



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:21 PM JST

PDB ID : 6JY4 / pdb_00006jy4
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 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:

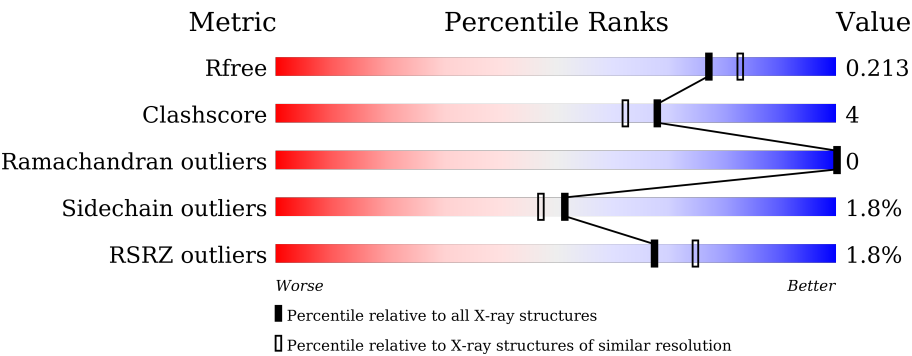
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	91%9%
2	B	227	2% 86%11% .
3	C	261	% 90%7% .
4	D	147	2% 88%7% ..
5	E	109	% 88%6% ..
6	F	98	4% 84%8% 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	NA	C	302	-	-	-	X

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			

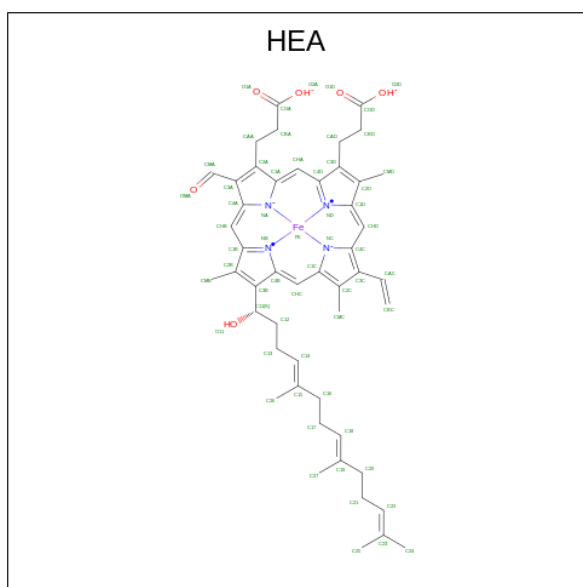
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 (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		

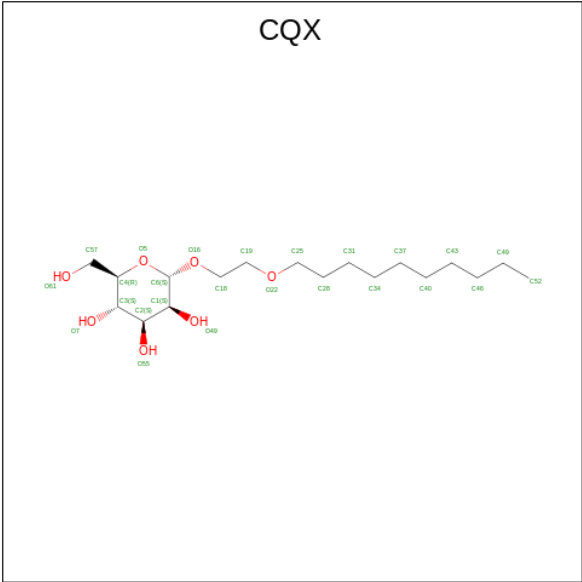
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

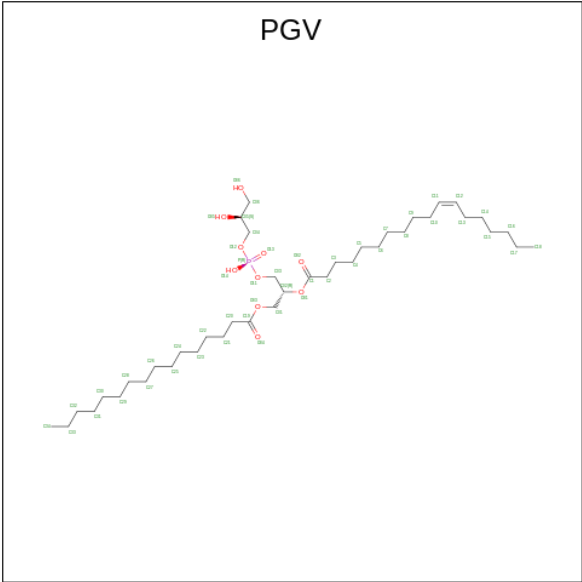
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		

- Molecule 18 is (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).



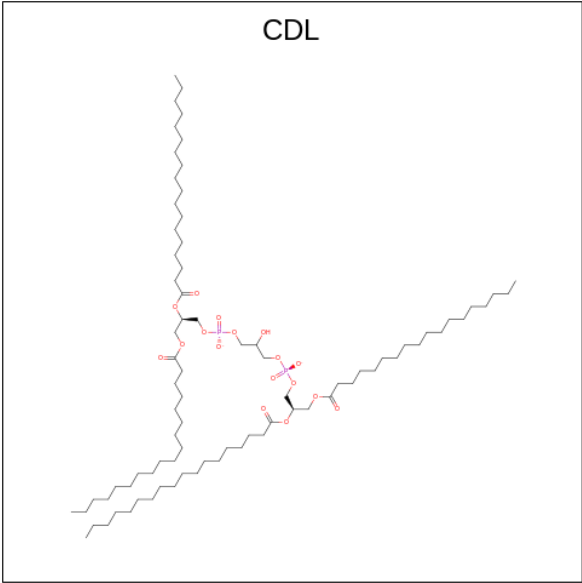
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			25	18	7		
18	A	1	Total	C	O	0	0
			25	18	7		
18	A	1	Total	C	O	0	0
			25	18	7		
18	B	1	Total	C	O	0	0
			16	9	7		
18	C	1	Total	C	O	0	0
			25	18	7		
18	C	1	Total	C	O	0	0
			25	18	7		
18	G	1	Total	C	O	0	0
			25	18	7		

- Molecule 19 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
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 (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



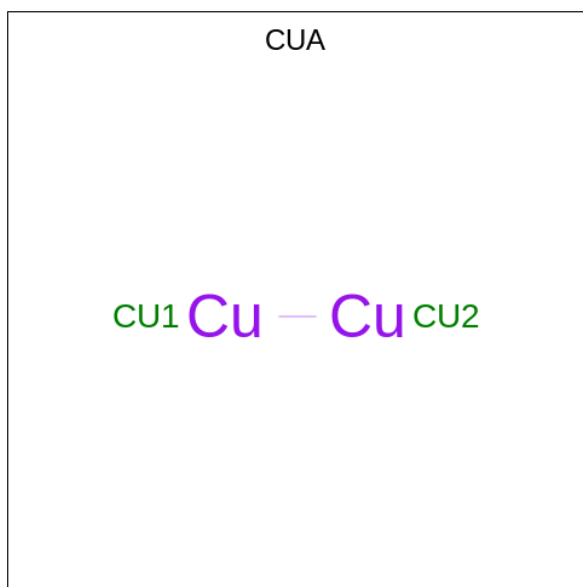
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	B	1	Total	C	O	P	0	0
			64	45	17	2		

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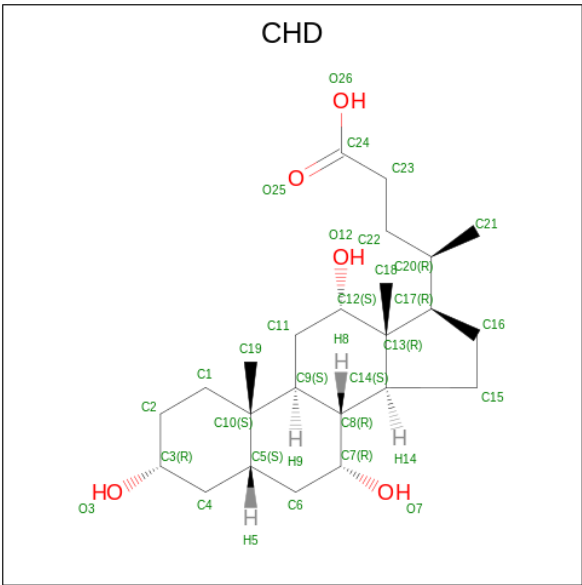
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			87	68	17	2		
20	L	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅) (labeled as "Ligand of Interest" by depositor).

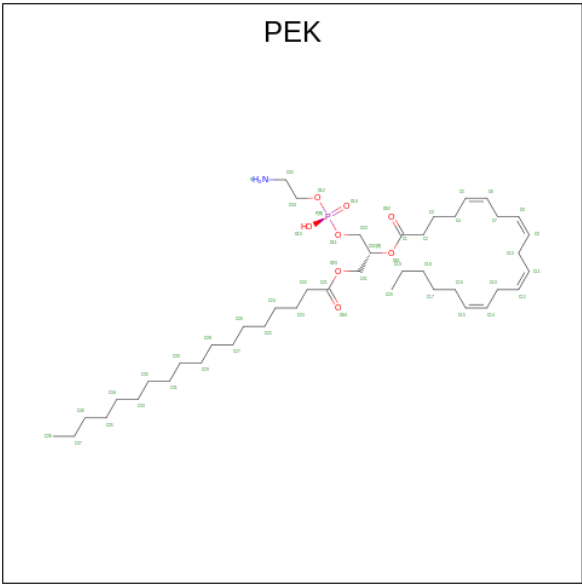


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	C	1	Total	C O	0	0
			29	24 5		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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	G	1	Total 43	C 33	N 1	O 8	P 1	0	0

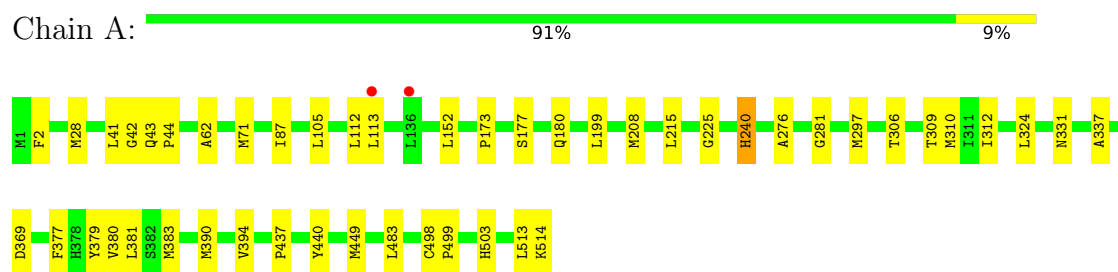
- Molecule 25 is water.

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

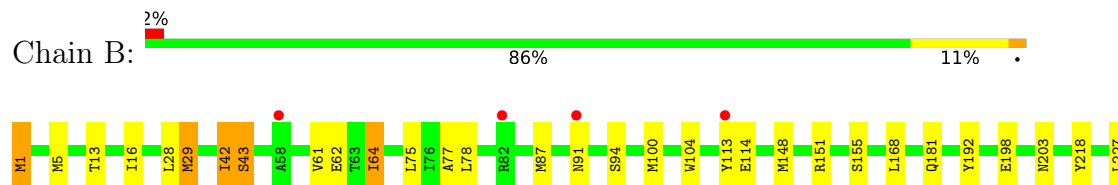
3 Residue-property plots

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.

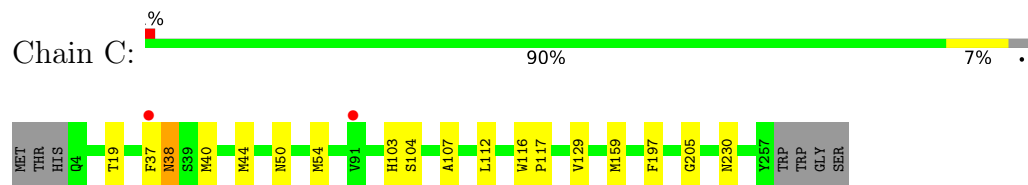
• Molecule 1: Cytochrome c oxidase subunit 1



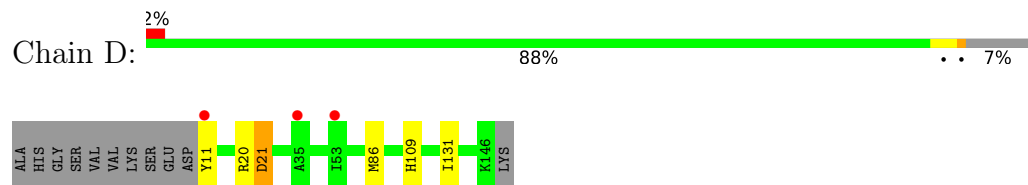
• Molecule 2: Cytochrome c oxidase subunit 2



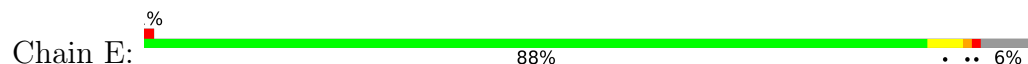
• Molecule 3: Cytochrome c oxidase subunit 3

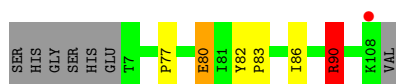


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

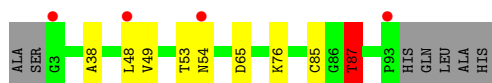
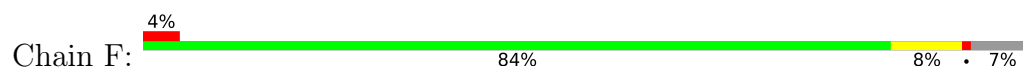


• Molecule 5: Cytochrome c oxidase subunit 5A

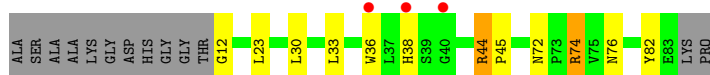




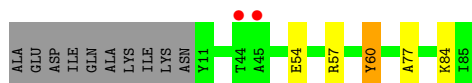
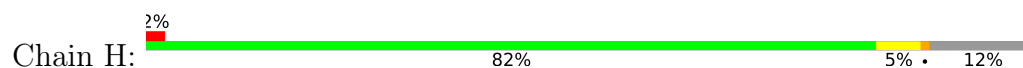
- Molecule 6: Cytochrome c oxidase subunit 5B



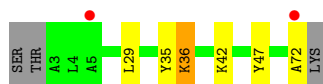
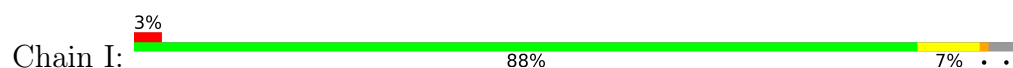
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



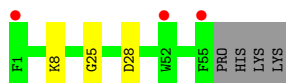
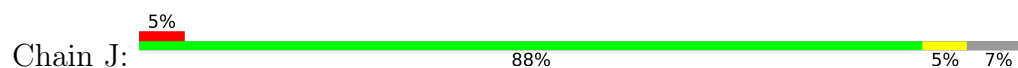
- Molecule 8: Cytochrome c oxidase subunit 6B1



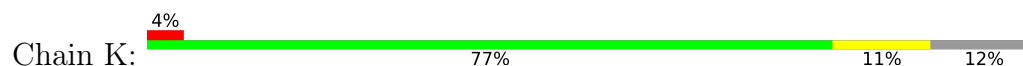
- Molecule 9: Cytochrome c oxidase subunit 6C



