



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 6HCP / pdb_00006hcp
Title : Crystal structure of BauA, the Ferric preacinetobactin receptor from *Acinetobacter baumannii*
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2018-08-16
Resolution : 1.83 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

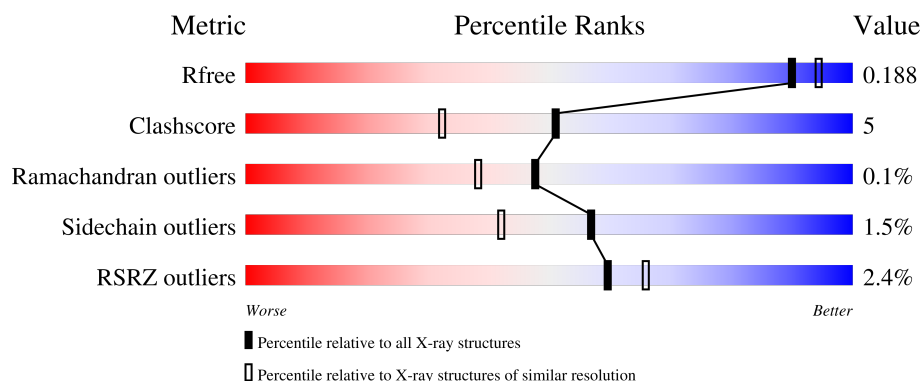
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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% 87% 8% 5%
1	B	706	3% 88% 6% 5%
1	C	706	3% 87% 8% 5%

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
2	EDO	A	825	-	-	X	-
3	C8E	C	836[A]	-	-	X	-
3	C8E	C	836[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18809 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	22	0
			5301	3345	885	1060	11			
1	B	671	Total	C	N	O	S	0	23	0
			5303	3350	885	1057	11			
1	C	671	Total	C	N	O	S	0	42	0
			5456	3448	913	1084	11			

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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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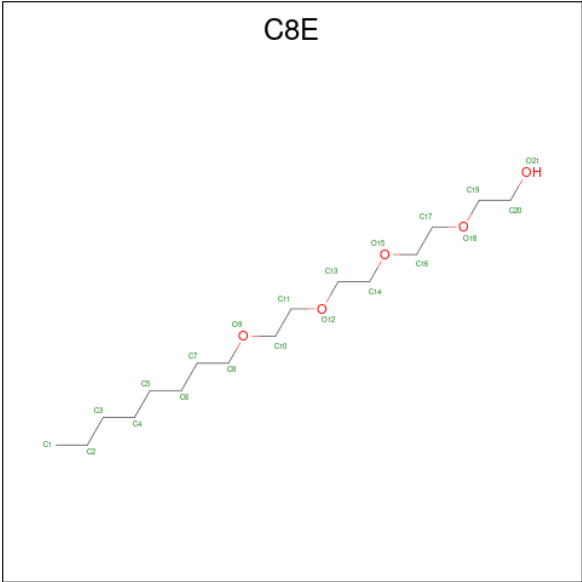
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



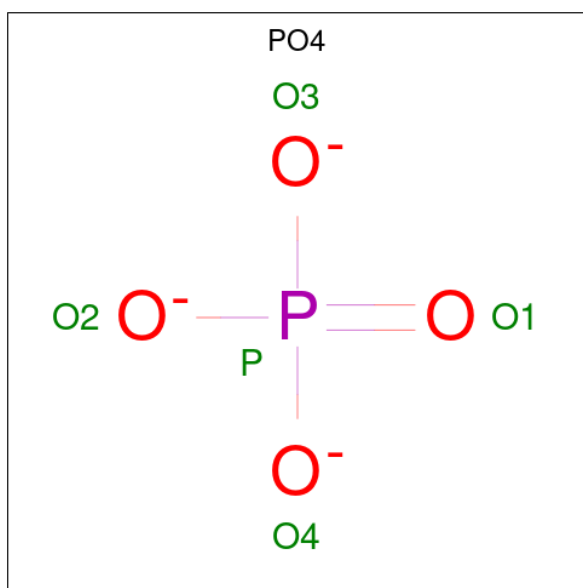
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	A	1	Total	C	O	0	0
			18	14	4		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C		0	0
			8	8			
3	A	1	Total	C	O	0	0
			19	15	4		
3	A	1	Total	C		0	0
			8	8			
3	A	1	Total	C	O	0	0
			10	9	1		
3	B	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			9	8	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 8 8	0	0
3	B	1	Total C O 9 8 1	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 9 8 1	0	0
3	B	1	Total C O 9 8 1	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C O 21 16 5	0	0
3	C	1	Total C O 18 14 4	0	0
3	C	1	Total C O 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0
3	C	1	Total C O 15 12 3	0	0
3	C	1	Total C O 15 12 3	0	0
3	C	1	Total C O 15 12 3	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C O 9 8 1	0	0
3	C	1	Total C O 15 12 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C O 42 32 10	0	1

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

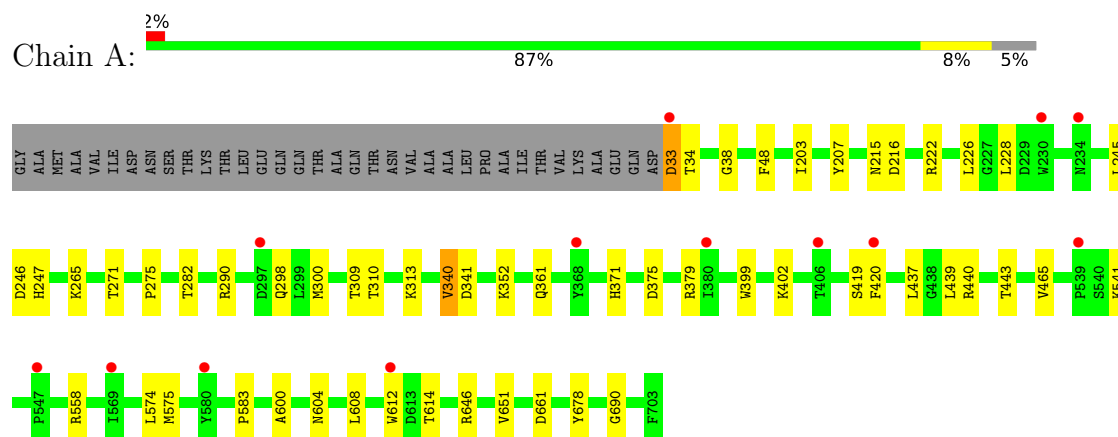
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	677	Total	O	0	0
			677	677		
5	B	620	Total	O	0	0
			620	620		
5	C	698	Total	O	0	0
			698	698		

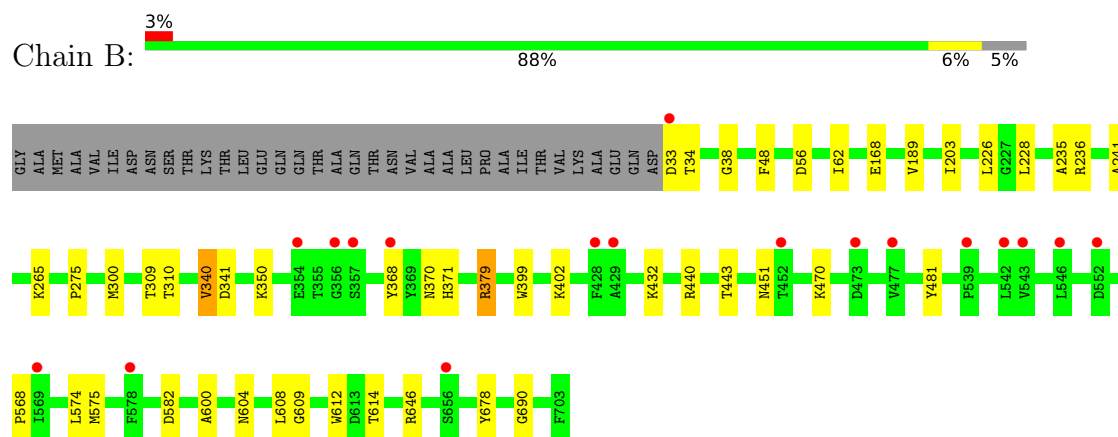
3 Residue-property plots [i](#)

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.

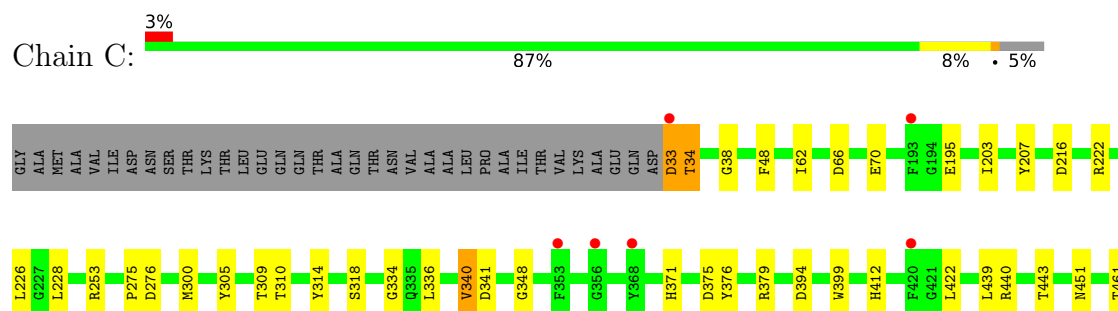
• Molecule 1: BauA



• 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	180.20Å 219.52Å 101.43Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	57.24 – 1.83 57.24 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.24-1.83) 99.7 (57.24-1.83)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.156 , 0.177 0.168 , 0.188	Depositor DCC
R_{free} test set	17140 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18809	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: EDO, C8E, PO4

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	0.67	0/5427	0.77	0/7385
1	B	0.69	0/5429	0.77	0/7389
1	C	0.69	0/5587	0.77	2/7607 (0.0%)
All	All	0.68	0/16443	0.77	2/22381 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	394	ASP	CA-CB-CG	5.38	117.98	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	ARG	Sidechain
1	B	379	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	440	ARG	Sidechain
1	C	440	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	5301	0	5094	47	0
1	B	5303	0	5113	37	0
1	C	5456	0	5262	66	0
2	A	100	0	150	14	0
2	B	96	0	144	4	0
2	C	88	0	132	7	0
3	A	153	0	254	8	0
3	B	90	0	157	5	0
3	C	222	0	367	45	0
4	B	5	0	0	0	0
5	A	677	0	0	11	0
5	B	620	0	0	8	1
5	C	698	0	0	11	1
All	All	18809	0	16673	174	1

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 5.

All (174) 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)
3:C:836[B]:C8E:O21	3:C:836[B]:C8E:C11	1.90	1.18
1:C:336[LEU]:HD22	3:C:836[B]:C8E:H102	1.20	1.15
1:A:574[LEU]:HD11	1:A:608[A]:LEU:HD11	1.25	1.11
1:B:574[A]:LEU:HD11	1:B:608[LEU]:HD11	1.19	1.10
1:C:253[B]:ARG:HH12	3:C:836[B]:C8E:H111	1.17	1.09
1:A:215[ASN]:ND2	2:A:825[EDO]:H12	1.70	1.06
1:C:574[B]:LEU:HD11	1:C:608[LEU]:HD11	1.37	1.06
1:C:336[LEU]:CD2	3:C:836[B]:C8E:H102	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:HD22	2:A:825:EDO:H12	0.87	1.02
1:B:574[A]:LEU:CD1	1:B:608:LEU:HD11	1.92	1.00
1:A:574:LEU:CD1	1:A:608[A]:LEU:HD11	1.94	0.97
3:C:836[B]:C8E:O21	3:C:836[B]:C8E:H112	1.68	0.94
1:C:318:SER:HB3	3:C:836[B]:C8E:H62	1.54	0.88
1:C:574[B]:LEU:CD1	1:C:608:LEU:HD11	2.04	0.87
3:C:836[B]:C8E:O21	3:C:836[B]:C8E:C10	2.24	0.85
3:C:836[B]:C8E:O21	3:C:836[B]:C8E:H111	1.76	0.82
1:C:253[B]:ARG:NH1	3:C:836[B]:C8E:H111	1.95	0.80
1:A:215:ASN:HD22	2:A:825:EDO:C1	1.84	0.80
3:C:825:C8E:H201	5:C:1431:HOH:O	1.81	0.79
3:C:836[B]:C8E:O21	3:C:836[B]:C8E:H101	1.83	0.77
1:C:207:TYR:HD1	1:C:222:ARG:HG2	1.53	0.74
1:B:56:ASP:OD1	1:B:470:LYS:HE2	1.88	0.72
1:C:318:SER:HB3	3:C:836[A]:C8E:H61	1.72	0.72
1:C:62:ILE:HD13	2:C:820:EDO:H21	1.73	0.71
3:C:836[B]:C8E:H41	3:C:836[B]:C8E:H81	1.73	0.70
1:A:207:TYR:HD1	1:A:222:ARG:HG2	1.57	0.69
3:A:831:C8E:H82	3:B:828:C8E:C8	2.23	0.69
1:B:402:LYS:HE3	5:B:1018:HOH:O	1.91	0.69
1:A:271:THR:HA	2:A:825:EDO:H11	1.76	0.68
2:C:808:EDO:O1	3:C:836[A]:C8E:H192	1.94	0.67
3:C:836[B]:C8E:H101	3:C:836[B]:C8E:C20	2.24	0.67
1:B:443:THR:HG22	2:B:815:EDO:H21	1.77	0.67
1:B:604:ASN:HB3	3:B:828:C8E:H51	1.77	0.67
1:C:580:TYR:CE2	3:C:827:C8E:H42	2.29	0.67
1:B:56:ASP:OD1	1:B:470:LYS:CE	2.45	0.65
1:C:253[A]:ARG:NE	1:C:318:SER:O	2.30	0.65
1:C:34:THR:CG2	1:C:38:GLY:HA2	2.26	0.64
1:C:318:SER:HB3	3:C:836[A]:C8E:C6	2.28	0.64
1:B:62[A]:ILE:HD13	2:B:804:EDO:H12	1.79	0.64
1:C:207:TYR:CD1	1:C:222:ARG:HG2	2.33	0.64
1:B:451:ASN:ND2	5:B:904:HOH:O	2.24	0.64
1:A:651:VAL:CG1	3:A:833:C8E:H12	2.28	0.63
3:C:836[B]:C8E:H202	5:C:1489:HOH:O	1.99	0.63
1:B:34:THR:CG2	1:B:38:GLY:HA2	2.28	0.63
3:C:836[B]:C8E:H112	3:C:836[B]:C8E:O15	1.99	0.61
1:C:568:PRO:HG3	1:C:574[A]:LEU:HD12	1.82	0.61
1:A:34:THR:CG2	1:A:38:GLY:HA2	2.30	0.61
3:A:836:C8E:C10	5:A:910:HOH:O	2.48	0.61
1:C:66:ASP:O	1:C:70[B]:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TYR:CD1	1:A:222:ARG:HG2	2.37	0.60
1:A:439:LEU:C	1:A:439:LEU:HD12	2.26	0.60
3:C:836[A]:C8E:H202	5:C:1413:HOH:O	2.02	0.59
1:C:203:ILE:HG12	1:C:226[B]:LEU:CD2	2.34	0.58
1:A:437:LEU:HD23	1:A:465:VAL:HG23	1.86	0.58
1:C:439[B]:LEU:HD11	1:C:461:THR:CG2	2.34	0.56
1:C:203:ILE:HG12	1:C:226[B]:LEU:HD23	1.88	0.56
1:C:539:PRO:CA	1:C:547[B]:PRO:HB3	2.37	0.54
1:A:352:LYS:HG2	1:A:361:GLN:HG3	1.89	0.54
3:C:836[B]:C8E:H101	3:C:836[B]:C8E:H201	1.89	0.54
1:A:247[A]:HIS:HE1	5:A:971:HOH:O	1.90	0.54
1:C:580:TYR:CE2	3:C:827:C8E:C4	2.91	0.54
1:B:189[B]:VAL:HG12	1:B:203:ILE:HB	1.90	0.54
1:C:439[B]:LEU:HD11	1:C:461:THR:HG22	1.90	0.53
1:B:168:GLU:O	5:B:901:HOH:O	2.18	0.53
1:C:494[A]:THR:O	1:C:494[A]:THR:CG2	2.57	0.53
1:C:563:SER:HB2	2:C:820:EDO:H11	1.89	0.53
1:C:412:HIS:HD2	2:C:822:EDO:H22	1.74	0.53
1:C:309:THR:HG22	1:C:341:ASP:OD1	2.09	0.52
1:C:616:VAL:O	1:C:616:VAL:CG2	2.57	0.52
1:B:568:PRO:HG3	1:B:574[B]:LEU:HD12	1.92	0.52
3:A:831:C8E:C8	3:B:828:C8E:C8	2.88	0.52
1:C:336:LEU:HB2	3:C:836[B]:C8E:H81	1.92	0.52
1:A:443:THR:HG22	2:A:811:EDO:H12	1.92	0.51
1:B:379:ARG:HG3	5:B:1449:HOH:O	2.10	0.51
1:B:612:TRP:CH2	1:B:614[B]:THR:HG21	2.45	0.51
1:C:253[B]:ARG:HH12	3:C:836[B]:C8E:C11	2.05	0.51
1:C:348:GLY:HA2	3:C:826:C8E:H71	1.92	0.51
1:A:216:ASP:OD2	1:B:265:LYS:NZ	2.37	0.50
1:A:282:THR:OG1	2:A:823:EDO:H12	2.11	0.50
1:B:432:LYS:HE2	5:B:1399:HOH:O	2.10	0.50
1:C:542[B]:LEU:HD21	5:C:1193:HOH:O	2.11	0.50
1:C:678:TYR:CZ	1:C:690:GLY:HA3	2.46	0.50
1:A:298:GLN:NE2	5:A:912:HOH:O	2.44	0.50
1:B:309:THR:HG22	1:B:341:ASP:OD1	2.12	0.50
1:A:678:TYR:CZ	1:A:690:GLY:HA3	2.48	0.49
1:C:539:PRO:HA	1:C:547[B]:PRO:HB3	1.93	0.49
1:C:253[B]:ARG:HH22	3:C:836[B]:C8E:C11	2.26	0.49
3:C:825:C8E:C20	5:C:1431:HOH:O	2.47	0.49
1:A:575[A]:MET:SD	2:A:806:EDO:O1	2.71	0.48
1:A:309:THR:HG22	1:A:341[A]:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:801:EDO:C2	5:C:1026:HOH:O	2.61	0.48
1:B:678:TYR:CZ	1:B:690:GLY:HA3	2.48	0.48
1:C:580:TYR:CZ	3:C:827:C8E:H42	2.48	0.48
1:B:310:THR:HB	1:B:340:VAL:HG13	1.95	0.48
1:C:495[B]:ALA:HB2	1:C:537:LEU:HD13	1.95	0.47
1:C:318:SER:CB	3:C:836[A]:C8E:C6	2.92	0.47
1:B:612:TRP:CH2	1:B:614[B]:THR:CG2	2.97	0.47
1:C:451:ASN:ND2	5:C:909:HOH:O	2.40	0.47
1:C:616:VAL:O	1:C:616:VAL:HG23	2.14	0.47
1:A:265:LYS:NZ	1:C:216:ASP:OD2	2.39	0.46
1:C:336:LEU:CD2	3:C:836[A]:C8E:H141	2.45	0.46
1:C:494[A]:THR:O	1:C:494[A]:THR:HG22	2.15	0.46
1:C:537:LEU:HG	1:C:547[B]:PRO:HB2	1.97	0.46
1:B:582:ASP:OD2	5:B:902:HOH:O	2.20	0.46
1:C:33:ASP:CG	1:C:33:ASP:O	2.59	0.46
2:A:813:EDO:C1	5:A:1376:HOH:O	2.63	0.46
1:C:568:PRO:HG3	1:C:574[A]:LEU:CD1	2.44	0.46
1:C:336:LEU:HD23	3:C:836[A]:C8E:H141	1.98	0.46
1:C:580:TYR:CZ	3:C:827:C8E:C4	2.98	0.46
3:C:836[A]:C8E:H42	3:C:836[A]:C8E:H71	1.55	0.45
1:A:558:ARG:HB3	3:A:830:C8E:H21	1.98	0.45
1:C:336:LEU:HD12	1:C:376:TYR:O	2.16	0.45
1:C:314:TYR:CE1	3:C:836[A]:C8E:H81	2.52	0.45
1:B:241:ALA:HB1	3:B:825:C8E:H32	1.97	0.45
1:C:305:TYR:HB2	3:C:835:C8E:H31	1.98	0.45
1:C:310:THR:HB	1:C:340:VAL:HG13	1.99	0.45
1:A:604:ASN:HB3	3:A:827:C8E:H72	1.98	0.45
1:B:575[B]:MET:SD	2:B:820:EDO:O1	2.75	0.45
1:A:361:GLN:HG2	5:A:1355:HOH:O	2.16	0.44
1:B:275:PRO:HA	1:B:399:TRP:CD2	2.52	0.44
1:A:310:THR:HB	1:A:340:VAL:HG13	1.99	0.44
1:A:379:ARG:HG3	5:A:1476:HOH:O	2.18	0.44
1:B:612:TRP:CZ2	1:B:614[B]:THR:HG22	2.52	0.44
1:C:336:LEU:HD23	3:C:836[B]:C8E:H102	1.90	0.44
1:C:318:SER:CB	3:C:836[A]:C8E:H62	2.47	0.44
1:A:612:TRP:CH2	1:A:614[B]:THR:HG21	2.52	0.44
1:B:481:TYR:OH	3:B:826:C8E:H191	2.17	0.44
1:C:684:LEU:HD13	5:C:1076:HOH:O	2.17	0.44
2:C:801:EDO:H22	5:C:1026:HOH:O	2.18	0.44
1:B:350:LYS:NZ	5:B:927:HOH:O	2.48	0.44
1:A:222:ARG:HG3	1:A:245:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:PRO:HA	1:C:399:TRP:CD2	2.53	0.44
1:C:539:PRO:HA	1:C:547[B]:PRO:HA	2.00	0.44
1:A:313:LYS:NZ	5:A:925:HOH:O	2.52	0.43
1:A:34:THR:HG21	1:A:38:GLY:HA2	1.99	0.43
1:B:568:PRO:HG3	1:B:574[B]:LEU:CD1	2.49	0.43
1:C:318:SER:CB	3:C:836[B]:C8E:H62	2.36	0.43
1:B:368:TYR:OH	1:B:370:ASN:HB2	2.19	0.43
3:C:826:C8E:H202	3:C:835:C8E:H11	2.01	0.43
1:B:226[A]:LEU:HD11	1:B:228:LEU:HD21	2.01	0.42
1:C:443:THR:HG22	2:C:811:EDO:H21	2.01	0.42
1:A:203:ILE:HG12	1:A:226[B]:LEU:HD23	2.00	0.42
1:A:271:THR:HA	2:A:825:EDO:C1	2.48	0.42
1:A:575[A]:MET:HG3	2:A:818:EDO:O1	2.19	0.42
1:A:419:SER:C	1:A:420:PHE:CD1	2.98	0.42
1:B:34:THR:HG21	1:B:38:GLY:HA2	1.98	0.42
1:A:290:ARG:HD2	2:A:819:EDO:C2	2.50	0.42
1:A:226[A]:LEU:HD11	1:A:228:LEU:HD21	2.00	0.42
1:B:235:ALA:C	1:B:236:ARG:HG3	2.45	0.42
1:A:541:LYS:NZ	5:A:922:HOH:O	2.51	0.42
1:A:651:VAL:HG12	3:A:833:C8E:H12	1.99	0.42
1:C:379:ARG:HG3	5:C:1572:HOH:O	2.20	0.42
1:B:33:ASP:O	1:B:33:ASP:CG	2.63	0.41
1:C:226[A]:LEU:HD11	1:C:228:LEU:HD21	2.01	0.41
1:C:568:PRO:C	1:C:569:ILE:HG13	2.45	0.41
1:C:510:GLN:OE1	3:C:824:C8E:H162	2.20	0.41
1:A:402:LYS:HE3	5:A:960:HOH:O	2.20	0.41
1:B:612:TRP:CZ2	1:B:614[B]:THR:CG2	3.04	0.41
1:C:34:THR:HG21	1:C:38:GLY:HA2	1.98	0.41
1:A:246:ASP:OD2	2:A:823:EDO:H21	2.20	0.41
2:A:813:EDO:H12	5:A:1376:HOH:O	2.19	0.41
1:A:33:ASP:O	1:A:33:ASP:CG	2.64	0.41
1:A:290:ARG:HD2	2:A:819:EDO:H22	2.02	0.41
1:C:422[A]:LEU:HG	3:C:826:C8E:H13	2.03	0.41
3:C:836[B]:C8E:C11	3:C:836[B]:C8E:HO2	2.20	0.41
1:B:609:GLY:C	2:B:820:EDO:H22	2.46	0.41
1:A:402:LYS:CE	5:A:960:HOH:O	2.68	0.40
1:A:612:TRP:CZ2	1:A:614[B]:THR:CG2	3.05	0.40
1:B:451:ASN:CB	5:B:904:HOH:O	2.69	0.40
3:C:826:C8E:C20	3:C:835:C8E:H11	2.51	0.40
3:C:836[A]:C8E:H192	5:C:916:HOH:O	2.22	0.40
1:A:222:ARG:HB3	3:A:832:C8E:H42	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HA	1:A:399:TRP:CD2	2.57	0.40
1:C:334:GLY:HA3	3:C:836[B]:C8E:C6	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1455:HOH:O	5:C:1074:HOH:O[4_757]	2.08	0.12

