



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:34 am BST

PDB ID : 6H7F
Title : Crystal structure of BauA, the Ferric preacinetobactin receptor from Acinetobacter baumannii in complex with Fe³⁺-Preacinetobactin-acinetobactin
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2018-07-31
Resolution : 2.26 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

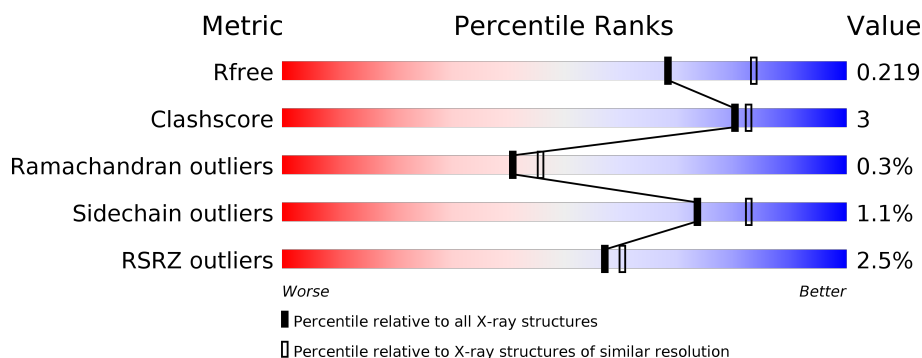
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	706	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>5% • 5%</div> </div> </div>
1	B	706	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>6% 5%</div> </div> </div>
1	C	706	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7% • 5%</div> </div> </div>

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
6	C8E	B	810	-	-	-	X
6	C8E	C	811	-	-	-	X
7	EDO	B	826	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17122 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 BauA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	13	0
			5229	3303	875	1041	10			
1	B	671	Total	C	N	O	S	0	9	0
			5199	3283	869	1037	10			
1	C	671	Total	C	N	O	S	0	15	0
			5251	3316	879	1046	10			

There are 9 discrepancies between the modelled and reference sequences:

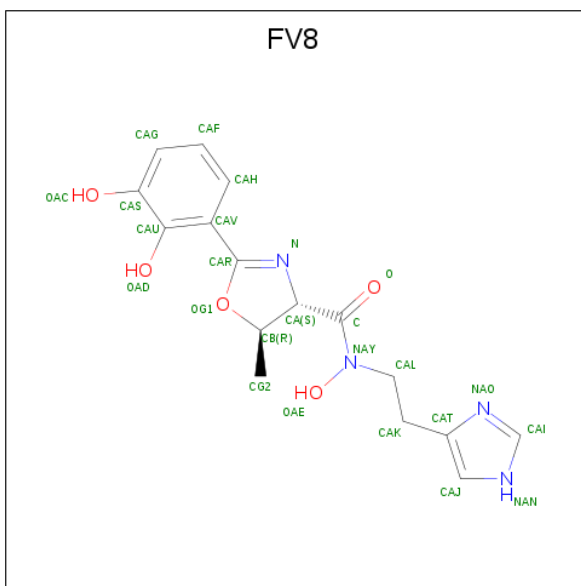
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q76HJ9
A	-1	ALA	-	expression tag	UNP Q76HJ9
A	0	MET	-	expression tag	UNP Q76HJ9
B	-2	GLY	-	expression tag	UNP Q76HJ9
B	-1	ALA	-	expression tag	UNP Q76HJ9
B	0	MET	-	expression tag	UNP Q76HJ9
C	-2	GLY	-	expression tag	UNP Q76HJ9
C	-1	ALA	-	expression tag	UNP Q76HJ9
C	0	MET	-	expression tag	UNP Q76HJ9

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

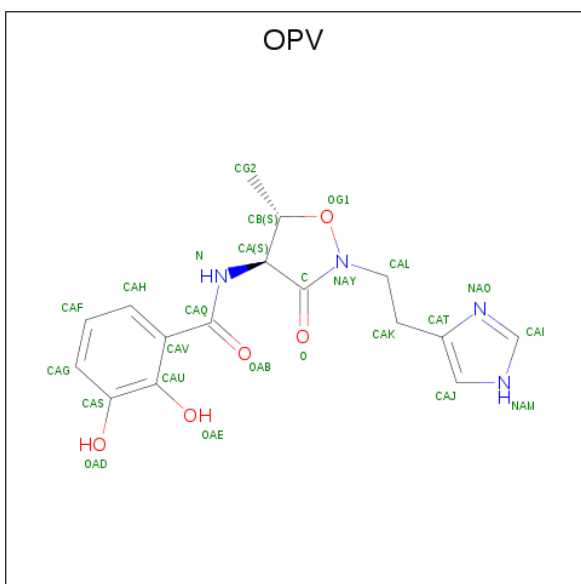
- Molecule 3 is (4 {S},5 {R})-2-[2,3-bis(oxidanyl)phenyl]- {N}-[2-(1 {H}-imidazol-4-yl)ethyl]-5-methyl- {N}-oxidanyl-4,5-dihydro-1,3-oxazole-4-carboxamide (three-letter code: FV8)

(formula: $C_{16}H_{18}N_4O_5$).



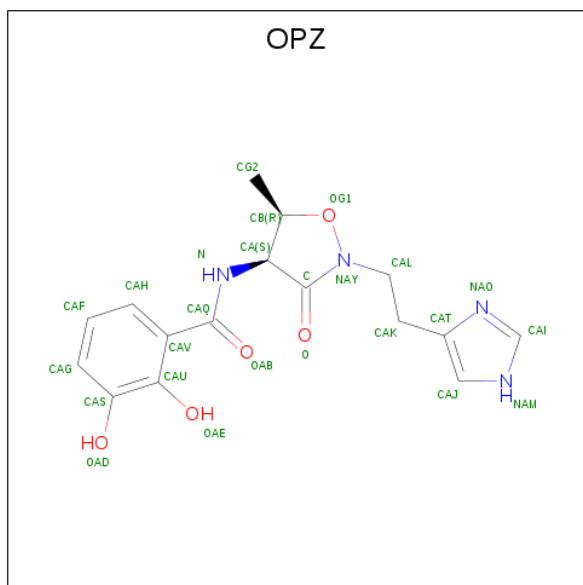
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	16	4	5		
3	B	1	Total	C	N	O	0	0
			25	16	4	5		
3	C	1	Total	C	N	O	0	0
			25	16	4	5		

- Molecule 4 is {N}-[(4 {S},5 {S})-2-[2-(1 {H}-imidazol-4-yl)ethyl]-5-methyl-3-oxidanylidene-1,2-oxazolidin-4-yl]-2,3-bis(oxidanyl)benzamide (three-letter code: OPV) (formula: $C_{16}H_{18}N_4O_5$).



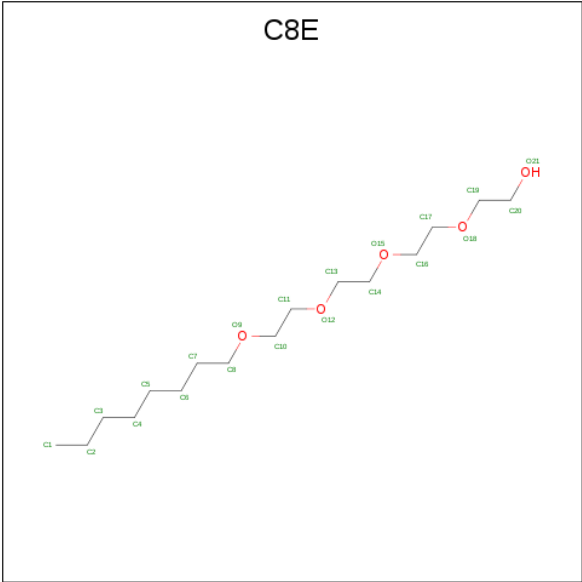
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			25	16	4	5		

- Molecule 5 is {N}-[(4 {S},5 {R})-2-[2-(1 {H}-imidazol-4-yl)ethyl]-5-methyl-3-oxidanyl idene-1,2-oxazolidin-4-yl]-2,3-bis(oxidanyl)benzamide (three-letter code: OPZ) (formula: C₁₆H₁₈N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			25	16	4	5		
5	B	1	Total	C	N	O	0	0
			25	16	4	5		
5	C	1	Total	C	N	O	0	0
			25	16	4	5		

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	10	1		
6	A	1	Total	C	O	0	0
			9	8	1		
6	A	1	Total	C		0	0
			8	8			
6	A	1	Total	C	O	0	0
			9	8	1		
6	A	1	Total	C		0	0
			7	7			
6	A	1	Total	C	O	0	0
			9	8	1		
6	B	1	Total	C	O	0	0
			16	11	5		
6	B	1	Total	C	O	0	0
			18	14	4		
6	B	1	Total	C	O	0	0
			13	11	2		
6	B	1	Total	C	O	0	0
			21	16	5		
6	B	1	Total	C	O	0	0
			9	8	1		
6	B	1	Total	C	O	0	0
			12	10	2		
6	B	1	Total	C		0	0
			8	8			
6	B	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 12 10 2	0	0
6	B	1	Total C O 12 10 2	0	0
6	B	1	Total C O 9 8 1	0	0
6	B	1	Total C 8 8	0	0
6	C	1	Total C O 16 11 5	0	0
6	C	1	Total C O 16 11 5	0	0
6	C	1	Total C O 14 10 4	0	0
6	C	1	Total C O 21 16 5	0	0
6	C	1	Total C O 15 12 3	0	0
6	C	1	Total C O 15 12 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 10 9 1	0	0
6	C	1	Total C 8 8	0	0
6	C	1	Total C 7 7	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

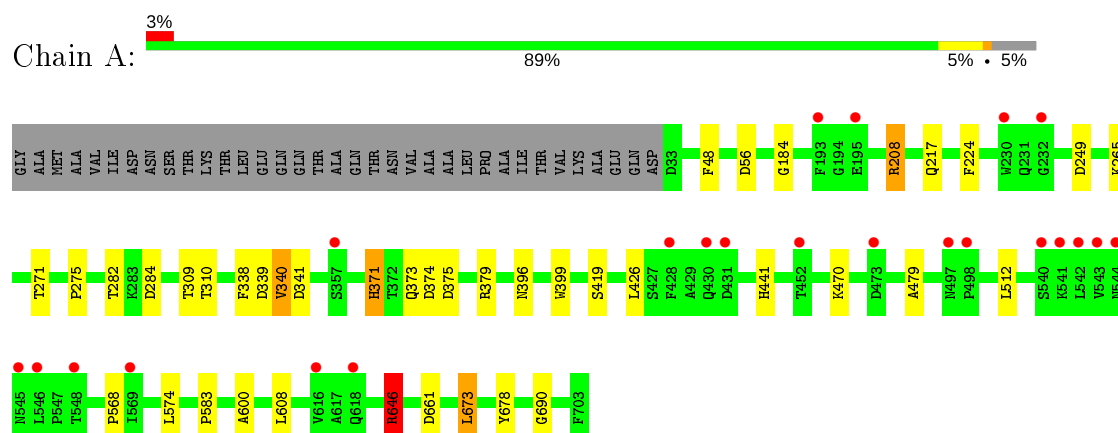
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	256	Total O 256 256	0	0
8	B	232	Total O 232 232	0	0
8	C	264	Total O 264 264	0	0

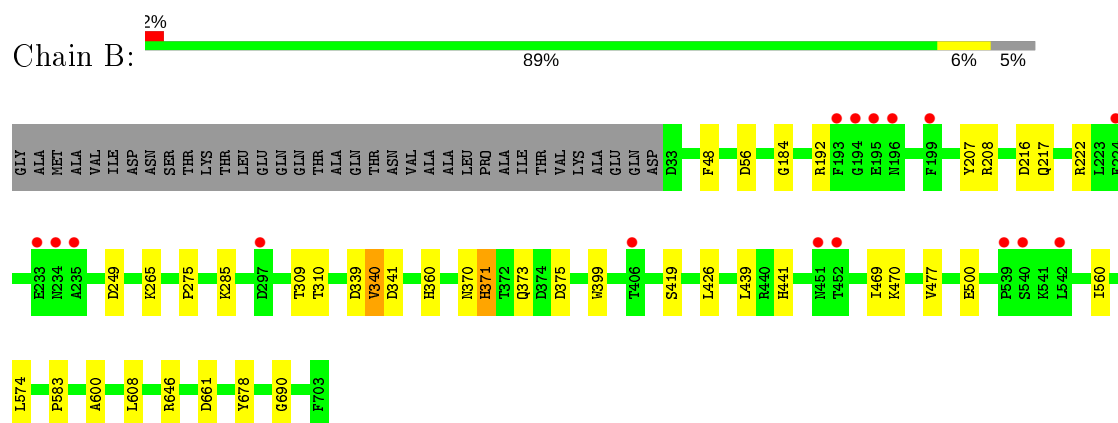
3 Residue-property plots [i](#)

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

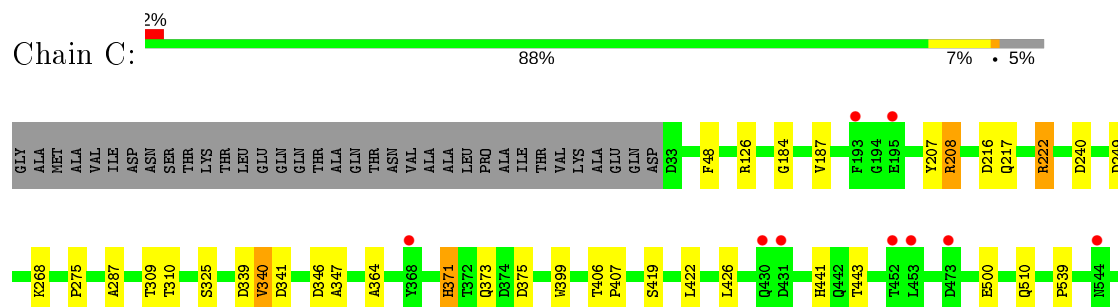
• Molecule 1: BauA

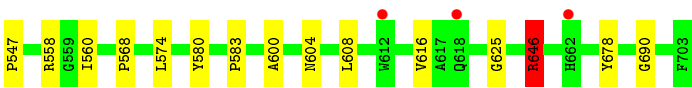


• Molecule 1: BauA



• Molecule 1: BauA





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.64Å 220.65Å 101.14Å 90.00° 99.09° 90.00°	Depositor
Resolution (Å)	49.93 – 2.26 49.93 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.93-2.26) 99.8 (49.93-2.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.186 , 0.217 0.192 , 0.219	Depositor DCC
R_{free} test set	8832 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17122	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: OPV, EDO, OPZ, C8E, FV8, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/5354	0.55	0/7287
1	B	0.43	0/5323	0.55	0/7243
1	C	0.45	0/5376	0.56	0/7315
All	All	0.44	0/16053	0.55	0/21845

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	3
1	B	0	1
1	C	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	646	ARG	Sidechain
1	B	192	ARG	Sidechain
1	C	126	ARG	Sidechain
1	C	208	ARG	Sidechain
1	C	222	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	646	ARG	Sidechain