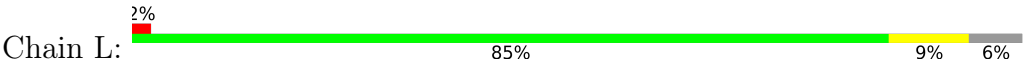
- Molecule 10: Cytochrome c oxidase subunit 7A1



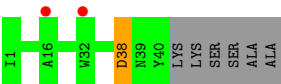
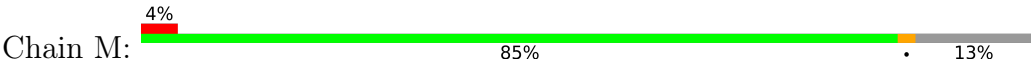
- Molecule 11: Cytochrome c oxidase subunit 7B



- 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	149.40Å 152.40Å 174.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.2 (40.00-1.95) 89.2 (40.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.38 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

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: NA, ZN, CUA, CDL, CQX, PEK, CHD, HEA, FME, PGV, MG, 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	1.28	8/4156 (0.2%)	1.12	9/5678 (0.2%)
2	B	1.25	3/1860 (0.2%)	1.14	2/2534 (0.1%)
3	C	1.17	4/2143 (0.2%)	1.01	5/2931 (0.2%)
4	D	1.01	0/1167	1.06	1/1577 (0.1%)
5	E	1.08	2/843 (0.2%)	1.03	0/1145
6	F	0.98	0/709	1.04	3/963 (0.3%)
7	G	1.17	1/621 (0.2%)	1.16	1/848 (0.1%)
8	H	1.16	1/648 (0.2%)	1.08	0/877
9	I	1.05	0/588	1.08	0/781
10	J	1.16	2/443 (0.5%)	1.02	0/598
11	K	1.10	1/398 (0.3%)	1.04	1/546 (0.2%)
12	L	1.19	0/372	1.09	0/500
13	M	1.14	0/321	1.04	0/440
All	All	1.18	22/14269 (0.2%)	1.08	22/19418 (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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	11.32	1.36	1.23
1	A	281	GLY	N-CA	7.25	1.54	1.45
11	K	21	GLY	N-CA	-6.87	1.37	1.45
5	E	80	GLU	C-O	-6.64	1.15	1.24
10	J	25	GLY	C-O	-6.20	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	77	ALA	C-O	-6.17	1.16	1.24
1	A	297	MET	SD-CE	5.93	1.94	1.79
3	C	107	ALA	CA-CB	5.91	1.60	1.53
3	C	19	THR	N-CA	5.87	1.53	1.46
10	J	28	ASP	N-CA	5.80	1.53	1.46
7	G	36	TRP	CB-CG	5.77	1.68	1.50
1	A	41	LEU	CA-C	5.60	1.60	1.52
1	A	42	GLY	N-CA	5.48	1.53	1.45
1	A	312	ILE	CA-C	5.47	1.60	1.52
1	A	306	THR	N-CA	5.37	1.52	1.46
2	B	43	SER	CB-OG	-5.26	1.31	1.42
1	A	208	MET	SD-CE	-5.10	1.66	1.79
3	C	197	PHE	N-CA	5.06	1.52	1.46
1	A	276	ALA	CA-C	5.04	1.59	1.52
3	C	104	SER	CA-CB	5.03	1.61	1.53
2	B	113	TYR	C-O	-5.03	1.17	1.24
5	E	90	ARG	N-CA	5.01	1.51	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	ILE	CB-CA-C	-7.85	101.54	112.14
1	A	71	MET	CG-SD-CE	-7.13	85.21	100.90
6	F	87	THR	N-CA-CB	6.51	119.61	110.04
1	A	240	HIS	N-CA-CB	6.50	119.99	110.30
1	A	105	LEU	CA-C-N	-6.29	113.91	120.38
1	A	105	LEU	C-N-CA	-6.29	113.91	120.38
3	C	129	VAL	CA-C-N	-6.25	112.41	119.28
3	C	129	VAL	C-N-CA	-6.25	112.41	119.28
1	A	199	LEU	CA-C-N	-6.06	112.76	119.19
1	A	199	LEU	C-N-CA	-6.06	112.76	119.19
1	A	240	HIS	CA-CB-CG	-5.87	107.93	113.80
7	G	38	HIS	N-CA-C	-5.77	106.05	112.57
4	D	20	ARG	NE-CZ-NH2	-5.59	114.17	119.20
2	B	29	MET	CG-SD-CE	-5.55	88.70	100.90
6	F	49	VAL	CA-C-N	-5.35	114.44	119.85
6	F	49	VAL	C-N-CA	-5.35	114.44	119.85
11	K	7	PRO	CB-CA-C	-5.13	104.84	111.46
1	A	71	MET	CA-C-N	-5.12	113.27	118.85
1	A	71	MET	C-N-CA	-5.12	113.27	118.85
3	C	38	ASN	N-CA-C	5.08	118.75	112.24
3	C	103	HIS	CA-C-N	5.05	127.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	103	HIS	C-N-CA	5.05	127.31	120.44

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	37	0
2	B	1824	0	1833	22	0
3	C	2061	0	1992	8	0
4	D	1133	0	1119	5	0
5	E	825	0	823	3	0
6	F	694	0	677	5	0
7	G	595	0	569	7	0
8	H	628	0	580	2	0
9	I	575	0	584	6	0
10	J	434	0	432	6	0
11	K	384	0	366	2	0
12	L	360	0	360	2	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	104	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 (104) 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
20:C:304:CDL:O1	10:J:8:LYS:CE	2.34	0.75
1:A:2:PHE:CZ	20:L:101:CDL:H712	2.22	0.73
2:B:29:MET:SD	18:B:303:CQX:O61	2.49	0.71
20:C:304:CDL:O1	10:J:8:LYS:HD2	1.93	0.68
2:B:29:MET:SD	9:I:36:LYS:HE2	2.35	0.67
7:G:76:ASN:HD21	24:G:101:PEK:HN2	1.41	0.67
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.75	0.67
2:B:13:THR:HB	2:B:168:LEU:HD23	1.78	0.65
20:C:304:CDL:O1	10:J:8:LYS:NZ	2.29	0.64
3:C:205:GLY:HA3	18:C:305:CQX:C52	2.27	0.64
20:C:304:CDL:OB4	20:C:304:CDL:OA6	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.81	0.62
7:G:72:ASN:H	7:G:76:ASN:HD22	1.44	0.62
1:A:113:LEU:HD12	20:L:101:CDL:H871	1.82	0.61
4:D:21:ASP:HB3	25:D:232:HOH:O	2.02	0.59
20:C:304:CDL:O1	10:J:8:LYS:CD	2.51	0.58
2:B:114:GLU:HB3	2:B:227:LEU:HD21	1.85	0.58
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.19	0.57
5:E:80:GLU:OE2	5:E:80:GLU:N	2.28	0.56
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.86	0.56
7:G:44:ARG:NH1	7:G:74:ARG:O	2.38	0.56
20:L:101:CDL:C41	20:L:101:CDL:H842	2.36	0.56
1:A:449:MET:SD	2:B:5:MET:HG2	2.47	0.54
2:B:28:LEU:HD23	9:I:35:TYR:OH	2.08	0.53
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.90	0.53
1:A:390:MET:HA	1:A:390:MET:HE3	1.90	0.53
20:L:101:CDL:H211	20:L:101:CDL:H822	1.90	0.53
1:A:113:LEU:CD1	20:L:101:CDL:H871	2.40	0.51
14:A:602:HEA:HMD1	14:A:602:HEA:HBD2	1.92	0.51
7:G:12:GLY:CA	25:G:201:HOH:O	2.59	0.50
7:G:12:GLY:N	25:G:201:HOH:O	2.44	0.50
13:M:38:ASP:HB2	25:M:102:HOH:O	2.11	0.50
20:C:304:CDL:OB2	10:J:8:LYS:HE3	2.11	0.50
20:C:304:CDL:PA1	20:C:304:CDL:CB2	3.00	0.50
1:A:310:MET:CE	2:B:77:ALA:HB2	2.42	0.50
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.93	0.49
5:E:82:TYR:O	5:E:83:PRO:C	2.56	0.49
1:A:112:LEU:HD11	25:A:785:HOH:O	2.12	0.49
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.13	0.49
3:C:40:MET:HE3	3:C:44:MET:HE2	1.95	0.49
11:K:13:TYR:O	11:K:17:VAL:HG23	2.13	0.48
20:B:301:CDL:H1	25:B:494:HOH:O	2.14	0.48
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.44	0.48
4:D:109:HIS:HD2	25:D:223:HOH:O	1.96	0.48
1:A:503:HIS:HE1	25:A:887:HOH:O	1.97	0.47
1:A:28:MET:HE3	12:L:29:PHE:CD1	2.49	0.47
3:C:205:GLY:CA	18:C:305:CQX:C52	2.92	0.47
7:G:45:PRO:O	7:G:82:TYR:OH	2.20	0.47
4:D:131:ILE:HD13	9:I:47:TYR:CE2	2.50	0.47
14:A:602:HEA:HMC1	14:A:602:HEA:HBC1	1.97	0.46
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.97	0.46
1:A:377:PHE:O	1:A:381:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ASN:OD1	6:F:76:LYS:CD	2.64	0.46
2:B:16:ILE:HG12	25:B:448:HOH:O	2.15	0.46
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.98	0.45
20:B:301:CDL:HB31	25:B:500:HOH:O	2.15	0.45
1:A:112:LEU:CD1	25:A:785:HOH:O	2.64	0.45
4:D:11:TYR:C	4:D:11:TYR:CD1	2.94	0.45
1:A:379:TYR:CZ	1:A:383:MET:HE1	2.51	0.45
19:A:607:PGV:H183	24:G:101:PEK:H332	1.98	0.45
2:B:61:VAL:O	2:B:62:GLU:C	2.57	0.45
2:B:94:SER:HB2	2:B:148:MET:HE3	1.99	0.45
1:A:215:LEU:HD11	24:G:101:PEK:H272	1.99	0.45
20:C:304:CDL:O1	10:J:8:LYS:HE3	2.16	0.44
4:D:86:MET:HE2	11:K:22:ALA:HA	2.00	0.44
2:B:28:LEU:HD23	9:I:35:TYR:CZ	2.53	0.43
1:A:177:SER:H	1:A:180:GLN:HE21	1.65	0.43
12:L:4:GLU:HB2	25:L:202:HOH:O	2.18	0.43
1:A:177:SER:H	1:A:180:GLN:NE2	2.17	0.43
2:B:100:MET:SD	2:B:155:SER:HB3	2.58	0.43
1:A:240:HIS:CD2	1:A:240:HIS:C	2.97	0.42
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.42
7:G:23:LEU:HD12	7:G:23:LEU:HA	1.88	0.42
20:L:101:CDL:OB7	20:L:101:CDL:H531	2.18	0.42
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.51	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.98	0.42
2:B:13:THR:HB	2:B:168:LEU:CD2	2.48	0.42
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.83	0.42
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.97	0.42
2:B:16:ILE:HD12	2:B:87:MET:HG2	2.01	0.42
1:A:2:PHE:HE1	20:L:101:CDL:H712	1.76	0.41
1:A:309:THR:CG2	14:A:602:HEA:HMB2	2.49	0.41
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.91	0.41
1:A:437:PRO:HG2	1:A:440:TYR:CZ	2.54	0.41
1:A:498:CYS:HA	1:A:499:PRO:HA	1.94	0.41
25:A:899:HOH:O	3:C:37:PHE:HE1	2.03	0.41
1:A:87:ILE:O	1:A:173:PRO:HD3	2.21	0.41
3:C:38:ASN:CG	3:C:38:ASN:O	2.63	0.41
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.01	0.41
2:B:218:TYR:CD2	9:I:72:ALA:HB2	2.56	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.46	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.40
5:E:86:ILE:O	5:E:90:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:FME:O1	2:B:192:TYR:HA	2.21	0.40
25:D:215:HOH:O	9:I:42:LYS:HE2	2.20	0.40
1:A:437:PRO:HG2	1:A:440:TYR:CE2	2.56	0.40
20:C:304:CDL:OB4	20:C:304:CDL:CA5	2.70	0.40
6:F:53:THR:HB	6:F:54:ASN:H	1.62	0.40
1:A:43:GLN:HB2	1:A:44:PRO:HD2	2.04	0.40
1:A:87:ILE:HD13	1:A:87:ILE:HG21	1.86	0.40
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 ⓘ

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%)	424 (100%)	2 (0%)	81	82
2	B	210/210 (100%)	204 (97%)	6 (3%)	37	29
3	C	220/226 (97%)	218 (99%)	2 (1%)	70	70
4	D	120/129 (93%)	119 (99%)	1 (1%)	73	74
5	E	89/95 (94%)	87 (98%)	2 (2%)	45	40
6	F	76/81 (94%)	74 (97%)	2 (3%)	40	33
7	G	62/69 (90%)	58 (94%)	4 (6%)	15	6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	27
9	I	55/58 (95%)	53 (96%)	2 (4%)	31	21
10	J	46/50 (92%)	46 (100%)	0	100	100
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	33
12	L	37/40 (92%)	35 (95%)	2 (5%)	20	9
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	29
All	All	1481/1543 (96%)	1454 (98%)	27 (2%)	51	47

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	A	369	ASP
2	B	42	ILE
2	B	43	SER
2	B	64	ILE
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
3	C	159	MET
3	C	230	ASN

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Mol	Chain	Res	Type
4	D	21	ASP
5	E	77	PRO
5	E	90	ARG
6	F	48	LEU
6	F	87	THR
7	G	30	LEU
7	G	33	LEU
7	G	44	ARG
7	G	74	ARG
8	H	60	TYR
8	H	84	LYS
9	I	29	LEU
9	I	36	LYS
11	K	12	LYS
12	L	16	GLU
12	L	26	THR
13	M	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
5	E	94	ASN
6	F	88	HIS
7	G	76	ASN
8	H	12	GLN
8	H	37	HIS

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	0.42	0	7,9,11	1.27	0
2	FME	B	1	2	8,9,10	1.31	1 (12%)	7,9,11	4.49	3 (42%)

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	-	3/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-

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(°)	Ideal(°)
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
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 oligosaccharides 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%)
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%)
18	CQX	G	102	-	25,25,25	0.69	1 (4%)	30,30,30	0.99	3 (10%)
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
19	PGV	C	303	-	50,50,50	0.88	3 (6%)	53,56,56	1.00	3 (5%)
14	HEA	A	602	1	66,67,67	1.81	16 (24%)	78,103,103	2.54	25 (32%)
20	CDL	B	301	-	63,63,99	1.42	4 (6%)	69,75,111	1.60	13 (18%)
20	CDL	C	304	-	86,86,99	1.09	4 (4%)	92,98,111	1.25	13 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CQX	B	303	-	16,16,25	1.23	1 (6%)	21,21,30	1.61	4 (19%)
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%)
19	PGV	A	607	-	50,50,50	0.91	2 (4%)	53,56,56	1.12	3 (5%)
20	CDL	L	101	-	93,93,99	0.95	5 (5%)	99,105,111	1.50	11 (11%)
24	PEK	G	101	-	42,42,52	0.91	3 (7%)	45,47,57	1.17	3 (6%)
14	HEA	A	601	1	66,67,67	2.35	18 (27%)	78,103,103	2.11	21 (26%)