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	691/706 (98%)	673 (97%)	16 (2%)	2 (0%)	36	25
1	B	692/706 (98%)	673 (97%)	18 (3%)	1 (0%)	48	38
1	C	711/706 (101%)	690 (97%)	21 (3%)	0	100	100
All	All	2094/2118 (99%)	2036 (97%)	55 (3%)	3 (0%)	48	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ALA
1	B	600	ALA
1	A	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	572/577 (99%)	564 (99%)	8 (1%)	59	45
1	B	573/577 (99%)	568 (99%)	5 (1%)	70	60
1	C	588/577 (102%)	576 (98%)	12 (2%)	48	32
All	All	1733/1731 (100%)	1708 (99%)	25 (1%)	57	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	48	PHE
1	A	300	MET
1	A	340	VAL
1	A	371	HIS
1	A	375	ASP
1	A	646	ARG
1	A	661	ASP
1	B	48	PHE
1	B	300	MET
1	B	340	VAL
1	B	371	HIS
1	B	646	ARG
1	C	33	ASP
1	C	34	THR
1	C	48	PHE
1	C	195	GLU
1	C	300	MET
1	C	340	VAL
1	C	371	HIS
1	C	375	ASP
1	C	494[A]	THR
1	C	494[B]	THR
1	C	616	VAL
1	C	646	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN

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Mol	Chain	Res	Type
1	A	626	ASN
1	A	681	GLN
1	A	683	GLN
1	B	234	ASN
1	B	373	GLN
1	B	683	GLN
1	C	234	ASN
1	C	361	GLN
1	C	373	GLN
1	C	683	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](#)

108 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	C	815	-	3,3,3	0.75	0	2,2,2	0.70	0
2	EDO	A	808	-	3,3,3	0.87	0	2,2,2	0.48	0
2	EDO	A	819	-	3,3,3	0.39	0	2,2,2	0.73	0
2	EDO	A	818	-	3,3,3	0.50	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	810	-	3,3,3	0.38	0	2,2,2	0.63	0
3	C8E	A	834	-	18,18,20	0.50	0	17,17,19	0.28	0
2	EDO	B	803	-	3,3,3	0.31	0	2,2,2	0.69	0
2	EDO	A	807	-	3,3,3	0.39	0	2,2,2	0.45	0
2	EDO	B	815	-	3,3,3	0.43	0	2,2,2	0.24	0
2	EDO	A	820	-	3,3,3	0.33	0	2,2,2	0.36	0
2	EDO	A	804	-	3,3,3	0.54	0	2,2,2	0.16	0
3	C8E	B	829	-	8,8,20	0.22	0	7,7,19	0.44	0
3	C8E	B	834	-	7,7,20	0.28	0	6,6,19	0.37	0
3	C8E	C	831	-	8,8,20	0.28	0	7,7,19	0.53	0
2	EDO	B	821	-	3,3,3	0.28	0	2,2,2	0.51	0
2	EDO	A	809	-	3,3,3	0.38	0	2,2,2	0.48	0
2	EDO	B	811	-	3,3,3	0.34	0	2,2,2	0.32	0
3	C8E	B	831	-	6,6,20	0.26	0	5,5,19	0.45	0
2	EDO	A	802	-	3,3,3	0.37	0	2,2,2	0.75	0
3	C8E	A	835	-	7,7,20	0.29	0	6,6,19	0.41	0
3	C8E	C	828	-	14,14,20	0.33	0	13,13,19	0.48	0
2	EDO	C	813	-	3,3,3	0.63	0	2,2,2	0.16	0
2	EDO	A	806	-	3,3,3	0.75	0	2,2,2	0.17	0
3	C8E	C	830	-	7,7,20	0.31	0	6,6,19	0.44	0
2	EDO	A	821	-	3,3,3	0.39	0	2,2,2	0.39	0
3	C8E	C	827	-	14,14,20	0.37	0	13,13,19	0.43	0
3	C8E	C	835	-	7,7,20	0.22	0	6,6,19	0.49	0
2	EDO	C	806	-	3,3,3	0.32	0	2,2,2	0.13	0
2	EDO	C	816	-	3,3,3	0.52	0	2,2,2	0.31	0
3	C8E	B	833	-	8,8,20	0.39	0	7,7,19	0.41	0
2	EDO	B	818	-	3,3,3	0.59	0	2,2,2	0.07	0
3	C8E	C	834	-	6,6,20	0.34	0	5,5,19	0.30	0
2	EDO	C	803	-	3,3,3	0.32	0	2,2,2	0.60	0
2	EDO	C	811	-	3,3,3	0.39	0	2,2,2	0.54	0
4	PO4	B	835	-	4,4,4	0.93	0	6,6,6	0.62	0
3	C8E	A	828	-	20,20,20	0.59	0	19,19,19	0.35	0
2	EDO	B	805	-	3,3,3	0.74	0	2,2,2	0.08	0
2	EDO	A	816	-	3,3,3	0.28	0	2,2,2	0.70	0
3	C8E	A	833	-	7,7,20	0.22	0	6,6,19	0.46	0
3	C8E	C	823	-	20,20,20	0.58	0	19,19,19	0.81	1 (5%)
2	EDO	B	809	-	3,3,3	0.42	0	2,2,2	0.55	0
2	EDO	B	812	-	3,3,3	0.44	0	2,2,2	0.41	0
3	C8E	B	832	-	8,8,20	0.20	0	7,7,19	0.52	0
2	EDO	B	824	-	3,3,3	0.57	0	2,2,2	0.12	0
2	EDO	B	802	-	3,3,3	0.31	0	2,2,2	0.76	0
3	C8E	B	827	-	8,8,20	0.30	0	7,7,19	0.42	0
2	EDO	A	812	-	3,3,3	0.34	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	C	836[B]	-	20,20,20	0.56	0	19,19,19	0.44	0
3	C8E	A	832	-	11,11,20	0.32	0	10,10,19	0.41	0
2	EDO	A	813	-	3,3,3	0.36	0	2,2,2	0.41	0
3	C8E	A	830	-	20,20,20	0.47	0	19,19,19	0.43	0
2	EDO	C	807	-	3,3,3	0.33	0	2,2,2	0.79	0
2	EDO	C	809	-	3,3,3	0.63	0	2,2,2	0.29	0
2	EDO	C	812	-	3,3,3	0.29	0	2,2,2	0.74	0
2	EDO	C	804	-	3,3,3	0.55	0	2,2,2	0.46	0
2	EDO	A	815	-	3,3,3	0.41	0	2,2,2	0.23	0
2	EDO	B	819	-	3,3,3	0.48	0	2,2,2	0.59	0
3	C8E	C	825	-	20,20,20	0.48	0	19,19,19	0.56	0
3	C8E	C	832	-	14,14,20	0.41	0	13,13,19	0.65	0
2	EDO	B	806	-	3,3,3	0.40	0	2,2,2	0.68	0
2	EDO	B	807	-	3,3,3	0.56	0	2,2,2	0.67	0
2	EDO	C	820	-	3,3,3	0.37	0	2,2,2	0.46	0
2	EDO	A	811	-	3,3,3	0.35	0	2,2,2	0.62	0
3	C8E	C	824	-	17,17,20	0.46	0	16,16,19	0.45	0
2	EDO	C	817	-	3,3,3	0.72	0	2,2,2	0.10	0
3	C8E	C	833	-	6,6,20	0.50	0	5,5,19	0.44	0
2	EDO	A	801	-	3,3,3	0.29	0	2,2,2	0.28	0
3	C8E	B	830	-	6,6,20	0.29	0	5,5,19	0.31	0
2	EDO	B	820	-	3,3,3	0.61	0	2,2,2	0.38	0
2	EDO	A	825	-	3,3,3	0.30	0	2,2,2	1.26	0
2	EDO	B	808	-	3,3,3	0.31	0	2,2,2	0.65	0
2	EDO	B	814	-	3,3,3	0.29	0	2,2,2	0.41	0
2	EDO	B	822	-	3,3,3	0.69	0	2,2,2	0.29	0
2	EDO	B	804	-	3,3,3	0.47	0	2,2,2	0.09	0
3	C8E	B	825	-	10,10,20	0.42	0	9,9,19	0.39	0
2	EDO	C	805	-	3,3,3	0.27	0	2,2,2	0.15	0
2	EDO	A	817	-	3,3,3	0.28	0	2,2,2	0.50	0
3	C8E	C	826	-	20,20,20	0.58	0	19,19,19	0.63	0
2	EDO	A	822	-	3,3,3	0.69	0	2,2,2	0.81	0
2	EDO	C	802	-	3,3,3	0.29	0	2,2,2	0.61	0
2	EDO	A	814	-	3,3,3	0.35	0	2,2,2	0.41	0
2	EDO	C	819	-	3,3,3	1.24	0	2,2,2	0.69	0
2	EDO	C	801	-	3,3,3	0.32	0	2,2,2	0.56	0
2	EDO	B	801	-	3,3,3	0.38	0	2,2,2	0.05	0
2	EDO	A	810	-	3,3,3	0.45	0	2,2,2	0.27	0
2	EDO	C	822	-	3,3,3	0.28	0	2,2,2	0.75	0
3	C8E	B	826	-	12,12,20	0.48	0	11,11,19	0.40	0
3	C8E	B	828	-	7,7,20	0.34	0	6,6,19	0.24	0
2	EDO	C	814	-	3,3,3	0.38	0	2,2,2	0.23	0
2	EDO	B	823	-	3,3,3	0.32	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	A	829	-	11,11,20	0.30	0	10,10,19	0.51	0
3	C8E	A	836	-	9,9,20	0.40	0	8,8,19	0.44	0
2	EDO	A	803	-	3,3,3	0.29	0	2,2,2	0.60	0
2	EDO	B	816	-	3,3,3	0.37	0	2,2,2	0.60	0
3	C8E	A	831	-	8,8,20	0.22	0	7,7,19	0.45	0
3	C8E	A	827	-	17,17,20	0.74	0	16,16,19	0.74	0
2	EDO	B	810	-	3,3,3	0.38	0	2,2,2	0.49	0
3	C8E	A	826	-	14,14,20	0.32	0	13,13,19	0.57	0
2	EDO	A	805	-	3,3,3	0.59	0	2,2,2	0.30	0
2	EDO	A	823	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	C	808	-	3,3,3	0.45	0	2,2,2	0.32	0
3	C8E	C	829	-	14,14,20	0.36	0	13,13,19	0.47	0
2	EDO	C	818	-	3,3,3	0.73	0	2,2,2	0.16	0
2	EDO	C	821	-	3,3,3	0.45	0	2,2,2	0.16	0
2	EDO	B	817	-	3,3,3	1.32	0	2,2,2	0.84	0
3	C8E	C	836[A]	-	20,20,20	0.51	0	19,19,19	0.71	1 (5%)
2	EDO	B	813	-	3,3,3	0.35	0	2,2,2	0.37	0
2	EDO	A	824	-	3,3,3	0.47	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	815	-	-	0/1/1/1	-
2	EDO	A	808	-	-	0/1/1/1	-
2	EDO	A	819	-	-	1/1/1/1	-
2	EDO	A	818	-	-	1/1/1/1	-
2	EDO	C	810	-	-	0/1/1/1	-
3	C8E	A	834	-	-	10/16/16/18	-
2	EDO	B	803	-	-	1/1/1/1	-
2	EDO	A	807	-	-	1/1/1/1	-
2	EDO	B	815	-	-	0/1/1/1	-
2	EDO	A	820	-	-	1/1/1/1	-
2	EDO	A	804	-	-	0/1/1/1	-
3	C8E	B	829	-	-	5/6/6/18	-
3	C8E	B	834	-	-	1/5/5/18	-
3	C8E	C	831	-	-	4/6/6/18	-
2	EDO	B	821	-	-	0/1/1/1	-
2	EDO	A	809	-	-	0/1/1/1	-
2	EDO	B	811	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	831	-	-	1/4/4/18	-
2	EDO	A	802	-	-	0/1/1/1	-
3	C8E	A	835	-	-	2/5/5/18	-
3	C8E	C	828	-	-	6/12/12/18	-
2	EDO	C	813	-	-	0/1/1/1	-
2	EDO	A	806	-	-	0/1/1/1	-
3	C8E	C	830	-	-	1/5/5/18	-
2	EDO	A	821	-	-	1/1/1/1	-
3	C8E	C	827	-	-	6/12/12/18	-
3	C8E	C	835	-	-	3/5/5/18	-
2	EDO	C	806	-	-	0/1/1/1	-
2	EDO	C	816	-	-	1/1/1/1	-
3	C8E	B	833	-	-	3/6/6/18	-
2	EDO	B	818	-	-	0/1/1/1	-
3	C8E	C	834	-	-	1/4/4/18	-
2	EDO	C	803	-	-	1/1/1/1	-
2	EDO	C	811	-	-	0/1/1/1	-
3	C8E	A	828	-	-	7/18/18/18	-
2	EDO	B	805	-	-	0/1/1/1	-
2	EDO	A	816	-	-	0/1/1/1	-
3	C8E	A	833	-	-	2/5/5/18	-
3	C8E	C	823	-	-	1/18/18/18	-
2	EDO	B	809	-	-	0/1/1/1	-
2	EDO	B	812	-	-	0/1/1/1	-
3	C8E	B	832	-	-	2/6/6/18	-
2	EDO	B	824	-	-	0/1/1/1	-
2	EDO	B	802	-	-	0/1/1/1	-
3	C8E	B	827	-	-	2/6/6/18	-
2	EDO	A	812	-	-	0/1/1/1	-
3	C8E	C	836[B]	-	-	9/18/18/18	-
3	C8E	A	832	-	-	3/9/9/18	-
2	EDO	A	813	-	-	1/1/1/1	-
3	C8E	A	830	-	-	8/18/18/18	-
2	EDO	C	807	-	-	0/1/1/1	-
2	EDO	C	809	-	-	1/1/1/1	-
2	EDO	C	812	-	-	0/1/1/1	-
2	EDO	C	804	-	-	0/1/1/1	-
2	EDO	A	815	-	-	1/1/1/1	-
2	EDO	B	819	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	C	825	-	-	6/18/18/18	-
3	C8E	C	832	-	-	4/12/12/18	-
2	EDO	B	806	-	-	0/1/1/1	-
2	EDO	B	807	-	-	1/1/1/1	-
2	EDO	C	820	-	-	1/1/1/1	-
2	EDO	A	811	-	-	0/1/1/1	-
3	C8E	C	824	-	-	5/15/15/18	-
2	EDO	C	817	-	-	1/1/1/1	-
3	C8E	C	833	-	-	2/4/4/18	-
2	EDO	A	801	-	-	0/1/1/1	-
3	C8E	B	830	-	-	4/4/4/18	-
2	EDO	B	820	-	-	1/1/1/1	-
2	EDO	A	825	-	-	1/1/1/1	-
2	EDO	B	808	-	-	0/1/1/1	-
2	EDO	B	814	-	-	1/1/1/1	-
2	EDO	B	822	-	-	1/1/1/1	-
2	EDO	B	804	-	-	1/1/1/1	-
3	C8E	B	825	-	-	3/8/8/18	-
2	EDO	C	805	-	-	0/1/1/1	-
2	EDO	A	817	-	-	1/1/1/1	-
3	C8E	C	826	-	-	8/18/18/18	-
2	EDO	A	822	-	-	1/1/1/1	-
2	EDO	C	802	-	-	0/1/1/1	-
2	EDO	A	814	-	-	1/1/1/1	-
2	EDO	C	819	-	-	0/1/1/1	-
2	EDO	C	801	-	-	0/1/1/1	-
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	A	810	-	-	1/1/1/1	-
2	EDO	C	822	-	-	0/1/1/1	-
3	C8E	B	826	-	-	5/10/10/18	-
3	C8E	B	828	-	-	3/5/5/18	-
2	EDO	C	814	-	-	0/1/1/1	-
2	EDO	B	823	-	-	1/1/1/1	-
3	C8E	A	829	-	-	4/9/9/18	-
3	C8E	A	836	-	-	1/7/7/18	-
2	EDO	A	803	-	-	1/1/1/1	-
2	EDO	B	816	-	-	1/1/1/1	-
3	C8E	A	831	-	-	2/6/6/18	-
3	C8E	A	827	-	-	6/15/15/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	810	-	-	0/1/1/1	-
3	C8E	A	826	-	-	7/12/12/18	-
2	EDO	A	805	-	-	0/1/1/1	-
2	EDO	A	823	-	-	0/1/1/1	-
2	EDO	C	808	-	-	0/1/1/1	-
3	C8E	C	829	-	-	3/12/12/18	-
2	EDO	C	818	-	-	0/1/1/1	-
2	EDO	C	821	-	-	0/1/1/1	-
2	EDO	B	817	-	-	1/1/1/1	-
3	C8E	C	836[A]	-	-	10/18/18/18	-
2	EDO	B	813	-	-	0/1/1/1	-
2	EDO	A	824	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	823	C8E	C6-C5-C4	-2.09	103.79	114.37
3	C	836[A]	C8E	C13-O12-C11	-2.08	104.14	113.26

