



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 6H7F / pdb_00006h7f
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 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

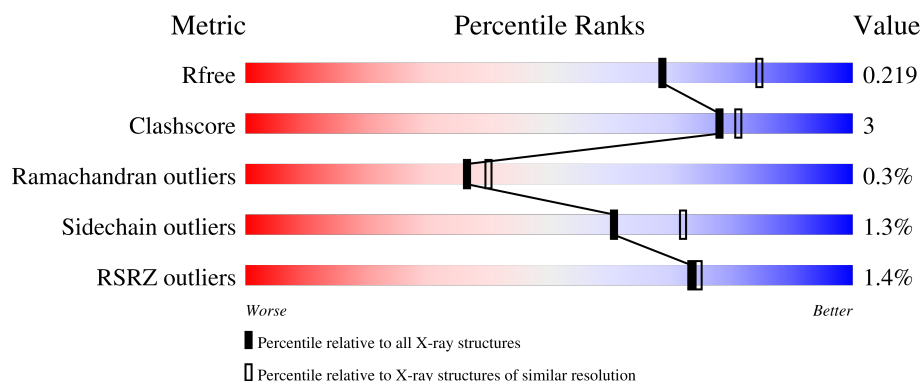
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

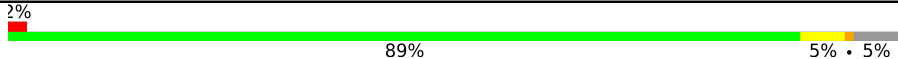
The reported resolution of this entry is 2.26 Å.

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	706	 2% 89% 5% • 5%
1	B	706	 % 89% 5% • 5%
1	C	706	 % 87% 7% • 5%

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:

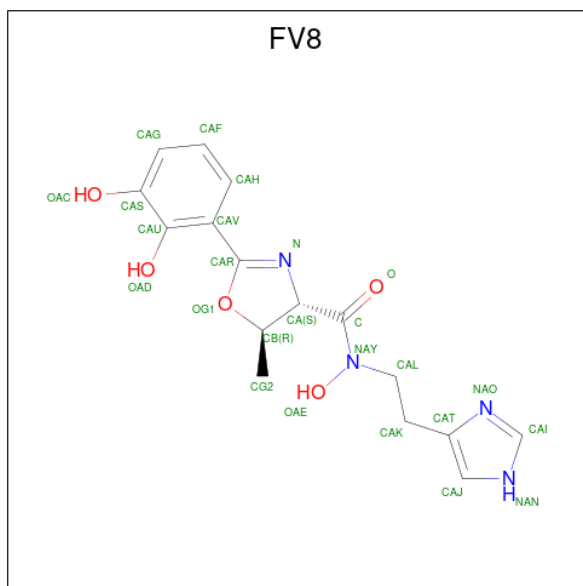
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q76HJ9
A	-1	ALA	-	expression tag	UNP Q76HJ9
A	0	MET	-	expression tag	UNP Q76HJ9
B	-2	GLY	-	expression tag	UNP Q76HJ9
B	-1	ALA	-	expression tag	UNP Q76HJ9
B	0	MET	-	expression tag	UNP Q76HJ9
C	-2	GLY	-	expression tag	UNP Q76HJ9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

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

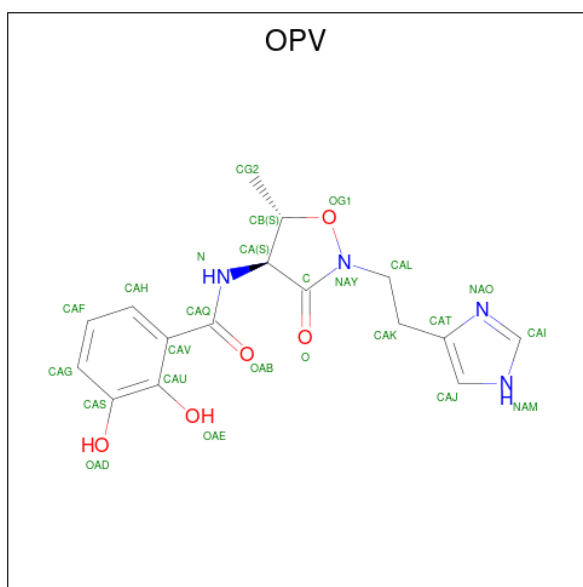
- Molecule 3 is (4 {S},5 {R})-2-[2,3-bis(oxidanyl)phenyl]- {N}-[2-(1 {H}-imidazol-4-yl)ethyl]-5-methyl- {N}-oxidanyl-4,5-dihydro-1,3-oxazole-4-carboxamide (CCD ID: FV8) (formula:

C₁₆H₁₈N₄O₅).



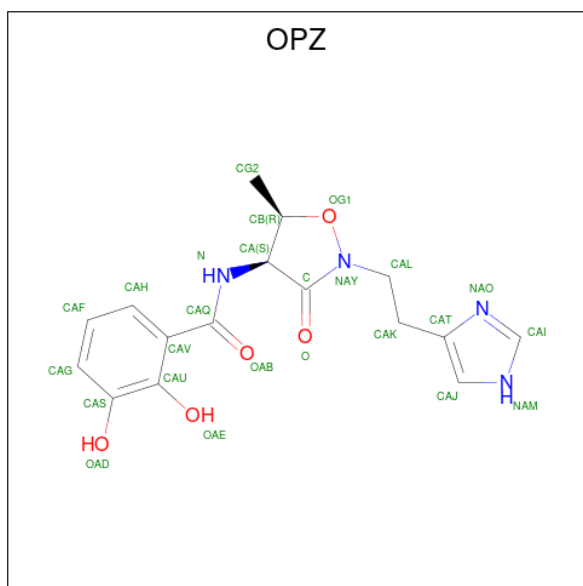
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	16	4	5		
3	B	1	Total	C	N	O	0	0
			25	16	4	5		
3	C	1	Total	C	N	O	0	0
			25	16	4	5		

- 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 (CCD ID: OPV) (formula: C₁₆H₁₈N₄O₅).



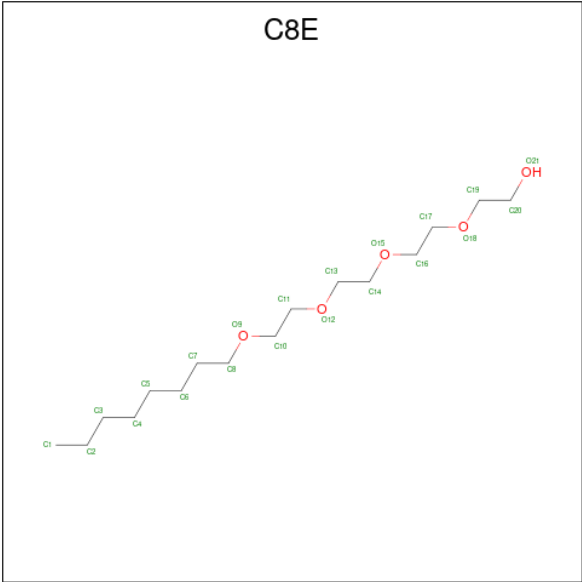
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			25	16	4	5		

- Molecule 5 is {N}-[(4 {S},5 {R})-2-[2-(1 {H}-imidazol-4-yl)ethyl]-5-methyl-3-oxidanylidene-1,2-oxazolidin-4-yl]-2,3-bis(oxidanyl)benzamide (CCD ID: 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 (CCD ID: 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 (CCD ID: 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	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

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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

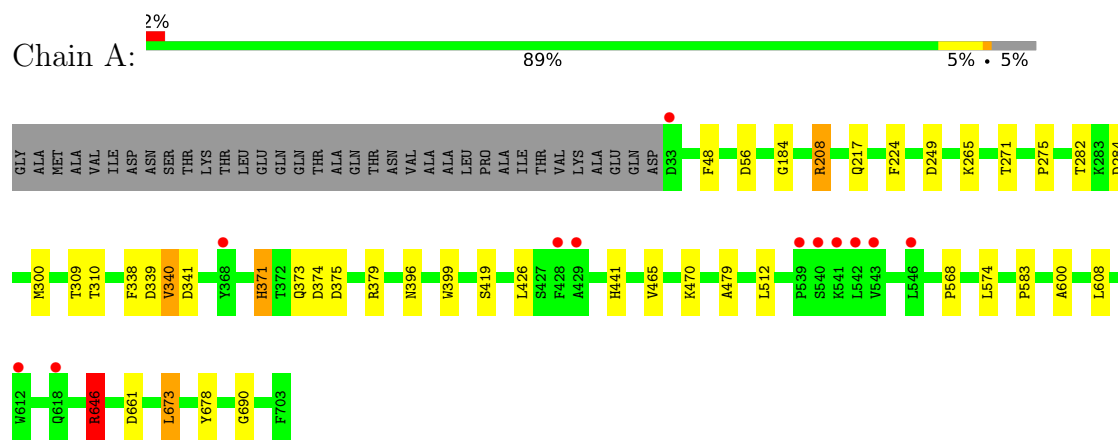
- Molecule 8 is water.

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

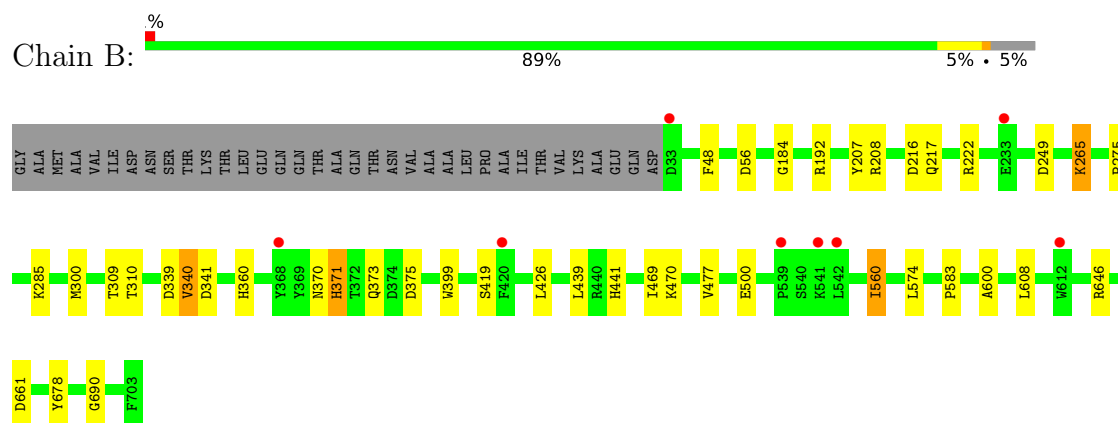
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

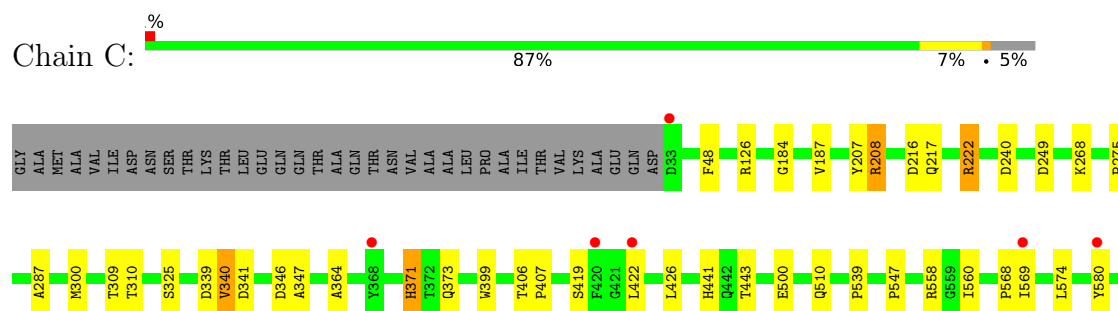
• Molecule 1: BauA

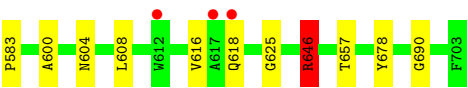


• Molecule 1: BauA



• 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 , 28.6	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: FE, EDO, OPV, OPZ, C8E, FV8

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	0.70	0/5354	0.76	0/7287
1	B	0.71	0/5323	0.76	0/7243
1	C	0.71	0/5376	0.76	0/7315
All	All	0.70	0/16053	0.76	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	24	0
1	B	5199	0	5014	26	0
1	C	5251	0	5062	40	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	91	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 (91) 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:OG1	5:B:803:OPZ:NAY	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
1:B:439:LEU:C	1:B:439:LEU:HD12	2.28	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:A:673:LEU:C	1:A:673:LEU:HD12	2.33	0.53
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:C:616:VAL:O	1:C:616:VAL:HG23	2.13	0.48
1:C:618:GLN:O	1:C:657:THR:OG1	2.26	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:678:TYR:CZ	1:C:690:GLY:HA3	2.49	0.48
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:C:300:MET:HB3	1:C:300:MET:HE2	1.76	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:O	4:A:803[A]:OPV:CAJ	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:N	1:A:426:LEU:HD12	2.34	0.42
1:C:406:THR:N	1:C:407:PRO:CD	2.82	0.42
1:A:265:LYS:NZ	1:B:216:ASP:OD2	2.39	0.42
1:C:347:ALA:HB1	6:C:807:C8E:H101	2.01	0.42
1:B:426:LEU:HD12	1:B:426:LEU:N	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:B:300:MET:HE2	1:B:300:MET:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:300:MET:HE2	1:A:300:MET:HB3	1.81	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%)	36	40
1	B	678/706 (96%)	657 (97%)	19 (3%)	2 (0%)	36	40
1	C	684/706 (97%)	663 (97%)	19 (3%)	2 (0%)	36	40
All	All	2044/2118 (96%)	1981 (97%)	57 (3%)	6 (0%)	36	40

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 ⓘ

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%)	555 (99%)	8 (1%)	59	70
1	B	559/577 (97%)	551 (99%)	8 (1%)	59	70
1	C	565/577 (98%)	560 (99%)	5 (1%)	70	79
All	All	1687/1731 (98%)	1666 (99%)	21 (1%)	61	74