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

All (63) 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	601	HEA	CHA-C1A	6.43	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4B-NB	-6.08	1.29	1.40
14	A	601	HEA	FE-ND	5.97	2.13	1.94
14	A	601	HEA	C1D-ND	-4.95	1.31	1.40
20	B	301	CDL	OB6-CB5	4.74	1.47	1.34
14	A	601	HEA	C1A-C2A	-4.59	1.37	1.45
20	B	301	CDL	OB8-CB7	4.58	1.46	1.33
20	C	304	CDL	OB8-CB7	4.54	1.46	1.33
20	C	304	CDL	OB6-CB5	4.53	1.47	1.34
14	A	601	HEA	C3A-C4A	-4.50	1.38	1.46
14	A	601	HEA	C1C-NC	-4.45	1.31	1.39
14	A	602	HEA	FE-ND	4.36	2.08	1.94
14	A	601	HEA	FE-NB	4.23	2.08	1.94
20	B	301	CDL	OA8-CA7	4.09	1.45	1.33
20	L	101	CDL	OB8-CB7	4.03	1.45	1.33
14	A	602	HEA	CHA-C1A	3.91	1.46	1.38
14	A	602	HEA	CHB-C4A	3.84	1.45	1.38
20	C	304	CDL	OA8-CA7	3.83	1.44	1.33
20	L	101	CDL	OA8-CA7	3.81	1.44	1.33
14	A	601	HEA	C1B-NB	-3.65	1.31	1.38
14	A	601	HEA	CHC-C1C	3.60	1.47	1.39
20	C	304	CDL	OA6-CA5	3.55	1.44	1.34
14	A	601	HEA	O11-C11	3.51	1.50	1.42
19	A	607	PGV	O01-C1	3.51	1.44	1.34
20	L	101	CDL	OA6-CA5	3.50	1.44	1.34
19	A	607	PGV	O03-C19	3.36	1.43	1.33
19	C	303	PGV	O01-C1	3.28	1.43	1.34
14	A	602	HEA	C3A-C4A	-3.23	1.40	1.46
14	A	602	HEA	C1A-C2A	-3.19	1.39	1.45
14	A	602	HEA	CHD-C4C	3.14	1.46	1.39
24	G	101	PEK	O01-C1	3.11	1.43	1.34
20	L	101	CDL	OB6-CB5	3.08	1.43	1.34
19	C	303	PGV	O03-C19	3.06	1.42	1.33
14	A	602	HEA	C1B-NB	-3.04	1.32	1.38
14	A	601	HEA	C4D-ND	-3.02	1.32	1.38
14	A	602	HEA	CMA-C3A	2.98	1.51	1.45
18	B	303	CQX	O16-C6	2.92	1.45	1.40
18	C	305	CQX	O16-C6	2.85	1.45	1.40
24	G	101	PEK	O03-C21	2.76	1.41	1.33
14	A	602	HEA	CHD-C1D	2.72	1.44	1.38
14	A	602	HEA	C4D-ND	-2.65	1.33	1.38
14	A	601	HEA	C3A-C2A	2.62	1.42	1.36
24	G	101	PEK	O01-C02	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C1A-NA	-2.51	1.34	1.39
14	A	601	HEA	CHC-C4B	2.42	1.43	1.38
18	G	102	CQX	O16-C6	2.41	1.44	1.40
18	A	609	CQX	O16-C6	2.40	1.44	1.40
18	C	305	CQX	O16-C18	2.34	1.49	1.43
14	A	601	HEA	C1B-C2B	-2.32	1.40	1.44
18	A	606	CQX	O7-C3	2.29	1.48	1.43
20	L	101	CDL	OB6-CB4	-2.27	1.40	1.46
14	A	601	HEA	C3C-C4C	-2.23	1.37	1.42
19	C	303	PGV	O01-C02	-2.21	1.41	1.46
14	A	602	HEA	FE-NB	2.19	2.01	1.94
14	A	602	HEA	C1D-ND	-2.14	1.36	1.40
14	A	601	HEA	CHB-C4A	2.13	1.42	1.38
14	A	602	HEA	CHA-C4D	2.12	1.44	1.39
22	C	301	CHD	O26-C24	-2.11	1.23	1.30
22	C	301	CHD	C13-C17	-2.04	1.52	1.55
14	A	602	HEA	C12-C11	2.03	1.56	1.52
14	A	602	HEA	C1C-C2C	-2.03	1.38	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C4C-NC-C1C	-9.35	96.19	105.35
14	A	602	HEA	C3C-C4C-NC	8.20	115.29	110.25
14	A	601	HEA	C13-C12-C11	-6.95	103.92	114.35
14	A	601	HEA	C3C-C4C-NC	6.13	114.02	110.25
20	B	301	CDL	CA4-OA6-CA5	6.03	132.63	117.79
14	A	602	HEA	C4A-NA-C1A	-5.72	99.75	105.35
20	L	101	CDL	OB6-CB5-C51	5.55	123.46	111.50
14	A	602	HEA	CHB-C4A-NA	-5.42	118.58	124.44
14	A	601	HEA	C4A-C3A-C2A	-5.23	102.45	106.75
20	C	304	CDL	OB6-CB5-C51	5.11	122.52	111.50
20	L	101	CDL	CB4-OB6-CB5	-5.09	105.25	117.79
20	L	101	CDL	OA6-CA5-C11	5.03	122.34	111.50
18	C	305	CQX	C18-O16-C6	4.92	122.00	113.84
14	A	601	HEA	OMA-CMA-C3A	-4.59	115.30	125.69
18	A	606	CQX	C18-O16-C6	-4.55	106.30	113.84
14	A	601	HEA	C1B-C2B-C3B	-4.52	101.39	106.80
14	A	602	HEA	C3B-C4B-NB	4.41	115.06	109.84
19	A	607	PGV	O03-C19-O04	-4.39	112.53	123.59
20	L	101	CDL	CA4-OA6-CA5	-4.37	107.04	117.79
14	A	602	HEA	C27-C19-C20	4.26	122.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	301	CDL	OA6-CA5-C11	4.26	120.69	111.50
22	C	301	CHD	C21-C20-C22	-4.18	103.80	110.36
14	A	602	HEA	C2C-C1C-NC	3.98	116.14	110.08
18	B	303	CQX	C18-O16-C6	3.90	120.30	113.84
14	A	601	HEA	C2B-C1B-NB	3.82	114.46	109.88
14	A	602	HEA	CMC-C2C-C1C	3.77	131.12	125.37
14	A	602	HEA	C20-C19-C18	-3.77	113.48	121.12
14	A	602	HEA	C4A-C3A-C2A	-3.74	103.68	106.75
20	B	301	CDL	OB6-CB5-C51	3.71	121.15	110.80
18	A	606	CQX	C6-O5-C4	3.69	120.94	113.69
14	A	602	HEA	C1D-C2D-C3D	-3.61	103.17	106.96
14	A	602	HEA	C4B-NB-C1B	-3.56	101.39	105.07
14	A	602	HEA	C2B-C1B-NB	3.53	114.11	109.88
18	A	606	CQX	O5-C4-C3	3.52	116.08	109.69
20	L	101	CDL	OA8-CA7-C31	3.51	122.93	111.91
14	A	602	HEA	C2A-C1A-NA	3.50	113.73	110.32
20	B	301	CDL	CA6-CA4-CA3	-3.47	103.58	111.79
20	L	101	CDL	OA6-CA5-OA7	-3.45	115.37	123.70
14	A	601	HEA	O11-C11-C12	3.44	119.02	109.42
14	A	602	HEA	CBD-CAD-C3D	3.43	122.15	112.63
14	A	602	HEA	C2D-C1D-ND	3.38	113.85	109.84
18	A	608	CQX	C34-C31-C28	-3.35	97.40	114.42
18	A	608	CQX	O16-C6-C1	-3.35	103.07	108.30
18	B	303	CQX	O5-C4-C3	3.33	115.73	109.69
22	C	301	CHD	C9-C11-C12	3.30	118.66	114.30
14	A	601	HEA	CHB-C4A-NA	-3.27	120.90	124.44
18	C	305	CQX	O16-C18-C19	-3.27	98.38	109.72
19	C	303	PGV	O03-C19-O04	-3.24	115.42	123.59
18	A	608	CQX	C6-C1-C2	-3.19	103.35	110.00
18	A	606	CQX	C37-C34-C31	-3.17	98.35	114.42
20	B	301	CDL	OB8-CB7-C71	3.16	121.81	111.91
19	A	607	PGV	O03-C19-C20	3.13	121.72	111.91
14	A	601	HEA	C4A-CHB-C1B	3.11	132.76	126.06
14	A	601	HEA	CAD-C3D-C2D	3.10	133.65	127.88
20	C	304	CDL	OB8-CB7-C71	3.08	121.57	111.91
14	A	601	HEA	C4C-NC-C1C	-3.08	102.33	105.35
20	L	101	CDL	C52-C51-CB5	-3.07	102.45	113.62
14	A	602	HEA	CHC-C1C-C2C	-3.06	118.58	127.24
14	A	601	HEA	C4D-C3D-C2D	-3.06	102.44	106.90
24	G	101	PEK	C24-C23-C22	-3.03	102.28	113.19
14	A	601	HEA	C17-C18-C19	-3.00	120.44	127.66
18	A	606	CQX	C31-C28-C25	-3.00	100.21	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C3C-C2C-C1C	-2.98	103.56	107.16
18	C	305	CQX	O7-C3-C2	-2.95	103.54	110.35
18	C	305	CQX	O49-C1-C6	2.94	117.19	110.05
20	L	101	CDL	OB6-CB5-OB7	-2.90	116.70	123.70
20	C	304	CDL	OA4-PA1-OA3	2.89	126.54	112.24
14	A	602	HEA	C4B-C3B-C2B	-2.88	102.49	107.41
18	C	305	CQX	O55-C2-C3	-2.87	103.72	110.35
22	C	301	CHD	C21-C20-C17	2.87	117.31	112.92
20	B	301	CDL	OA8-CA7-C31	2.84	120.82	111.91
20	C	304	CDL	OA6-CA5-OA7	-2.80	116.93	123.70
14	A	601	HEA	C4A-NA-C1A	-2.80	102.61	105.35
20	C	304	CDL	OA8-CA7-C31	2.76	120.56	111.91
20	B	301	CDL	OA6-CA4-CA6	2.75	118.34	108.40
14	A	602	HEA	CHB-C1B-C2B	-2.73	120.72	124.98
14	A	602	HEA	CHA-C1A-C2A	-2.71	120.55	124.94
14	A	601	HEA	C26-C15-C16	2.69	119.80	115.27
18	A	609	CQX	C31-C28-C25	-2.66	101.69	113.49
18	A	606	CQX	C43-C40-C37	-2.65	100.95	114.42
20	L	101	CDL	OA8-CA7-OA9	-2.64	116.92	123.59
20	B	301	CDL	OA8-CA7-OA9	-2.64	116.92	123.59
19	C	303	PGV	O03-C19-C20	2.63	120.16	111.91
14	A	601	HEA	C2C-C1C-NC	2.61	114.06	110.08
20	C	304	CDL	CA4-OA6-CA5	-2.61	111.36	117.79
14	A	601	HEA	C3D-C4D-ND	2.59	112.86	110.36
19	C	303	PGV	C22-C21-C20	-2.59	103.90	113.19
20	L	101	CDL	OB8-CB6-CB4	2.58	115.94	108.43
20	B	301	CDL	OA7-CA5-C11	-2.56	113.76	123.73
14	A	602	HEA	C1D-ND-C4D	-2.55	102.43	105.07
14	A	602	HEA	CAD-C3D-C4D	-2.55	120.20	124.66
18	A	609	CQX	O7-C3-C2	2.52	116.17	110.35
18	C	305	CQX	O5-C4-C57	2.50	112.65	106.44
22	C	301	CHD	C9-C8-C7	-2.50	108.89	111.88
14	A	601	HEA	C2A-C1A-NA	2.45	112.70	110.32
20	B	301	CDL	OB8-CB7-OB9	-2.44	117.43	123.59
18	A	606	CQX	C2-C3-C4	2.43	114.57	110.24
18	G	102	CQX	C3-C2-C1	-2.43	106.59	110.82
18	A	606	CQX	O55-C2-C1	-2.41	104.78	110.35
18	B	303	CQX	O5-C6-O16	2.40	115.66	109.97
20	C	304	CDL	OB5-PB2-OB3	2.38	118.38	109.07
20	B	301	CDL	OA6-CA4-CA3	2.33	116.85	108.40
22	C	301	CHD	C11-C12-C13	-2.33	108.85	111.24
18	A	608	CQX	O49-C1-C2	2.33	115.73	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	PGV	C32-C31-C30	-2.32	102.65	114.42
20	L	101	CDL	OB6-CB4-CB3	-2.30	100.07	108.40
18	A	606	CQX	C3-C2-C1	2.29	114.83	110.82
20	B	301	CDL	OB4-PB2-OB3	2.29	123.57	112.24
18	A	609	CQX	C2-C3-C4	-2.29	106.15	110.24
18	B	303	CQX	C6-O5-C4	2.29	118.18	113.69
14	A	601	HEA	C1A-CHA-C4D	-2.27	121.16	126.06
24	G	101	PEK	C31-C30-C29	-2.27	102.90	114.42
14	A	601	HEA	CHB-C1B-NB	-2.26	121.96	124.42
18	G	102	CQX	C18-O16-C6	-2.26	110.10	113.84
20	C	304	CDL	OA6-CA5-C11	2.22	116.28	111.50
14	A	602	HEA	CAD-C3D-C2D	2.21	131.99	127.88
18	A	608	CQX	C40-C37-C34	-2.20	103.25	114.42
20	C	304	CDL	O1-C1-CA2	-2.16	101.99	109.56
20	C	304	CDL	OA4-PA1-OA2	-2.14	97.81	107.75
18	A	606	CQX	O5-C6-C1	2.13	114.86	110.35
18	A	609	CQX	C6-O5-C4	2.13	117.87	113.69
14	A	602	HEA	CAA-CBA-CGA	2.13	118.18	113.60
18	A	608	CQX	C31-C28-C25	-2.11	104.16	113.49
14	A	601	HEA	C16-C17-C18	2.11	118.80	111.88
20	B	301	CDL	CB2-C1-CA2	-2.09	106.65	112.79
18	G	102	CQX	C2-C3-C4	2.08	113.95	110.24
20	C	304	CDL	OA8-CA7-OA9	-2.07	118.37	123.59
18	A	606	CQX	O16-C6-C1	-2.06	105.08	108.30
22	C	301	CHD	C1-C10-C9	2.05	114.58	111.35
18	A	606	CQX	O16-C18-C19	-2.04	102.63	109.72
20	C	304	CDL	C12-C11-CA5	-2.02	106.27	113.62
20	C	304	CDL	OB8-CB7-OB9	-2.02	118.50	123.59
24	G	101	PEK	O13-P-O12	-2.01	98.42	107.75

There are no chirality outliers.

