2.63	106.24	110.36
18	C	305	CDL	OA6-CA5-OA7	-2.63	117.35	123.70
21	B	304	CQX	C18-O16-C6	2.55	118.08	113.84
23	C	301	CHD	C1-C2-C3	-2.54	107.20	110.47
14	A	601	HEA	CMB-C2B-C1B	2.54	128.91	125.04
14	A	601	HEA	C3D-C4D-ND	2.52	112.79	110.36
14	A	601	HEA	C1A-CHA-C4D	-2.51	120.64	126.06
18	A	606	CDL	C52-C51-CB5	-2.50	104.54	113.62
21	A	611	CQX	O49-C1-C2	2.49	116.12	110.35
14	A	601	HEA	CHA-C4D-C3D	-2.48	121.19	124.84
18	A	606	CDL	C79-C78-C77	-2.46	101.93	114.42
21	B	303	CQX	C3-C2-C1	2.44	115.09	110.82
14	A	602	HEA	C21-C20-C19	2.44	121.00	112.98
21	A	611	CQX	C6-O5-C4	2.42	118.44	113.69
18	A	606	CDL	OB8-CB6-CB4	2.40	115.43	108.43
18	B	301	CDL	OB4-PB2-OB3	2.40	124.11	112.24
21	A	609	CQX	C3-C2-C1	2.39	115.00	110.82
21	B	303	CQX	O49-C1-C2	2.38	115.85	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C2D-C1D-ND	2.38	112.66	109.84
14	A	601	HEA	O1A-CGA-CBA	-2.38	115.45	123.08
21	B	303	CQX	O5-C6-C1	2.36	115.35	110.35
21	A	610	CQX	C37-C34-C31	-2.35	102.48	114.42
18	C	305	CDL	OB6-CB5-OB7	-2.33	118.06	123.70
14	A	602	HEA	C16-C15-C14	-2.33	116.40	121.12
14	A	601	HEA	C4A-NA-C1A	-2.31	103.09	105.35
18	B	301	CDL	OA6-CA4-CA3	2.29	116.69	108.40
14	A	602	HEA	C27-C19-C20	2.29	119.12	115.27
18	A	606	CDL	C84-C83-C82	-2.29	102.82	114.42
14	A	601	HEA	CAA-CBA-CGA	-2.28	108.69	113.60
18	A	606	CDL	C65-C64-C63	-2.28	102.85	114.42
18	A	606	CDL	OB4-PB2-OB2	2.25	118.17	107.75
23	C	301	CHD	C5-C6-C7	-2.24	111.99	114.46
23	C	301	CHD	C22-C20-C17	-2.22	105.69	110.28
14	A	601	HEA	CAD-C3D-C2D	2.22	132.01	127.88
14	A	602	HEA	CHC-C1C-C2C	-2.20	121.02	127.24
21	C	307	CQX	O49-C1-C2	2.20	115.44	110.35
18	C	305	CDL	O1-C1-CB2	2.19	117.24	109.56
14	A	602	HEA	C13-C14-C15	-2.19	122.39	127.66
21	A	609	CQX	O22-C19-C18	-2.19	100.53	110.39
18	B	301	CDL	OB8-CB7-OB9	-2.18	118.09	123.59
20	C	304	PGV	O14-P-O13	2.17	122.99	112.24
20	A	608	PGV	C25-C24-C23	2.16	125.38	114.42
21	B	304	CQX	O5-C4-C3	2.14	113.58	109.69
23	C	301	CHD	C4-C3-C2	-2.14	108.00	110.55
18	B	301	CDL	CB6-OB8-CB7	2.13	125.00	117.12
21	A	609	CQX	C6-O5-C4	2.12	117.86	113.69
18	A	606	CDL	C78-C77-C76	-2.12	103.66	114.42
21	A	610	CQX	C31-C28-C25	-2.11	104.15	113.49
23	C	301	CHD	C11-C12-C13	-2.07	109.11	111.24
18	C	305	CDL	CA6-CA4-CA3	2.05	116.64	111.79
18	A	606	CDL	OA8-CA7-OA9	-2.05	118.42	123.59
21	B	303	CQX	O22-C19-C18	-2.05	101.17	110.39
14	A	601	HEA	C2A-C1A-NA	2.04	112.31	110.32
21	C	306	CQX	O7-C3-C2	-2.03	105.67	110.35
20	C	304	PGV	O01-C1-O02	-2.02	118.81	123.70
18	C	305	CDL	OA6-CA5-C11	2.01	115.83	111.50
21	A	611	CQX	C18-O16-C6	-2.01	110.51	113.84
14	A	601	HEA	CHC-C1C-C2C	-2.00	121.58	127.24

There are no chirality outliers.