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	5229	0	5045	23	0
1	B	5199	0	5014	25	0
1	C	5251	0	5062	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
4	A	25	0	0	2	0
5	A	25	0	0	1	0
5	B	25	0	0	1	0
5	C	25	0	0	0	0
6	A	53	0	95	1	0
6	B	159	0	266	3	0
6	C	129	0	192	8	0
7	A	52	0	78	1	0
7	B	52	0	78	1	0
7	C	68	0	102	4	0
8	A	256	0	0	1	0
8	B	232	0	0	1	0
8	C	264	0	0	2	0
All	All	17122	0	15932	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (87) 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)
5:B:803:OPZ:NAY	5:B:803:OPZ:OG1	1.57	1.09
4:A:803[A]:OPV:OG1	4:A:803[A]:OPV:NAY	1.56	1.08
1:C:574[A]:LEU:HD11	1:C:608:LEU:HD11	1.57	0.86
1:C:574[A]:LEU:CD1	1:C:608:LEU:HD11	2.19	0.73
1:B:207:TYR:HD1	1:B:222:ARG:HG2	1.58	0.69
1:A:271:THR:HG23	7:A:814:EDO:H22	1.76	0.67
1:B:309:THR:HG22	1:B:341:ASP:OD1	1.95	0.66
1:C:309:THR:HG22	1:C:341:ASP:OD1	1.95	0.66
1:C:207:TYR:HD1	1:C:222:ARG:HG2	1.60	0.66
1:C:268:LYS:HG2	7:C:828:EDO:H21	1.79	0.65
1:A:309:THR:HG22	1:A:341:ASP:OD1	1.98	0.64
1:C:625:GLY:HA3	6:C:809:C8E:H112	1.81	0.62
1:C:310:THR:HB	1:C:340:VAL:HG13	1.80	0.61
1:B:560:ILE:HD11	6:B:807:C8E:H31	1.83	0.61
1:B:310:THR:HB	1:B:340:VAL:HG13	1.84	0.60
1:A:310:THR:HB	1:A:340:VAL:HG13	1.83	0.59
1:A:479:ALA:HB2	1:A:512[B]:LEU:HD23	1.85	0.58
1:C:580:TYR:HD1	1:C:604:ASN:OD1	1.85	0.58
1:A:396:ASN:ND2	1:C:325:SER:O	2.36	0.58
5:A:804[B]:OPZ:N	5:A:804[B]:OPZ:OAE	2.38	0.57
1:B:56:ASP:OD1	1:B:470:LYS:HE2	2.06	0.56
1:C:558:ARG:HD2	8:C:947:HOH:O	2.06	0.55
1:B:439:LEU:C	1:B:439:LEU:HD12	2.28	0.54
1:C:568:PRO:HG3	1:C:574[B]:LEU:HD12	1.90	0.53
1:C:346:ASP:OD2	7:C:824:EDO:H21	2.09	0.53
1:A:568:PRO:HG3	1:A:574[B]:LEU:HD12	1.91	0.52
1:A:56:ASP:OD1	1:A:470:LYS:HE2	2.09	0.52
1:B:217:GLN:HA	1:B:249:ASP:O	2.10	0.52
1:A:217:GLN:HA	1:A:249:ASP:O	2.10	0.52
1:C:580:TYR:CE1	6:C:808:C8E:H42	2.46	0.51
1:B:574:LEU:HD11	1:B:608[A]:LEU:HD11	1.93	0.50
1:C:646:ARG:HD3	8:C:983:HOH:O	2.12	0.50
1:B:341:ASP:O	1:B:371:HIS:HA	2.12	0.50
1:B:500:GLU:HA	7:B:818:EDO:H21	1.94	0.50
1:C:539:PRO:HA	1:C:547:PRO:HB3	1.93	0.49
1:C:364:ALA:HB2	1:C:422[B]:LEU:HD23	1.94	0.49
1:B:678:TYR:CZ	1:B:690:GLY:HA3	2.48	0.49
1:C:187[A]:VAL:HG23	6:C:806:C8E:C6	2.43	0.48
1:A:673:LEU:C	1:A:673:LEU:HD12	2.33	0.48
1:C:616:VAL:HG23	1:C:616:VAL:O	2.13	0.48
1:C:678:TYR:CZ	1:C:690:GLY:HA3	2.49	0.48
1:C:510:GLN:HG3	6:C:804:C8E:C20	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLN:HG3	6:C:804:C8E:H201	1.96	0.48
1:B:285:LYS:HB3	6:B:814:C8E:H71	1.94	0.47
1:C:419:SER:HA	1:C:441:HIS:O	2.14	0.47
1:B:419:SER:HA	1:B:441:HIS:O	2.14	0.47
1:C:275:PRO:HA	1:C:399:TRP:CD2	2.49	0.47
1:A:341:ASP:O	1:A:371:HIS:HA	2.15	0.47
1:C:500:GLU:HA	7:C:818:EDO:H21	1.97	0.47
1:A:275:PRO:HA	1:A:399:TRP:CD2	2.50	0.47
1:A:574[A]:LEU:HD11	1:A:608:LEU:HD11	1.96	0.46
1:C:604:ASN:HB3	6:C:808:C8E:H82	1.97	0.46
1:C:217:GLN:HA	1:C:249:ASP:O	2.14	0.46
1:A:419:SER:HA	1:A:441:HIS:O	2.16	0.46
1:B:574:LEU:CD1	1:B:608[A]:LEU:HD11	2.46	0.46
1:C:426:LEU:HD12	1:C:426:LEU:N	2.32	0.45
1:A:678:TYR:CZ	1:A:690:GLY:HA3	2.51	0.45
1:B:370:ASN:ND2	8:B:907:HOH:O	2.45	0.45
1:C:443:THR:HG22	7:C:820:EDO:H12	1.99	0.44
1:A:646:ARG:HD3	8:A:979:HOH:O	2.16	0.44
4:A:803[A]:OPV:CAJ	4:A:803[A]:OPV:O	2.66	0.44
1:B:339:ASP:O	1:B:373:GLN:HA	2.18	0.43
1:B:275:PRO:HA	1:B:399:TRP:CD2	2.53	0.43
1:B:184:GLY:HA3	1:B:208:ARG:HB3	2.00	0.43
1:A:338:PHE:HA	1:A:374:ASP:O	2.19	0.42
1:B:207:TYR:CD1	1:B:222:ARG:HG2	2.46	0.42
1:A:426:LEU:HD12	1:A:426:LEU:N	2.34	0.42
1:C:406:THR:N	1:C:407:PRO:CD	2.82	0.42
1:C:347:ALA:HB1	6:C:807:C8E:H101	2.01	0.42
1:B:426:LEU:N	1:B:426:LEU:HD12	2.35	0.42
1:A:339:ASP:O	1:A:373:GLN:HA	2.19	0.42
1:A:282[A]:THR:HG22	1:A:284:ASP:OD2	2.19	0.41
1:C:184:GLY:HA3	1:C:208:ARG:HB3	2.02	0.41
1:C:207:TYR:CD1	1:C:222:ARG:HG2	2.47	0.41
1:C:339:ASP:O	1:C:373:GLN:HA	2.21	0.41
1:A:265:LYS:NZ	1:B:216:ASP:OD2	2.39	0.41
1:B:469:ILE:HB	1:B:477[A]:VAL:HG13	2.03	0.41
1:C:560:ILE:HD11	6:C:804:C8E:H132	2.03	0.41
1:C:580:TYR:CD1	1:C:604:ASN:OD1	2.71	0.41
1:A:184:GLY:HA3	1:A:208:ARG:HB3	2.02	0.41
1:A:574[A]:LEU:CD1	1:A:608:LEU:HD11	2.51	0.41
1:B:265:LYS:HE3	1:C:216:ASP:OD2	2.21	0.41
1:A:224:PHE:CD2	6:A:805:C8E:H11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HH11	6:B:809:C8E:H12	1.86	0.41
1:C:240:ASP:O	1:C:287:ALA:HA	2.21	0.40
1:C:341:ASP:O	1:C:371:HIS:HA	2.21	0.40
1:B:360:HIS:CE1	1:B:426:LEU:HG	2.56	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	682/706 (97%)	661 (97%)	19 (3%)	2 (0%)	41	46
1	B	678/706 (96%)	657 (97%)	19 (3%)	2 (0%)	41	46
1	C	684/706 (97%)	663 (97%)	19 (3%)	2 (0%)	41	46
All	All	2044/2118 (96%)	1981 (97%)	57 (3%)	6 (0%)	41	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ALA
1	B	600	ALA
1	C	600	ALA
1	A	583	PRO
1	B	583	PRO
1	C	583	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/577 (98%)	556 (99%)	7 (1%)	71	80
1	B	559/577 (97%)	553 (99%)	6 (1%)	73	82
1	C	565/577 (98%)	560 (99%)	5 (1%)	78	86
All	All	1687/1731 (98%)	1669 (99%)	18 (1%)	73	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	340	VAL
1	A	371	HIS
1	A	375	ASP
1	A	646	ARG
1	A	661	ASP
1	A	673	LEU
1	B	48	PHE
1	B	340	VAL
1	B	371	HIS
1	B	375	ASP
1	B	646	ARG
1	B	661	ASP
1	C	48	PHE
1	C	340	VAL
1	C	371	HIS
1	C	375	ASP
1	C	646	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	C	234	ASN
1	C	361	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 81 ligands modelled in this entry, 3 are monoatomic - leaving 78 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	$\# Z > 2$
7	EDO	C	826	-	3,3,3	0.44	0	2,2,2	0.57	0
7	EDO	C	819	-	3,3,3	0.29	0	2,2,2	0.83	0
6	C8E	B	813	-	11,11,20	0.53	0	10,10,19	0.32	0
3	FV8	A	802	2	22,27,27	2.37	8 (36%)	27,38,38	2.33	5 (18%)
7	EDO	B	819	-	3,3,3	0.38	0	2,2,2	0.52	0
6	C8E	B	804	-	15,15,20	0.52	0	14,14,19	0.26	0
7	EDO	B	818	-	3,3,3	0.32	0	2,2,2	0.93	0
7	EDO	C	814	-	3,3,3	0.55	0	2,2,2	0.24	0
7	EDO	C	815	-	3,3,3	0.42	0	2,2,2	0.13	0
6	C8E	A	807	-	7,7,20	0.44	0	6,6,19	0.37	0
7	EDO	B	825	-	3,3,3	0.45	0	2,2,2	0.35	0
6	C8E	B	805	-	17,17,20	0.69	0	16,16,19	0.43	0
6	C8E	C	806	-	13,13,20	0.62	0	12,12,19	0.29	0
6	C8E	B	811	-	20,20,20	0.64	0	19,19,19	0.28	0
6	C8E	B	806	-	12,12,20	0.49	0	11,11,19	0.33	0
6	C8E	B	808	-	8,8,20	0.32	0	7,7,19	0.41	0
7	EDO	C	818	-	3,3,3	0.32	0	2,2,2	0.68	0
7	EDO	A	821	-	3,3,3	0.43	0	2,2,2	0.44	0
7	EDO	C	829	-	3,3,3	0.43	0	2,2,2	0.43	0
7	EDO	C	822	-	3,3,3	0.50	0	2,2,2	0.46	0
3	FV8	B	802	2	22,27,27	4.19	3 (13%)	27,38,38	2.32	8 (29%)
7	EDO	C	828	-	3,3,3	0.52	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	C8E	B	809	-	11,11,20	0.47	0	10,10,19	0.39	0
7	EDO	A	814	-	3,3,3	0.25	0	2,2,2	0.51	0
6	C8E	C	808	-	14,14,20	0.65	0	13,13,19	0.49	0
5	OPZ	B	803	2	23,27,27	2.65	5 (21%)	25,38,38	1.80	3 (12%)
6	C8E	A	810	-	8,8,20	0.34	0	7,7,19	0.47	0
6	C8E	B	812	-	11,11,20	0.49	0	10,10,19	0.44	0
7	EDO	B	817	-	3,3,3	0.28	0	2,2,2	0.69	0
6	C8E	C	807	-	20,20,20	0.69	0	19,19,19	0.48	0
7	EDO	C	827	-	3,3,3	0.60	0	2,2,2	0.22	0
7	EDO	A	815	-	3,3,3	0.42	0	2,2,2	0.64	0
7	EDO	B	827	-	3,3,3	0.39	0	2,2,2	0.41	0
7	EDO	C	823	-	3,3,3	0.58	0	2,2,2	0.25	0
7	EDO	A	813	-	3,3,3	0.45	0	2,2,2	0.42	0
7	EDO	A	816	-	3,3,3	0.38	0	2,2,2	0.39	0
7	EDO	B	823	-	3,3,3	0.45	0	2,2,2	0.46	0
7	EDO	A	818	-	3,3,3	0.40	0	2,2,2	0.41	0
6	C8E	B	814	-	8,8,20	0.54	0	7,7,19	0.38	0
6	C8E	C	805	-	15,15,20	0.56	0	14,14,19	0.28	0
6	C8E	C	811	-	9,9,20	0.50	0	8,8,19	0.35	0
6	C8E	A	805	-	10,10,20	0.54	0	9,9,19	0.34	0
6	C8E	C	809	-	14,14,20	0.52	0	13,13,19	0.41	0
7	EDO	C	825	-	3,3,3	0.43	0	2,2,2	0.32	0
7	EDO	C	821	-	3,3,3	0.41	0	2,2,2	0.42	0
7	EDO	C	824	-	3,3,3	0.41	0	2,2,2	0.41	0
7	EDO	B	828	-	3,3,3	0.81	0	2,2,2	0.41	0
7	EDO	B	826	-	3,3,3	0.52	0	2,2,2	0.32	0
7	EDO	C	820	-	3,3,3	0.29	0	2,2,2	0.51	0
7	EDO	A	822	-	3,3,3	0.54	0	2,2,2	0.22	0
7	EDO	A	820	-	3,3,3	0.44	0	2,2,2	0.33	0
5	OPZ	A	804[B]	2	23,27,27	2.29	4 (17%)	25,38,38	1.58	4 (16%)
6	C8E	A	808	-	8,8,20	0.43	0	7,7,19	0.33	0
6	C8E	B	815	-	7,7,20	0.44	0	6,6,19	0.32	0
6	C8E	C	812	-	7,7,20	0.29	0	6,6,19	0.47	0
5	OPZ	C	803	2	23,27,27	1.95	4 (17%)	25,38,38	1.87	4 (16%)
7	EDO	B	824	-	3,3,3	0.33	0	2,2,2	0.50	0
7	EDO	B	820	-	3,3,3	0.41	0	2,2,2	0.28	0
7	EDO	C	817	-	3,3,3	0.53	0	2,2,2	0.45	0
6	C8E	A	809	-	6,6,20	0.54	0	5,5,19	0.38	0
6	C8E	C	813	-	6,6,20	0.51	0	5,5,19	0.25	0
6	C8E	B	810	-	7,7,20	0.52	0	6,6,19	0.27	0
7	EDO	B	821	-	3,3,3	0.38	0	2,2,2	0.43	0
4	OPV	A	803[A]	2	23,27,27	2.37	4 (17%)	25,38,38	2.05	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	C8E	C	804	-	15,15,20	0.57	0	14,14,19	0.34	0
7	EDO	B	816	-	3,3,3	0.53	0	2,2,2	0.31	0
6	C8E	C	810	-	6,6,20	0.54	0	5,5,19	0.22	0
7	EDO	A	811	-	3,3,3	0.71	0	2,2,2	0.12	0
7	EDO	B	822	-	3,3,3	0.35	0	2,2,2	0.36	0
7	EDO	C	830	-	3,3,3	0.45	0	2,2,2	0.33	0
7	EDO	A	819	-	3,3,3	0.39	0	2,2,2	0.43	0
7	EDO	A	812	-	3,3,3	0.33	0	2,2,2	0.58	0
3	FV8	C	802	2	22,27,27	2.61	6 (27%)	27,38,38	2.20	6 (22%)
7	EDO	C	816	-	3,3,3	0.34	0	2,2,2	0.77	0
7	EDO	A	817	-	3,3,3	0.43	0	2,2,2	0.23	0
7	EDO	A	823	-	3,3,3	0.44	0	2,2,2	0.58	0
6	C8E	A	806	-	8,8,20	0.47	0	7,7,19	0.33	0
6	C8E	B	807	-	20,20,20	0.58	0	19,19,19	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	826	-	-	0/1/1/1	-
7	EDO	C	819	-	-	1/1/1/1	-
6	C8E	B	813	-	-	5/9/9/18	-
3	FV8	A	802	2	-	3/15/29/29	0/3/3/3
7	EDO	B	819	-	-	1/1/1/1	-
6	C8E	B	804	-	-	9/13/13/18	-
7	EDO	B	818	-	-	1/1/1/1	-
7	EDO	C	814	-	-	1/1/1/1	-
7	EDO	C	815	-	-	0/1/1/1	-
6	C8E	A	807	-	-	1/5/5/18	-
7	EDO	B	825	-	-	1/1/1/1	-
6	C8E	B	805	-	-	5/15/15/18	-
6	C8E	C	806	-	-	7/11/11/18	-
6	C8E	B	811	-	-	8/18/18/18	-
6	C8E	B	806	-	-	3/10/10/18	-
6	C8E	B	808	-	-	3/6/6/18	-
7	EDO	C	818	-	-	0/1/1/1	-
7	EDO	A	821	-	-	1/1/1/1	-
7	EDO	C	829	-	-	1/1/1/1	-
7	EDO	C	822	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FV8	B	802	2	-	4/15/29/29	0/3/3/3
7	EDO	C	828	-	-	0/1/1/1	-
6	C8E	B	809	-	-	2/9/9/18	-
7	EDO	A	814	-	-	1/1/1/1	-
6	C8E	C	808	-	-	5/12/12/18	-
5	OPZ	B	803	2	-	3/12/29/29	0/3/3/3
6	C8E	A	810	-	-	3/6/6/18	-
6	C8E	B	812	-	-	7/9/9/18	-
7	EDO	B	817	-	-	0/1/1/1	-
6	C8E	C	807	-	-	11/18/18/18	-
7	EDO	C	827	-	-	1/1/1/1	-
7	EDO	A	815	-	-	0/1/1/1	-
7	EDO	B	827	-	-	1/1/1/1	-
7	EDO	C	823	-	-	0/1/1/1	-
7	EDO	A	813	-	-	1/1/1/1	-
7	EDO	A	816	-	-	0/1/1/1	-
7	EDO	B	823	-	-	0/1/1/1	-
7	EDO	A	818	-	-	0/1/1/1	-
6	C8E	B	814	-	-	2/6/6/18	-
6	C8E	C	805	-	-	5/13/13/18	-
6	C8E	C	811	-	-	3/7/7/18	-
6	C8E	A	805	-	-	6/8/8/18	-
6	C8E	C	809	-	-	5/12/12/18	-
7	EDO	C	825	-	-	1/1/1/1	-
7	EDO	C	821	-	-	0/1/1/1	-
7	EDO	C	824	-	-	0/1/1/1	-
7	EDO	B	828	-	-	1/1/1/1	-
7	EDO	B	826	-	-	0/1/1/1	-
7	EDO	C	820	-	-	0/1/1/1	-
7	EDO	A	822	-	-	0/1/1/1	-
7	EDO	A	820	-	-	0/1/1/1	-
5	OPZ	A	804[B]	2	-	1/12/29/29	0/3/3/3
6	C8E	A	808	-	-	5/6/6/18	-
6	C8E	B	815	-	-	1/5/5/18	-
6	C8E	C	812	-	-	2/5/5/18	-
5	OPZ	C	803	2	-	0/12/29/29	0/3/3/3
7	EDO	B	824	-	-	1/1/1/1	-
7	EDO	B	820	-	-	1/1/1/1	-
7	EDO	C	817	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C8E	A	809	-	-	1/4/4/18	-
6	C8E	C	813	-	-	0/4/4/18	-
6	C8E	B	810	-	-	3/5/5/18	-
7	EDO	B	821	-	-	0/1/1/1	-
4	OPV	A	803[A]	2	-	0/12/29/29	0/3/3/3
6	C8E	C	804	-	-	6/13/13/18	-
7	EDO	B	816	-	-	0/1/1/1	-
6	C8E	C	810	-	-	3/4/4/18	-
7	EDO	A	811	-	-	0/1/1/1	-
7	EDO	B	822	-	-	0/1/1/1	-
7	EDO	C	830	-	-	0/1/1/1	-
7	EDO	A	819	-	-	0/1/1/1	-
7	EDO	A	812	-	-	0/1/1/1	-
3	FV8	C	802	2	-	3/15/29/29	0/3/3/3
7	EDO	C	816	-	-	1/1/1/1	-
7	EDO	A	817	-	-	1/1/1/1	-
7	EDO	A	823	-	-	1/1/1/1	-
6	C8E	A	806	-	-	3/6/6/18	-
6	C8E	B	807	-	-	10/18/18/18	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	FV8	OAE-NAY	16.80	1.53	1.40
5	B	803	OPZ	OG1-NAY	8.73	1.57	1.46
4	A	803[A]	OPV	OG1-NAY	8.08	1.56	1.46
5	A	804[B]	OPZ	OG1-NAY	7.43	1.55	1.46
3	C	802	FV8	CAV-CAR	-7.28	1.34	1.47
3	B	802	FV8	CAV-CAR	-6.41	1.36	1.47
3	A	802	FV8	CAV-CAR	-6.41	1.36	1.47
3	B	802	FV8	CAR-N	6.15	1.36	1.27
3	C	802	FV8	CAR-N	5.89	1.35	1.27
3	A	802	FV8	CAR-N	5.62	1.35	1.27
5	C	803	OPZ	CAV-CAQ	-5.10	1.39	1.50
5	B	803	OPZ	CAL-NAY	4.98	1.55	1.47
5	A	804[B]	OPZ	CAV-CAQ	-4.94	1.40	1.50
5	B	803	OPZ	CAV-CAQ	-4.92	1.40	1.50
4	A	803[A]	OPV	CA-C	-4.80	1.39	1.52
4	A	803[A]	OPV	CAV-CAQ	-4.75	1.40	1.50
5	A	804[B]	OPZ	CA-C	-4.31	1.40	1.52
3	C	802	FV8	CA-N	4.19	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	OPZ	OG1-NAY	4.13	1.51	1.46
3	C	802	FV8	C-NAY	-3.91	1.30	1.35
5	C	803	OPZ	CA-C	-3.72	1.42	1.52
5	B	803	OPZ	CA-C	-3.67	1.42	1.52
3	A	802	FV8	OAE-NAY	-3.59	1.37	1.40
3	C	802	FV8	CB-CA	-3.13	1.50	1.54
3	A	802	FV8	C-NAY	-2.88	1.32	1.35
5	C	803	OPZ	CAL-NAY	2.83	1.52	1.47
3	C	802	FV8	OAE-NAY	2.82	1.42	1.40
3	A	802	FV8	O-C	2.45	1.26	1.22
5	B	803	OPZ	CAK-CAT	2.44	1.56	1.51
4	A	803[A]	OPV	CAL-NAY	2.43	1.51	1.47
5	A	804[B]	OPZ	CAK-CAT	2.36	1.56	1.51
3	A	802	FV8	CB-CA	-2.13	1.52	1.54
3	A	802	FV8	OG1-CB	-2.12	1.43	1.46
3	A	802	FV8	CA-N	2.01	1.50	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	FV8	OG1-CAR-N	-8.83	112.29	118.14
3	B	802	FV8	OG1-CAR-N	-8.48	112.53	118.14
3	C	802	FV8	OG1-CAR-N	-7.82	112.96	118.14
4	A	803[A]	OPV	OG1-NAY-CAL	7.25	126.67	114.06
5	B	803	OPZ	OG1-NAY-CAL	6.68	125.67	114.06
5	C	803	OPZ	OG1-NAY-CAL	6.07	124.62	114.06
5	A	804[B]	OPZ	OG1-NAY-CAL	5.60	123.81	114.06
3	C	802	FV8	OG1-CB-CA	4.29	106.34	102.53
5	C	803	OPZ	CAV-CAU-CAS	4.27	122.69	119.99
3	A	802	FV8	CAV-CAU-CAS	4.19	122.64	119.99
3	B	802	FV8	CAV-CAU-CAS	4.14	122.62	119.99
3	C	802	FV8	CAV-CAU-CAS	3.82	122.41	119.99
3	A	802	FV8	OG1-CB-CA	3.71	105.82	102.53
3	B	802	FV8	OG1-CB-CA	3.27	105.43	102.53
4	A	803[A]	OPV	O-C-CA	-3.23	123.19	127.53
4	A	803[A]	OPV	C-CA-N	-2.83	108.87	113.06
5	A	804[B]	OPZ	CAV-CAU-CAS	2.74	121.72	119.99
3	C	802	FV8	CB-CA-N	-2.69	102.68	104.86
3	C	802	FV8	OAE-NAY-CAL	2.50	119.84	113.59
3	B	802	FV8	CAH-CAV-CAU	-2.45	116.33	118.74
4	A	803[A]	OPV	CG2-CB-CA	-2.44	111.36	114.80
5	B	803	OPZ	O-C-CA	-2.42	124.28	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	FV8	CB-CA-N	-2.36	102.94	104.86
5	A	804[B]	OPZ	O-C-CA	-2.36	124.36	127.53
3	A	802	FV8	CA-N-CAR	2.36	108.68	106.83
3	C	802	FV8	C-CA-N	-2.34	108.25	111.96
5	B	803	OPZ	CAV-CAU-CAS	2.24	121.41	119.99
3	A	802	FV8	OG1-CB-CG2	-2.20	105.73	108.70
3	B	802	FV8	CA-N-CAR	2.18	108.54	106.83
5	A	804[B]	OPZ	CG2-CB-CA	-2.17	111.75	114.80
5	C	803	OPZ	OAD-CAS-CAG	2.16	125.20	119.33
3	B	802	FV8	CAU-CAV-CAR	2.06	123.86	121.21
5	C	803	OPZ	O-C-CA	-2.06	124.76	127.53
4	A	803[A]	OPV	CB-CA-N	-2.04	110.86	114.44
3	B	802	FV8	CAF-CAG-CAS	-2.00	117.52	120.05