All (207) 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
20	B	301	CDL	C11-CA5-OA6-CA4
20	B	301	CDL	C51-CB5-OB6-CB4
20	C	304	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	C	304	CDL	O1-C1-CB2-OB2
20	C	304	CDL	CA2-C1-CB2-OB2
20	C	304	CDL	C1-CA2-OA2-PA1
20	C	304	CDL	CA2-OA2-PA1-OA3
20	C	304	CDL	CA3-OA5-PA1-OA3
20	C	304	CDL	CA3-OA5-PA1-OA4
20	C	304	CDL	C11-CA5-OA6-CA4
20	C	304	CDL	CB3-OB5-PB2-OB4
20	C	304	CDL	OB7-CB5-OB6-CB4
20	C	304	CDL	C51-CB5-OB6-CB4
20	L	101	CDL	CA2-C1-CB2-OB2
20	L	101	CDL	C11-CA5-OA6-CA4
20	L	101	CDL	CB2-OB2-PB2-OB5
20	L	101	CDL	CB3-OB5-PB2-OB3
20	L	101	CDL	CB3-OB5-PB2-OB4
20	L	101	CDL	OA9-CA7-OA8-CA6
20	L	101	CDL	C31-CA7-OA8-CA6
20	B	301	CDL	OB7-CB5-OB6-CB4
20	L	101	CDL	OA7-CA5-OA6-CA4
18	A	606	CQX	O5-C4-C57-O61
14	A	602	HEA	C4D-C3D-CAD-CBD
20	B	301	CDL	OA7-CA5-OA6-CA4
20	C	304	CDL	OA7-CA5-OA6-CA4
18	B	303	CQX	O5-C4-C57-O61
20	B	301	CDL	O1-C1-CA2-OA2
20	B	301	CDL	O1-C1-CB2-OB2
20	C	304	CDL	C51-C52-C53-C54
20	B	301	CDL	CB2-C1-CA2-OA2
20	B	301	CDL	C71-CB7-OB8-CB6
20	C	304	CDL	C71-CB7-OB8-CB6
18	A	606	CQX	C3-C4-C57-O61
18	B	303	CQX	C3-C4-C57-O61
20	L	101	CDL	O1-C1-CB2-OB2
18	C	306	CQX	O16-C18-C19-O22
14	A	601	HEA	C14-C15-C16-C17
18	C	305	CQX	O16-C18-C19-O22
20	B	301	CDL	OB9-CB7-OB8-CB6
20	B	301	CDL	CB7-C71-C72-C73
20	C	304	CDL	CA7-C31-C32-C33
20	L	101	CDL	CA5-C11-C12-C13
20	L	101	CDL	CA7-C31-C32-C33
18	A	609	CQX	O16-C18-C19-O22

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Mol	Chain	Res	Type	Atoms
20	C	304	CDL	CB5-C51-C52-C53
20	B	301	CDL	CA5-C11-C12-C13
20	C	304	CDL	OB9-CB7-OB8-CB6
20	B	301	CDL	CB2-OB2-PB2-OB5
20	C	304	CDL	CA2-OA2-PA1-OA5
20	C	304	CDL	CA3-OA5-PA1-OA2
20	L	101	CDL	CB3-OB5-PB2-OB2
14	A	601	HEA	C26-C15-C16-C17
20	L	101	CDL	C52-C53-C54-C55
20	B	301	CDL	C18-C19-C20-C21
20	L	101	CDL	C19-C20-C21-C22
18	C	306	CQX	C31-C34-C37-C40
20	C	304	CDL	O1-C1-CA2-OA2
20	C	304	CDL	C73-C74-C75-C76
20	L	101	CDL	C14-C15-C16-C17
20	L	101	CDL	C62-C63-C64-C65
20	B	301	CDL	C71-C72-C73-C74
20	C	304	CDL	C71-C72-C73-C74
19	C	303	PGV	C27-C28-C29-C30
20	C	304	CDL	C14-C15-C16-C17
20	C	304	CDL	C13-C14-C15-C16
20	C	304	CDL	C21-C22-C23-C24
24	G	101	PEK	C24-C25-C26-C27
20	B	301	CDL	C77-C78-C79-C80
20	C	304	CDL	C56-C57-C58-C59
20	L	101	CDL	C59-C60-C61-C62
20	B	301	CDL	C72-C73-C74-C75
20	L	101	CDL	C22-C23-C24-C25
20	L	101	CDL	C76-C77-C78-C79
20	B	301	CDL	C78-C79-C80-C81
19	C	303	PGV	C11-C10-C9-C8
18	C	305	CQX	C31-C34-C37-C40
20	C	304	CDL	C54-C55-C56-C57
20	L	101	CDL	C71-C72-C73-C74
18	C	305	CQX	C28-C31-C34-C37
20	C	304	CDL	C35-C36-C37-C38
20	B	301	CDL	C32-C33-C34-C35
20	C	304	CDL	C57-C58-C59-C60
20	C	304	CDL	C82-C83-C84-C85
20	L	101	CDL	C13-C14-C15-C16
19	C	303	PGV	C25-C26-C27-C28
19	C	303	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	L	101	CDL	C20-C21-C22-C23
18	C	305	CQX	C40-C43-C46-C49
18	A	608	CQX	C34-C37-C40-C43
18	C	305	CQX	O22-C25-C28-C31
18	A	606	CQX	C40-C43-C46-C49
18	C	306	CQX	C28-C31-C34-C37
20	L	101	CDL	C79-C80-C81-C82
24	G	101	PEK	C35-C36-C37-C38
20	C	304	CDL	C77-C78-C79-C80
20	B	301	CDL	C79-C80-C81-C82
20	B	301	CDL	CA6-CA4-OA6-CA5
18	C	305	CQX	C43-C46-C49-C52
20	B	301	CDL	CB4-CB3-OB5-PB2
19	A	607	PGV	C27-C28-C29-C30
20	C	304	CDL	C75-C76-C77-C78
18	C	306	CQX	O22-C25-C28-C31
20	C	304	CDL	C83-C84-C85-C86
20	C	304	CDL	C78-C79-C80-C81
24	G	101	PEK	C27-C28-C29-C30
20	C	304	CDL	C80-C81-C82-C83
20	L	101	CDL	OB5-CB3-CB4-CB6
19	C	303	PGV	C14-C15-C16-C17
19	C	303	PGV	C22-C23-C24-C25
20	C	304	CDL	C18-C19-C20-C21
20	L	101	CDL	C32-C33-C34-C35
20	L	101	CDL	C54-C55-C56-C57
18	A	608	CQX	C43-C46-C49-C52
20	L	101	CDL	C63-C64-C65-C66
20	B	301	CDL	CB3-CB4-CB6-OB8
20	C	304	CDL	C24-C25-C26-C27
14	A	602	HEA	C2A-C3A-CMA-OMA
20	C	304	CDL	C79-C80-C81-C82
20	L	101	CDL	OB5-CB3-CB4-OB6
19	C	303	PGV	C28-C29-C30-C31
20	C	304	CDL	C59-C60-C61-C62
20	B	301	CDL	OA6-CA4-CA6-OA8
20	L	101	CDL	OB6-CB4-CB6-OB8
20	C	304	CDL	C22-C23-C24-C25
20	L	101	CDL	C58-C59-C60-C61
20	B	301	CDL	CA4-CA3-OA5-PA1
20	B	301	CDL	C1-CB2-OB2-PB2
20	B	301	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	B	301	CDL	OA5-CA3-CA4-CA6
18	C	306	CQX	C18-C19-O22-C25
19	A	607	PGV	C26-C27-C28-C29
20	B	301	CDL	OB6-CB4-CB6-OB8
24	G	101	PEK	C26-C27-C28-C29
20	L	101	CDL	OB9-CB7-OB8-CB6
20	C	304	CDL	C32-C33-C34-C35
19	C	303	PGV	C7-C8-C9-C10
20	L	101	CDL	C71-CB7-OB8-CB6
19	C	303	PGV	C13-C14-C15-C16
19	C	303	PGV	C02-C03-O11-P
20	B	301	CDL	CB2-OB2-PB2-OB4
20	C	304	CDL	CA2-OA2-PA1-OA4
20	L	101	CDL	CB2-OB2-PB2-OB4
20	B	301	CDL	C19-C20-C21-C22
24	G	101	PEK	C23-C24-C25-C26
18	A	608	CQX	C37-C40-C43-C46
20	B	301	CDL	C52-C51-CB5-OB7
18	A	608	CQX	C28-C31-C34-C37
20	C	304	CDL	C12-C13-C14-C15
20	C	304	CDL	C84-C85-C86-C87
18	A	606	CQX	C28-C25-O22-C19
20	L	101	CDL	CA2-OA2-PA1-OA5
18	C	306	CQX	C34-C37-C40-C43
20	C	304	CDL	C19-C20-C21-C22
20	B	301	CDL	C1-CA2-OA2-PA1
18	C	305	CQX	C18-C19-O22-C25
14	A	601	HEA	CAD-CBD-CGD-O1D
24	G	101	PEK	C25-C26-C27-C28
18	A	606	CQX	C37-C40-C43-C46
14	A	602	HEA	CAA-CBA-CGA-O1A
19	A	607	PGV	O03-C19-C20-C21
20	B	301	CDL	C52-C51-CB5-OB6
18	A	609	CQX	C18-C19-O22-C25
20	B	301	CDL	OB5-CB3-CB4-OB6
20	C	304	CDL	C76-C77-C78-C79
14	A	602	HEA	CAA-CBA-CGA-O2A
18	C	306	CQX	C43-C46-C49-C52
14	A	601	HEA	CAD-CBD-CGD-O2D
20	B	301	CDL	C72-C71-CB7-OB8
20	L	101	CDL	C77-C78-C79-C80
19	A	607	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	C	301	CHD	C22-C23-C24-O26
20	B	301	CDL	C32-C31-CA7-OA8
14	A	602	HEA	C26-C15-C16-C17
20	L	101	CDL	C72-C73-C74-C75
20	L	101	CDL	C12-C13-C14-C15
20	C	304	CDL	C12-C11-CA5-OA6
20	L	101	CDL	C72-C71-CB7-OB8
20	C	304	CDL	C72-C71-CB7-OB8
20	L	101	CDL	C32-C31-CA7-OA8
18	B	303	CQX	O16-C18-C19-O22
22	C	301	CHD	C22-C23-C24-O25
20	C	304	CDL	C52-C51-CB5-OB6
18	A	608	CQX	C28-C25-O22-C19
18	A	609	CQX	C40-C43-C46-C49
14	A	601	HEA	CAA-CBA-CGA-O2A
14	A	601	HEA	CAA-CBA-CGA-O1A
18	A	606	CQX	O5-C6-O16-C18
20	L	101	CDL	C32-C31-CA7-OA9
20	L	101	CDL	C72-C71-CB7-OB9
20	B	301	CDL	C32-C31-CA7-OA9
20	C	304	CDL	C72-C71-CB7-OB9
20	C	304	CDL	C52-C51-CB5-OB7
19	C	303	PGV	C05-C04-O12-P
18	A	609	CQX	C1-C6-O16-C18
20	C	304	CDL	CB2-OB2-PB2-OB3
20	C	304	CDL	CB3-OB5-PB2-OB3
20	L	101	CDL	CA2-OA2-PA1-OA3
20	L	101	CDL	CA3-OA5-PA1-OA4
20	B	301	CDL	C74-C75-C76-C77
20	C	304	CDL	OA5-CA3-CA4-OA6
18	A	609	CQX	O5-C6-O16-C18

There are no ring outliers.

9 monomers are involved in 31 short contacts:

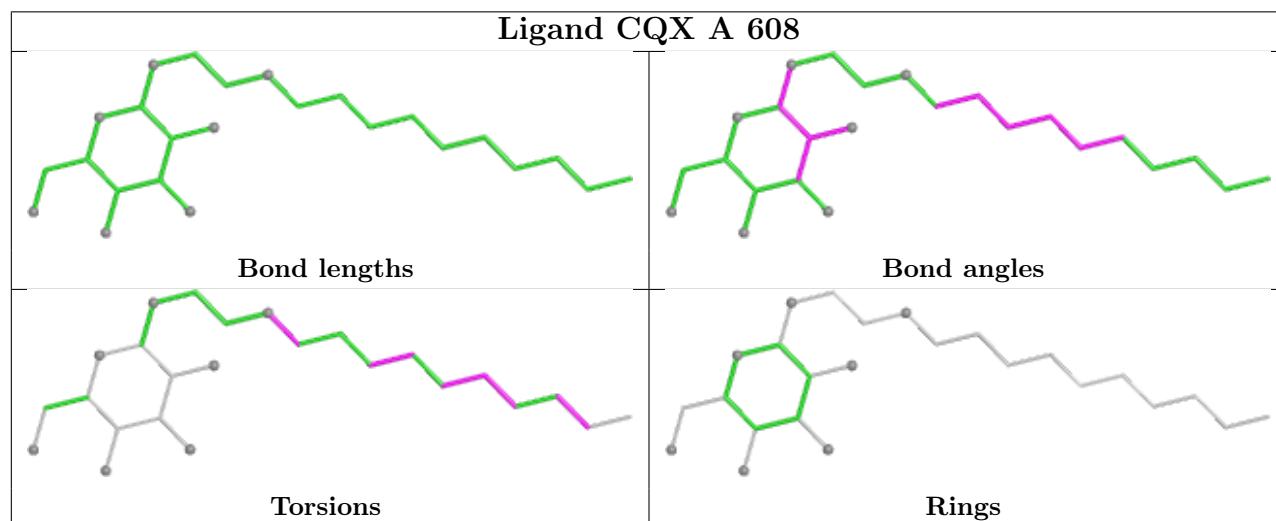
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	602	HEA	4	0
20	B	301	CDL	2	0
20	C	304	CDL	9	0
18	B	303	CQX	1	0
18	C	305	CQX	2	0
19	A	607	PGV	1	0