All (21) 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	465	VAL
1	A	646	ARG
1	A	661	ASP
1	A	673	LEU
1	B	48	PHE
1	B	265	LYS
1	B	340	VAL
1	B	371	HIS
1	B	375	ASP
1	B	560	ILE
1	B	646	ARG
1	B	661	ASP
1	C	48	PHE
1	C	340	VAL
1	C	371	HIS
1	C	569	ILE
1	C	646	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	234	ASN
1	A	298	GLN
1	A	370	ASN
1	A	373	GLN
1	A	669	ASN
1	A	683	GLN
1	B	73	GLN
1	B	298	GLN
1	B	669	ASN
1	B	683	GLN
1	C	215	ASN
1	C	234	ASN
1	C	615	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
6	C8E	C	807	-	20,20,20	0.69	0	19,19,19	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	C	817	-	3,3,3	0.51	0	2,2,2	0.49	0
6	C8E	A	806	-	8,8,20	0.49	0	7,7,19	0.33	0
6	C8E	A	805	-	10,10,20	0.56	0	9,9,19	0.34	0
6	C8E	B	805	-	17,17,20	0.70	0	16,16,19	0.43	0
6	C8E	C	813	-	6,6,20	0.55	0	5,5,19	0.25	0
6	C8E	B	809	-	11,11,20	0.47	0	10,10,19	0.39	0
6	C8E	B	806	-	12,12,20	0.50	0	11,11,19	0.33	0
6	C8E	B	812	-	11,11,20	0.50	0	10,10,19	0.44	0
7	EDO	C	818	-	3,3,3	0.30	0	2,2,2	0.71	0
7	EDO	B	816	-	3,3,3	0.51	0	2,2,2	0.35	0
7	EDO	A	822	-	3,3,3	0.51	0	2,2,2	0.27	0
7	EDO	C	814	-	3,3,3	0.52	0	2,2,2	0.29	0
7	EDO	A	821	-	3,3,3	0.40	0	2,2,2	0.48	0
7	EDO	A	816	-	3,3,3	0.36	0	2,2,2	0.43	0
7	EDO	A	819	-	3,3,3	0.36	0	2,2,2	0.47	0
6	C8E	C	809	-	14,14,20	0.53	0	13,13,19	0.41	0
6	C8E	B	815	-	7,7,20	0.46	0	6,6,19	0.32	0
7	EDO	C	829	-	3,3,3	0.39	0	2,2,2	0.47	0
7	EDO	C	830	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	C	826	-	3,3,3	0.43	0	2,2,2	0.60	0
7	EDO	C	827	-	3,3,3	0.56	0	2,2,2	0.15	0
7	EDO	B	827	-	3,3,3	0.36	0	2,2,2	0.45	0
7	EDO	A	812	-	3,3,3	0.31	0	2,2,2	0.61	0
5	OPZ	A	804[B]	2	27,27,27	2.11	4 (14%)	30,38,38	1.41	3 (10%)
6	C8E	A	809	-	6,6,20	0.58	0	5,5,19	0.41	0
6	C8E	A	810	-	8,8,20	0.34	0	7,7,19	0.47	0
3	FV8	A	802	2	26,27,27	2.28	9 (34%)	31,38,38	2.28	7 (22%)
7	EDO	C	824	-	3,3,3	0.38	0	2,2,2	0.45	0
7	EDO	B	818	-	3,3,3	0.31	0	2,2,2	0.95	0
7	EDO	A	823	-	3,3,3	0.42	0	2,2,2	0.61	0
7	EDO	C	828	-	3,3,3	0.48	0	2,2,2	0.41	0
7	EDO	B	828	-	3,3,3	0.78	0	2,2,2	0.44	0
7	EDO	A	814	-	3,3,3	0.23	0	2,2,2	0.54	0
6	C8E	A	807	-	7,7,20	0.47	0	6,6,19	0.37	0
7	EDO	A	820	-	3,3,3	0.41	0	2,2,2	0.37	0
7	EDO	A	817	-	3,3,3	0.40	0	2,2,2	0.28	0
7	EDO	B	822	-	3,3,3	0.33	0	2,2,2	0.40	0
3	FV8	B	802	2	26,27,27	3.98	4 (15%)	31,38,38	2.25	8 (25%)
6	C8E	B	807	-	20,20,20	0.58	0	19,19,19	0.37	0
6	C8E	B	811	-	20,20,20	0.65	0	19,19,19	0.28	0
7	EDO	A	815	-	3,3,3	0.41	0	2,2,2	0.67	0
7	EDO	A	813	-	3,3,3	0.42	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	C8E	B	814	-	8,8,20	0.56	0	7,7,19	0.38	0
7	EDO	C	822	-	3,3,3	0.46	0	2,2,2	0.49	0
6	C8E	C	810	-	6,6,20	0.55	0	5,5,19	0.22	0
3	FV8	C	802	2	26,27,27	2.51	8 (30%)	31,38,38	2.16	6 (19%)
6	C8E	C	812	-	7,7,20	0.30	0	6,6,19	0.48	0
7	EDO	C	821	-	3,3,3	0.38	0	2,2,2	0.46	0
5	OPZ	C	803	2	27,27,27	1.90	6 (22%)	30,38,38	1.73	5 (16%)
6	C8E	C	805	-	15,15,20	0.56	0	14,14,19	0.28	0
7	EDO	A	818	-	3,3,3	0.37	0	2,2,2	0.45	0
6	C8E	B	810	-	7,7,20	0.56	0	6,6,19	0.28	0
7	EDO	C	819	-	3,3,3	0.26	0	2,2,2	0.85	0
7	EDO	B	825	-	3,3,3	0.42	0	2,2,2	0.39	0
7	EDO	C	823	-	3,3,3	0.55	0	2,2,2	0.28	0
7	EDO	C	815	-	3,3,3	0.40	0	2,2,2	0.18	0
6	C8E	B	813	-	11,11,20	0.55	0	10,10,19	0.32	0
5	OPZ	B	803	2	27,27,27	2.43	6 (22%)	30,38,38	1.63	4 (13%)
7	EDO	B	823	-	3,3,3	0.42	0	2,2,2	0.50	0
6	C8E	C	804	-	15,15,20	0.57	0	14,14,19	0.34	0
6	C8E	C	808	-	14,14,20	0.67	0	13,13,19	0.49	0
7	EDO	B	817	-	3,3,3	0.27	0	2,2,2	0.71	0
7	EDO	A	811	-	3,3,3	0.69	0	2,2,2	0.06	0
7	EDO	B	819	-	3,3,3	0.34	0	2,2,2	0.56	0
7	EDO	B	820	-	3,3,3	0.38	0	2,2,2	0.33	0
7	EDO	B	821	-	3,3,3	0.36	0	2,2,2	0.46	0
6	C8E	B	808	-	8,8,20	0.32	0	7,7,19	0.40	0
7	EDO	B	826	-	3,3,3	0.49	0	2,2,2	0.37	0
4	OPV	A	803[A]	2	27,27,27	2.17	6 (22%)	30,38,38	1.80	3 (10%)
7	EDO	B	824	-	3,3,3	0.31	0	2,2,2	0.53	0
6	C8E	A	808	-	8,8,20	0.44	0	7,7,19	0.33	0
7	EDO	C	820	-	3,3,3	0.27	0	2,2,2	0.54	0
6	C8E	C	806	-	13,13,20	0.62	0	12,12,19	0.29	0
7	EDO	C	825	-	3,3,3	0.40	0	2,2,2	0.36	0
6	C8E	C	811	-	9,9,20	0.50	0	8,8,19	0.36	0
6	C8E	B	804	-	15,15,20	0.53	0	14,14,19	0.26	0
7	EDO	C	816	-	3,3,3	0.32	0	2,2,2	0.79	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
6	C8E	C	807	-	-	11/18/18/18	-
7	EDO	C	817	-	-	1/1/1/1	-
6	C8E	A	806	-	-	3/6/6/18	-
6	C8E	A	805	-	-	6/8/8/18	-
6	C8E	B	805	-	-	5/15/15/18	-
6	C8E	C	813	-	-	0/4/4/18	-
6	C8E	B	809	-	-	2/9/9/18	-
6	C8E	B	806	-	-	3/10/10/18	-
6	C8E	B	812	-	-	7/9/9/18	-
7	EDO	C	818	-	-	0/1/1/1	-
7	EDO	B	816	-	-	0/1/1/1	-
7	EDO	A	822	-	-	0/1/1/1	-
7	EDO	C	814	-	-	1/1/1/1	-
7	EDO	A	821	-	-	1/1/1/1	-
7	EDO	A	816	-	-	0/1/1/1	-
7	EDO	A	819	-	-	0/1/1/1	-
6	C8E	C	809	-	-	5/12/12/18	-
6	C8E	B	815	-	-	1/5/5/18	-
7	EDO	C	829	-	-	1/1/1/1	-
7	EDO	C	830	-	-	0/1/1/1	-
7	EDO	C	826	-	-	0/1/1/1	-
7	EDO	C	827	-	-	1/1/1/1	-
7	EDO	B	827	-	-	1/1/1/1	-
7	EDO	A	812	-	-	0/1/1/1	-
5	OPZ	A	804[B]	2	-	1/13/29/29	0/3/3/3
6	C8E	A	809	-	-	1/4/4/18	-
6	C8E	A	810	-	-	3/6/6/18	-
3	FV8	A	802	2	-	4/16/29/29	0/3/3/3
7	EDO	C	824	-	-	0/1/1/1	-
7	EDO	B	818	-	-	1/1/1/1	-
7	EDO	A	823	-	-	1/1/1/1	-
7	EDO	C	828	-	-	0/1/1/1	-
7	EDO	B	828	-	-	1/1/1/1	-
7	EDO	A	814	-	-	1/1/1/1	-
6	C8E	A	807	-	-	1/5/5/18	-
7	EDO	A	820	-	-	0/1/1/1	-
7	EDO	A	817	-	-	1/1/1/1	-
7	EDO	B	822	-	-	0/1/1/1	-
3	FV8	B	802	2	-	3/16/29/29	0/3/3/3
6	C8E	B	807	-	-	10/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C8E	B	811	-	-	8/18/18/18	-
7	EDO	A	815	-	-	0/1/1/1	-
7	EDO	A	813	-	-	1/1/1/1	-
6	C8E	B	814	-	-	2/6/6/18	-
7	EDO	C	822	-	-	1/1/1/1	-
6	C8E	C	810	-	-	3/4/4/18	-
3	FV8	C	802	2	-	3/16/29/29	0/3/3/3
6	C8E	C	812	-	-	2/5/5/18	-
7	EDO	C	821	-	-	0/1/1/1	-
5	OPZ	C	803	2	-	0/13/29/29	0/3/3/3
6	C8E	C	805	-	-	5/13/13/18	-
7	EDO	A	818	-	-	0/1/1/1	-
6	C8E	B	810	-	-	3/5/5/18	-
7	EDO	C	819	-	-	1/1/1/1	-
7	EDO	B	825	-	-	1/1/1/1	-
7	EDO	C	823	-	-	0/1/1/1	-
7	EDO	C	815	-	-	0/1/1/1	-
6	C8E	B	813	-	-	5/9/9/18	-
5	OPZ	B	803	2	-	5/13/29/29	0/3/3/3
7	EDO	B	823	-	-	0/1/1/1	-
6	C8E	C	804	-	-	7/13/13/18	-
6	C8E	C	808	-	-	5/12/12/18	-
7	EDO	B	817	-	-	0/1/1/1	-
7	EDO	A	811	-	-	0/1/1/1	-
7	EDO	B	819	-	-	1/1/1/1	-
7	EDO	B	820	-	-	1/1/1/1	-
7	EDO	B	821	-	-	0/1/1/1	-
6	C8E	B	808	-	-	4/6/6/18	-
7	EDO	B	826	-	-	0/1/1/1	-
4	OPV	A	803[A]	2	-	0/13/29/29	0/3/3/3
7	EDO	B	824	-	-	1/1/1/1	-
6	C8E	A	808	-	-	5/6/6/18	-
7	EDO	C	820	-	-	0/1/1/1	-
6	C8E	C	806	-	-	7/11/11/18	-
7	EDO	C	825	-	-	1/1/1/1	-
6	C8E	C	811	-	-	3/7/7/18	-
6	C8E	B	804	-	-	10/13/13/18	-
7	EDO	C	816	-	-	1/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	FV8	OAE-NAY	17.32	1.53	1.40
5	B	803	OPZ	OG1-NAY	7.65	1.57	1.46
3	C	802	FV8	CAV-CAR	-7.14	1.34	1.47
4	A	803[A]	OPV	OG1-NAY	7.08	1.56	1.46
5	A	804[B]	OPZ	OG1-NAY	6.50	1.55	1.46
3	B	802	FV8	CAV-CAR	-6.28	1.36	1.47
3	A	802	FV8	CAV-CAR	-6.28	1.36	1.47
3	B	802	FV8	CAR-N	6.20	1.36	1.27
3	C	802	FV8	CAR-N	5.94	1.35	1.27
3	A	802	FV8	CAR-N	5.66	1.35	1.27
5	C	803	OPZ	CAV-CAQ	-5.23	1.39	1.50
5	A	804[B]	OPZ	CAV-CAQ	-5.05	1.40	1.50
5	B	803	OPZ	CAV-CAQ	-5.04	1.40	1.50
5	B	803	OPZ	CAL-NAY	5.02	1.55	1.47
4	A	803[A]	OPV	CA-C	-4.95	1.39	1.52
4	A	803[A]	OPV	CAV-CAQ	-4.86	1.40	1.50
5	A	804[B]	OPZ	CA-C	-4.45	1.40	1.52
3	C	802	FV8	CA-N	4.42	1.53	1.47
3	C	802	FV8	C-NAY	-4.00	1.30	1.35
5	C	803	OPZ	CA-C	-3.83	1.42	1.52
5	B	803	OPZ	CA-C	-3.79	1.42	1.52
5	C	803	OPZ	OG1-NAY	3.60	1.51	1.46
3	A	802	FV8	OAE-NAY	-3.56	1.37	1.40
3	C	802	FV8	CB-CA	-3.23	1.50	1.54
5	B	803	OPZ	CAK-CAT	3.02	1.56	1.50
3	C	802	FV8	OAE-NAY	3.00	1.42	1.40
3	A	802	FV8	C-NAY	-2.95	1.32	1.35
5	A	804[B]	OPZ	CAK-CAT	2.94	1.56	1.50
5	C	803	OPZ	CAL-NAY	2.86	1.52	1.47
4	A	803[A]	OPV	CAL-NAY	2.45	1.51	1.47
3	A	802	FV8	O-C	2.44	1.26	1.22
4	A	803[A]	OPV	CAK-CAT	2.38	1.54	1.50
3	C	802	FV8	CAT-NAO	-2.28	1.32	1.38
5	C	803	OPZ	CAK-CAT	2.25	1.54	1.50
3	B	802	FV8	CAK-CAT	2.24	1.54	1.50
3	A	802	FV8	CB-CA	-2.18	1.52	1.54
3	A	802	FV8	CAI-NAO	2.18	1.37	1.33
3	C	802	FV8	CAK-CAT	2.15	1.54	1.50
3	A	802	FV8	CA-N	2.15	1.50	1.47
5	B	803	OPZ	CAL-CAK	2.14	1.56	1.52
5	C	803	OPZ	CAF-CAH	2.10	1.42	1.38
3	A	802	FV8	OG1-CB	-2.03	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803[A]	OPV	CAT-NAO	-2.01	1.33	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	FV8	OG1-CAR-N	-8.95	112.29	118.21
3	B	802	FV8	OG1-CAR-N	-8.59	112.53	118.21
3	C	802	FV8	OG1-CAR-N	-7.94	112.96	118.21
4	A	803[A]	OPV	OG1-NAY-CAL	6.90	126.67	113.99
5	B	803	OPZ	OG1-NAY-CAL	6.36	125.67	113.99
5	C	803	OPZ	OG1-NAY-CAL	5.79	124.62	113.99
5	A	804[B]	OPZ	OG1-NAY-CAL	5.34	123.81	113.99
3	C	802	FV8	OG1-CB-CA	4.53	106.34	102.57
5	C	803	OPZ	CAV-CAU-CAS	4.43	122.69	119.99
3	A	802	FV8	CAV-CAU-CAS	4.35	122.64	119.99
3	B	802	FV8	CAV-CAU-CAS	4.30	122.62	119.99
3	C	802	FV8	CAV-CAU-CAS	3.96	122.41	119.99
3	A	802	FV8	OG1-CB-CA	3.90	105.82	102.57
3	B	802	FV8	OG1-CB-CA	3.44	105.43	102.57
4	A	803[A]	OPV	O-C-CA	-3.19	123.19	127.46
3	C	802	FV8	CB-CA-N	-2.89	102.68	104.87
5	C	803	OPZ	CAL-CAK-CAT	-2.84	108.07	113.49
5	A	804[B]	OPZ	CAV-CAU-CAS	2.84	121.72	119.99
4	A	803[A]	OPV	C-CA-N	-2.83	108.87	113.06
3	C	802	FV8	OAE-NAY-CAL	2.60	119.84	113.76
3	B	802	FV8	CB-CA-N	-2.54	102.94	104.87
3	B	802	FV8	CAH-CAV-CAU	-2.51	116.33	118.76
3	A	802	FV8	CA-N-CAR	2.49	108.68	106.79
5	B	803	OPZ	O-C-CA	-2.37	124.28	127.46
3	C	802	FV8	C-CA-N	-2.35	108.25	111.97
5	B	803	OPZ	CAV-CAU-CAS	2.33	121.41	119.99
5	A	804[B]	OPZ	O-C-CA	-2.31	124.36	127.46
3	B	802	FV8	CA-N-CAR	2.31	108.54	106.79
3	A	802	FV8	OG1-CB-CG2	-2.27	105.73	108.68
3	A	802	FV8	CAK-CAT-CAJ	-2.23	122.93	128.44
5	C	803	OPZ	OAD-CAS-CAG	2.18	125.20	119.36
5	B	803	OPZ	O-C-NAY	-2.17	123.42	126.00
3	B	802	FV8	CAK-CAT-CAJ	-2.13	123.19	128.44
3	A	802	FV8	CB-CA-N	-2.07	103.29	104.87
3	B	802	FV8	CAF-CAG-CAS	-2.05	117.52	120.05
5	C	803	OPZ	O-C-CA	-2.01	124.76	127.46

There are no chirality outliers.

All (163) 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
3	C	802	FV8	CAK-CAL-NAY-OAE
5	B	803	OPZ	CAL-CAK-CAT-CAJ
5	B	803	OPZ	CAL-CAK-CAT-NAO
5	B	803	OPZ	CAT-CAK-CAL-NAY
5	B	803	OPZ	CAK-CAL-NAY-C
5	B	803	OPZ	CAK-CAL-NAY-OG1
6	C	806	C8E	O15-C16-C17-O18
6	C	810	C8E	O12-C13-C14-O15
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	O18-C19-C20-O21
6	C	807	C8E	O18-C19-C20-O21
6	A	805	C8E	C6-C7-C8-O9
6	C	807	C8E	C6-C7-C8-O9
6	B	804	C8E	O15-C16-C17-O18
6	B	806	C8E	C6-C7-C8-O9
6	C	804	C8E	O15-C16-C17-O18
6	C	807	C8E	O15-C16-C17-O18
6	C	807	C8E	O9-C10-C11-O12
6	B	811	C8E	O18-C19-C20-O21
6	C	810	C8E	O9-C10-C11-O12
6	C	806	C8E	O9-C10-C11-O12
6	B	810	C8E	C4-C5-C6-C7
6	B	804	C8E	O12-C13-C14-O15
6	B	808	C8E	C5-C6-C7-C8
6	B	812	C8E	C5-C6-C7-C8
6	B	808	C8E	C4-C5-C6-C7
7	C	819	EDO	O1-C1-C2-O2
6	A	810	C8E	C3-C4-C5-C6
6	C	807	C8E	C3-C4-C5-C6
6	B	812	C8E	C6-C7-C8-O9
6	B	814	C8E	C3-C4-C5-C6
6	C	808	C8E	O12-C13-C14-O15
6	B	805	C8E	O12-C13-C14-O15
6	B	807	C8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	B	810	C8E	C2-C3-C4-C5
6	B	806	C8E	C3-C4-C5-C6
6	C	811	C8E	C5-C6-C7-C8
6	C	804	C8E	O9-C10-C11-O12
6	B	813	C8E	C6-C7-C8-O9
5	A	804[B]	OPZ	CAT-CAK-CAL-NAY
6	A	806	C8E	C6-C7-C8-O9
6	A	810	C8E	C6-C7-C8-O9
7	B	818	EDO	O1-C1-C2-O2
7	C	822	EDO	O1-C1-C2-O2
7	C	827	EDO	O1-C1-C2-O2
7	C	829	EDO	O1-C1-C2-O2
6	A	808	C8E	C3-C4-C5-C6
6	B	807	C8E	C2-C3-C4-C5
6	A	805	C8E	C2-C3-C4-C5
6	B	810	C8E	C5-C6-C7-C8
6	B	811	C8E	C1-C2-C3-C4
6	A	805	C8E	C5-C6-C7-C8
6	C	807	C8E	C1-C2-C3-C4
6	A	807	C8E	C2-C3-C4-C5
6	C	811	C8E	C11-C10-O9-C8
6	B	811	C8E	O12-C13-C14-O15
6	B	807	C8E	O12-C13-C14-O15
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	B	811	C8E	O15-C16-C17-O18
6	B	807	C8E	C1-C2-C3-C4
6	C	808	C8E	C3-C4-C5-C6
6	A	808	C8E	C1-C2-C3-C4
6	B	813	C8E	C1-C2-C3-C4
6	C	811	C8E	C4-C5-C6-C7
6	A	808	C8E	C6-C7-C8-O9
6	C	805	C8E	O18-C19-C20-O21
6	B	814	C8E	C2-C3-C4-C5
6	C	804	C8E	C13-C14-O15-C16
6	B	811	C8E	C16-C17-O18-C19
6	B	815	C8E	C3-C4-C5-C6
6	C	809	C8E	C14-C13-O12-C11
3	B	802	FV8	CAK-CAL-NAY-C
3	C	802	FV8	CAK-CAL-NAY-C
6	B	807	C8E	O18-C19-C20-O21

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Mol	Chain	Res	Type	Atoms
6	C	809	C8E	O12-C13-C14-O15
6	B	804	C8E	C17-C16-O15-C14
6	B	804	C8E	C13-C14-O15-C16
6	B	811	C8E	C17-C16-O15-C14
6	C	806	C8E	C13-C14-O15-C16
6	C	806	C8E	C17-C16-O15-C14
6	B	805	C8E	C7-C8-O9-C10
6	B	812	C8E	O9-C10-C11-O12
6	B	812	C8E	C7-C8-O9-C10
6	A	806	C8E	C3-C4-C5-C6
6	A	806	C8E	C5-C6-C7-C8
6	B	813	C8E	O9-C10-C11-O12
6	A	809	C8E	C5-C6-C7-C8
6	B	805	C8E	C10-C11-O12-C13
6	C	805	C8E	C14-C13-O12-C11
6	A	810	C8E	C1-C2-C3-C4
6	C	807	C8E	C14-C13-O12-C11
6	B	807	C8E	C13-C14-O15-C16
6	C	808	C8E	C14-C13-O12-C11
6	B	811	C8E	O9-C10-C11-O12
6	B	804	C8E	C6-C7-C8-O9
6	B	813	C8E	C7-C8-O9-C10
6	C	807	C8E	C16-C17-O18-C19
6	B	812	C8E	C2-C3-C4-C5
6	C	805	C8E	O12-C13-C14-O15
6	C	808	C8E	C11-C10-O9-C8
6	A	808	C8E	C4-C5-C6-C7
6	B	807	C8E	C14-C13-O12-C11
6	C	809	C8E	C10-C11-O12-C13
6	B	807	C8E	C10-C11-O12-C13
7	C	814	EDO	O1-C1-C2-O2
7	C	816	EDO	O1-C1-C2-O2
7	C	817	EDO	O1-C1-C2-O2
6	C	809	C8E	C2-C3-C4-C5
6	B	808	C8E	C3-C4-C5-C6
6	B	806	C8E	C11-C10-O9-C8
6	C	804	C8E	C17-C16-O15-C14
6	B	809	C8E	C4-C5-C6-C7
6	B	805	C8E	C14-C13-O12-C11
6	B	804	C8E	C14-C13-O12-C11
6	C	812	C8E	C3-C4-C5-C6
7	A	817	EDO	O1-C1-C2-O2

