Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:56 am BST

PDB ID	:	6HCP
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 following versions of software and data (see references ⓘ) were used in the production of this report:

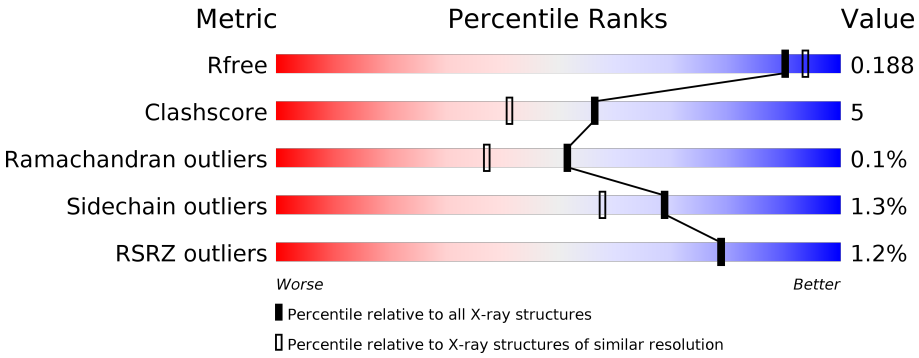
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	87% 8% 5%
1	B	706	2% 89% 6% 5%
1	C	706	% 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.

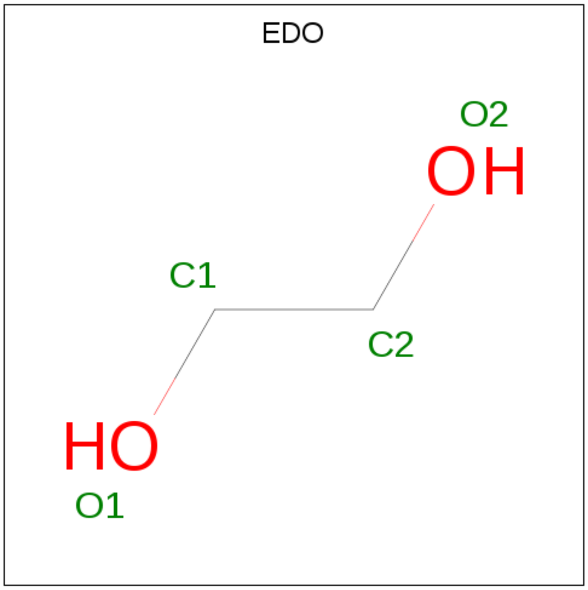
- Molecule 1 is a protein called BauA.

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

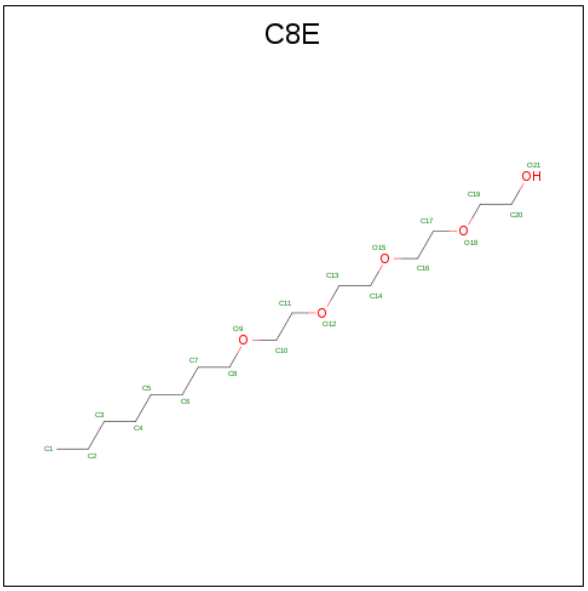
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

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 (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



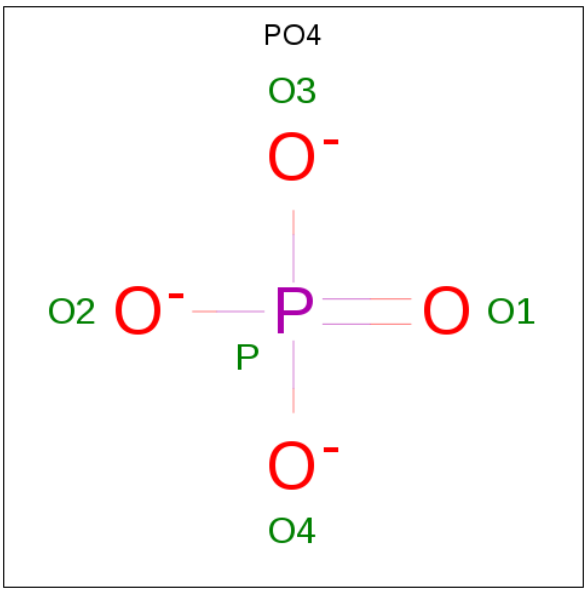
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 15 12 3	0	0
3	A	1	Total C O 18 14 4	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 9 8 1	0	0
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 19 15 4	0	0
3	A	1	Total C 8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

Continued on next page...

Continued from previous page...

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 (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

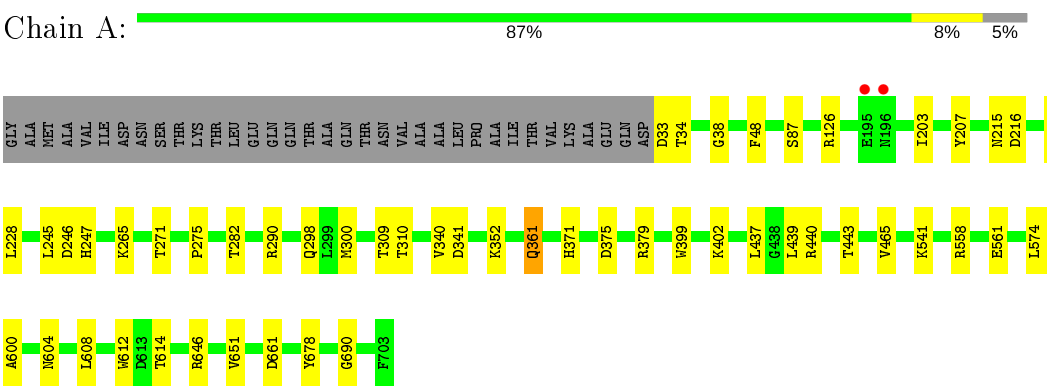
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	677	Total O 677 677	0	0
5	B	620	Total O 620 620	0	0
5	C	698	Total O 698 698	0	0

3 Residue-property plots (i)

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

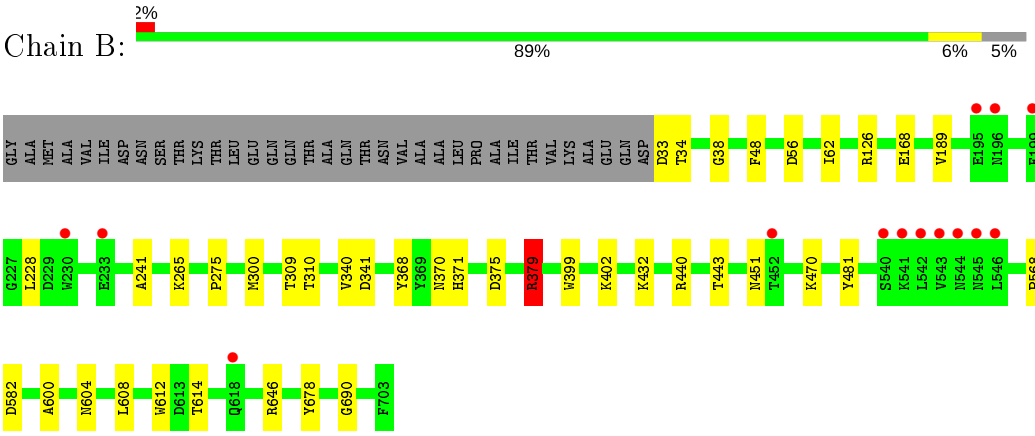
- Molecule 1: BauA

Chain A:



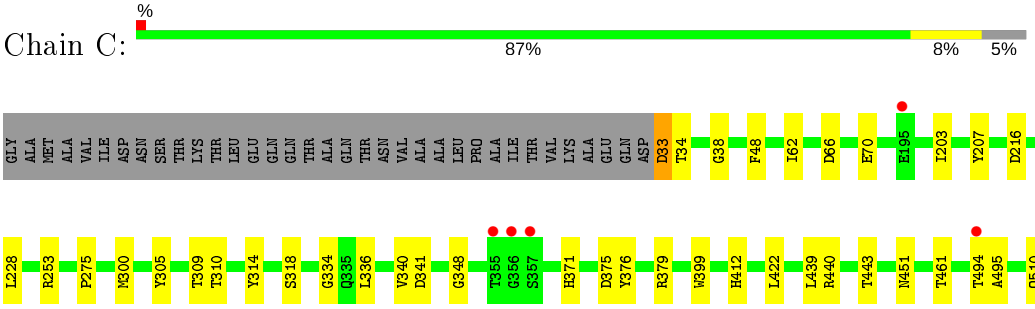
- Molecule 1: BauA

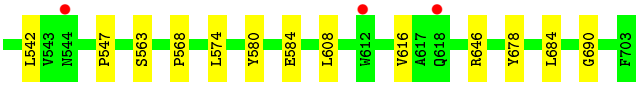
Chain B:



- Molecule 1: BauA

Chain C:




L542
V543
N544
P547
S563
P568
L574
Y580
E584
L608
W612
V616
A617
Q618
R646
Y678
L684
G690
F703

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, C8E, EDO

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	0.46	0/5427	0.63	1/7385 (0.0%)
1	B	0.46	0/5429	0.64	1/7389 (0.0%)
1	C	0.49	1/5587 (0.0%)	0.65	0/7607
All	All	0.47	1/16443 (0.0%)	0.64	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	584	GLU	CD-OE1	-5.78	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	126	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	126	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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
1	B	440	ARG	Sidechain
1	C	440	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5301	0	5094	46	0
1	B	5303	0	5113	33	0
1	C	5456	0	5262	65	0
2	A	100	0	150	15	0
2	B	96	0	144	3	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	10	0
5	B	620	0	0	7	1
5	C	698	0	0	11	1
All	All	18809	0	16673	168	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 (168) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:CD2	3:C:836[B]:C8E:H102	1.88	1.03
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:H81	3:C:836[B]:C8E:H41	1.73	0.70
1:A:207:TYR:HD1	1:A:222:ARG:HG2	1.57	0.69
1:B:402:LYS:HE3	5:B:1018:HOH:O	1.91	0.69
3:A:831:C8E:H82	3:B:828:C8E:C8	2.23	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:C20	3:C:836[B]:C8E:H101	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:O15	3:C:836[B]:C8E:H112	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:O	1:C:70[B]:GLU:HG3	2.00	0.61
1:A:207:TYR:CD1	1:A:222:ARG:HG2	2.37	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:A:439:LEU:C	1:A:439:LEU:HD12	2.26	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:H201	3:C:836[B]:C8E:H101	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:CG2	1:C:494[A]:THR:O	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: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:A:87:SER:OG	1:A:561[B]:GLU:OE1	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG22	1:A:341[A]:ASP:OD1	2.14	0.48
1:A:575[A]:MET:HG3	2:A:818:EDO:HO1	1.78	0.48
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:494[A]:THR:HG22	1:C:494[A]:THR:O	2.15	0.46
1:C:537:LEU:HG	1:C:547[B]:PRO:HB2	1.97	0.46
1:C:336:LEU:CD2	3:C:836[A]:C8E:H141	2.45	0.46
1:B:582:ASP:OD2	5:B:902:HOH:O	2.20	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:A:216:ASP:OD2	1:B:265:LYS:NZ	2.37	0.45
1:B:241:ALA:HB1	3:B:825:C8E:H32	1.97	0.45
1:C:310:THR:HB	1:C:340:VAL:HG13	1.99	0.45
1:C:305:TYR:HB2	3:C:835:C8E:H31	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HG3	1:A:245:LEU:HD23	2.00	0.44
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: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: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: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
3:C:836[B]:C8E:HO2	3:C:836[B]:C8E:C11	2.22	0.41
1:C:226[A]:LEU:HD11	1:C:228:LEU:HD21	2.01	0.41
1:C:33:ASP:CG	1:C:33:ASP:O	2.59	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
2:A:813:EDO:H12	5:A:1376:HOH:O	2.19	0.41
1:A:246:ASP:OD2	2:A:823:EDO:H21	2.20	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
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
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%)	41 27
1	B	692/706 (98%)	673 (97%)	18 (3%)	1 (0%)	51 37
1	C	711/706 (101%)	690 (97%)	21 (3%)	0	100 100
All	All	2094/2118 (99%)	2036 (97%)	55 (3%)	3 (0%)	51 37

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%)	67 55
1	B	573/577 (99%)	566 (99%)	7 (1%)	71 61
1	C	588/577 (102%)	582 (99%)	6 (1%)	76 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1733/1731 (100%)	1712 (99%)	21 (1%)	69 61