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	FV8	CAK-CAL-NAY-OAE
3	A	802	FV8	CAK-CAL-NAY-C
3	B	802	FV8	CAK-CAL-NAY-OAE
5	B	803	OPZ	CAT-CAK-CAL-NAY
5	B	803	OPZ	CAK-CAL-NAY-C
5	B	803	OPZ	CAK-CAL-NAY-OG1
3	C	802	FV8	CAK-CAL-NAY-OAE
6	C	810	C8E	O12-C13-C14-O15
6	C	806	C8E	O15-C16-C17-O18
6	C	805	C8E	C6-C7-C8-O9
6	C	805	C8E	O15-C16-C17-O18
6	C	806	C8E	O12-C13-C14-O15
6	B	804	C8E	O9-C10-C11-O12
6	B	804	C8E	O15-C16-C17-O18
6	C	807	C8E	O15-C16-C17-O18
6	B	804	C8E	O18-C19-C20-O21
6	C	807	C8E	O18-C19-C20-O21
6	C	804	C8E	O15-C16-C17-O18
6	C	807	C8E	C6-C7-C8-O9
6	A	805	C8E	C6-C7-C8-O9
6	B	806	C8E	C6-C7-C8-O9
6	C	807	C8E	O9-C10-C11-O12
6	B	811	C8E	O18-C19-C20-O21
6	C	810	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
6	C	806	C8E	O9-C10-C11-O12
6	B	810	C8E	C4-C5-C6-C7
6	A	810	C8E	C3-C4-C5-C6
6	C	807	C8E	C3-C4-C5-C6
6	B	804	C8E	O12-C13-C14-O15
6	B	814	C8E	C3-C4-C5-C6
6	B	808	C8E	C4-C5-C6-C7
6	B	810	C8E	C2-C3-C4-C5
6	B	806	C8E	C3-C4-C5-C6
6	B	805	C8E	O12-C13-C14-O15
6	B	808	C8E	C5-C6-C7-C8
6	B	812	C8E	C5-C6-C7-C8
6	B	812	C8E	C6-C7-C8-O9
6	C	808	C8E	O12-C13-C14-O15
7	C	819	EDO	O1-C1-C2-O2
7	B	818	EDO	O1-C1-C2-O2
7	C	829	EDO	O1-C1-C2-O2
7	C	822	EDO	O1-C1-C2-O2
7	C	827	EDO	O1-C1-C2-O2
6	A	808	C8E	C3-C4-C5-C6
6	B	807	C8E	C2-C3-C4-C5
6	B	807	C8E	C5-C6-C7-C8
6	A	805	C8E	C2-C3-C4-C5
6	C	811	C8E	C5-C6-C7-C8
6	C	804	C8E	O9-C10-C11-O12
6	B	811	C8E	C1-C2-C3-C4
6	B	813	C8E	C6-C7-C8-O9
6	B	810	C8E	C5-C6-C7-C8
6	C	807	C8E	C1-C2-C3-C4
6	A	807	C8E	C2-C3-C4-C5
6	B	811	C8E	O12-C13-C14-O15
6	A	810	C8E	C6-C7-C8-O9
6	A	806	C8E	C6-C7-C8-O9
6	B	811	C8E	O15-C16-C17-O18
6	B	807	C8E	O12-C13-C14-O15
5	A	804[B]	OPZ	CAT-CAK-CAL-NAY
6	B	807	C8E	C1-C2-C3-C4
6	A	805	C8E	C5-C6-C7-C8
6	C	811	C8E	C11-C10-O9-C8
6	C	808	C8E	C3-C4-C5-C6
6	C	811	C8E	C4-C5-C6-C7
6	A	808	C8E	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	B	813	C8E	C1-C2-C3-C4
6	B	814	C8E	C2-C3-C4-C5
6	A	808	C8E	C6-C7-C8-O9
3	A	802	FV8	O-C-CA-N
3	B	802	FV8	O-C-CA-N
3	C	802	FV8	O-C-CA-N
6	C	805	C8E	O18-C19-C20-O21
6	B	815	C8E	C3-C4-C5-C6
6	C	809	C8E	O12-C13-C14-O15
6	B	807	C8E	O18-C19-C20-O21
6	C	804	C8E	C13-C14-O15-C16
3	B	802	FV8	CAK-CAL-NAY-C
3	C	802	FV8	CAK-CAL-NAY-C
6	B	811	C8E	C16-C17-O18-C19
6	B	805	C8E	C7-C8-O9-C10
6	C	809	C8E	C14-C13-O12-C11
6	B	804	C8E	C13-C14-O15-C16
6	B	804	C8E	C17-C16-O15-C14
6	C	806	C8E	C13-C14-O15-C16
6	B	811	C8E	C17-C16-O15-C14
6	A	806	C8E	C3-C4-C5-C6
6	A	810	C8E	C1-C2-C3-C4
6	C	806	C8E	C17-C16-O15-C14
6	A	806	C8E	C5-C6-C7-C8
6	B	812	C8E	C7-C8-O9-C10
6	B	813	C8E	O9-C10-C11-O12
6	B	812	C8E	O9-C10-C11-O12
7	B	825	EDO	O1-C1-C2-O2
7	C	817	EDO	O1-C1-C2-O2
7	C	816	EDO	O1-C1-C2-O2
6	A	809	C8E	C5-C6-C7-C8
6	C	805	C8E	C14-C13-O12-C11
6	B	811	C8E	O9-C10-C11-O12
6	C	807	C8E	C14-C13-O12-C11
6	B	805	C8E	C10-C11-O12-C13
6	B	812	C8E	C2-C3-C4-C5
6	B	807	C8E	C13-C14-O15-C16
6	C	808	C8E	C14-C13-O12-C11
6	B	804	C8E	C6-C7-C8-O9
6	C	807	C8E	C16-C17-O18-C19
6	C	805	C8E	O12-C13-C14-O15
6	C	808	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
6	A	808	C8E	C4-C5-C6-C7
6	C	809	C8E	C10-C11-O12-C13
6	B	807	C8E	C14-C13-O12-C11
6	B	807	C8E	C10-C11-O12-C13
6	B	813	C8E	C7-C8-O9-C10
7	B	819	EDO	O1-C1-C2-O2
7	B	828	EDO	O1-C1-C2-O2
7	B	824	EDO	O1-C1-C2-O2
7	A	817	EDO	O1-C1-C2-O2
6	C	809	C8E	C2-C3-C4-C5
6	B	808	C8E	C3-C4-C5-C6
6	B	809	C8E	C4-C5-C6-C7
6	B	806	C8E	C11-C10-O9-C8
6	C	804	C8E	C17-C16-O15-C14
6	B	804	C8E	C14-C13-O12-C11
6	C	812	C8E	C3-C4-C5-C6
6	B	805	C8E	C14-C13-O12-C11
6	A	805	C8E	C3-C4-C5-C6
6	C	807	C8E	C7-C8-O9-C10
7	C	814	EDO	O1-C1-C2-O2
7	C	825	EDO	O1-C1-C2-O2
7	B	820	EDO	O1-C1-C2-O2
6	B	809	C8E	C2-C3-C4-C5
6	C	807	C8E	O12-C13-C14-O15
6	B	807	C8E	C17-C16-O15-C14
6	B	805	C8E	C3-C4-C5-C6
6	B	807	C8E	O15-C16-C17-O18
6	C	806	C8E	C16-C17-O18-C19
6	C	806	C8E	C6-C7-C8-O9
6	A	805	C8E	C11-C10-O9-C8
7	A	821	EDO	O1-C1-C2-O2
6	B	812	C8E	C1-C2-C3-C4
6	C	809	C8E	O9-C10-C11-O12
6	C	804	C8E	C16-C17-O18-C19
6	A	805	C8E	C1-C2-C3-C4
6	B	813	C8E	C2-C3-C4-C5
6	B	812	C8E	C3-C4-C5-C6
6	C	808	C8E	C7-C8-O9-C10
6	B	804	C8E	C16-C17-O18-C19
7	A	814	EDO	O1-C1-C2-O2
7	B	827	EDO	O1-C1-C2-O2
7	A	813	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	823	EDO	O1-C1-C2-O2
6	C	807	C8E	C10-C11-O12-C13
6	B	811	C8E	C4-C5-C6-C7
3	B	802	FV8	NAY-C-CA-CB
6	C	812	C8E	C1-C2-C3-C4
6	C	810	C8E	C10-C11-O12-C13
6	C	804	C8E	O12-C13-C14-O15
6	A	808	C8E	C2-C3-C4-C5

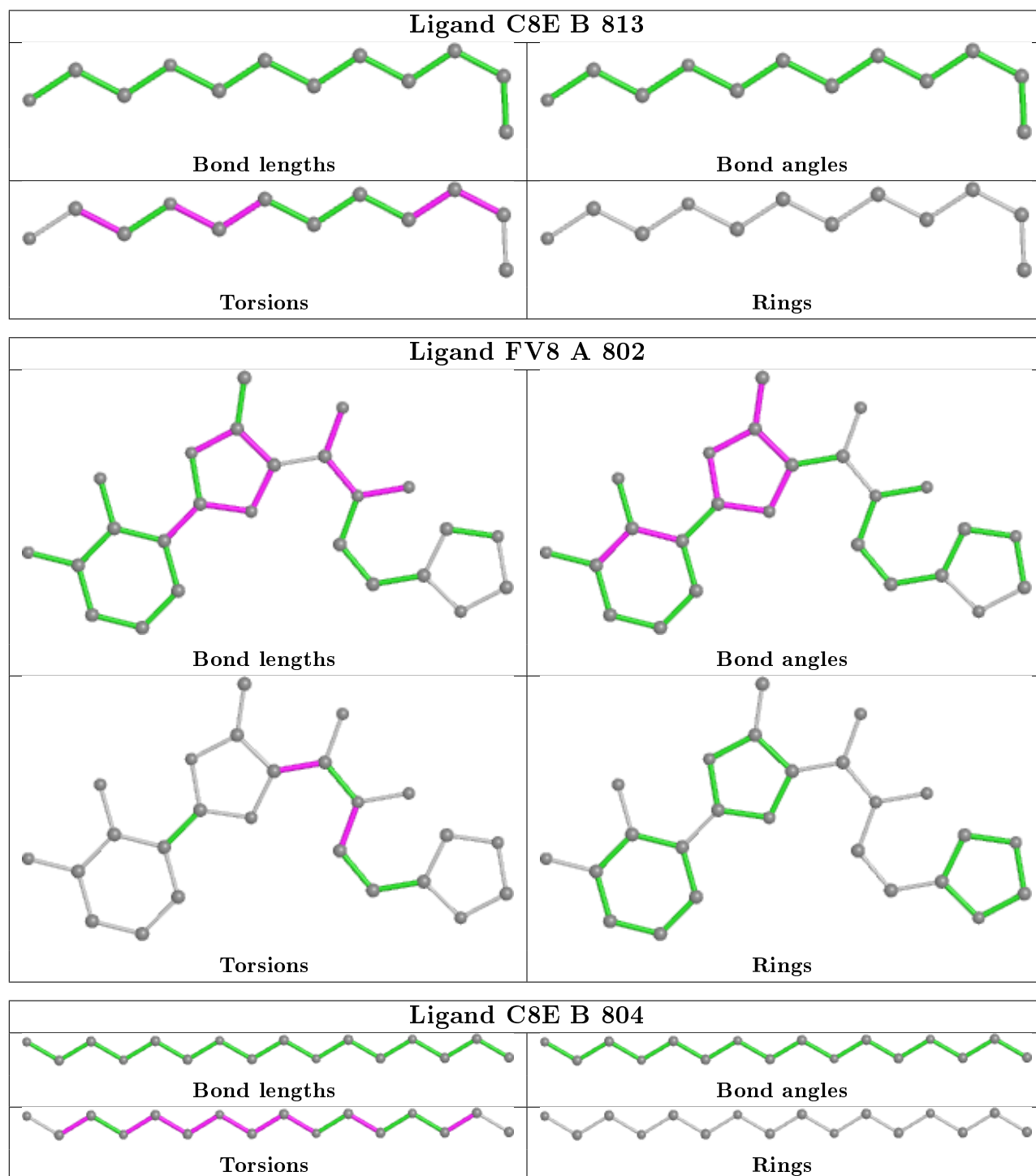
There are no ring outliers.

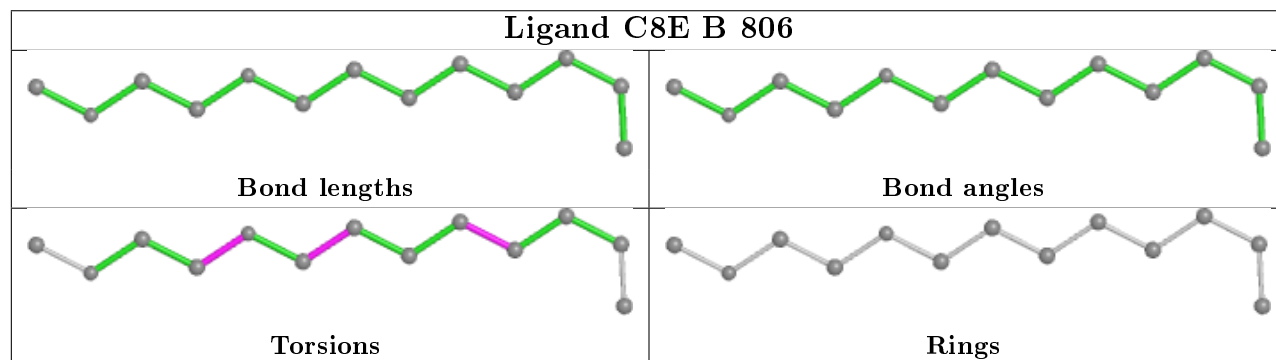
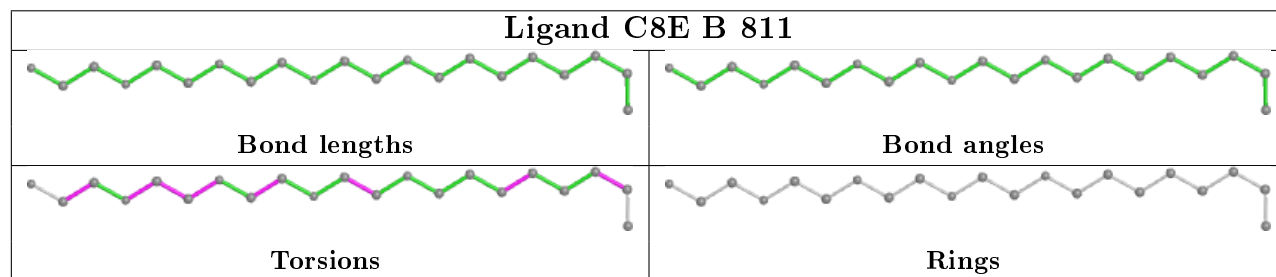
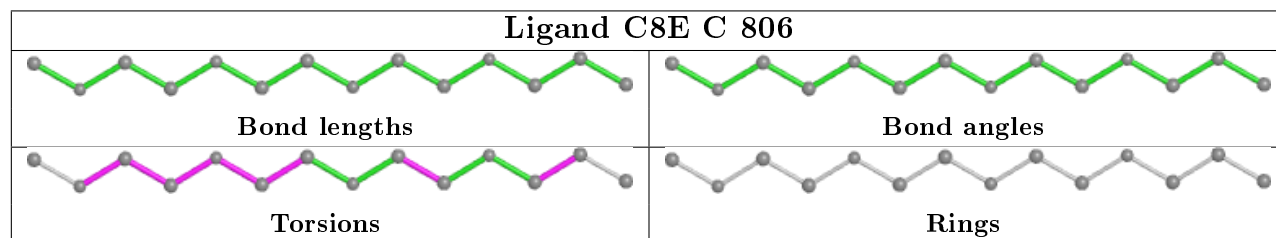
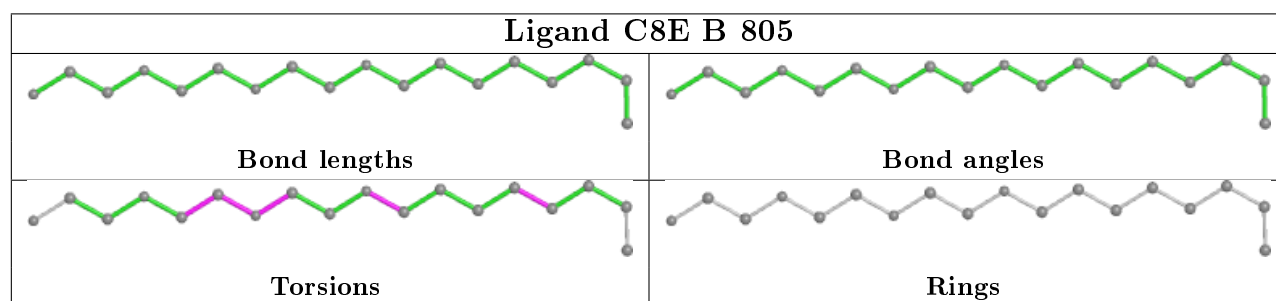
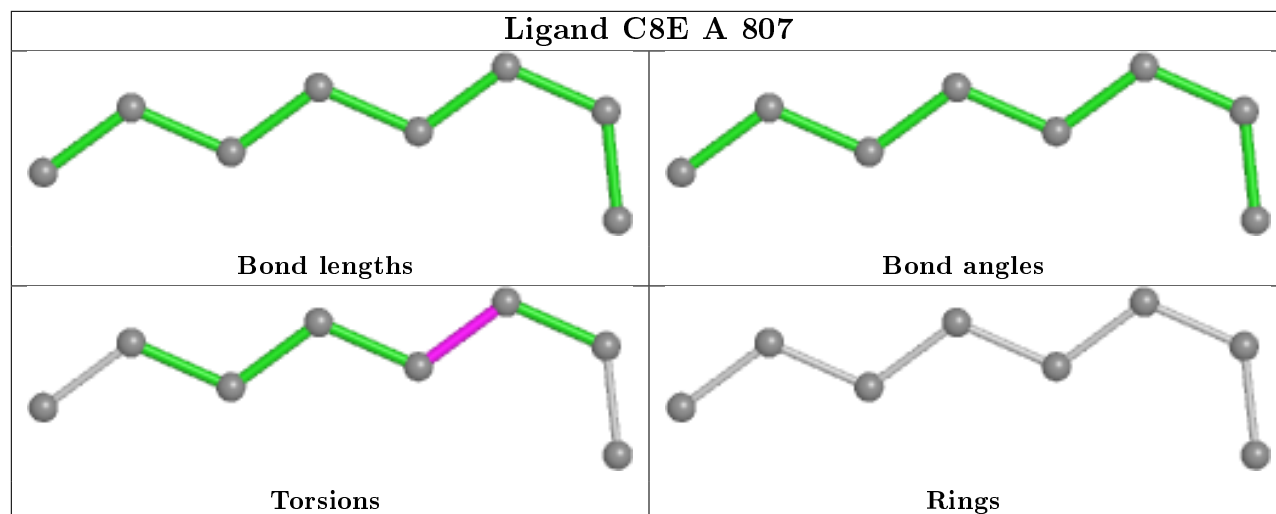
18 monomers are involved in 22 short contacts:

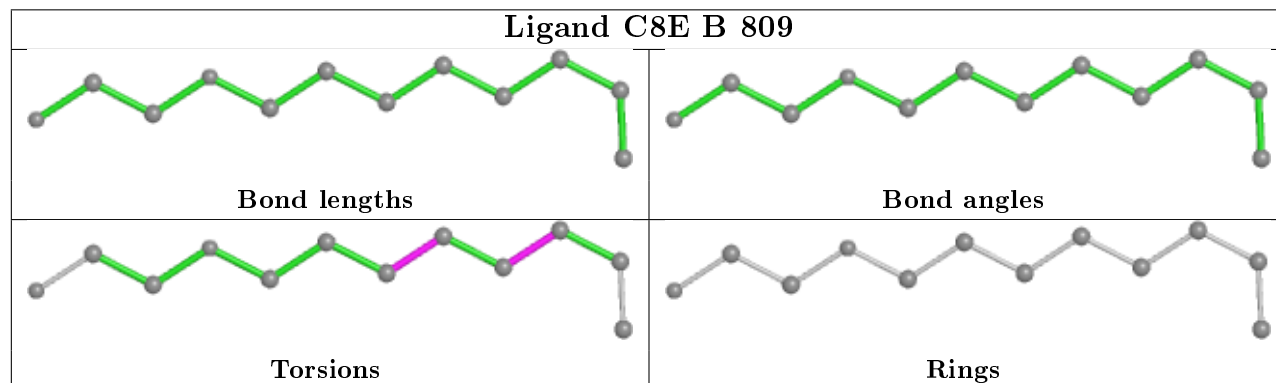
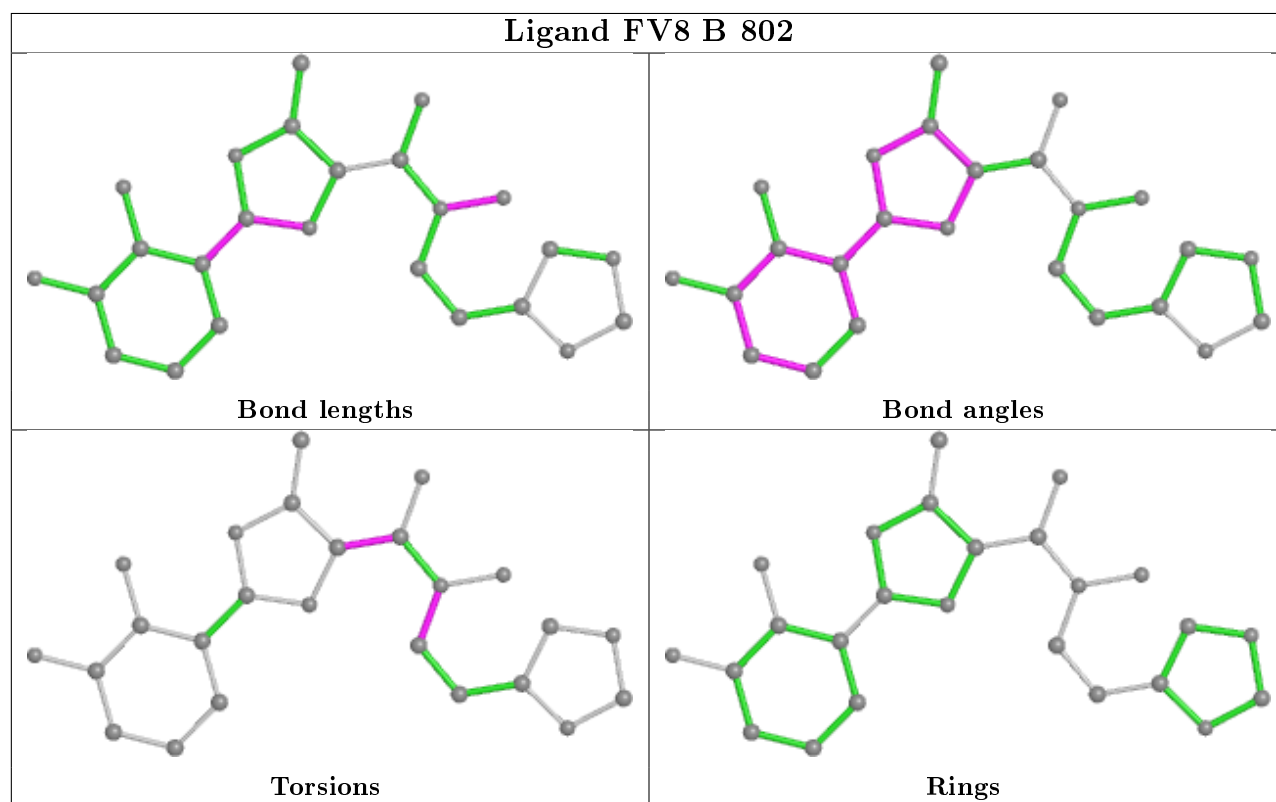
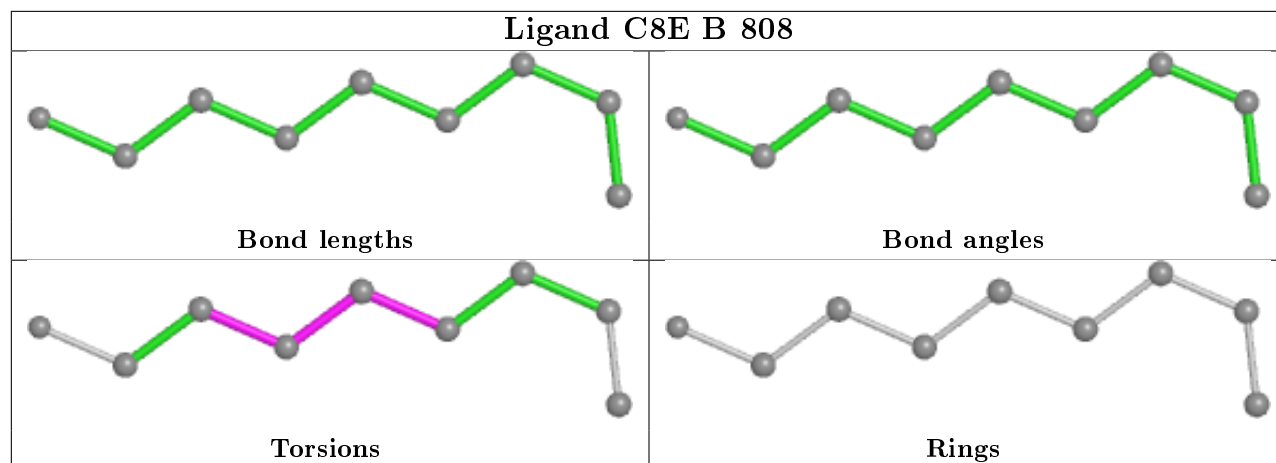
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	818	EDO	1	0
6	C	806	C8E	1	0
7	C	818	EDO	1	0
7	C	828	EDO	1	0
6	B	809	C8E	1	0
7	A	814	EDO	1	0
6	C	808	C8E	2	0
5	B	803	OPZ	1	0
6	C	807	C8E	1	0
6	B	814	C8E	1	0
6	A	805	C8E	1	0
6	C	809	C8E	1	0
7	C	824	EDO	1	0
7	C	820	EDO	1	0
5	A	804[B]	OPZ	1	0
4	A	803[A]	OPV	2	0
6	C	804	C8E	3	0
6	B	807	C8E	1	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.