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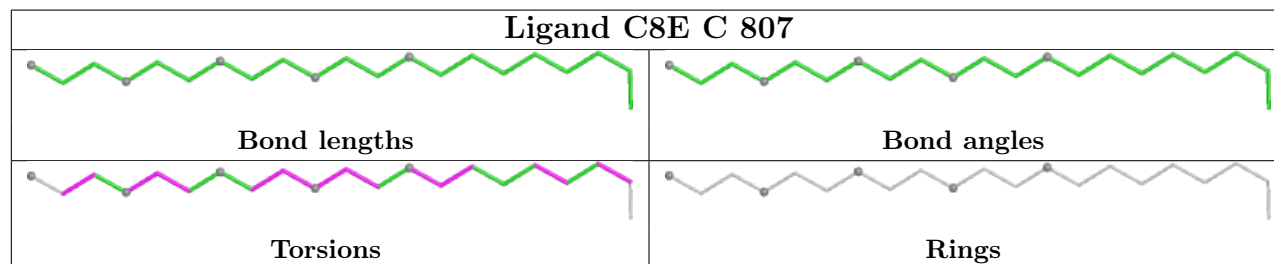
Mol	Chain	Res	Type	Atoms
7	A	821	EDO	O1-C1-C2-O2
7	B	819	EDO	O1-C1-C2-O2
7	B	824	EDO	O1-C1-C2-O2
7	B	825	EDO	O1-C1-C2-O2
6	C	806	C8E	C16-C17-O18-C19
6	A	805	C8E	C3-C4-C5-C6
6	B	809	C8E	C2-C3-C4-C5
6	C	806	C8E	C6-C7-C8-O9
6	A	805	C8E	C11-C10-O9-C8
6	B	807	C8E	C17-C16-O15-C14
6	B	807	C8E	O15-C16-C17-O18
6	C	807	C8E	C7-C8-O9-C10
6	B	805	C8E	C3-C4-C5-C6
6	C	807	C8E	O12-C13-C14-O15
7	A	823	EDO	O1-C1-C2-O2
7	B	820	EDO	O1-C1-C2-O2
7	B	827	EDO	O1-C1-C2-O2
7	B	828	EDO	O1-C1-C2-O2
7	C	825	EDO	O1-C1-C2-O2
6	C	804	C8E	C16-C17-O18-C19
6	C	809	C8E	O9-C10-C11-O12
6	C	808	C8E	C7-C8-O9-C10
6	B	812	C8E	C1-C2-C3-C4
6	B	804	C8E	C16-C17-O18-C19
6	B	813	C8E	C2-C3-C4-C5
6	A	805	C8E	C1-C2-C3-C4
6	B	812	C8E	C3-C4-C5-C6
6	C	807	C8E	C10-C11-O12-C13
6	B	811	C8E	C4-C5-C6-C7
7	A	813	EDO	O1-C1-C2-O2
7	A	814	EDO	O1-C1-C2-O2
6	C	810	C8E	C10-C11-O12-C13
6	C	812	C8E	C1-C2-C3-C4
6	B	808	C8E	C6-C7-C8-O9
3	A	802	FV8	O-C-CA-CB
6	B	804	C8E	C10-C11-O12-C13
6	C	804	C8E	O12-C13-C14-O15
6	C	804	C8E	C6-C7-C8-O9
6	A	808	C8E	C2-C3-C4-C5

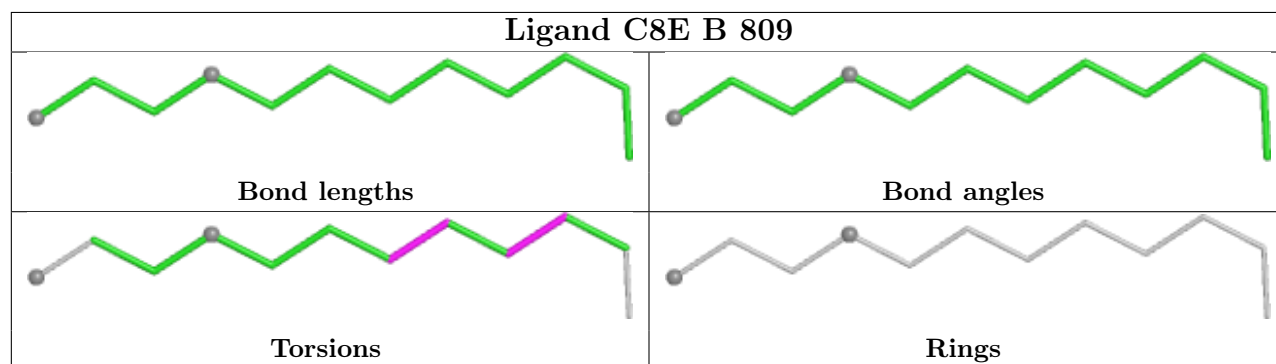
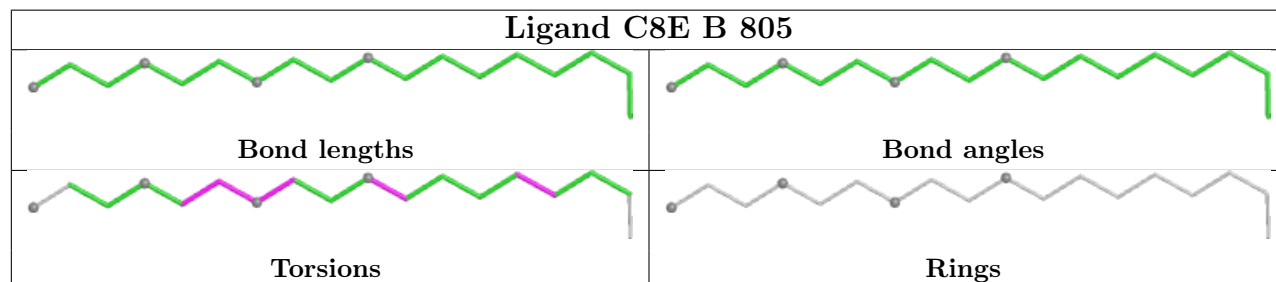
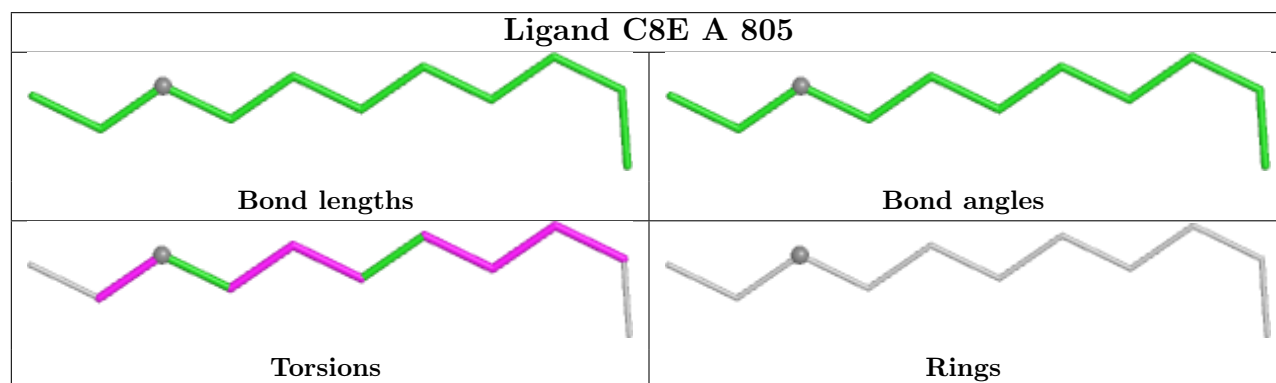
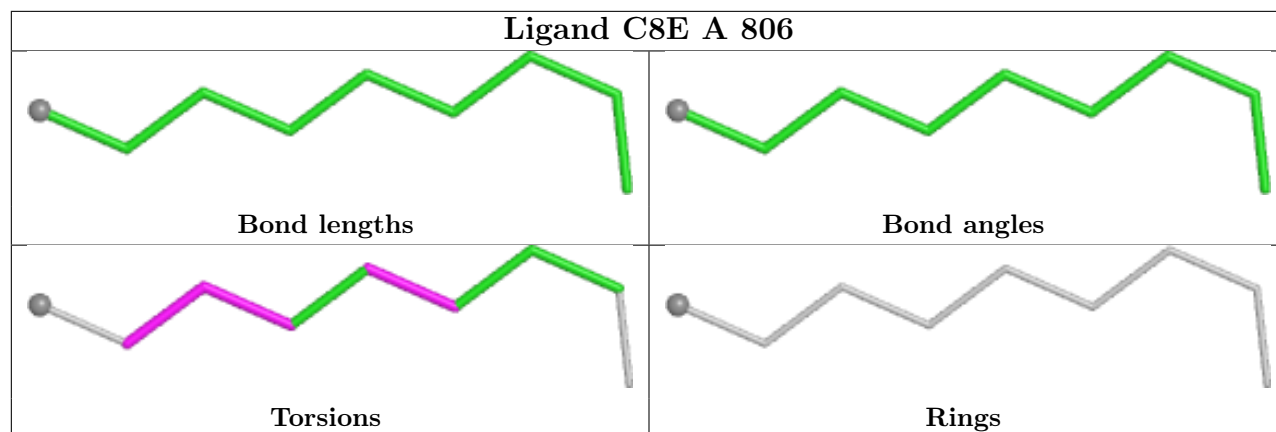
There are no ring outliers.

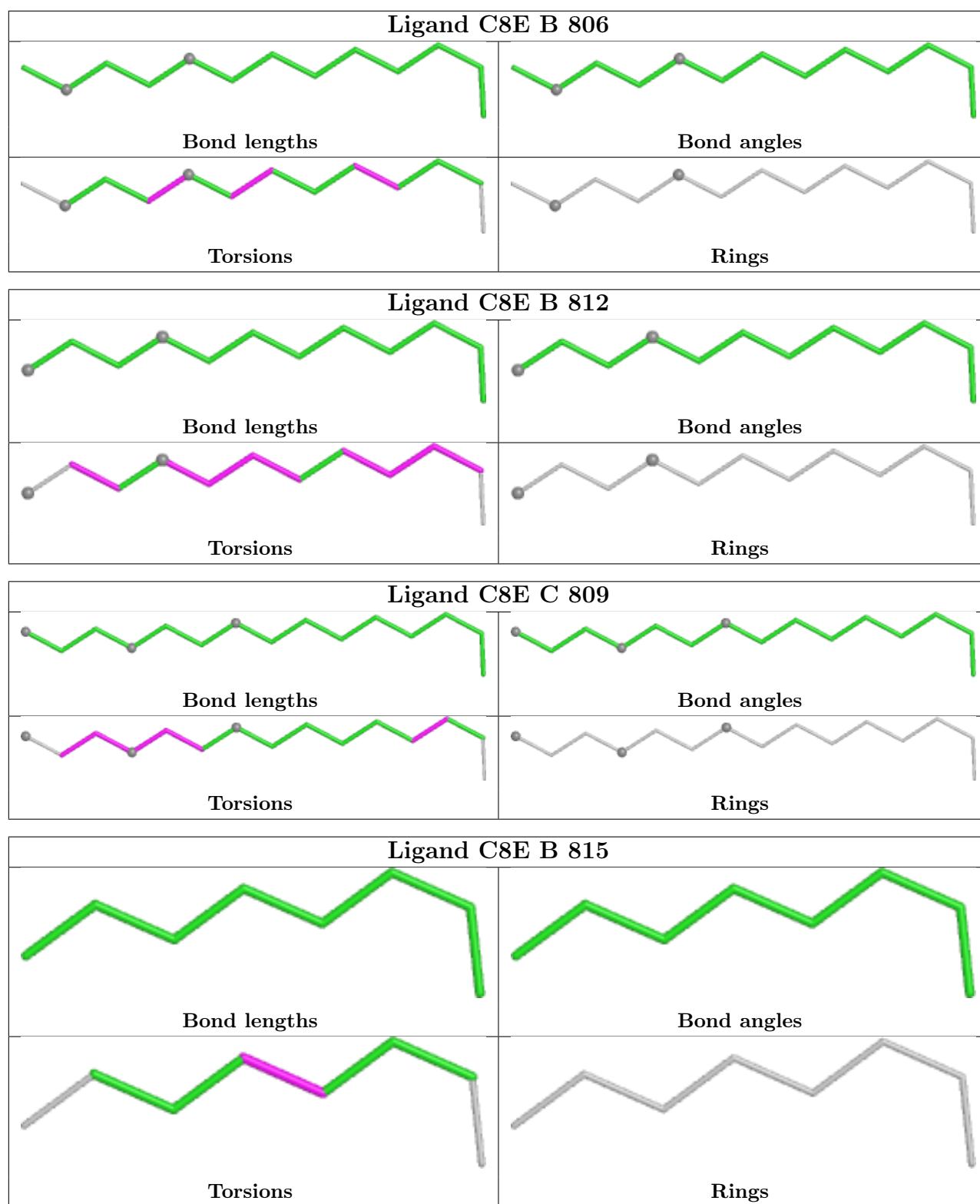
18 monomers are involved in 22 short contacts:

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

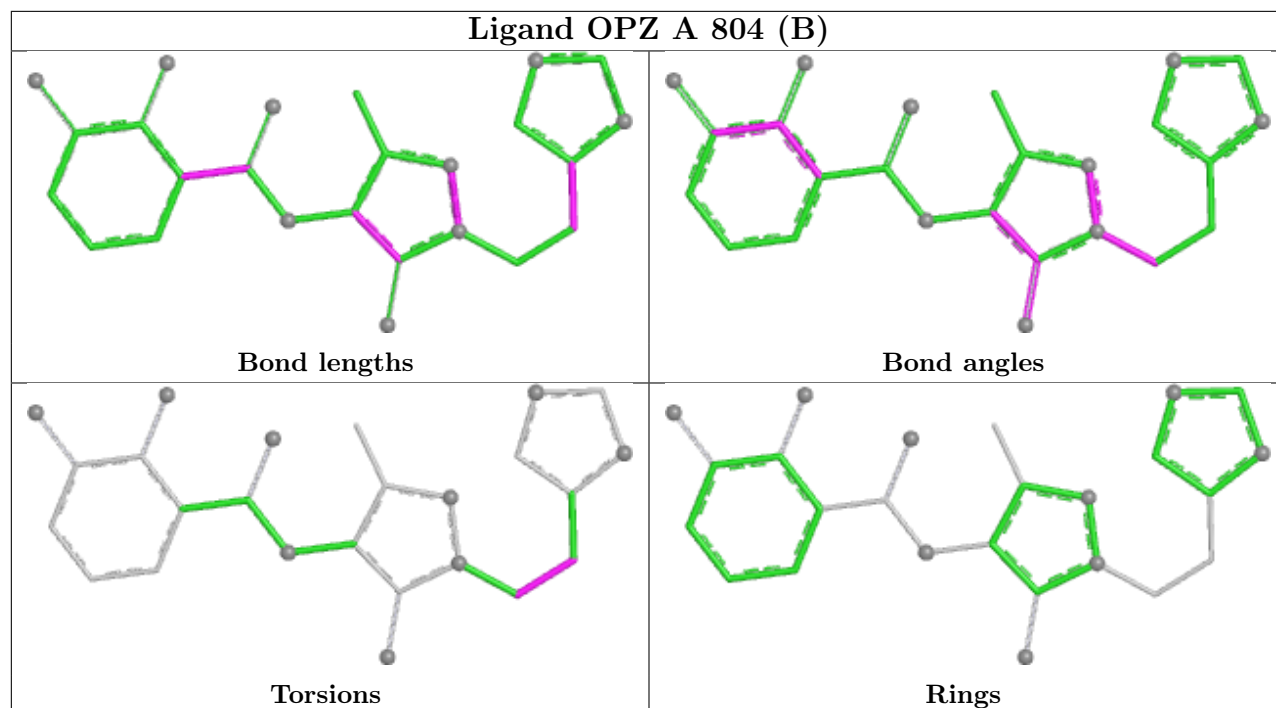
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



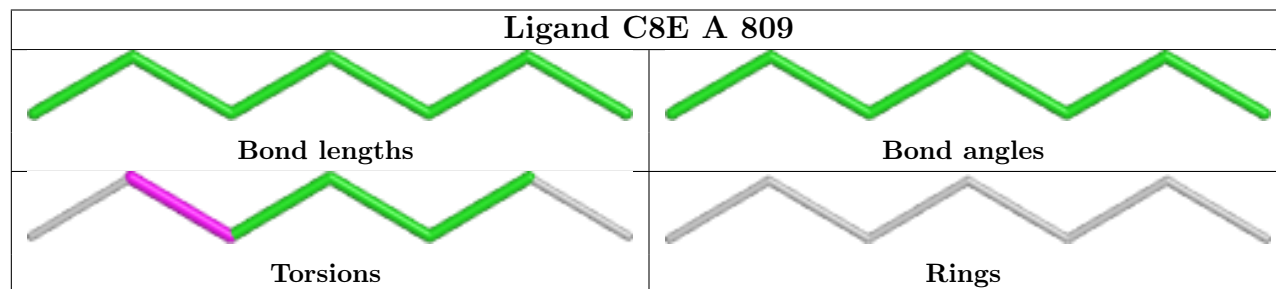




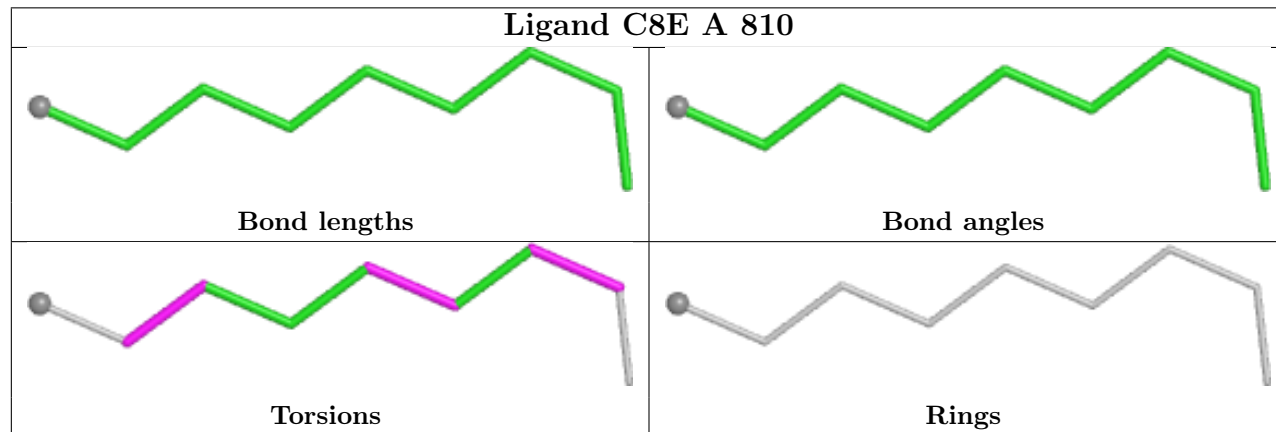
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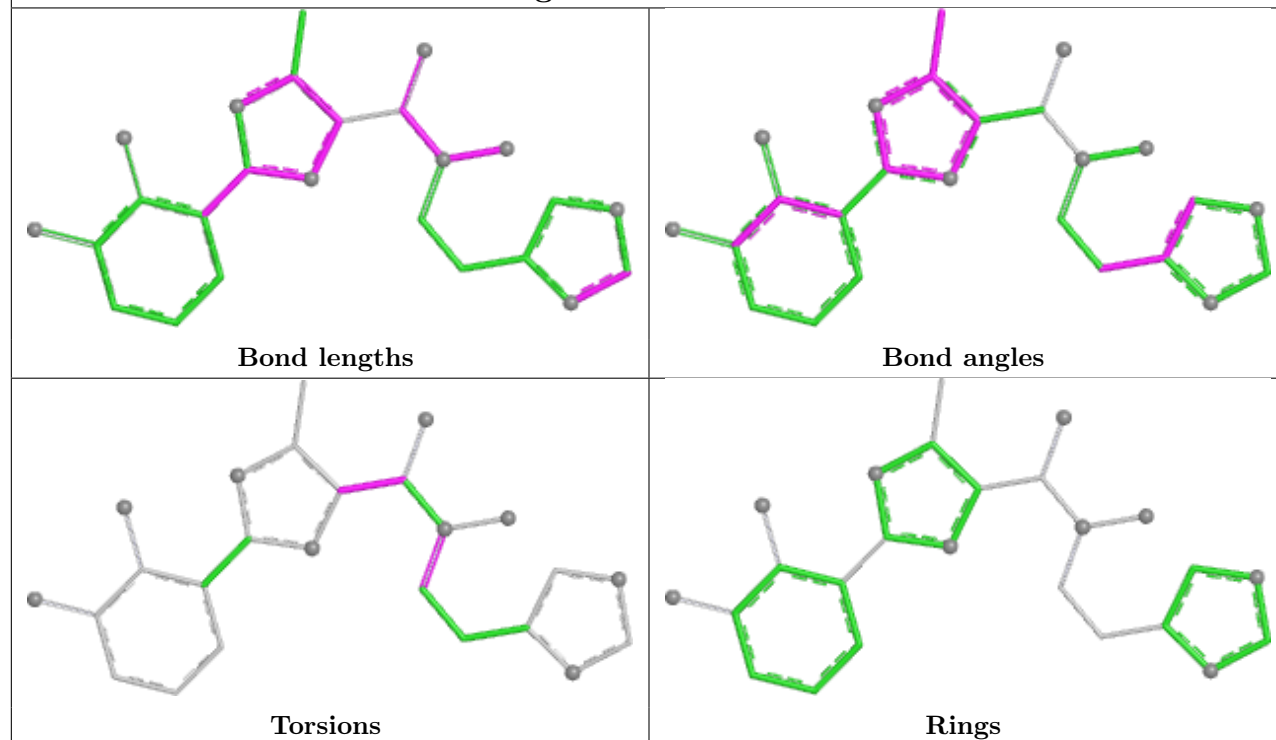
Ligand C8E A 809