All (213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	CDL	CA2-C1-CB2-OB2
18	A	606	CDL	CA2-OA2-PA1-OA3
18	A	606	CDL	CA3-OA5-PA1-OA3
18	A	606	CDL	C11-CA5-OA6-CA4
18	A	606	CDL	CB2-OB2-PB2-OB5
18	A	606	CDL	CB3-OB5-PB2-OB3
18	A	606	CDL	CB3-OB5-PB2-OB4
18	B	301	CDL	CA2-C1-CB2-OB2
18	B	301	CDL	CA3-OA5-PA1-OA2
18	B	301	CDL	CA3-OA5-PA1-OA3
18	B	301	CDL	CA3-OA5-PA1-OA4
18	B	301	CDL	C11-CA5-OA6-CA4
18	B	301	CDL	CB2-OB2-PB2-OB4
18	C	305	CDL	C1-CA2-OA2-PA1
18	C	305	CDL	CA2-OA2-PA1-OA3
18	C	305	CDL	CA3-OA5-PA1-OA3
18	C	305	CDL	C11-CA5-OA6-CA4
18	C	305	CDL	CB2-OB2-PB2-OB4
18	C	305	CDL	OB7-CB5-OB6-CB4
18	C	305	CDL	C51-CB5-OB6-CB4
18	A	606	CDL	OA9-CA7-OA8-CA6
18	A	606	CDL	OA7-CA5-OA6-CA4
18	B	301	CDL	OA7-CA5-OA6-CA4
18	C	305	CDL	OA7-CA5-OA6-CA4
18	A	606	CDL	C31-CA7-OA8-CA6
18	B	301	CDL	C71-CB7-OB8-CB6
21	B	303	CQX	O5-C4-C57-O61
18	B	301	CDL	O1-C1-CB2-OB2
18	C	305	CDL	O1-C1-CB2-OB2
18	B	301	CDL	OB9-CB7-OB8-CB6
18	C	305	CDL	C51-C52-C53-C54
18	B	301	CDL	CB2-C1-CA2-OA2
18	C	305	CDL	CA2-C1-CB2-OB2
18	C	305	CDL	C71-CB7-OB8-CB6
21	C	307	CQX	O16-C18-C19-O22
21	B	303	CQX	C3-C4-C57-O61
18	A	606	CDL	O1-C1-CB2-OB2
18	B	301	CDL	CB7-C71-C72-C73
20	C	304	PGV	C19-C20-C21-C22
21	A	611	CQX	O16-C18-C19-O22
18	C	305	CDL	CB5-C51-C52-C53
18	A	606	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
18	C	305	CDL	CA7-C31-C32-C33
18	C	305	CDL	OB9-CB7-OB8-CB6
18	C	305	CDL	C31-CA7-OA8-CA6
18	B	301	CDL	C51-CB5-OB6-CB4
18	A	606	CDL	CA3-OA5-PA1-OA2
18	A	606	CDL	CB3-OB5-PB2-OB2
18	B	301	CDL	CB2-OB2-PB2-OB5
18	C	305	CDL	CA2-OA2-PA1-OA5
18	C	305	CDL	CA3-OA5-PA1-OA2
18	B	301	CDL	OB7-CB5-OB6-CB4
18	B	301	CDL	CA5-C11-C12-C13
18	A	606	CDL	C76-C77-C78-C79
20	C	304	PGV	C20-C21-C22-C23
20	C	304	PGV	C27-C28-C29-C30
21	C	307	CQX	C28-C31-C34-C37
18	A	606	CDL	C71-CB7-OB8-CB6
18	C	305	CDL	C82-C83-C84-C85
18	A	606	CDL	CA5-C11-C12-C13
18	A	606	CDL	C19-C20-C21-C22
21	C	306	CQX	O22-C25-C28-C31
18	C	305	CDL	C35-C36-C37-C38
18	A	606	CDL	C62-C63-C64-C65
18	C	305	CDL	C71-C72-C73-C74
21	C	307	CQX	C34-C37-C40-C43
18	A	606	CDL	C52-C53-C54-C55
24	C	303	PEK	C28-C29-C30-C31
18	B	301	CDL	C71-C72-C73-C74
18	C	305	CDL	C73-C74-C75-C76
21	A	610	CQX	C31-C34-C37-C40
18	C	305	CDL	C14-C15-C16-C17
18	C	305	CDL	C78-C79-C80-C81
21	A	609	CQX	C37-C40-C43-C46
18	C	305	CDL	C13-C14-C15-C16
18	C	305	CDL	C21-C22-C23-C24
24	C	303	PEK	C34-C35-C36-C37
18	A	606	CDL	OB9-CB7-OB8-CB6
18	C	305	CDL	OA9-CA7-OA8-CA6
21	B	303	CQX	C40-C43-C46-C49
18	C	305	CDL	C12-C13-C14-C15
21	B	303	CQX	O22-C25-C28-C31
21	C	307	CQX	C40-C43-C46-C49
18	A	606	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
21	C	307	CQX	C31-C34-C37-C40
18	B	301	CDL	C18-C19-C20-C21
18	C	305	CDL	C56-C57-C58-C59
18	C	305	CDL	C77-C78-C79-C80
18	A	606	CDL	C54-C55-C56-C57
18	B	301	CDL	C77-C78-C79-C80
18	A	606	CDL	C20-C21-C22-C23
21	C	306	CQX	C28-C31-C34-C37
18	C	305	CDL	C54-C55-C56-C57
18	A	606	CDL	C22-C23-C24-C25
24	C	303	PEK	C26-C27-C28-C29
18	B	301	CDL	C72-C73-C74-C75
20	A	608	PGV	C28-C29-C30-C31
18	A	606	CDL	C14-C15-C16-C17
18	B	301	CDL	C73-C74-C75-C76
18	B	301	CDL	C78-C79-C80-C81
18	C	305	CDL	C75-C76-C77-C78
20	A	608	PGV	C31-C32-C33-C34
18	A	606	CDL	C79-C80-C81-C82
18	A	606	CDL	C71-C72-C73-C74
18	A	606	CDL	C72-C73-C74-C75
21	A	609	CQX	O16-C18-C19-O22
18	B	301	CDL	CA6-CA4-OA6-CA5
20	C	304	PGV	C28-C29-C30-C31
21	A	609	CQX	C28-C31-C34-C37
24	C	303	PEK	C25-C26-C27-C28
18	C	305	CDL	OA5-CA3-CA4-OA6
18	B	301	CDL	O1-C1-CA2-OA2
21	C	306	CQX	C40-C43-C46-C49
21	C	306	CQX	C43-C46-C49-C52
18	A	606	CDL	C13-C14-C15-C16
18	A	606	CDL	OB5-CB3-CB4-CB6
18	C	305	CDL	OA5-CA3-CA4-CA6
18	A	606	CDL	C58-C59-C60-C61
18	B	301	CDL	C79-C80-C81-C82
18	B	301	CDL	CB3-CB4-CB6-OB8
18	C	305	CDL	C18-C19-C20-C21
18	B	301	CDL	C74-C75-C76-C77
14	A	602	HEA	C2A-C3A-CMA-OMA
24	C	303	PEK	C27-C28-C29-C30
20	C	304	PGV	C31-C32-C33-C34
18	C	305	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
18	A	606	CDL	C35-C36-C37-C38
18	B	301	CDL	OA5-CA3-CA4-CA6
21	A	609	CQX	C34-C37-C40-C43
21	B	303	CQX	C28-C25-O22-C19
18	A	606	CDL	OB5-CB3-CB4-OB6
21	A	610	CQX	O16-C18-C19-O22
21	C	307	CQX	C18-C19-O22-C25
18	A	606	CDL	OB6-CB4-CB6-OB8
18	B	301	CDL	OB6-CB4-CB6-OB8
20	A	608	PGV	C11-C10-C9-C8
18	B	301	CDL	C1-CB2-OB2-PB2
18	B	301	CDL	CB4-CB3-OB5-PB2
20	C	304	PGV	C02-C03-O11-P
18	A	606	CDL	CA3-OA5-PA1-OA4
18	C	305	CDL	CA2-OA2-PA1-OA4
18	C	305	CDL	CB2-OB2-PB2-OB3
21	C	306	CQX	C31-C34-C37-C40
21	A	611	CQX	C18-C19-O22-C25
18	A	606	CDL	C24-C25-C26-C27
18	C	305	CDL	C79-C80-C81-C82
14	A	601	HEA	C11-C12-C13-C14
18	B	301	CDL	C76-C77-C78-C79
18	B	301	CDL	OB5-CB3-CB4-OB6
18	A	606	CDL	CA2-OA2-PA1-OA5
24	C	303	PEK	C30-C31-C32-C33
20	A	608	PGV	C30-C31-C32-C33
24	C	303	PEK	C29-C30-C31-C32
18	B	301	CDL	C1-CA2-OA2-PA1
18	A	606	CDL	C84-C85-C86-C87
20	A	608	PGV	C19-C20-C21-C22
21	A	609	CQX	C43-C46-C49-C52
18	B	301	CDL	CA4-CA3-OA5-PA1
14	A	601	HEA	C26-C15-C16-C17
18	C	305	CDL	C12-C11-CA5-OA6
18	C	305	CDL	C57-C58-C59-C60
21	C	306	CQX	O16-C18-C19-O22
18	B	301	CDL	C52-C51-CB5-OB6
21	C	307	CQX	C37-C40-C43-C46
21	B	303	CQX	C31-C34-C37-C40
21	G	101	CQX	C40-C43-C46-C49
14	A	602	HEA	CAD-CBD-CGD-O2D
18	B	301	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	C	305	CDL	C83-C84-C85-C86
18	A	606	CDL	C77-C78-C79-C80
14	A	602	HEA	CAD-CBD-CGD-O1D
21	B	303	CQX	C28-C31-C34-C37
20	A	608	PGV	O03-C19-C20-C21
18	A	606	CDL	C34-C35-C36-C37
18	C	305	CDL	C76-C77-C78-C79
21	A	609	CQX	C28-C25-O22-C19
14	A	601	HEA	C14-C15-C16-C17
24	C	303	PEK	C23-C24-C25-C26
21	A	611	CQX	C1-C6-O16-C18
20	C	304	PGV	C05-C04-O12-P
18	C	305	CDL	C22-C23-C24-C25
14	A	601	HEA	CAD-CBD-CGD-O1D
18	C	305	CDL	C36-C37-C38-C39
18	A	606	CDL	OB7-CB5-OB6-CB4
18	B	301	CDL	C52-C51-CB5-OB7
14	A	602	HEA	CAA-CBA-CGA-O1A
18	A	606	CDL	C32-C31-CA7-OA8
18	B	301	CDL	C72-C71-CB7-OB8
18	A	606	CDL	OA5-CA3-CA4-OA6
14	A	601	HEA	CAA-CBA-CGA-O1A
18	B	301	CDL	OA6-CA4-CA6-OA8
14	A	602	HEA	CAA-CBA-CGA-O2A
18	C	305	CDL	C52-C51-CB5-OB6
18	A	606	CDL	C64-C65-C66-C67
20	C	304	PGV	C26-C27-C28-C29
20	A	608	PGV	C11-C12-C13-C14
18	C	305	CDL	C33-C34-C35-C36
14	A	601	HEA	CAD-CBD-CGD-O2D
18	A	606	CDL	C51-CB5-OB6-CB4
18	A	606	CDL	C63-C64-C65-C66
18	A	606	CDL	CB2-OB2-PB2-OB4
18	C	305	CDL	CB3-OB5-PB2-OB3
18	C	305	CDL	CB3-OB5-PB2-OB4
18	C	305	CDL	C74-C75-C76-C77
23	C	301	CHD	C22-C23-C24-O26
18	A	606	CDL	C32-C31-CA7-OA9
20	C	304	PGV	C30-C31-C32-C33
23	C	301	CHD	C22-C23-C24-O25
21	C	306	CQX	C18-C19-O22-C25
21	A	611	CQX	O5-C6-O16-C18

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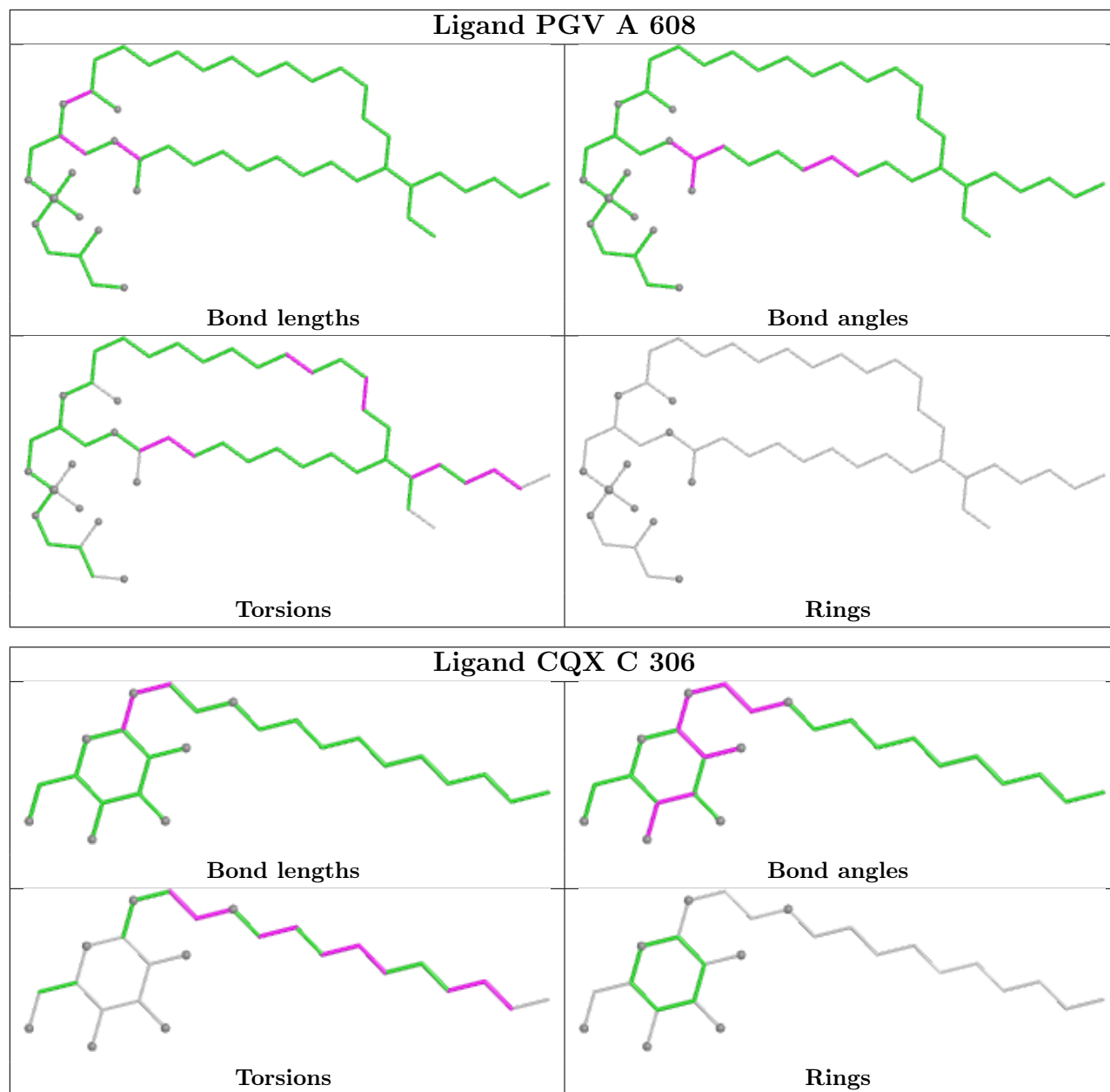
Mol	Chain	Res	Type	Atoms
18	C	305	CDL	C52-C51-CB5-OB7
18	A	606	CDL	C72-C71-CB7-OB8
14	A	601	HEA	CAA-CBA-CGA-O2A