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	834	C8E	O9-C10-C11-O12
3	C	825	C8E	O9-C10-C11-O12
3	A	826	C8E	O9-C10-C11-O12
3	C	832	C8E	O9-C10-C11-O12
3	C	824	C8E	O12-C13-C14-O15
3	A	827	C8E	O12-C13-C14-O15
3	A	830	C8E	O18-C19-C20-O21
2	A	820	EDO	O1-C1-C2-O2
3	B	825	C8E	C6-C7-C8-O9
3	C	836[A]	C8E	C4-C5-C6-C7
3	C	827	C8E	C6-C7-C8-O9
3	C	836[A]	C8E	O15-C16-C17-O18
3	C	836[A]	C8E	C6-C7-C8-O9
3	C	836[B]	C8E	O18-C19-C20-O21
3	A	833	C8E	C5-C6-C7-C8
3	C	826	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	C	826	C8E	O18-C19-C20-O21
3	C	836[A]	C8E	O18-C19-C20-O21
3	B	832	C8E	C3-C4-C5-C6
3	A	829	C8E	C6-C7-C8-O9
3	C	827	C8E	C5-C6-C7-C8
3	C	828	C8E	C5-C6-C7-C8
3	A	828	C8E	O12-C13-C14-O15
3	B	829	C8E	C4-C5-C6-C7
3	C	827	C8E	C3-C4-C5-C6
2	A	810	EDO	O1-C1-C2-O2
2	B	816	EDO	O1-C1-C2-O2
3	A	835	C8E	C4-C5-C6-C7
3	C	824	C8E	O9-C10-C11-O12
3	B	826	C8E	O18-C19-C20-O21
3	A	830	C8E	C2-C3-C4-C5
3	B	832	C8E	C6-C7-C8-O9
3	A	830	C8E	O12-C13-C14-O15
3	C	836[A]	C8E	C2-C3-C4-C5
3	B	828	C8E	C2-C3-C4-C5
3	B	829	C8E	C6-C7-C8-O9
3	A	828	C8E	O18-C19-C20-O21
3	A	832	C8E	O9-C10-C11-O12
3	C	836[B]	C8E	O15-C16-C17-O18
3	C	825	C8E	C2-C3-C4-C5
3	A	829	C8E	O9-C10-C11-O12
3	C	833	C8E	O9-C10-C11-O12
3	A	835	C8E	C3-C4-C5-C6
3	A	831	C8E	C6-C7-C8-O9
2	B	804	EDO	O1-C1-C2-O2
2	B	811	EDO	O1-C1-C2-O2
3	A	827	C8E	C6-C7-C8-O9
3	A	829	C8E	C5-C6-C7-C8
3	B	830	C8E	C2-C3-C4-C5
3	B	825	C8E	C11-C10-O9-C8
3	A	826	C8E	C4-C5-C6-C7
3	A	834	C8E	O12-C13-C14-O15
3	A	830	C8E	C4-C5-C6-C7
3	B	831	C8E	C5-C6-C7-C8
3	C	828	C8E	C1-C2-C3-C4
3	B	833	C8E	C1-C2-C3-C4
3	B	828	C8E	C5-C6-C7-C8
3	C	825	C8E	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	836[B]	C8E	C5-C6-C7-C8
3	A	826	C8E	C2-C3-C4-C5
3	A	834	C8E	C5-C6-C7-C8
3	A	827	C8E	O9-C10-C11-O12
3	B	830	C8E	C4-C5-C6-C7
3	A	826	C8E	C3-C4-C5-C6
2	A	807	EDO	O1-C1-C2-O2
2	C	820	EDO	O1-C1-C2-O2
3	C	826	C8E	C10-C11-O12-C13
3	C	831	C8E	C2-C3-C4-C5
3	A	834	C8E	C20-C19-O18-C17
3	C	835	C8E	C4-C5-C6-C7
3	B	834	C8E	C2-C3-C4-C5
3	B	830	C8E	C3-C4-C5-C6
3	A	827	C8E	C10-C11-O12-C13
3	C	826	C8E	C17-C16-O15-C14
3	C	836[B]	C8E	C3-C4-C5-C6
3	C	836[A]	C8E	C3-C4-C5-C6
3	C	832	C8E	C10-C11-O12-C13
3	A	830	C8E	C17-C16-O15-C14
3	A	826	C8E	C10-C11-O12-C13
3	A	830	C8E	C13-C14-O15-C16
3	C	833	C8E	C14-C13-O12-C11
3	B	833	C8E	C3-C4-C5-C6
3	C	824	C8E	O15-C16-C17-O18
3	A	831	C8E	C1-C2-C3-C4
3	C	831	C8E	C3-C4-C5-C6
3	C	827	C8E	C1-C2-C3-C4
3	A	834	C8E	C6-C7-C8-O9
3	A	833	C8E	C3-C4-C5-C6
3	C	831	C8E	C4-C5-C6-C7
3	A	834	C8E	O15-C16-C17-O18
3	B	826	C8E	C17-C16-O15-C14
3	C	825	C8E	C11-C10-O9-C8
3	A	827	C8E	C14-C13-O12-C11
3	B	830	C8E	C1-C2-C3-C4
3	A	828	C8E	C2-C3-C4-C5
3	A	832	C8E	C6-C7-C8-O9
3	B	829	C8E	C1-C2-C3-C4
3	C	827	C8E	O12-C13-C14-O15
3	C	824	C8E	C13-C14-O15-C16
3	B	826	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	C	830	C8E	C2-C3-C4-C5
3	A	829	C8E	C7-C8-O9-C10
3	C	836[B]	C8E	C17-C16-O15-C14
2	A	824	EDO	O1-C1-C2-O2
3	A	826	C8E	C7-C8-O9-C10
3	A	827	C8E	C7-C8-O9-C10
3	C	836[A]	C8E	C7-C8-O9-C10
3	C	823	C8E	C5-C6-C7-C8
3	C	835	C8E	C5-C6-C7-C8
3	C	836[B]	C8E	C14-C13-O12-C11
3	A	834	C8E	C14-C13-O12-C11
3	B	825	C8E	C7-C8-O9-C10
3	C	824	C8E	C1-C2-C3-C4
3	A	828	C8E	C13-C14-O15-C16
3	A	828	C8E	C10-C11-O12-C13
3	C	832	C8E	O12-C13-C14-O15
3	C	825	C8E	C16-C17-O18-C19
3	C	836[B]	C8E	C20-C19-O18-C17
2	A	813	EDO	O1-C1-C2-O2
2	A	825	EDO	O1-C1-C2-O2
2	B	803	EDO	O1-C1-C2-O2
3	C	836[B]	C8E	C10-C11-O12-C13
3	C	829	C8E	C2-C3-C4-C5
3	A	834	C8E	C11-C10-O9-C8
3	C	828	C8E	C3-C4-C5-C6
3	C	831	C8E	C6-C7-C8-O9
3	C	828	C8E	C6-C7-C8-O9
3	A	834	C8E	C13-C14-O15-C16
2	A	814	EDO	O1-C1-C2-O2
2	A	817	EDO	O1-C1-C2-O2
2	A	819	EDO	O1-C1-C2-O2
2	A	822	EDO	O1-C1-C2-O2
2	B	819	EDO	O1-C1-C2-O2
3	B	827	C8E	C3-C4-C5-C6
3	B	829	C8E	C2-C3-C4-C5
3	C	835	C8E	C2-C3-C4-C5
3	B	833	C8E	C6-C7-C8-O9
3	C	829	C8E	O12-C13-C14-O15
3	C	826	C8E	C16-C17-O18-C19
3	B	828	C8E	C1-C2-C3-C4
3	C	827	C8E	C4-C5-C6-C7
3	A	832	C8E	C3-C4-C5-C6

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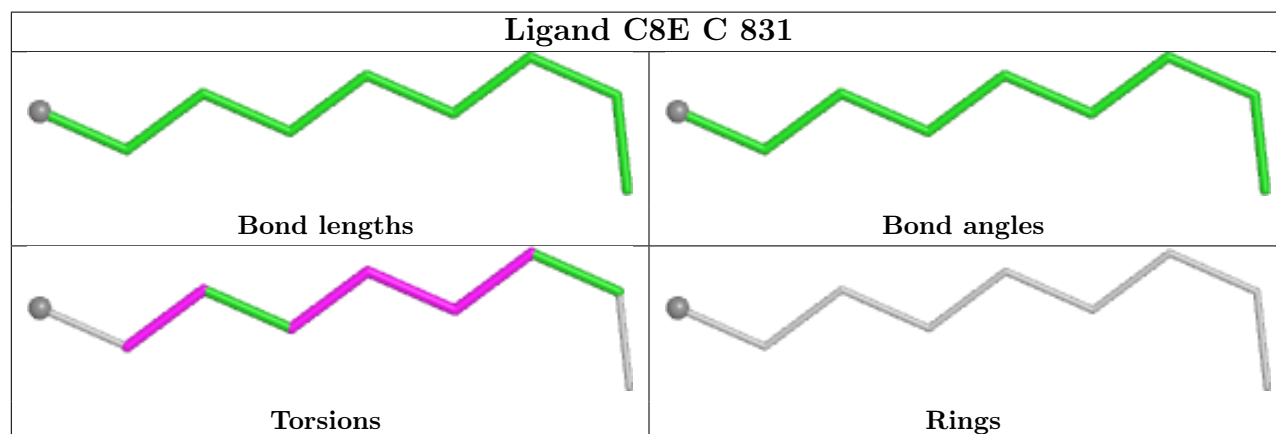
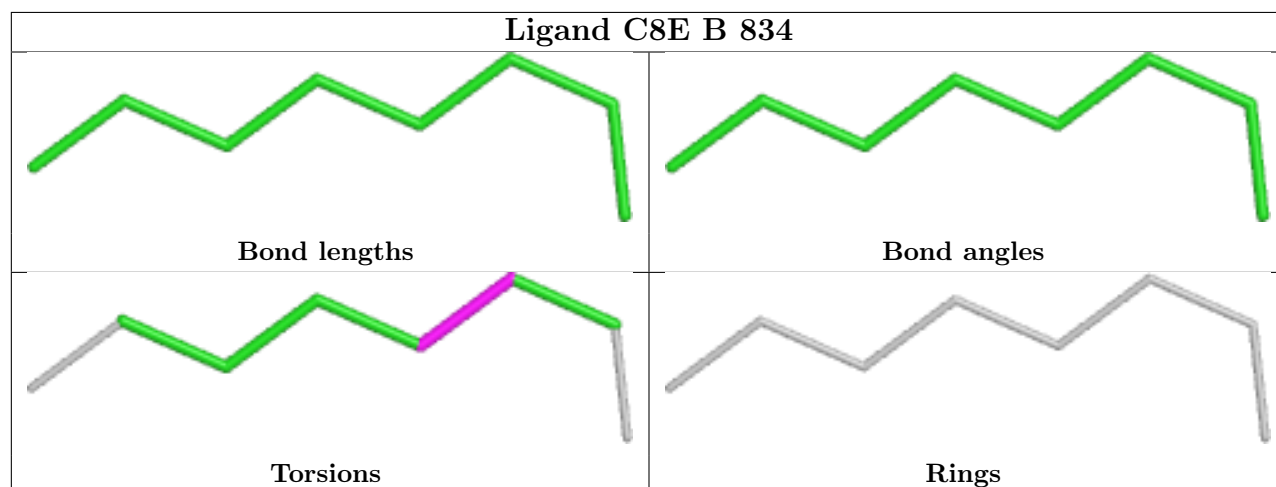
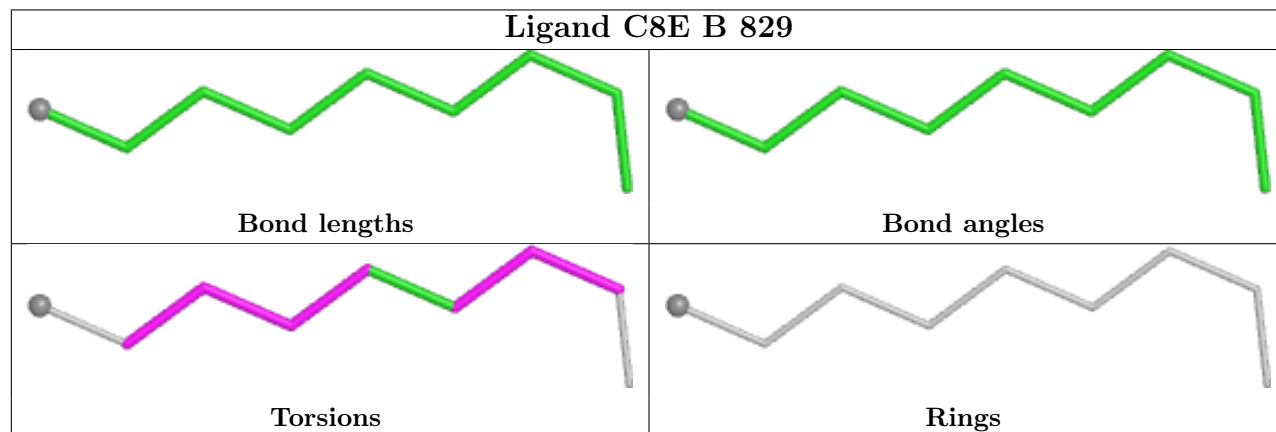
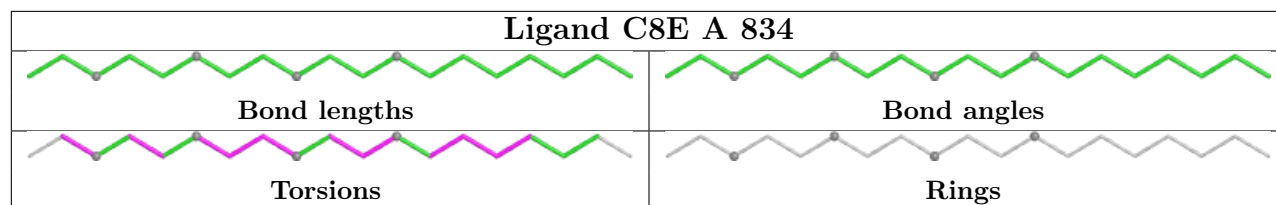
Mol	Chain	Res	Type	Atoms
2	A	803	EDO	O1-C1-C2-O2
2	A	815	EDO	O1-C1-C2-O2
2	A	818	EDO	O1-C1-C2-O2
2	B	807	EDO	O1-C1-C2-O2
2	B	820	EDO	O1-C1-C2-O2
2	C	803	EDO	O1-C1-C2-O2
2	C	817	EDO	O1-C1-C2-O2
3	B	826	C8E	O15-C16-C17-O18
3	A	834	C8E	C4-C5-C6-C7
3	C	826	C8E	C13-C14-O15-C16
3	A	830	C8E	C11-C10-O9-C8
3	C	828	C8E	C14-C13-O12-C11
2	B	814	EDO	O1-C1-C2-O2
2	B	817	EDO	O1-C1-C2-O2
2	B	822	EDO	O1-C1-C2-O2
2	C	816	EDO	O1-C1-C2-O2
3	C	826	C8E	O9-C10-C11-O12
3	C	836[B]	C8E	C11-C10-O9-C8
3	C	836[A]	C8E	C20-C19-O18-C17
3	C	832	C8E	C5-C6-C7-C8
3	C	828	C8E	O12-C13-C14-O15
3	C	834	C8E	C2-C3-C4-C5
3	B	829	C8E	C5-C6-C7-C8
3	B	826	C8E	C14-C13-O12-C11
2	A	821	EDO	O1-C1-C2-O2
2	B	823	EDO	O1-C1-C2-O2
2	C	809	EDO	O1-C1-C2-O2
3	A	836	C8E	C4-C5-C6-C7
3	C	836[A]	C8E	C14-C13-O12-C11
3	A	828	C8E	O15-C16-C17-O18
3	C	826	C8E	O15-C16-C17-O18
3	C	836[A]	C8E	C17-C16-O15-C14
3	B	827	C8E	C1-C2-C3-C4
3	A	828	C8E	O9-C10-C11-O12
3	A	826	C8E	C14-C13-O12-C11
3	C	829	C8E	C6-C7-C8-O9
3	A	830	C8E	O9-C10-C11-O12
3	C	825	C8E	C13-C14-O15-C16