All (21) 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	361	GLN
1	A	371	HIS
1	A	375	ASP
1	A	646	ARG
1	A	661	ASP
1	B	33	ASP
1	B	48	PHE
1	B	300	MET
1	B	371	HIS
1	B	375	ASP
1	B	379	ARG
1	B	646	ARG
1	C	33	ASP
1	C	48	PHE
1	C	300	MET
1	C	371	HIS
1	C	375	ASP
1	C	646	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	818	-	3,3,3	0.53	0	2,2,2	0.48	0
2	EDO	A	804	-	3,3,3	0.56	0	2,2,2	0.11	0
2	EDO	C	803	-	3,3,3	0.35	0	2,2,2	0.57	0
2	EDO	C	819	-	3,3,3	1.25	0	2,2,2	0.80	0
2	EDO	B	807	-	3,3,3	0.60	0	2,2,2	0.66	0
2	EDO	B	808	-	3,3,3	0.33	0	2,2,2	0.62	0
2	EDO	A	808	-	3,3,3	0.89	0	2,2,2	0.44	0
2	EDO	B	811	-	3,3,3	0.37	0	2,2,2	0.29	0
3	C8E	A	831	-	8,8,20	0.23	0	7,7,19	0.45	0
2	EDO	A	803	-	3,3,3	0.32	0	2,2,2	0.57	0
2	EDO	A	807	-	3,3,3	0.42	0	2,2,2	0.42	0
2	EDO	A	809	-	3,3,3	0.40	0	2,2,2	0.45	0
2	EDO	A	820	-	3,3,3	0.35	0	2,2,2	0.31	0
3	C8E	C	830	-	7,7,20	0.30	0	6,6,19	0.43	0
3	C8E	A	829	-	11,11,20	0.30	0	10,10,19	0.52	0
3	C8E	A	827	-	17,17,20	0.74	0	16,16,19	0.74	0
2	EDO	B	815	-	3,3,3	0.47	0	2,2,2	0.19	0
2	EDO	B	803	-	3,3,3	0.34	0	2,2,2	0.67	0
2	EDO	C	807	-	3,3,3	0.34	0	2,2,2	0.78	0
2	EDO	B	814	-	3,3,3	0.32	0	2,2,2	0.38	0
2	EDO	C	805	-	3,3,3	0.28	0	2,2,2	0.18	0
2	EDO	B	824	-	3,3,3	0.58	0	2,2,2	0.18	0
3	C8E	C	835	-	7,7,20	0.22	0	6,6,19	0.48	0
2	EDO	A	811	-	3,3,3	0.37	0	2,2,2	0.59	0
2	EDO	A	814	-	3,3,3	0.38	0	2,2,2	0.37	0
3	C8E	B	833	-	8,8,20	0.38	0	7,7,19	0.41	0
2	EDO	B	820	-	3,3,3	0.63	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	A	822	-	3,3,3	0.70	0	2,2,2	0.79	0
3	C8E	B	826	-	12,12,20	0.48	0	11,11,19	0.40	0
2	EDO	B	810	-	3,3,3	0.40	0	2,2,2	0.45	0
2	EDO	C	814	-	3,3,3	0.40	0	2,2,2	0.18	0
3	C8E	C	825	-	20,20,20	0.47	0	19,19,19	0.56	0
3	C8E	B	831	-	6,6,20	0.26	0	5,5,19	0.43	0
2	EDO	C	802	-	3,3,3	0.30	0	2,2,2	0.58	0
2	EDO	B	812	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	C	801	-	3,3,3	0.34	0	2,2,2	0.53	0
3	C8E	C	824	-	17,17,20	0.46	0	16,16,19	0.46	0
2	EDO	A	805	-	3,3,3	0.62	0	2,2,2	0.25	0
2	EDO	C	804	-	3,3,3	0.57	0	2,2,2	0.42	0
3	C8E	C	827	-	14,14,20	0.36	0	13,13,19	0.44	0
2	EDO	A	825	-	3,3,3	0.32	0	2,2,2	1.27	0
2	EDO	A	821	-	3,3,3	0.42	0	2,2,2	0.35	0
3	C8E	B	828	-	7,7,20	0.33	0	6,6,19	0.24	0
2	EDO	B	817	-	3,3,3	1.33	0	2,2,2	0.96	0
2	EDO	C	806	-	3,3,3	0.33	0	2,2,2	0.12	0
3	C8E	A	830	-	20,20,20	0.47	0	19,19,19	0.43	0
3	C8E	A	834	-	18,18,20	0.50	0	17,17,19	0.28	0
3	C8E	A	833	-	7,7,20	0.22	0	6,6,19	0.43	0
2	EDO	C	821	-	3,3,3	0.47	0	2,2,2	0.11	0
2	EDO	C	811	-	3,3,3	0.41	0	2,2,2	0.50	0
2	EDO	A	812	-	3,3,3	0.38	0	2,2,2	0.38	0
2	EDO	A	816	-	3,3,3	0.29	0	2,2,2	0.68	0
2	EDO	B	802	-	3,3,3	0.33	0	2,2,2	0.74	0
3	C8E	C	836[A]	-	20,20,20	0.51	0	19,19,19	0.72	1 (5%)
3	C8E	B	830	-	6,6,20	0.28	0	5,5,19	0.29	0
2	EDO	A	815	-	3,3,3	0.44	0	2,2,2	0.18	0
2	EDO	C	809	-	3,3,3	0.64	0	2,2,2	0.30	0
2	EDO	B	822	-	3,3,3	0.73	0	2,2,2	0.25	0
2	EDO	C	815	-	3,3,3	0.76	0	2,2,2	0.74	0
3	C8E	C	834	-	6,6,20	0.33	0	5,5,19	0.29	0
2	EDO	B	806	-	3,3,3	0.44	0	2,2,2	0.65	0
2	EDO	A	823	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	C	822	-	3,3,3	0.30	0	2,2,2	0.73	0
2	EDO	A	813	-	3,3,3	0.39	0	2,2,2	0.36	0
3	C8E	C	832	-	14,14,20	0.41	0	13,13,19	0.65	0
2	EDO	A	802	-	3,3,3	0.40	0	2,2,2	0.73	0
2	EDO	C	820	-	3,3,3	0.39	0	2,2,2	0.43	0
2	EDO	B	823	-	3,3,3	0.34	0	2,2,2	0.62	0
2	EDO	C	817	-	3,3,3	0.75	0	2,2,2	0.17	0
2	EDO	A	817	-	3,3,3	0.30	0	2,2,2	0.46	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	0.40	0	2,2,2	0.60	0
3	C8E	A	826	-	14,14,20	0.32	0	13,13,19	0.56	0
2	EDO	B	818	-	3,3,3	0.61	0	2,2,2	0.07	0
2	EDO	A	819	-	3,3,3	0.42	0	2,2,2	0.70	0
3	C8E	C	823	-	20,20,20	0.57	0	19,19,19	0.81	1 (5%)
2	EDO	A	810	-	3,3,3	0.48	0	2,2,2	0.23	0
3	C8E	C	826	-	20,20,20	0.58	0	19,19,19	0.63	0
2	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.04	0
3	C8E	B	834	-	7,7,20	0.28	0	6,6,19	0.36	0
3	C8E	B	827	-	8,8,20	0.30	0	7,7,19	0.42	0
3	C8E	C	828	-	14,14,20	0.33	0	13,13,19	0.48	0
3	C8E	B	832	-	8,8,20	0.21	0	7,7,19	0.52	0
2	EDO	B	821	-	3,3,3	0.30	0	2,2,2	0.48	0
2	EDO	A	801	-	3,3,3	0.30	0	2,2,2	0.25	0
2	EDO	C	813	-	3,3,3	0.65	0	2,2,2	0.23	0
2	EDO	C	816	-	3,3,3	0.53	0	2,2,2	0.26	0
3	C8E	B	829	-	8,8,20	0.23	0	7,7,19	0.44	0
2	EDO	C	818	-	3,3,3	0.75	0	2,2,2	0.19	0
3	C8E	A	835	-	7,7,20	0.28	0	6,6,19	0.39	0
2	EDO	A	824	-	3,3,3	0.51	0	2,2,2	0.29	0
2	EDO	A	806	-	3,3,3	0.76	0	2,2,2	0.25	0
2	EDO	B	813	-	3,3,3	0.38	0	2,2,2	0.33	0
2	EDO	B	805	-	3,3,3	0.76	0	2,2,2	0.13	0
3	C8E	A	828	-	20,20,20	0.59	0	19,19,19	0.35	0
2	EDO	B	819	-	3,3,3	0.50	0	2,2,2	0.56	0
4	PO4	B	835	-	4,4,4	0.88	0	6,6,6	0.59	0
3	C8E	A	832	-	11,11,20	0.32	0	10,10,19	0.41	0
3	C8E	A	836	-	9,9,20	0.39	0	8,8,19	0.44	0
3	C8E	C	833	-	6,6,20	0.50	0	5,5,19	0.45	0
2	EDO	C	808	-	3,3,3	0.48	0	2,2,2	0.27	0
3	C8E	C	836[B]	-	20,20,20	0.56	0	19,19,19	0.44	0
2	EDO	C	812	-	3,3,3	0.31	0	2,2,2	0.72	0
2	EDO	B	809	-	3,3,3	0.45	0	2,2,2	0.52	0
3	C8E	B	825	-	10,10,20	0.42	0	9,9,19	0.40	0
3	C8E	C	831	-	8,8,20	0.29	0	7,7,19	0.53	0
2	EDO	B	801	-	3,3,3	0.40	0	2,2,2	0.07	0
2	EDO	B	816	-	3,3,3	0.40	0	2,2,2	0.57	0
3	C8E	C	829	-	14,14,20	0.36	0	13,13,19	0.47	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	A	818	-	-	1/1/1/1	-
2	EDO	A	804	-	-	0/1/1/1	-
2	EDO	C	803	-	-	1/1/1/1	-
2	EDO	C	819	-	-	0/1/1/1	-
2	EDO	B	807	-	-	1/1/1/1	-
2	EDO	B	808	-	-	0/1/1/1	-
2	EDO	A	808	-	-	0/1/1/1	-
2	EDO	B	811	-	-	1/1/1/1	-
3	C8E	A	831	-	-	2/6/6/18	-
2	EDO	A	803	-	-	1/1/1/1	-
2	EDO	A	807	-	-	1/1/1/1	-
2	EDO	A	809	-	-	0/1/1/1	-
2	EDO	A	820	-	-	1/1/1/1	-
3	C8E	C	830	-	-	1/5/5/18	-
3	C8E	A	829	-	-	4/9/9/18	-
3	C8E	A	827	-	-	6/15/15/18	-
2	EDO	B	815	-	-	0/1/1/1	-
2	EDO	B	803	-	-	1/1/1/1	-
2	EDO	C	807	-	-	0/1/1/1	-
2	EDO	B	814	-	-	1/1/1/1	-
2	EDO	C	805	-	-	0/1/1/1	-
2	EDO	B	824	-	-	0/1/1/1	-
3	C8E	C	835	-	-	3/5/5/18	-
2	EDO	A	811	-	-	0/1/1/1	-
2	EDO	A	814	-	-	1/1/1/1	-
3	C8E	B	833	-	-	3/6/6/18	-
2	EDO	B	820	-	-	1/1/1/1	-
2	EDO	A	822	-	-	1/1/1/1	-
3	C8E	B	826	-	-	5/10/10/18	-
2	EDO	B	810	-	-	0/1/1/1	-
2	EDO	C	814	-	-	0/1/1/1	-
3	C8E	C	825	-	-	5/18/18/18	-
3	C8E	B	831	-	-	1/4/4/18	-
2	EDO	C	802	-	-	0/1/1/1	-
2	EDO	B	812	-	-	0/1/1/1	-
2	EDO	C	801	-	-	0/1/1/1	-
3	C8E	C	824	-	-	5/15/15/18	-
2	EDO	A	805	-	-	0/1/1/1	-
2	EDO	C	804	-	-	0/1/1/1	-
3	C8E	C	827	-	-	6/12/12/18	-
2	EDO	A	825	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	821	-	-	1/1/1/1	-
3	C8E	B	828	-	-	3/5/5/18	-
2	EDO	B	817	-	-	1/1/1/1	-
2	EDO	C	806	-	-	0/1/1/1	-
3	C8E	A	830	-	-	8/18/18/18	-
3	C8E	A	834	-	-	10/16/16/18	-
3	C8E	A	833	-	-	2/5/5/18	-
2	EDO	C	821	-	-	0/1/1/1	-
2	EDO	C	811	-	-	0/1/1/1	-
2	EDO	A	812	-	-	0/1/1/1	-
2	EDO	A	816	-	-	0/1/1/1	-
2	EDO	B	802	-	-	0/1/1/1	-
3	C8E	C	836[A]	-	-	9/18/18/18	-
3	C8E	B	830	-	-	4/4/4/18	-
2	EDO	A	815	-	-	1/1/1/1	-
2	EDO	C	809	-	-	1/1/1/1	-
2	EDO	B	822	-	-	1/1/1/1	-
2	EDO	C	815	-	-	0/1/1/1	-
3	C8E	C	834	-	-	1/4/4/18	-
2	EDO	B	806	-	-	0/1/1/1	-
2	EDO	A	823	-	-	0/1/1/1	-
2	EDO	C	822	-	-	0/1/1/1	-
2	EDO	A	813	-	-	1/1/1/1	-
3	C8E	C	832	-	-	4/12/12/18	-
2	EDO	A	802	-	-	0/1/1/1	-
2	EDO	C	820	-	-	1/1/1/1	-
2	EDO	B	823	-	-	1/1/1/1	-
2	EDO	C	817	-	-	1/1/1/1	-
2	EDO	A	817	-	-	1/1/1/1	-
2	EDO	C	810	-	-	0/1/1/1	-
3	C8E	A	826	-	-	7/12/12/18	-
2	EDO	B	818	-	-	0/1/1/1	-
2	EDO	A	819	-	-	1/1/1/1	-
3	C8E	C	823	-	-	1/18/18/18	-
2	EDO	A	810	-	-	1/1/1/1	-
3	C8E	C	826	-	-	8/18/18/18	-
2	EDO	B	804	-	-	1/1/1/1	-
3	C8E	B	834	-	-	1/5/5/18	-
3	C8E	B	827	-	-	2/6/6/18	-
3	C8E	C	828	-	-	7/12/12/18	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	832	-	-	2/6/6/18	-
2	EDO	B	821	-	-	0/1/1/1	-
2	EDO	A	801	-	-	0/1/1/1	-
2	EDO	C	813	-	-	0/1/1/1	-
2	EDO	C	816	-	-	1/1/1/1	-
3	C8E	B	829	-	-	5/6/6/18	-
2	EDO	C	818	-	-	0/1/1/1	-
3	C8E	A	835	-	-	2/5/5/18	-
2	EDO	A	824	-	-	1/1/1/1	-
2	EDO	A	806	-	-	0/1/1/1	-
2	EDO	B	813	-	-	0/1/1/1	-
2	EDO	B	805	-	-	0/1/1/1	-
3	C8E	A	828	-	-	7/18/18/18	-
2	EDO	B	819	-	-	1/1/1/1	-
3	C8E	A	832	-	-	3/9/9/18	-
3	C8E	A	836	-	-	1/7/7/18	-
3	C8E	C	833	-	-	2/4/4/18	-
2	EDO	C	808	-	-	0/1/1/1	-
3	C8E	C	836[B]	-	-	9/18/18/18	-
2	EDO	C	812	-	-	0/1/1/1	-
2	EDO	B	809	-	-	0/1/1/1	-
3	C8E	B	825	-	-	3/8/8/18	-
3	C8E	C	831	-	-	4/6/6/18	-
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	B	816	-	-	1/1/1/1	-
3	C8E	C	829	-	-	2/12/12/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	836[A]	C8E	C13-O12-C11	-2.11	104.14	113.29
3	C	823	C8E	C6-C5-C4	-2.09	103.79	114.42

There are no chirality outliers.

All (178) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	820	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	828	C8E	O18-C19-C20-O21
3	A	832	C8E	O9-C10-C11-O12
3	C	833	C8E	O9-C10-C11-O12
3	B	829	C8E	C6-C7-C8-O9
3	A	830	C8E	C4-C5-C6-C7
3	A	827	C8E	C6-C7-C8-O9
3	A	834	C8E	O12-C13-C14-O15
3	C	828	C8E	C1-C2-C3-C4
3	C	825	C8E	C1-C2-C3-C4
2	C	820	EDO	O1-C1-C2-O2
3	B	833	C8E	C1-C2-C3-C4
3	B	828	C8E	C5-C6-C7-C8
3	A	826	C8E	C2-C3-C4-C5
3	A	831	C8E	C6-C7-C8-O9
3	A	829	C8E	C5-C6-C7-C8
3	B	825	C8E	C11-C10-O9-C8
3	B	831	C8E	C5-C6-C7-C8
3	C	836[B]	C8E	C5-C6-C7-C8
3	C	826	C8E	C10-C11-O12-C13
3	A	826	C8E	C3-C4-C5-C6
3	A	834	C8E	C5-C6-C7-C8
3	A	827	C8E	O9-C10-C11-O12
3	C	831	C8E	C2-C3-C4-C5
3	B	830	C8E	C4-C5-C6-C7
3	C	835	C8E	C4-C5-C6-C7
3	A	834	C8E	C20-C19-O18-C17
3	B	834	C8E	C2-C3-C4-C5
3	B	830	C8E	C3-C4-C5-C6
3	C	836[B]	C8E	C3-C4-C5-C6
2	A	807	EDO	O1-C1-C2-O2
2	A	813	EDO	O1-C1-C2-O2
3	C	836[A]	C8E	C3-C4-C5-C6
3	C	827	C8E	C1-C2-C3-C4
3	A	834	C8E	O15-C16-C17-O18
3	B	833	C8E	C3-C4-C5-C6
3	C	831	C8E	C3-C4-C5-C6
3	C	831	C8E	C4-C5-C6-C7
3	A	827	C8E	C10-C11-O12-C13
3	C	826	C8E	C17-C16-O15-C14
3	A	833	C8E	C3-C4-C5-C6
3	A	830	C8E	C13-C14-O15-C16
3	C	832	C8E	C10-C11-O12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	830	C8E	C17-C16-O15-C14
3	A	831	C8E	C1-C2-C3-C4
3	A	826	C8E	C10-C11-O12-C13
3	C	833	C8E	C14-C13-O12-C11
3	A	834	C8E	C6-C7-C8-O9
3	A	828	C8E	C2-C3-C4-C5
3	C	824	C8E	O15-C16-C17-O18
3	B	830	C8E	C1-C2-C3-C4
3	C	825	C8E	C11-C10-O9-C8
3	B	826	C8E	C17-C16-O15-C14
3	A	827	C8E	C14-C13-O12-C11
3	B	826	C8E	O12-C13-C14-O15
3	B	829	C8E	C1-C2-C3-C4
3	C	827	C8E	O12-C13-C14-O15
2	B	803	EDO	O1-C1-C2-O2
2	A	825	EDO	O1-C1-C2-O2
2	A	817	EDO	O1-C1-C2-O2
2	A	824	EDO	O1-C1-C2-O2
3	C	824	C8E	C13-C14-O15-C16
3	A	832	C8E	C6-C7-C8-O9
3	C	830	C8E	C2-C3-C4-C5
3	C	835	C8E	C5-C6-C7-C8
3	C	836[B]	C8E	C14-C13-O12-C11
3	C	836[B]	C8E	C17-C16-O15-C14
3	C	823	C8E	C5-C6-C7-C8
3	A	829	C8E	C7-C8-O9-C10
3	C	824	C8E	C1-C2-C3-C4
3	A	834	C8E	C14-C13-O12-C11
3	A	828	C8E	C10-C11-O12-C13
3	A	828	C8E	C13-C14-O15-C16
3	A	827	C8E	C7-C8-O9-C10
3	C	836[A]	C8E	C7-C8-O9-C10
3	A	826	C8E	C7-C8-O9-C10
2	A	814	EDO	O1-C1-C2-O2
2	B	820	EDO	O1-C1-C2-O2
2	A	822	EDO	O1-C1-C2-O2
2	C	817	EDO	O1-C1-C2-O2
2	A	819	EDO	O1-C1-C2-O2
2	B	819	EDO	O1-C1-C2-O2
3	C	825	C8E	C16-C17-O18-C19
3	C	836[B]	C8E	C20-C19-O18-C17
3	C	829	C8E	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	836[B]	C8E	C10-C11-O12-C13
3	B	825	C8E	C7-C8-O9-C10
3	A	834	C8E	C11-C10-O9-C8
3	C	828	C8E	C3-C4-C5-C6
3	C	832	C8E	O12-C13-C14-O15
3	B	827	C8E	C3-C4-C5-C6
3	B	829	C8E	C2-C3-C4-C5
2	C	803	EDO	O1-C1-C2-O2
3	C	828	C8E	C6-C7-C8-O9
3	C	835	C8E	C2-C3-C4-C5
3	A	834	C8E	C13-C14-O15-C16
3	C	831	C8E	C6-C7-C8-O9
3	C	827	C8E	C4-C5-C6-C7
3	A	832	C8E	C3-C4-C5-C6
3	B	826	C8E	O15-C16-C17-O18
3	B	828	C8E	C1-C2-C3-C4
3	B	833	C8E	C6-C7-C8-O9
3	C	826	C8E	C16-C17-O18-C19
3	C	829	C8E	O12-C13-C14-O15
2	A	803	EDO	O1-C1-C2-O2
2	A	815	EDO	O1-C1-C2-O2
3	C	826	C8E	C13-C14-O15-C16
3	A	834	C8E	C4-C5-C6-C7
3	C	826	C8E	O9-C10-C11-O12
3	C	828	C8E	C14-C13-O12-C11
3	A	830	C8E	C11-C10-O9-C8
3	C	832	C8E	C5-C6-C7-C8
2	A	818	EDO	O1-C1-C2-O2
2	B	807	EDO	O1-C1-C2-O2
2	A	821	EDO	O1-C1-C2-O2
2	C	809	EDO	O1-C1-C2-O2
2	B	823	EDO	O1-C1-C2-O2
3	C	836[B]	C8E	C11-C10-O9-C8
3	C	836[A]	C8E	C20-C19-O18-C17
3	B	829	C8E	C5-C6-C7-C8
3	C	834	C8E	C2-C3-C4-C5
3	A	828	C8E	O15-C16-C17-O18
3	C	826	C8E	O15-C16-C17-O18
3	C	828	C8E	O12-C13-C14-O15
3	B	826	C8E	C14-C13-O12-C11
3	A	836	C8E	C4-C5-C6-C7
3	A	828	C8E	O9-C10-C11-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	836[A]	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	A	830	C8E	O9-C10-C11-O12
3	B	827	C8E	C1-C2-C3-C4
3	C	828	C8E	O9-C10-C11-O12
3	A	826	C8E	C14-C13-O12-C11