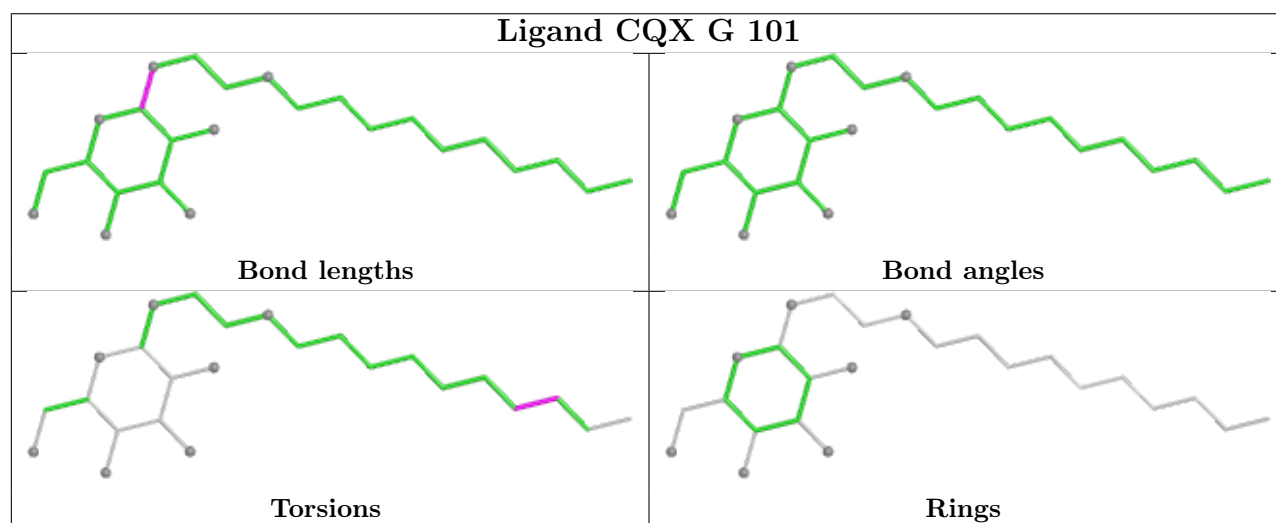
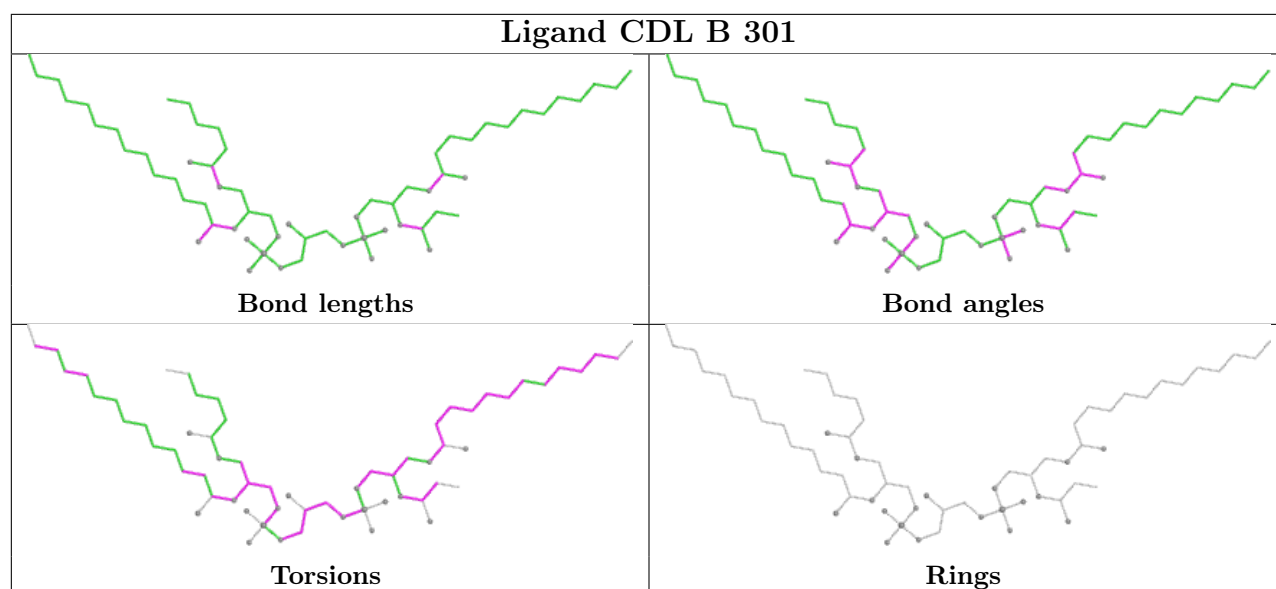
There are no ring outliers.

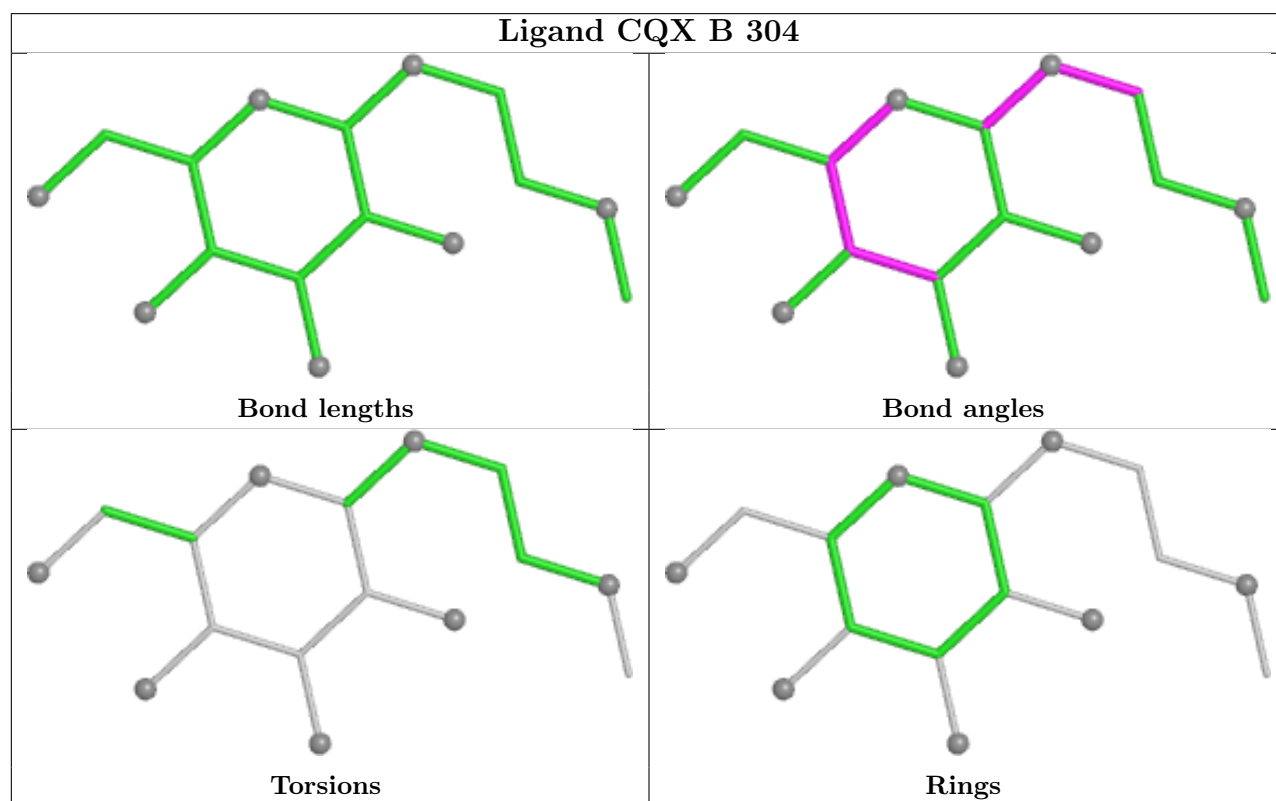
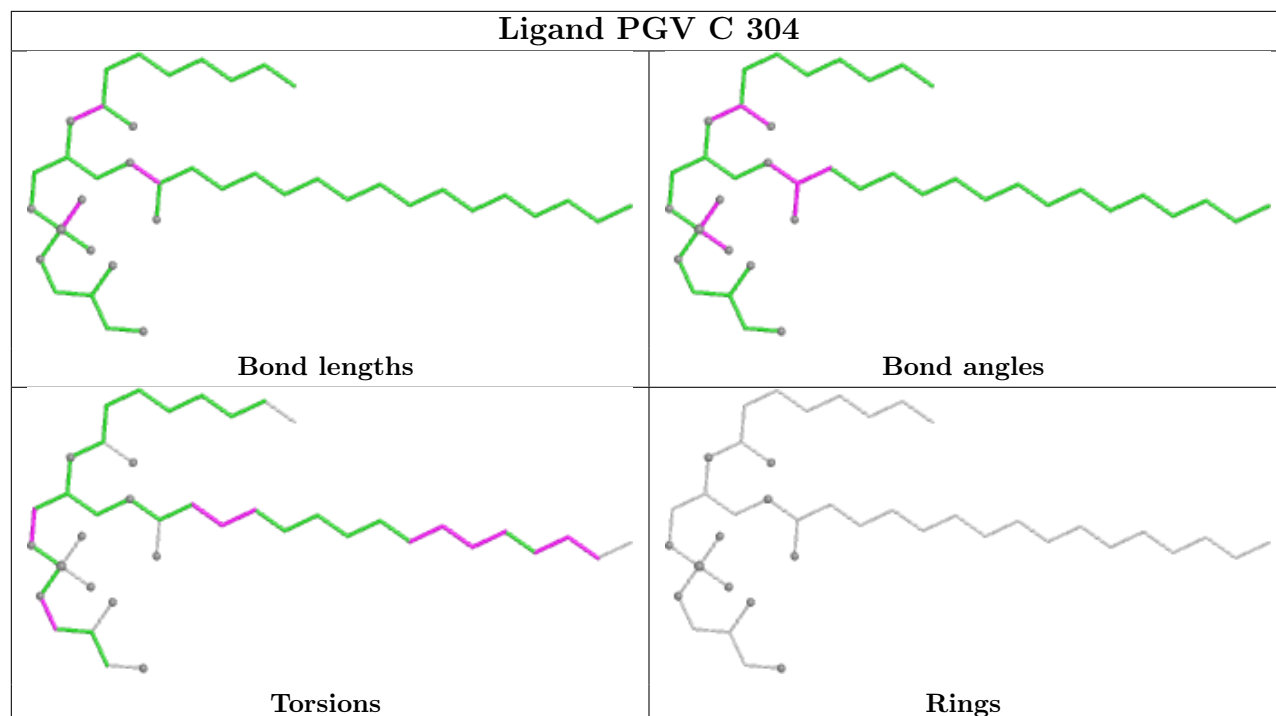
10 monomers are involved in 30 short contacts:

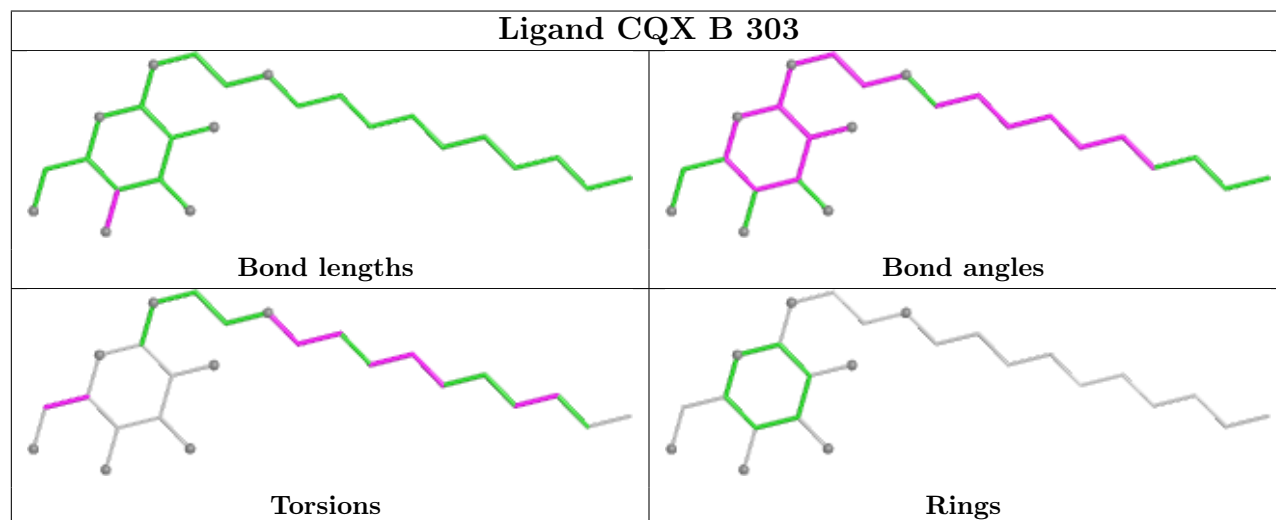
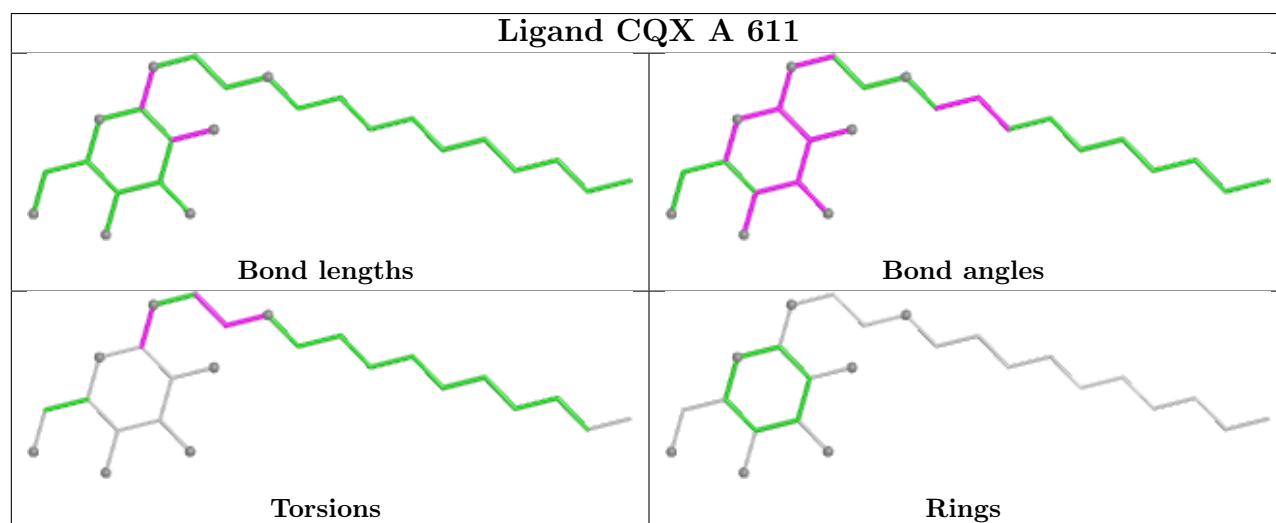
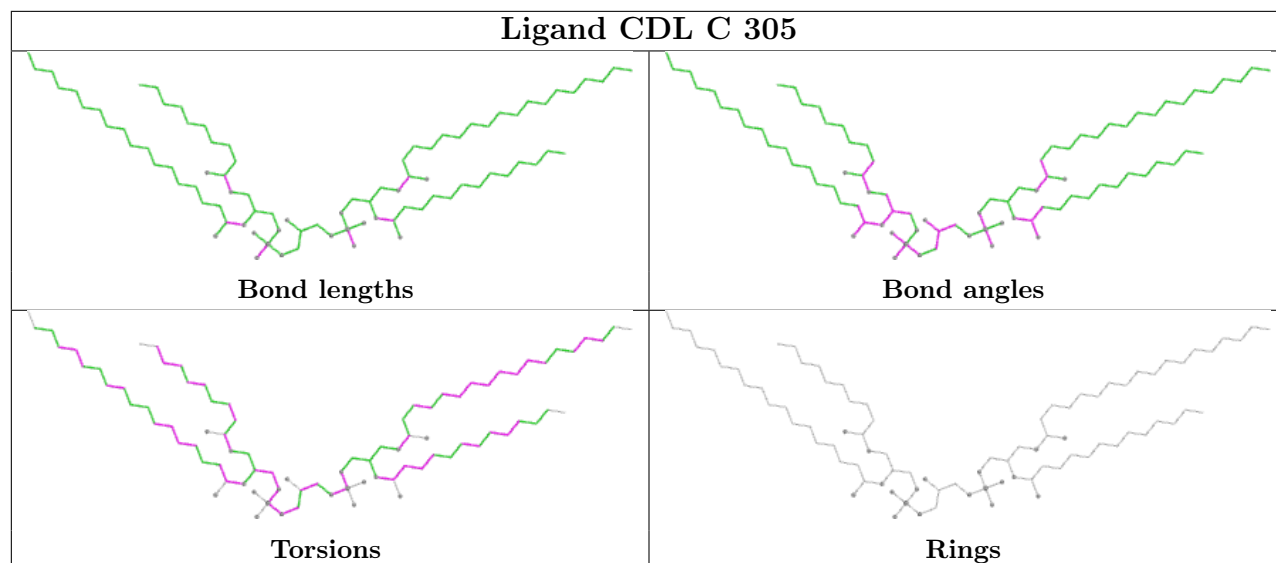
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	608	PGV	1	0
21	C	306	CQX	1	0
18	C	305	CDL	9	0
19	A	607	PER	1	0
23	C	301	CHD	1	0
24	C	303	PEK	2	0
14	A	601	HEA	3	0
14	A	602	HEA	1	0
21	A	610	CQX	2	0
18	A	606	CDL	10	0

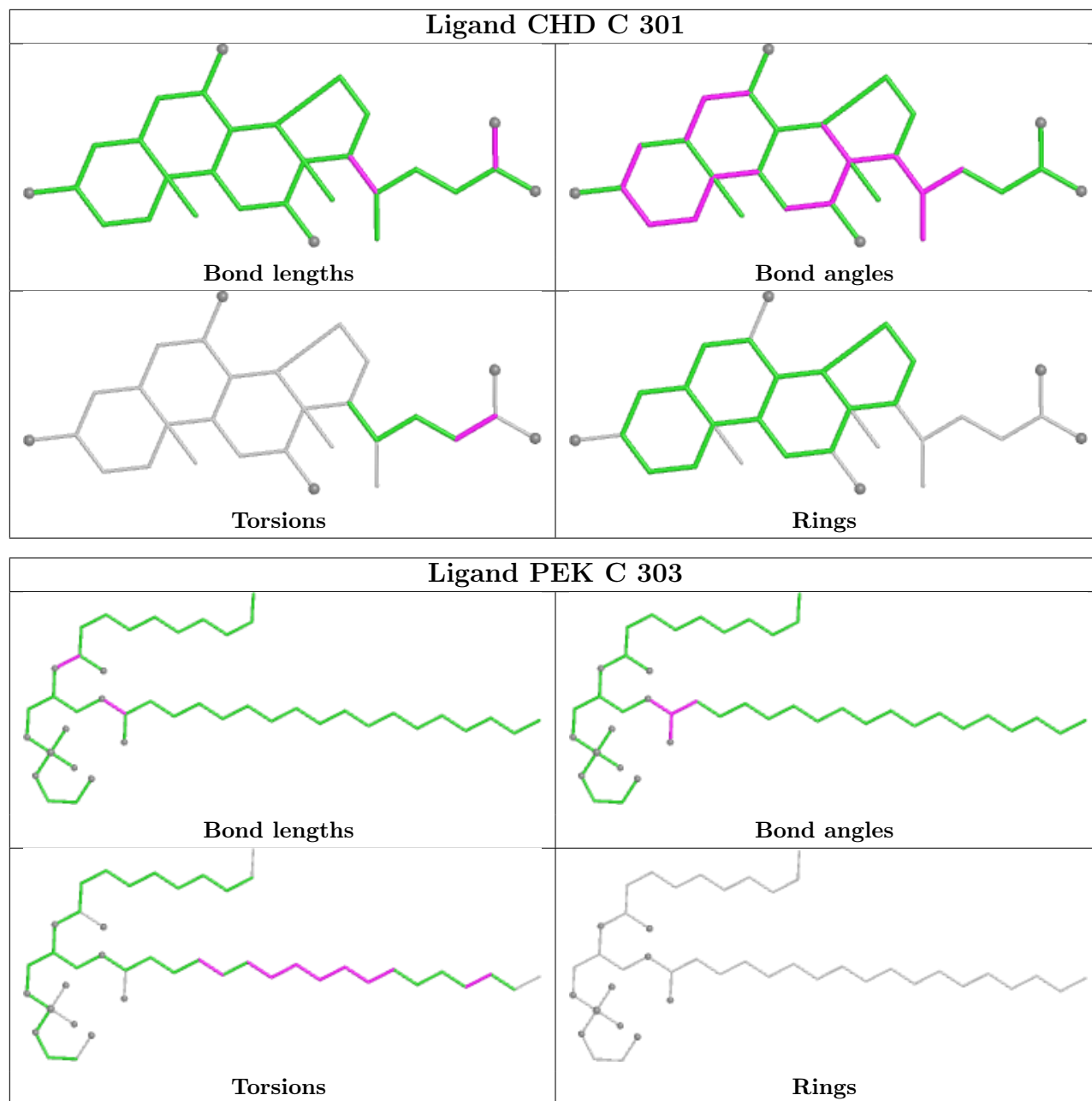
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