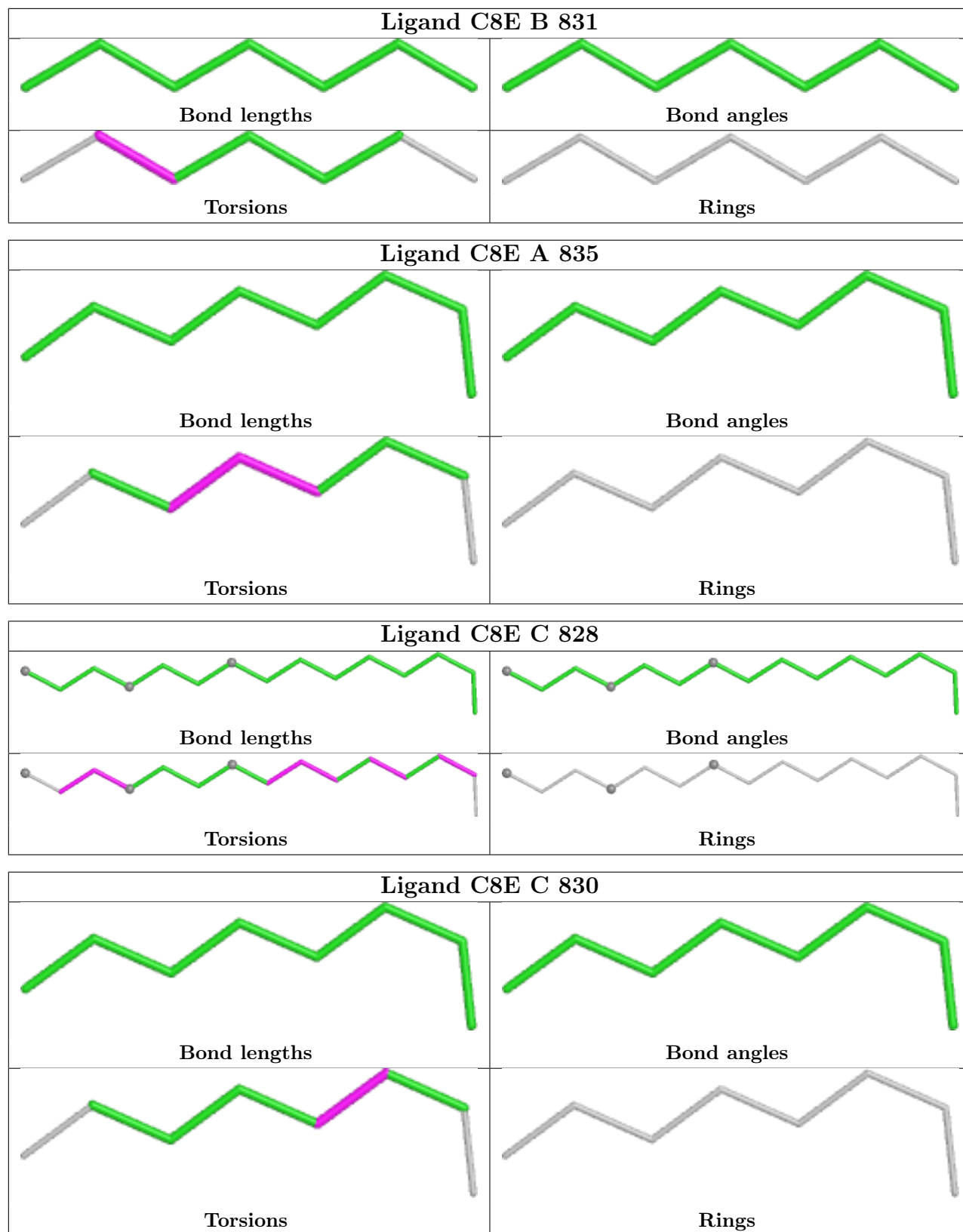
There are no ring outliers.

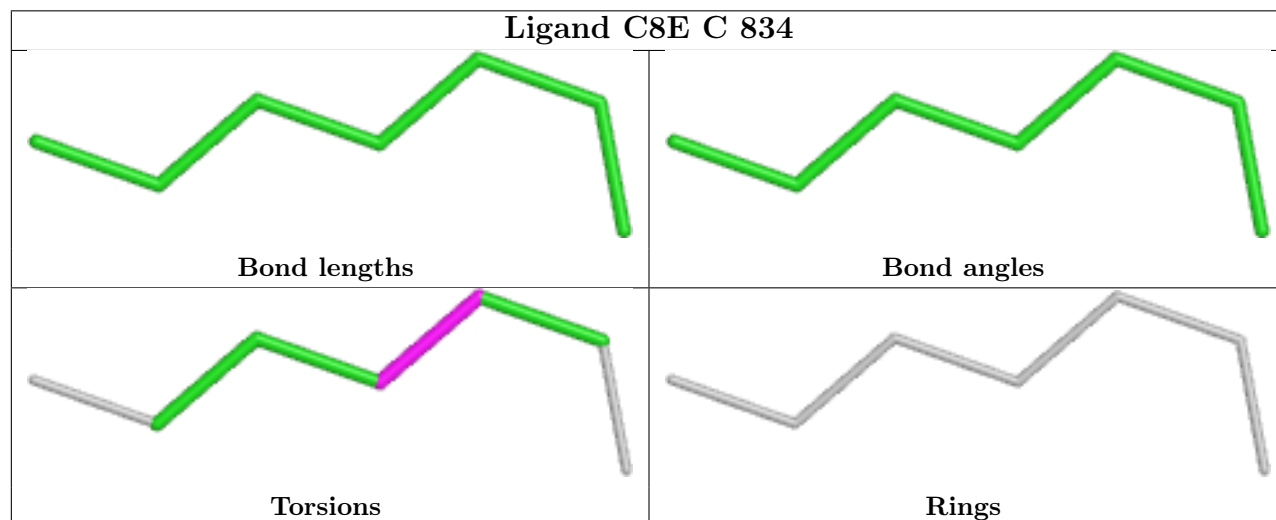
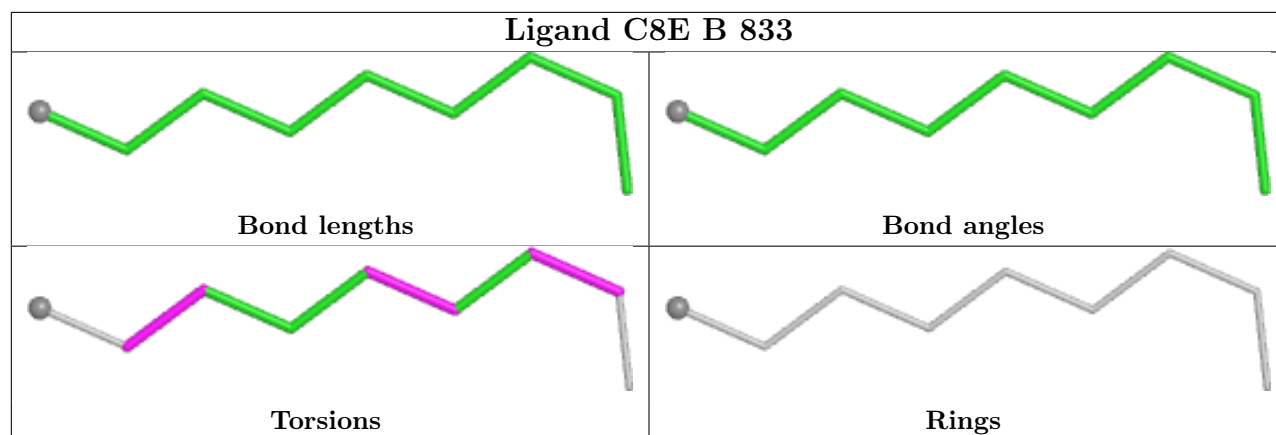
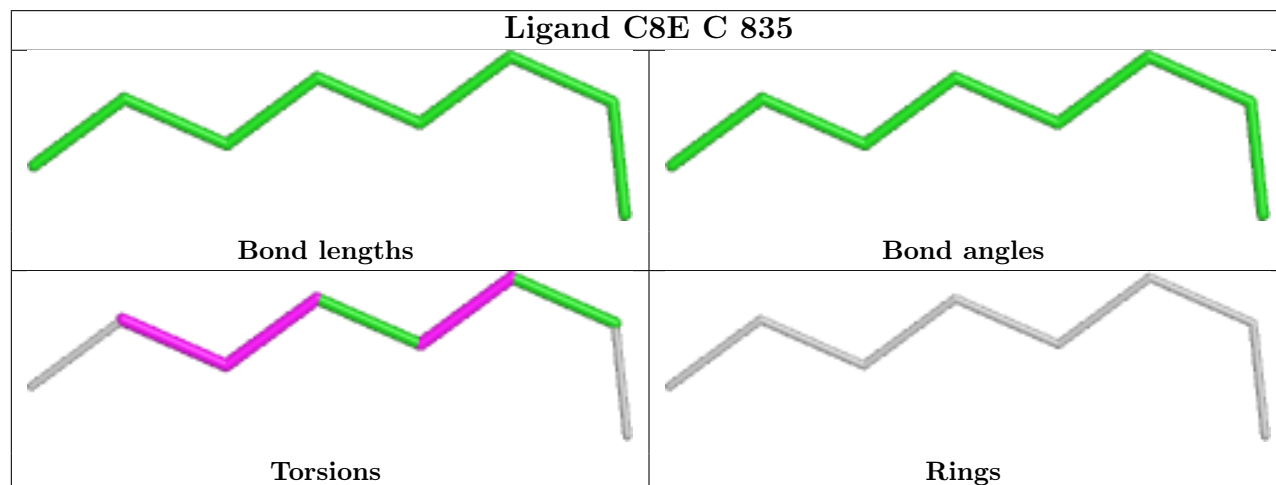
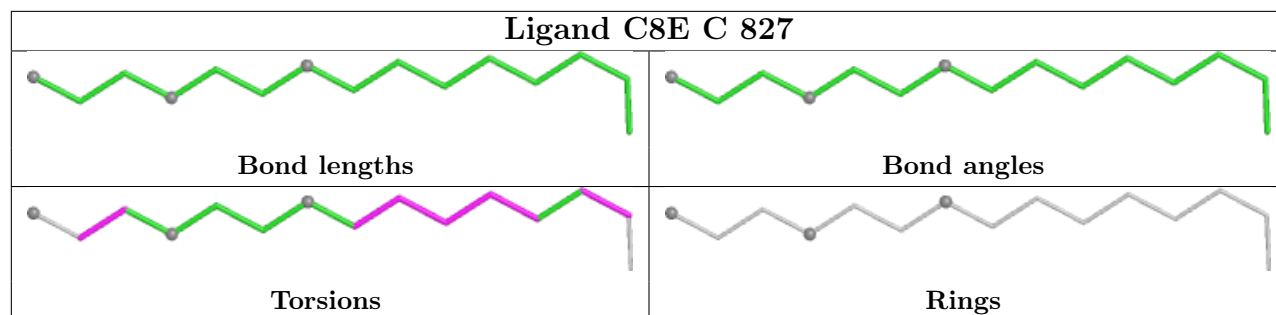
31 monomers are involved in 80 short contacts:

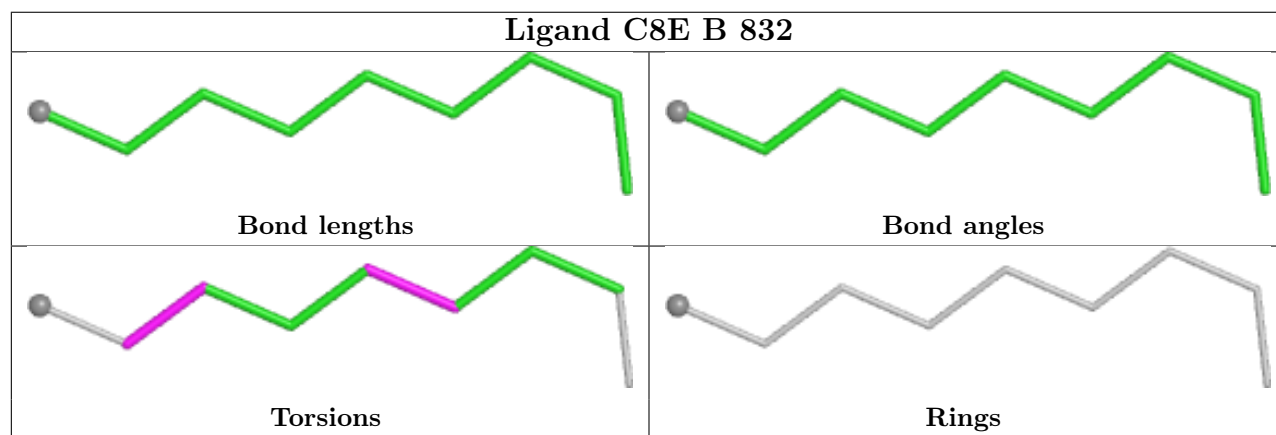
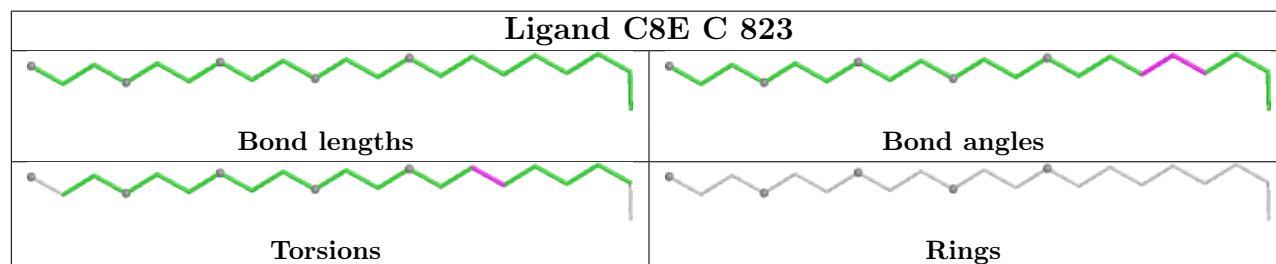
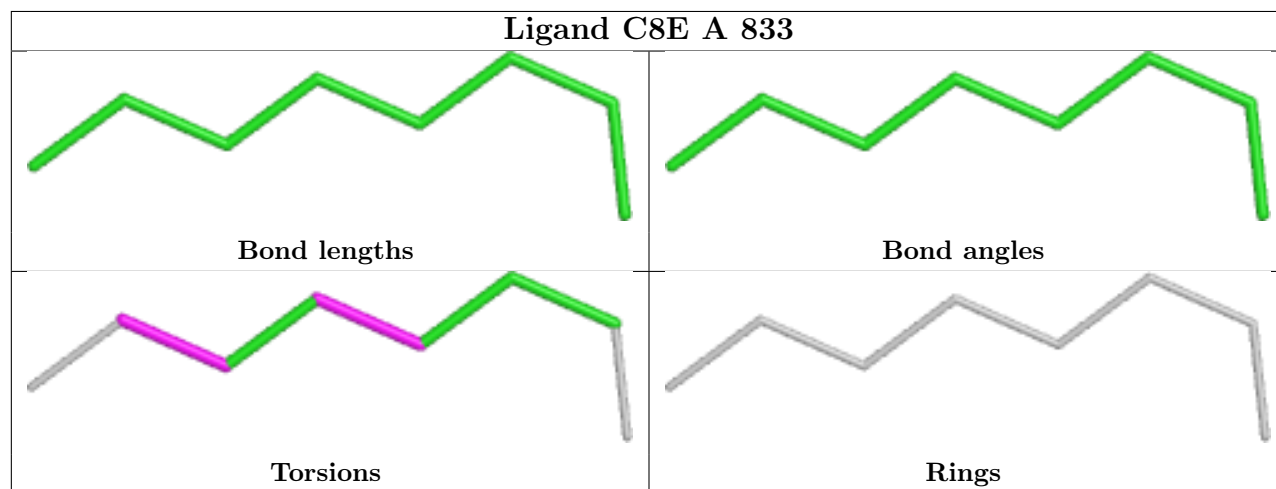
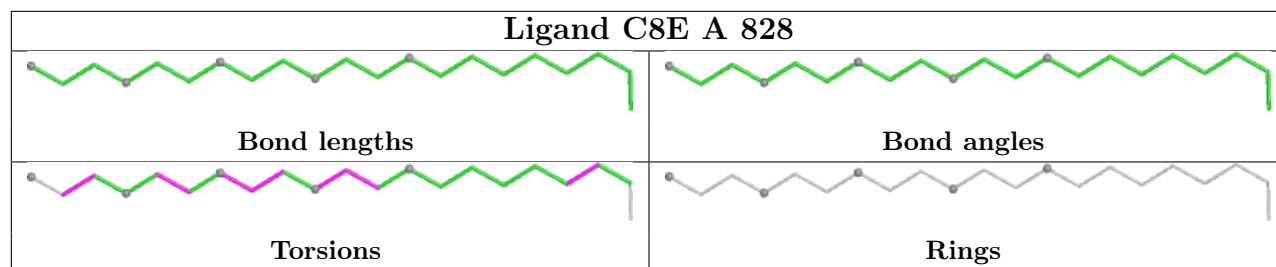
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	819	EDO	2	0
2	A	818	EDO	1	0
2	B	815	EDO	1	0
2	A	806	EDO	1	0
3	C	827	C8E	4	0
3	C	835	C8E	3	0
2	C	811	EDO	1	0
3	A	833	C8E	2	0
3	C	836[B]	C8E	22	0
3	A	832	C8E	1	0
2	A	813	EDO	2	0
3	A	830	C8E	1	0
3	C	825	C8E	2	0
2	C	820	EDO	2	0
2	A	811	EDO	1	0
3	C	824	C8E	1	0
2	B	820	EDO	2	0
2	A	825	EDO	5	0
2	B	804	EDO	1	0
3	B	825	C8E	1	0
3	C	826	C8E	4	0
2	C	801	EDO	2	0
2	C	822	EDO	1	0
3	B	826	C8E	1	0
3	B	828	C8E	3	0
3	A	836	C8E	1	0
3	A	831	C8E	2	0
3	A	827	C8E	1	0
2	A	823	EDO	2	0
2	C	808	EDO	1	0
3	C	836[A]	C8E	11	0