There are no ring outliers.

31 monomers are involved in 80 short contacts:

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

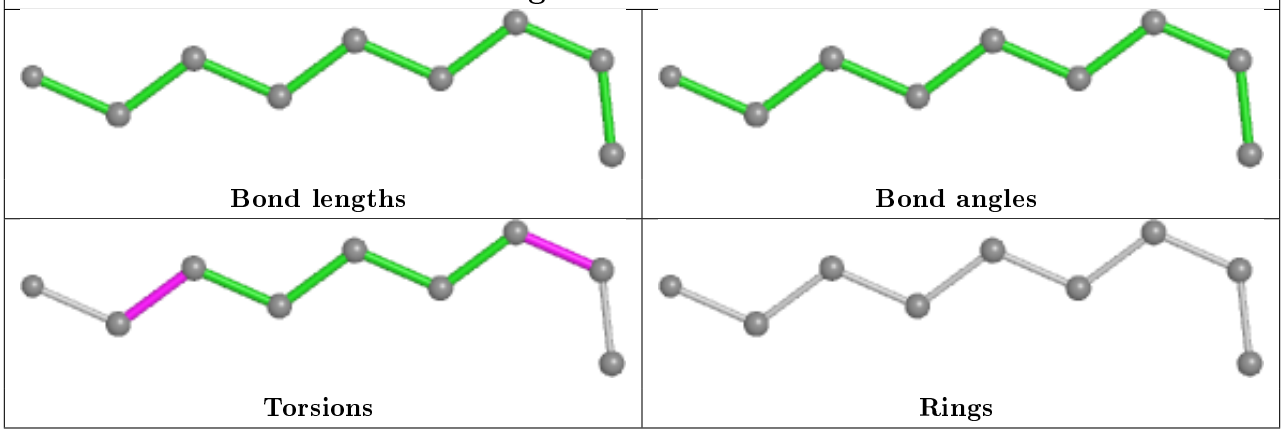
Continued on next page...

Continued from previous page...

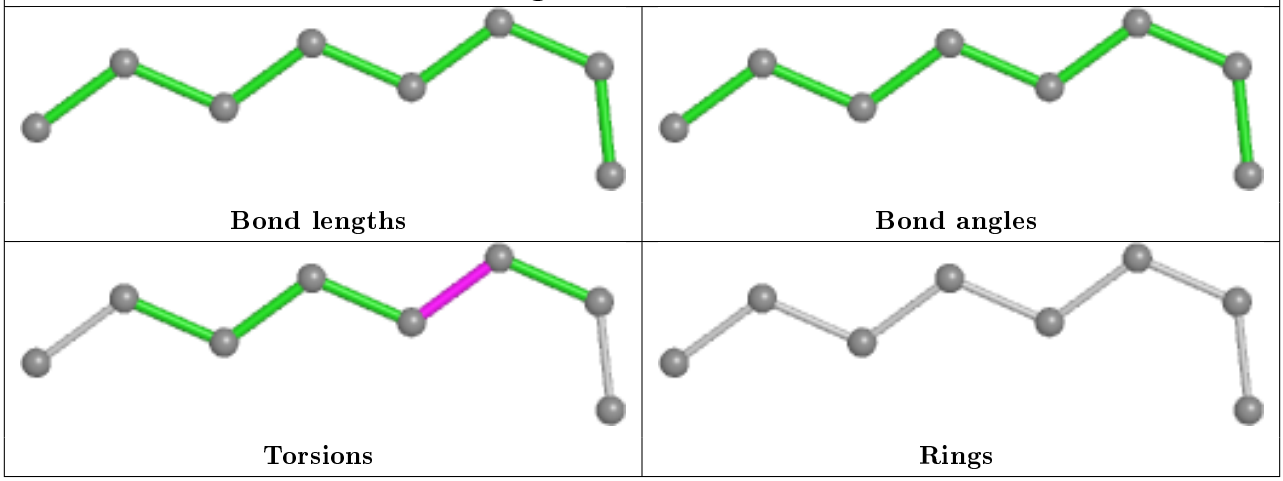
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	808	EDO	1	0
3	C	836[B]	C8E	22	0
3	B	825	C8E	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