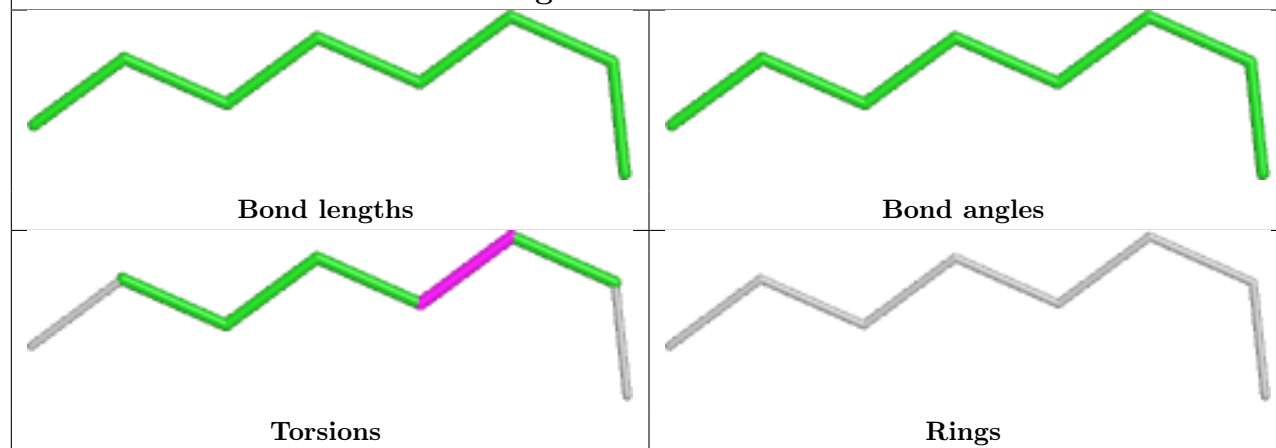
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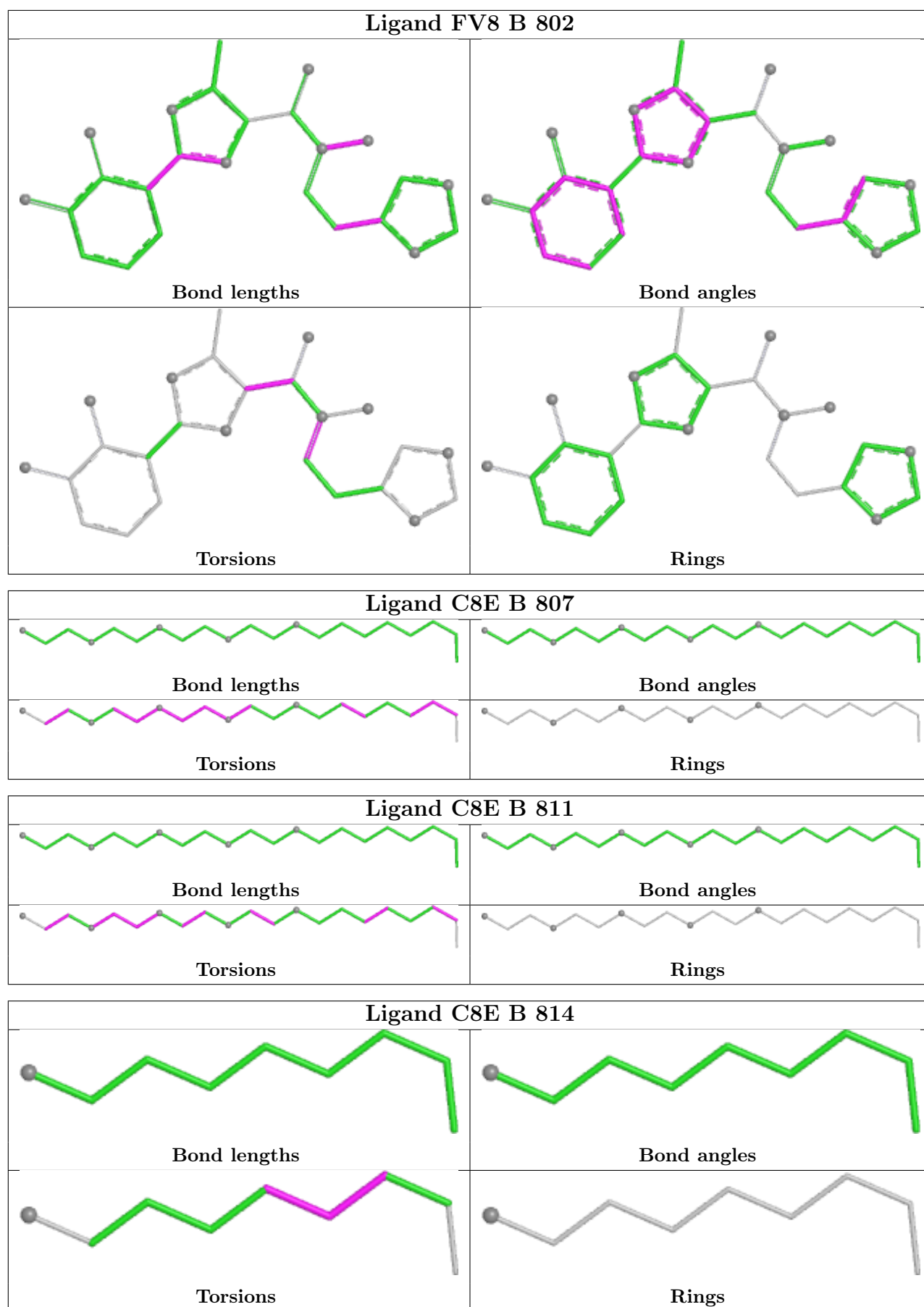


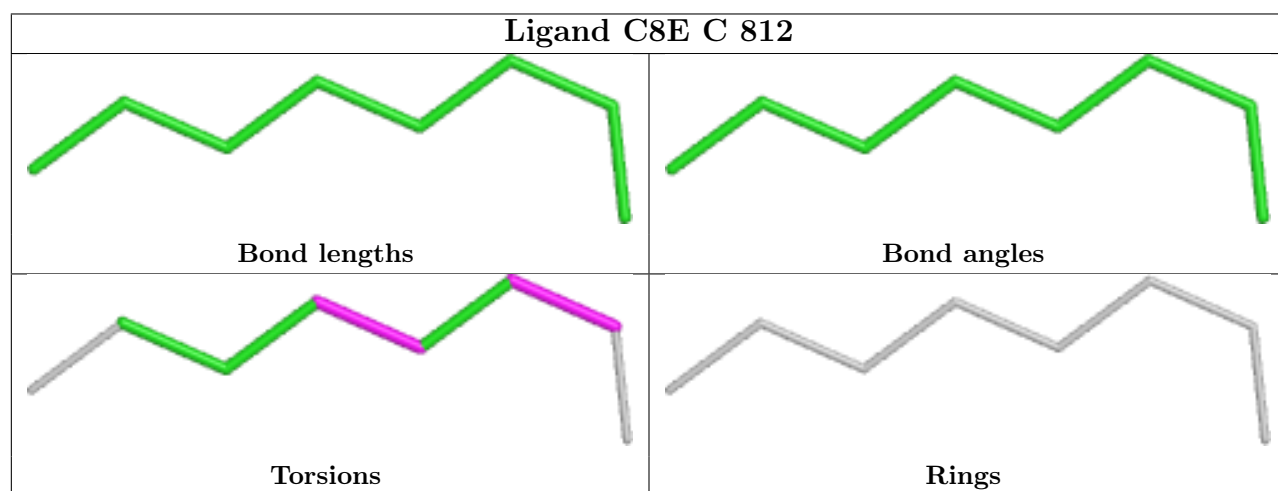
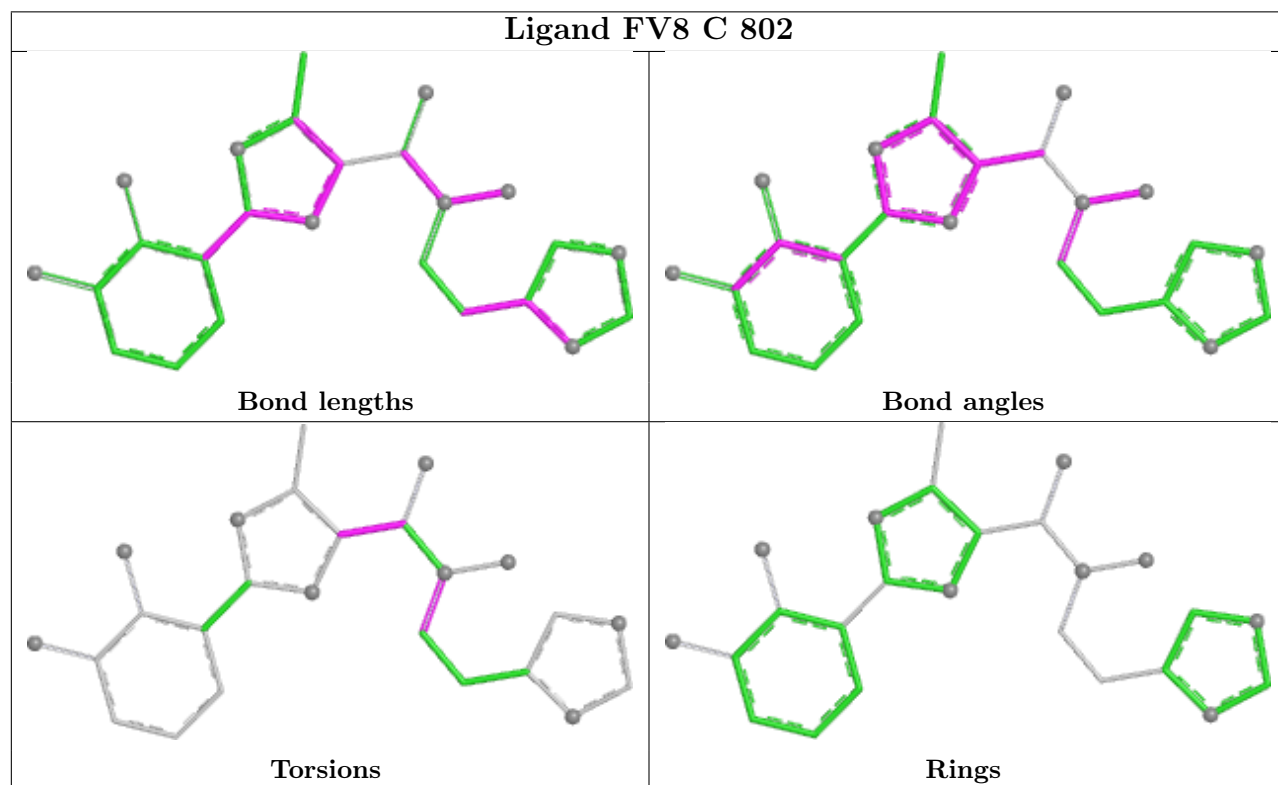
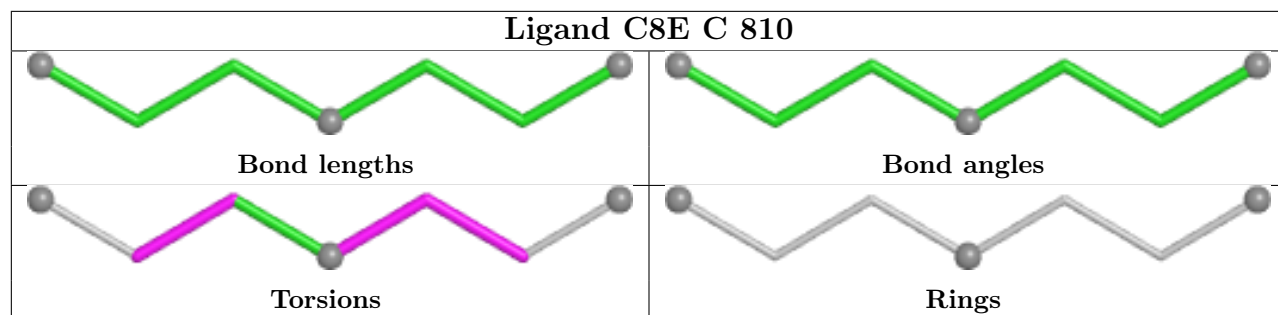
Ligand FV8 A 802

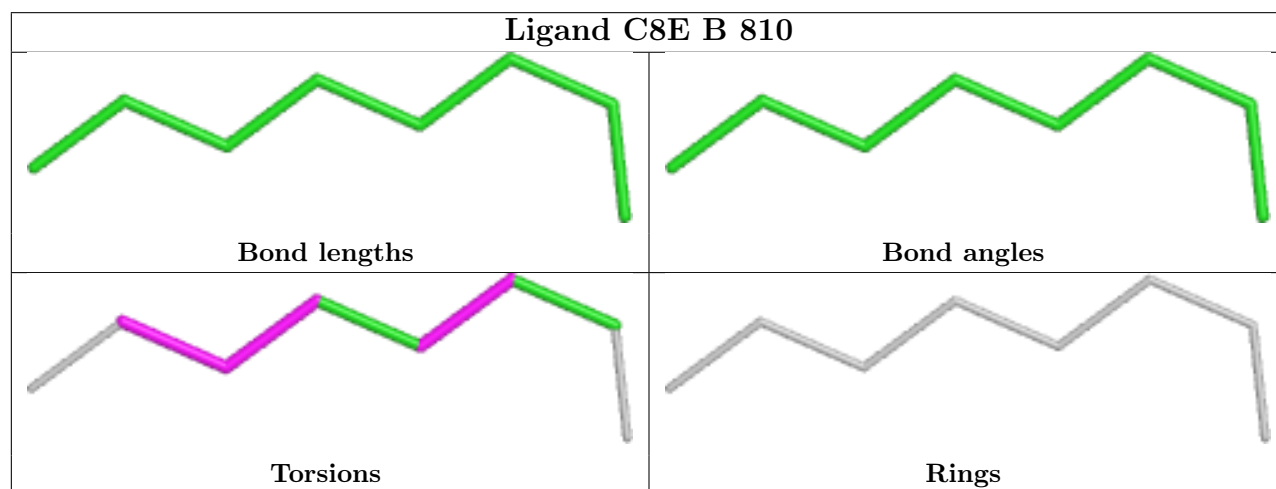
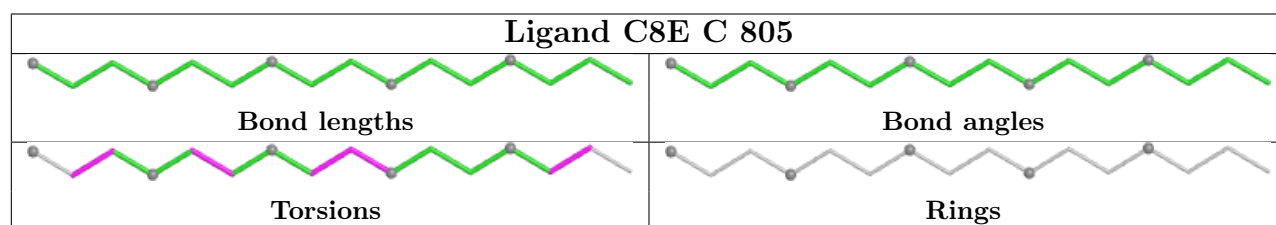
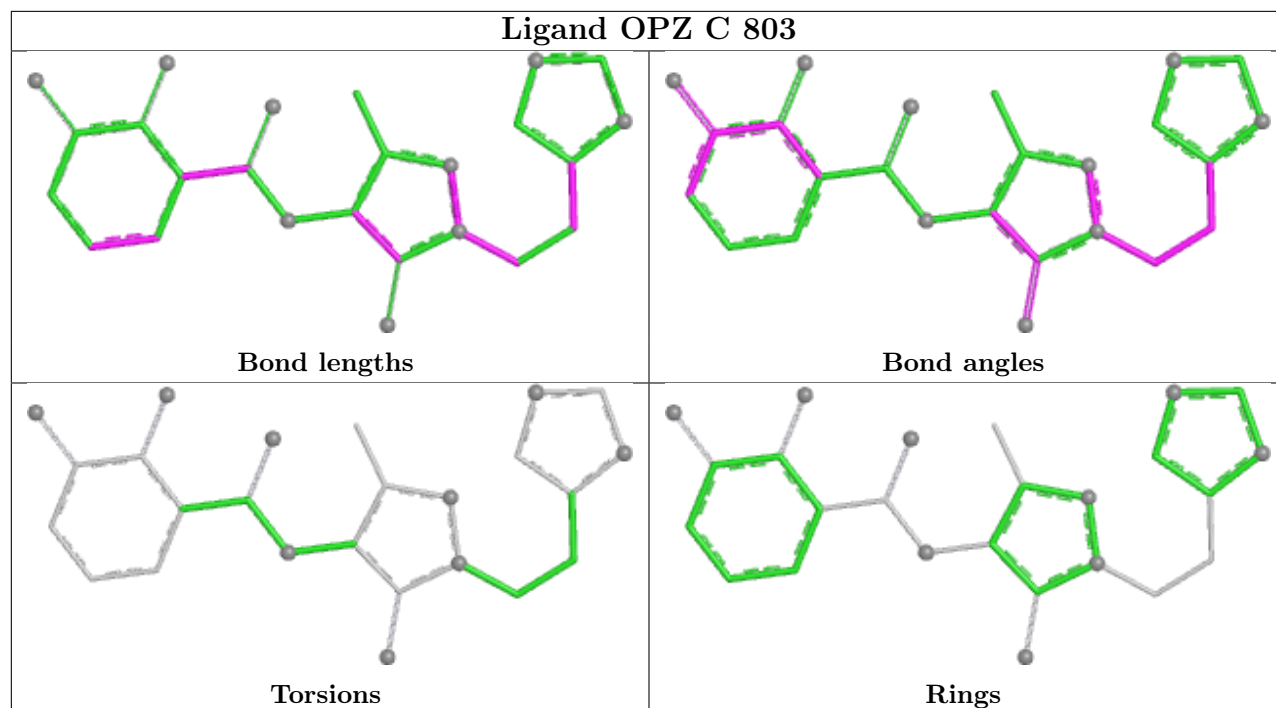