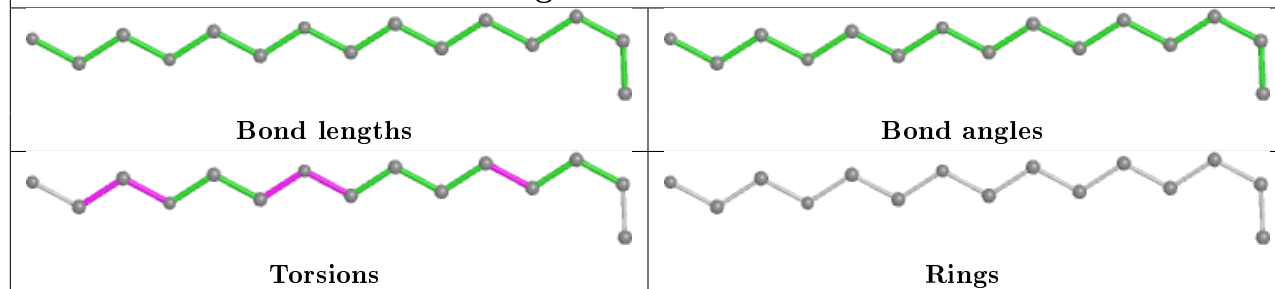
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



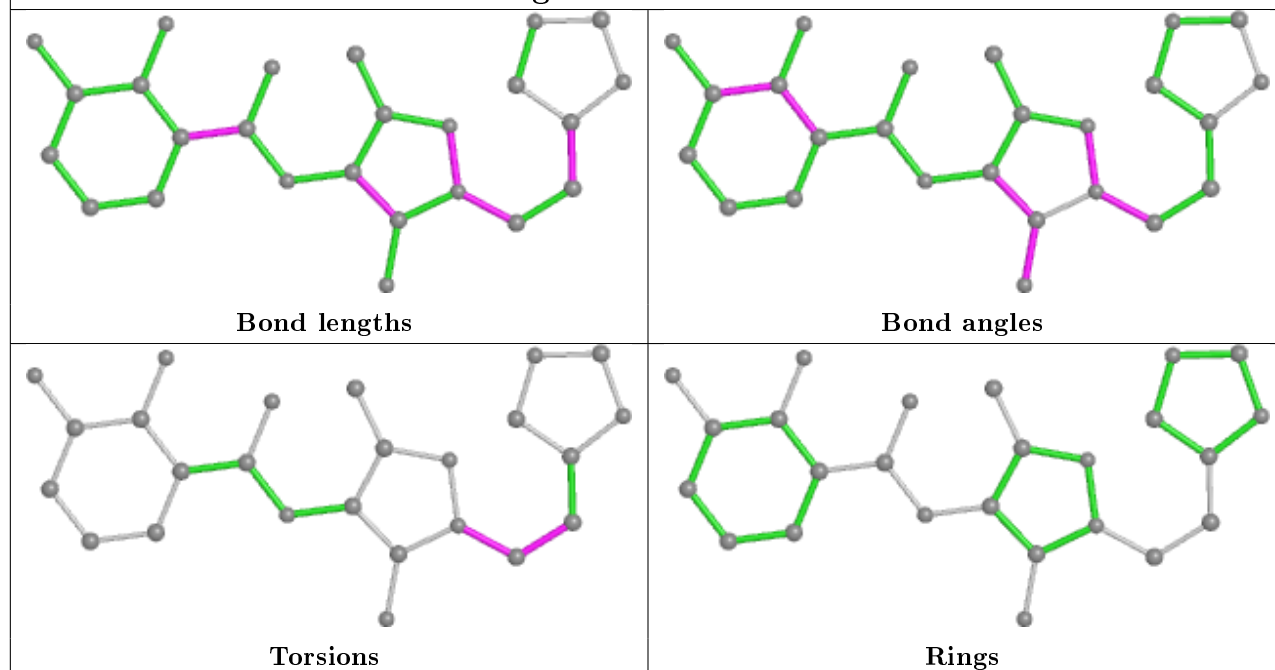




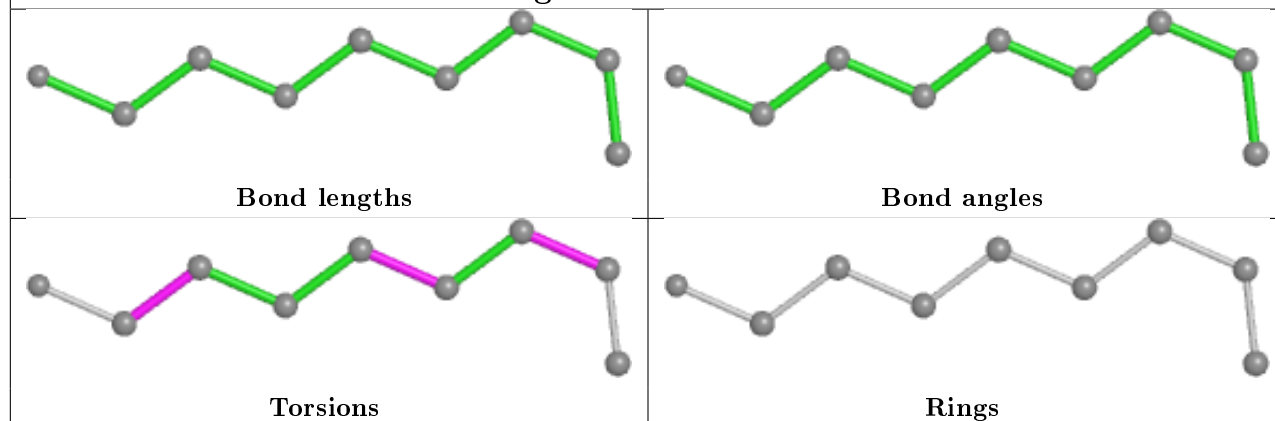
Ligand C8E C 808

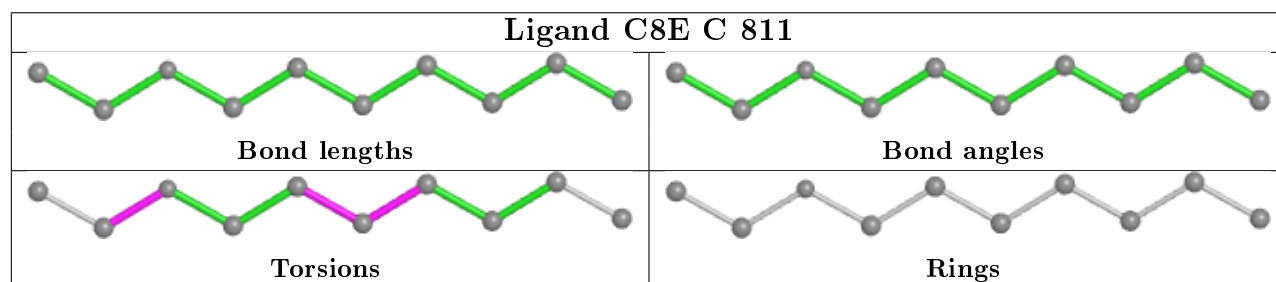
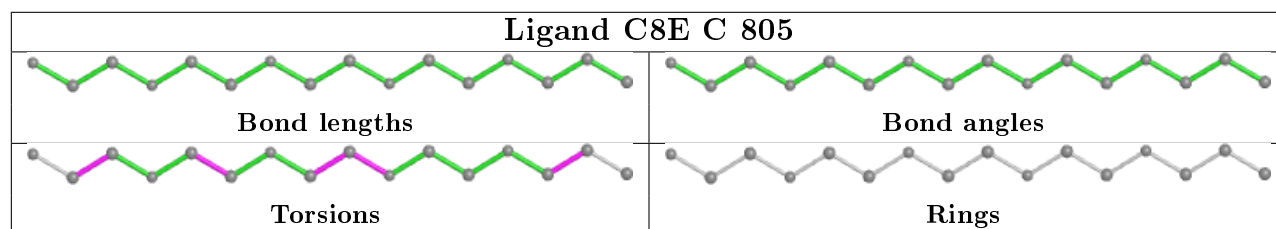
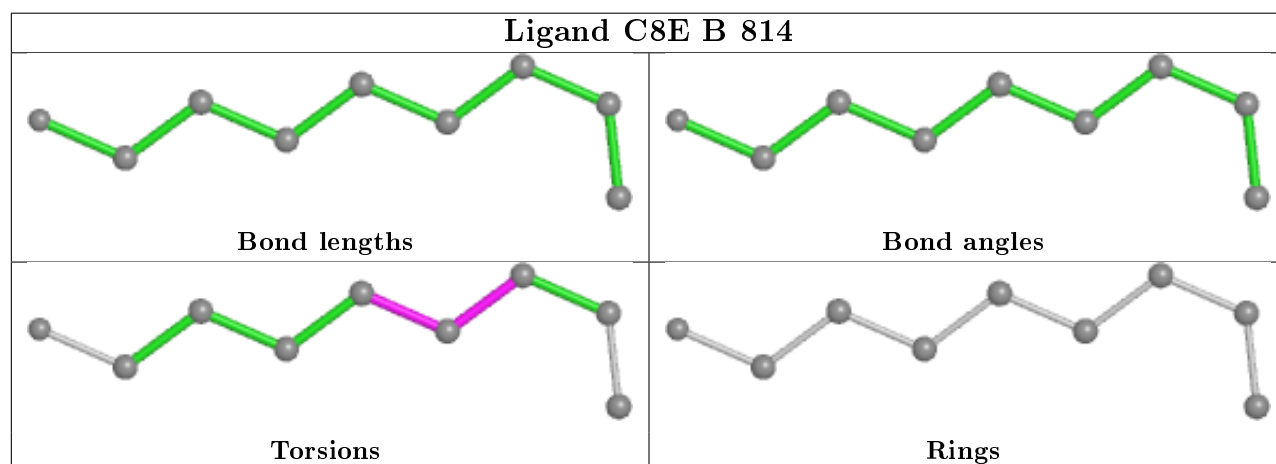
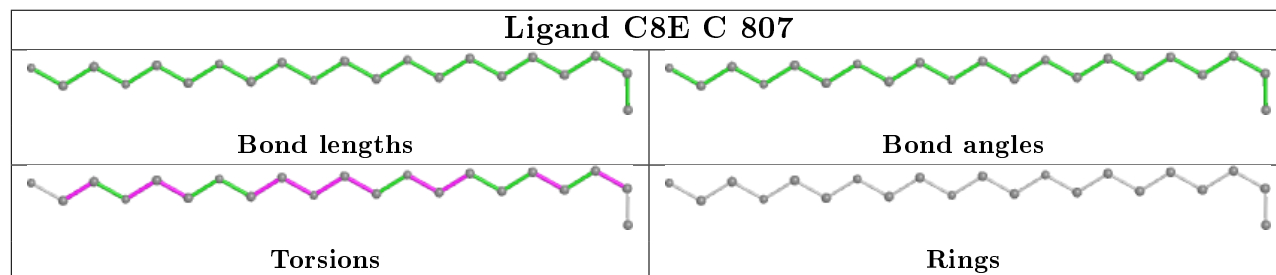
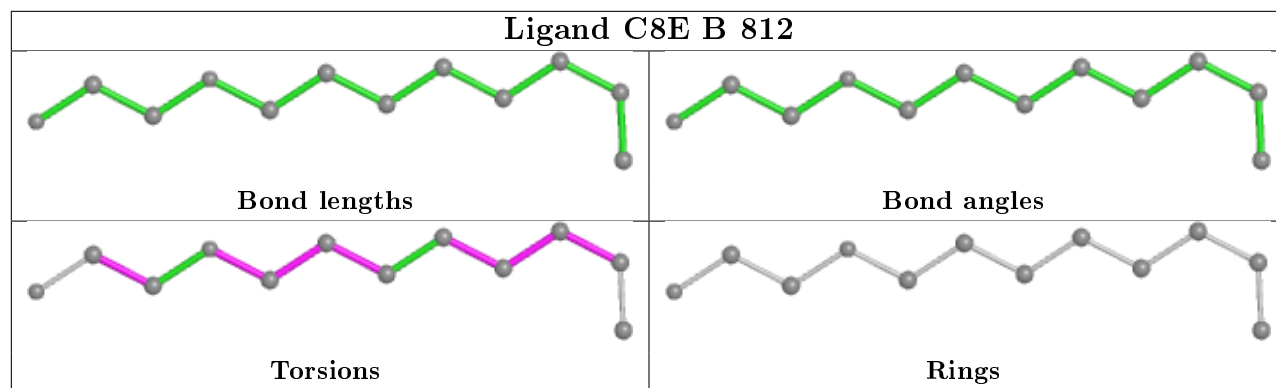


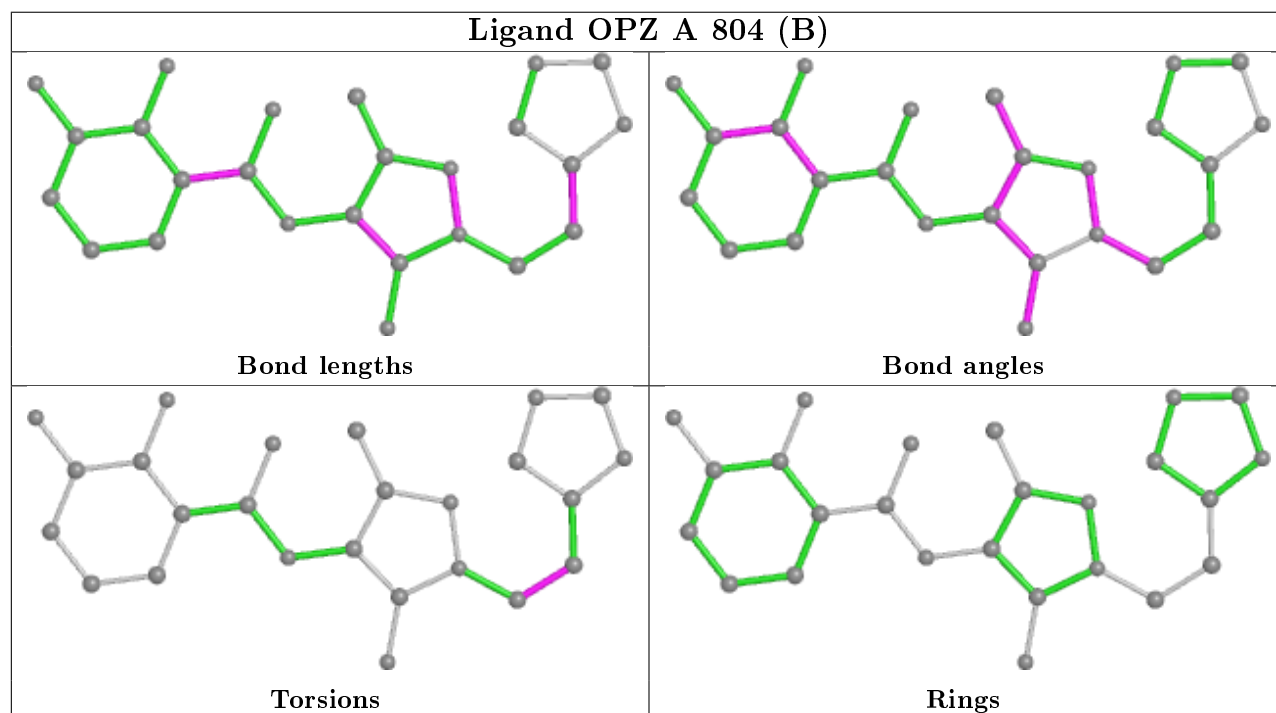
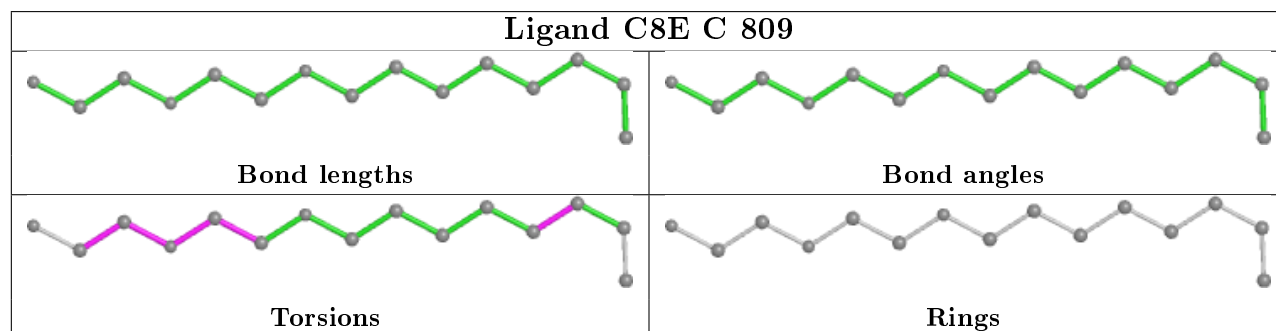
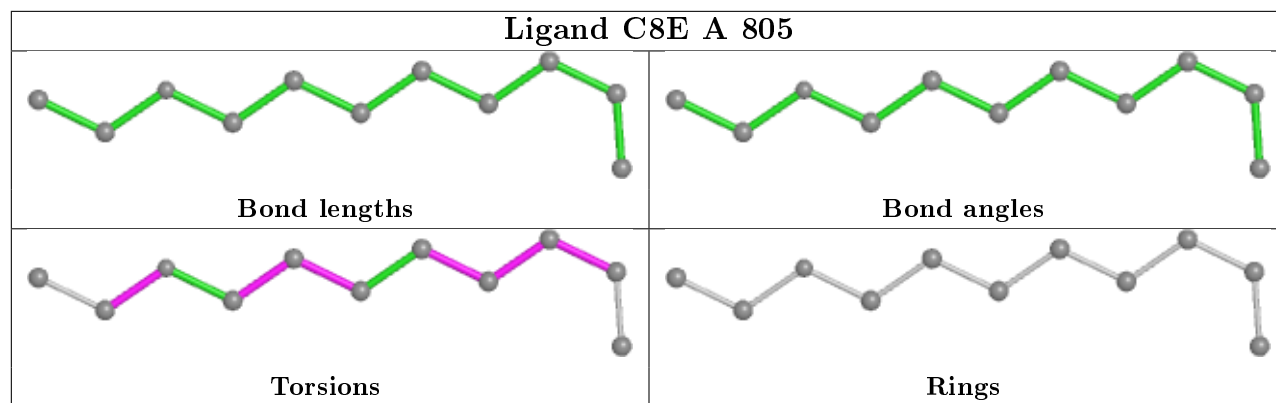
Ligand OPZ B 803