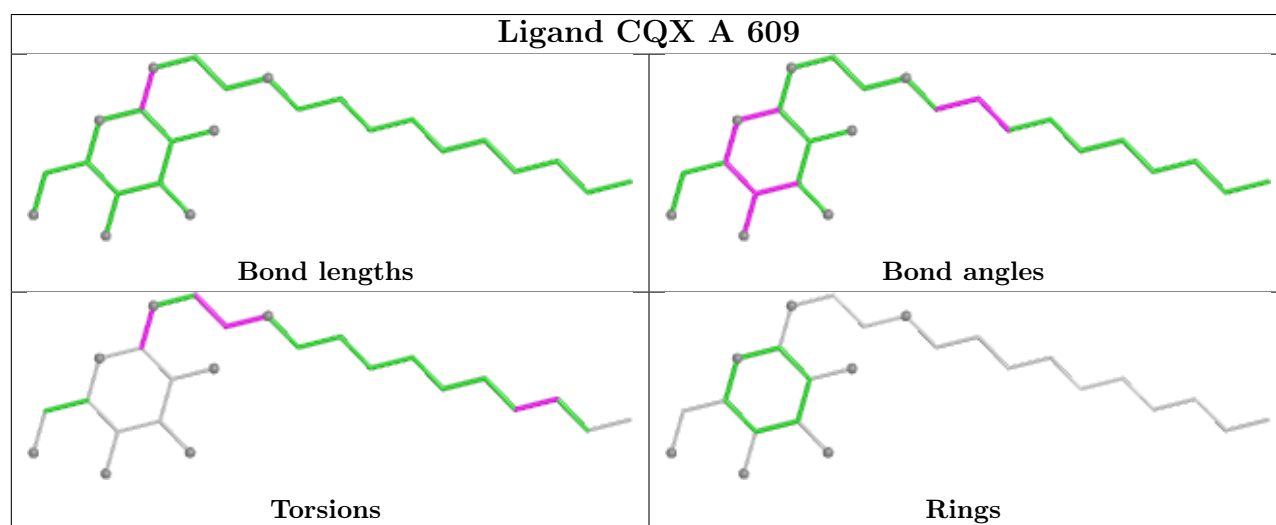
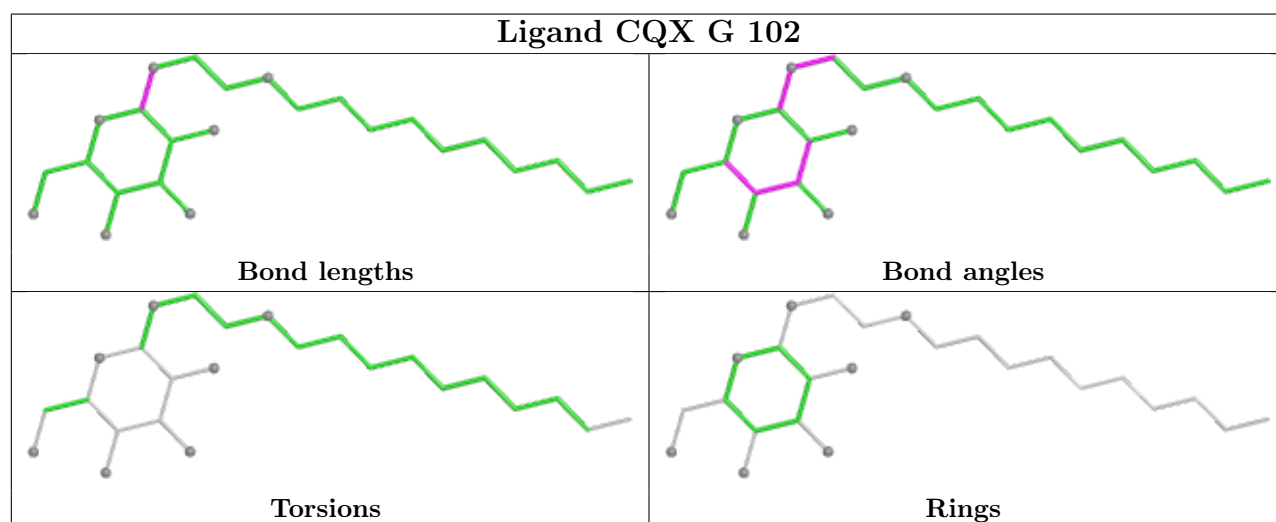
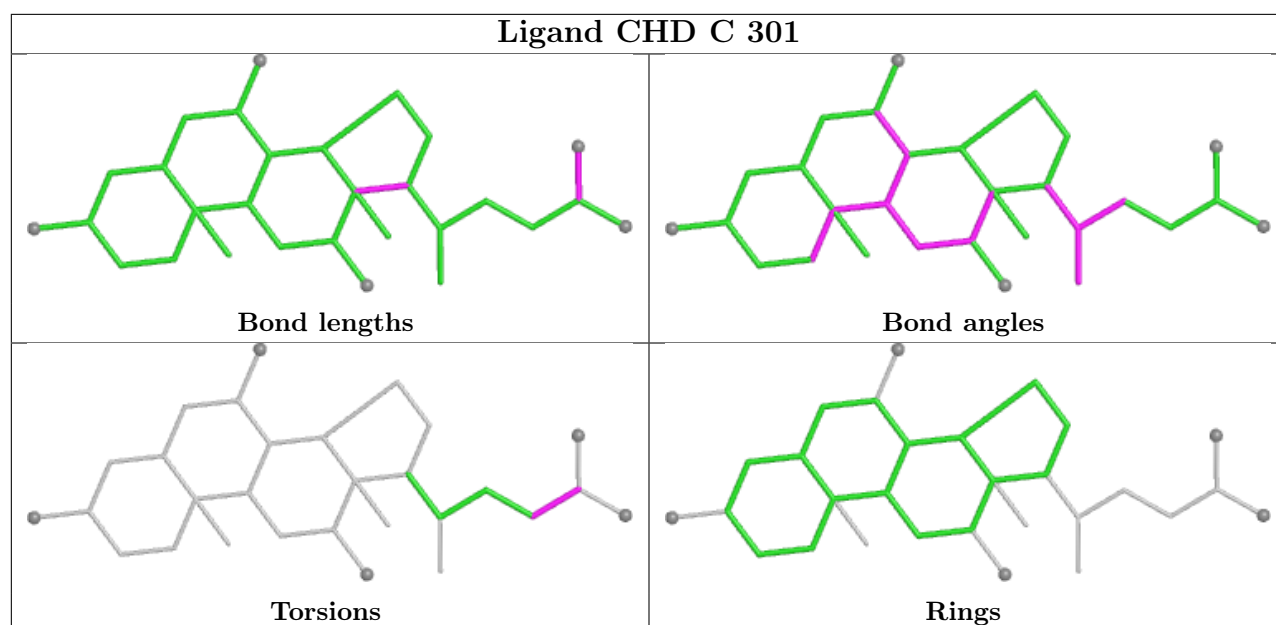
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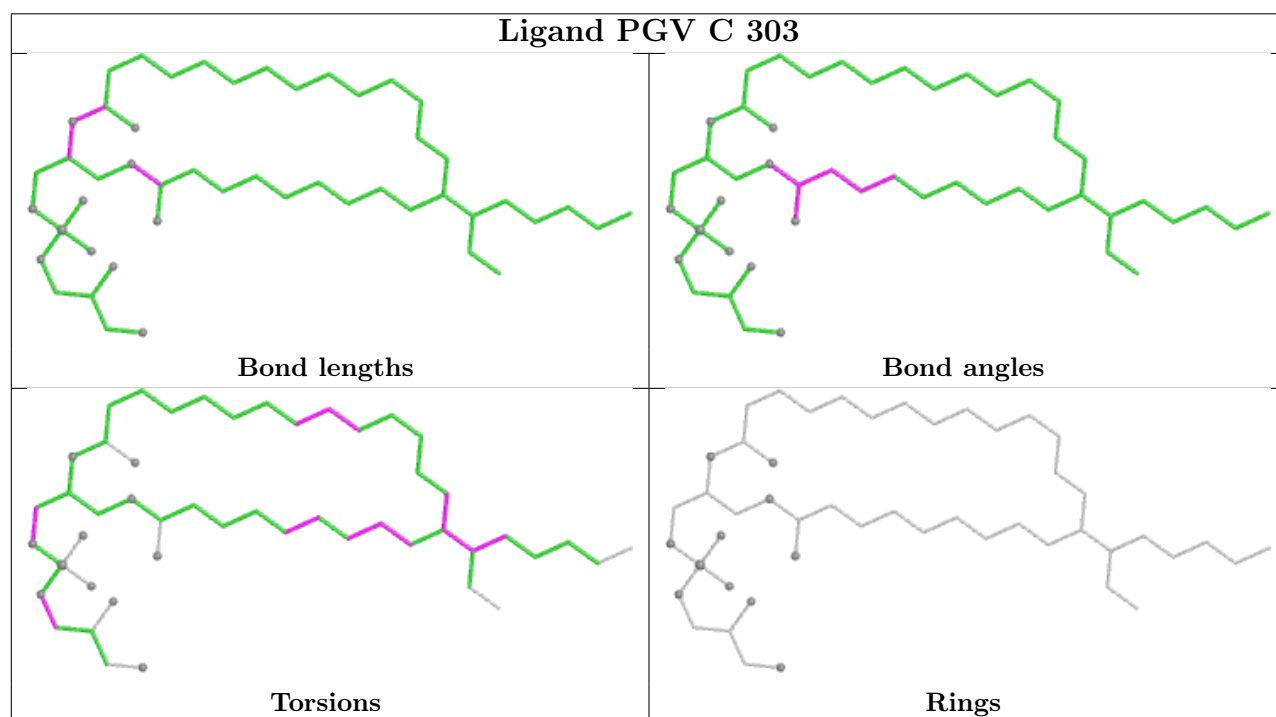
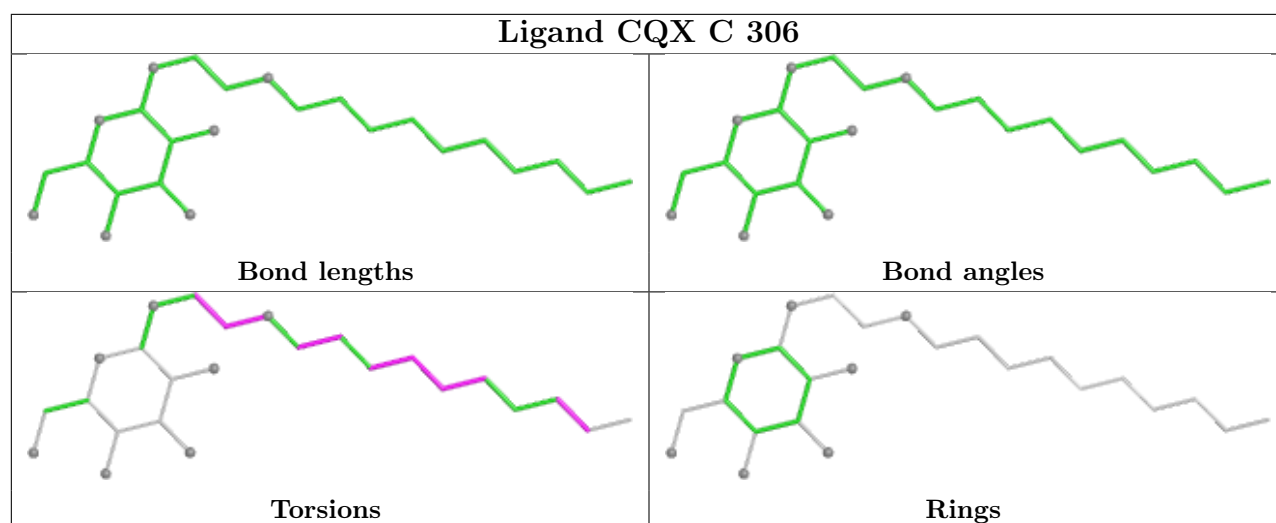
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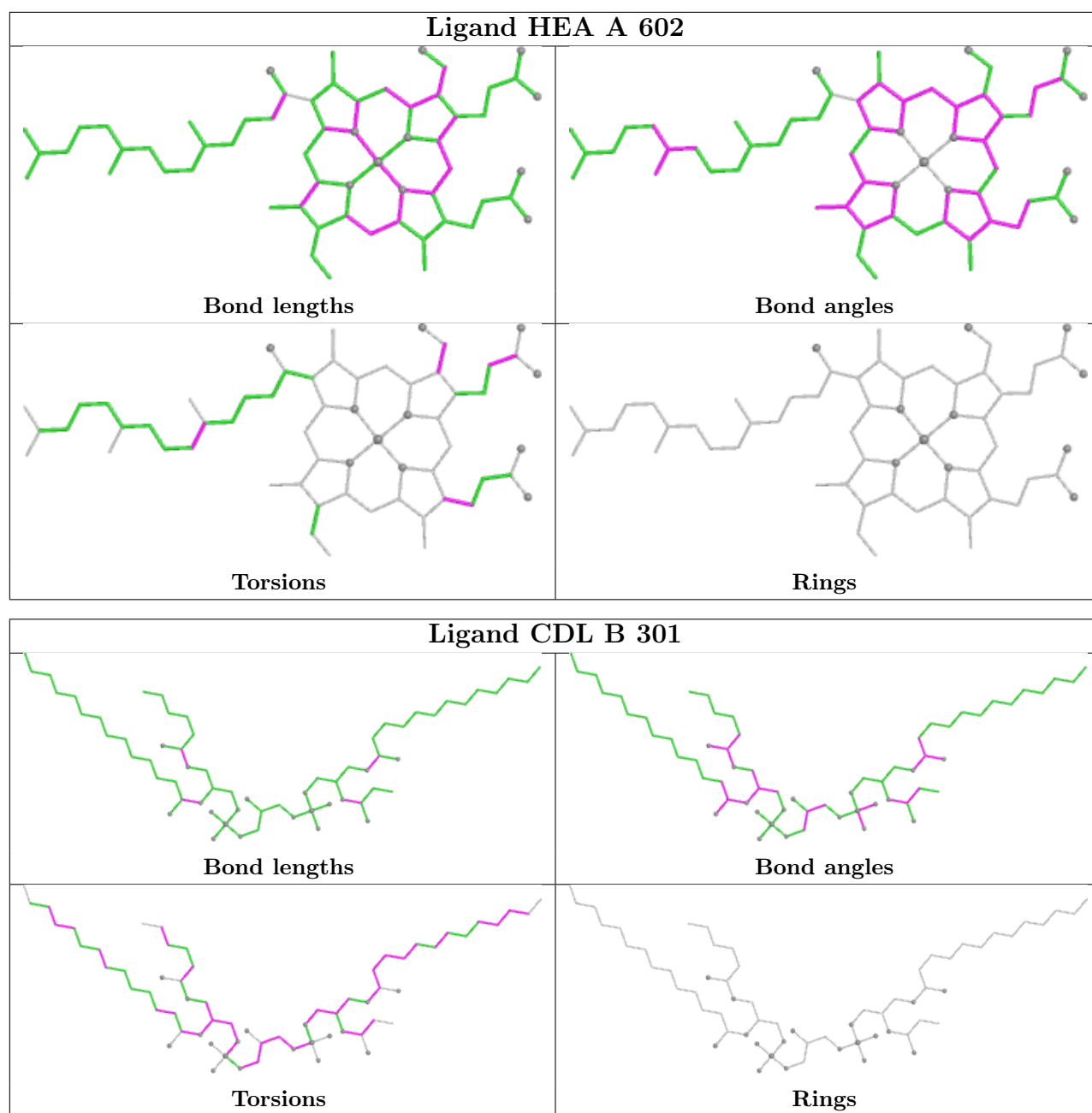
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	101	CDL	8	0
24	G	101	PEK	3	0
14	A	601	HEA	2	0