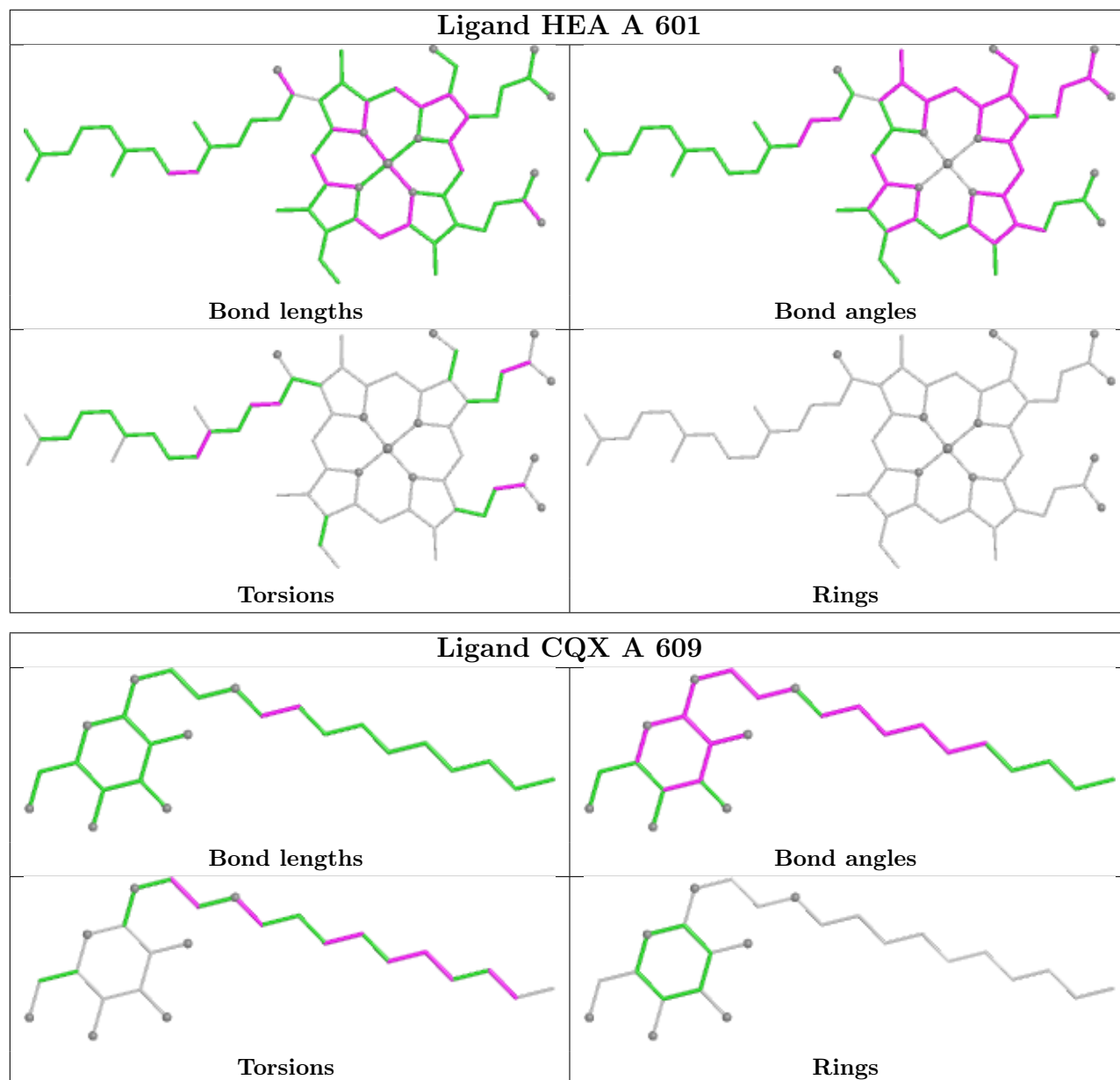


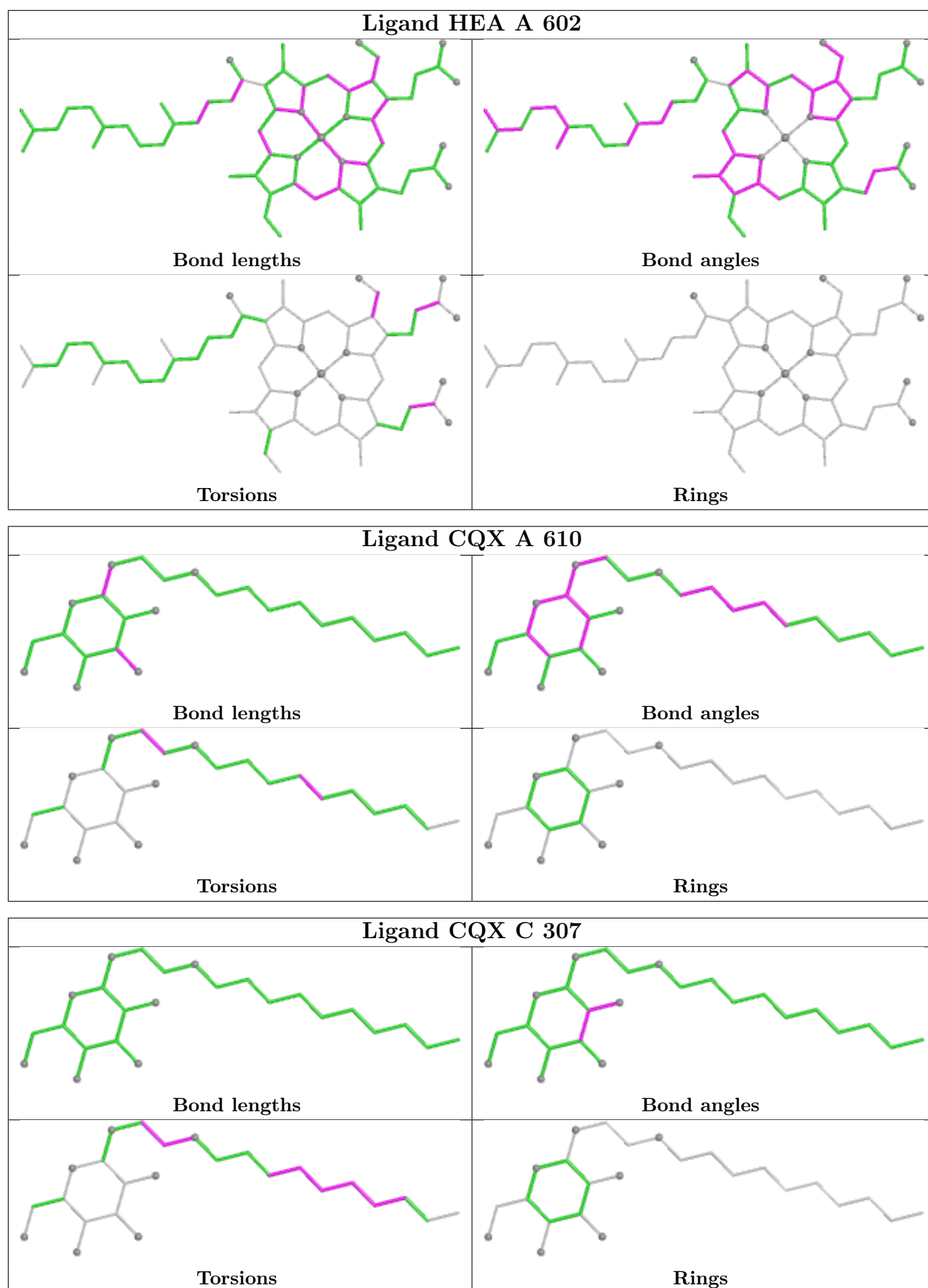


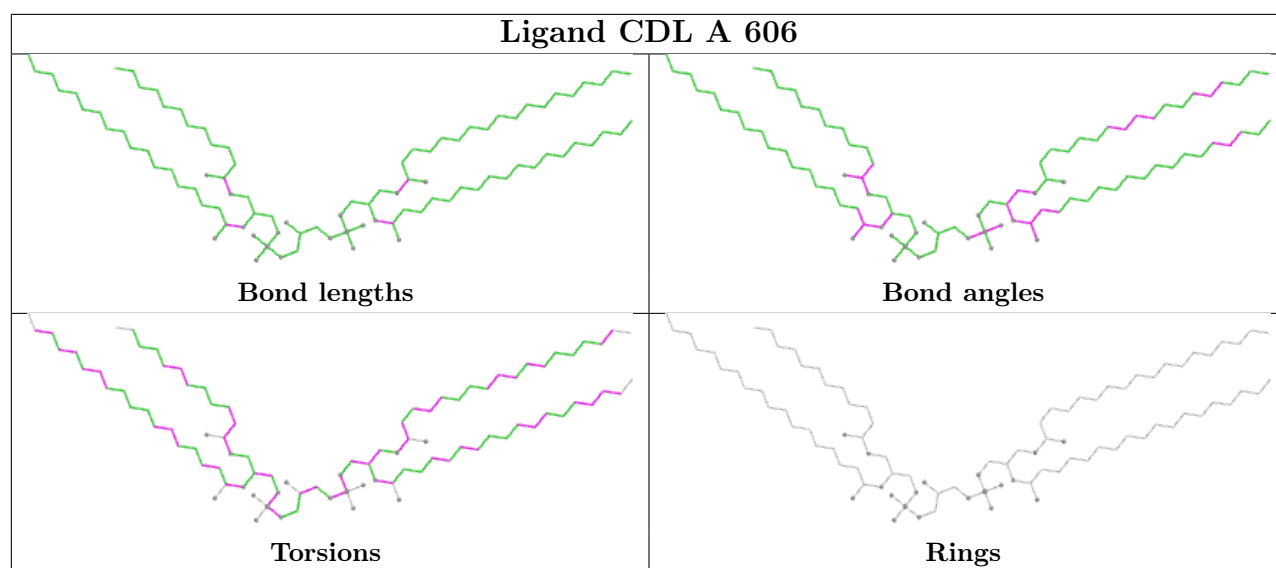












5.7 Other polymers [i](#)

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%)	-0.25	7 (1%) 73 77	25, 32, 42, 96	0
2	B	226/227 (99%)	0.14	8 (3%) 47 51	29, 38, 63, 95	0
3	C	254/261 (97%)	0.03	3 (1%) 76 80	28, 37, 51, 80	0
4	D	136/147 (92%)	0.48	5 (3%) 45 49	37, 50, 77, 84	0
5	E	102/109 (93%)	0.42	3 (2%) 53 57	39, 52, 71, 86	0
6	F	91/98 (92%)	0.37	5 (5%) 30 33	34, 49, 72, 93	0
7	G	72/85 (84%)	0.64	7 (9%) 13 13	35, 45, 89, 102	0
8	H	75/85 (88%)	0.31	3 (4%) 42 46	33, 43, 76, 84	0
9	I	70/73 (95%)	0.38	5 (7%) 22 24	36, 46, 68, 81	0
10	J	55/59 (93%)	0.63	4 (7%) 21 23	38, 48, 77, 86	0
11	K	49/56 (87%)	0.66	2 (4%) 41 45	42, 52, 69, 83	0
12	L	44/47 (93%)	0.11	1 (2%) 61 64	34, 41, 58, 67	0
13	M	40/46 (86%)	0.51	0 100 100	39, 47, 62, 71	0
All	All	1727/1807 (95%)	0.14	53 (3%) 51 55	25, 39, 68, 102	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	36	TRP	8.8
2	B	113	TYR	6.3
11	K	6	ALA	4.5
4	D	11	TYR	4.2
1	A	136	LEU	3.6
8	H	45	ALA	3.5
2	B	91	ASN	3.4
10	J	55	PHE	3.3
2	B	58	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	37	PHE	3.3
12	L	3	TYR	3.2
6	F	93	PRO	3.2
2	B	64	ILE	3.1
4	D	53	ILE	2.9
4	D	87	PHE	2.9
9	I	3	ALA	2.9
8	H	52	VAL	2.9
1	A	514	LYS	2.9
7	G	39	SER	2.9
1	A	483	LEU	2.8
7	G	38	HIS	2.7
7	G	40	GLY	2.7
2	B	221	LYS	2.7
10	J	1	PHE	2.6
5	E	108	LYS	2.6
6	F	24	ALA	2.6
2	B	87	MET	2.4
2	B	61	VAL	2.4
2	B	82	ARG	2.3
6	F	65	ASP	2.3
7	G	14	ARG	2.3
6	F	3	GLY	2.3
10	J	52	TRP	2.3
9	I	64	ARG	2.2
9	I	72	ALA	2.2
1	A	331	ASN	2.2
3	C	243	HIS	2.2
5	E	100	THR	2.2
10	J	53	ALA	2.2
9	I	31	PHE	2.2
7	G	42	ARG	2.2
1	A	275	TRP	2.2
1	A	298	ASP	2.2
11	K	7	PRO	2.1
7	G	34	ASN	2.1