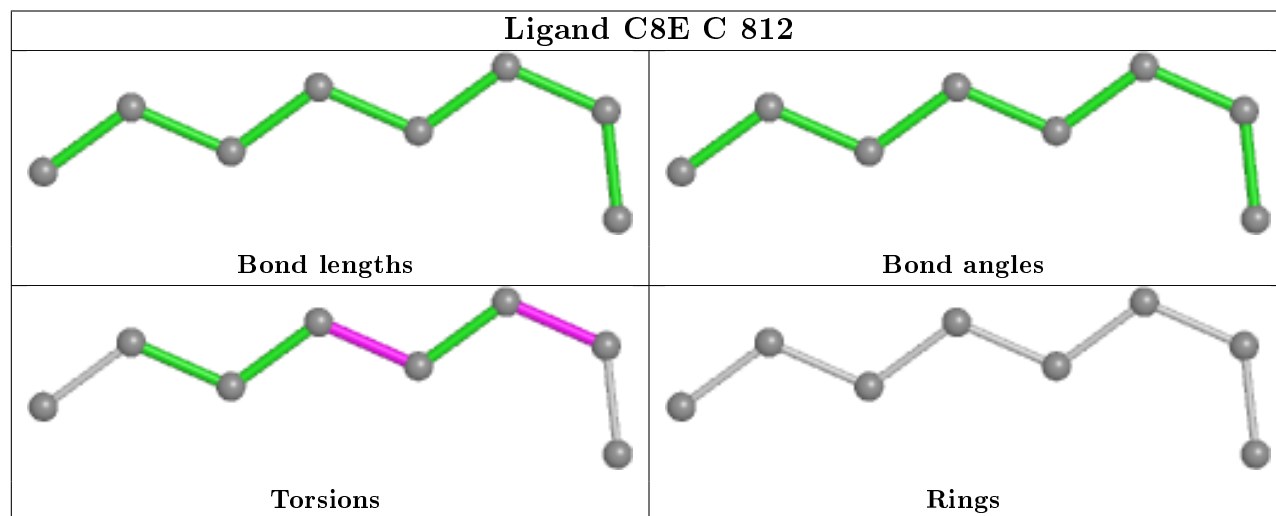
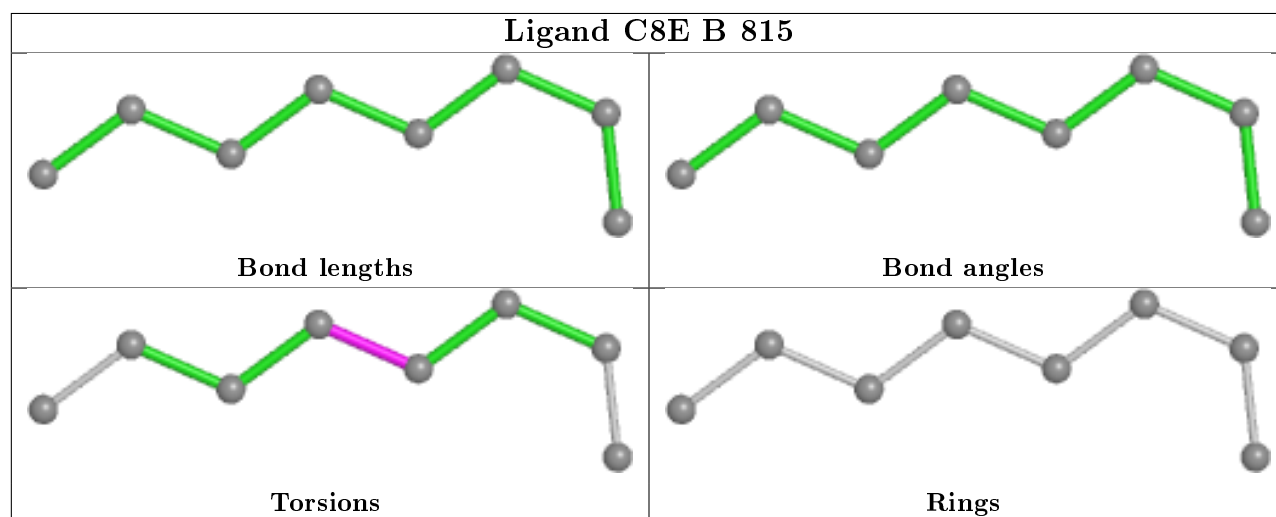
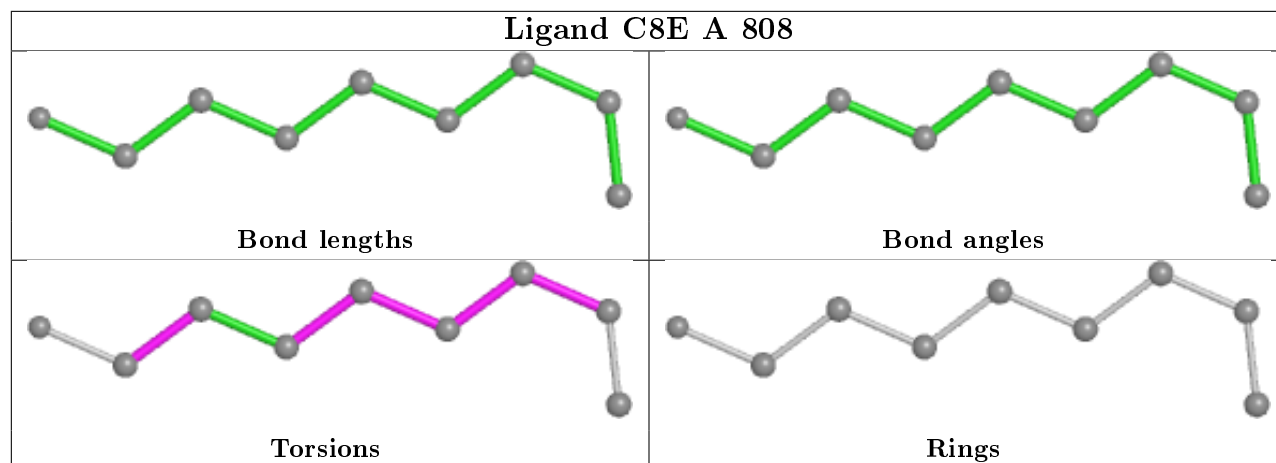


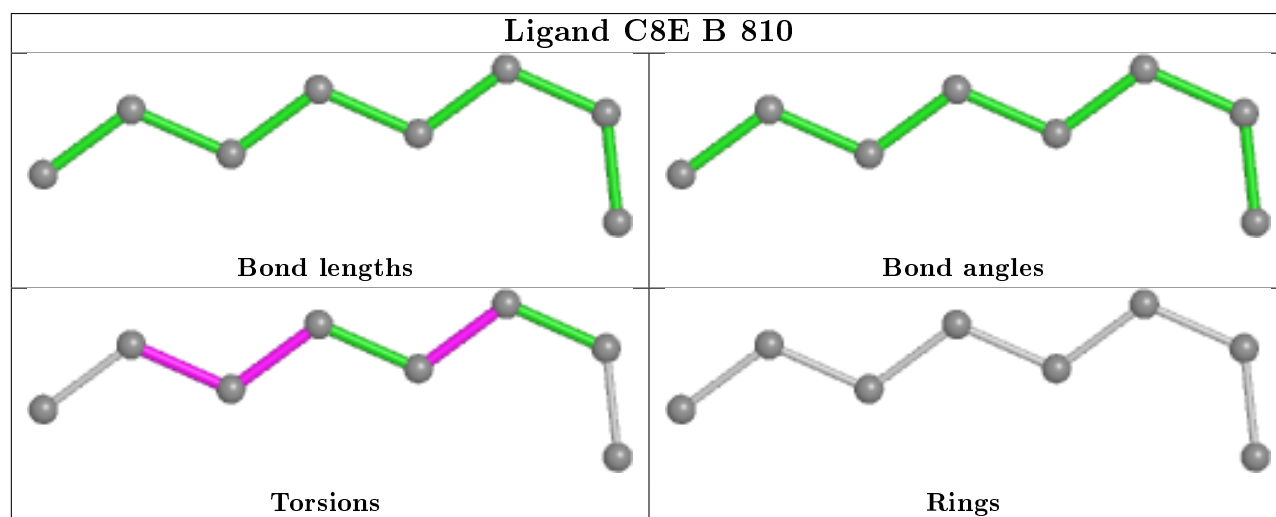
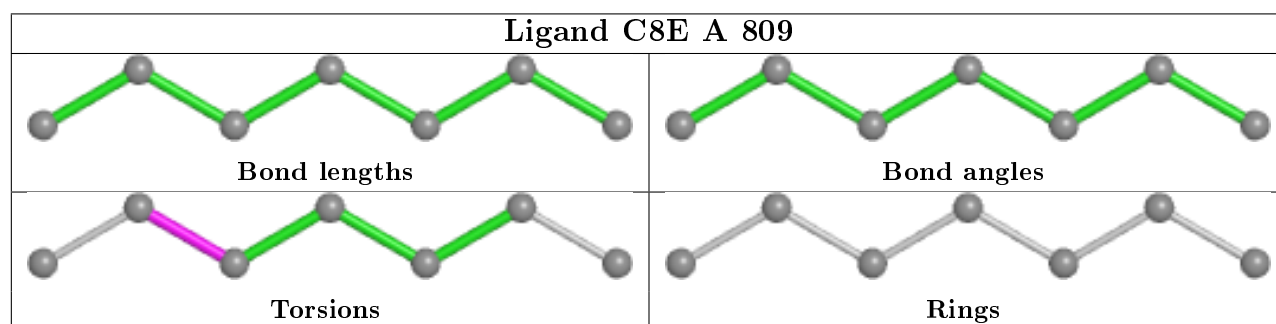
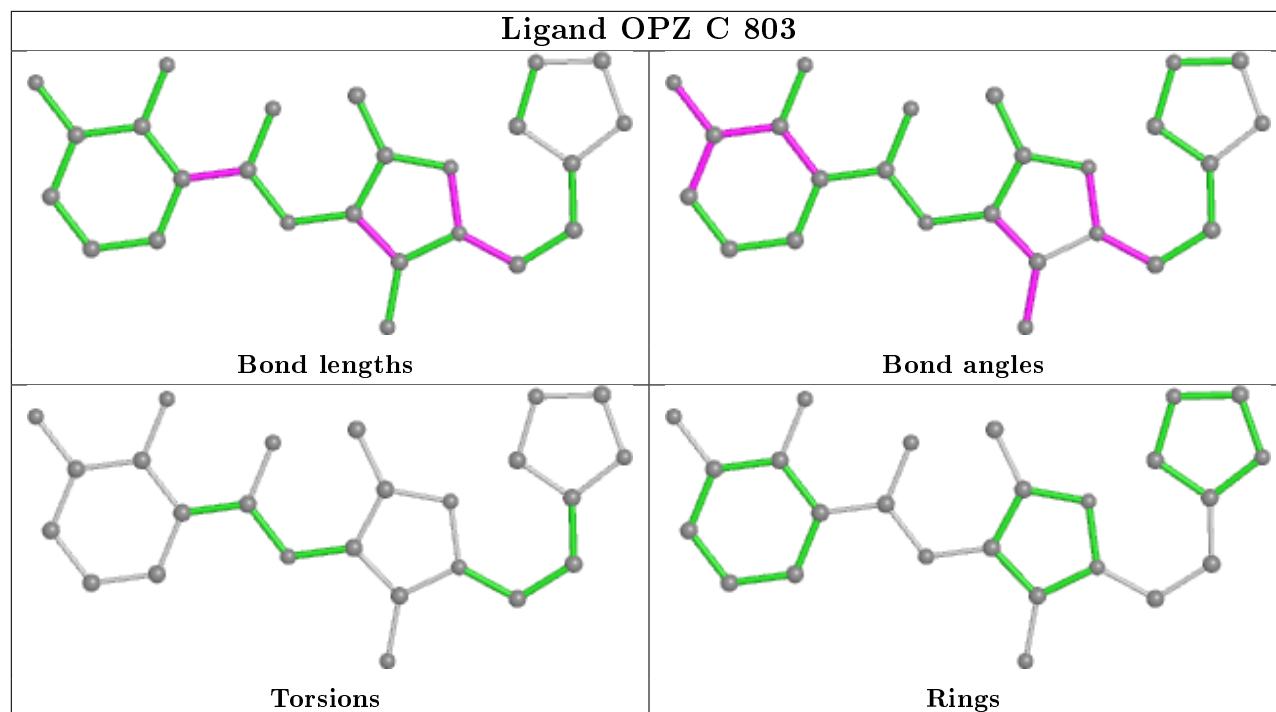
Ligand C8E A 810

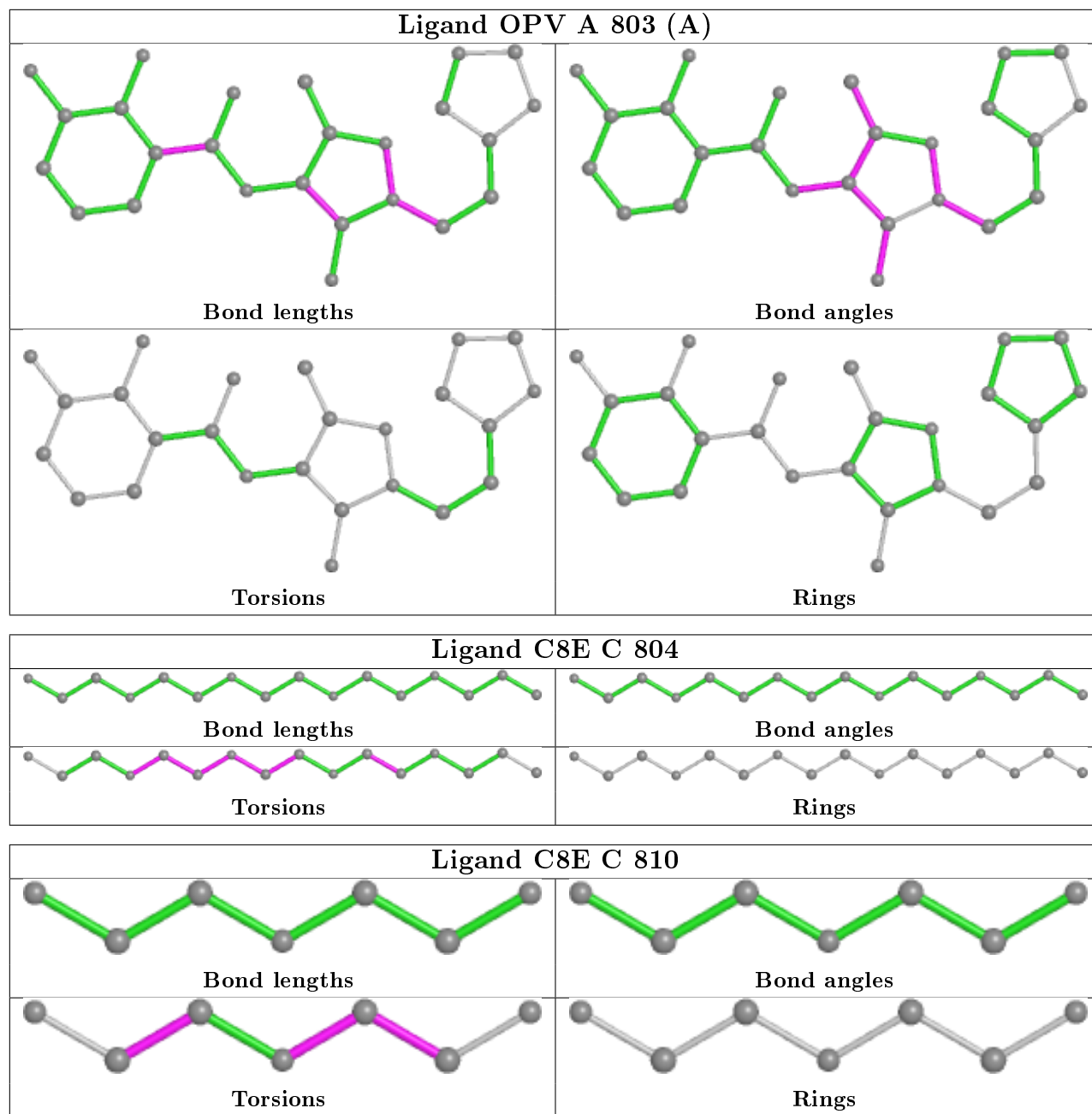


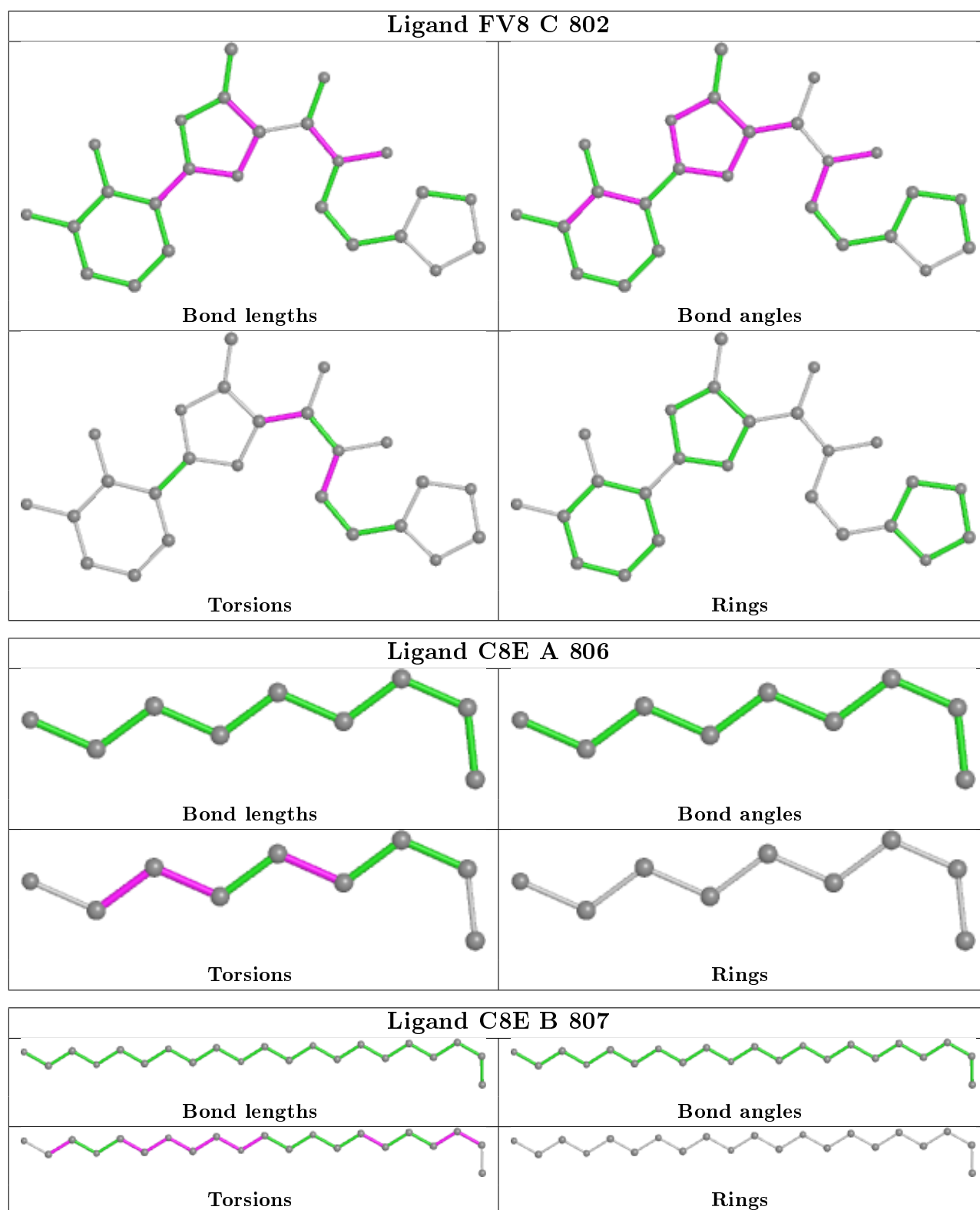












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	671/706 (95%)	0.03	23 (3%)	45 47	25, 38, 66, 106	0
1	B	671/706 (95%)	-0.00	16 (2%)	59 62	26, 37, 61, 87	0
1	C	671/706 (95%)	-0.13	12 (1%)	68 71	22, 34, 59, 91	0
All	All	2013/2118 (95%)	-0.04	51 (2%)	57 60	22, 36, 62, 106	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	ASN	4.8
1	A	543	VAL	4.5
1	A	542	LEU	4.4
1	A	546	LEU	3.7
1	A	618	GLN	3.7
1	A	195	GLU	3.4
1	B	195	GLU	3.2
1	C	430	GLN	3.2
1	C	544	ASN	3.2
1	C	431	ASP	3.0
1	A	540	SER	3.0
1	C	195	GLU	3.0
1	C	193	PHE	2.8
1	C	662	HIS	2.8
1	A	545	ASN	2.7
1	B	193	PHE	2.7
1	A	357	SER	2.7
1	A	428	PHE	2.7
1	A	497	ASN	2.6
1	C	368	TYR	2.6
1	A	541	LYS	2.6
1	B	194	GLY	2.6
1	B	540	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	2.5
1	B	235	ALA	2.4
1	B	196	ASN	2.4
1	B	452	THR	2.4
1	A	193	PHE	2.4
1	B	406	THR	2.4
1	B	224	PHE	2.4
1	B	542	LEU	2.3
1	A	452	THR	2.3
1	B	234	ASN	2.3
1	A	548	THR	2.3
1	B	297	ASP	2.3
1	A	498	PRO	2.3
1	A	616	VAL	2.2
1	A	473	ASP	2.2
1	B	233	GLU	2.2
1	B	199	PHE	2.2
1	B	451	ASN	2.2
1	A	569	ILE	2.2
1	C	612	TRP	2.2
1	C	618	GLN	2.1
1	C	452	THR	2.1
1	B	539	PRO	2.1
1	A	430	GLN	2.1
1	C	473	ASP	2.0
1	C	453	LEU	2.0
1	A	230	TRP	2.0
1	A	431	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	B	826	4/4	0.62	0.43	64,68,74,75	0
6	C8E	B	810	8/21	0.71	0.46	52,68,80,82	0
6	C8E	C	809	15/21	0.74	0.33	57,77,91,96	0
6	C8E	C	811	10/21	0.76	0.51	58,71,77,83	0
6	C8E	B	805	18/21	0.76	0.30	43,67,99,102	0
6	C8E	B	807	21/21	0.78	0.25	65,79,93,122	0
6	C8E	C	808	15/21	0.80	0.25	50,68,79,80	0
6	C8E	A	808	9/21	0.80	0.22	59,68,73,77	0
6	C8E	B	811	21/21	0.80	0.24	65,79,92,94	0
7	EDO	B	827	4/4	0.81	0.35	56,60,65,72	0
6	C8E	C	805	16/21	0.81	0.26	47,61,77,81	0
6	C8E	B	813	12/21	0.81	0.35	52,67,73,77	0
7	EDO	A	821	4/4	0.81	0.18	66,71,81,83	0
6	C8E	C	810	7/21	0.81	0.23	60,65,77,79	0
6	C8E	B	812	12/21	0.81	0.21	51,59,74,77	0
6	C8E	A	806	9/21	0.82	0.15	61,69,77,80	0
6	C8E	B	808	9/21	0.82	0.34	63,71,78,79	0
6	C8E	C	813	7/21	0.83	0.18	61,63,69,71	0
6	C8E	B	806	13/21	0.84	0.18	41,69,83,86	0
6	C8E	B	804	16/21	0.85	0.26	53,65,98,106	0
7	EDO	C	828	4/4	0.85	0.25	44,51,56,59	0
7	EDO	C	830	4/4	0.86	0.29	56,64,73,74	0
6	C8E	A	805	11/21	0.86	0.24	47,54,62,64	0
6	C8E	B	815	8/21	0.86	0.28	62,65,75,79	0
6	C8E	A	809	7/21	0.86	0.38	48,50,53,58	0
7	EDO	A	811	4/4	0.86	0.20	35,46,51,51	0
6	C8E	C	807	21/21	0.87	0.21	45,60,74,79	0
7	EDO	A	815	4/4	0.87	0.23	45,52,59,63	0
7	EDO	C	816	4/4	0.87	0.19	57,59,62,63	0
6	C8E	A	810	9/21	0.87	0.20	59,62,71,71	0
6	C8E	A	807	8/21	0.87	0.30	45,52,57,58	0
6	C8E	B	809	12/21	0.88	0.20	48,74,80,85	0
7	EDO	B	825	4/4	0.88	0.17	59,64,69,73	0
6	C8E	B	814	9/21	0.88	0.24	46,63,71,73	0
6	C8E	C	806	14/21	0.89	0.19	54,62,72,82	0
7	EDO	B	817	4/4	0.89	0.18	40,41,48,60	0
7	EDO	A	813	4/4	0.90	0.23	41,60,62,67	0
6	C8E	C	812	8/21	0.90	0.31	50,64,67,69	0
7	EDO	B	816	4/4	0.90	0.15	40,47,47,50	0
7	EDO	C	820	4/4	0.90	0.19	46,50,58,60	0
7	EDO	A	818	4/4	0.91	0.26	57,64,72,82	0