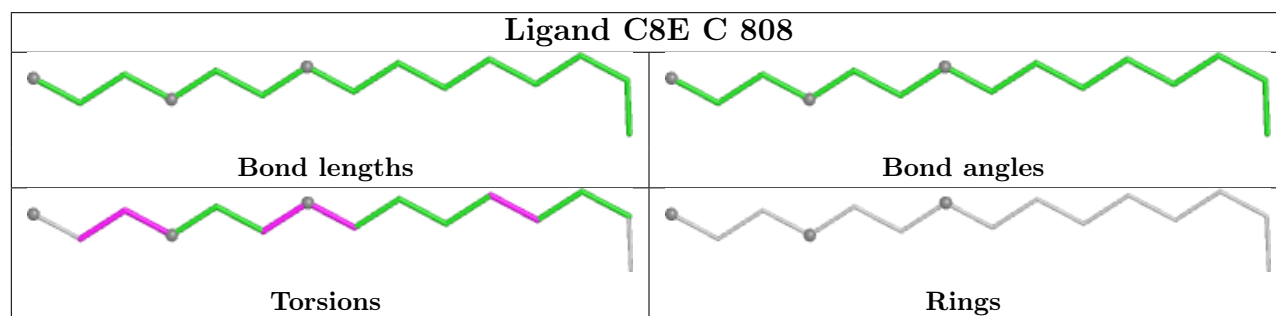
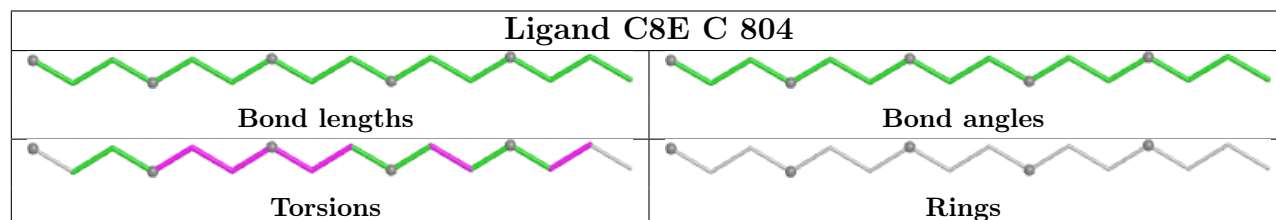
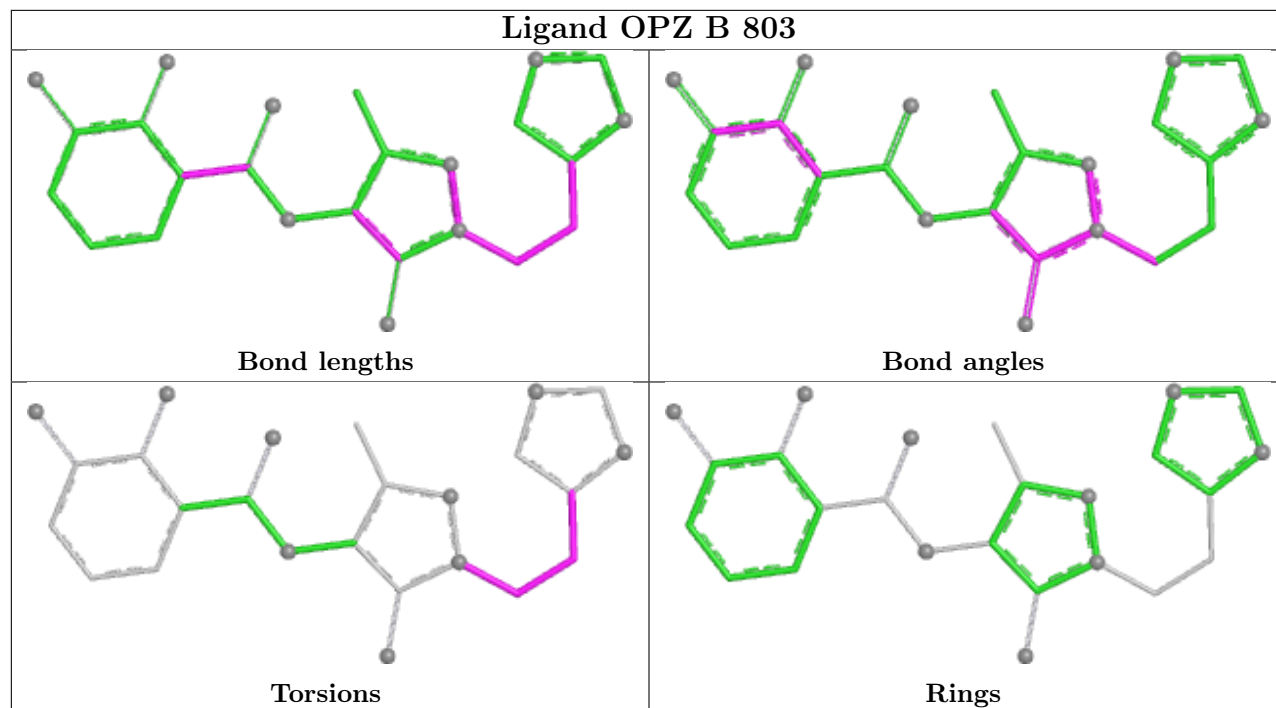
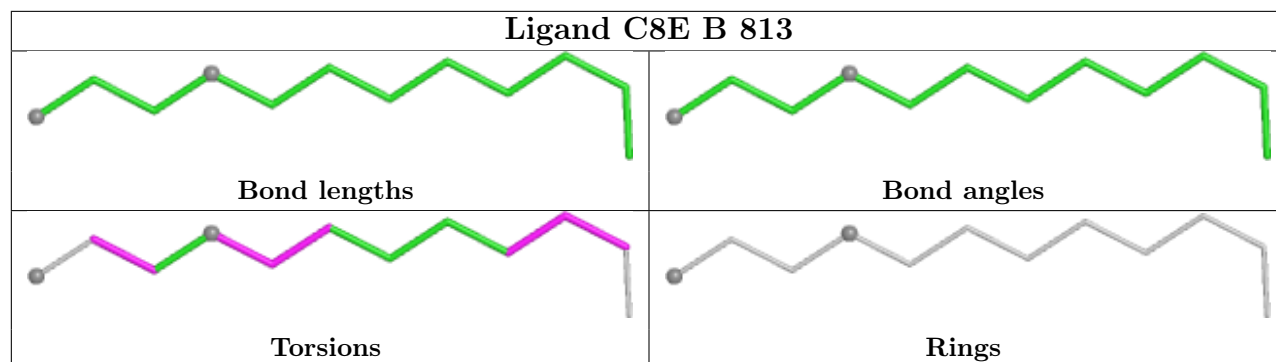
Ligand C8E A 807

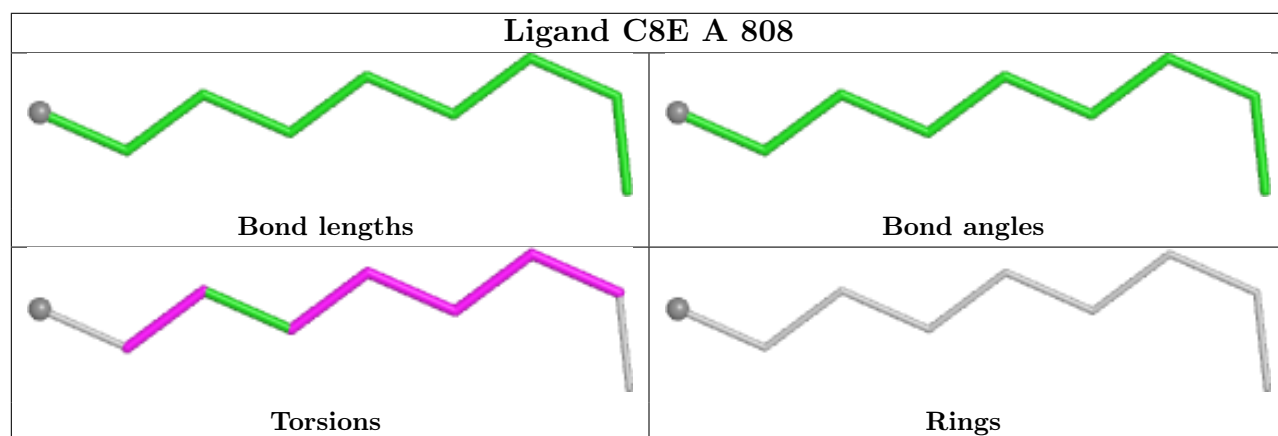
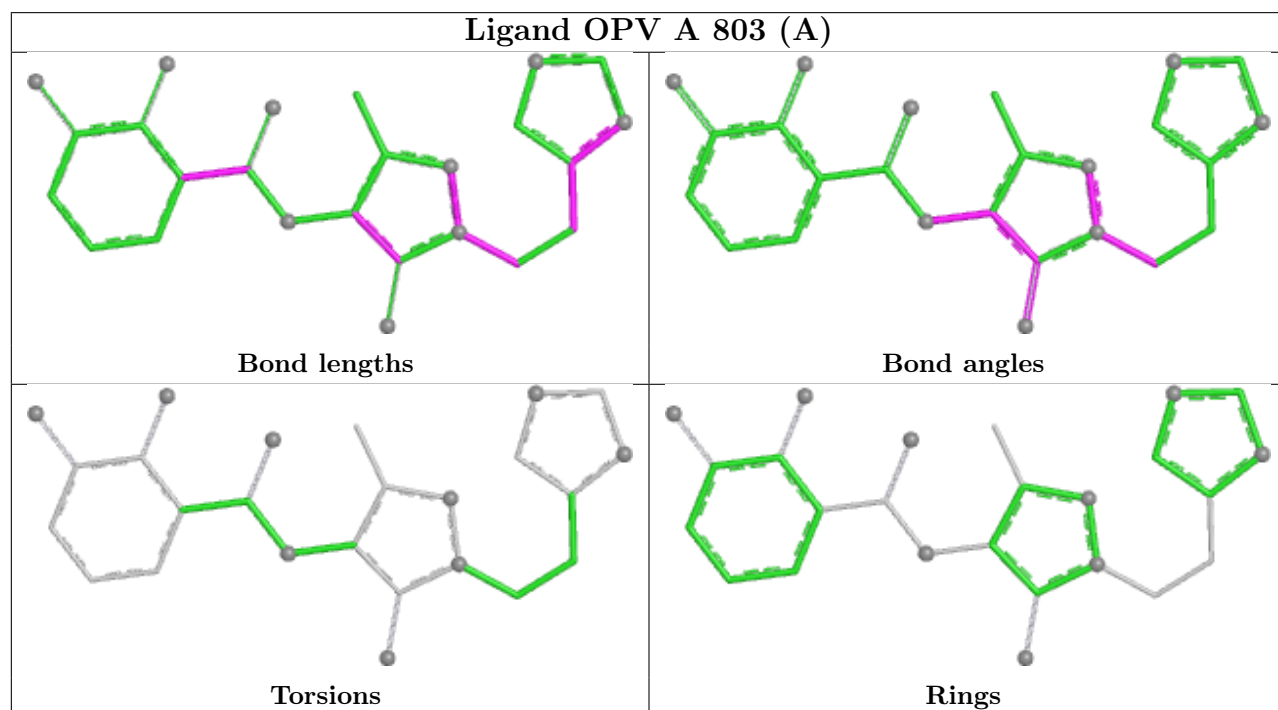
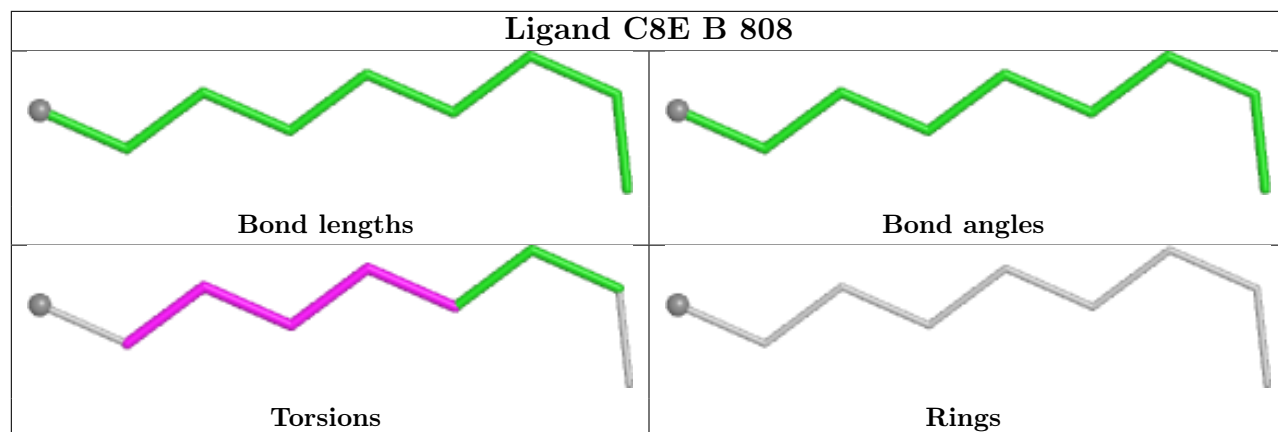