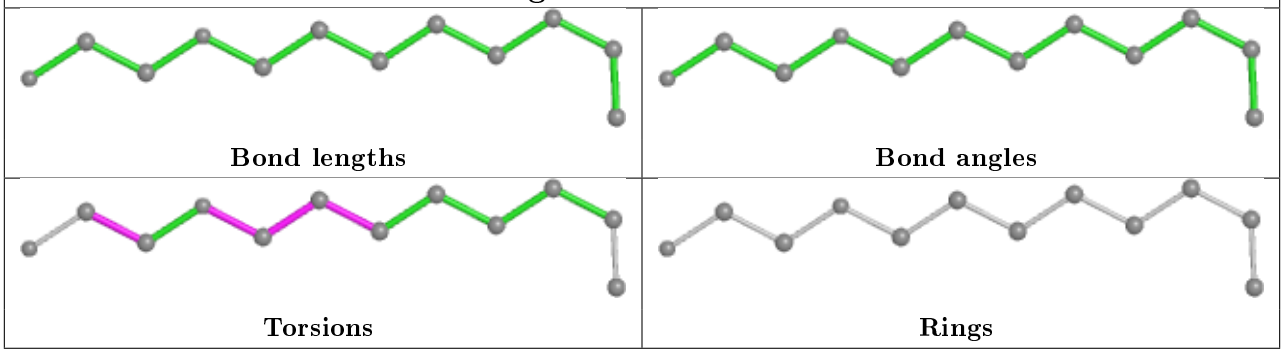
Ligand C8E A 831



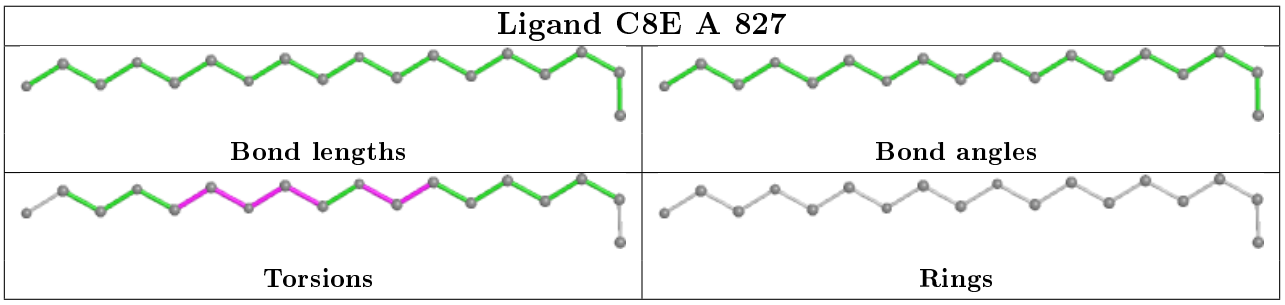
Ligand C8E C 830



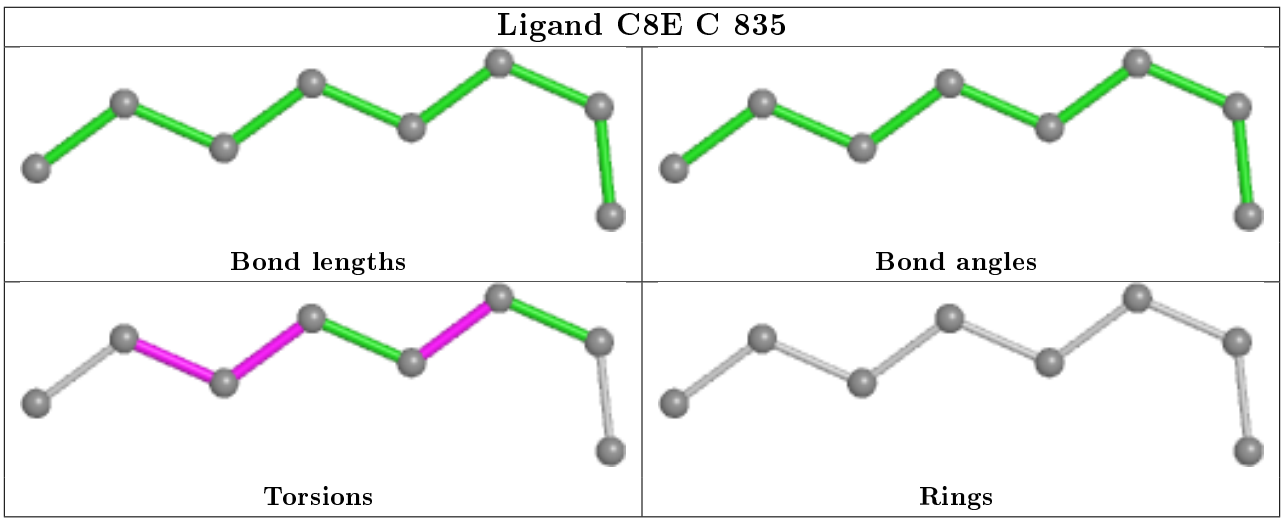
Ligand C8E A 829



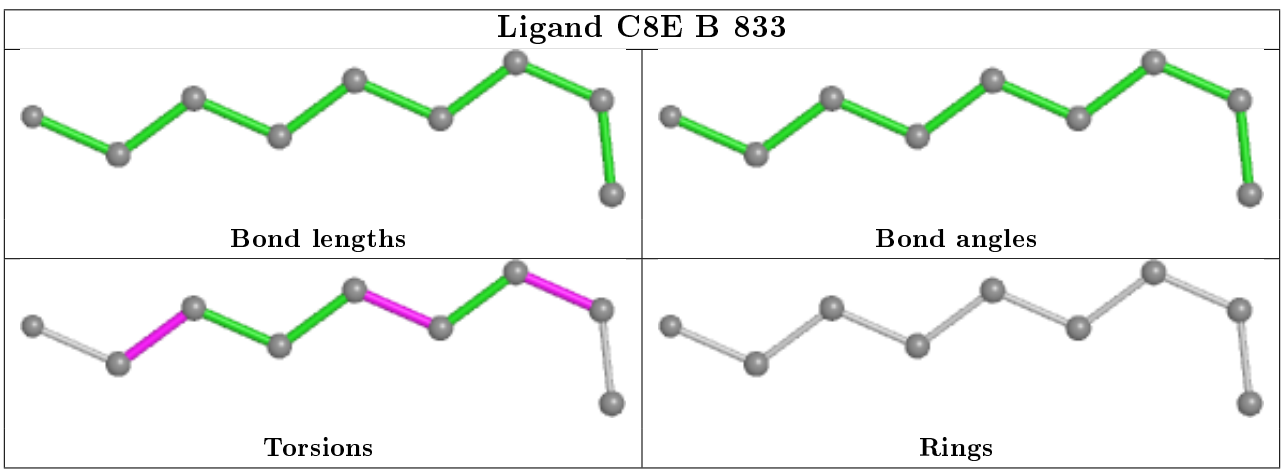
Ligand C8E A 827



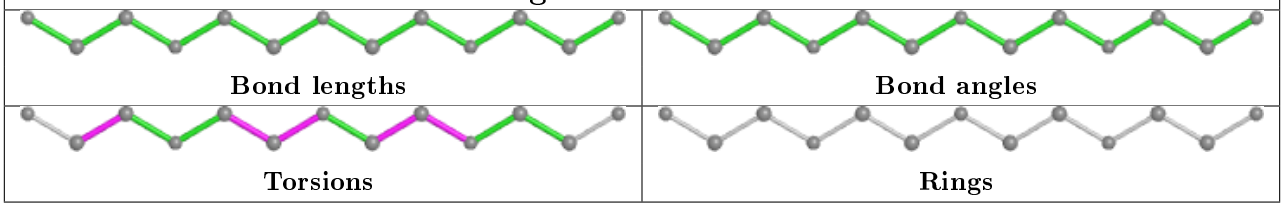
Ligand C8E C 835



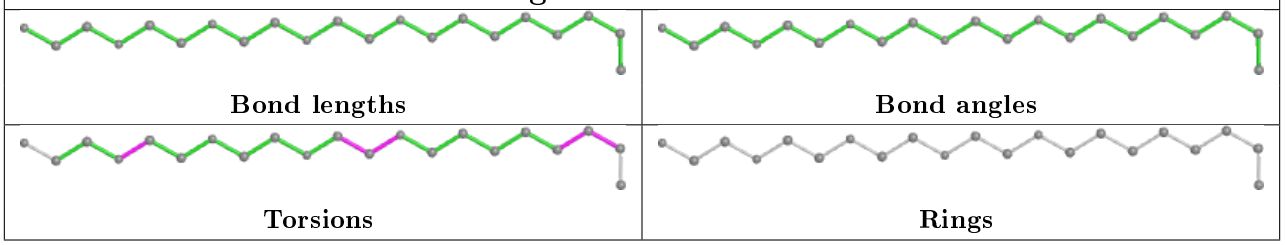
Ligand C8E B 833



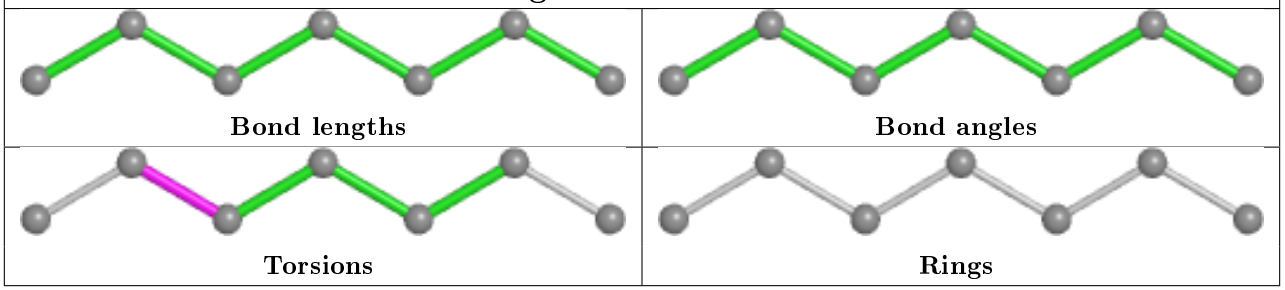
Ligand C8E B 826



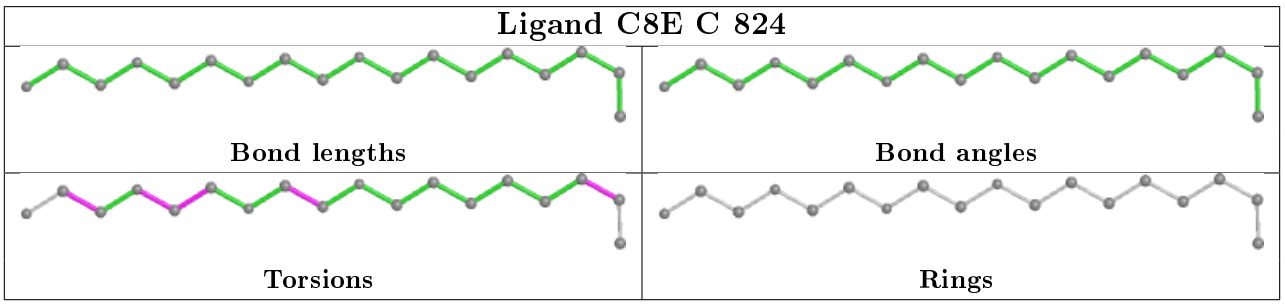
Ligand C8E C 825



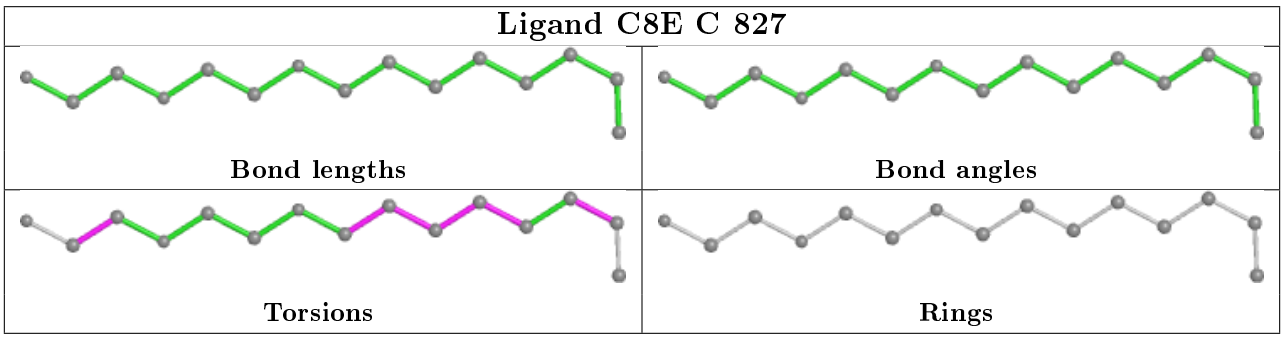
Ligand C8E B 831



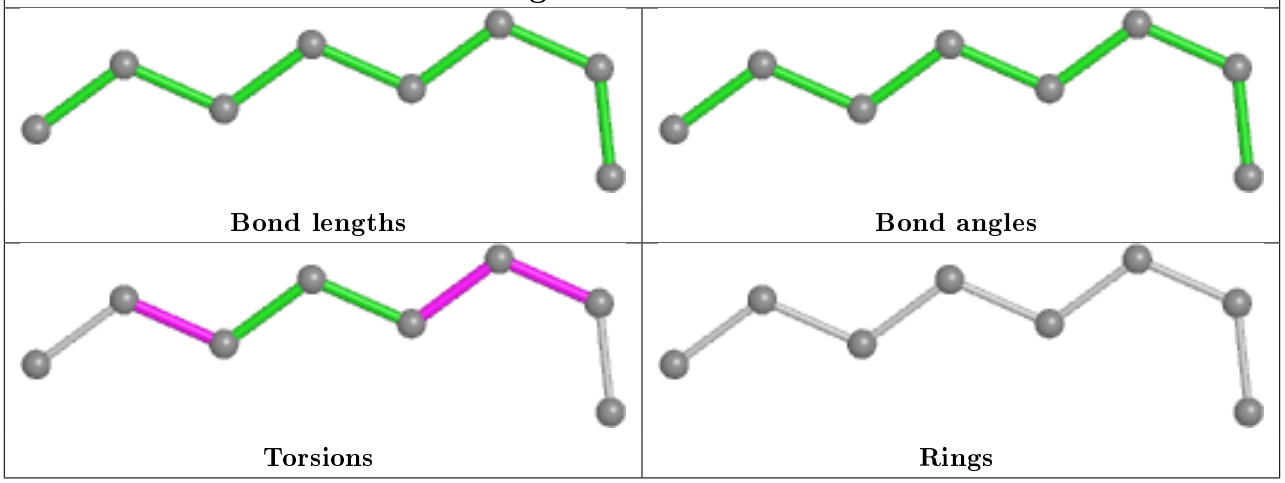
Ligand C8E C 824



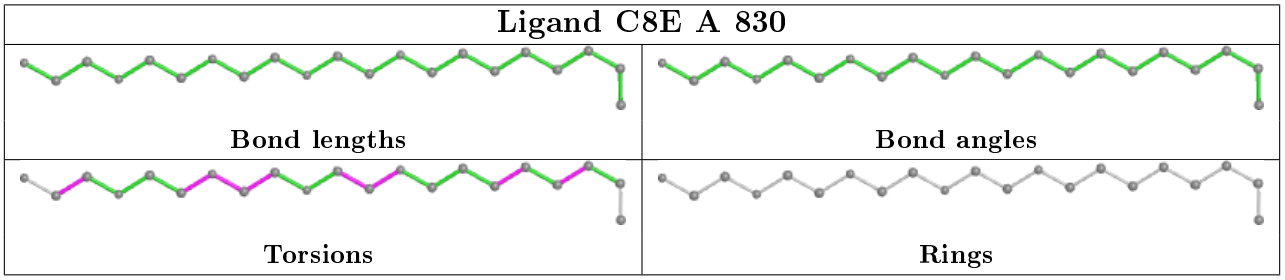
Ligand C8E C 827



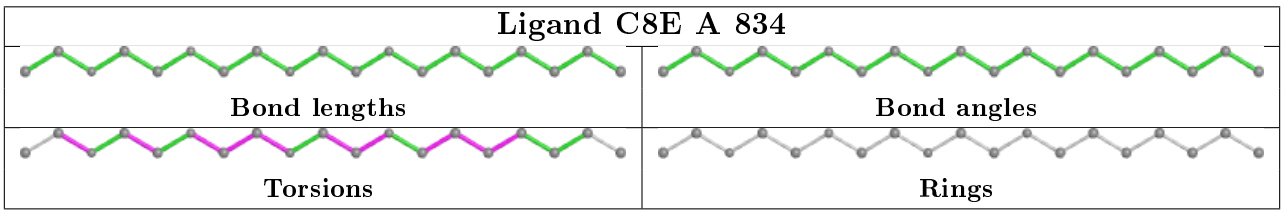
Ligand C8E B 828



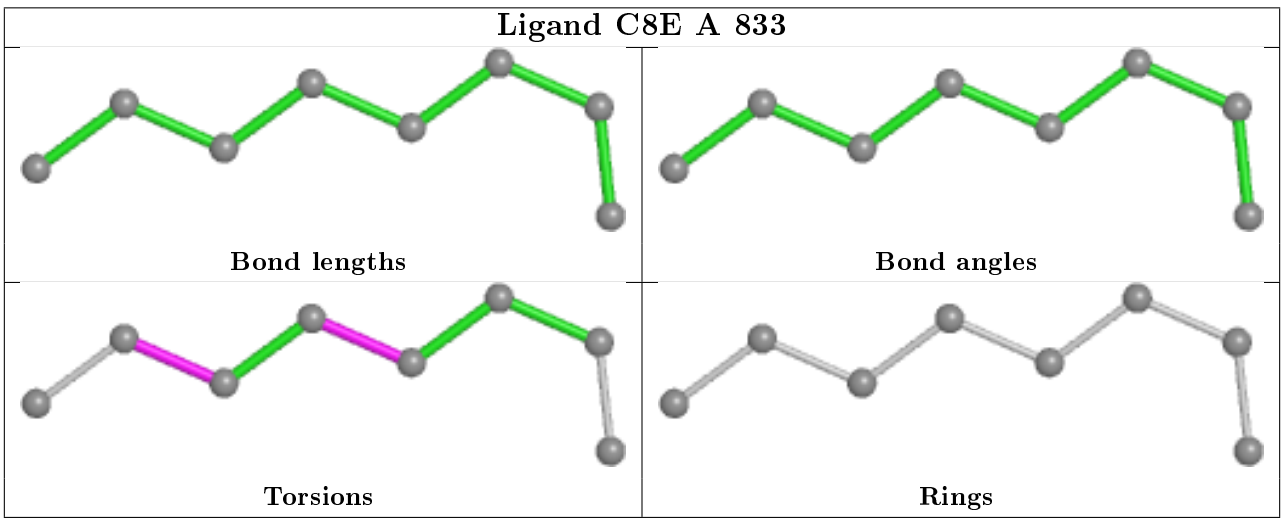
Ligand C8E A 830



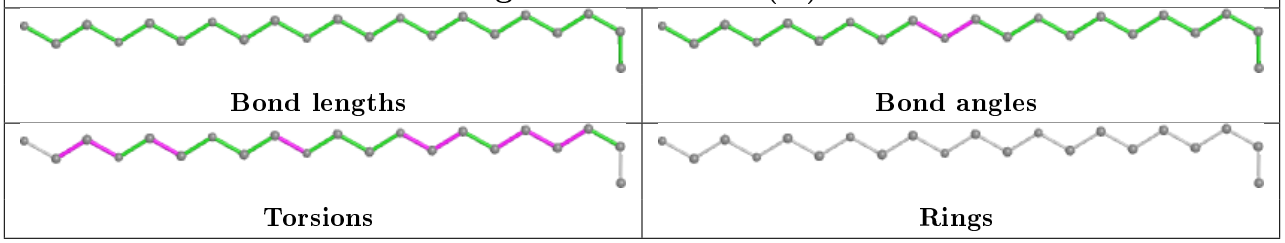
Ligand C8E A 834



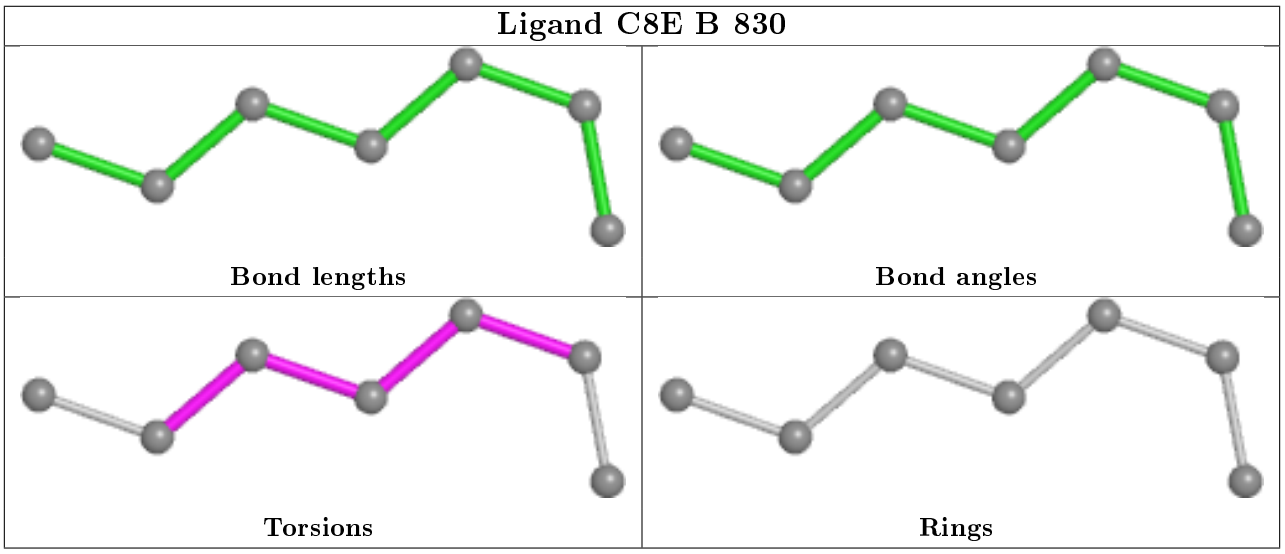
Ligand C8E A 833



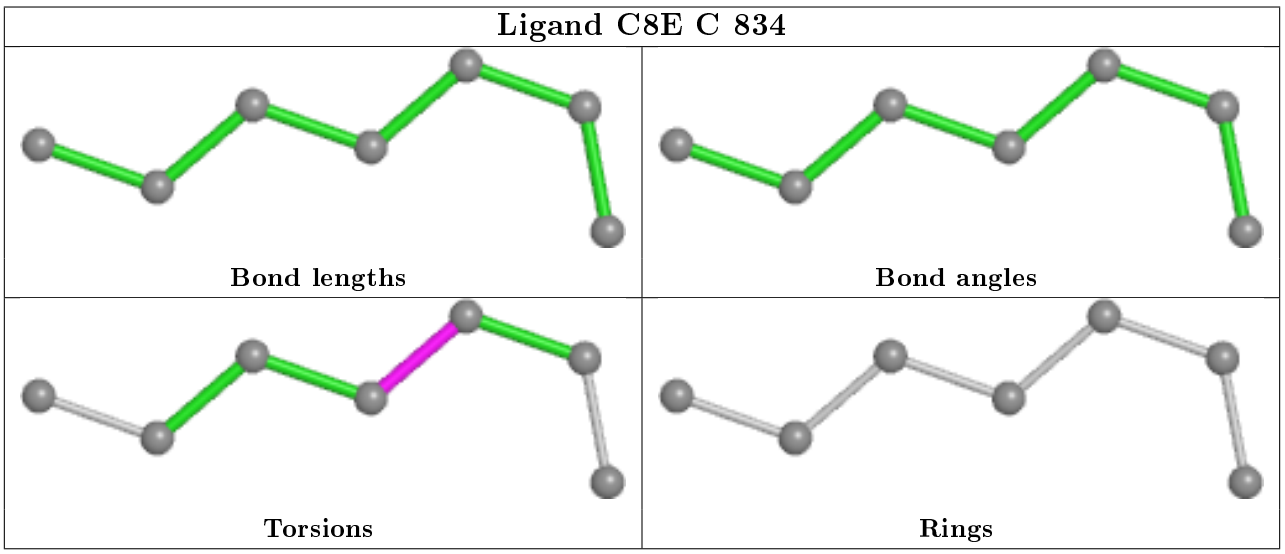
Ligand C8E C 836 (A)