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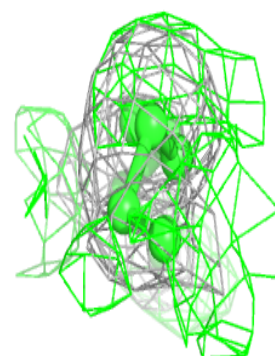
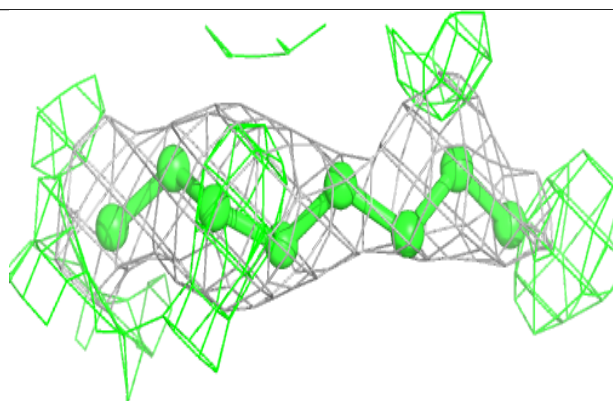
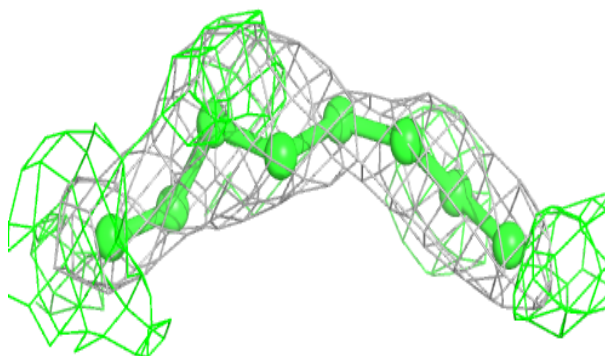
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	B	818	4/4	0.91	0.26	52,52,63,67	0
7	EDO	C	819	4/4	0.91	0.23	47,49,51,66	0
7	EDO	A	823	4/4	0.91	0.15	44,45,52,55	0
7	EDO	C	822	4/4	0.91	0.29	47,67,67,67	0
7	EDO	B	828	4/4	0.91	0.13	45,48,52,52	0
7	EDO	B	819	4/4	0.92	0.26	57,62,64,68	0
7	EDO	A	816	4/4	0.92	0.21	53,57,60,62	0
7	EDO	C	829	4/4	0.92	0.23	52,54,58,62	0
7	EDO	A	819	4/4	0.93	0.17	49,50,51,59	0
7	EDO	C	827	4/4	0.93	0.13	32,47,48,49	0
7	EDO	C	826	4/4	0.93	0.16	36,38,39,49	0
7	EDO	C	824	4/4	0.93	0.21	56,62,64,69	0
7	EDO	C	814	4/4	0.93	0.16	36,41,48,54	0
7	EDO	B	824	4/4	0.93	0.22	43,57,62,72	0
6	C8E	C	804	16/21	0.94	0.20	45,53,91,94	0
7	EDO	B	820	4/4	0.94	0.40	63,64,68,71	0
7	EDO	C	823	4/4	0.94	0.17	47,56,61,62	0
3	FV8	C	802	25/25	0.95	0.13	22,26,31,32	0
7	EDO	B	823	4/4	0.95	0.21	43,47,48,48	0
7	EDO	B	821	4/4	0.95	0.17	49,50,50,62	0
7	EDO	C	818	4/4	0.95	0.16	51,57,60,66	0
3	FV8	A	802	25/25	0.95	0.13	20,26,31,36	0
3	FV8	B	802	25/25	0.95	0.12	26,32,41,44	0
7	EDO	B	822	4/4	0.95	0.14	45,48,52,57	0
5	OPZ	A	804[B]	25/25	0.96	0.13	27,44,74,77	25
7	EDO	A	822	4/4	0.96	0.15	51,52,57,57	0
7	EDO	C	825	4/4	0.96	0.22	38,41,46,61	0
7	EDO	C	821	4/4	0.96	0.14	50,52,56,57	0
7	EDO	A	814	4/4	0.96	0.20	43,48,49,65	0
5	OPZ	B	803	25/25	0.96	0.17	24,60,89,98	0
4	OPV	A	803[A]	25/25	0.96	0.14	29,52,116,121	25
7	EDO	C	815	4/4	0.96	0.14	42,42,44,50	0
5	OPZ	C	803	25/25	0.96	0.14	26,67,87,96	0
7	EDO	C	817	4/4	0.97	0.14	37,52,55,58	0
7	EDO	A	812	4/4	0.97	0.18	33,39,42,43	0
7	EDO	A	817	4/4	0.97	0.16	42,43,49,49	0
7	EDO	A	820	4/4	0.98	0.17	48,56,58,60	0
2	FE	C	801	1/1	0.99	0.07	26,26,26,26	0
2	FE	A	801	1/1	1.00	0.06	28,28,28,28	0
2	FE	B	801	1/1	1.00	0.06	32,32,32,32	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.

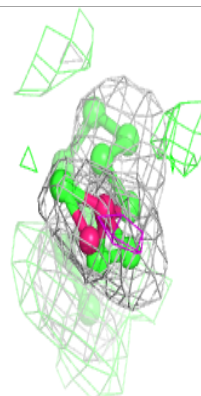
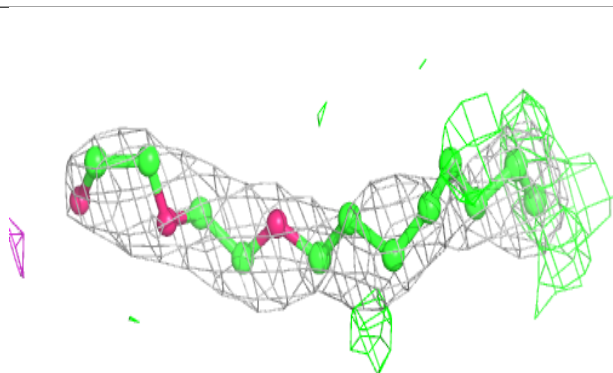
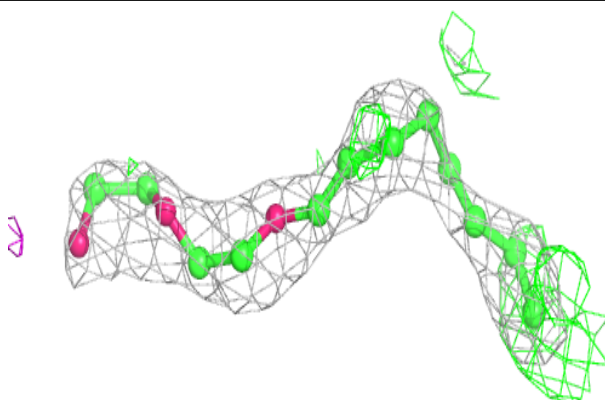
Electron density around C8E B 810:

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



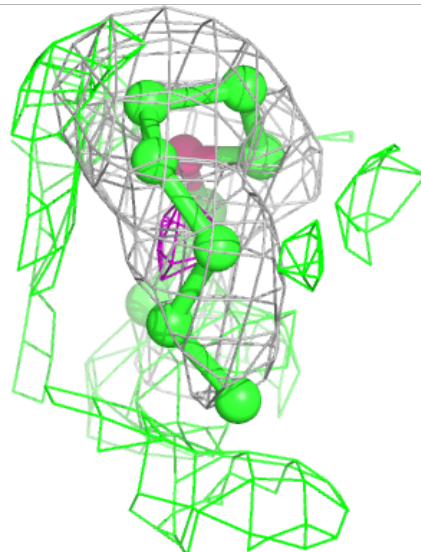
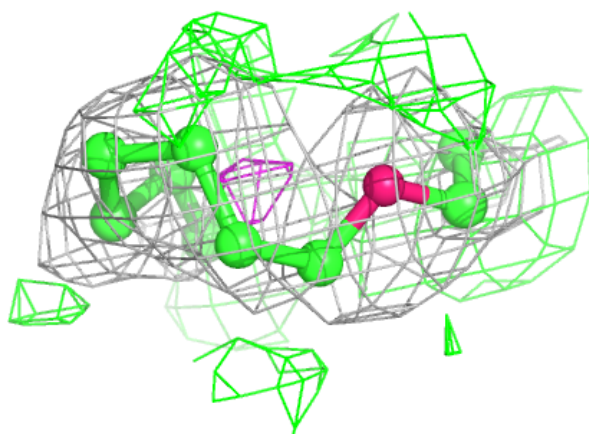
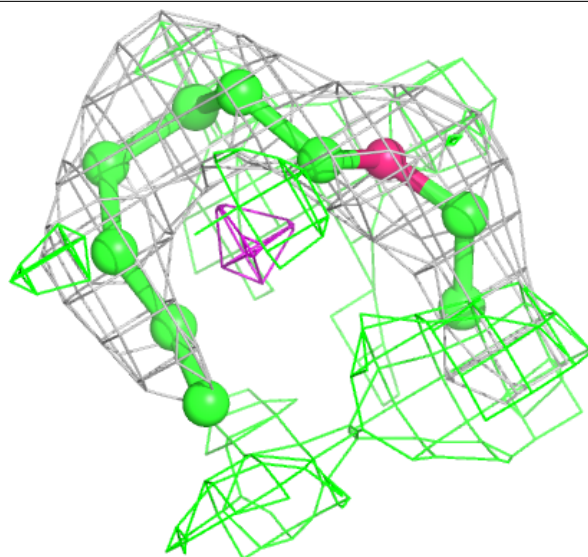
Electron density around C8E C 809:

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



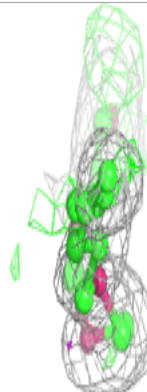
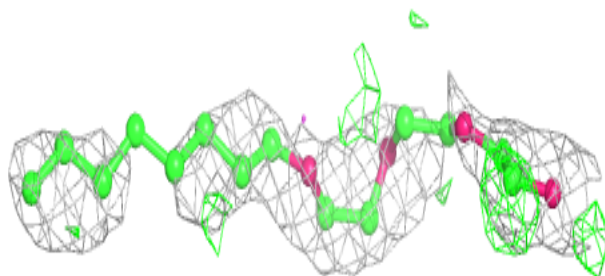
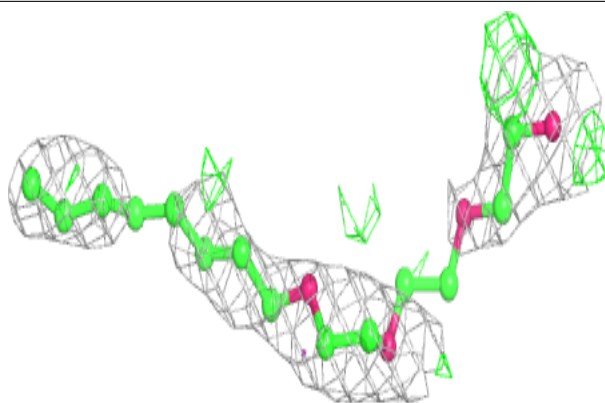
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and green (positive)

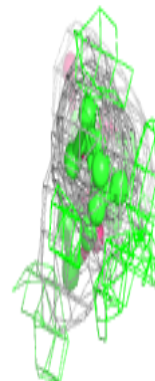
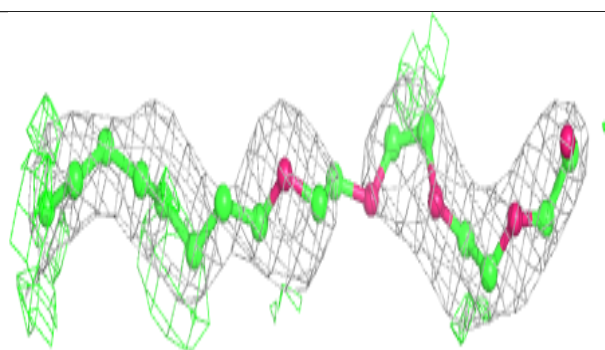
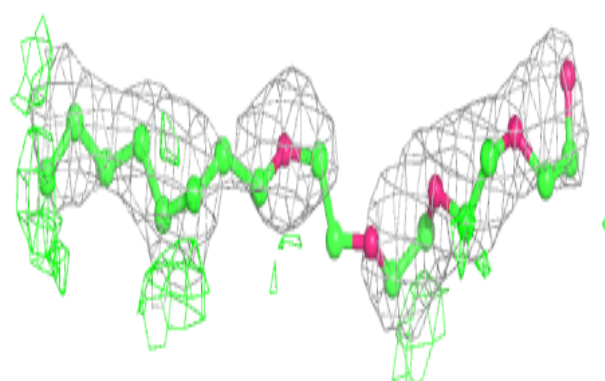


Electron density around C8E B 805:

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

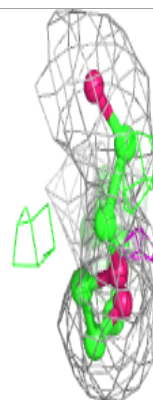
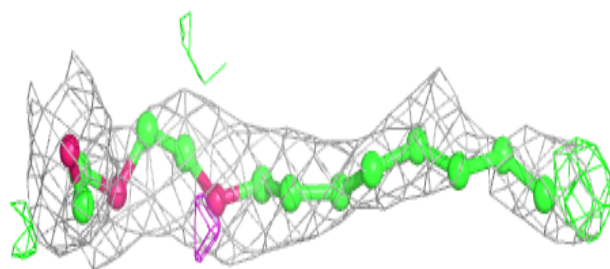
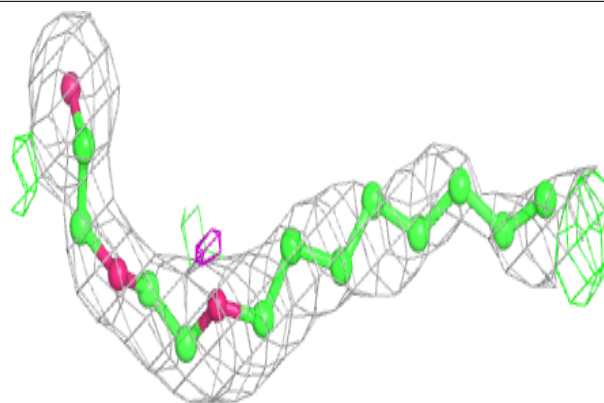
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

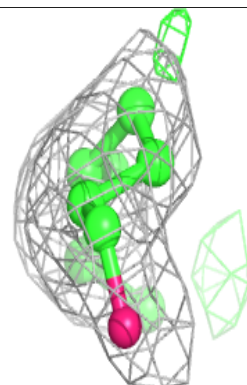
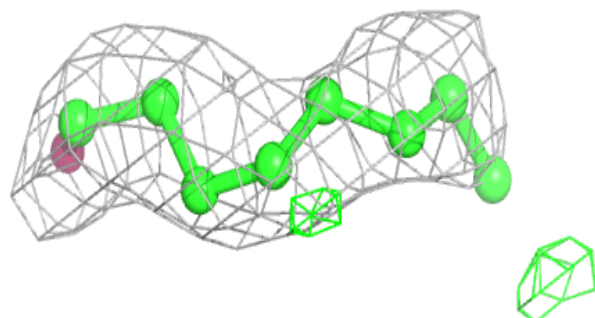
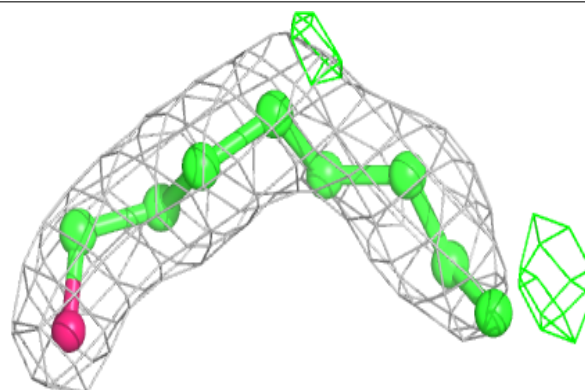


Electron density around C8E C 808:

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and green (positive)

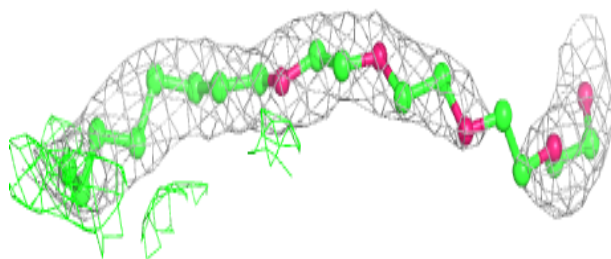
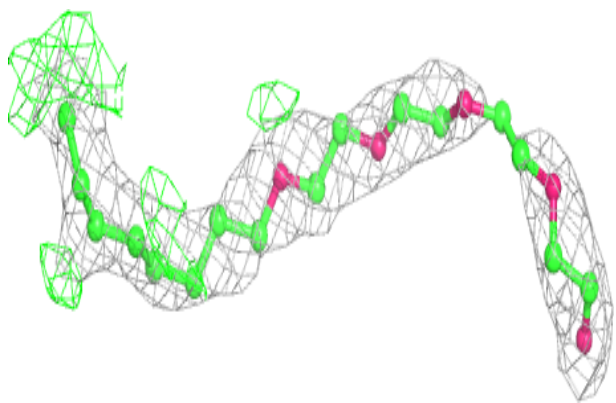
**Electron density around C8E A 808:**

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and green (positive)

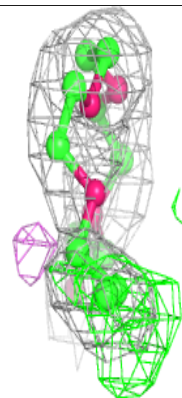
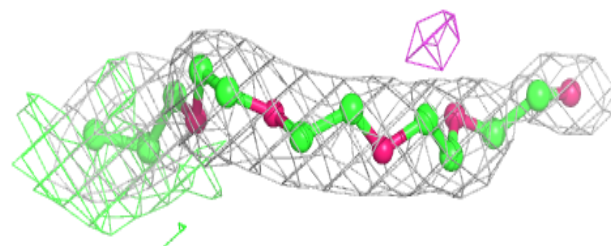
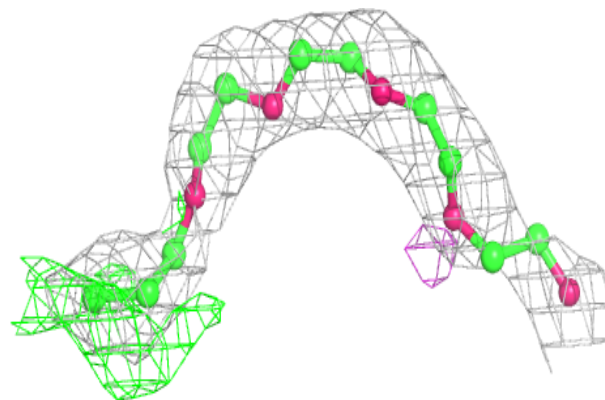


Electron density around C8E B 811:

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and green (positive)

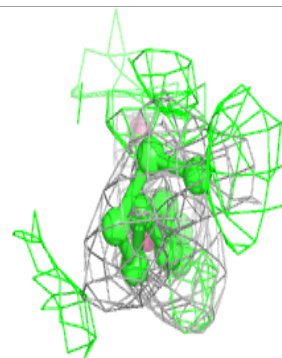
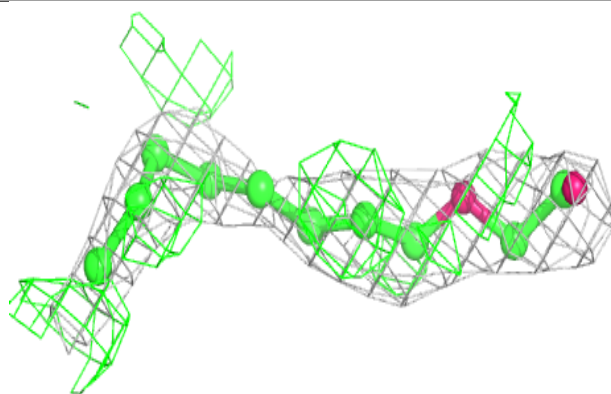
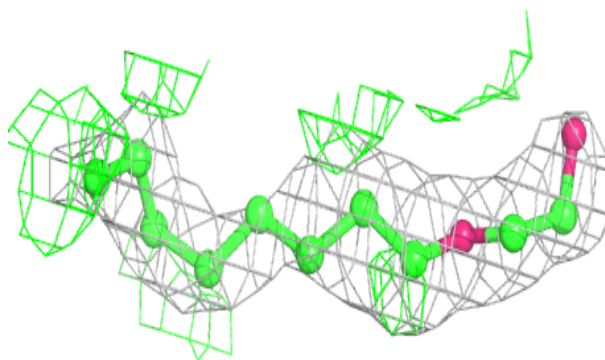
**Electron density around C8E C 805:**