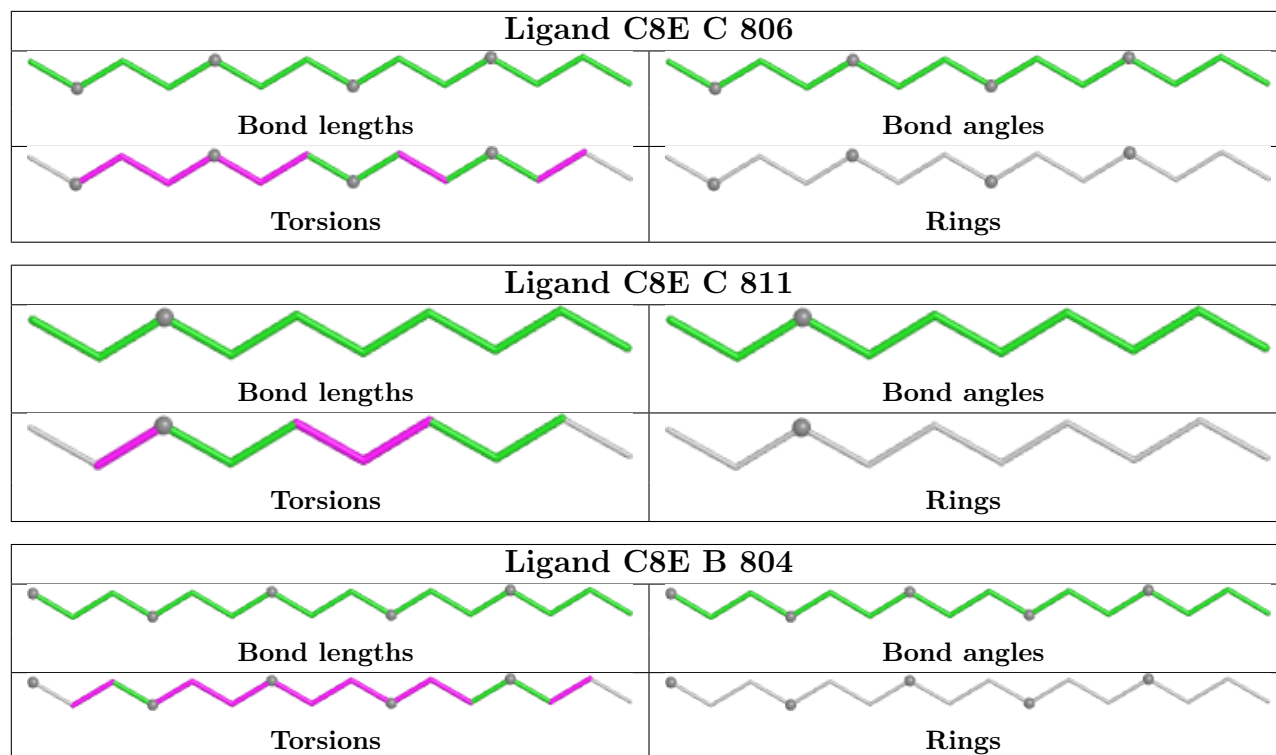












5.7 Other polymers [i](#)

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	671/706 (95%)	-0.17	12 (1%) 67 68	17, 37, 66, 106	13 (1%)
1	B	671/706 (95%)	-0.17	8 (1%) 76 77	18, 37, 61, 87	9 (1%)
1	C	671/706 (95%)	-0.30	9 (1%) 75 76	13, 33, 59, 91	15 (2%)
All	All	2013/2118 (95%)	-0.21	29 (1%) 73 74	13, 36, 62, 106	37 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	612	TRP	4.7
1	A	541	LYS	3.7
1	C	569	ILE	3.6
1	C	420	PHE	3.6
1	B	420	PHE	3.5
1	A	539	PRO	3.4
1	C	33	ASP	3.4
1	B	33	ASP	3.3
1	A	428	PHE	3.2
1	A	368	TYR	3.1
1	C	368	TYR	3.0
1	C	580	TYR	2.9
1	A	543	VAL	2.9
1	B	612	TRP	2.8
1	A	33	ASP	2.8
1	C	617	ALA	2.7
1	A	618	GLN	2.7
1	A	540	SER	2.6
1	B	542	LEU	2.5
1	C	618	GLN	2.4
1	A	546	LEU	2.3
1	B	539	PRO	2.3
1	B	233	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	429	ALA	2.2
1	B	541	LYS	2.2
1	A	542	LEU	2.2
1	B	368	TYR	2.2
1	C	422[A]	LEU	2.1
1	A	612	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	C8E	B	811	21/21	0.81	0.28	65,79,92,94	0
7	EDO	A	821	4/4	0.82	0.28	66,71,81,83	0
6	C8E	B	809	12/21	0.83	0.25	48,74,80,85	0
6	C8E	B	810	8/21	0.83	0.30	52,68,80,82	0
6	C8E	A	810	9/21	0.83	0.26	59,62,71,71	0
6	C8E	B	813	12/21	0.83	0.26	52,67,73,77	0
6	C8E	B	807	21/21	0.83	0.28	65,79,93,122	0
6	C8E	B	815	8/21	0.84	0.29	62,65,75,79	0
6	C8E	B	808	9/21	0.84	0.29	63,71,78,79	0
6	C8E	C	811	10/21	0.85	0.27	58,71,77,83	0
6	C8E	C	813	7/21	0.85	0.25	61,63,69,71	0
6	C8E	C	809	15/21	0.85	0.27	57,77,91,96	0
6	C8E	B	806	13/21	0.86	0.21	41,69,83,86	0
6	C8E	C	808	15/21	0.86	0.22	50,68,79,80	0
7	EDO	B	828	4/4	0.86	0.20	45,48,52,52	0
7	EDO	A	815	4/4	0.87	0.17	45,52,59,63	0
6	C8E	A	806	9/21	0.87	0.23	61,69,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	823	4/4	0.87	0.15	44,45,52,55	0
7	EDO	B	818	4/4	0.87	0.22	52,52,63,67	0
7	EDO	B	826	4/4	0.87	0.26	64,68,74,75	0
6	C8E	B	805	18/21	0.87	0.23	43,67,99,102	0
6	C8E	A	809	7/21	0.88	0.20	48,50,53,58	0
7	EDO	B	819	4/4	0.88	0.22	57,62,64,68	0
6	C8E	C	805	16/21	0.88	0.17	47,61,77,81	0
6	C8E	B	804	16/21	0.88	0.21	53,65,98,106	0
7	EDO	C	822	4/4	0.88	0.22	47,67,67,67	0
6	C8E	C	807	21/21	0.89	0.18	45,60,74,79	0
6	C8E	C	810	7/21	0.89	0.19	60,65,77,79	0
6	C8E	C	804	16/21	0.89	0.19	45,53,91,94	0
7	EDO	C	830	4/4	0.89	0.22	56,64,73,74	0
6	C8E	A	807	8/21	0.90	0.20	45,52,57,58	0
7	EDO	B	817	4/4	0.90	0.15	40,41,48,60	0
7	EDO	C	816	4/4	0.90	0.18	57,59,62,63	0
7	EDO	C	819	4/4	0.90	0.19	47,49,51,66	0
6	C8E	A	808	9/21	0.90	0.19	59,68,73,77	0
4	OPV	A	803[A]	25/25	0.90	0.20	29,52,116,121	25
7	EDO	C	817	4/4	0.91	0.15	37,52,55,58	0
7	EDO	C	828	4/4	0.91	0.17	44,51,56,59	0
6	C8E	C	806	14/21	0.91	0.17	54,62,72,82	0
7	EDO	C	818	4/4	0.92	0.18	51,57,60,66	0
5	OPZ	A	804[B]	25/25	0.92	0.14	27,44,74,77	25
7	EDO	A	813	4/4	0.92	0.17	41,60,62,67	0
6	C8E	B	812	12/21	0.92	0.17	51,59,74,77	0
7	EDO	C	829	4/4	0.92	0.16	52,54,58,62	0
6	C8E	A	805	11/21	0.92	0.17	47,54,62,64	0
7	EDO	C	820	4/4	0.93	0.14	46,50,58,60	0
7	EDO	B	825	4/4	0.93	0.15	59,64,69,73	0
7	EDO	C	826	4/4	0.93	0.11	36,38,39,49	0
6	C8E	C	812	8/21	0.93	0.17	50,64,67,69	0
7	EDO	B	827	4/4	0.93	0.16	56,60,65,72	0
7	EDO	B	820	4/4	0.93	0.17	63,64,68,71	0
7	EDO	A	819	4/4	0.94	0.12	49,50,51,59	0
7	EDO	B	824	4/4	0.94	0.17	43,57,62,72	0
5	OPZ	C	803	25/25	0.94	0.14	26,67,87,96	0
7	EDO	C	821	4/4	0.94	0.11	50,52,56,57	0
7	EDO	A	811	4/4	0.94	0.10	35,46,51,51	0
7	EDO	C	823	4/4	0.94	0.13	47,56,61,62	0
7	EDO	C	824	4/4	0.94	0.14	56,62,64,69	0
7	EDO	B	816	4/4	0.94	0.12	40,47,47,50	0

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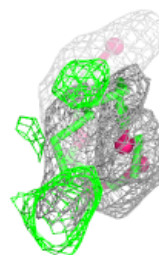
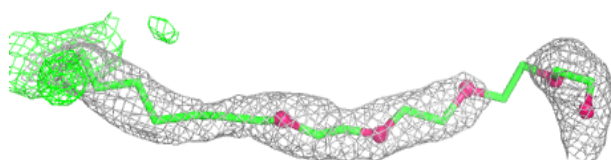
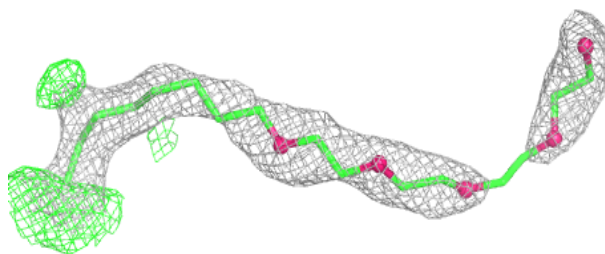
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	C8E	B	814	9/21	0.94	0.18	46,63,71,73	0
5	OPZ	B	803	25/25	0.94	0.13	24,60,89,98	0
7	EDO	A	818	4/4	0.94	0.15	57,64,72,82	0
7	EDO	C	825	4/4	0.95	0.16	38,41,46,61	0
7	EDO	A	816	4/4	0.95	0.16	53,57,60,62	0
7	EDO	C	827	4/4	0.95	0.11	32,47,48,49	0
7	EDO	B	823	4/4	0.95	0.11	43,47,48,48	0
7	EDO	A	814	4/4	0.95	0.13	43,48,49,65	0
7	EDO	A	812	4/4	0.95	0.10	33,39,42,43	0
7	EDO	C	815	4/4	0.96	0.09	42,42,44,50	0
7	EDO	A	822	4/4	0.96	0.14	51,52,57,57	0
7	EDO	B	821	4/4	0.96	0.10	49,50,50,62	0
7	EDO	B	822	4/4	0.96	0.10	45,48,52,57	0
7	EDO	C	814	4/4	0.97	0.09	36,41,48,54	0
3	FV8	A	802	25/25	0.98	0.04	20,26,31,36	0
3	FV8	B	802	25/25	0.98	0.05	26,32,41,44	0
7	EDO	A	820	4/4	0.98	0.07	48,56,58,60	0
7	EDO	A	817	4/4	0.98	0.07	42,43,49,49	0
3	FV8	C	802	25/25	0.99	0.04	22,26,31,32	0
2	FE	A	801	1/1	1.00	0.02	28,28,28,28	0
2	FE	B	801	1/1	1.00	0.01	32,32,32,32	0
2	FE	C	801	1/1	1.00	0.02	26,26,26,26	0

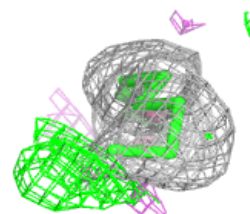
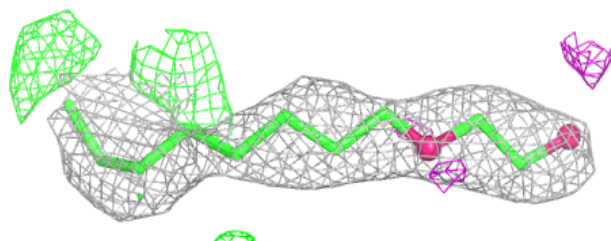
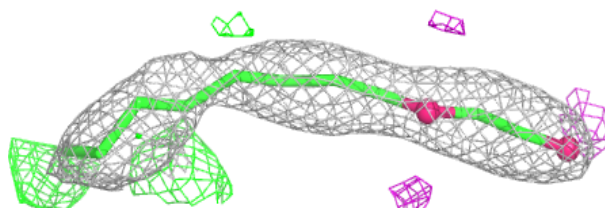
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E B 811:

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

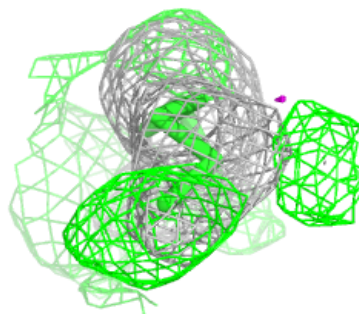
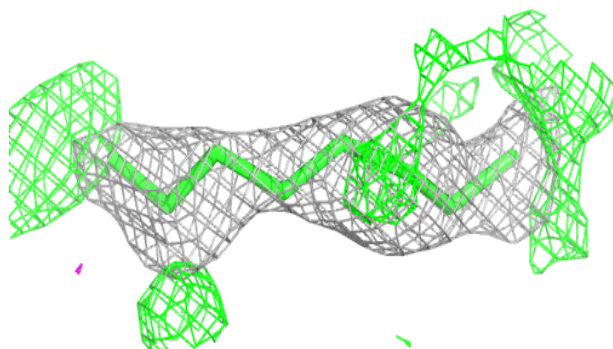
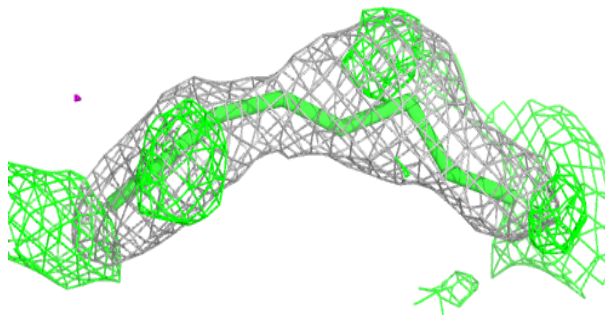
**Electron density around C8E B 809:**

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

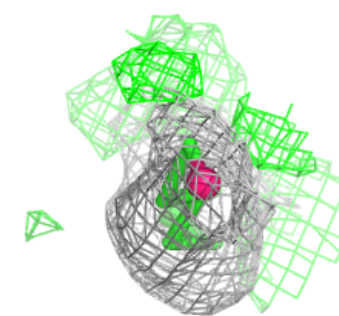
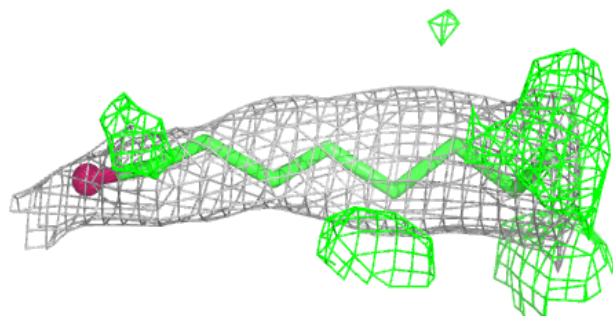
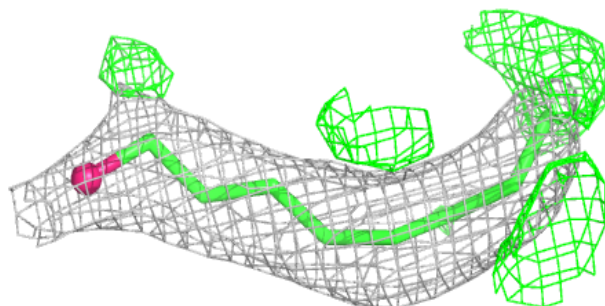


Electron density around C8E B 810:

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

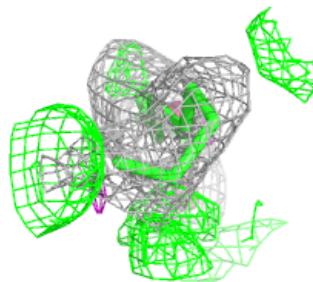
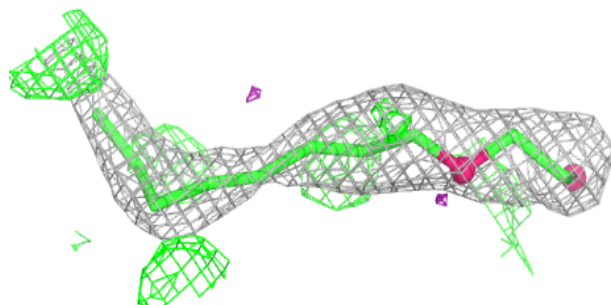
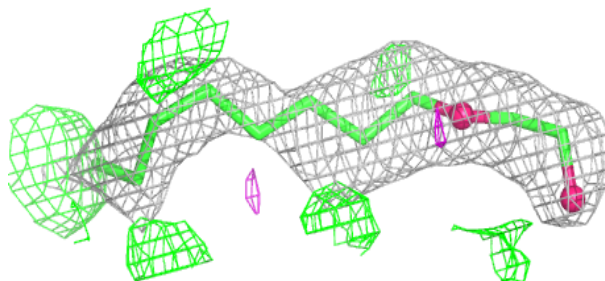
**Electron density around C8E A 810:**

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and green (positive)

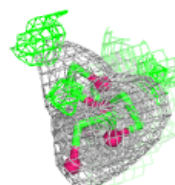
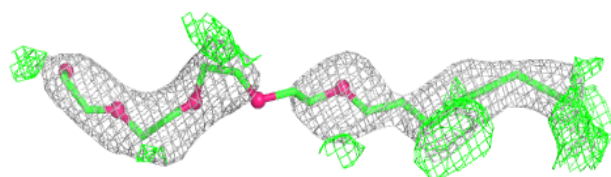
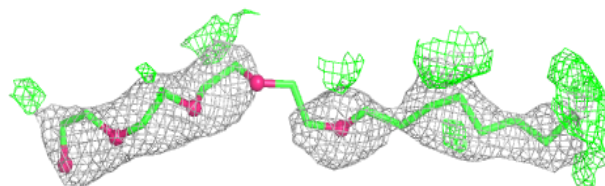


Electron density around C8E B 813:

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and green (positive)

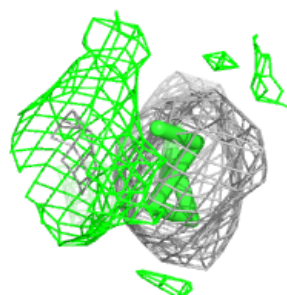
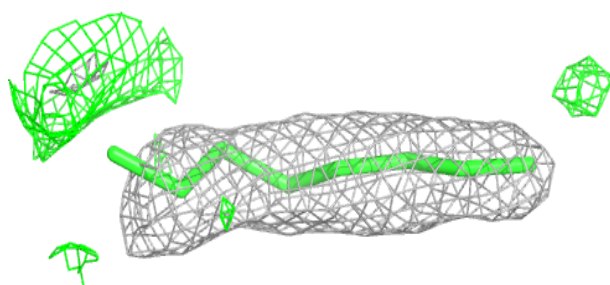
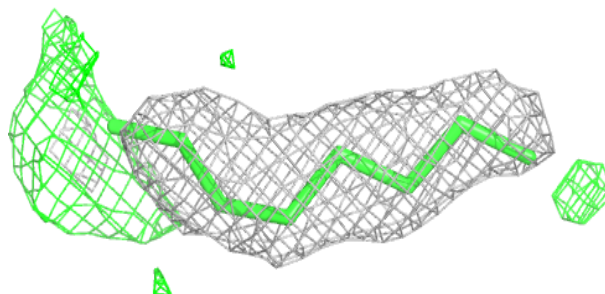
**Electron density around C8E B 807:**

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and green (positive)

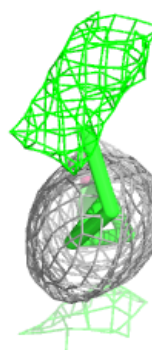
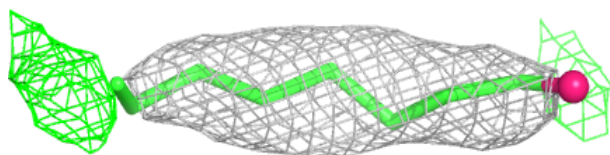
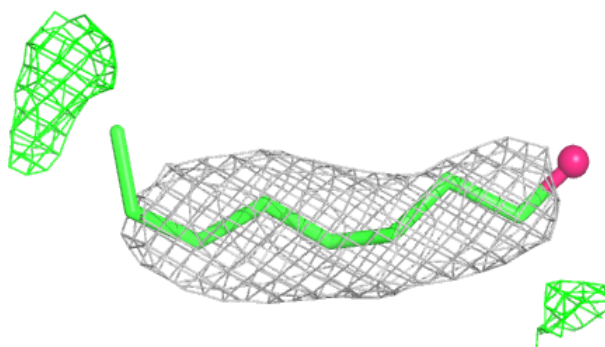


Electron density around C8E B 815:

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and green (positive)

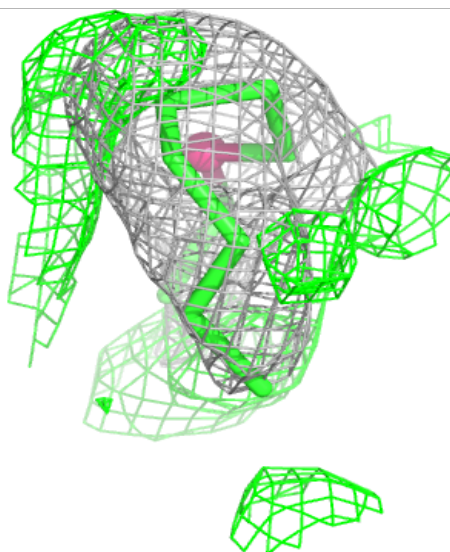
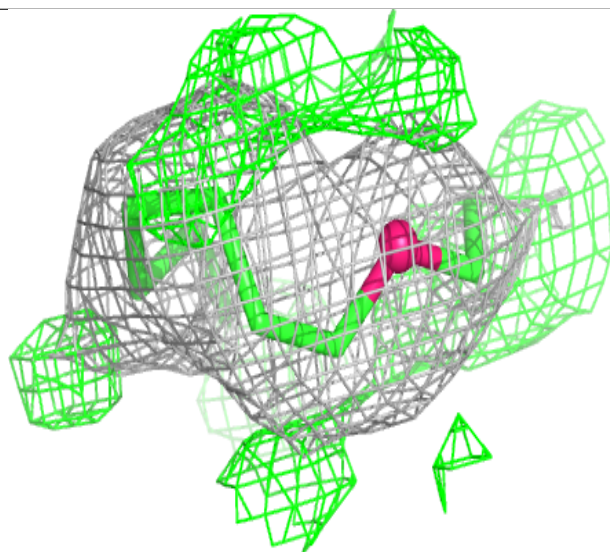
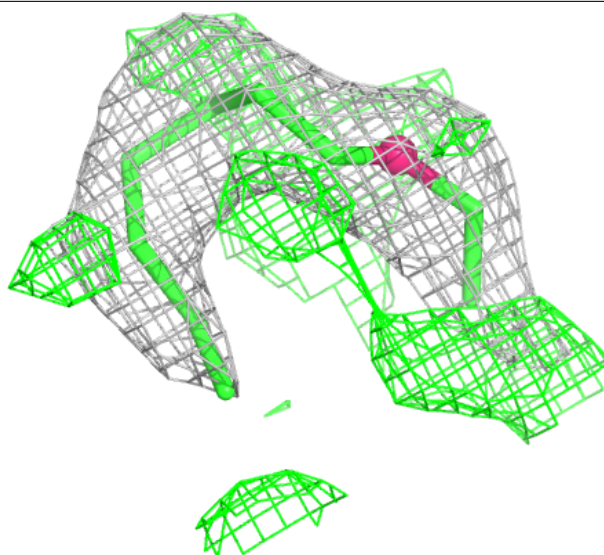
**Electron density around C8E B 808:**

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and green (positive)