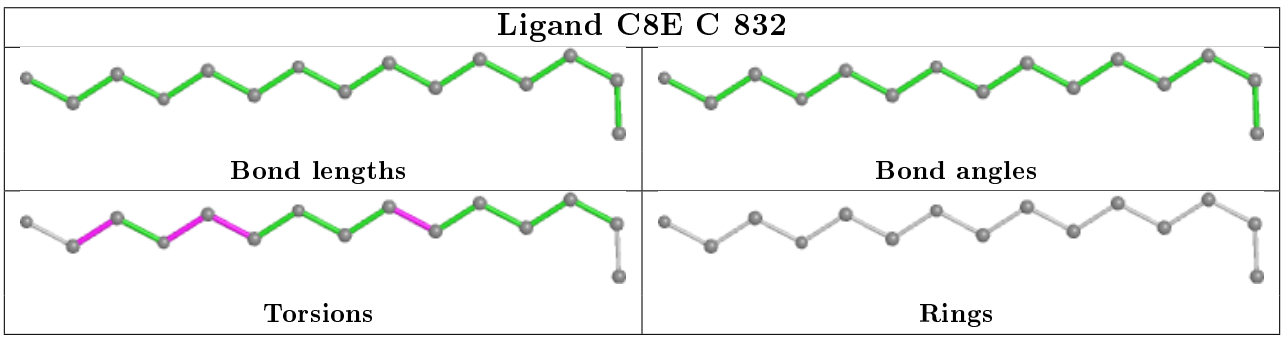
Ligand C8E B 830

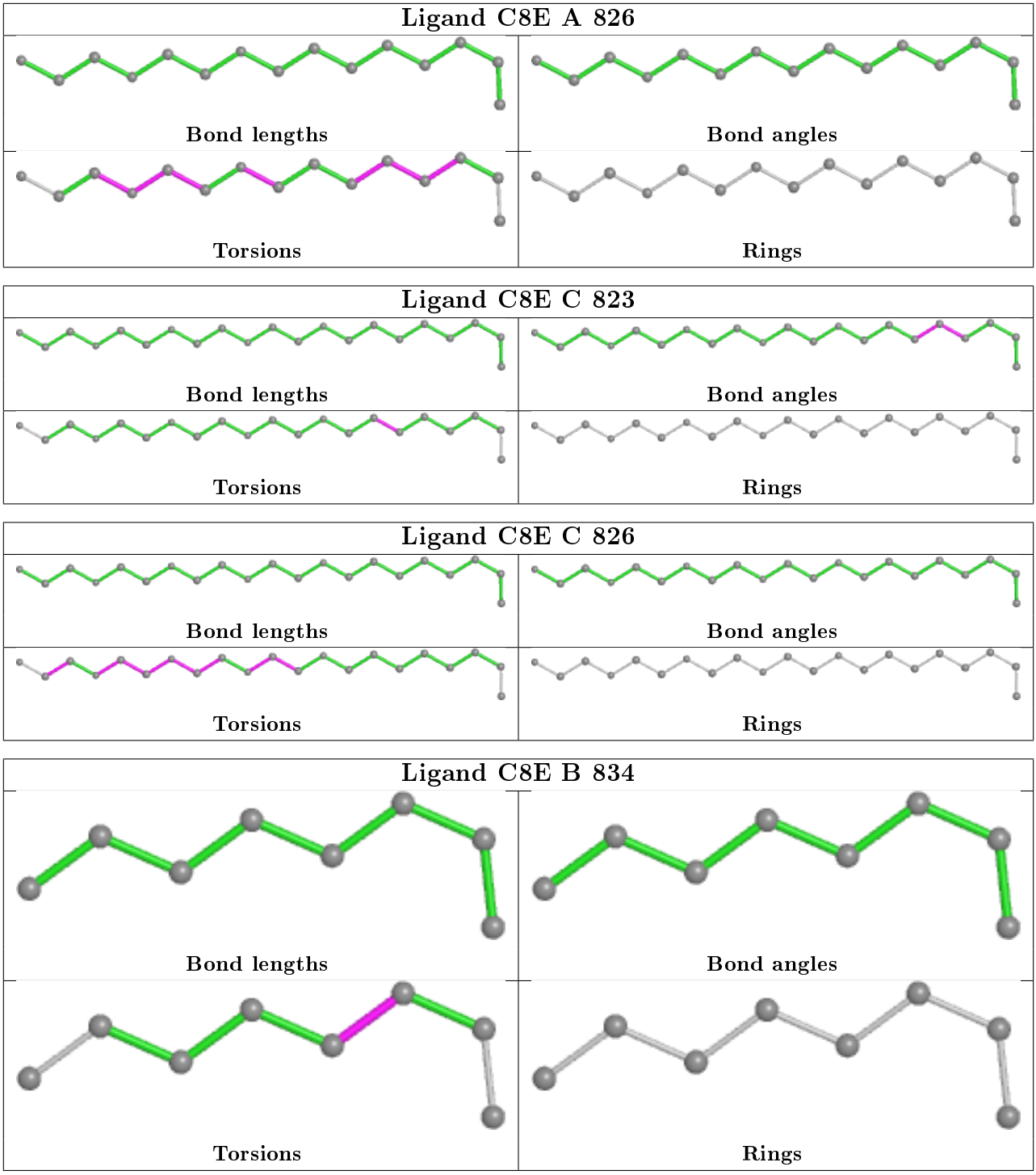


Ligand C8E C 834

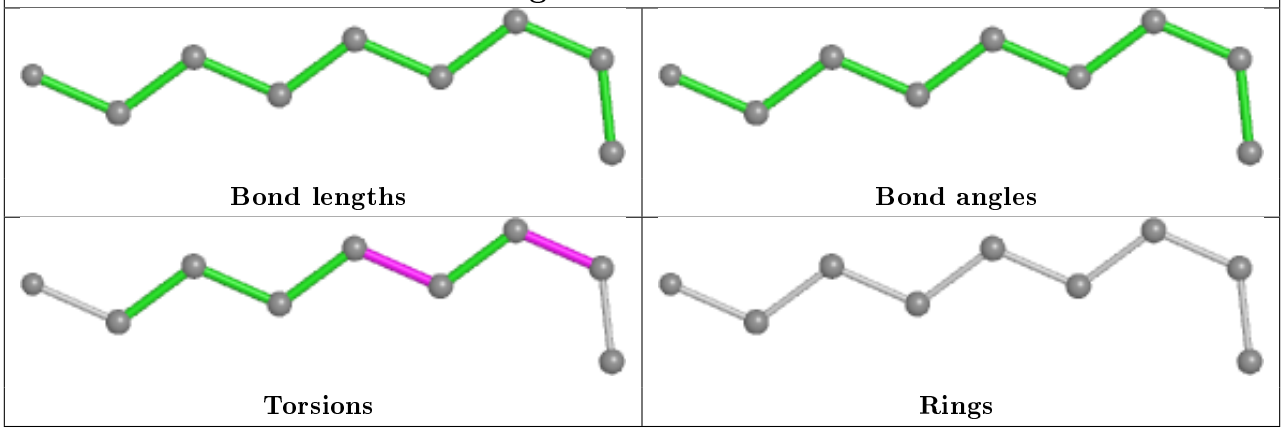


Ligand C8E C 832

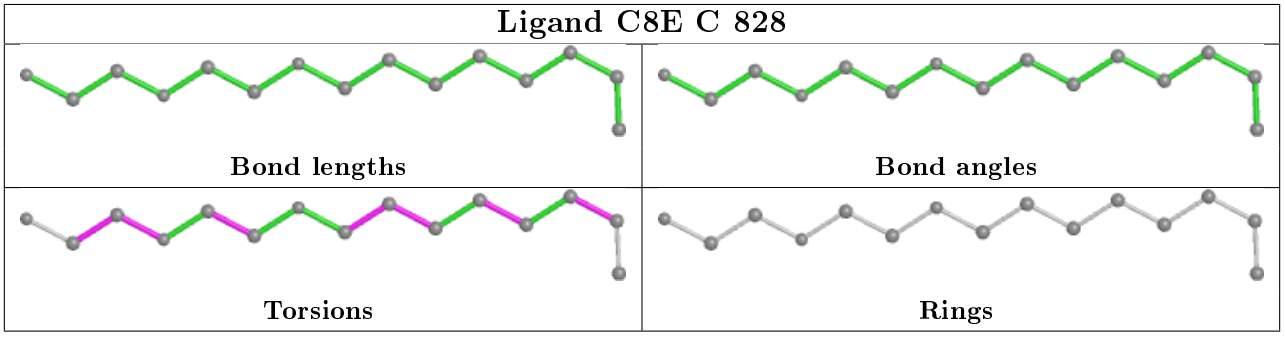



Ligand C8E A 826
Bond lengths
Bond angles
Torsions
Rings
Ligand C8E C 823
Bond lengths
Bond angles
Torsions
Rings
Ligand C8E C 826
Bond lengths
Bond angles
Torsions
Rings
Ligand C8E B 834
Bond lengths
Bond angles
Torsions
Rings