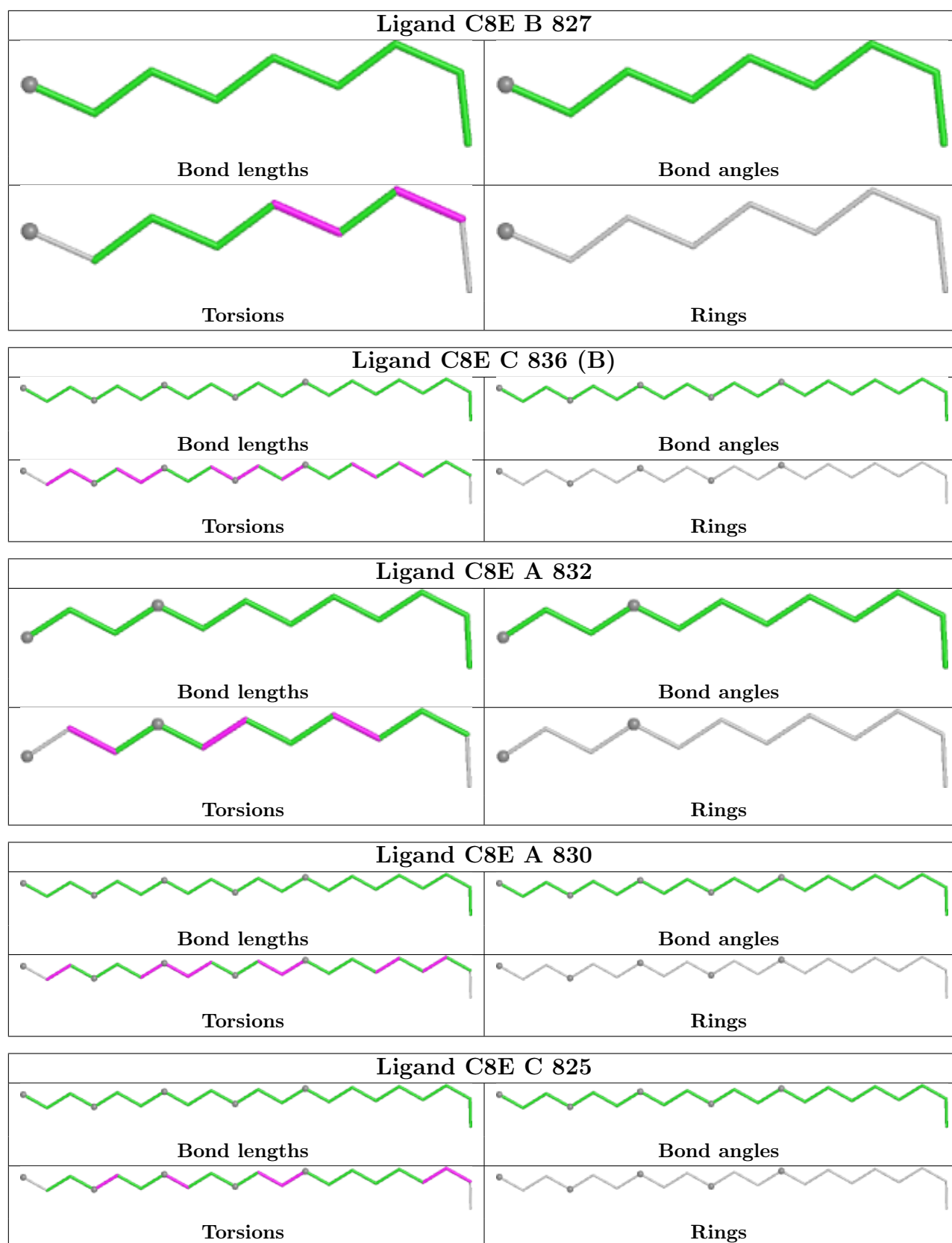
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

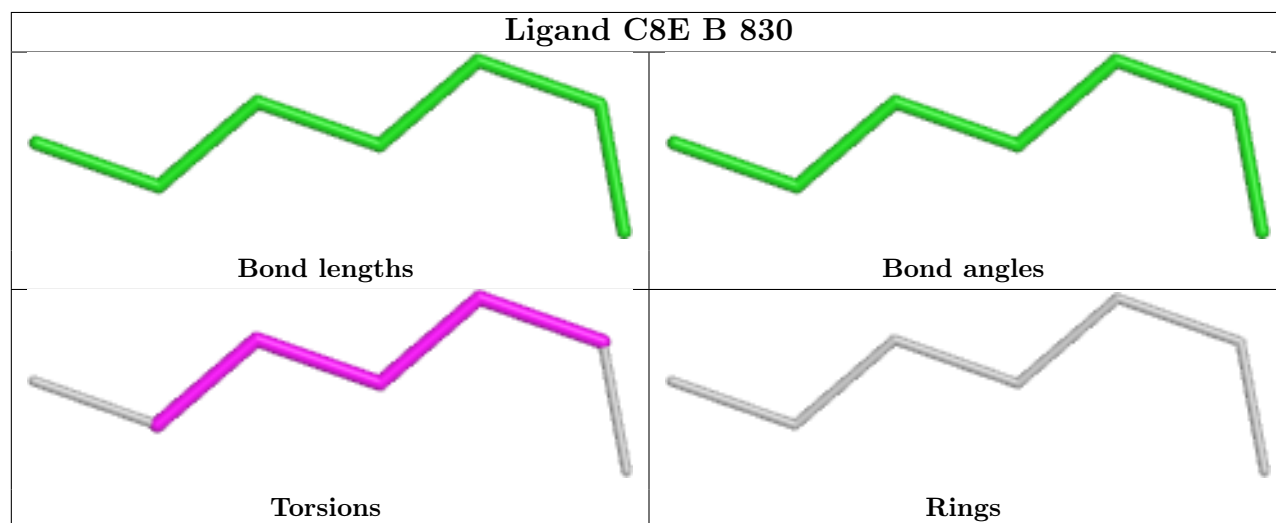
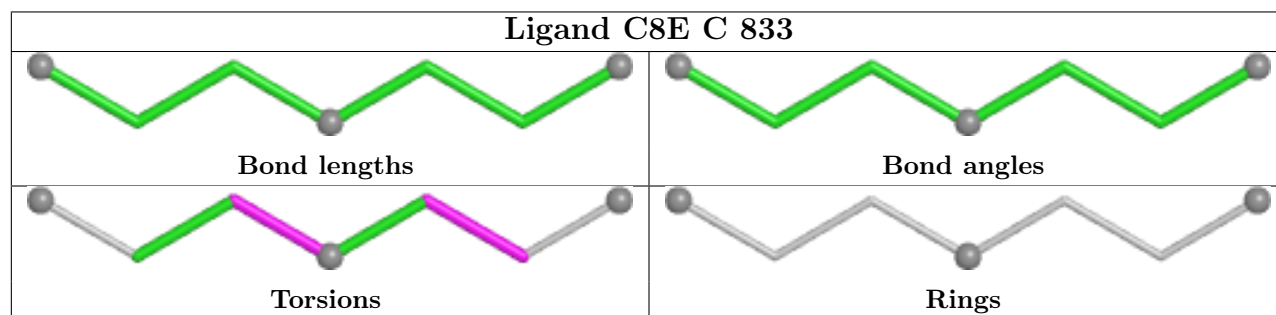
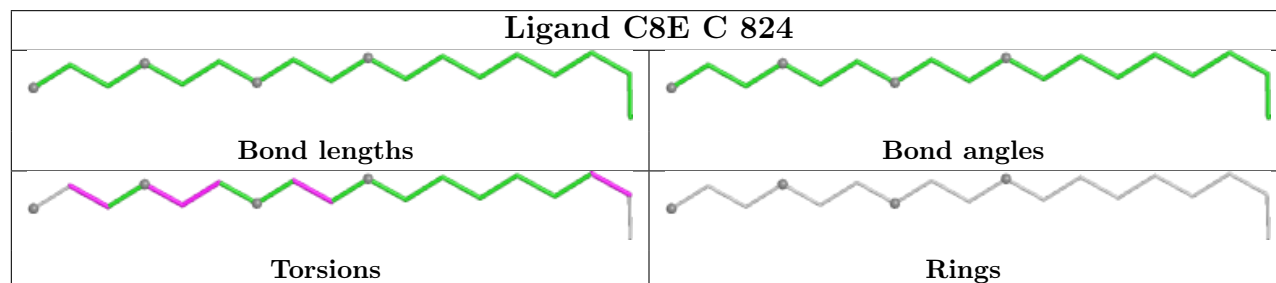
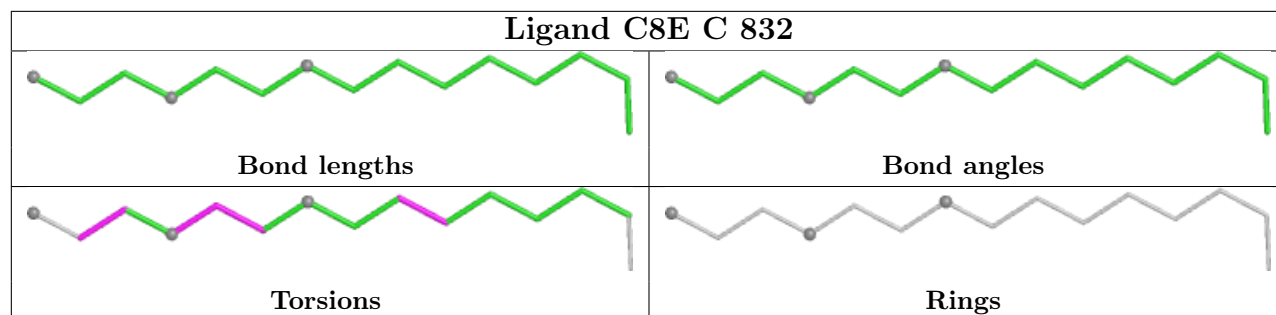