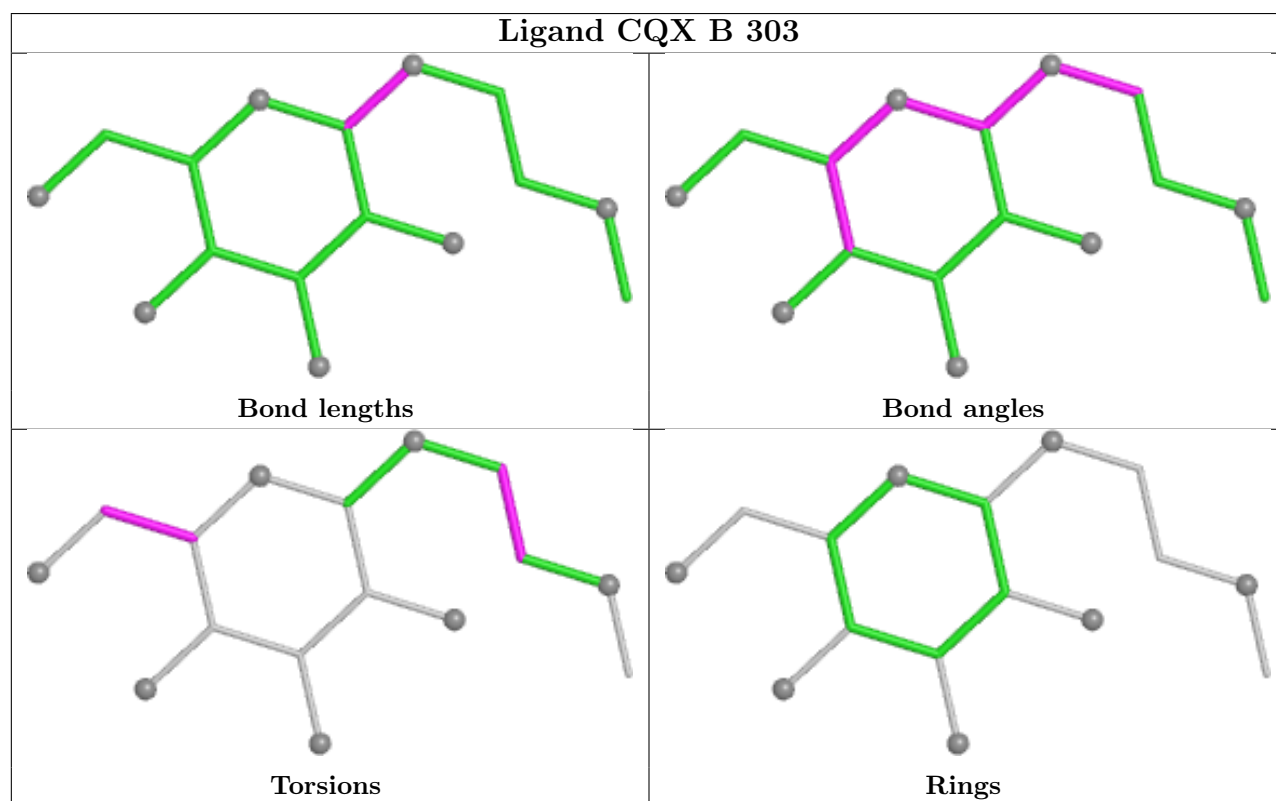
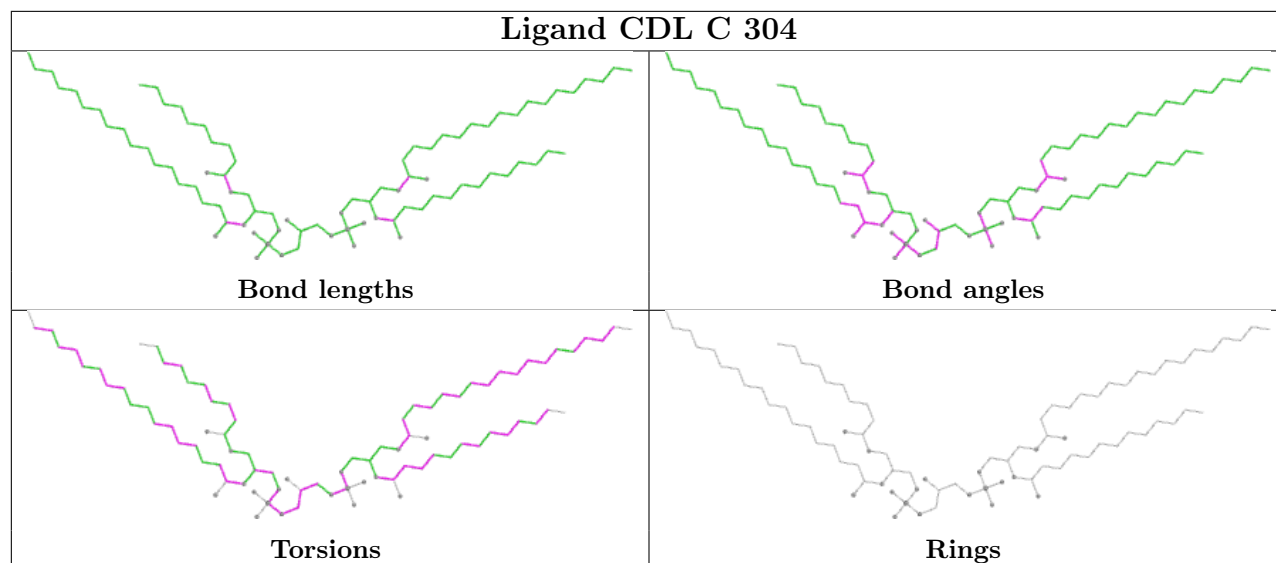
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

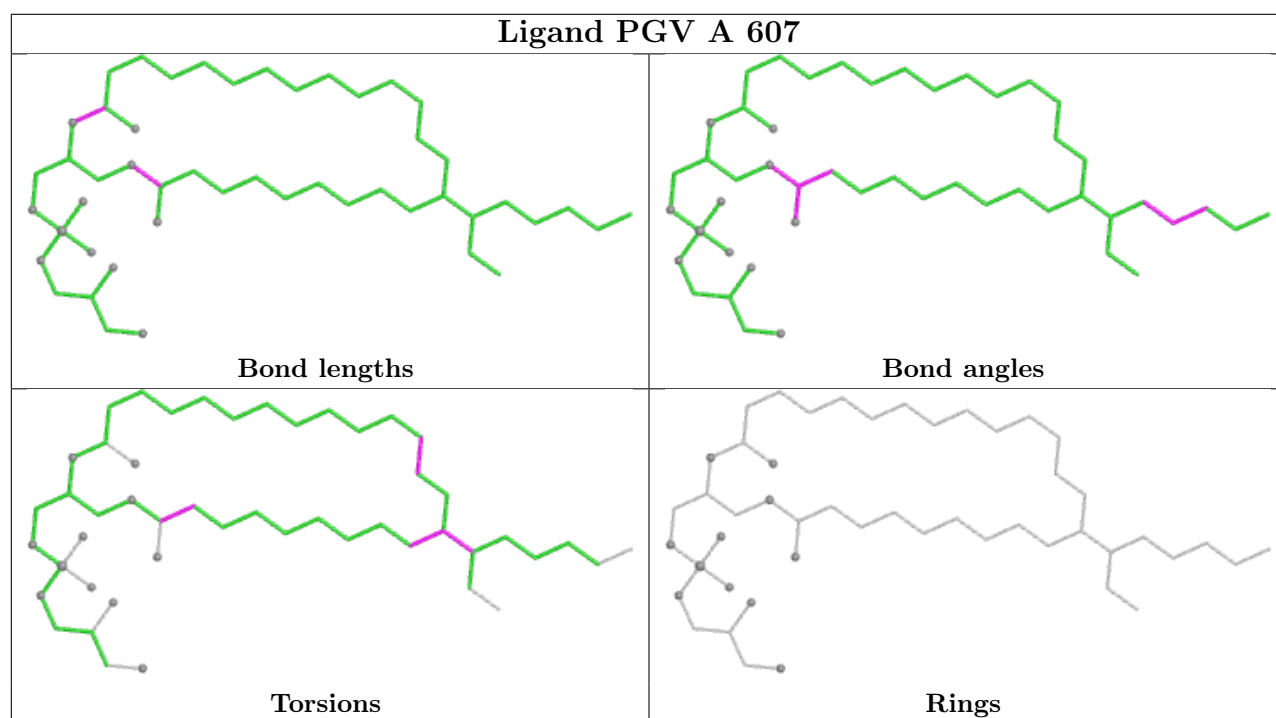
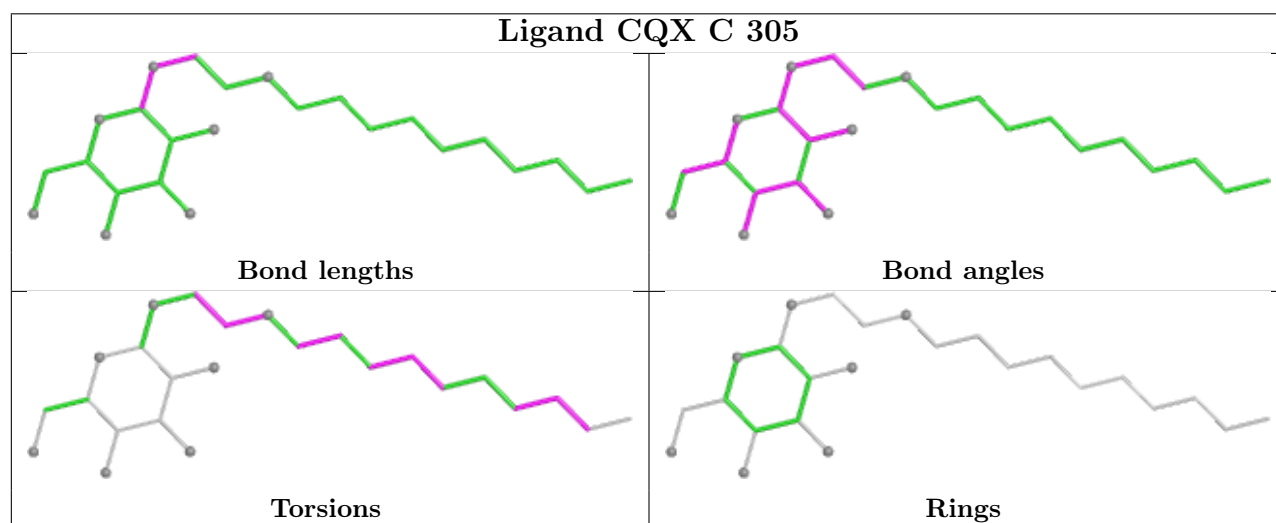
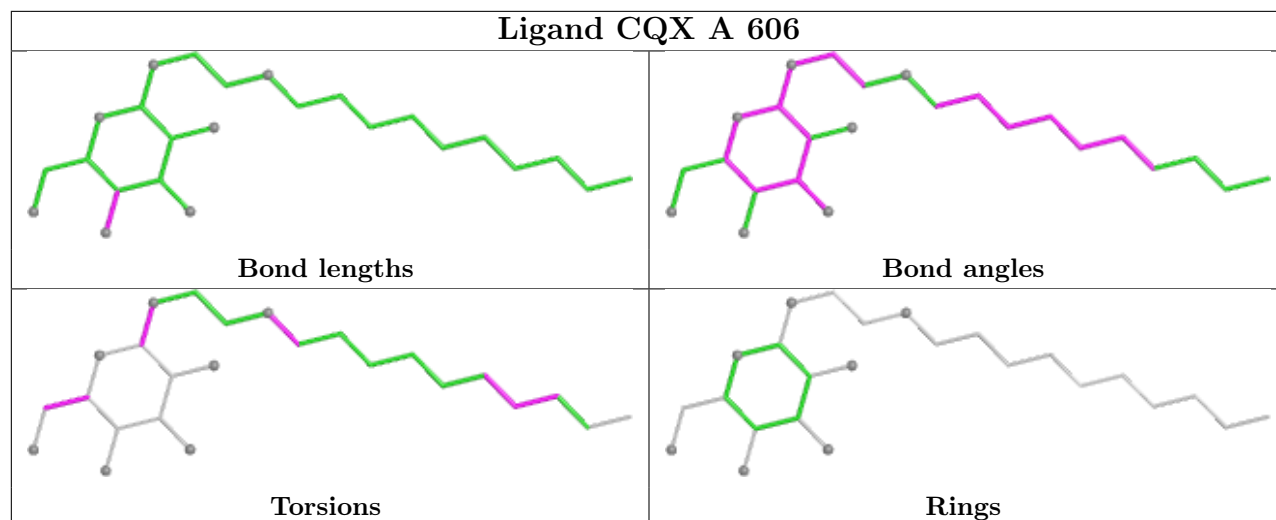


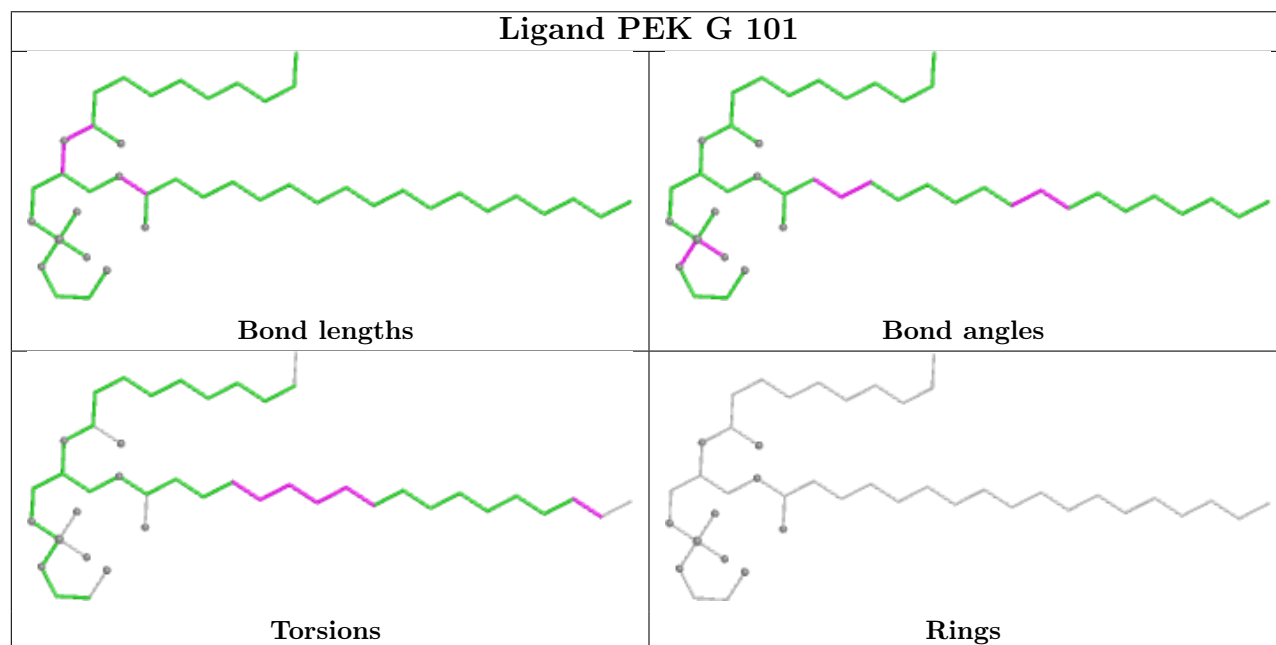
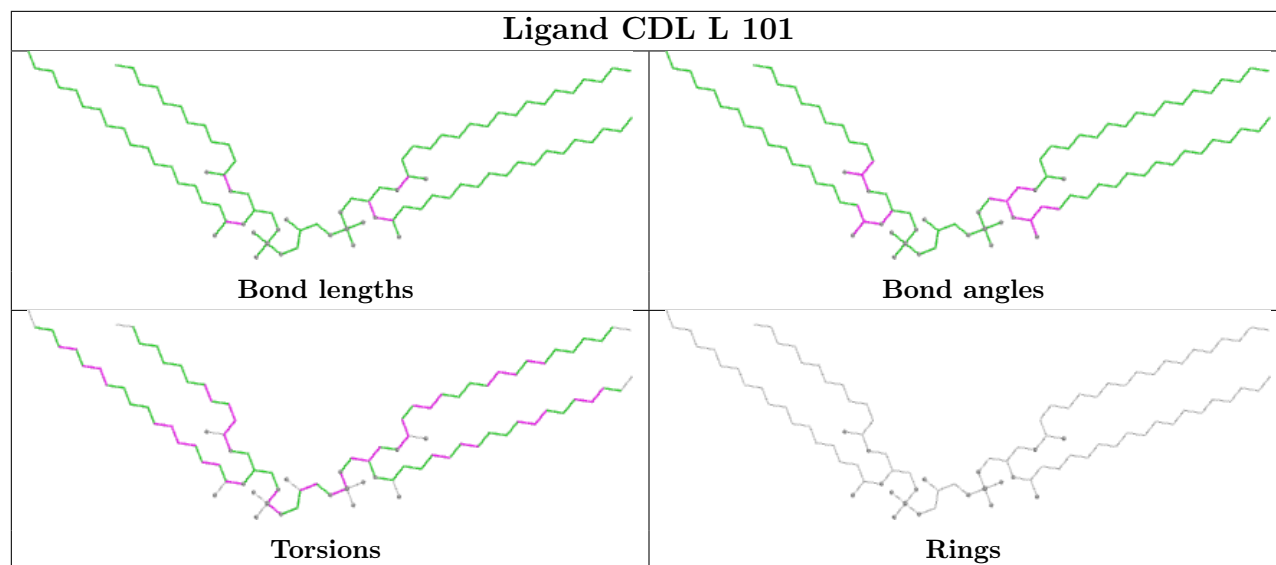