8	H	44	THR	2.1
3	C	91	VAL	2.1
4	D	35	ALA	2.1
9	I	5	ALA	2.1
5	E	9	GLU	2.0
4	D	60	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	4	GLY	2.0
1	A	513	LEU	2.0

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	0.90	0.21	47,60,99,117	0
2	FME	B	1	10/11	0.97	0.07	28,42,55,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

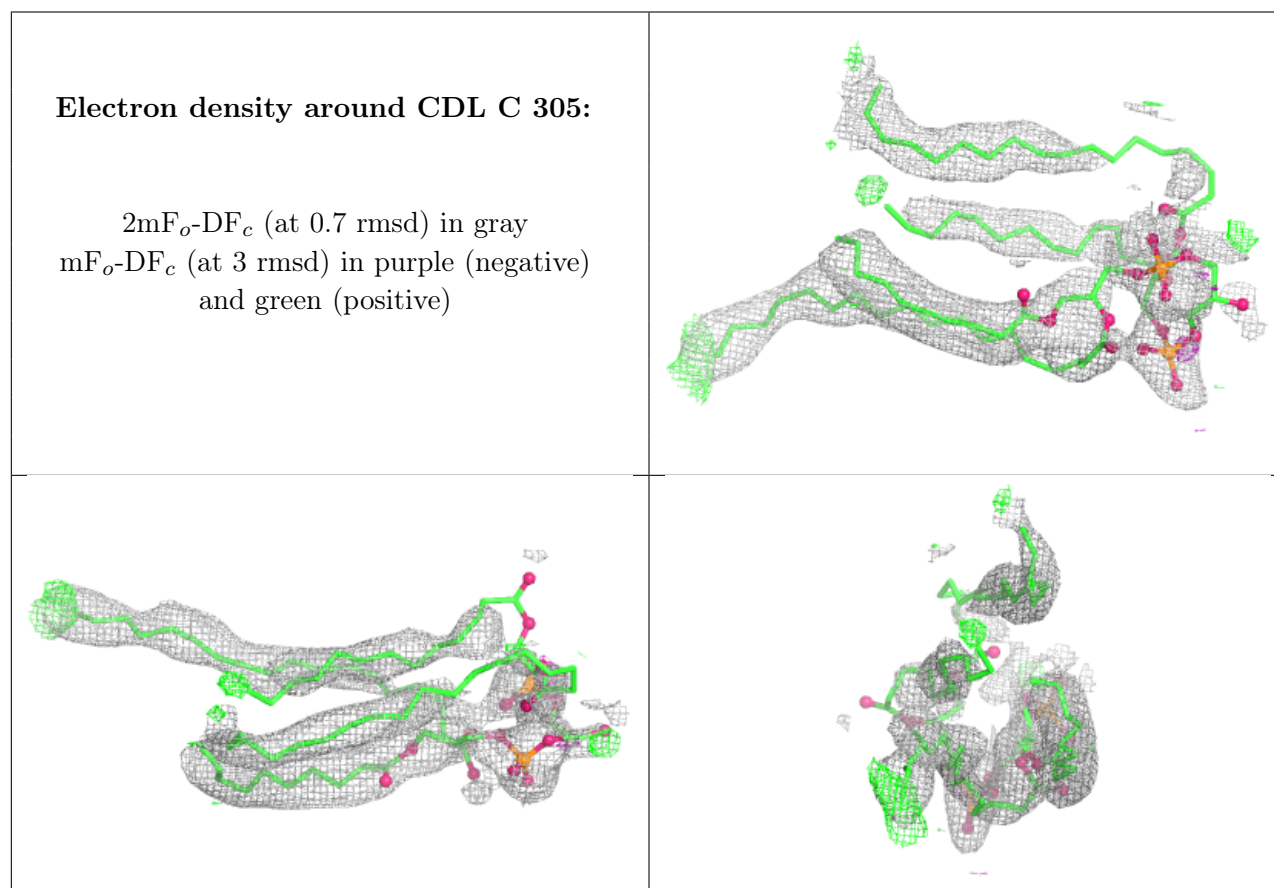
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	NA	C	302	1/1	0.75	0.30	64,64,64,64	0
18	CDL	C	305	87/100	0.89	0.18	44,87,139,152	0
21	CQX	A	611	25/25	0.89	0.17	49,63,92,102	0
18	CDL	A	606	94/100	0.90	0.17	46,79,133,139	0
18	CDL	B	301	64/100	0.92	0.15	52,88,124,138	0
21	CQX	B	304	16/25	0.92	0.12	46,54,81,83	0
21	CQX	B	303	25/25	0.94	0.11	40,53,73,75	0
21	CQX	A	609	25/25	0.94	0.11	40,60,74,99	0
21	CQX	C	307	25/25	0.94	0.14	40,57,89,98	0
21	CQX	C	306	25/25	0.95	0.12	38,49,93,95	0
21	CQX	A	610	25/25	0.96	0.09	47,57,72,80	0
21	CQX	G	101	25/25	0.96	0.08	43,49,59,61	0
23	CHD	C	301	29/29	0.96	0.08	29,34,39,48	0
19	PER	A	607	2/2	0.97	0.09	25,25,25,33	0

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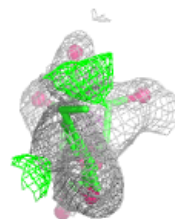
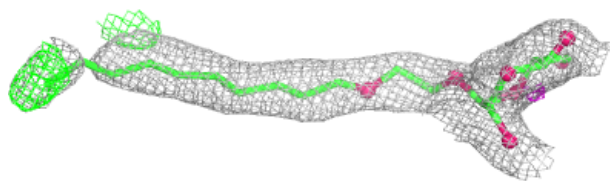
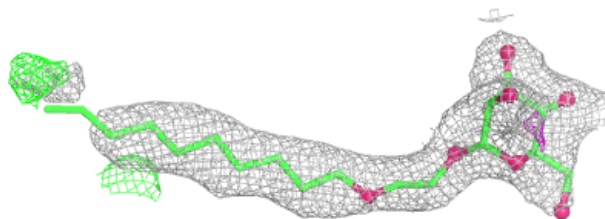
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	PGV	A	608	51/51	0.97	0.09	28,38,78,102	0
20	PGV	C	304	41/51	0.97	0.09	32,39,68,84	0
24	PEK	C	303	43/53	0.97	0.09	31,42,69,97	0
16	MG	A	604	1/1	0.99	0.03	31,31,31,31	0
14	HEA	A	601	60/60	0.99	0.06	24,29,49,60	0
14	HEA	A	602	60/60	0.99	0.05	21,26,34,45	0
22	CUA	B	302	2/2	1.00	0.01	30,30,30,31	0
17	NA	A	605	1/1	1.00	0.07	35,35,35,35	0
15	CU	A	603	1/1	1.00	0.01	26,26,26,26	0
25	ZN	F	101	1/1	1.00	0.04	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.