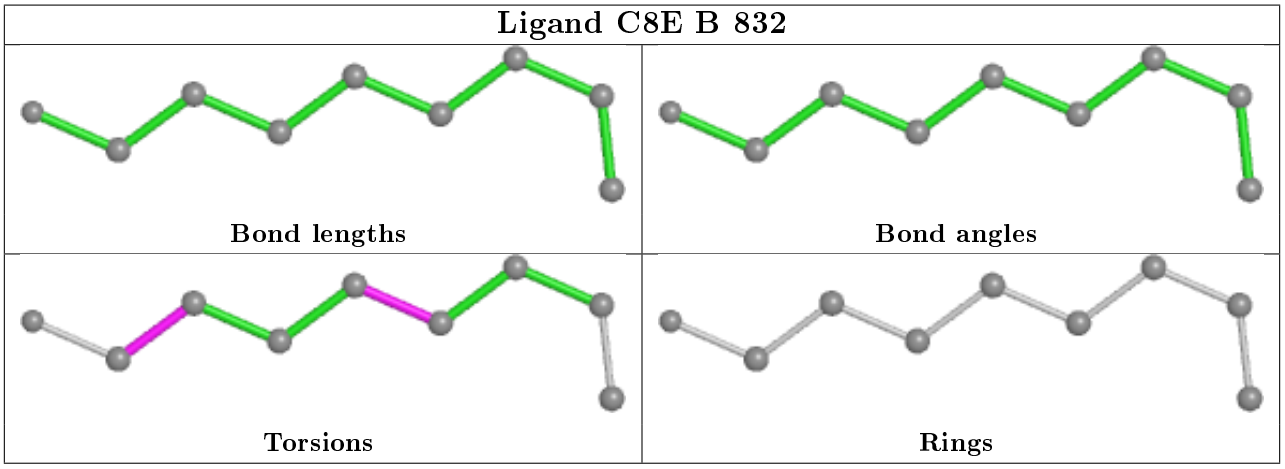
Ligand C8E B 827



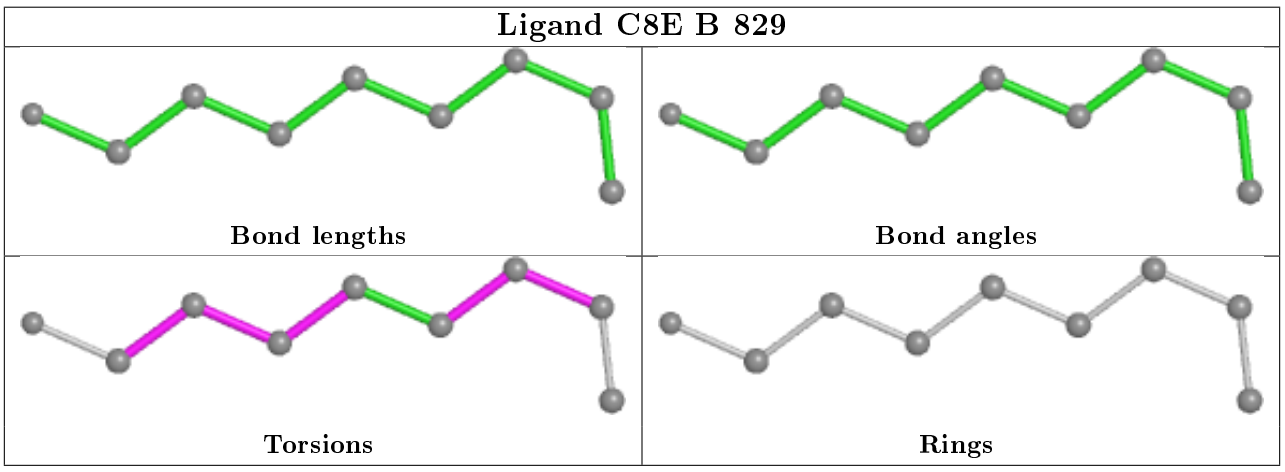
Ligand C8E C 828



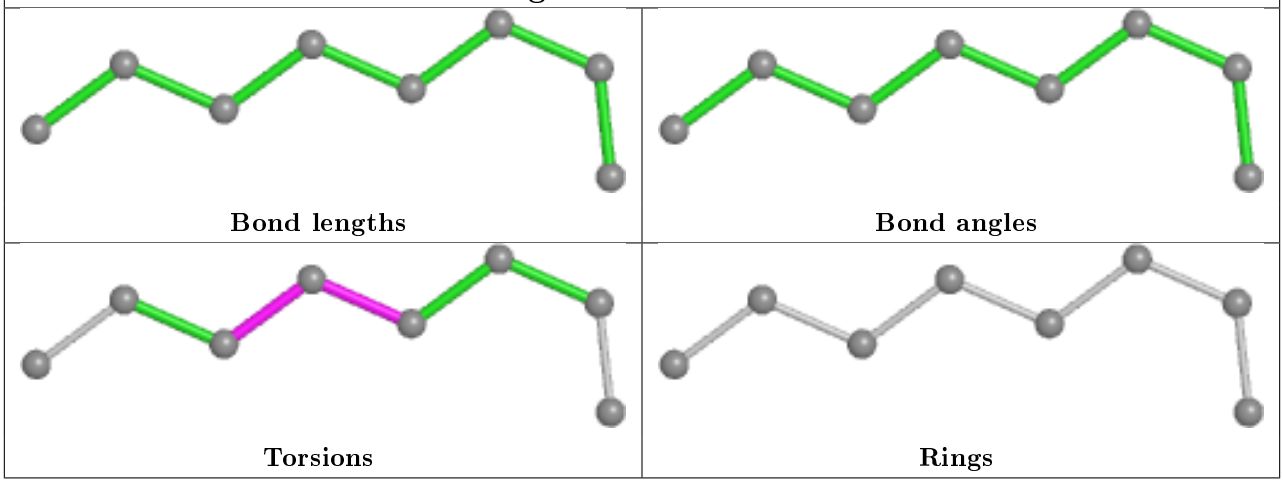
Ligand C8E B 832



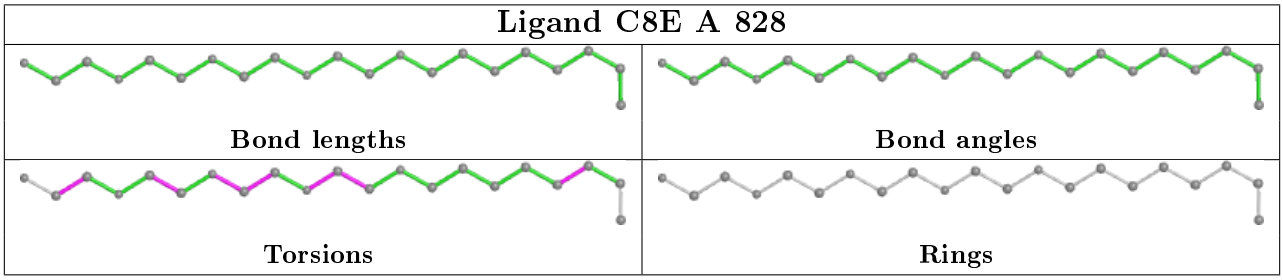
Ligand C8E B 829



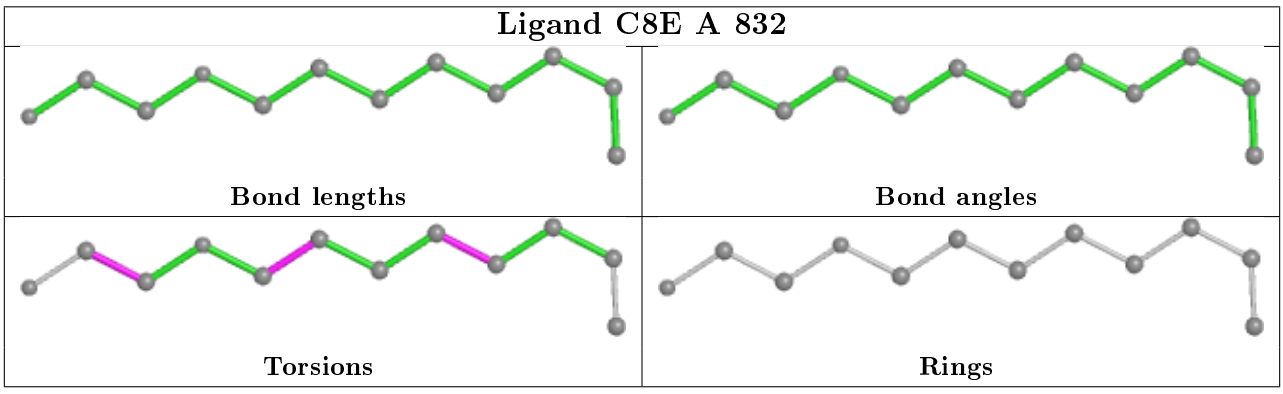
Ligand C8E A 835



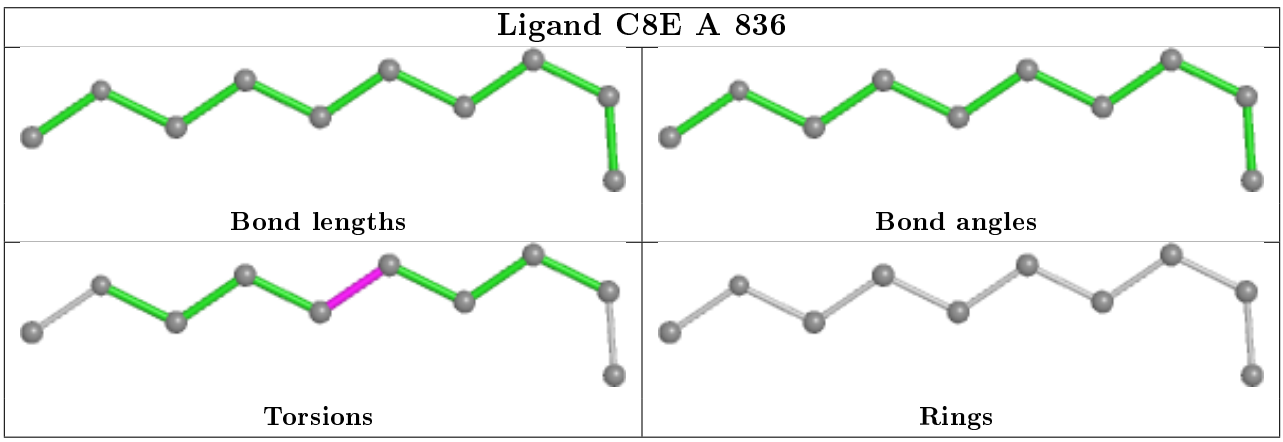
Ligand C8E A 828



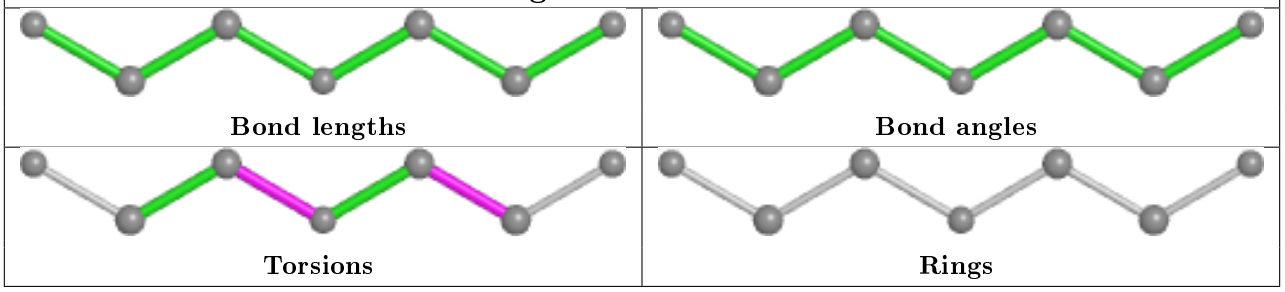
Ligand C8E A 832



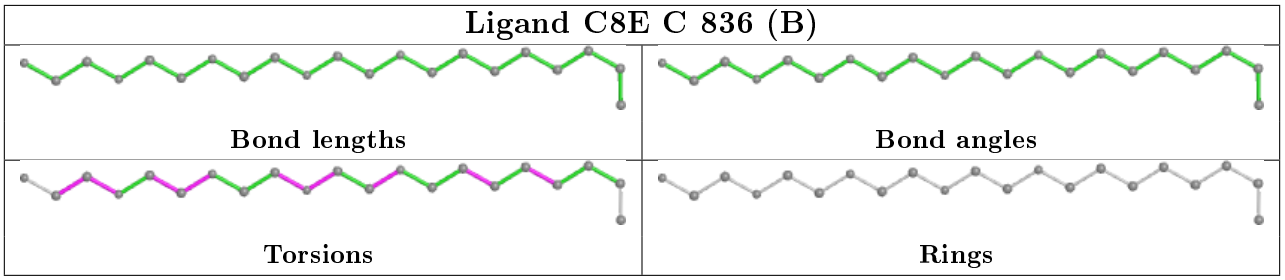
Ligand C8E A 836



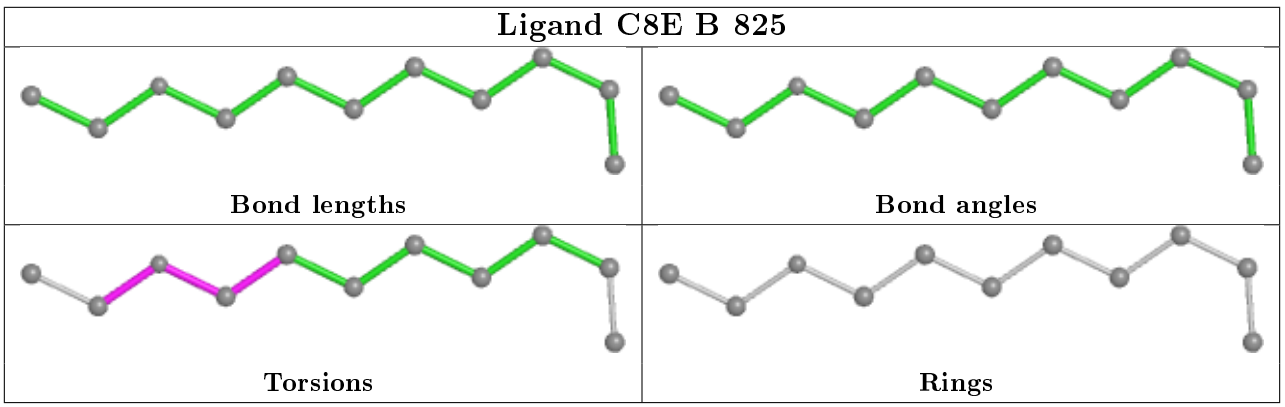
Ligand C8E C 833



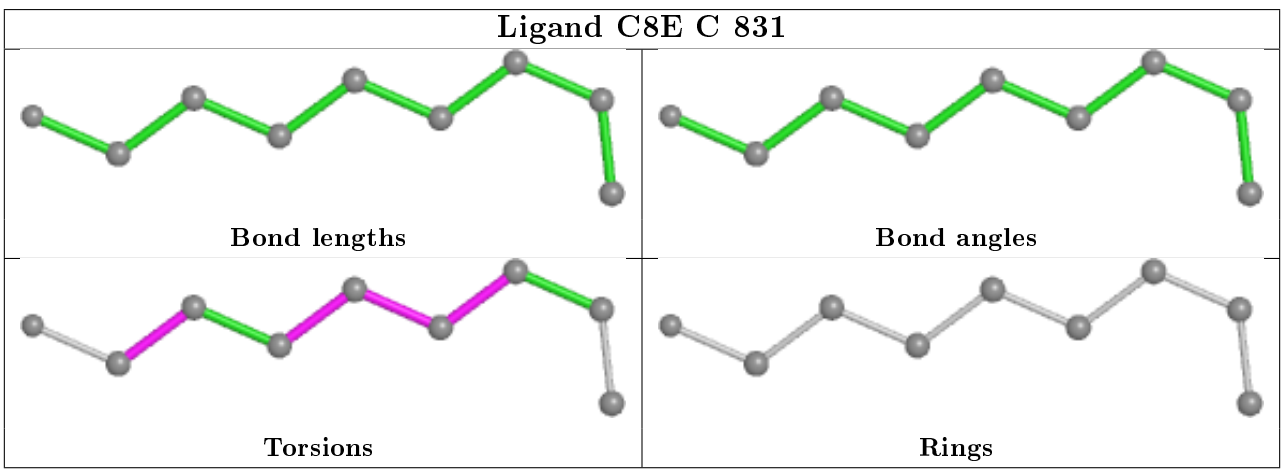
Ligand C8E C 836 (B)

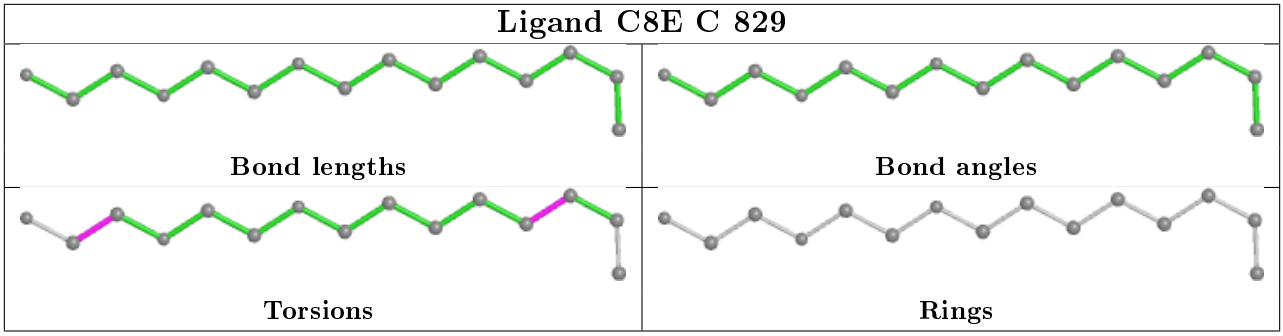


Ligand C8E B 825



Ligand C8E C 831





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.54	2 (0%) 94 93	23, 31, 51, 80	0
1	B	671/706 (95%)	-0.45	14 (2%) 63 62	23, 32, 55, 89	0
1	C	671/706 (95%)	-0.59	8 (1%) 79 79	21, 28, 46, 88	0
All	All	2013/2118 (95%)	-0.53	24 (1%) 79 79	21, 31, 52, 89	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	VAL	4.9
1	B	542	LEU	4.6
1	B	195	GLU	3.7
1	B	546	LEU	3.7
1	B	544	ASN	3.4
1	A	195	GLU	3.1
1	B	452	THR	3.0
1	B	545	ASN	2.9
1	B	618	GLN	2.8
1	B	541	LYS	2.7
1	C	618	GLN	2.6
1	B	196	ASN	2.5
1	B	199	PHE	2.5
1	A	196	ASN	2.3
1	C	544[A]	ASN	2.3
1	C	494[A]	THR	2.2
1	C	195	GLU	2.2
1	C	357	SER	2.2
1	C	356	GLY	2.1
1	C	355	THR	2.1
1	B	540	SER	2.1
1	B	233	GLU	2.1
1	B	230	TRP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	612[A]	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	C8E	A	836	10/21	0.68	0.20	58,64,70,76	0
3	C8E	A	834	19/21	0.72	0.34	64,82,100,105	0
3	C8E	B	826	13/21	0.74	0.21	58,70,89,94	0
2	EDO	A	824	4/4	0.78	0.20	59,71,72,75	0
2	EDO	B	808	4/4	0.81	0.14	44,53,53,54	0
3	C8E	B	833	9/21	0.81	0.19	52,61,66,68	0
3	C8E	C	833	7/21	0.81	0.12	55,57,70,74	0
3	C8E	C	832	15/21	0.82	0.18	46,66,74,75	0
3	C8E	B	834	8/21	0.83	0.24	41,55,63,67	0
3	C8E	A	830	21/21	0.83	0.21	52,63,75,92	0
2	EDO	C	817	4/4	0.84	0.19	37,55,64,71	0
3	C8E	C	834	7/21	0.84	0.12	56,60,64,65	0
2	EDO	A	808	4/4	0.84	0.13	37,39,46,51	0
2	EDO	B	818	4/4	0.84	0.14	38,64,70,73	0
3	C8E	A	828	21/21	0.85	0.14	53,70,77,83	0
3	C8E	C	836[A]	21/21	0.85	0.20	30,47,60,66	21
2	EDO	C	814	4/4	0.85	0.18	51,57,63,65	0
3	C8E	A	827	18/21	0.85	0.15	38,54,79,87	0
3	C8E	C	836[B]	21/21	0.85	0.20	30,42,53,59	21
3	C8E	B	825	11/21	0.85	0.16	40,55,61,64	0
3	C8E	C	826	21/21	0.86	0.16	39,60,106,112	0
3	C8E	C	830	8/21	0.86	0.21	51,54,60,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	818	4/4	0.86	0.15	37,48,51,52	0
3	C8E	C	831	9/21	0.86	0.15	56,62,67,70	0
3	C8E	A	832	12/21	0.87	0.15	52,64,69,76	0
3	C8E	A	831	9/21	0.88	0.21	57,61,82,106	0
3	C8E	C	835	8/21	0.88	0.15	48,51,67,72	0
2	EDO	A	806	4/4	0.88	0.14	38,44,49,52	0
2	EDO	B	819	4/4	0.88	0.28	47,65,66,74	0
3	C8E	A	829	12/21	0.88	0.15	47,54,67,71	0
2	EDO	C	808	4/4	0.89	0.13	39,45,49,63	0
3	C8E	B	830	7/21	0.89	0.12	48,53,59,62	0
4	PO4	B	835	5/5	0.89	0.17	60,73,80,89	0
3	C8E	C	825	21/21	0.89	0.19	34,66,122,127	0
2	EDO	B	816	4/4	0.89	0.10	61,67,70,72	0
2	EDO	B	820	4/4	0.90	0.11	42,45,47,50	0
3	C8E	C	823	21/21	0.90	0.15	38,42,73,84	0
2	EDO	A	810	4/4	0.90	0.18	57,62,68,79	0
2	EDO	A	822	4/4	0.90	0.20	32,33,60,61	0
2	EDO	B	811	4/4	0.90	0.12	51,58,62,69	0
3	C8E	C	828	15/21	0.90	0.16	43,67,78,79	0
2	EDO	A	819	4/4	0.90	0.12	65,66,67,67	0
2	EDO	B	810	4/4	0.90	0.11	50,55,55,70	0
2	EDO	C	803	4/4	0.90	0.18	48,51,65,66	0
2	EDO	A	820	4/4	0.90	0.21	49,62,71,72	0
2	EDO	A	823	4/4	0.91	0.19	32,44,49,55	0
3	C8E	B	832	9/21	0.91	0.12	56,61,71,73	0
3	C8E	B	828	8/21	0.91	0.21	41,49,68,69	0
2	EDO	B	823	4/4	0.91	0.18	49,55,55,73	0
2	EDO	B	813	4/4	0.92	0.13	64,70,73,78	0
2	EDO	A	815	4/4	0.92	0.16	50,59,62,69	0
2	EDO	C	806	4/4	0.92	0.13	37,47,49,53	0
3	C8E	C	824	18/21	0.92	0.12	35,53,66,71	0
3	C8E	B	827	9/21	0.92	0.10	57,61,75,86	0
2	EDO	C	804	4/4	0.92	0.13	31,35,36,38	0
2	EDO	C	820	4/4	0.92	0.13	35,44,52,57	0
2	EDO	C	811	4/4	0.92	0.14	40,41,49,58	0
2	EDO	B	809	4/4	0.92	0.12	42,47,48,55	0
2	EDO	A	812	4/4	0.92	0.21	62,64,66,68	0
3	C8E	C	827	15/21	0.92	0.14	40,60,69,74	0
2	EDO	C	807	4/4	0.92	0.13	43,48,54,66	0
3	C8E	C	829	15/21	0.92	0.13	47,53,77,87	0
3	C8E	B	829	9/21	0.93	0.14	50,63,68,72	0
3	C8E	B	831	7/21	0.93	0.24	44,48,54,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C8E	A	835	8/21	0.93	0.17	56,62,69,70	0
2	EDO	C	809	4/4	0.93	0.10	32,37,40,44	0
2	EDO	B	814	4/4	0.93	0.20	59,61,62,73	0
2	EDO	B	821	4/4	0.93	0.10	52,53,53,64	0
2	EDO	B	805	4/4	0.94	0.08	31,38,39,45	0
2	EDO	C	822	4/4	0.94	0.21	42,54,54,55	0
2	EDO	B	807	4/4	0.94	0.10	36,37,38,40	0
2	EDO	A	814	4/4	0.94	0.37	56,63,63,82	0
2	EDO	B	815	4/4	0.94	0.15	48,50,54,57	0
2	EDO	A	809	4/4	0.94	0.20	44,48,51,61	0
2	EDO	A	801	4/4	0.94	0.08	35,38,38,46	0
3	C8E	A	826	15/21	0.94	0.14	42,53,78,81	0
2	EDO	A	818	4/4	0.94	0.13	40,42,46,48	0
2	EDO	C	802	4/4	0.94	0.10	35,45,46,51	0
2	EDO	B	812	4/4	0.94	0.17	39,48,50,51	0
2	EDO	B	806	4/4	0.94	0.18	34,52,58,61	0
3	C8E	A	833	8/21	0.94	0.20	45,50,53,55	0
2	EDO	A	803	4/4	0.95	0.13	58,60,60,61	0
2	EDO	A	811	4/4	0.95	0.09	47,49,54,69	0
2	EDO	A	813	4/4	0.95	0.17	60,62,75,90	0
2	EDO	B	817	4/4	0.95	0.10	24,24,28,35	0
2	EDO	A	802	4/4	0.95	0.10	38,38,41,49	0
2	EDO	C	812	4/4	0.95	0.10	53,55,63,69	0
2	EDO	B	822	4/4	0.95	0.09	36,42,46,46	0
2	EDO	C	815	4/4	0.95	0.08	33,40,43,43	0
2	EDO	A	805	4/4	0.95	0.09	34,40,42,45	0
2	EDO	A	817	4/4	0.95	0.10	51,53,60,68	0
2	EDO	B	803	4/4	0.95	0.08	49,49,53,66	0
2	EDO	C	821	4/4	0.96	0.13	30,41,44,47	0
2	EDO	B	804	4/4	0.96	0.10	38,55,59,68	0
2	EDO	B	802	4/4	0.96	0.10	32,41,49,70	0
2	EDO	B	824	4/4	0.96	0.16	33,40,44,48	0
2	EDO	C	816	4/4	0.96	0.11	29,39,39,45	0
2	EDO	A	825	4/4	0.97	0.09	35,54,60,62	0
2	EDO	A	816	4/4	0.97	0.06	40,43,45,51	0
2	EDO	C	813	4/4	0.97	0.09	26,43,44,44	0
2	EDO	C	810	4/4	0.97	0.09	42,48,56,66	0
2	EDO	A	821	4/4	0.97	0.11	30,47,55,57	0
2	EDO	C	819	4/4	0.97	0.08	22,23,27,28	0
2	EDO	A	807	4/4	0.97	0.12	44,47,50,59	0
2	EDO	A	804	4/4	0.97	0.09	31,37,41,47	0
2	EDO	B	801	4/4	0.98	0.06	36,36,38,40	0