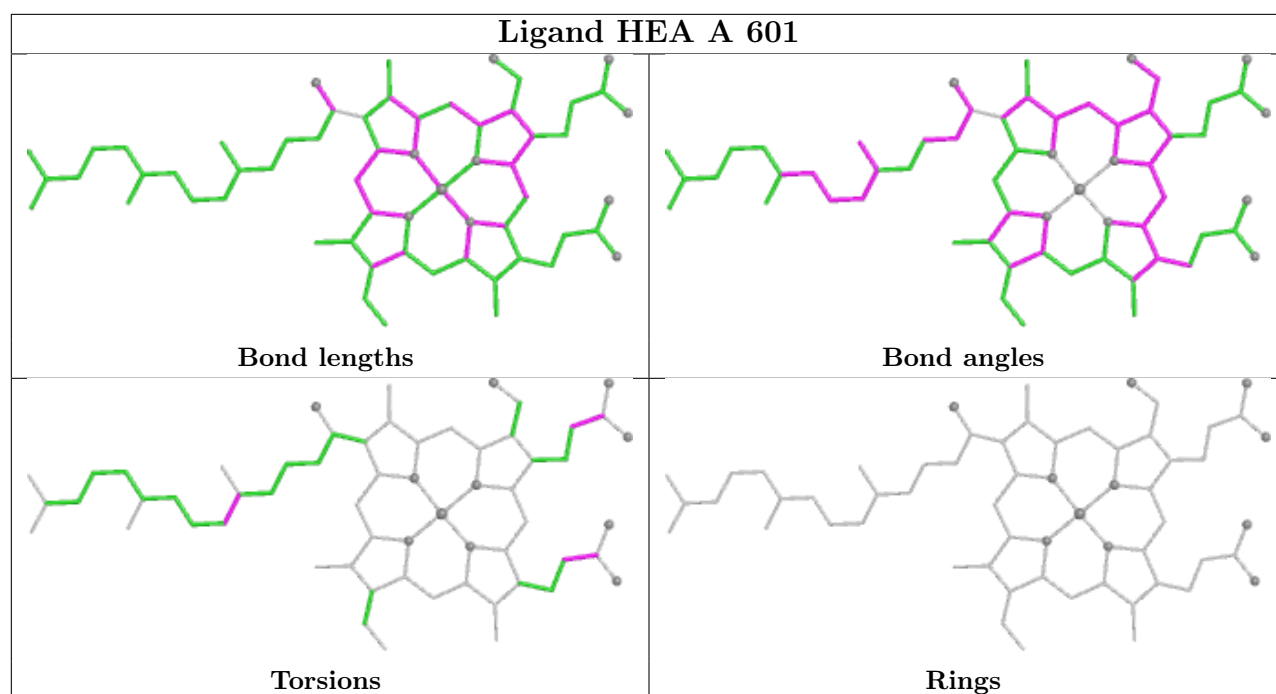












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.24	2 (0%) 88 91	28, 35, 47, 94	0
2	B	226/227 (99%)	0.09	4 (1%) 67 75	31, 42, 69, 97	0
3	C	254/261 (97%)	-0.02	2 (0%) 82 86	31, 40, 53, 82	0
4	D	136/147 (92%)	0.28	3 (2%) 62 69	41, 53, 76, 82	0
5	E	102/109 (93%)	0.28	1 (0%) 79 84	42, 55, 76, 89	0
6	F	91/98 (92%)	0.22	4 (4%) 39 45	38, 52, 75, 95	0
7	G	72/85 (84%)	0.43	3 (4%) 40 47	38, 48, 89, 105	0
8	H	75/85 (88%)	0.16	2 (2%) 56 62	37, 47, 77, 83	0
9	I	70/73 (95%)	0.32	2 (2%) 53 60	37, 50, 70, 74	0
10	J	55/59 (93%)	0.42	3 (5%) 30 36	43, 51, 76, 87	0
11	K	49/56 (87%)	0.48	2 (4%) 41 48	47, 55, 69, 82	0
12	L	44/47 (93%)	0.14	1 (2%) 61 68	37, 46, 63, 68	0
13	M	40/46 (86%)	0.53	2 (5%) 34 40	44, 50, 69, 77	0
All	All	1727/1807 (95%)	0.07	31 (1%) 67 75	28, 43, 70, 105	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	113	TYR	5.9
7	G	36	TRP	5.7
11	K	6	ALA	3.9
6	F	93	PRO	3.8
4	D	11	TYR	3.7
1	A	136	LEU	3.5
9	I	72	ALA	3.3
4	D	53	ILE	3.1
8	H	45	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
6	F	3	GLY	2.9
2	B	91	ASN	2.9
10	J	52	TRP	2.9
10	J	1	PHE	2.6
7	G	40	GLY	2.6
8	H	44	THR	2.6
3	C	37	PHE	2.6
10	J	55	PHE	2.6
7	G	38	HIS	2.5
12	L	3	TYR	2.5
13	M	32	TRP	2.5
5	E	108	LYS	2.5
4	D	35	ALA	2.3
2	B	82	ARG	2.3
6	F	54	ASN	2.3
1	A	113	LEU	2.3
13	M	16	ALA	2.2
2	B	58	ALA	2.2
3	C	91	VAL	2.1
6	F	48	LEU	2.1
11	K	26	VAL	2.0
9	I	5	ALA	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	0.20	50,69,103,115	0
2	FME	B	1	10/11	0.98	0.07	35,46,57,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

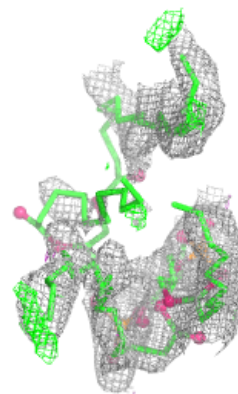
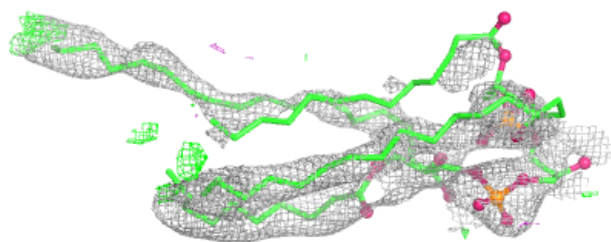
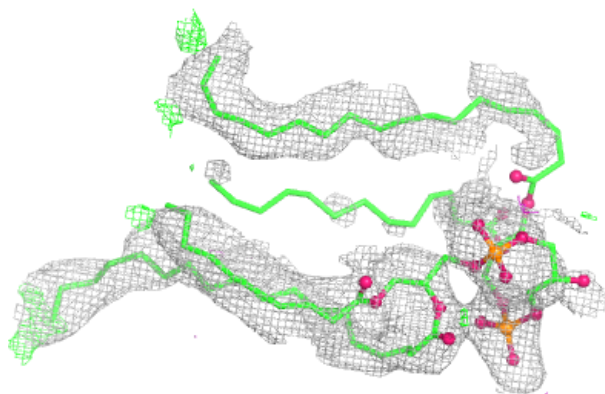
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	NA	C	302	1/1	0.76	0.50	42,42,42,42	1
20	CDL	C	304	87/100	0.90	0.16	50,96,139,153	0
18	CQX	B	303	16/25	0.91	0.11	53,74,86,92	0
20	CDL	L	101	94/100	0.92	0.14	48,83,125,140	0
20	CDL	B	301	64/100	0.93	0.15	54,89,130,135	0
18	CQX	A	609	25/25	0.94	0.12	55,70,87,108	0
18	CQX	C	306	25/25	0.96	0.11	43,63,101,108	0
18	CQX	G	102	25/25	0.96	0.08	46,54,61,67	0
18	CQX	A	606	25/25	0.96	0.10	41,55,68,81	0
18	CQX	A	608	25/25	0.96	0.11	49,65,75,92	0
18	CQX	C	305	25/25	0.96	0.10	44,54,91,100	0
22	CHD	C	301	29/29	0.96	0.07	31,37,42,57	0
19	PGV	C	303	51/51	0.97	0.09	35,45,107,132	0
24	PEK	G	101	43/53	0.97	0.08	34,46,65,86	0
16	MG	A	604	1/1	0.98	0.03	32,32,32,32	0
17	NA	A	605	1/1	0.98	0.12	40,40,40,40	0
19	PGV	A	607	51/51	0.98	0.08	30,43,75,83	0
14	HEA	A	602	60/60	0.99	0.05	25,30,38,49	0
14	HEA	A	601	60/60	0.99	0.06	26,33,51,54	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0
23	ZN	F	101	1/1	1.00	0.02	47,47,47,47	0
21	CUA	B	302	2/2	1.00	0.02	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.

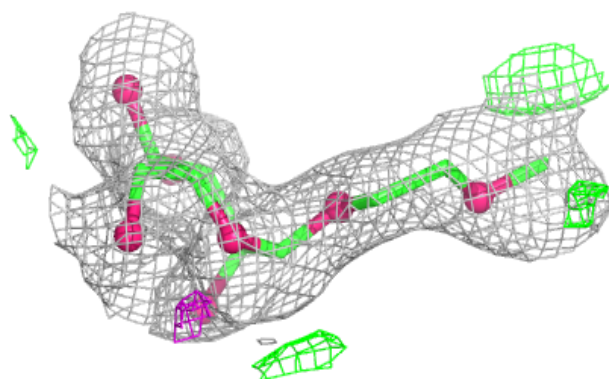
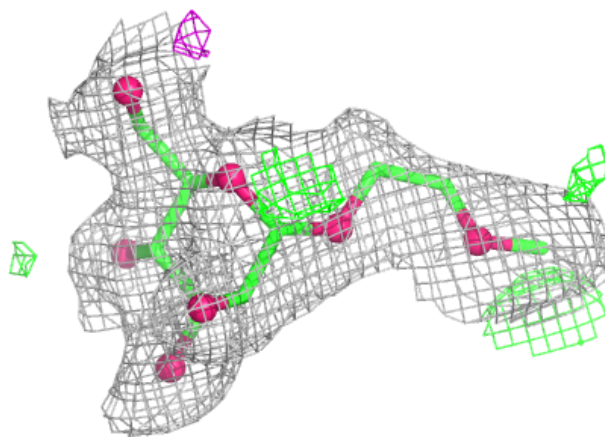
Electron density around CDL C 304:

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



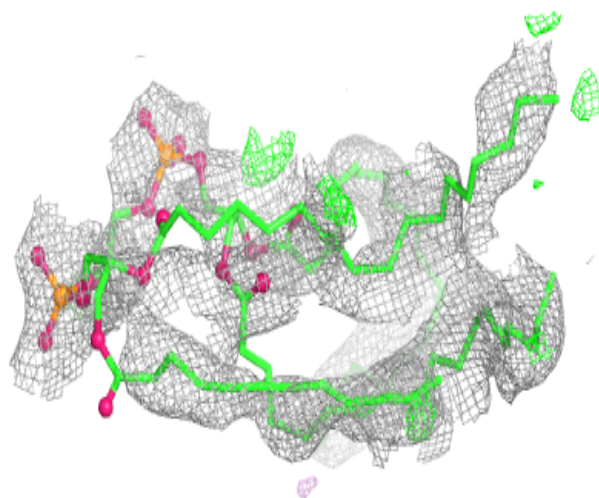
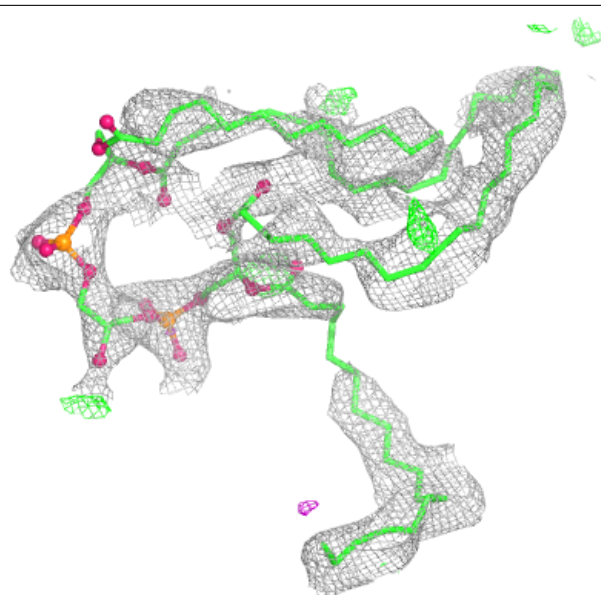
Electron density around CQX B 303:

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



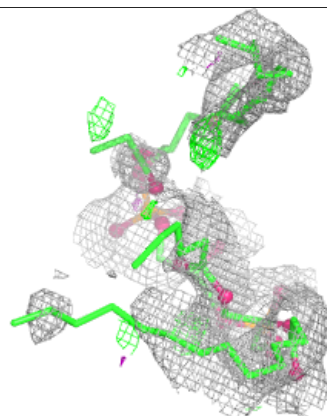
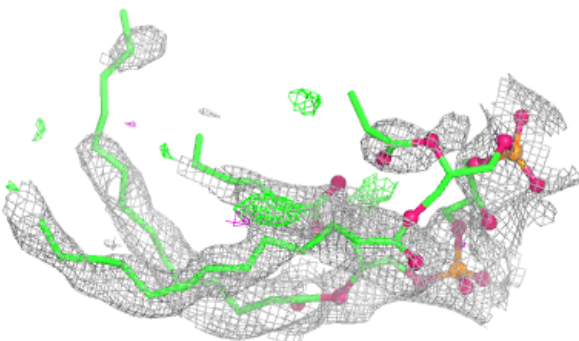
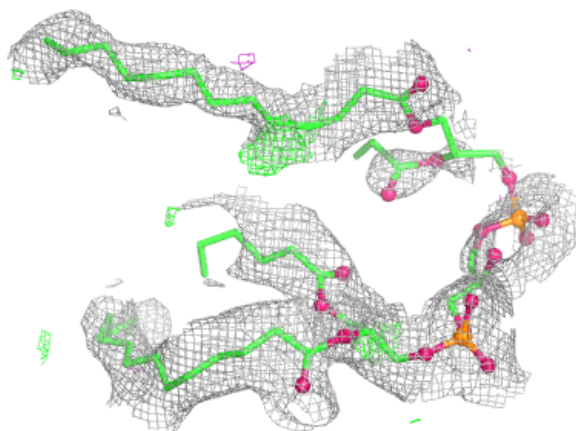
Electron density around CDL L 101:

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

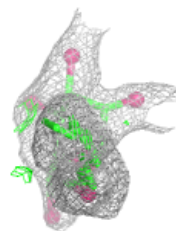
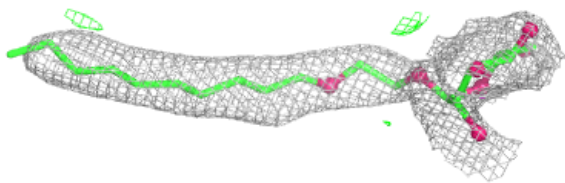
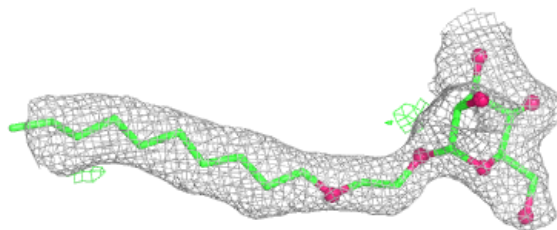


Electron density around CDL B 301:

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

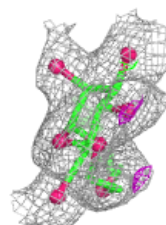
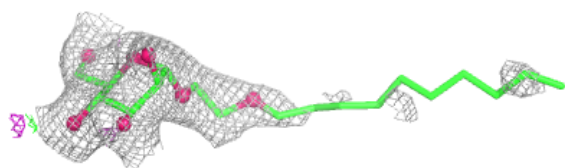
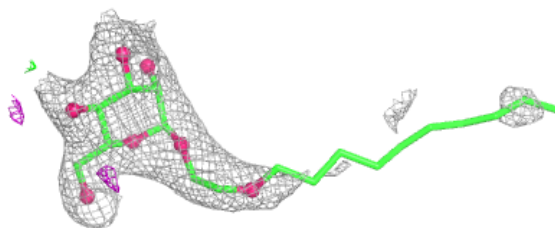
**Electron density around CQX A 609:**

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

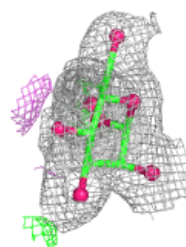
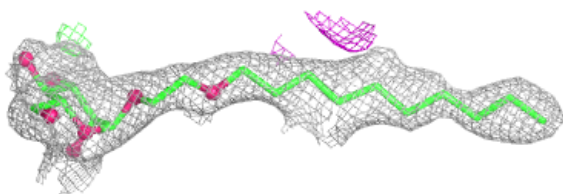
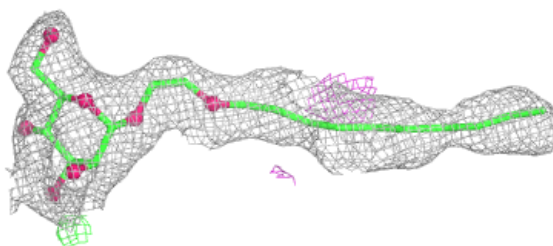


Electron density around CQX C 306:

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

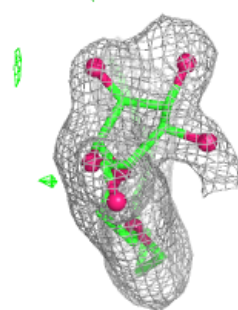
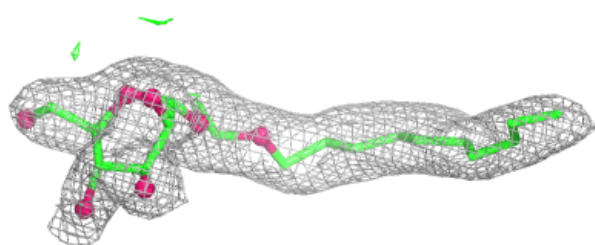
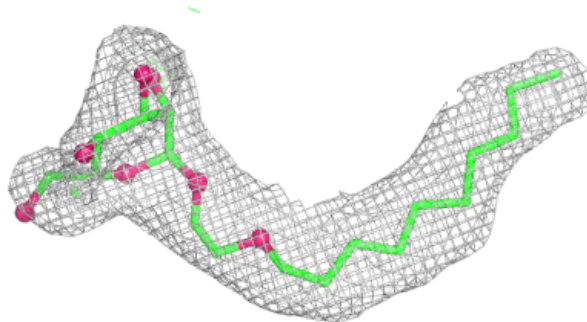
**Electron density around CQX G 102:**

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

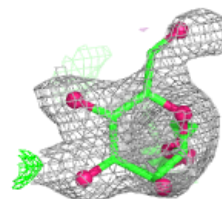
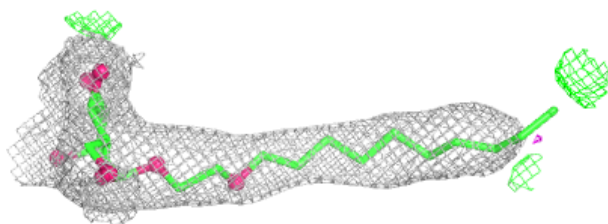
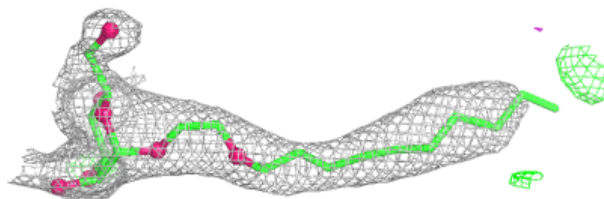


Electron density around CQX A 606:

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

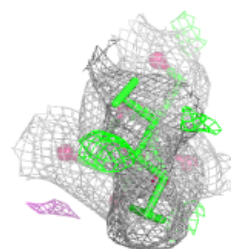
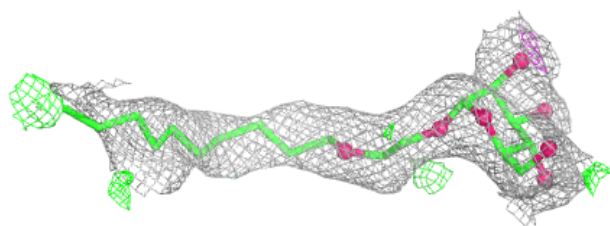
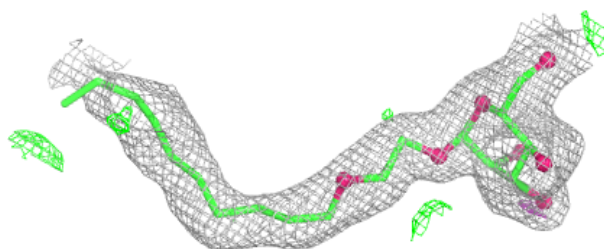
**Electron density around CQX A 608:**

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

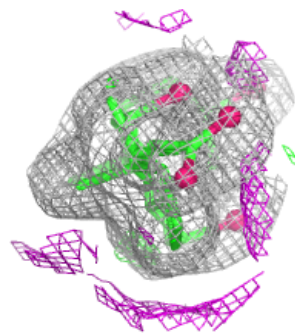
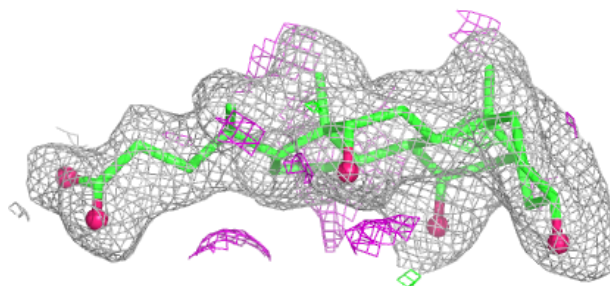
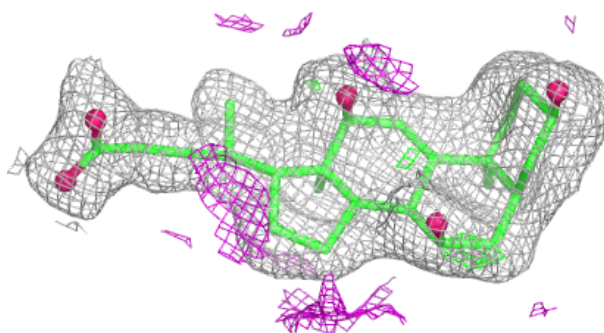


Electron density around CQX C 305:

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

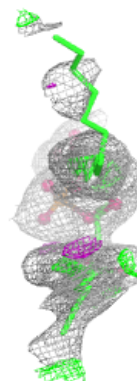
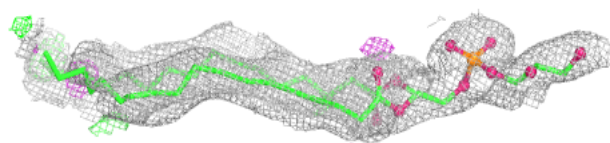
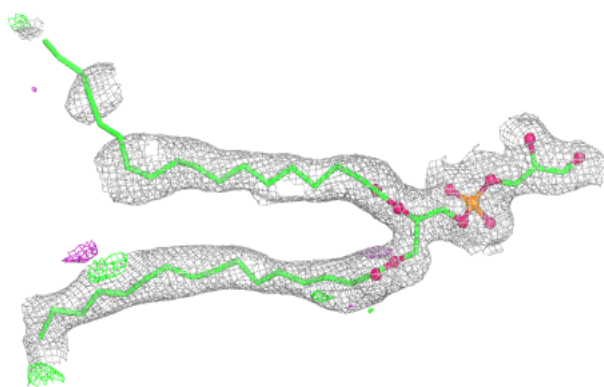
**Electron density around CHD C 301:**

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

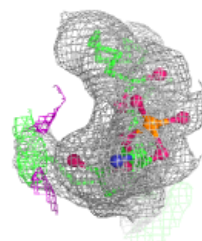
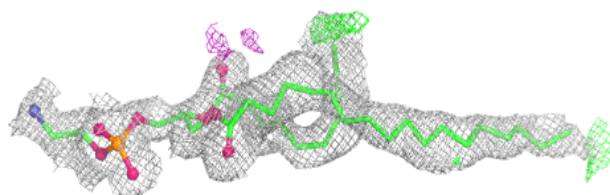
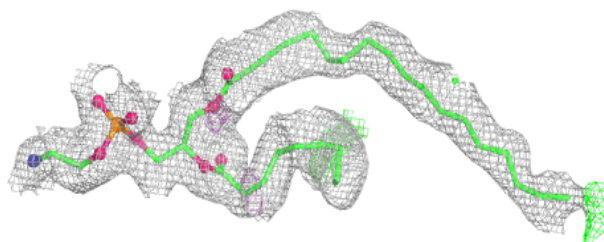


Electron density around PGV C 303:

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

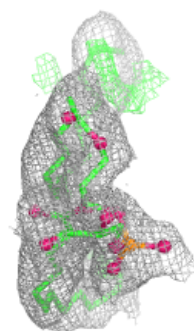
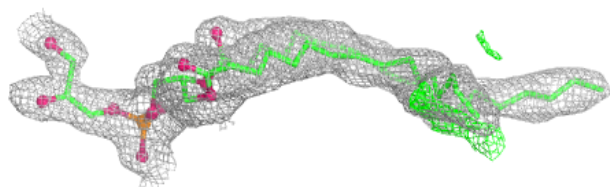
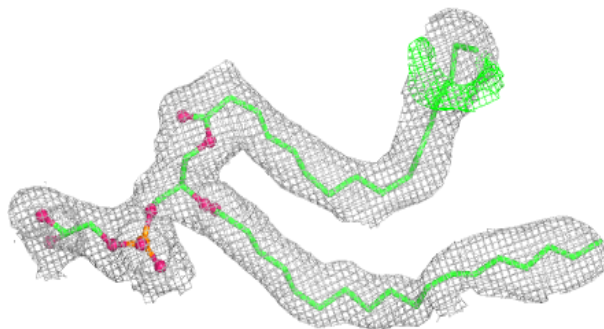
**Electron density around PEK G 101:**

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

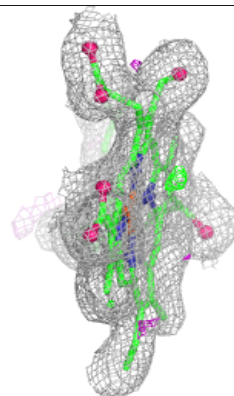
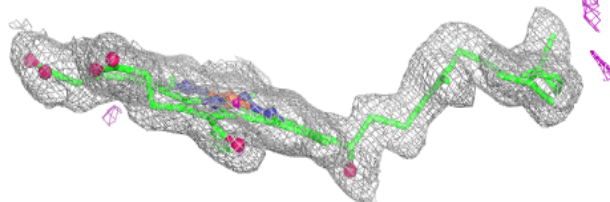
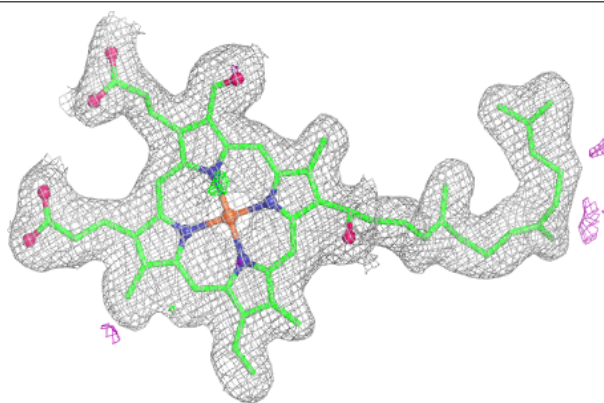


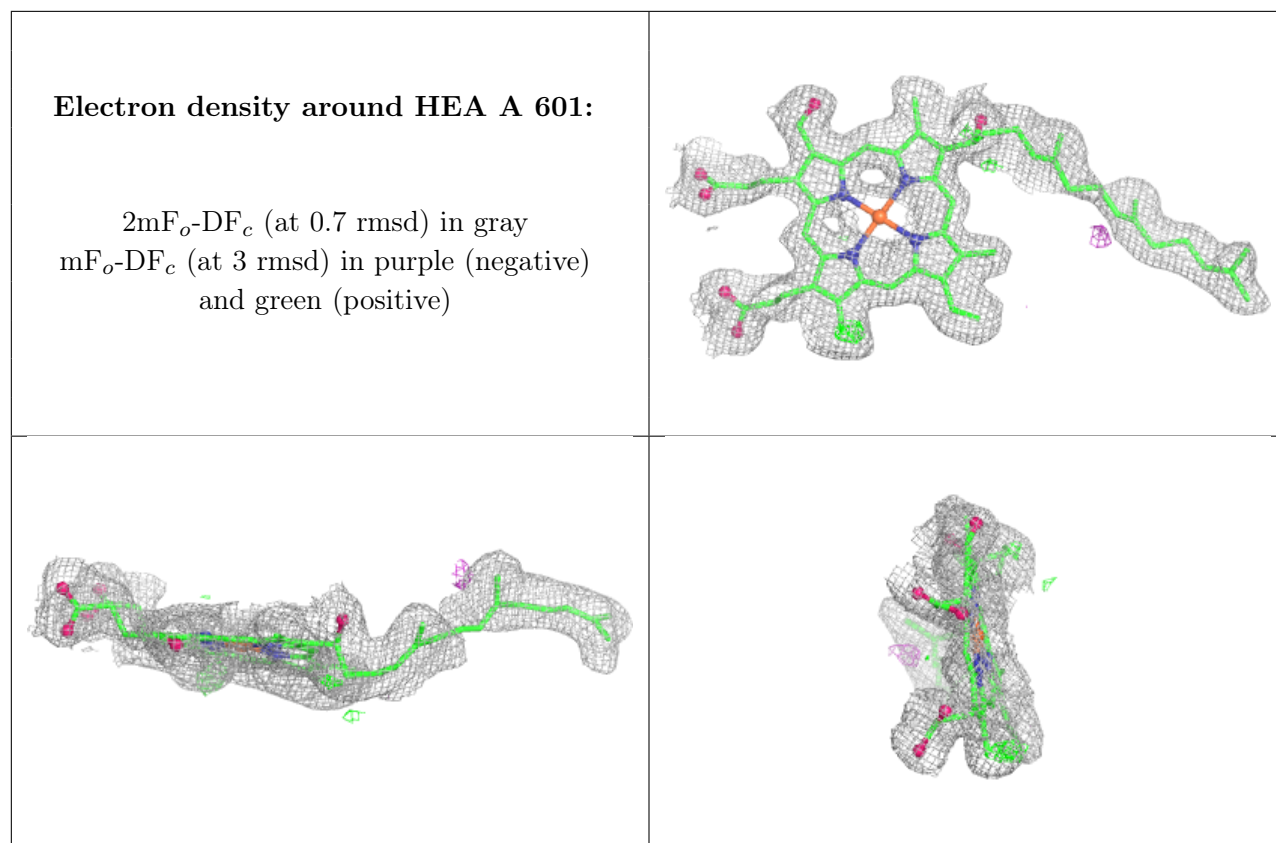
Electron density around PGV A 607:

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

**Electron density around HEA A 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.