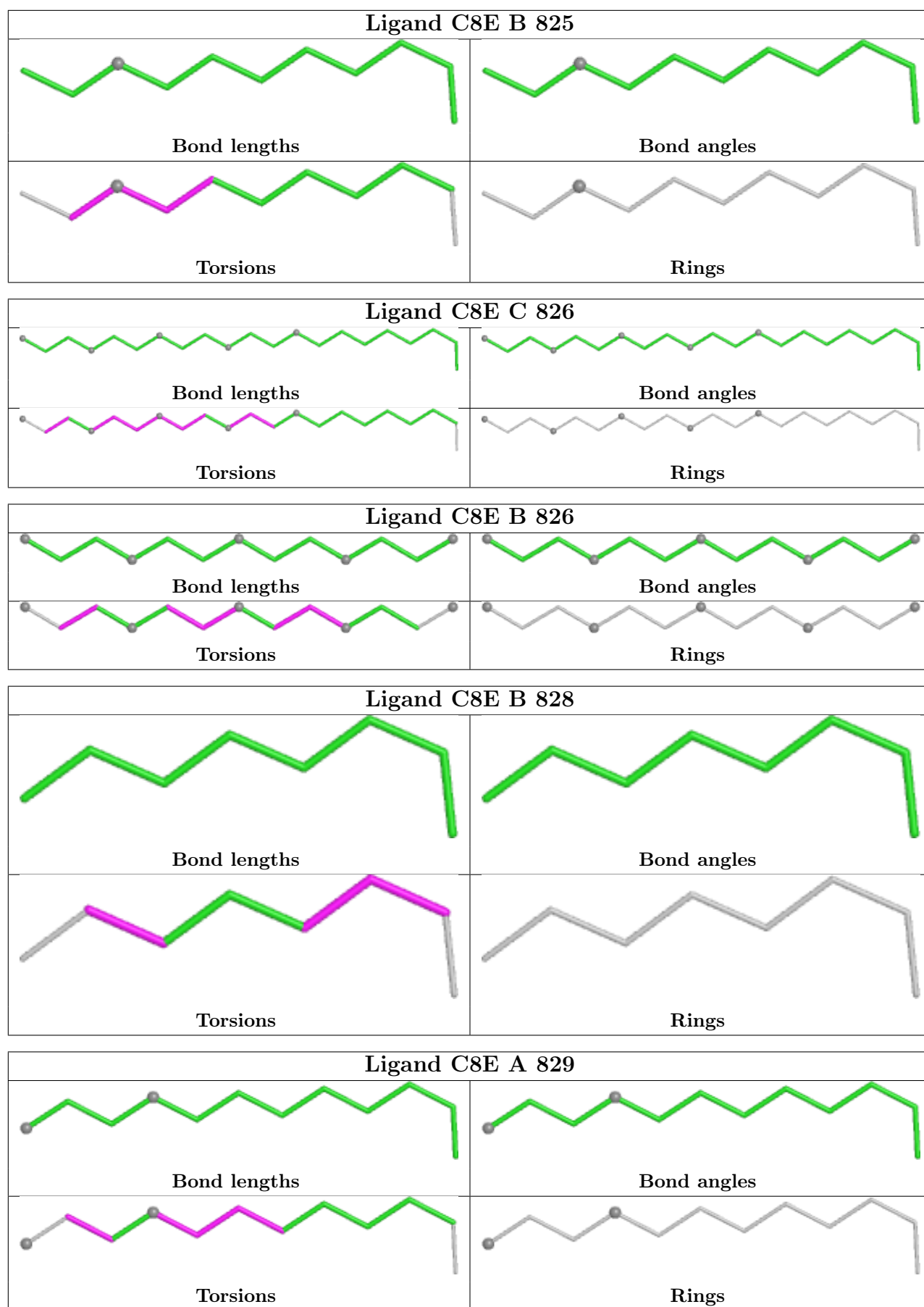


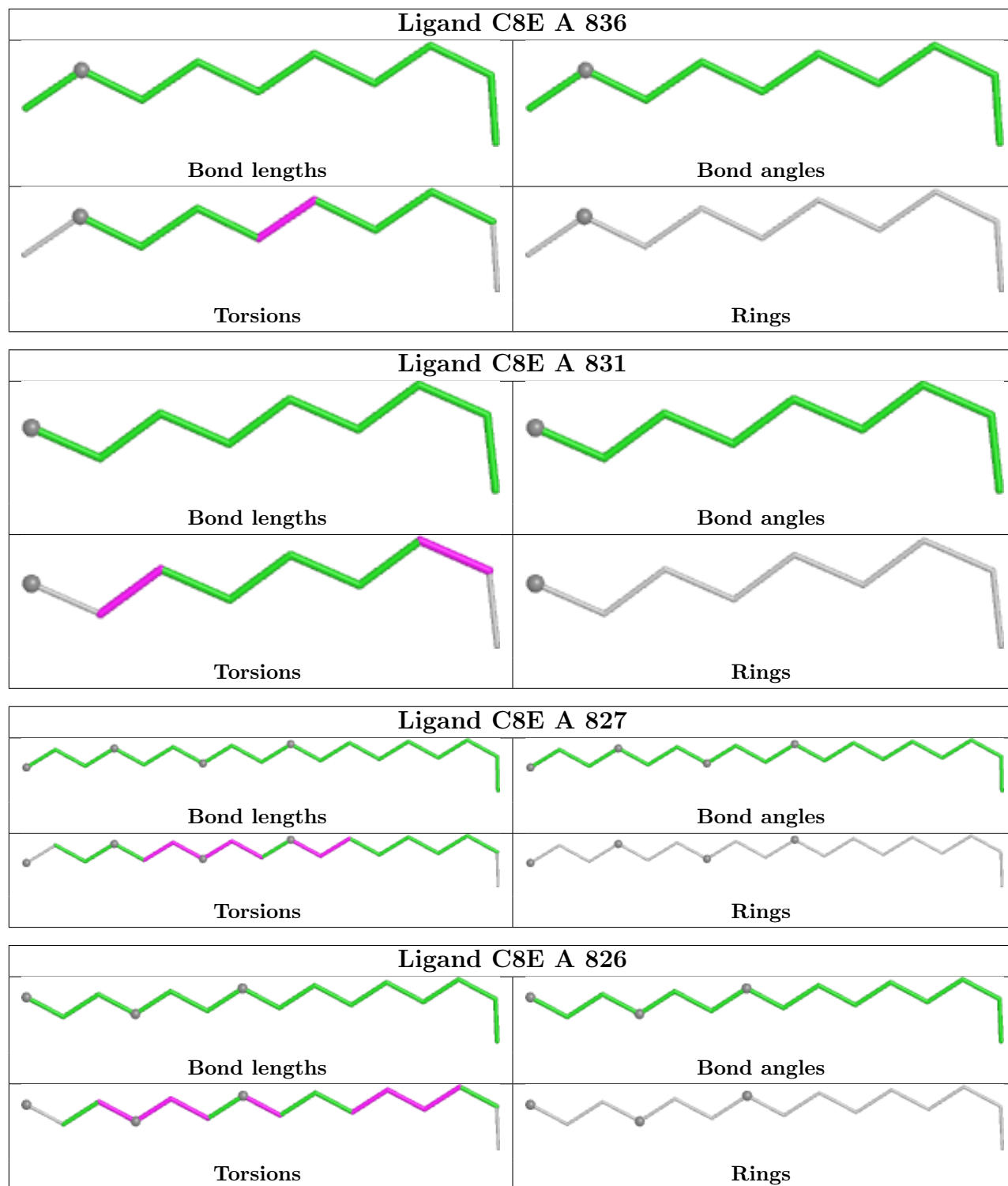


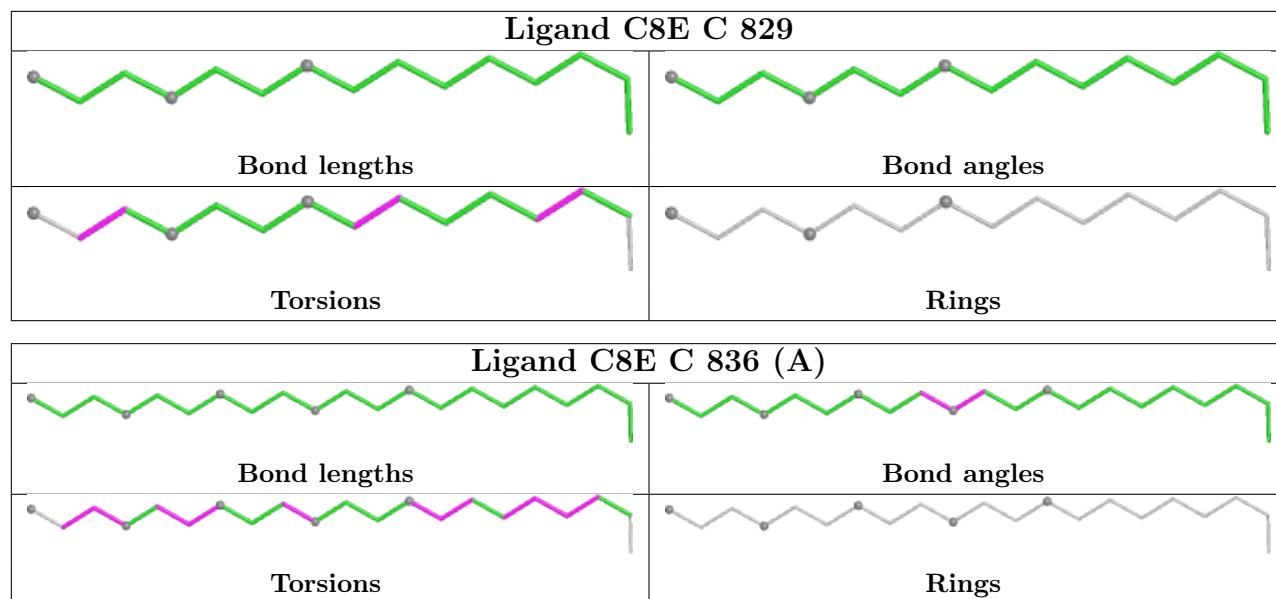












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	671/706 (95%)	-0.01	13 (1%) 66 73	13, 31, 51, 80	22 (3%)
1	B	671/706 (95%)	0.05	18 (2%) 56 61	12, 31, 55, 89	23 (3%)
1	C	671/706 (95%)	-0.12	18 (2%) 56 61	12, 28, 46, 88	42 (6%)
All	All	2013/2118 (95%)	-0.03	49 (2%) 59 66	12, 30, 52, 89	87 (4%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	569	ILE	5.4
1	C	612[A]	TRP	4.5
1	B	368	TYR	4.0
1	C	617	ALA	3.8
1	C	493[A]	ALA	3.7
1	B	428	PHE	3.7
1	B	539	PRO	3.7
1	A	33	ASP	3.6
1	A	368	TYR	3.4
1	A	420	PHE	3.4
1	C	33	ASP	3.4
1	C	498[A]	PRO	3.4
1	C	368	TYR	3.2
1	B	429	ALA	3.0
1	C	494[A]	THR	3.0
1	B	33	ASP	3.0
1	C	580	TYR	3.0
1	C	420	PHE	2.9
1	C	539	PRO	2.8
1	B	546	LEU	2.8
1	A	612	TRP	2.8
1	B	543	VAL	2.8
1	C	616	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	552	ASP	2.5
1	C	353	PHE	2.5
1	C	659	VAL	2.5
1	A	539	PRO	2.5
1	B	452	THR	2.4
1	B	477[A]	VAL	2.4
1	B	356	GLY	2.4
1	B	542	LEU	2.4
1	A	297	ASP	2.3
1	B	354	GLU	2.3
1	A	234	ASN	2.3
1	C	356	GLY	2.3
1	B	473	ASP	2.3
1	B	569	ILE	2.3
1	A	569	ILE	2.2
1	A	580	TYR	2.2
1	A	547	PRO	2.2
1	B	578	PHE	2.2
1	A	230	TRP	2.2
1	C	570	GLU	2.2
1	B	656[A]	SER	2.1
1	A	380	ILE	2.1
1	B	357	SER	2.1
1	C	193	PHE	2.0
1	A	406	THR	2.0
1	C	618	GLN	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	822	4/4	0.78	0.24	32,33,60,61	0
3	C8E	A	828	21/21	0.81	0.26	53,70,77,83	0
3	C8E	A	834	19/21	0.82	0.29	64,82,100,105	0
3	C8E	A	832	12/21	0.83	0.24	52,64,69,76	0
2	EDO	A	824	4/4	0.84	0.19	59,71,72,75	0
3	C8E	A	830	21/21	0.84	0.23	52,63,75,92	0
3	C8E	A	827	18/21	0.85	0.20	38,54,79,87	0
3	C8E	A	836	10/21	0.85	0.25	58,64,70,76	0
2	EDO	C	807	4/4	0.86	0.20	43,48,54,66	0
3	C8E	B	834	8/21	0.86	0.20	41,55,63,67	0
3	C8E	C	832	15/21	0.86	0.25	46,66,74,75	0
2	EDO	A	819	4/4	0.87	0.19	65,66,67,67	0
2	EDO	B	823	4/4	0.87	0.18	49,55,55,73	0
3	C8E	C	826	21/21	0.87	0.24	39,60,106,112	0
2	EDO	C	803	4/4	0.87	0.17	48,51,65,66	0
3	C8E	B	826	13/21	0.88	0.19	58,70,89,94	0
2	EDO	A	808	4/4	0.88	0.21	37,39,46,51	0
3	C8E	A	835	8/21	0.88	0.27	56,62,69,70	0
3	C8E	C	828	15/21	0.88	0.23	43,67,78,79	0
3	C8E	C	831	9/21	0.88	0.19	56,62,67,70	0
2	EDO	C	812	4/4	0.88	0.22	53,55,63,69	0
3	C8E	C	835	8/21	0.88	0.22	48,51,67,72	0
3	C8E	C	836[A]	21/21	0.88	0.21	30,47,60,66	21
3	C8E	C	836[B]	21/21	0.88	0.21	30,42,53,59	21
3	C8E	B	832	9/21	0.89	0.21	56,61,71,73	0
2	EDO	A	810	4/4	0.89	0.23	57,62,68,79	0
2	EDO	C	817	4/4	0.89	0.18	37,55,64,71	0
3	C8E	C	827	15/21	0.89	0.17	40,60,69,74	0
2	EDO	B	806	4/4	0.89	0.17	34,52,58,61	0
2	EDO	C	804	4/4	0.89	0.14	31,35,36,38	0
2	EDO	B	821	4/4	0.89	0.14	52,53,53,64	0
3	C8E	C	833	7/21	0.89	0.20	55,57,70,74	0
3	C8E	C	834	7/21	0.89	0.21	56,60,64,65	0
3	C8E	B	827	9/21	0.89	0.22	57,61,75,86	0
3	C8E	B	828	8/21	0.89	0.23	41,49,68,69	0
3	C8E	B	830	7/21	0.89	0.23	48,53,59,62	0
4	PO4	B	835	5/5	0.89	0.13	60,73,80,89	0
3	C8E	C	825	21/21	0.90	0.20	34,66,122,127	0
2	EDO	B	818	4/4	0.90	0.19	38,64,70,73	0
3	C8E	B	825	11/21	0.90	0.20	40,55,61,64	0
2	EDO	B	819	4/4	0.90	0.17	47,65,66,74	0
3	C8E	B	833	9/21	0.90	0.20	52,61,66,68	0
2	EDO	B	808	4/4	0.90	0.18	44,53,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	823	4/4	0.91	0.23	32,44,49,55	0
2	EDO	C	818	4/4	0.91	0.16	37,48,51,52	0
3	C8E	C	829	15/21	0.91	0.18	47,53,77,87	0
3	C8E	C	830	8/21	0.91	0.21	51,54,60,67	0
2	EDO	A	815	4/4	0.91	0.16	50,59,62,69	0
2	EDO	A	817	4/4	0.91	0.21	51,53,60,68	0
3	C8E	A	829	12/21	0.91	0.18	47,54,67,71	0
2	EDO	A	806	4/4	0.91	0.15	38,44,49,52	0
2	EDO	B	813	4/4	0.91	0.20	64,70,73,78	0
2	EDO	B	816	4/4	0.91	0.20	61,67,70,72	0
2	EDO	C	811	4/4	0.91	0.14	40,41,49,58	0
2	EDO	A	812	4/4	0.91	0.22	62,64,66,68	0
2	EDO	A	807	4/4	0.92	0.15	44,47,50,59	0
2	EDO	A	809	4/4	0.92	0.13	44,48,51,61	0
2	EDO	B	803	4/4	0.92	0.16	49,49,53,66	0
3	C8E	B	831	7/21	0.92	0.20	44,48,54,61	0
2	EDO	A	813	4/4	0.92	0.22	60,62,75,90	0
2	EDO	C	814	4/4	0.92	0.18	51,57,63,65	0
2	EDO	A	820	4/4	0.92	0.15	49,62,71,72	0
3	C8E	C	823	21/21	0.92	0.15	38,42,73,84	0
2	EDO	C	802	4/4	0.92	0.13	35,45,46,51	0
2	EDO	C	822	4/4	0.92	0.12	42,54,54,55	0
2	EDO	A	814	4/4	0.92	0.14	56,63,63,82	0
2	EDO	B	809	4/4	0.93	0.12	42,47,48,55	0
2	EDO	B	820	4/4	0.93	0.13	42,45,47,50	0
3	C8E	B	829	9/21	0.93	0.17	50,63,68,72	0
2	EDO	B	811	4/4	0.93	0.18	51,58,62,69	0
3	C8E	A	831	9/21	0.93	0.19	57,61,82,106	0
2	EDO	B	804	4/4	0.93	0.15	38,55,59,68	0
2	EDO	B	814	4/4	0.93	0.17	59,61,62,73	0
2	EDO	A	811	4/4	0.93	0.12	47,49,54,69	0
2	EDO	C	820	4/4	0.93	0.14	35,44,52,57	0
3	C8E	C	824	18/21	0.93	0.15	35,53,66,71	0
2	EDO	A	821	4/4	0.93	0.14	30,47,55,57	0
2	EDO	C	806	4/4	0.93	0.15	37,47,49,53	0
2	EDO	C	808	4/4	0.94	0.13	39,45,49,63	0
2	EDO	C	809	4/4	0.94	0.10	32,37,40,44	0
2	EDO	C	810	4/4	0.94	0.13	42,48,56,66	0
2	EDO	B	822	4/4	0.94	0.11	36,42,46,46	0
2	EDO	B	815	4/4	0.94	0.11	48,50,54,57	0
2	EDO	B	810	4/4	0.94	0.15	50,55,55,70	0
3	C8E	A	833	8/21	0.94	0.15	45,50,53,55	0

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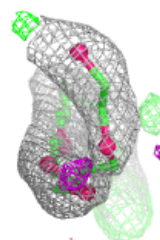
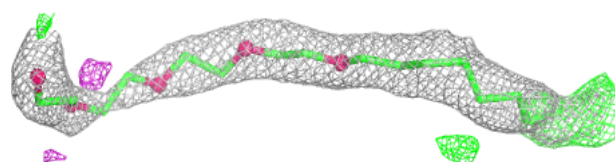
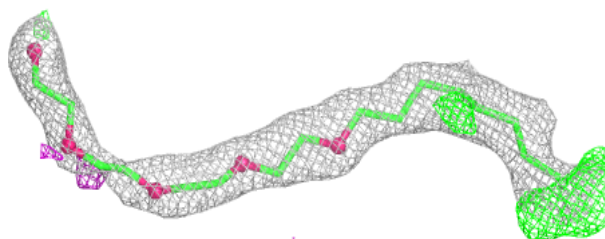
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	818	4/4	0.94	0.14	40,42,46,48	0
2	EDO	B	812	4/4	0.94	0.11	39,48,50,51	0
2	EDO	A	816	4/4	0.94	0.10	40,43,45,51	0
2	EDO	A	803	4/4	0.94	0.15	58,60,60,61	0
3	C8E	A	826	15/21	0.94	0.17	42,53,78,81	0
2	EDO	B	817	4/4	0.95	0.12	24,24,28,35	0
2	EDO	B	805	4/4	0.95	0.10	31,38,39,45	0
2	EDO	A	825	4/4	0.95	0.13	35,54,60,62	0
2	EDO	C	815	4/4	0.95	0.11	33,40,43,43	0
2	EDO	B	807	4/4	0.95	0.12	36,37,38,40	0
2	EDO	B	802	4/4	0.95	0.15	32,41,49,70	0
2	EDO	A	805	4/4	0.95	0.10	34,40,42,45	0
2	EDO	A	802	4/4	0.95	0.12	38,38,41,49	0
2	EDO	B	824	4/4	0.95	0.20	33,40,44,48	0
2	EDO	C	821	4/4	0.96	0.19	30,41,44,47	0
2	EDO	C	816	4/4	0.97	0.09	29,39,39,45	0
2	EDO	A	801	4/4	0.97	0.07	35,38,38,46	0
2	EDO	C	813	4/4	0.97	0.11	26,43,44,44	0
2	EDO	C	819	4/4	0.97	0.09	22,23,27,28	0
2	EDO	C	801	4/4	0.98	0.11	29,32,48,49	0
2	EDO	C	805	4/4	0.98	0.06	31,31,32,35	0
2	EDO	B	801	4/4	0.98	0.06	36,36,38,40	0
2	EDO	A	804	4/4	0.98	0.09	31,37,41,47	0

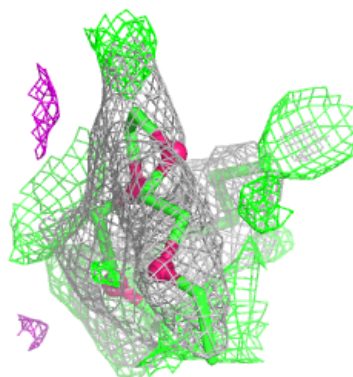
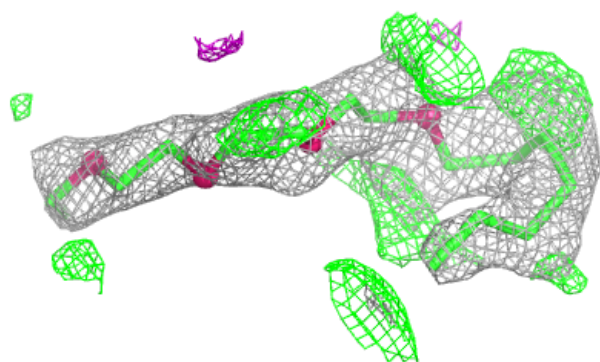
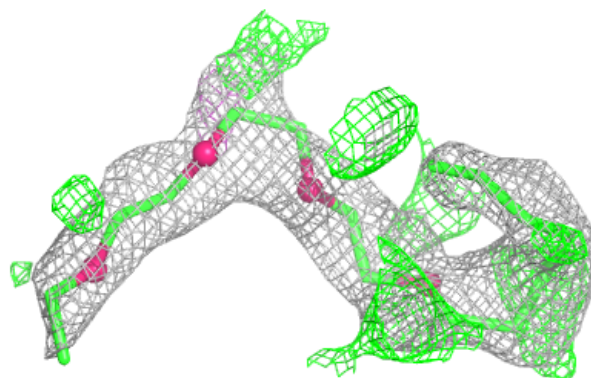
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 828:

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

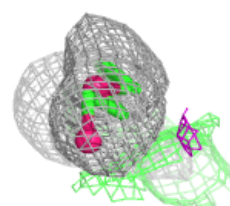
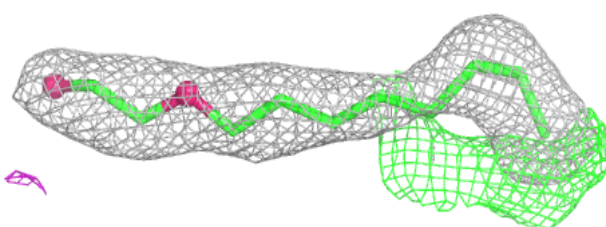
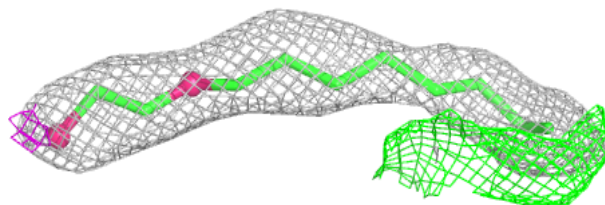
**Electron density around C8E A 834:**

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

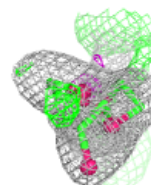
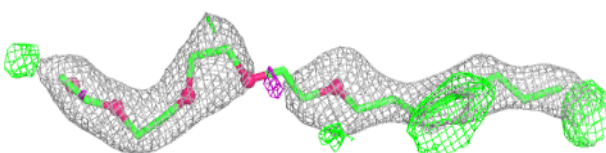
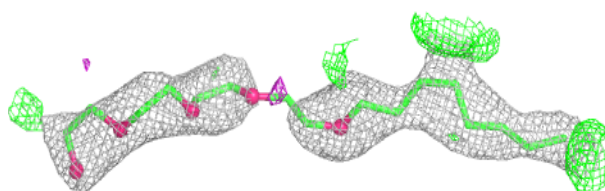


Electron density around C8E A 832:

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

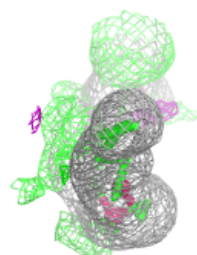
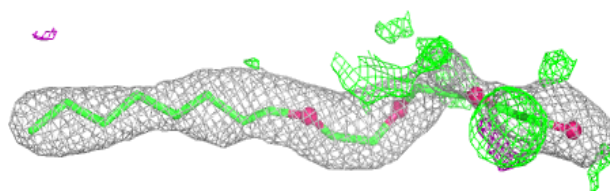
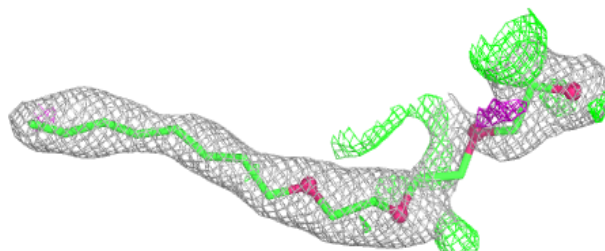
**Electron density around C8E A 830:**

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

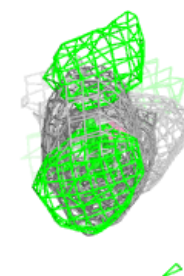
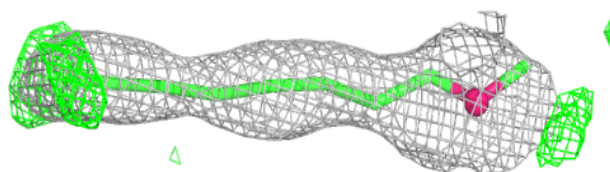
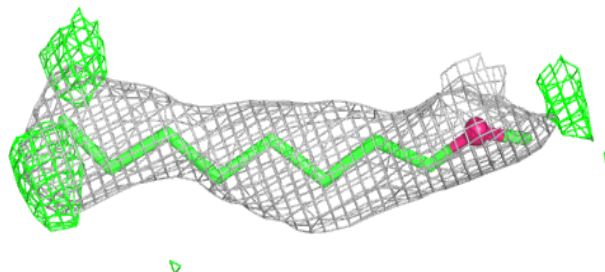


Electron density around C8E A 827:

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

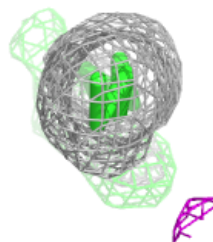
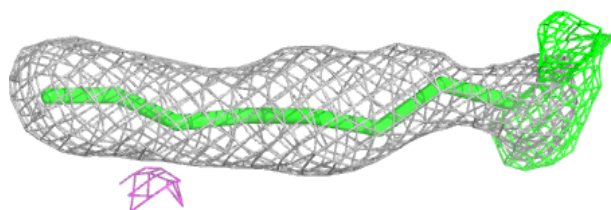
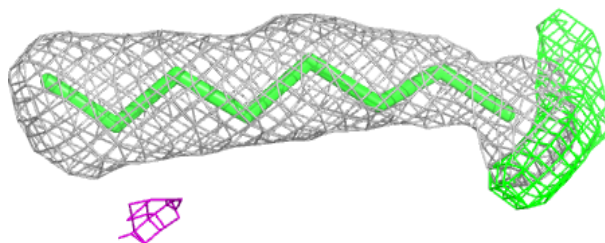
**Electron density around C8E A 836:**

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

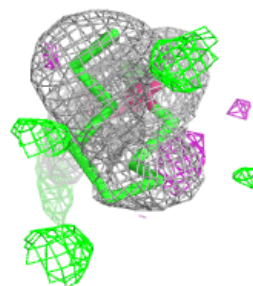
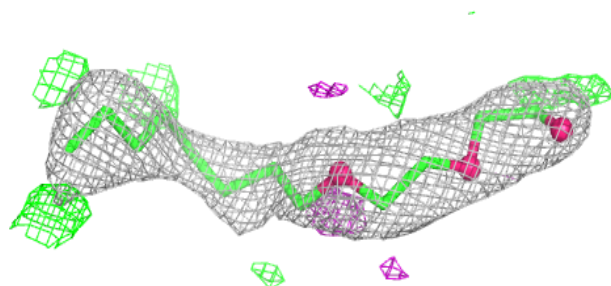
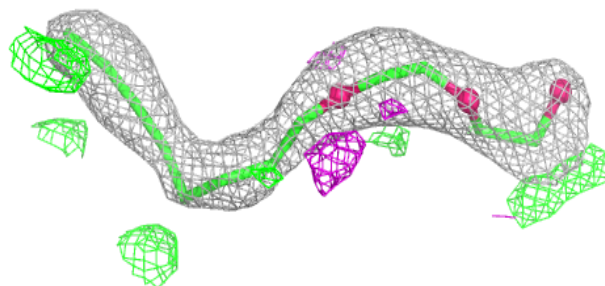