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and green (positive)

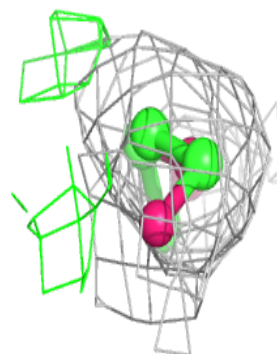
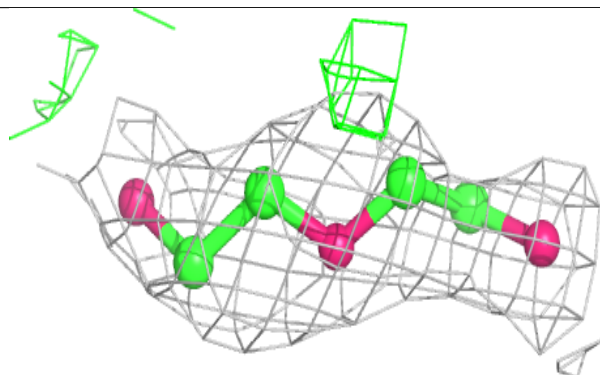
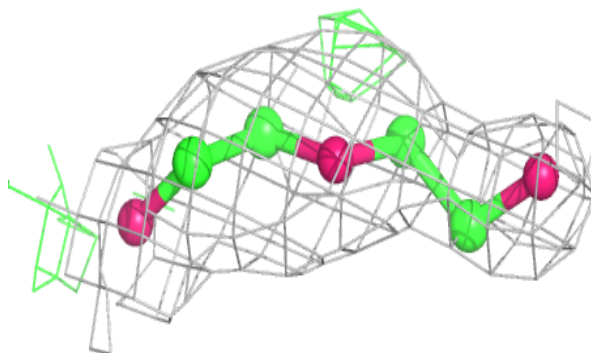


Electron density around C8E B 813:

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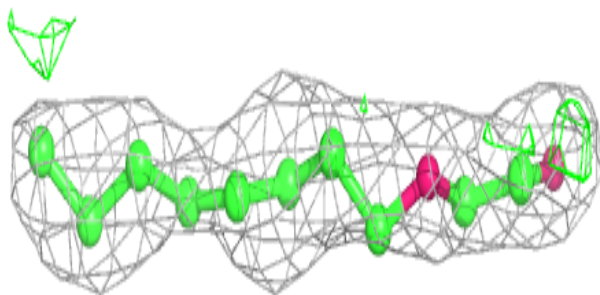
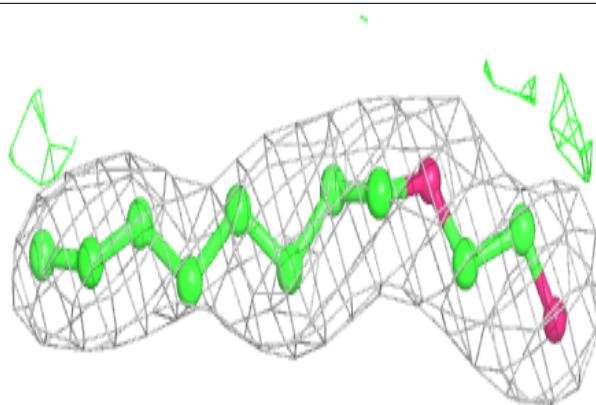
**Electron density around C8E C 810:**

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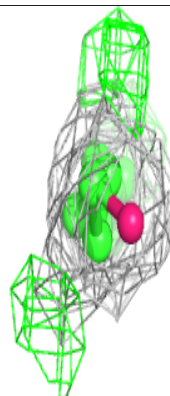
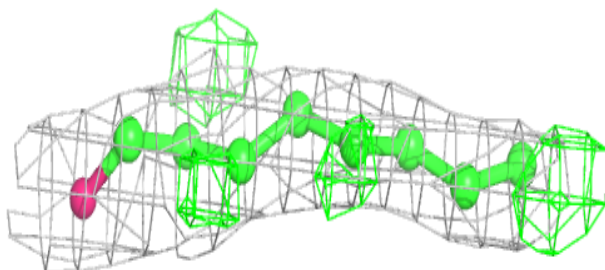
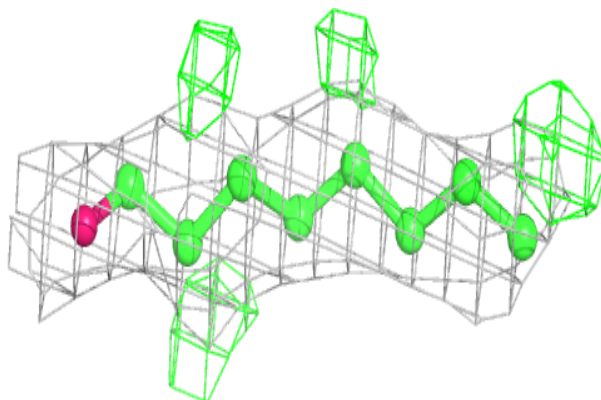


Electron density around C8E B 812:

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

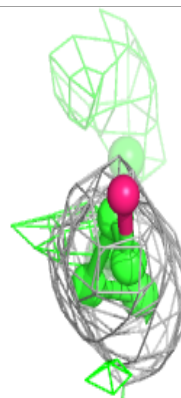
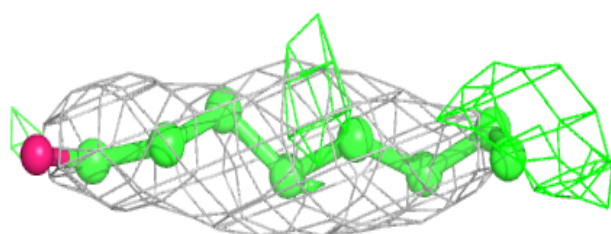
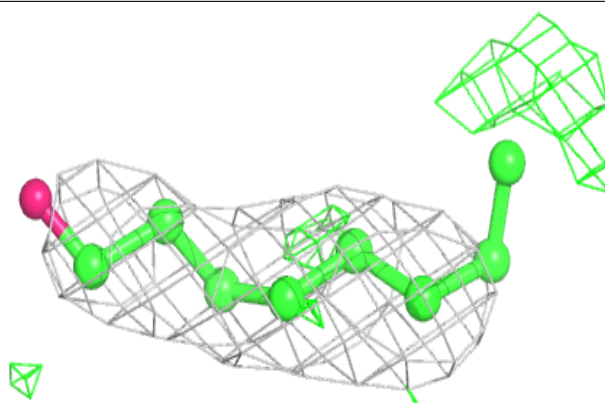
**Electron density around C8E A 806:**

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

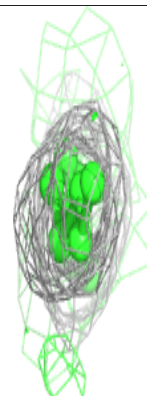
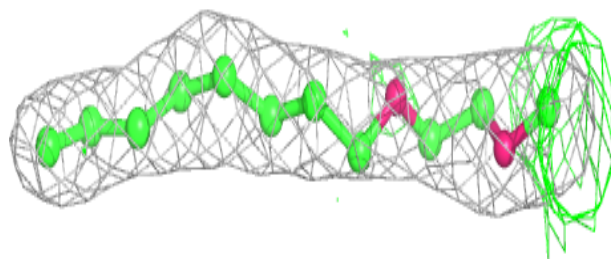
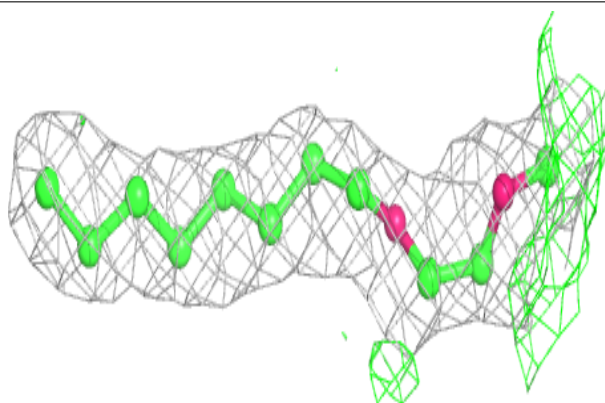


Electron density around C8E B 808:

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

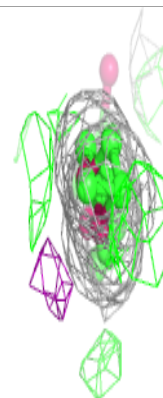
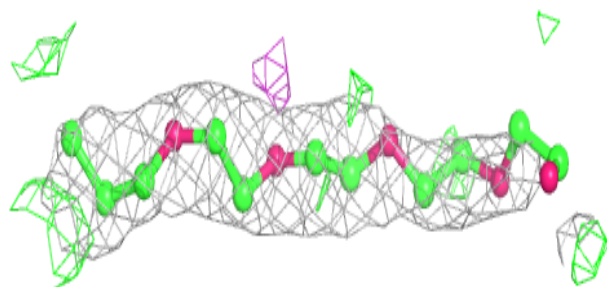
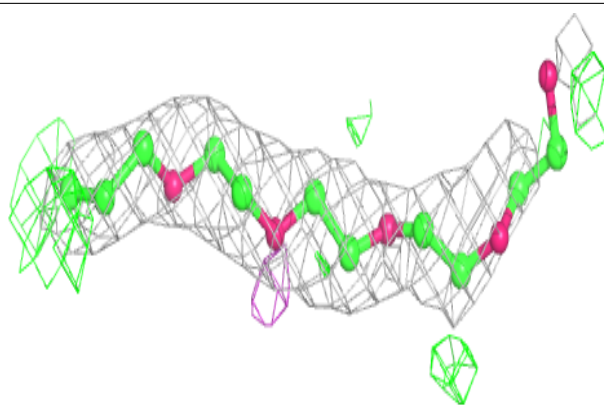
**Electron density around C8E B 806:**

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

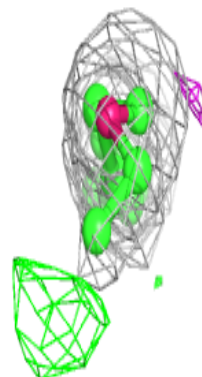
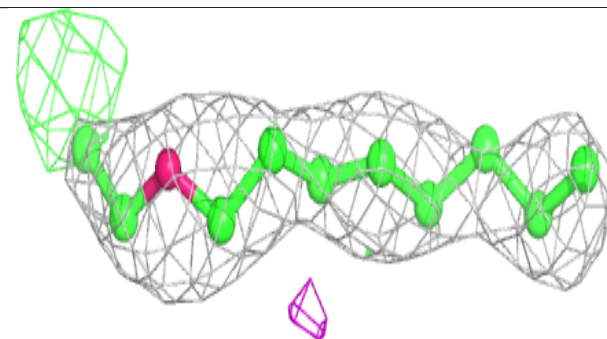
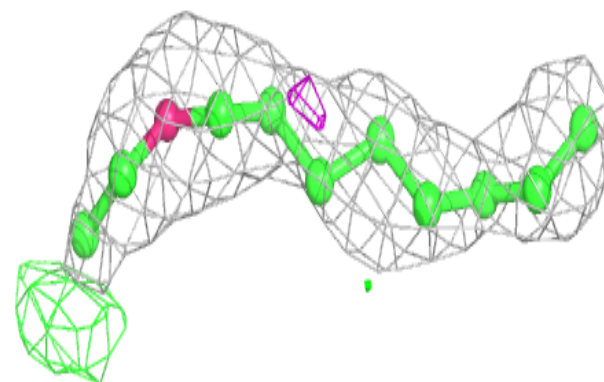


Electron density around C8E B 804:

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

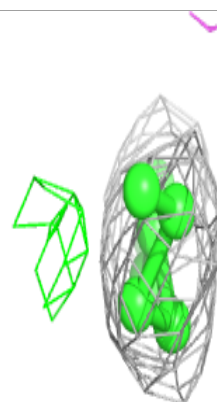
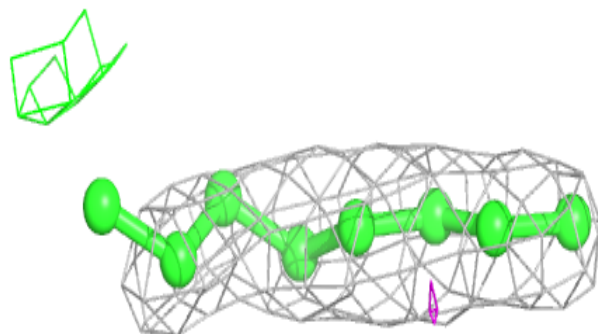
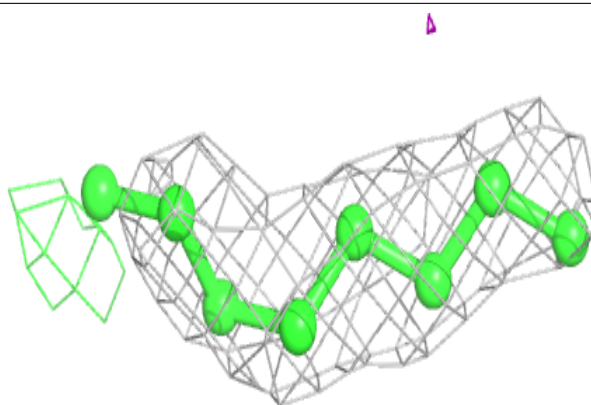
**Electron density around C8E A 805:**

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

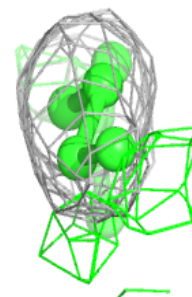
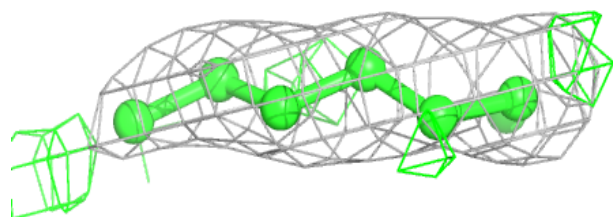
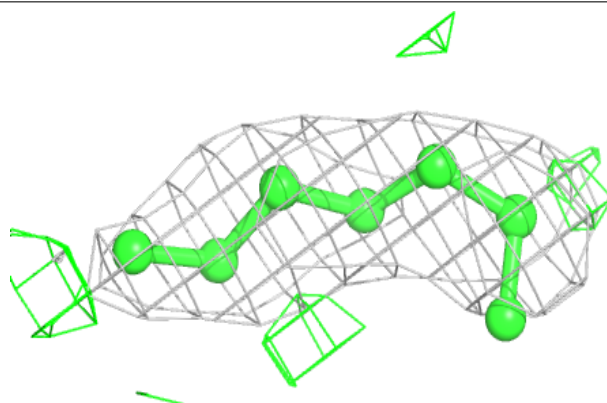


Electron density around C8E B 815:

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

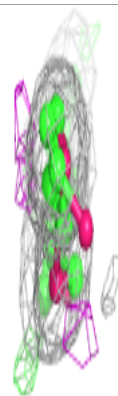
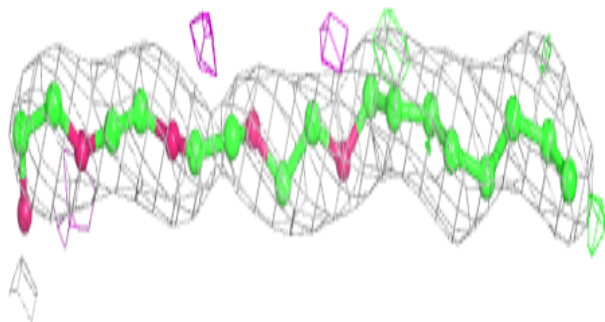
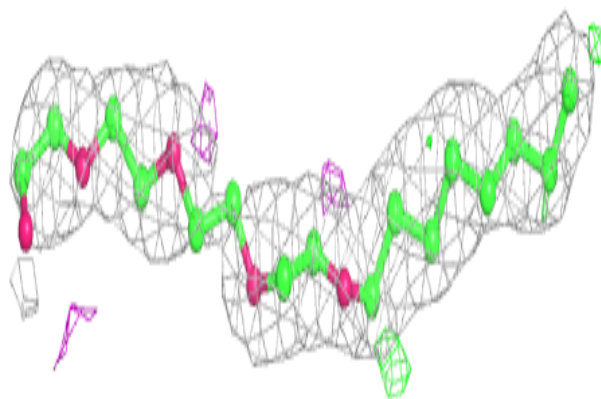
**Electron density around C8E A 809:**

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

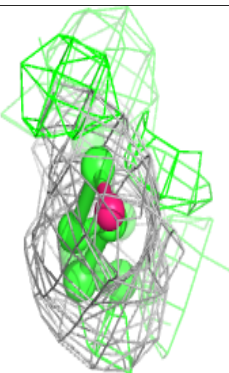
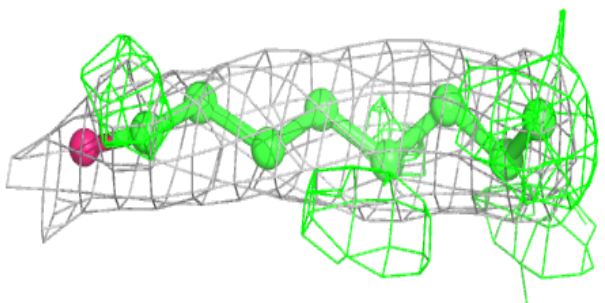
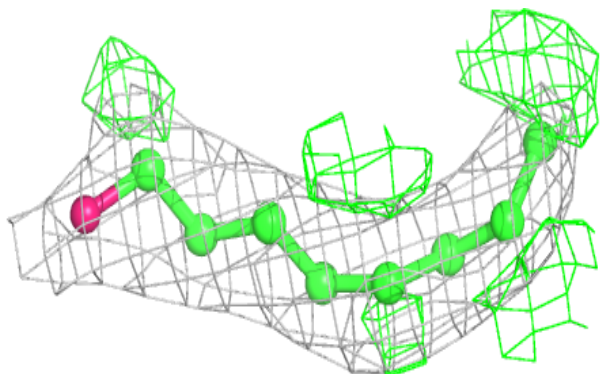


Electron density around C8E C 807:

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

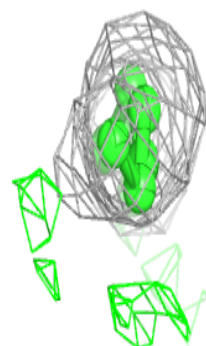
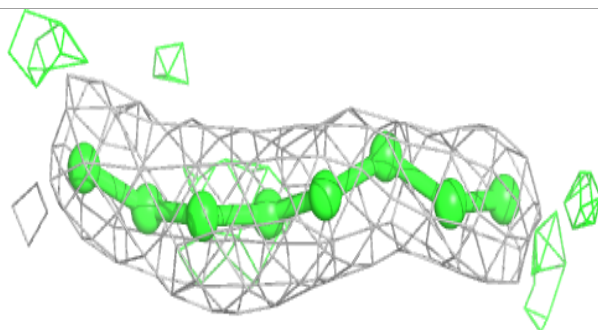
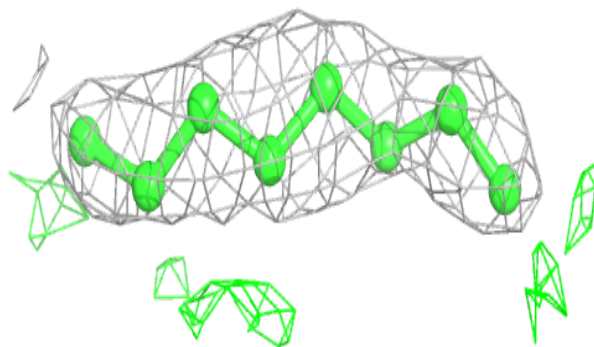
**Electron density around C8E A 810:**

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

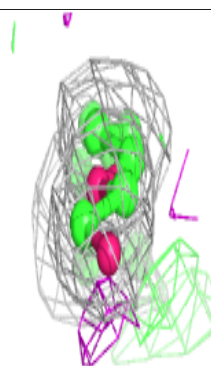
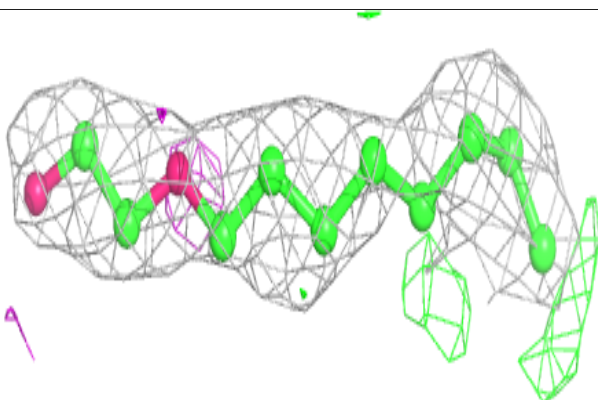
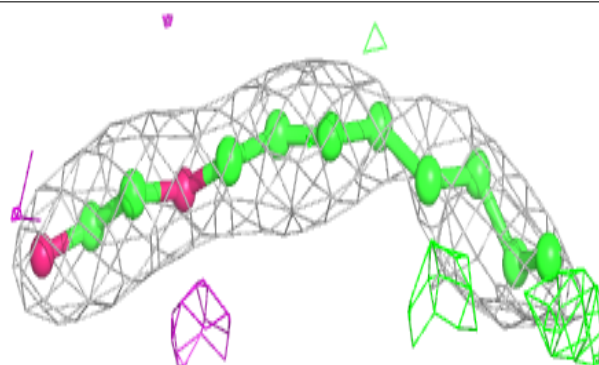