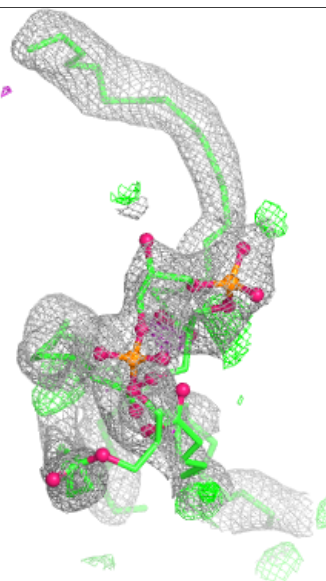
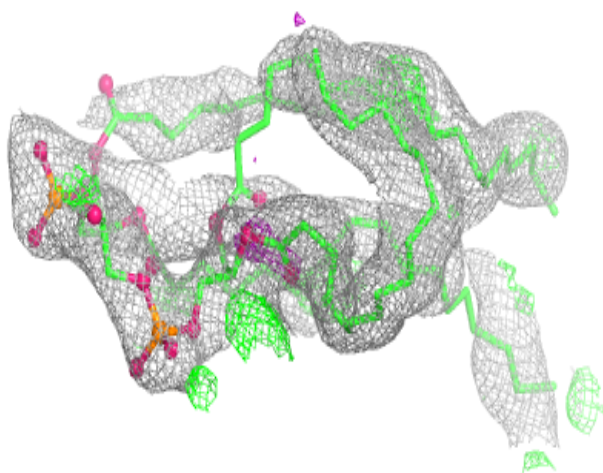
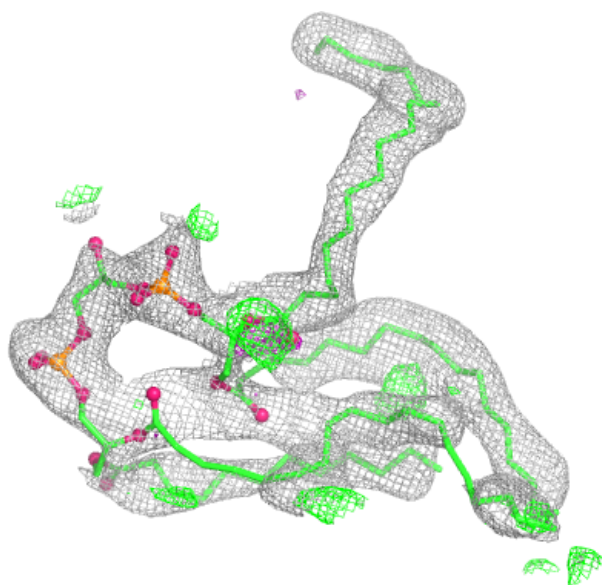
Electron density around CQX A 611:

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



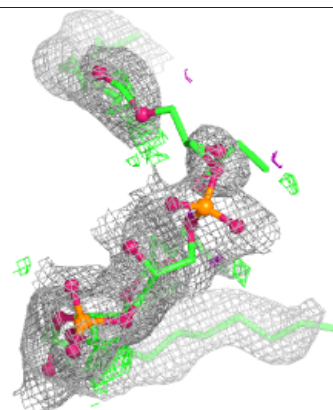
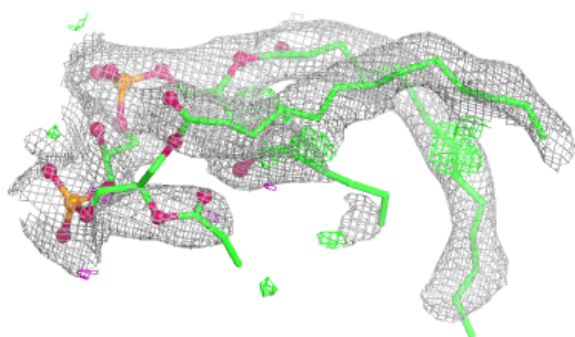
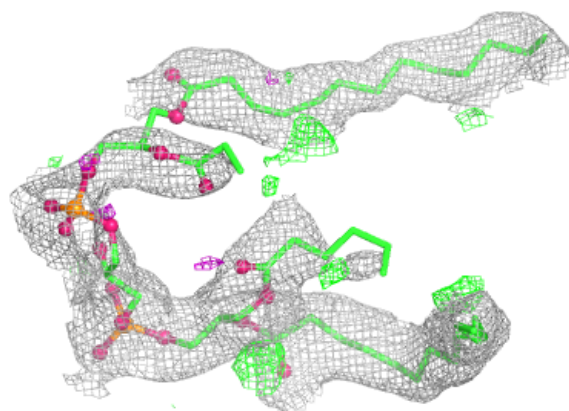
Electron density around CDL A 606:

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

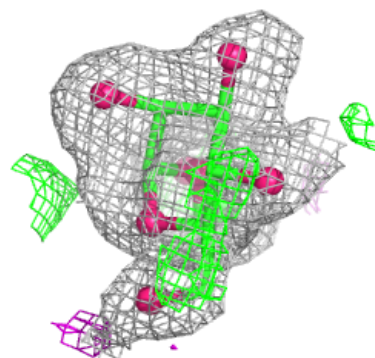
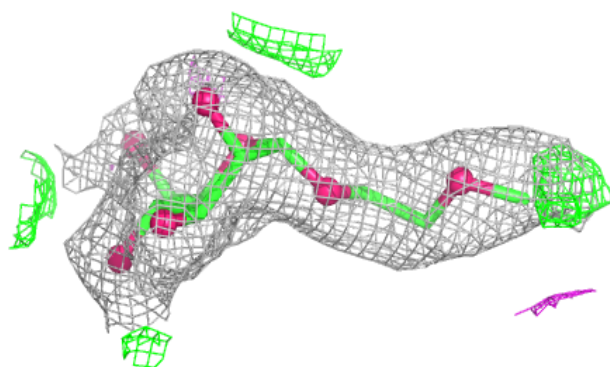
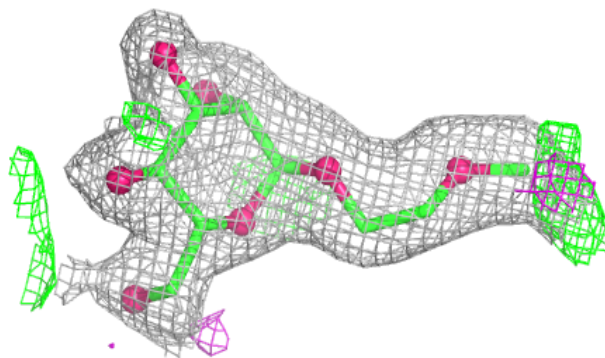


Electron density around CDL B 301:

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

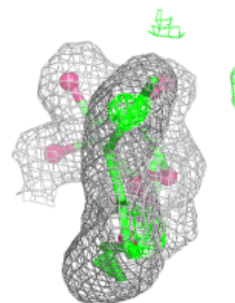
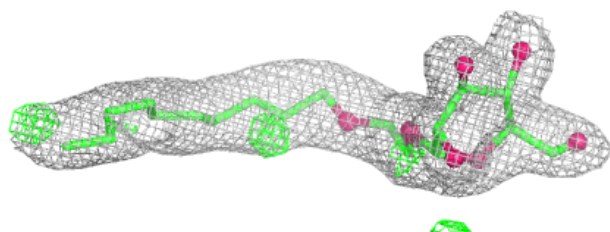
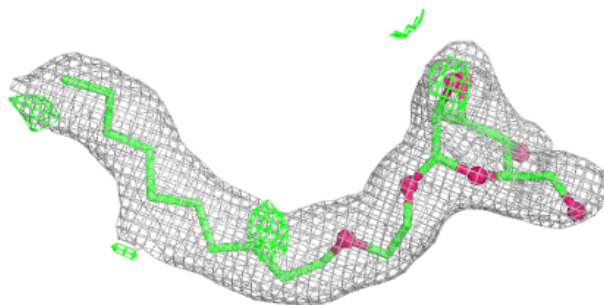
**Electron density around CQX B 304:**

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

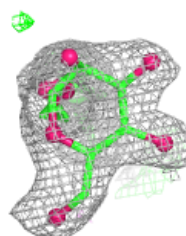
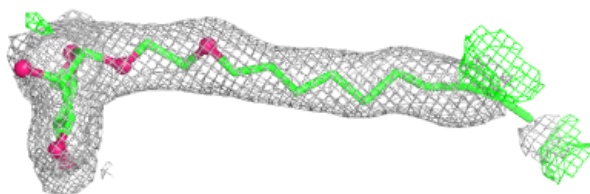
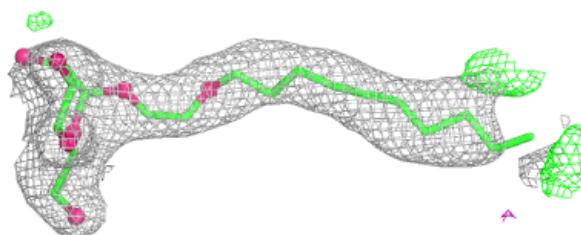


Electron density around CQX B 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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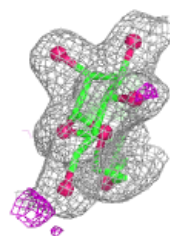
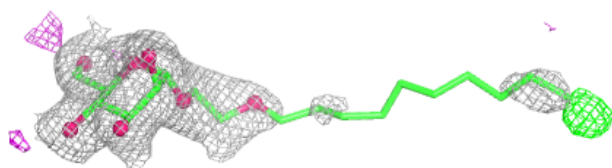
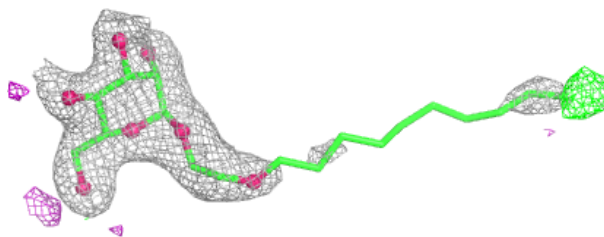
**Electron density around CQX A 609:**