Electron density around C8E B 834:

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

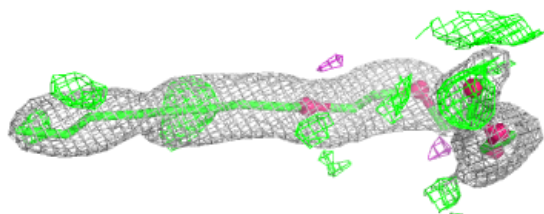
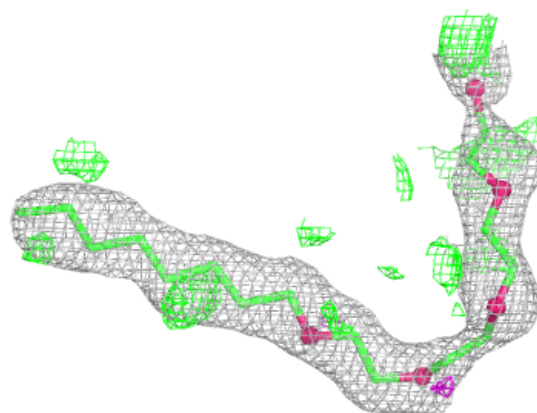
**Electron density around C8E C 832:**

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

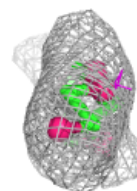
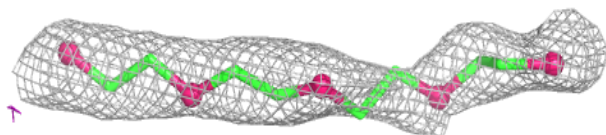
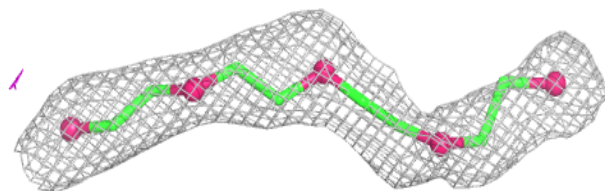


Electron density around C8E C 826:

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

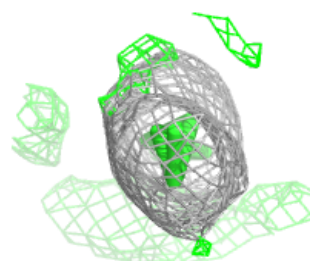
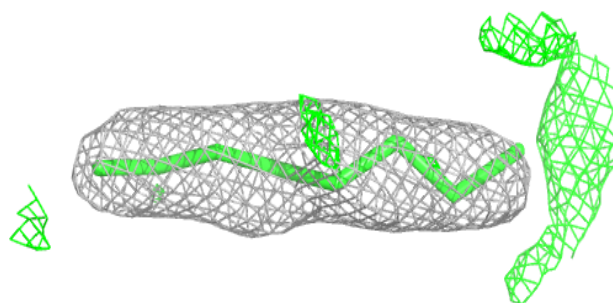
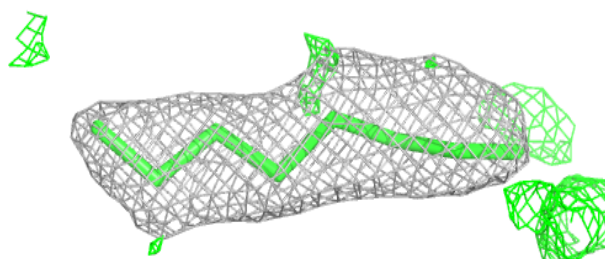
**Electron density around C8E B 826:**

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

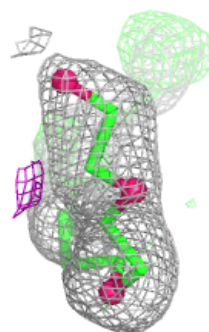
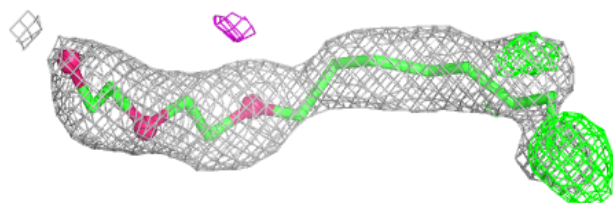
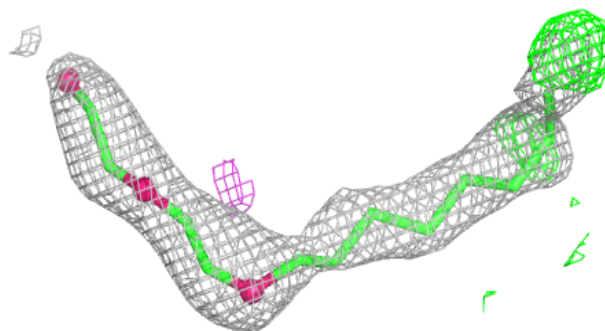


Electron density around C8E A 835:

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

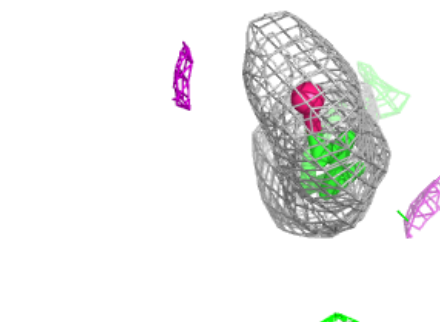
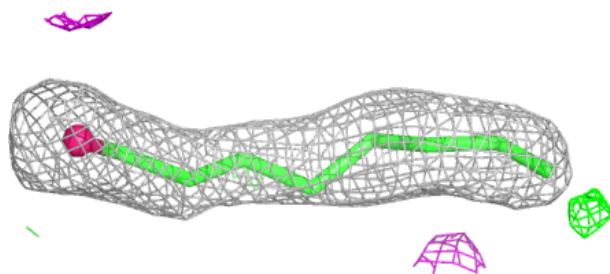
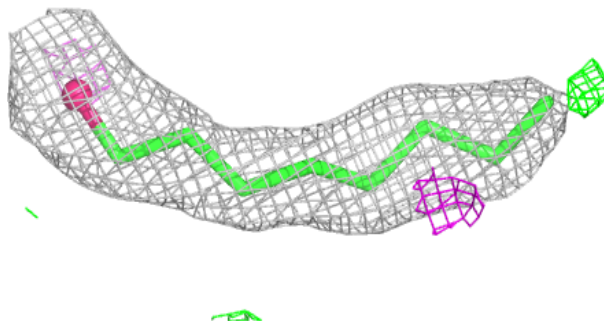
**Electron density around C8E C 828:**

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

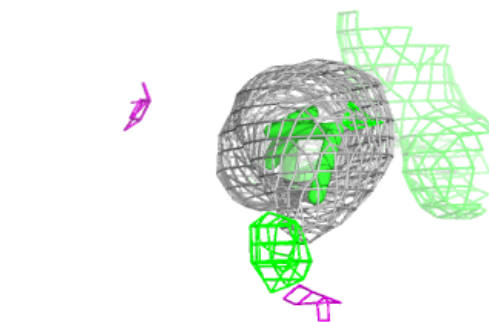
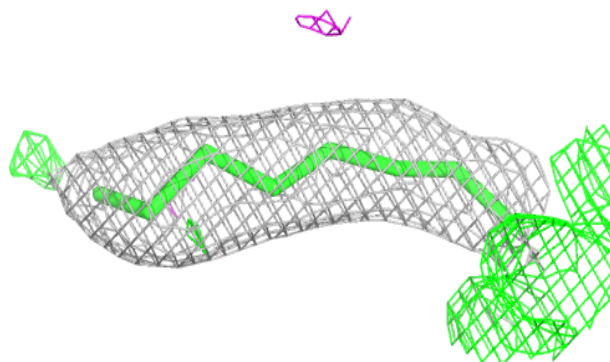
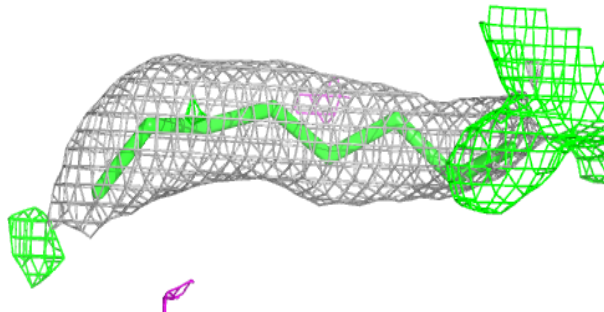


Electron density around C8E C 831:

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

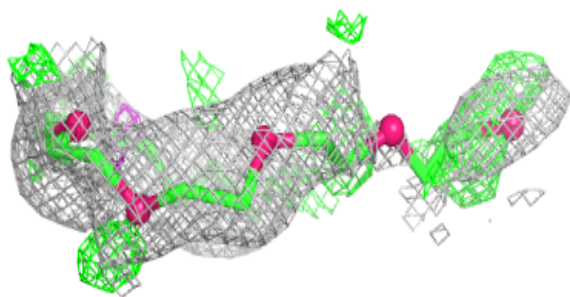
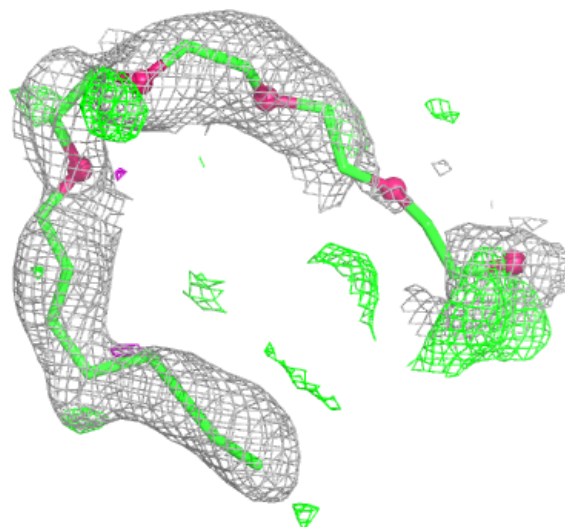
**Electron density around C8E C 835:**

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



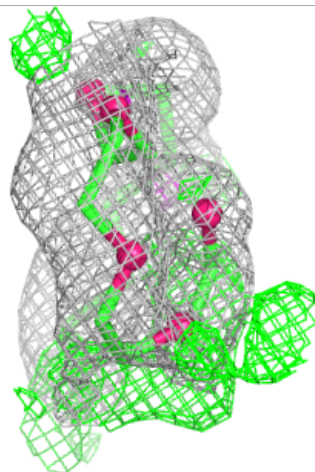
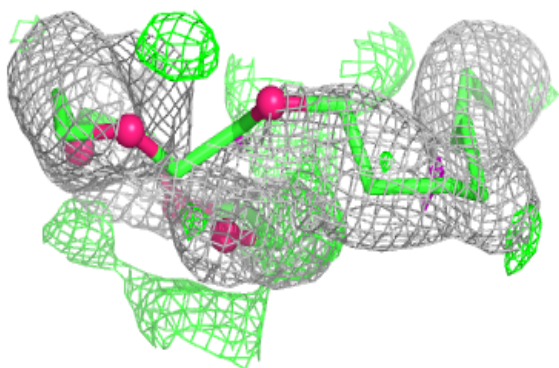
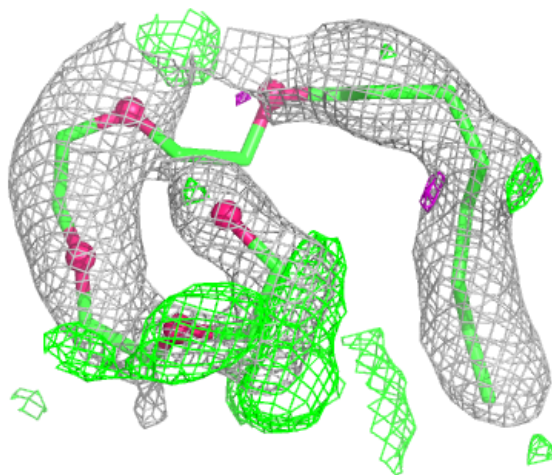
Electron density around C8E C 836 (A):

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



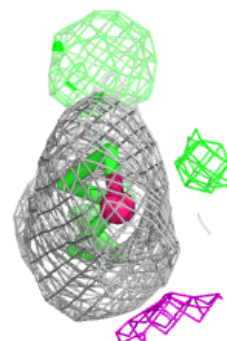
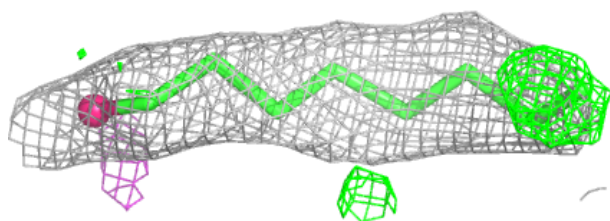
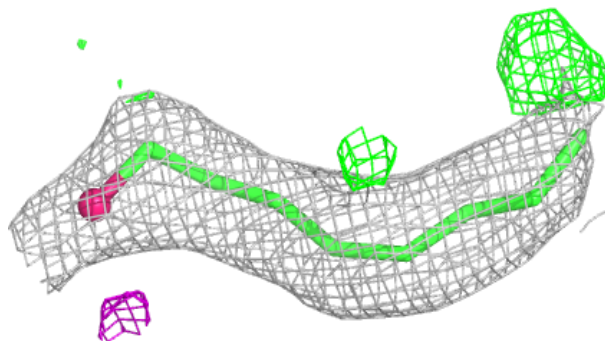
Electron density around C8E C 836 (B):

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and green (positive)

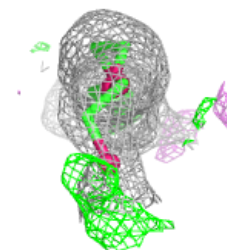
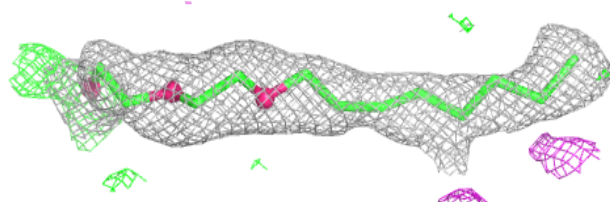
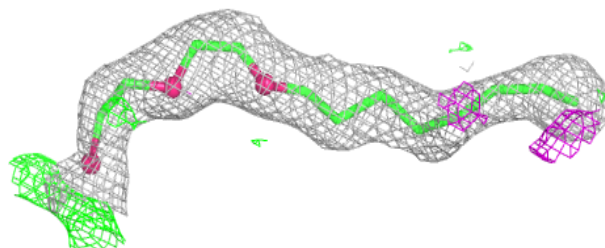


Electron density around C8E B 832:

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

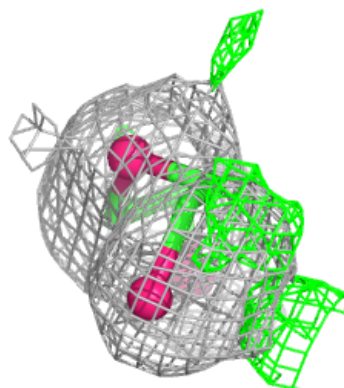
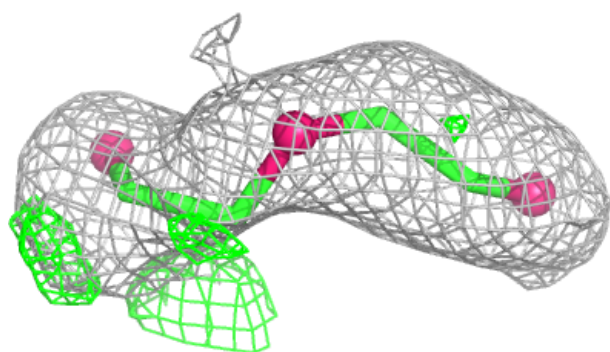
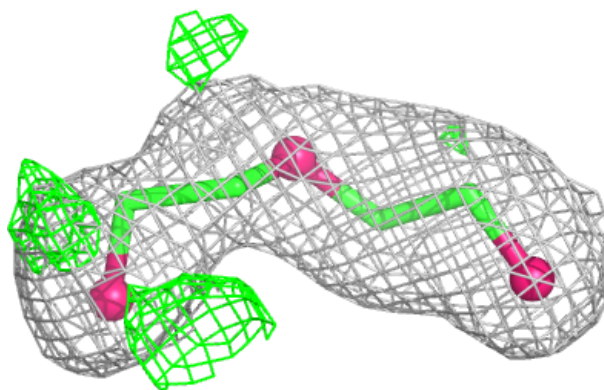
**Electron density around C8E C 827:**

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

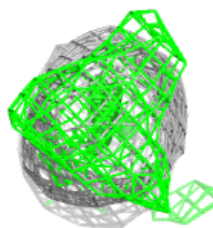
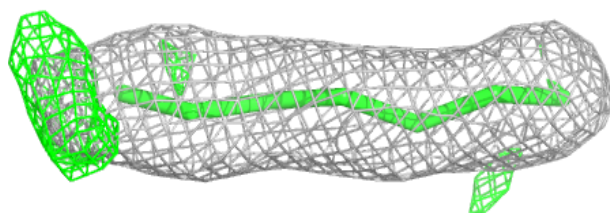
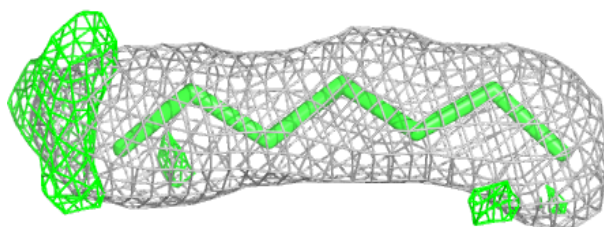


Electron density around C8E C 833:

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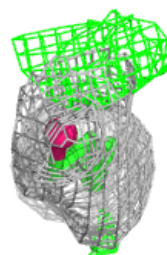
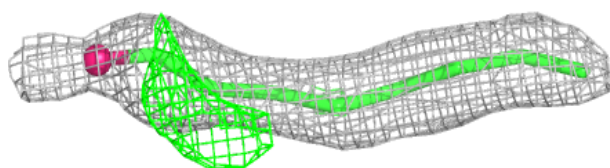
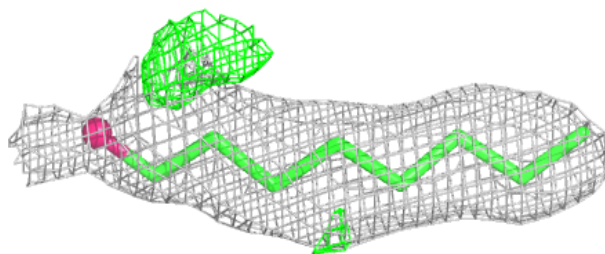
**Electron density around C8E C 834:**