Electron density around C8E A 807:

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

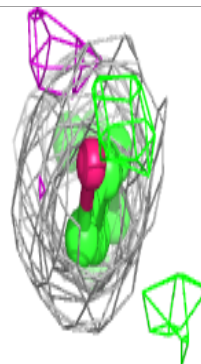
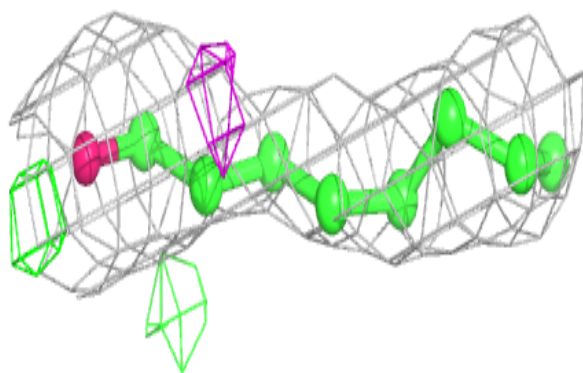
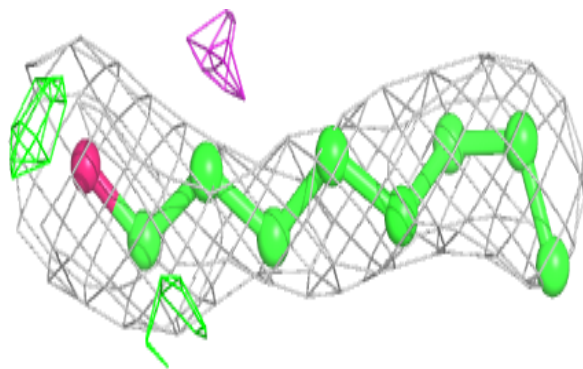
**Electron density around C8E B 809:**

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

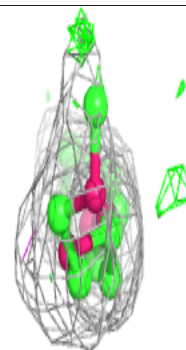
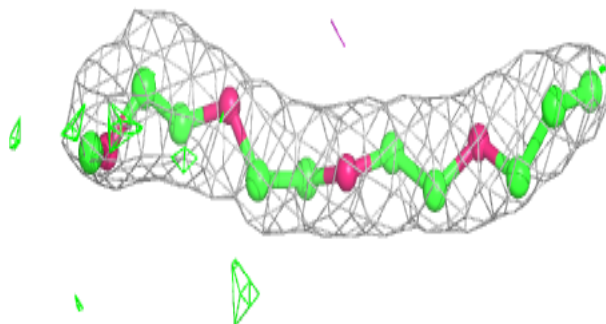
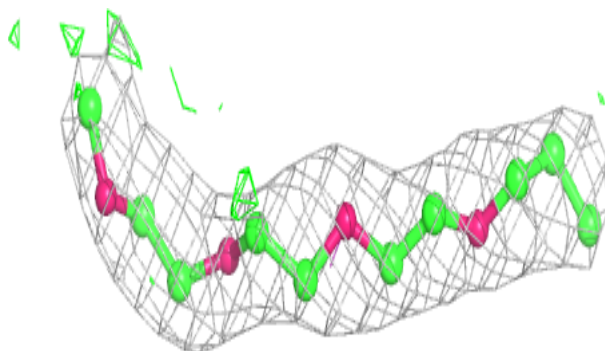


Electron density around C8E B 814:

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

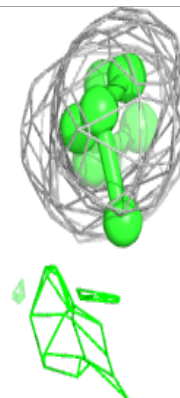
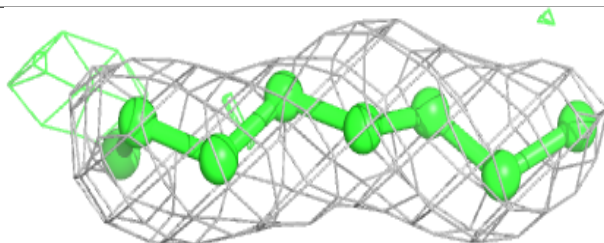
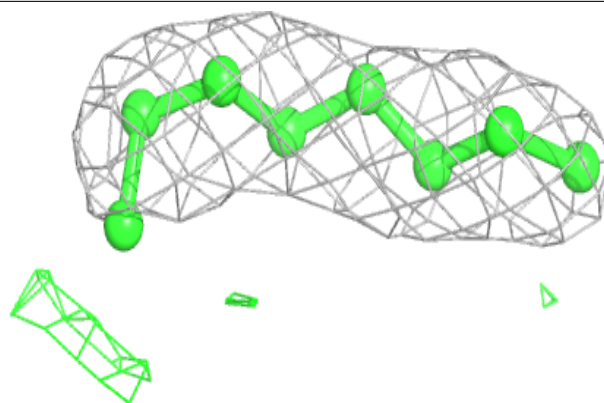
**Electron density around C8E C 806:**

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

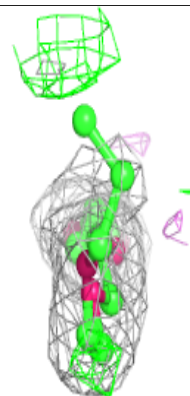
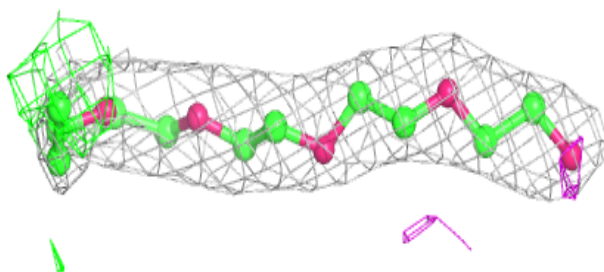
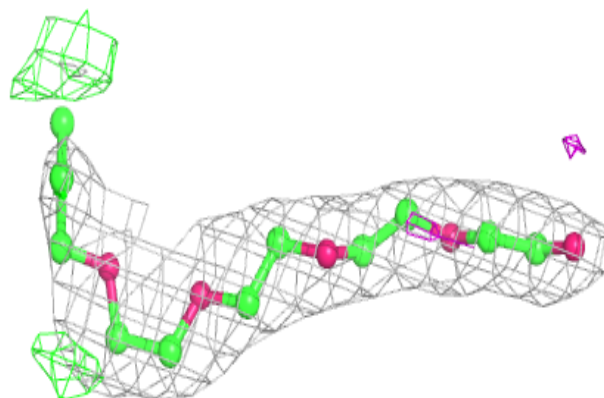


Electron density around C8E C 812:

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

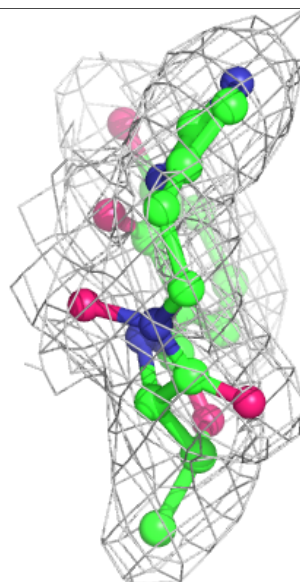
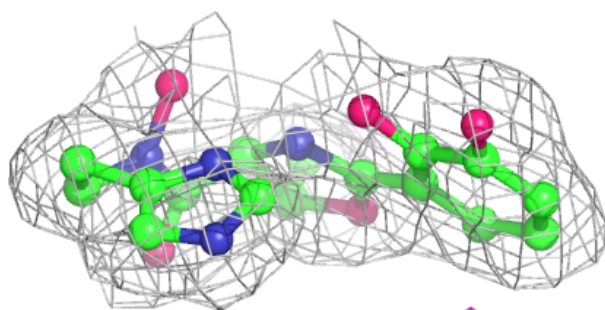
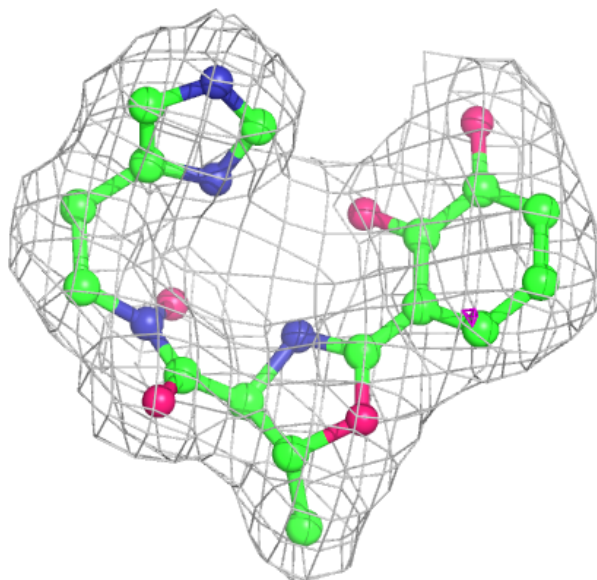
**Electron density around C8E C 804:**

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



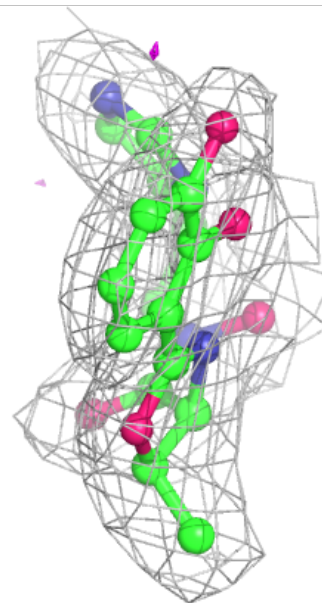
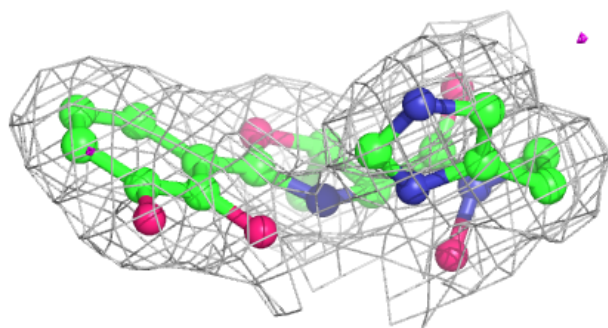
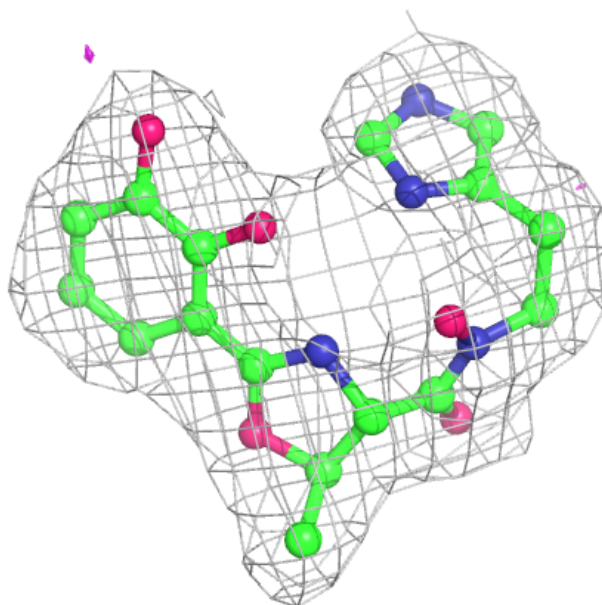
Electron density around FV8 C 802:

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



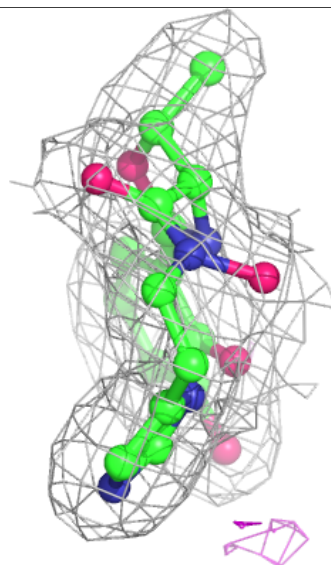
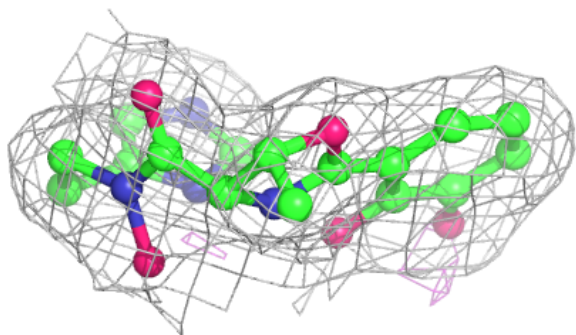
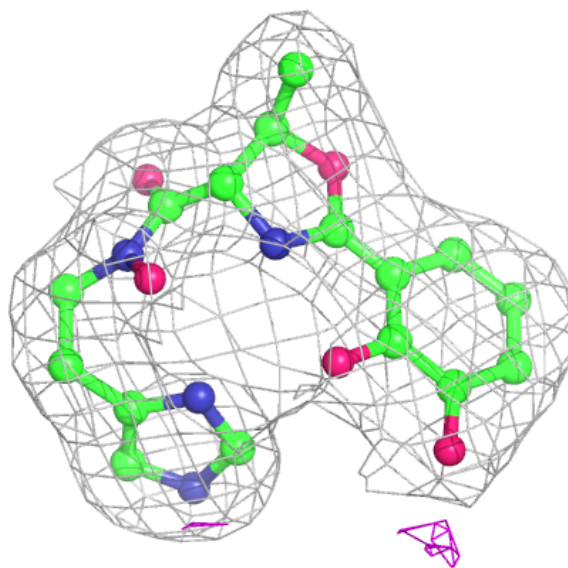
Electron density around FV8 A 802:

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



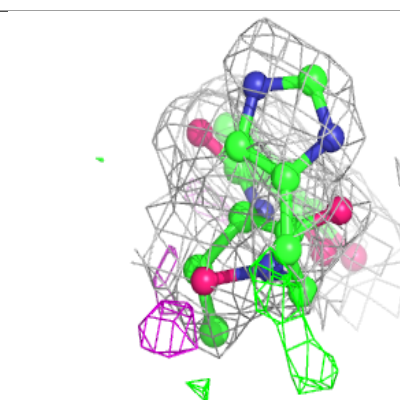
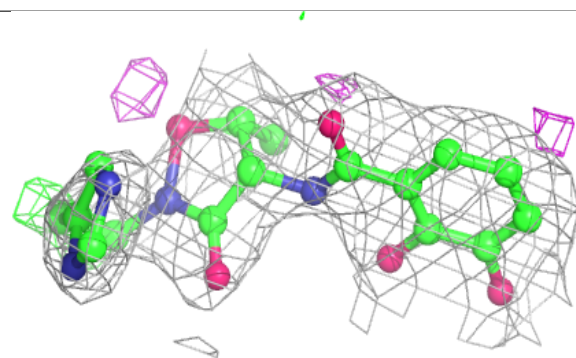
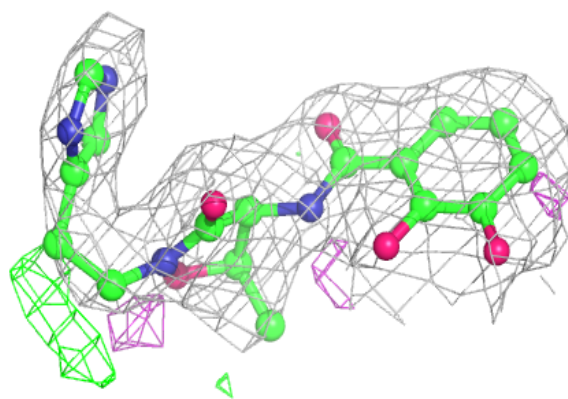
Electron density around FV8 B 802:

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

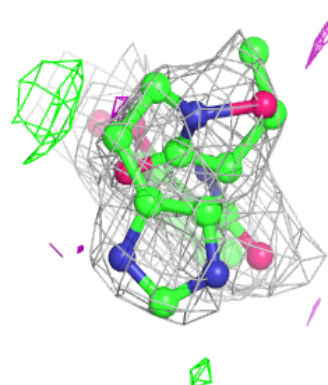
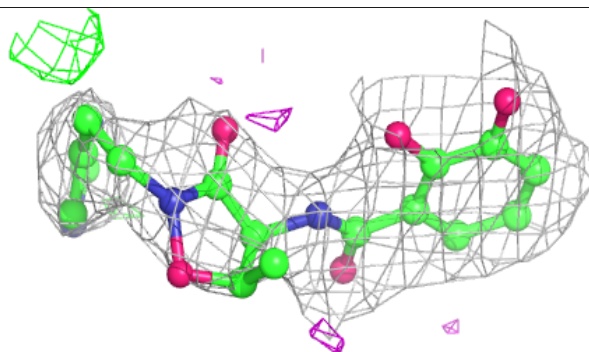
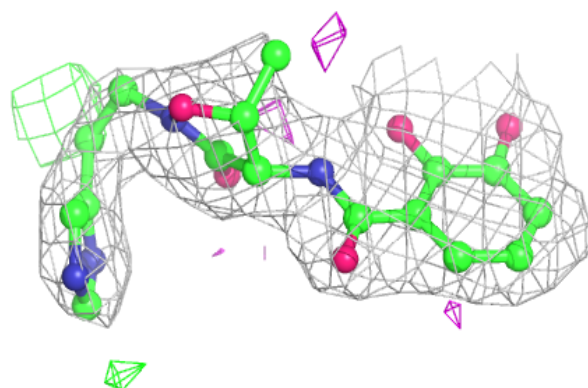


Electron density around OPZ A 804 (B):

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

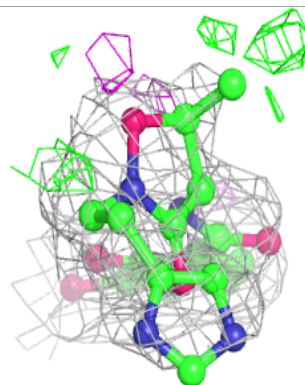
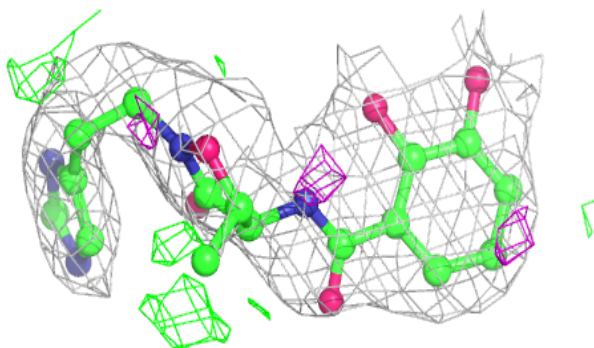
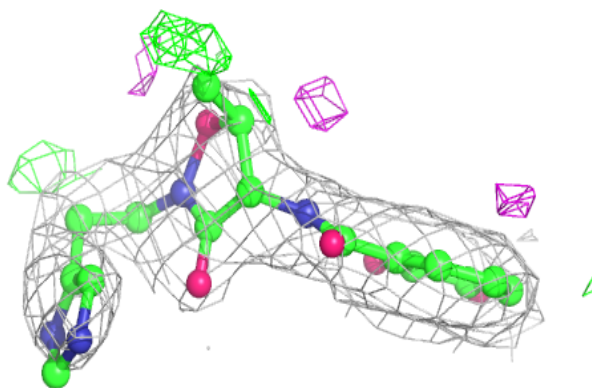
**Electron density around OPZ B 803:**

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

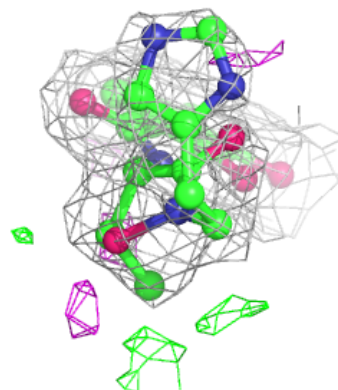
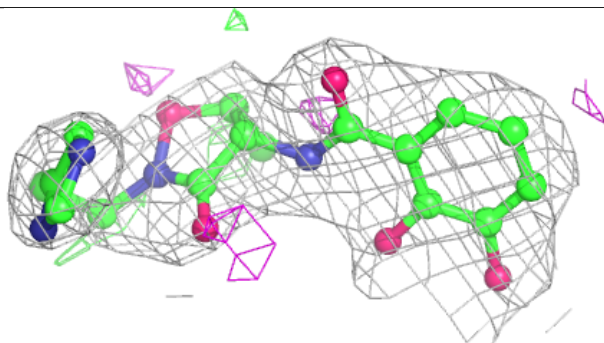
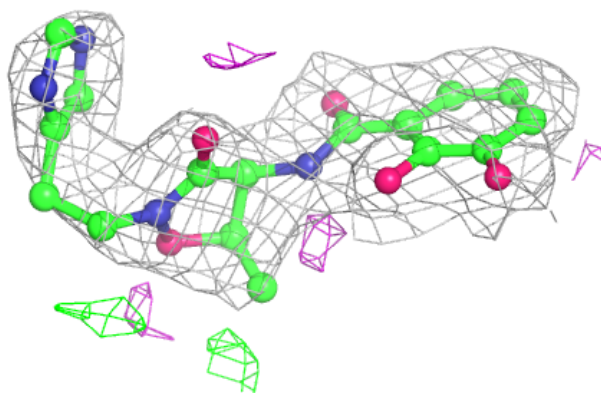


Electron density around OPV A 803 (A):

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

**Electron density around OPZ C 803:**

$2mF_o-DF_c$ (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.