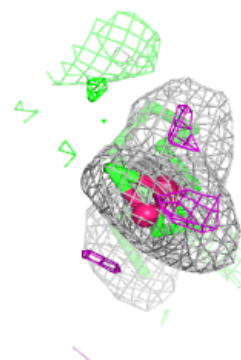
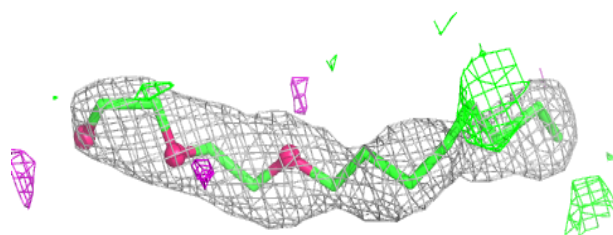
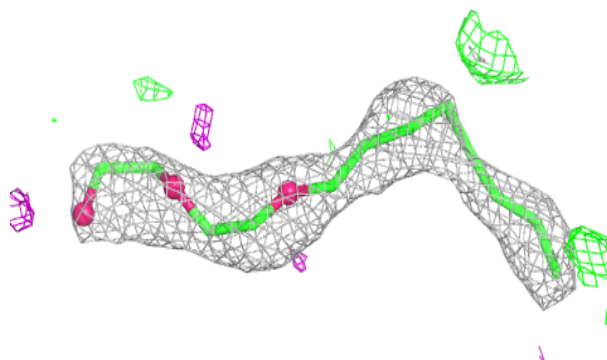
Electron density around C8E C 811:

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and green (positive)

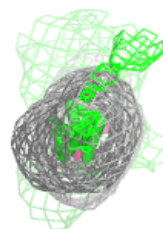
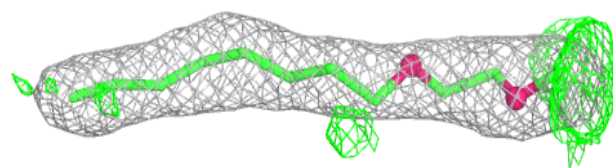
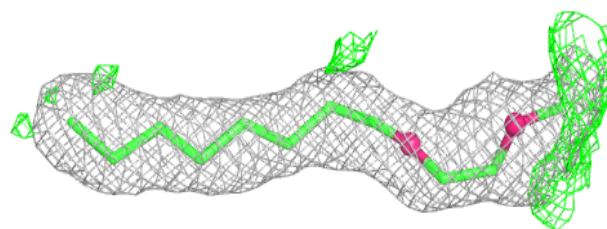


Electron density around C8E C 809:

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

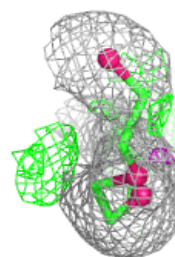
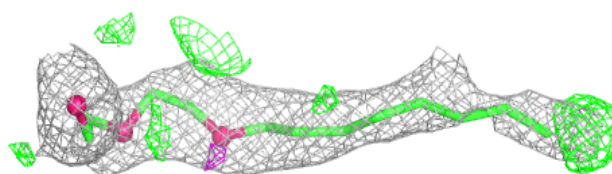
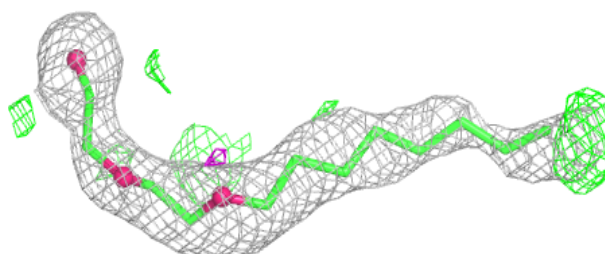
**Electron density around C8E B 806:**

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

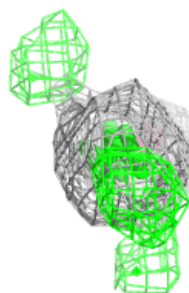
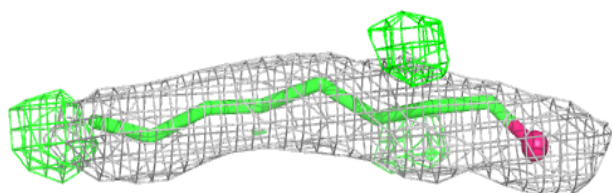
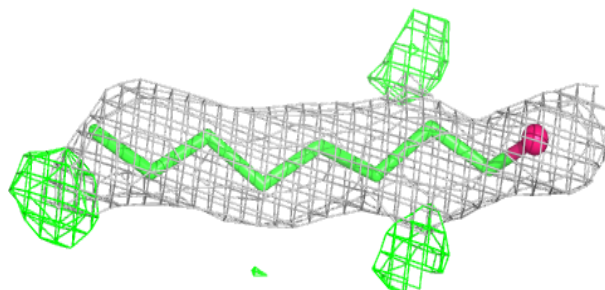


Electron density around C8E C 808:

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

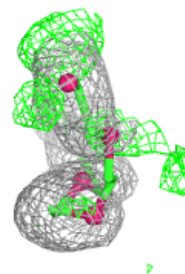
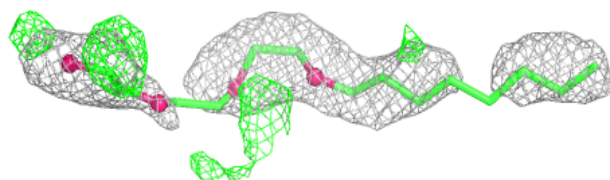
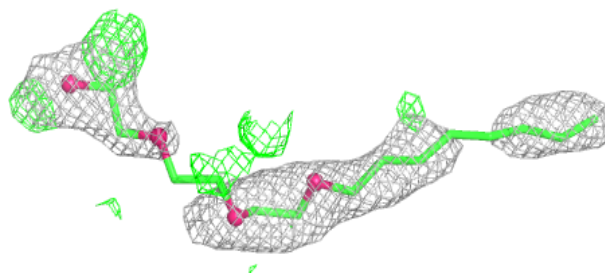
**Electron density around C8E A 806:**

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

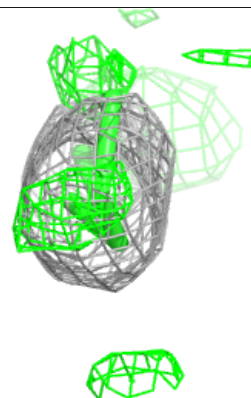
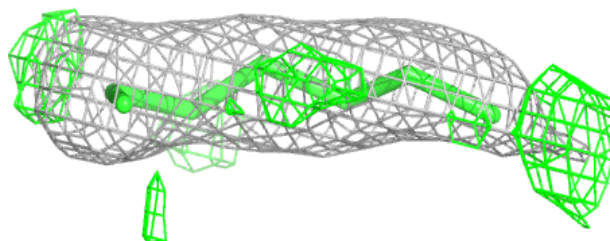
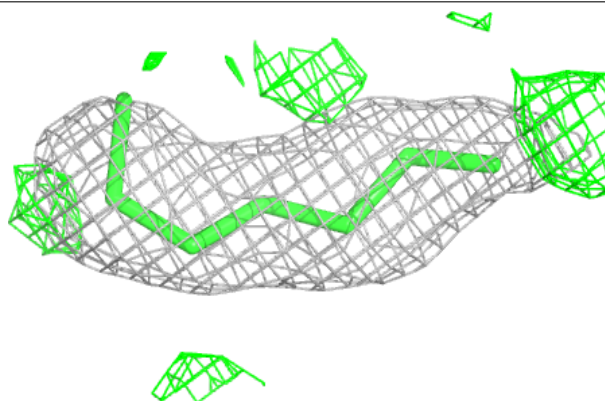


Electron density around C8E B 805:

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

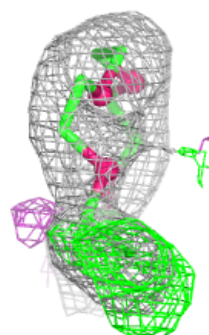
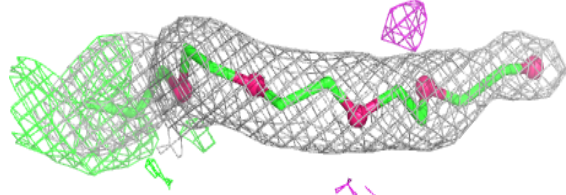
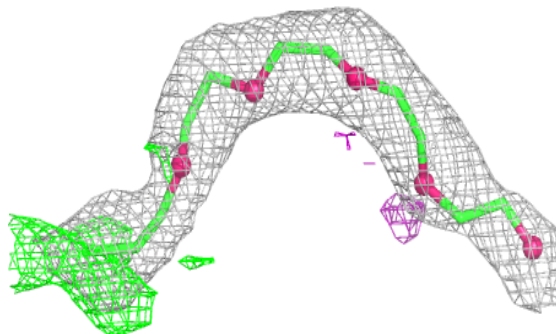
**Electron density around C8E A 809:**

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

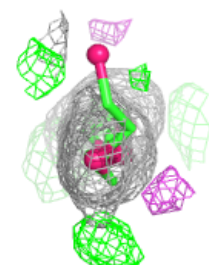
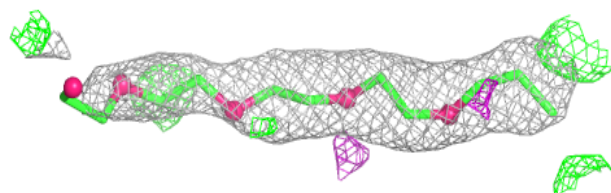
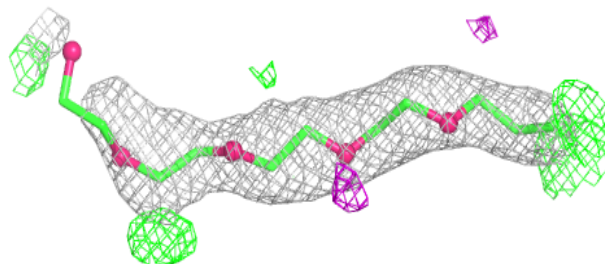


Electron density around C8E C 805:

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

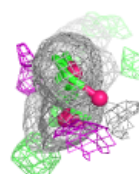
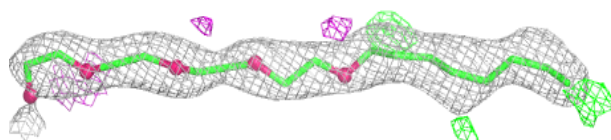
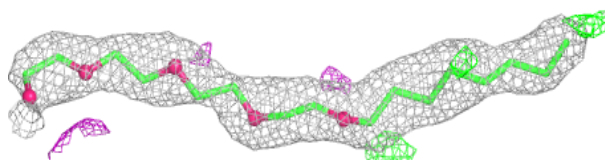
**Electron density around C8E B 804:**

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

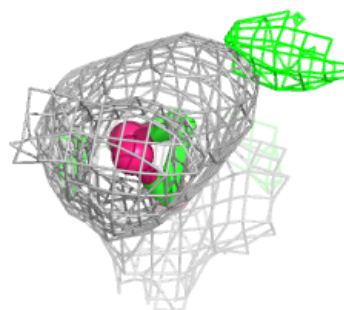
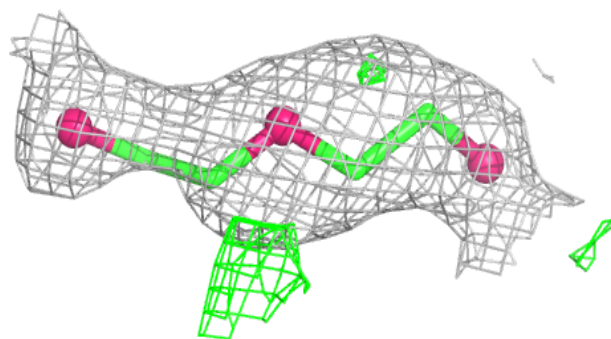
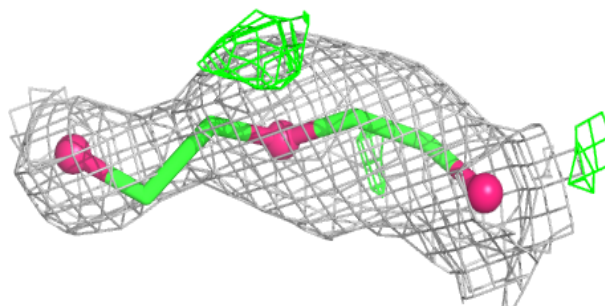


Electron density around C8E C 807:

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

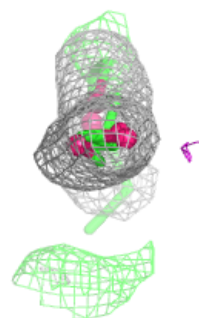
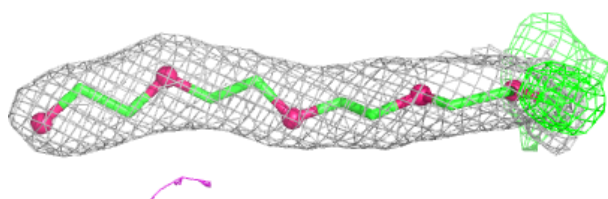
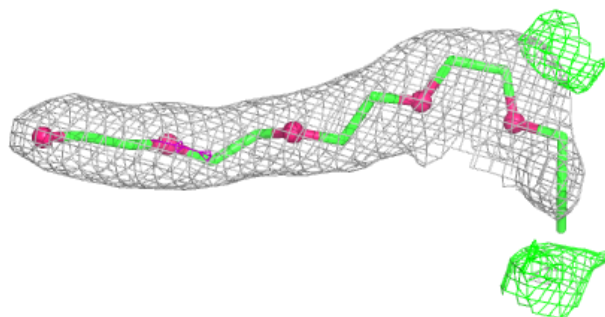
**Electron density around C8E C 810:**

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

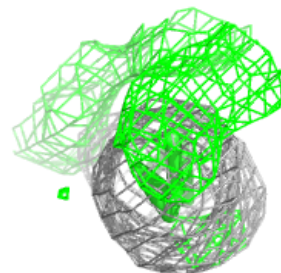
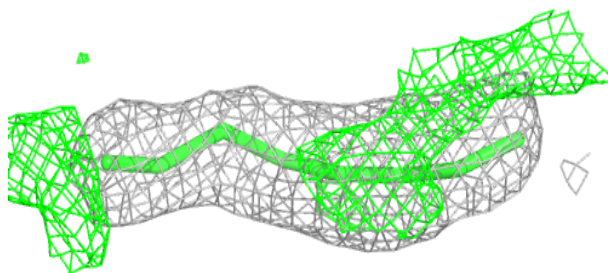
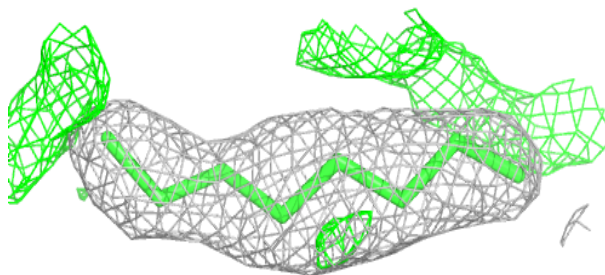


Electron density around C8E C 804:

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

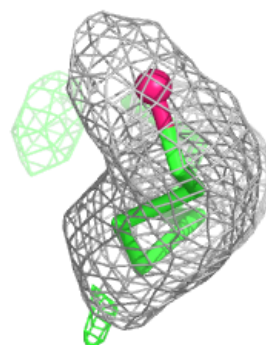
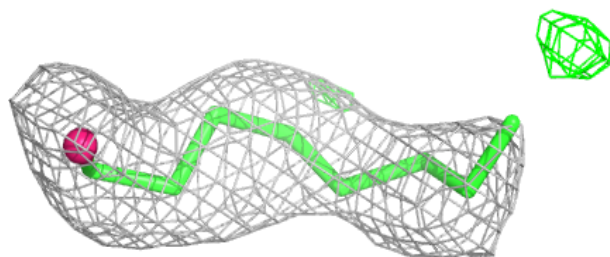
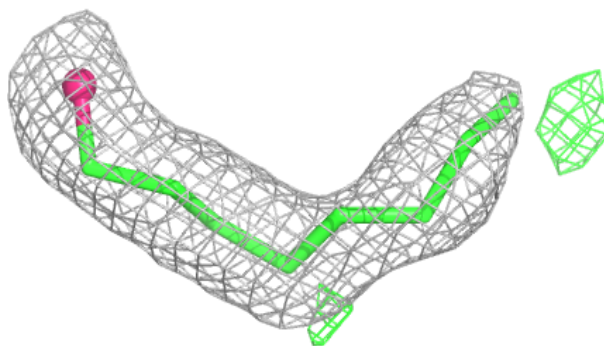
**Electron density around C8E A 807:**

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

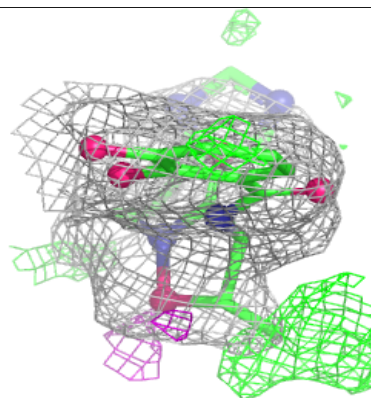
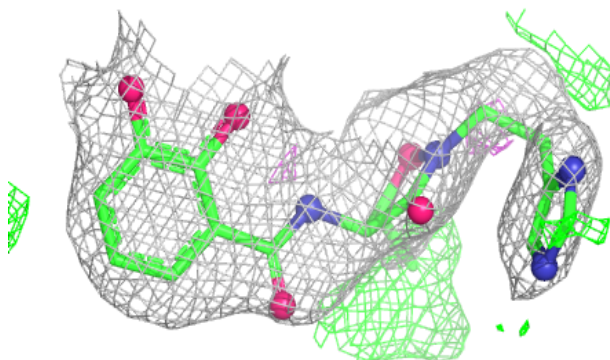
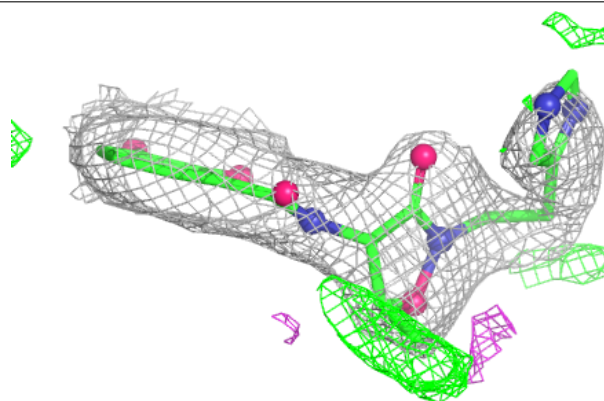


Electron density around C8E A 808:

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

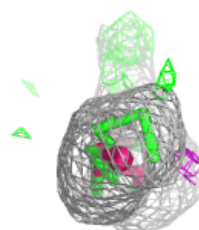
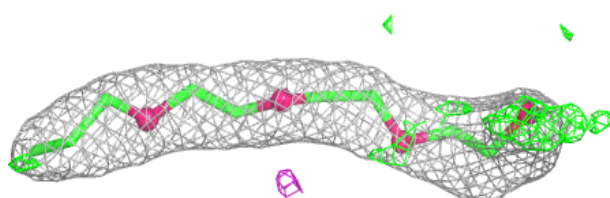
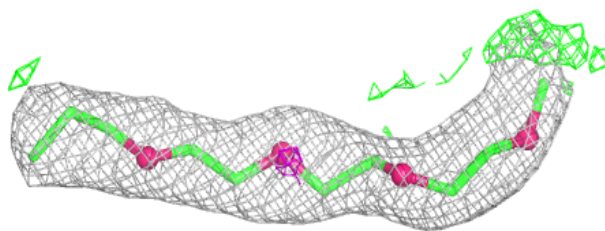
**Electron density around OPV A 803 (A):**