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and green (positive)

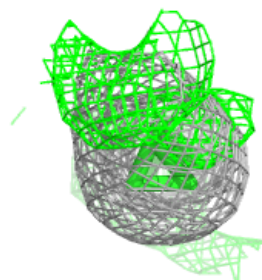
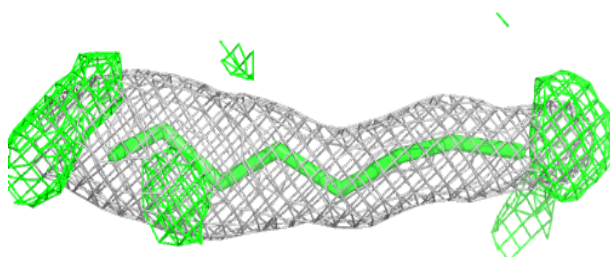
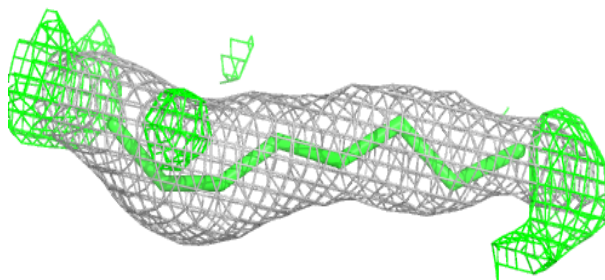


Electron density around C8E B 827:

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

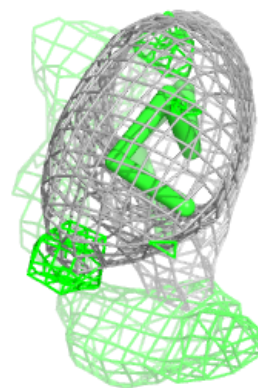
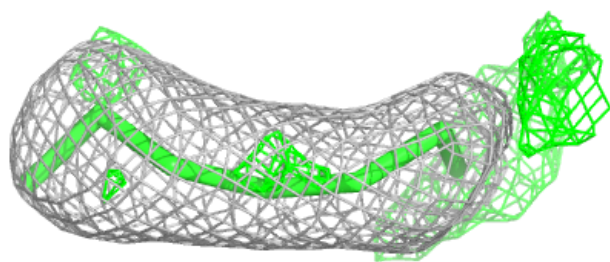
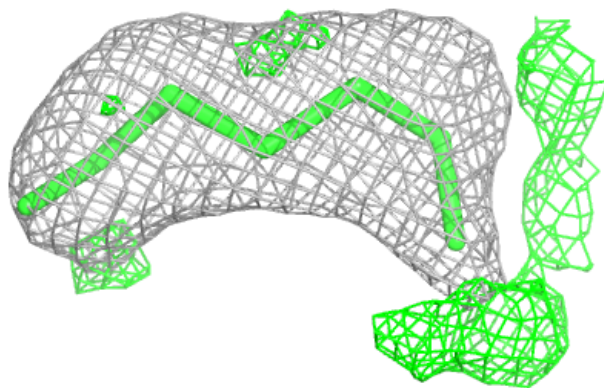
**Electron density around C8E B 828:**

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

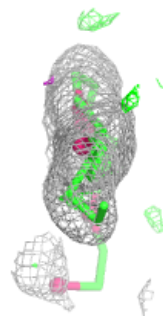
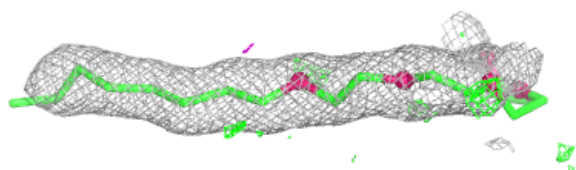
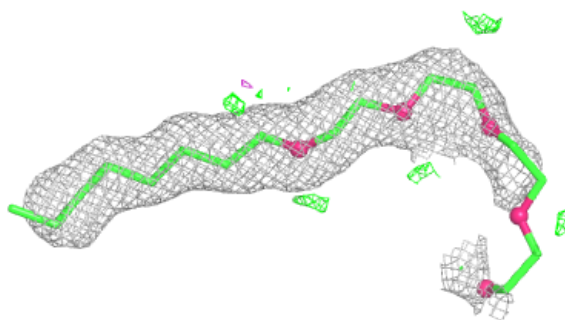


Electron density around C8E B 830:

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

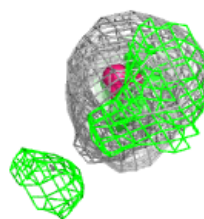
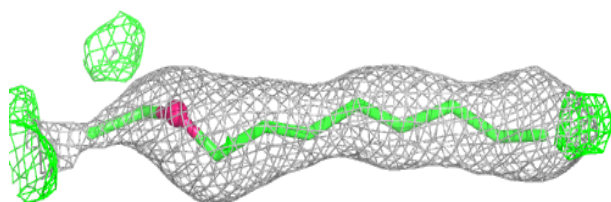
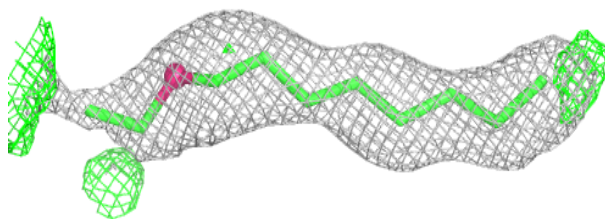
**Electron density around C8E C 825:**

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

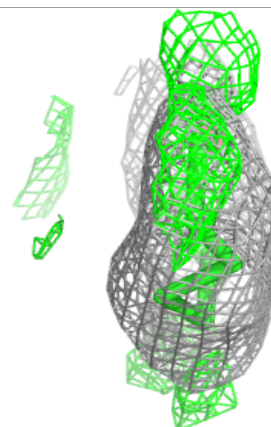
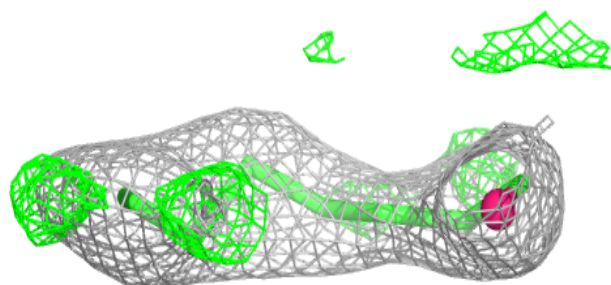
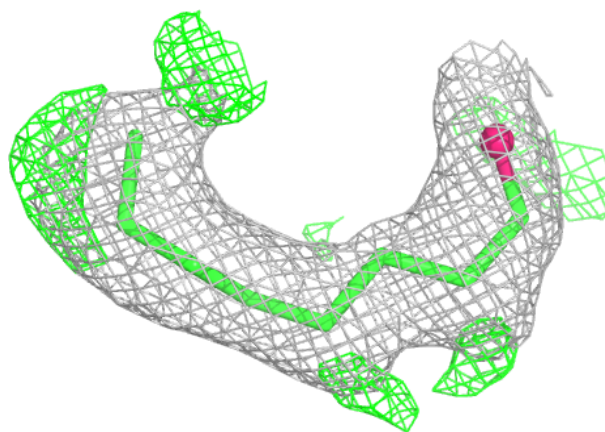


Electron density around C8E B 825:

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

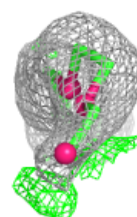
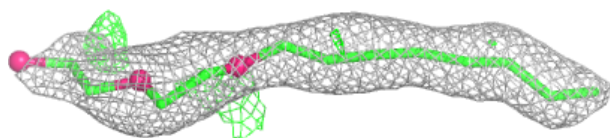
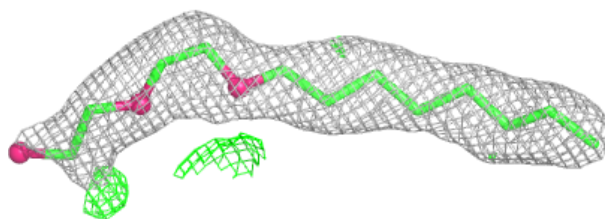
**Electron density around C8E B 833:**

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

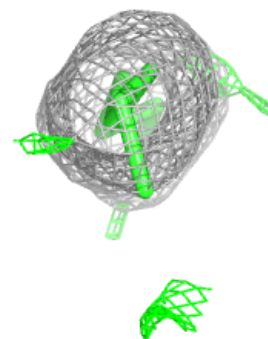
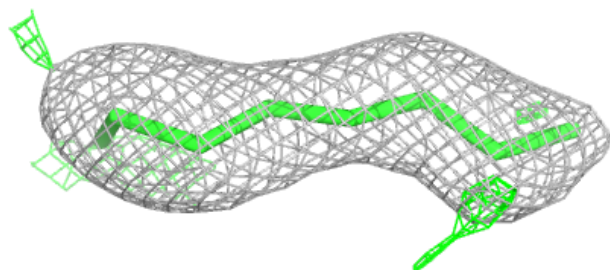
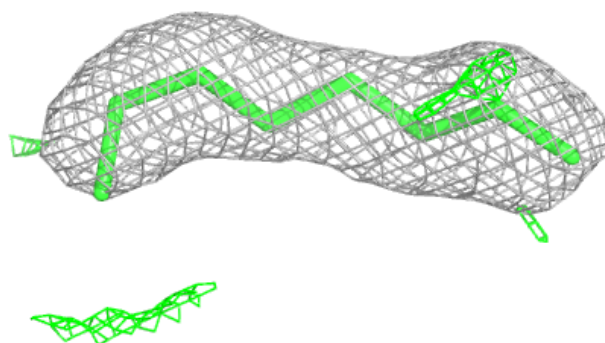


Electron density around C8E C 829:

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

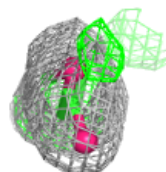
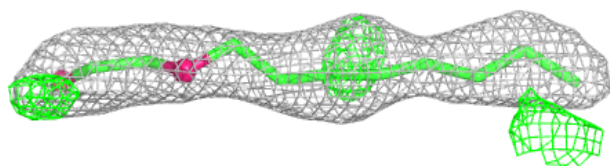
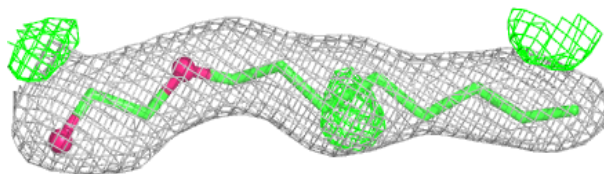
**Electron density around C8E C 830:**

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

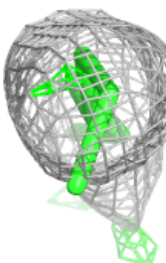
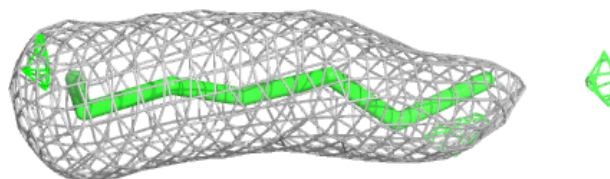
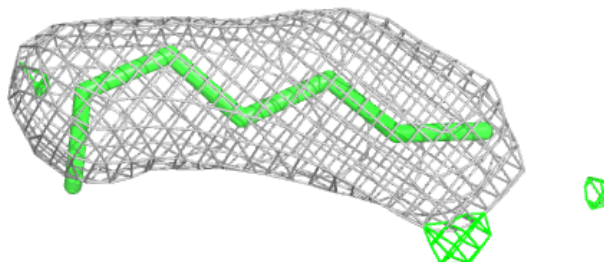


Electron density around C8E A 829:

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

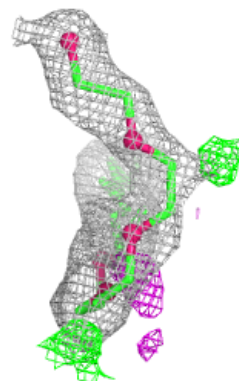
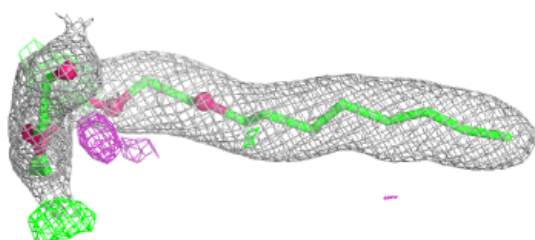
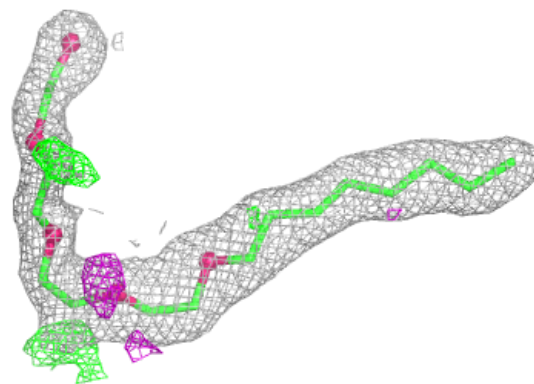
**Electron density around C8E B 831:**

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

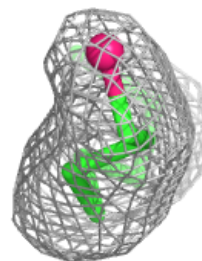
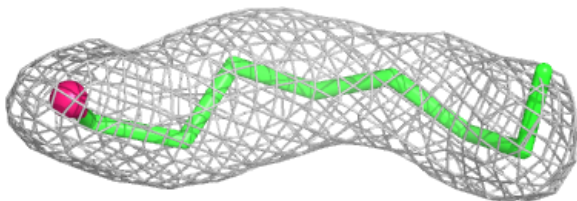
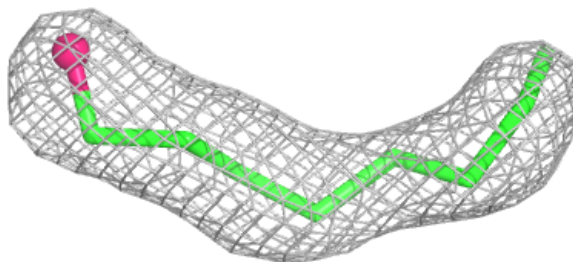


Electron density around C8E C 823:

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

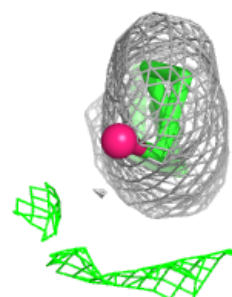
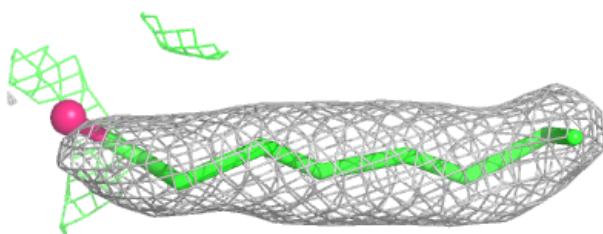
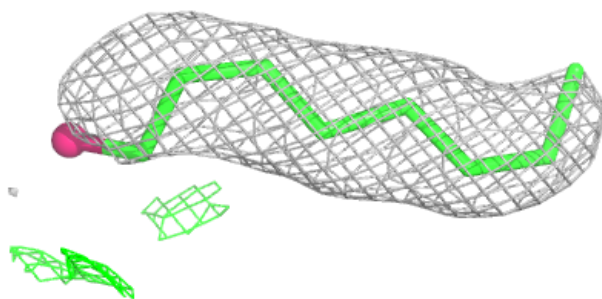
**Electron density around C8E B 829:**

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

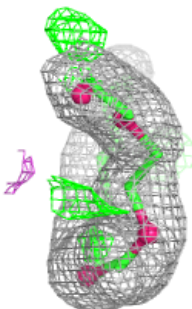
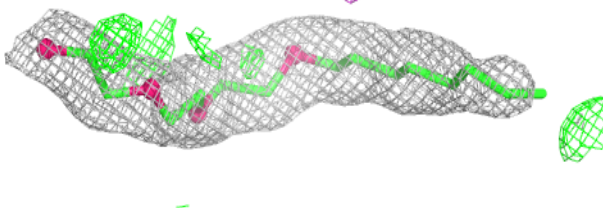
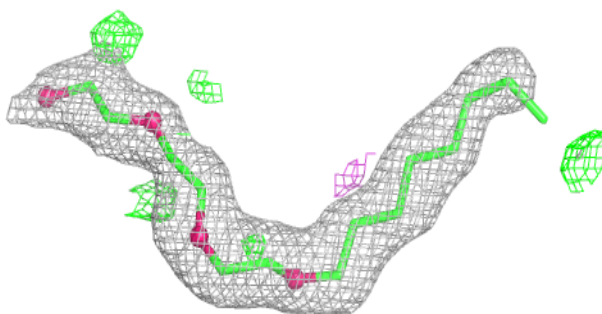


Electron density around C8E A 831:

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

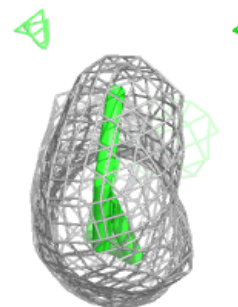
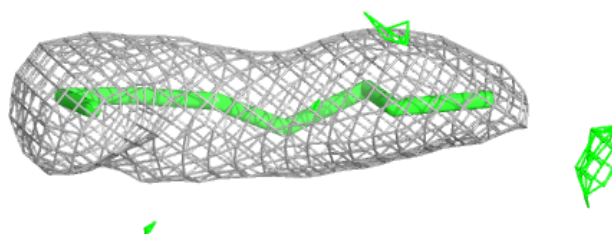
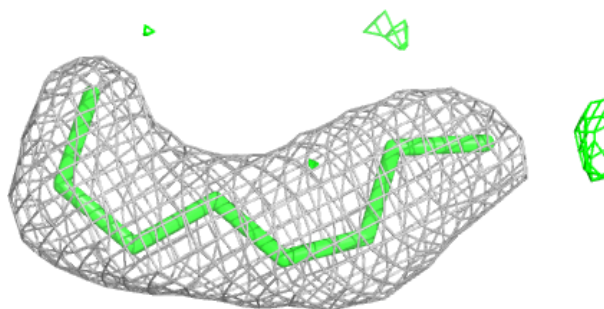
**Electron density around C8E C 824:**

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

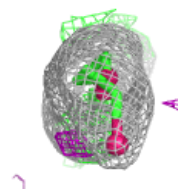
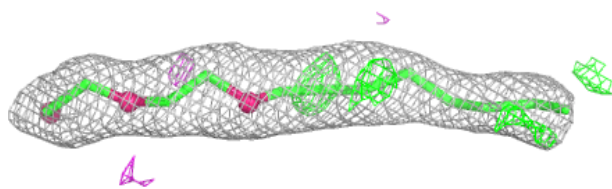
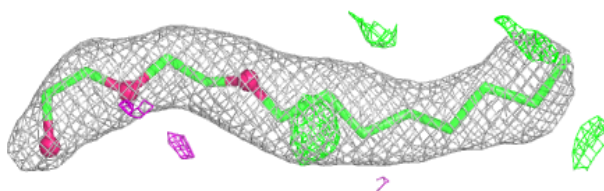


Electron density around C8E A 833:

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

**Electron density around C8E A 826:**

$2mF_o-DF_c$ (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.