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

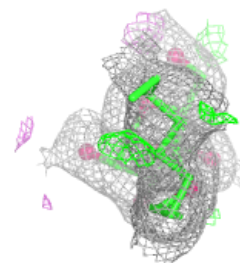
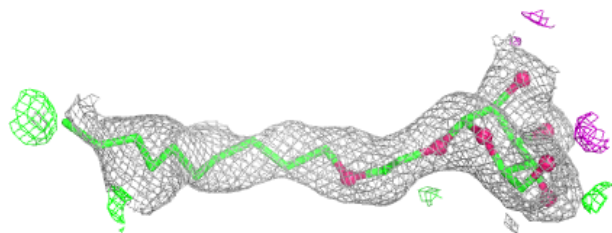
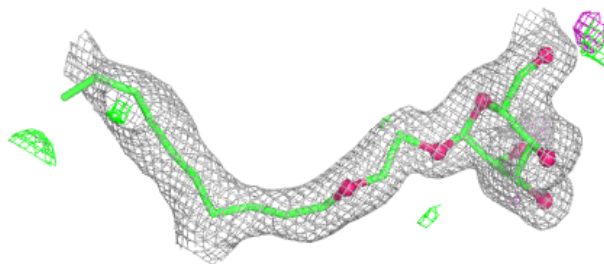


Electron density around CQX C 307:

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

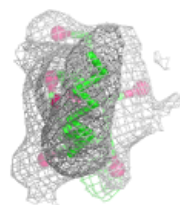
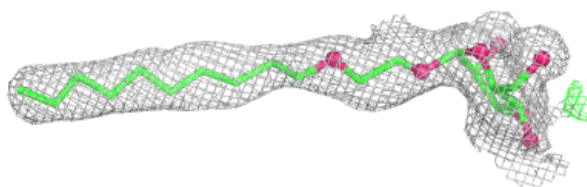
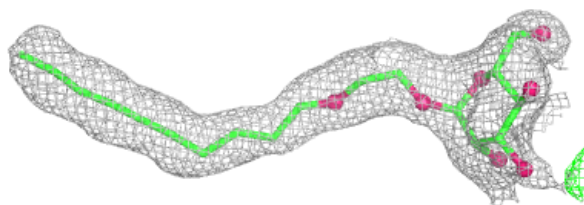
**Electron density around CQX C 306:**

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

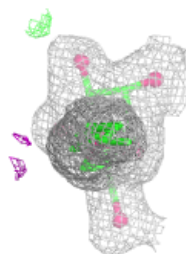
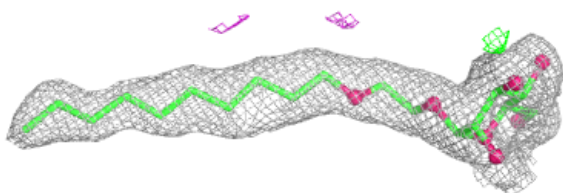
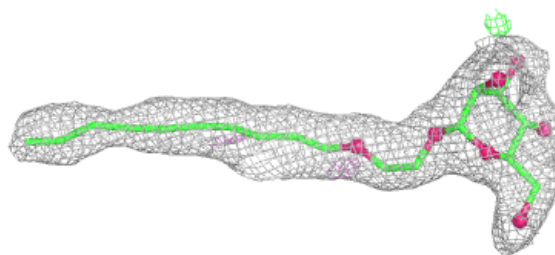


Electron density around CQX A 610:

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

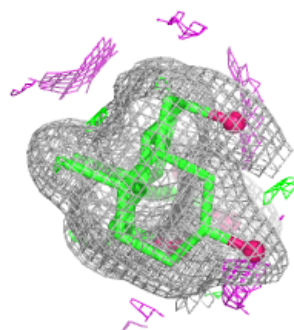
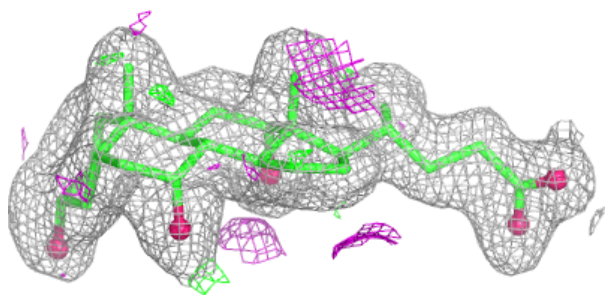
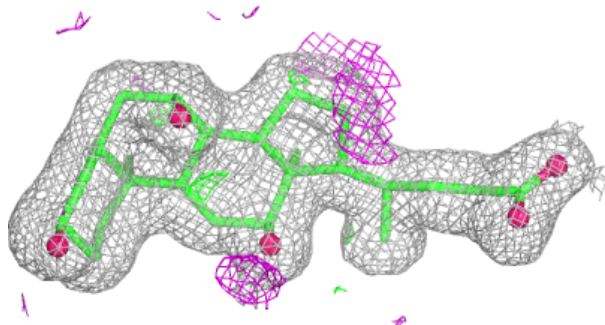
**Electron density around CQX G 101:**

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

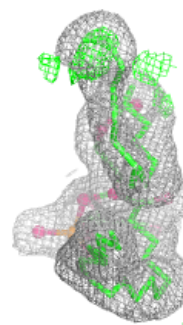
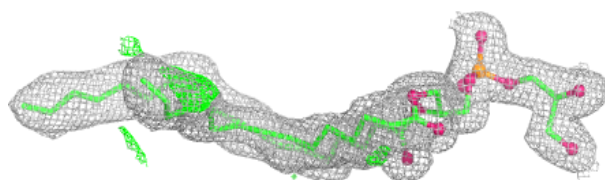
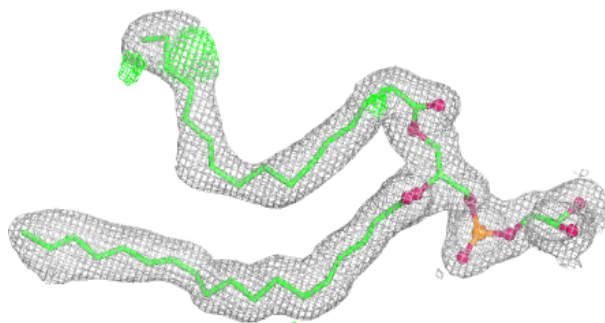


Electron density around CHD C 301:

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and green (positive)

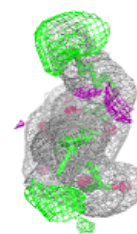
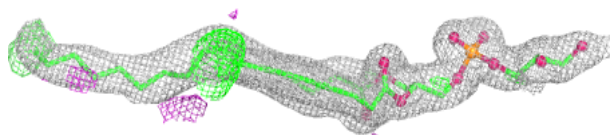
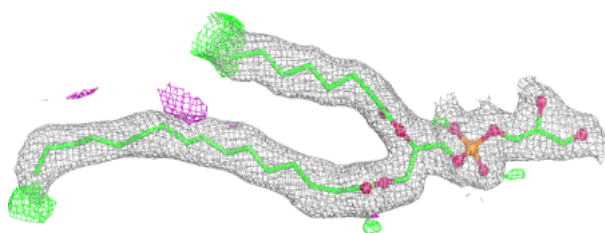
**Electron density around PGV A 608:**

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

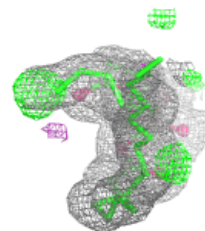
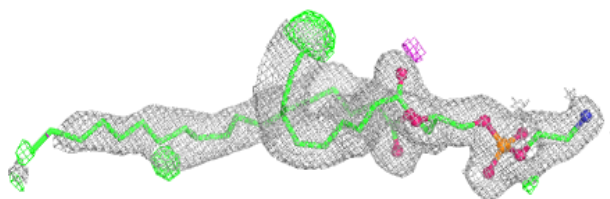
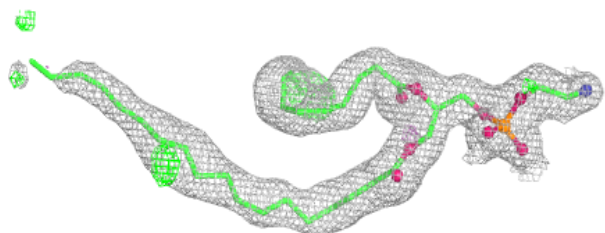


Electron density around PGV C 304:

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

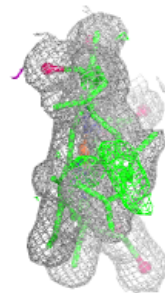
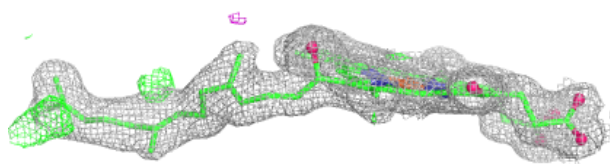
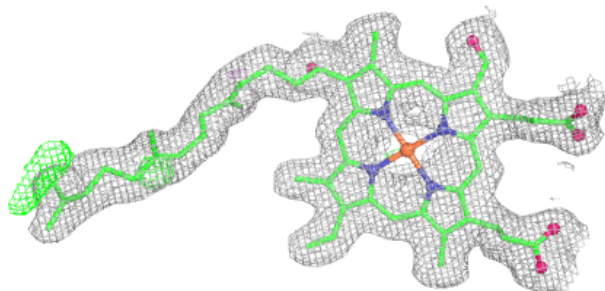
**Electron density around PEK C 303:**

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

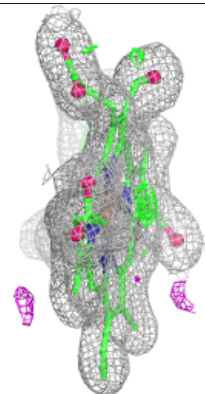
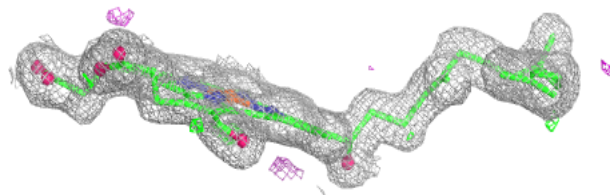
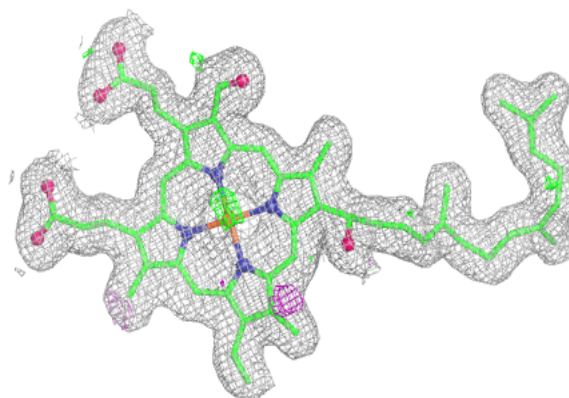


Electron density around HEA A 601:

$2mF_o-DF_c$ (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.