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

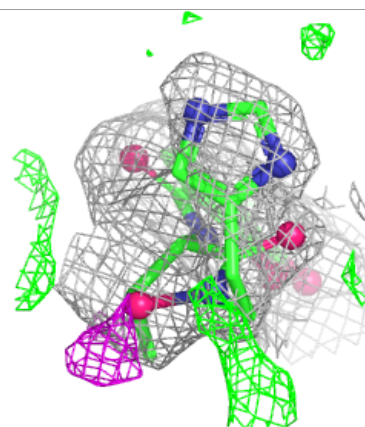
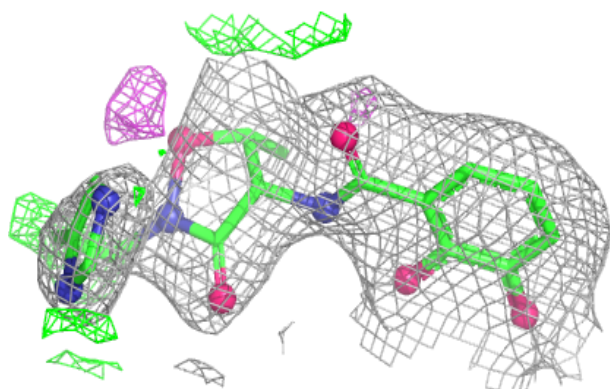
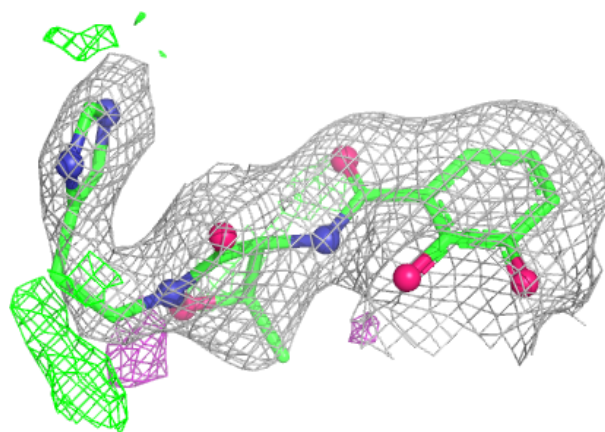


Electron density around C8E C 806:

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

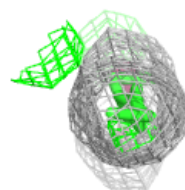
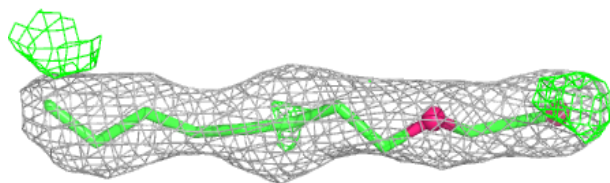
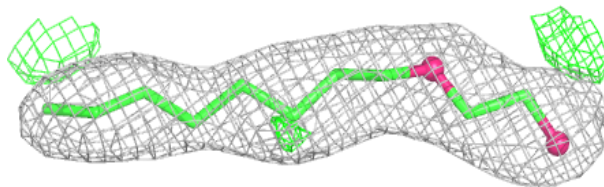
**Electron density around OPZ A 804 (B):**

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

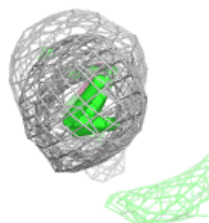
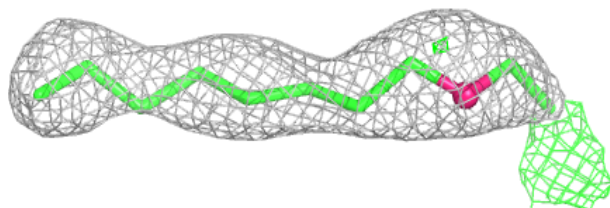
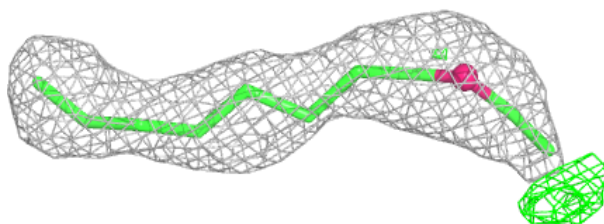


Electron density around C8E B 812:

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

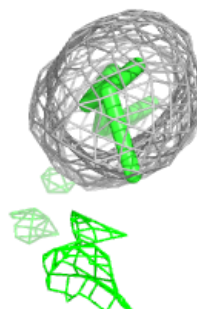
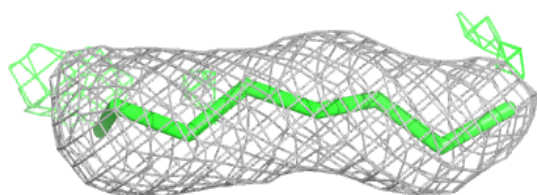
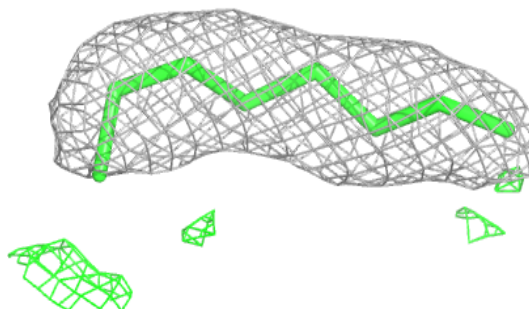
**Electron density around C8E A 805:**

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

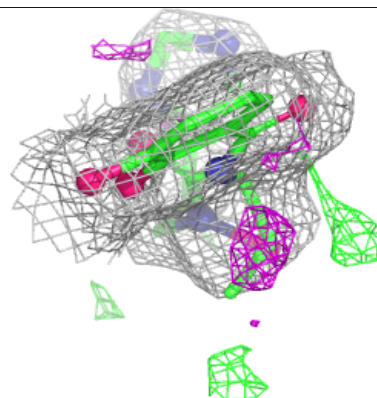
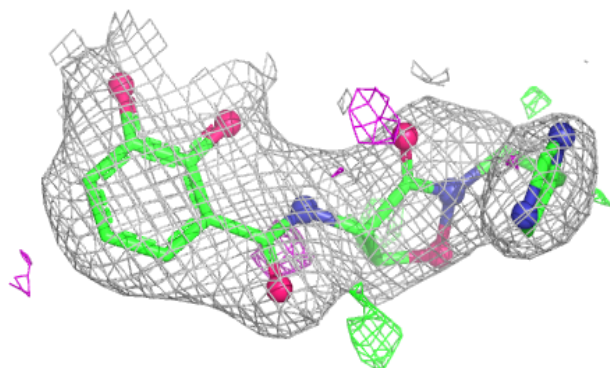
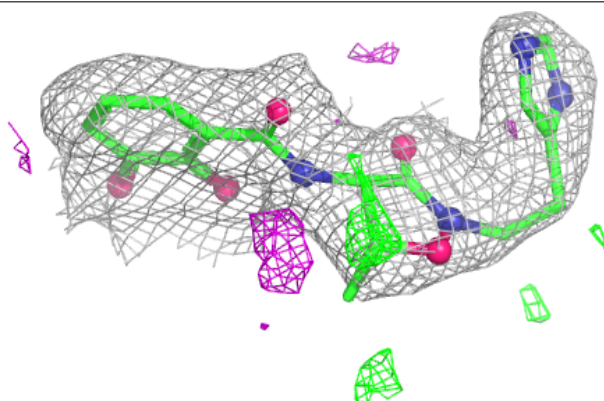


Electron density around C8E C 812:

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

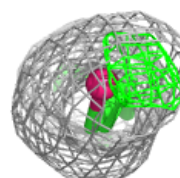
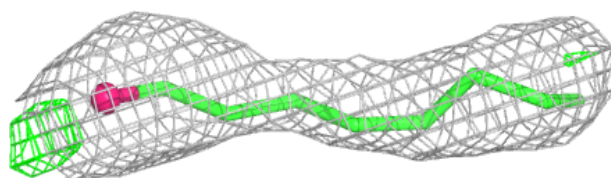
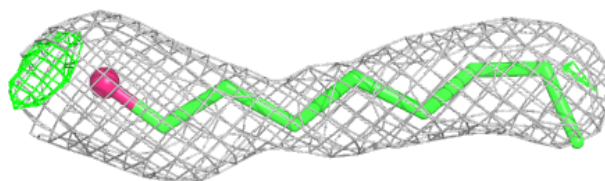
**Electron density around OPZ C 803:**

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

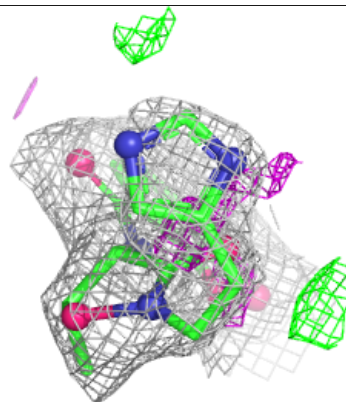
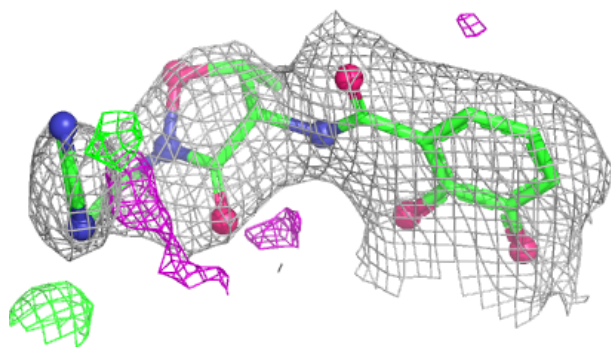
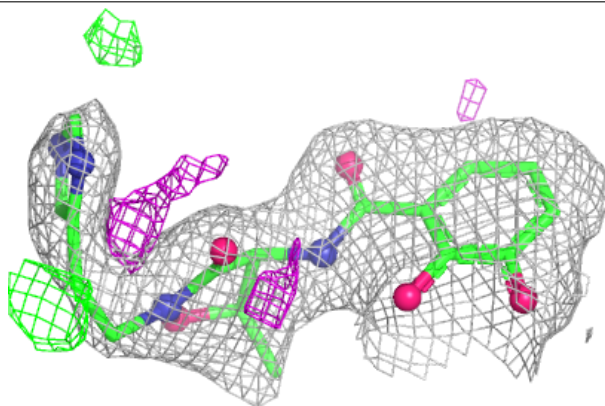


Electron density around C8E B 814:

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

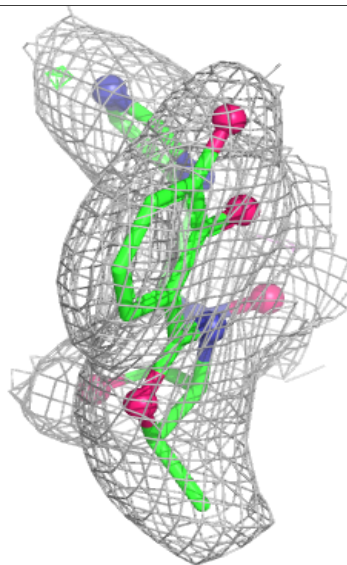
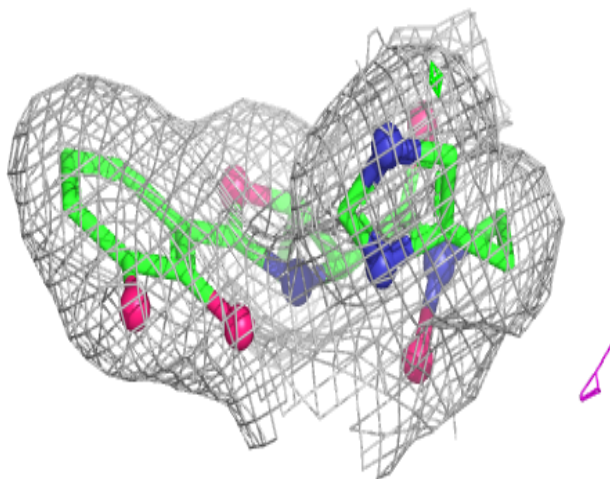
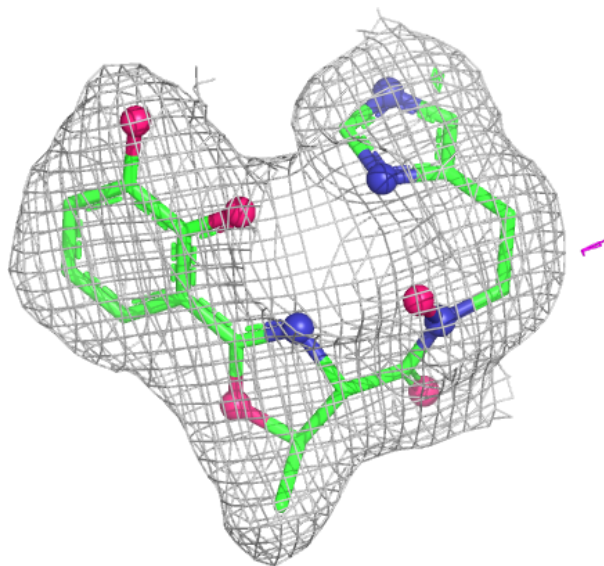
**Electron density around OPZ B 803:**

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



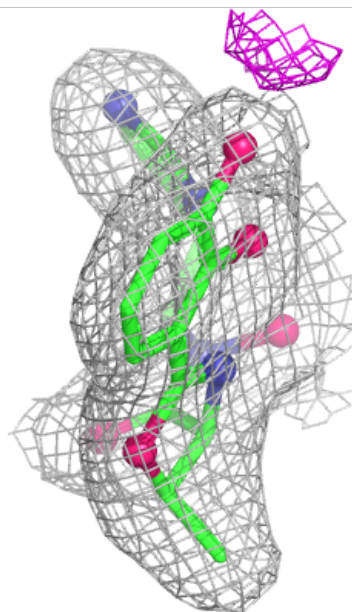
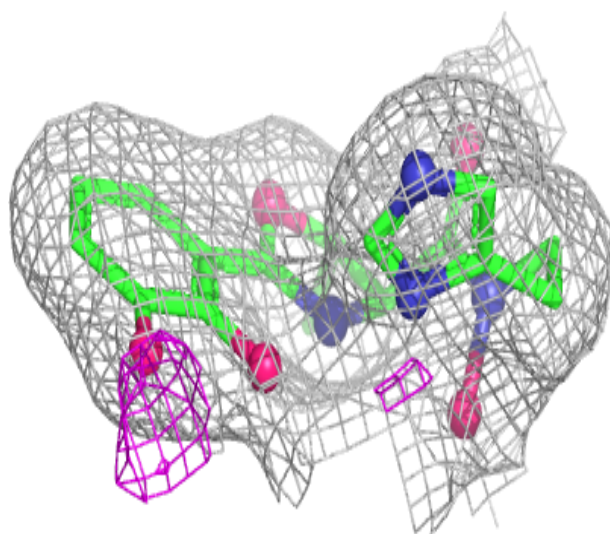
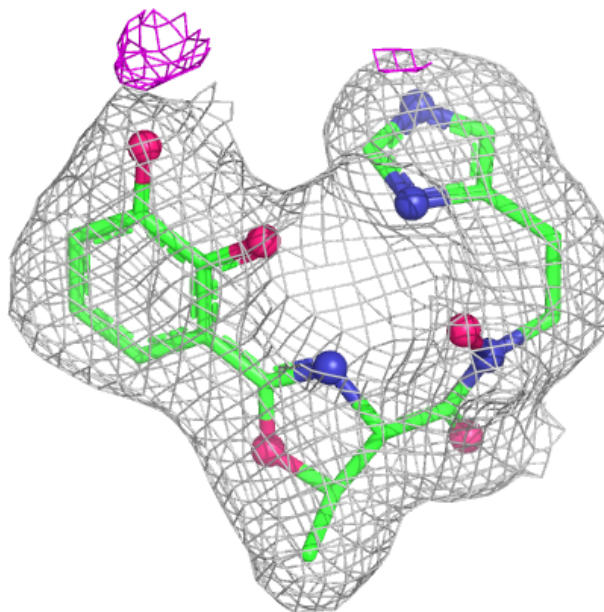
Electron density around FV8 A 802:

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



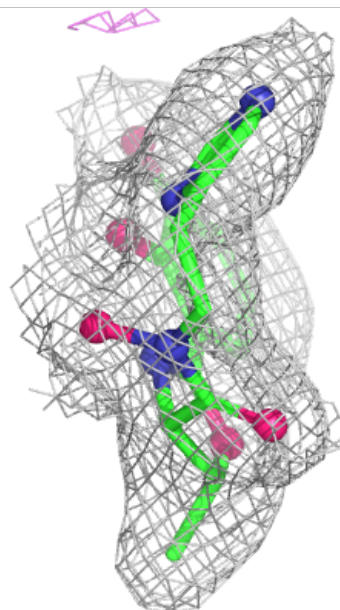
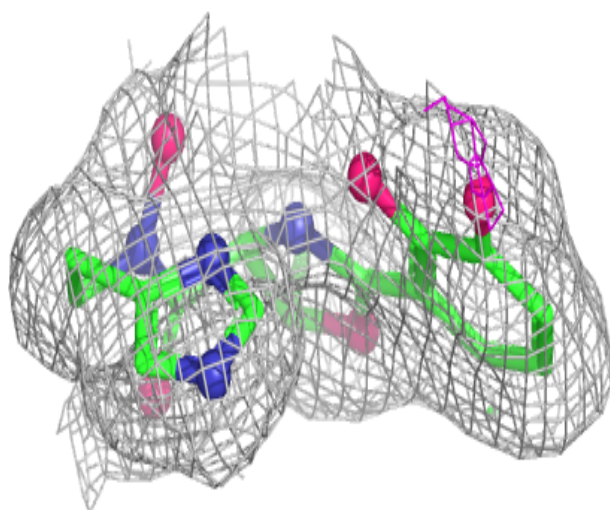
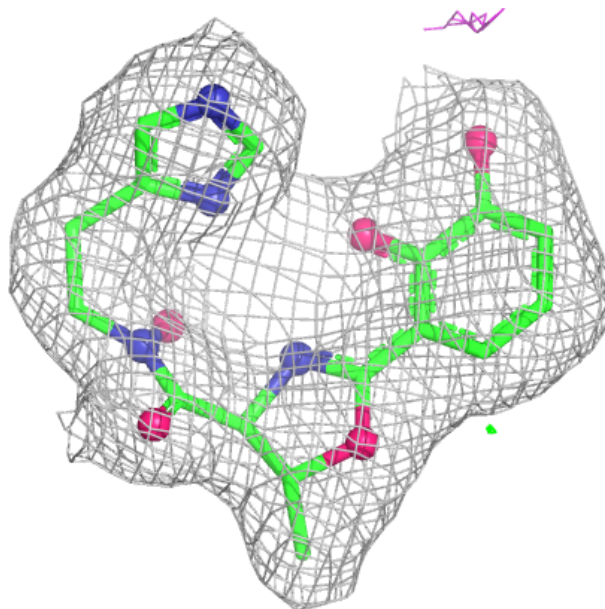
Electron density around FV8 B 802:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.