Continued on next page...

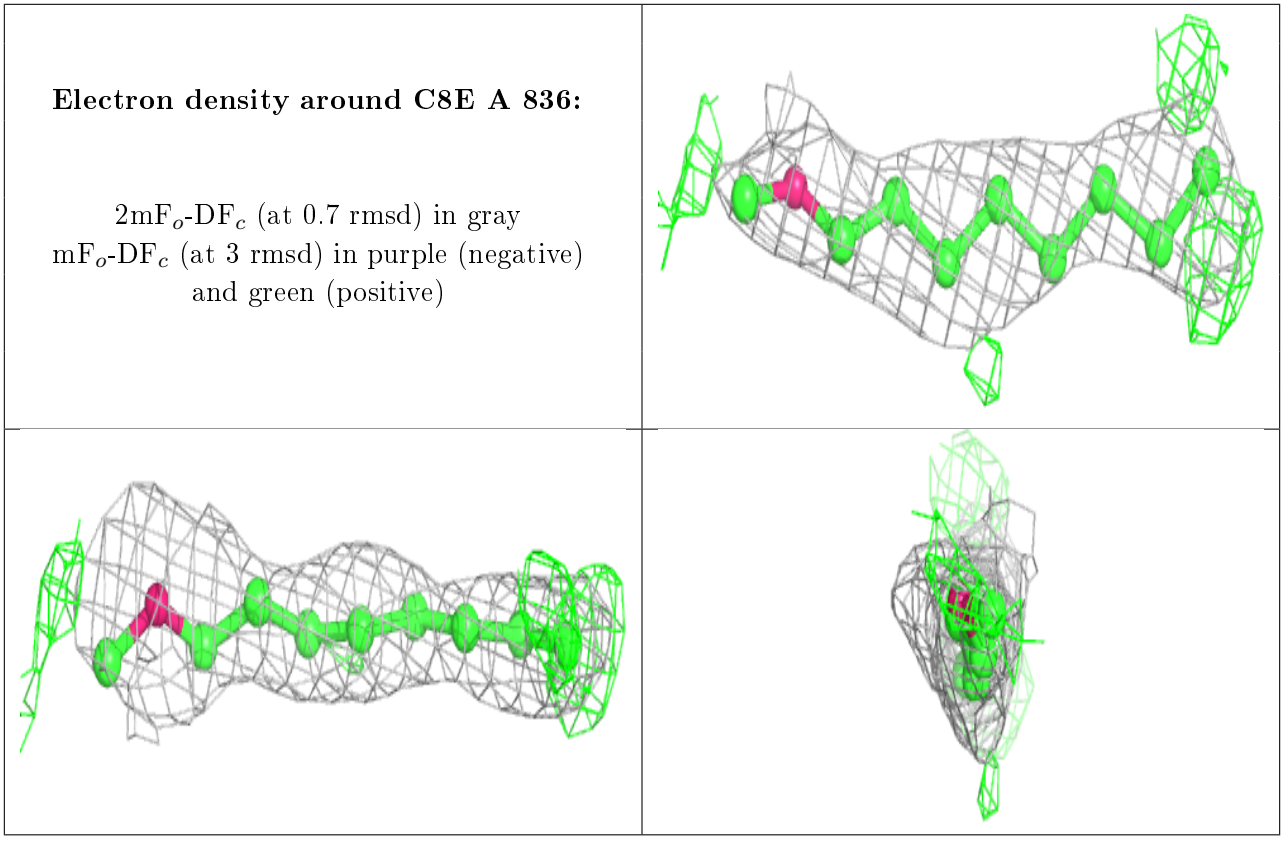
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	801	4/4	0.98	0.09	29,32,48,49	0
2	EDO	C	805	4/4	0.99	0.09	31,31,32,35	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.

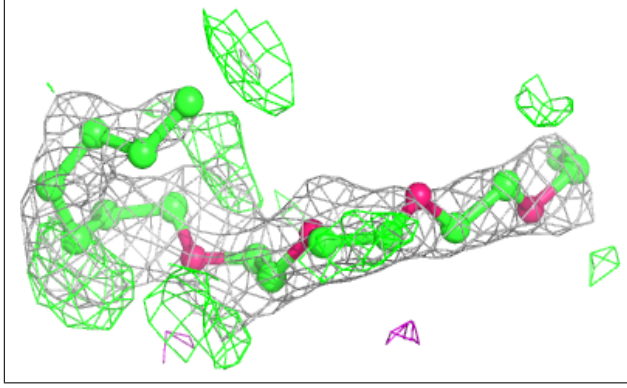
Electron density around C8E A 836:

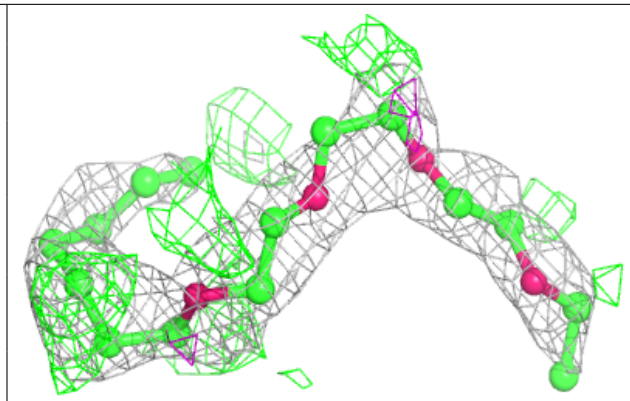
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

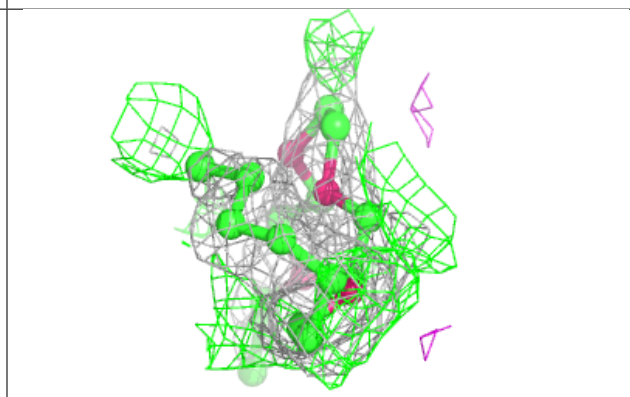


Electron density around C8E A 834:

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

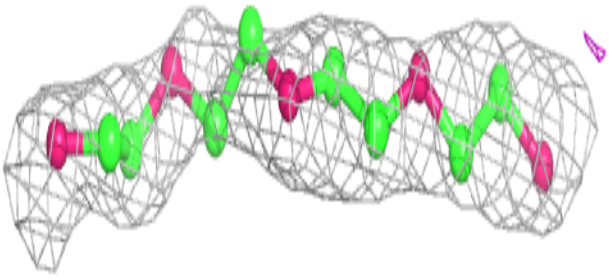


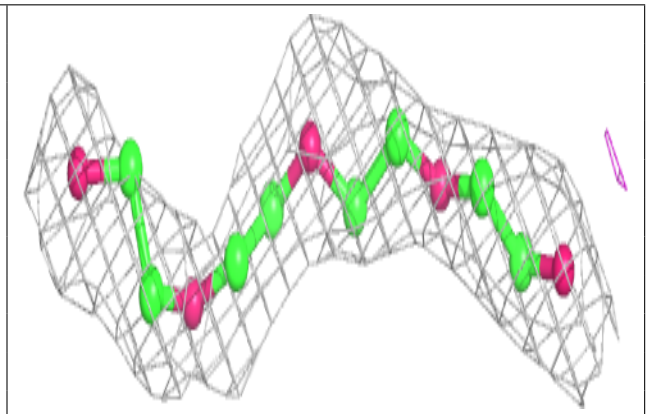


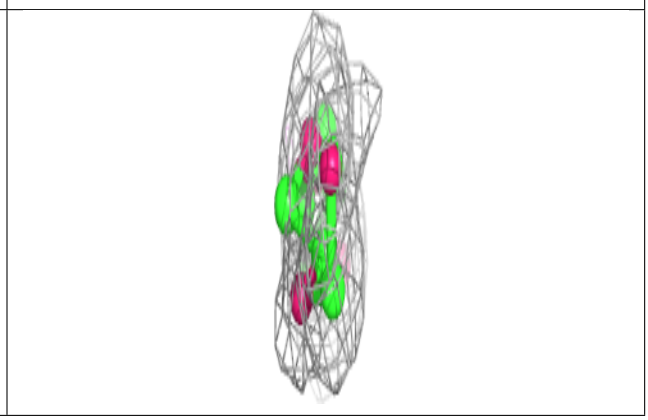


Electron density around C8E B 826:

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

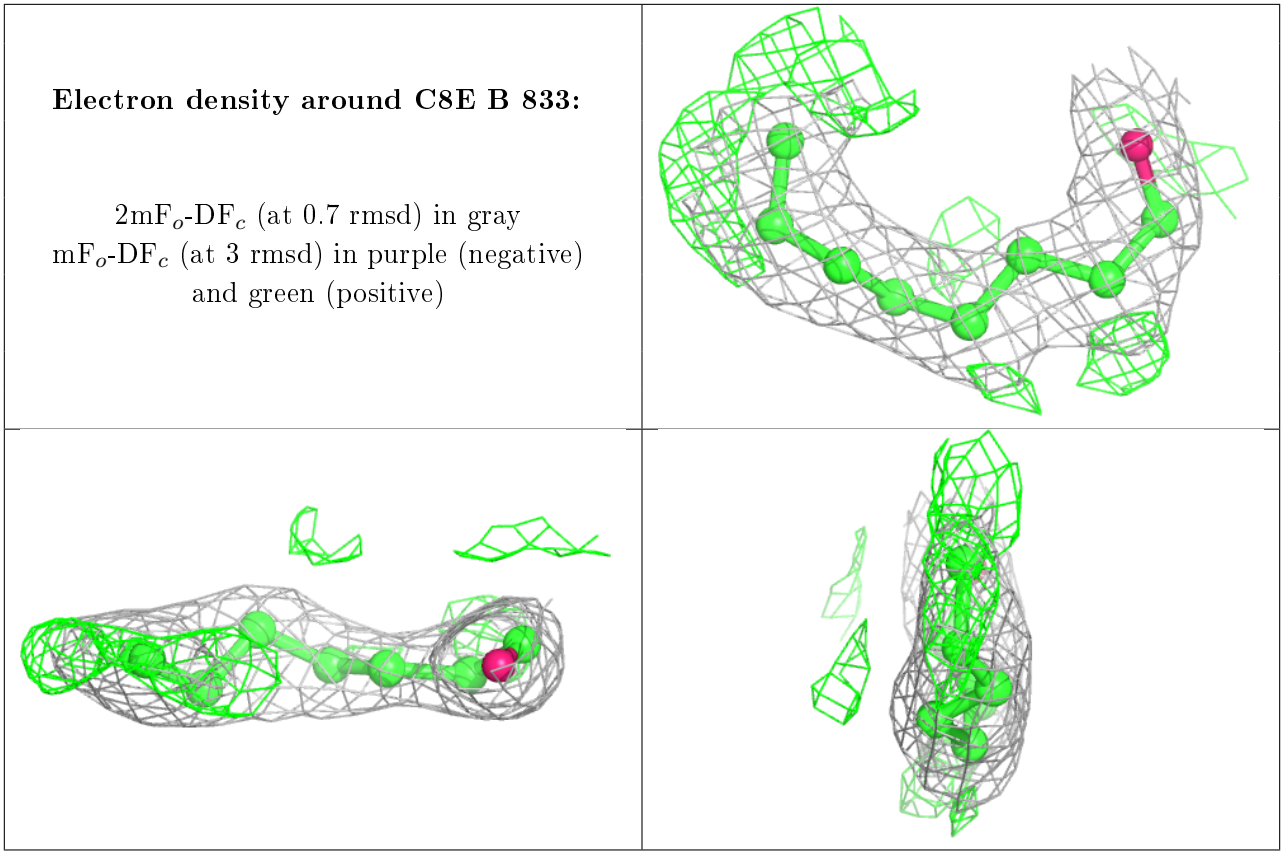






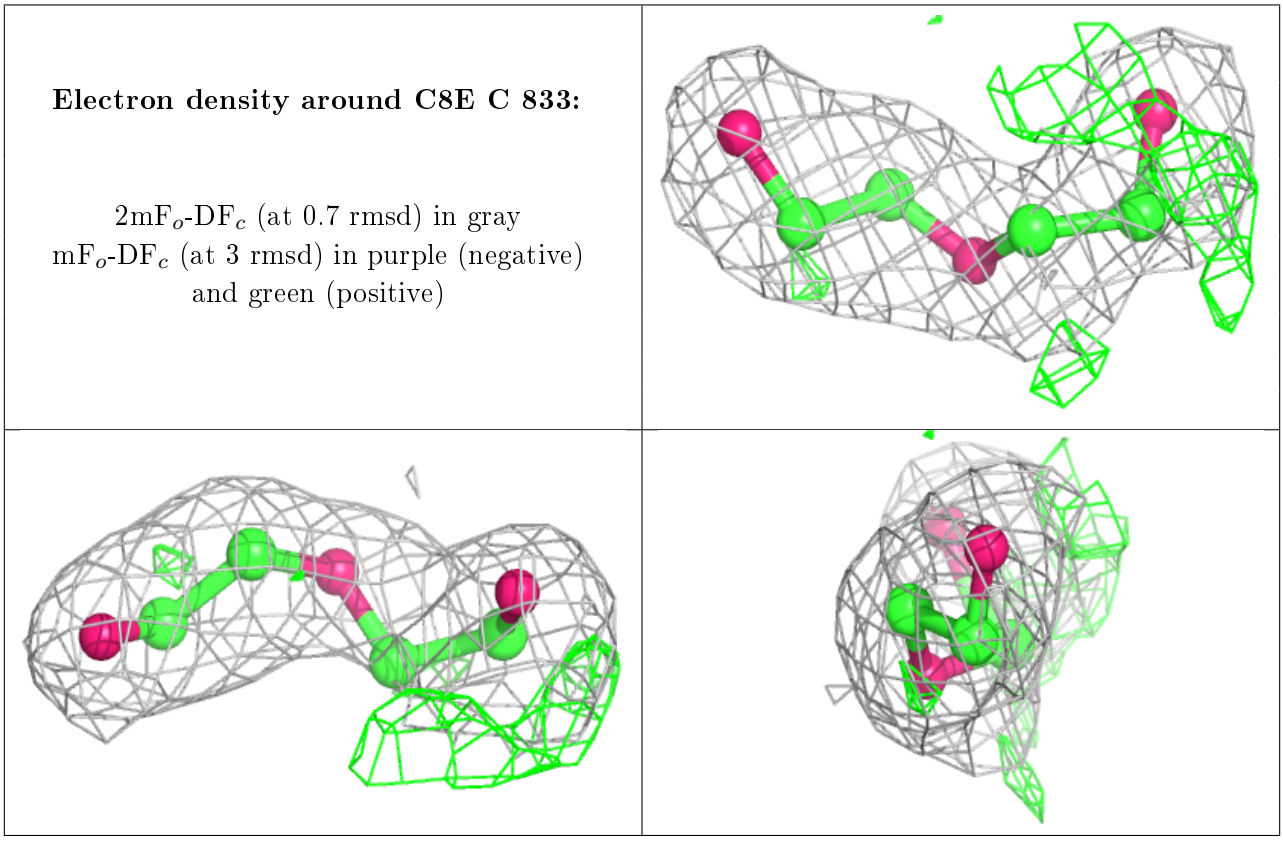
Electron density around C8E B 833:

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



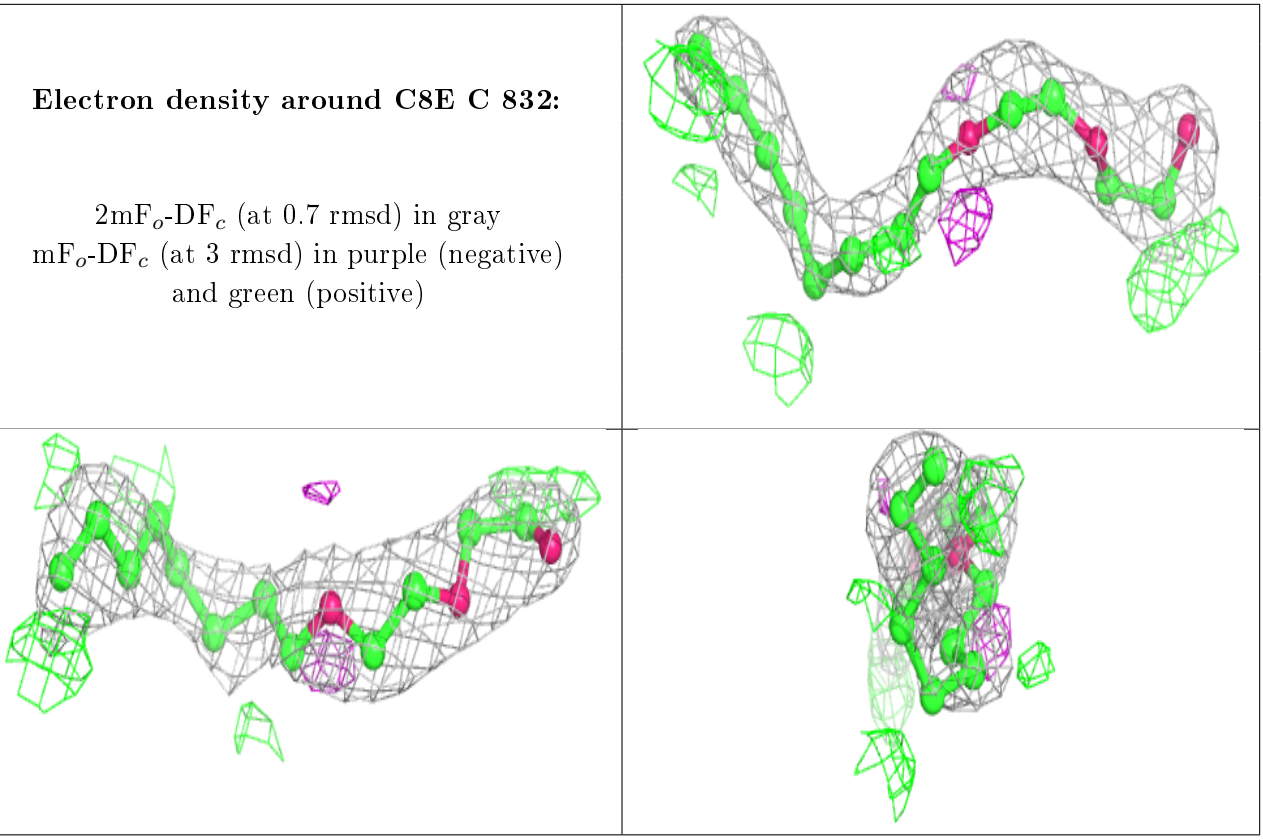
Electron density around C8E C 833:

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



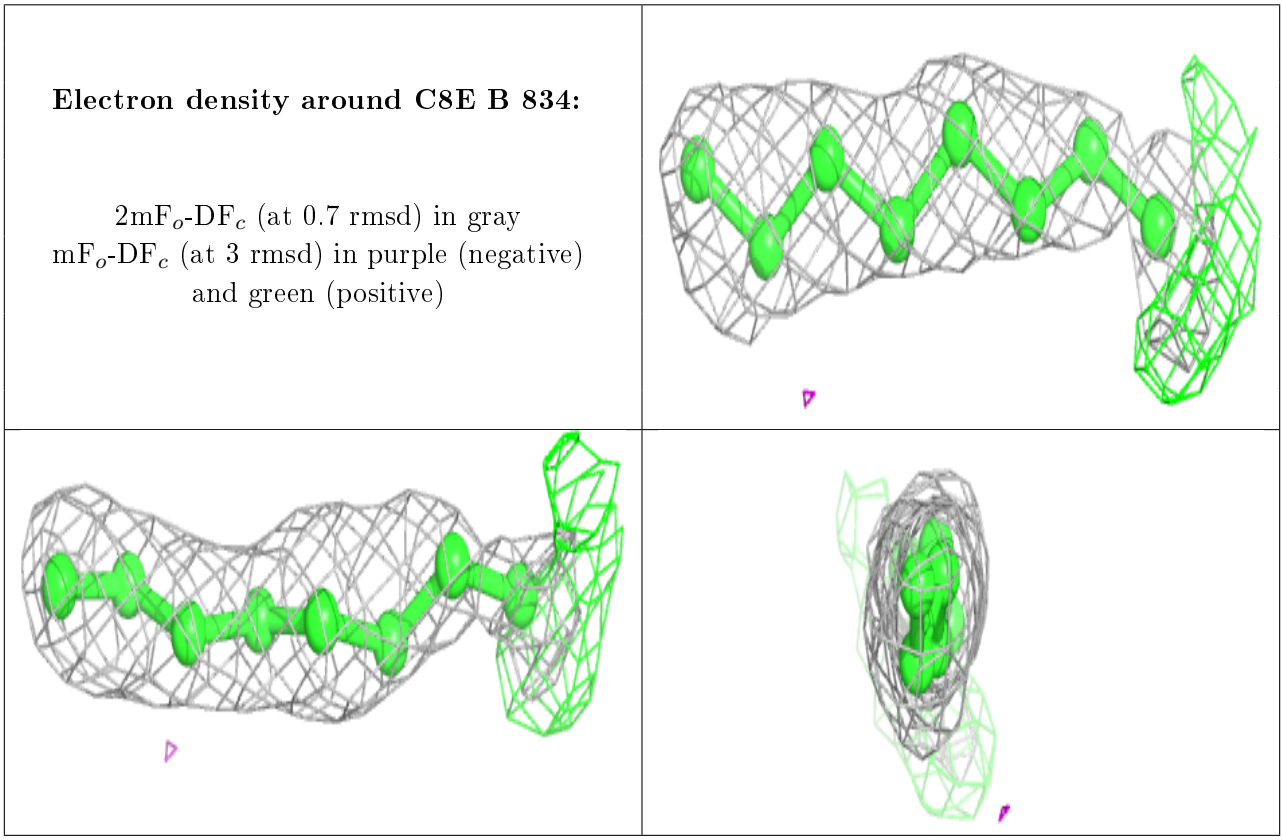
Electron density around C8E C 832:

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



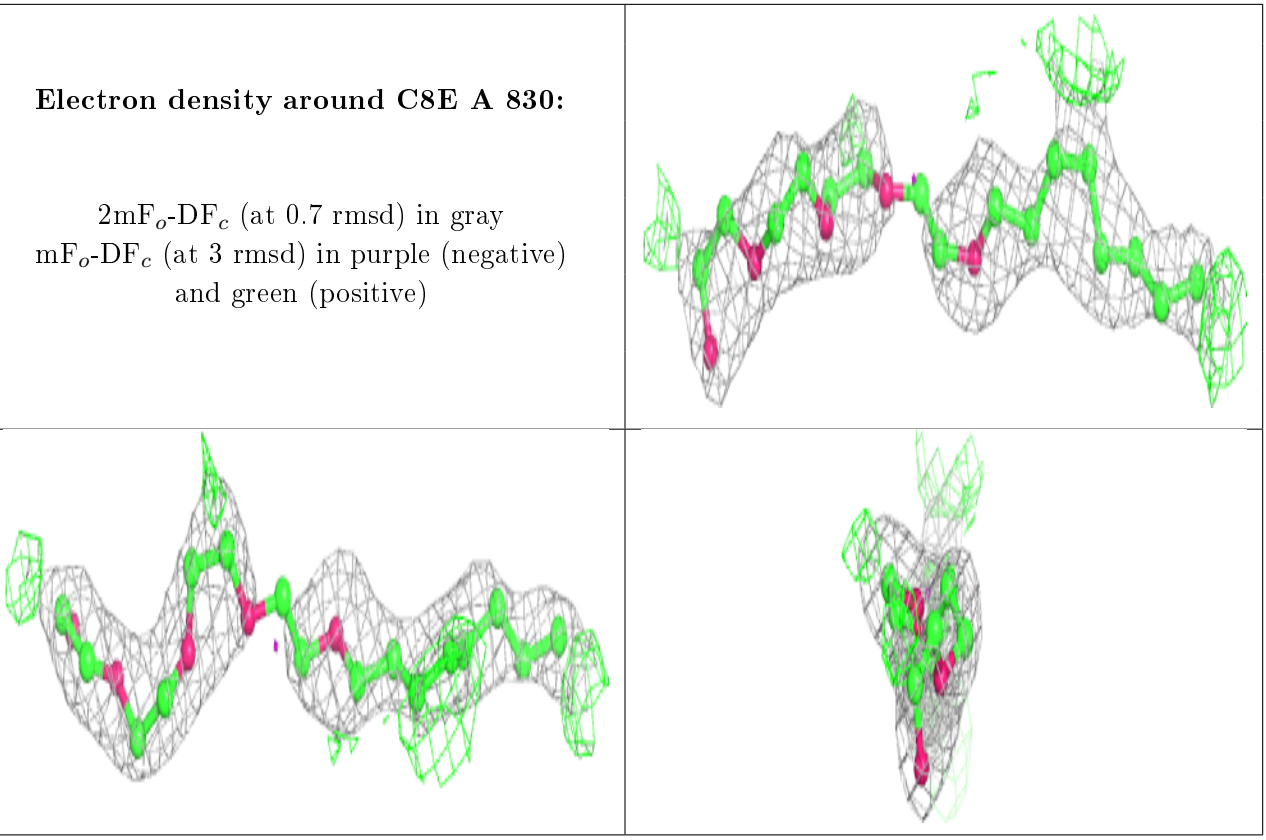
Electron density around C8E B 834:

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



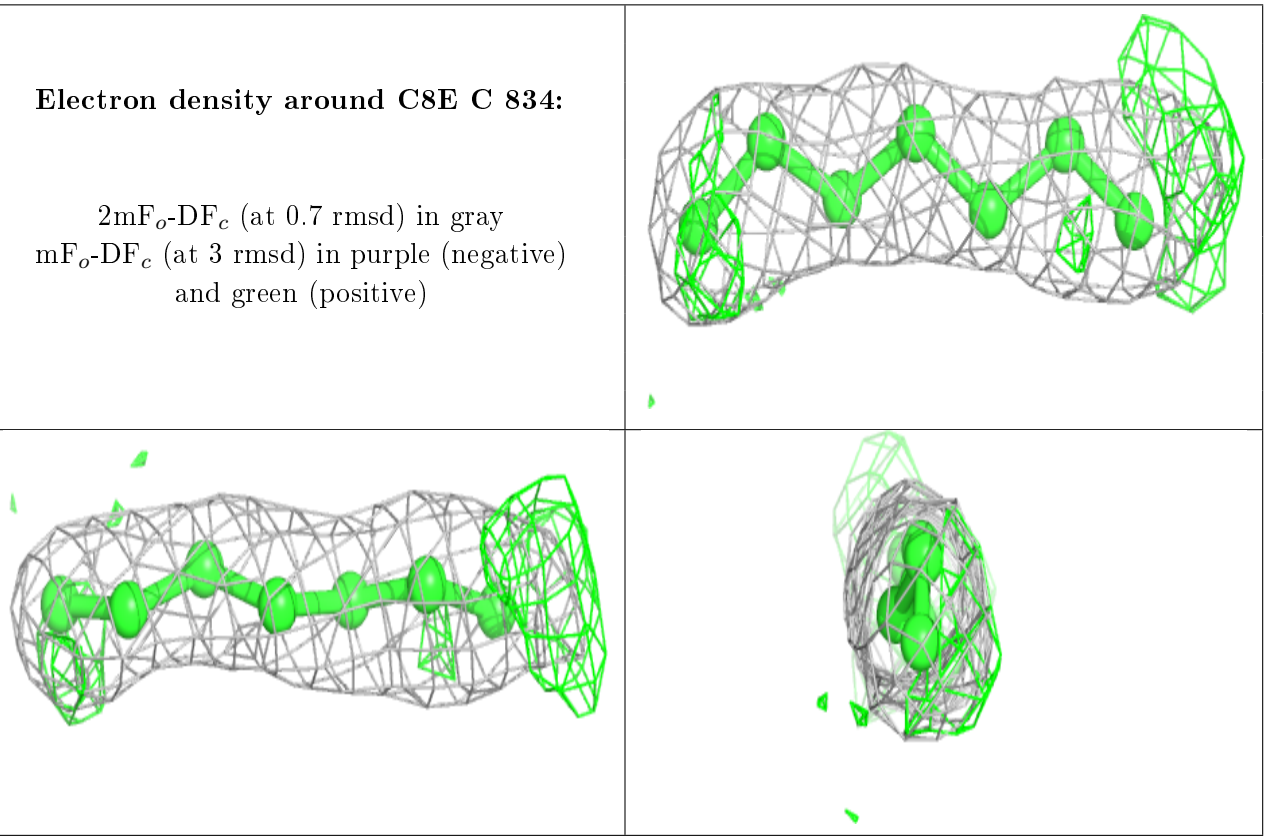
Electron density around C8E A 830:

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



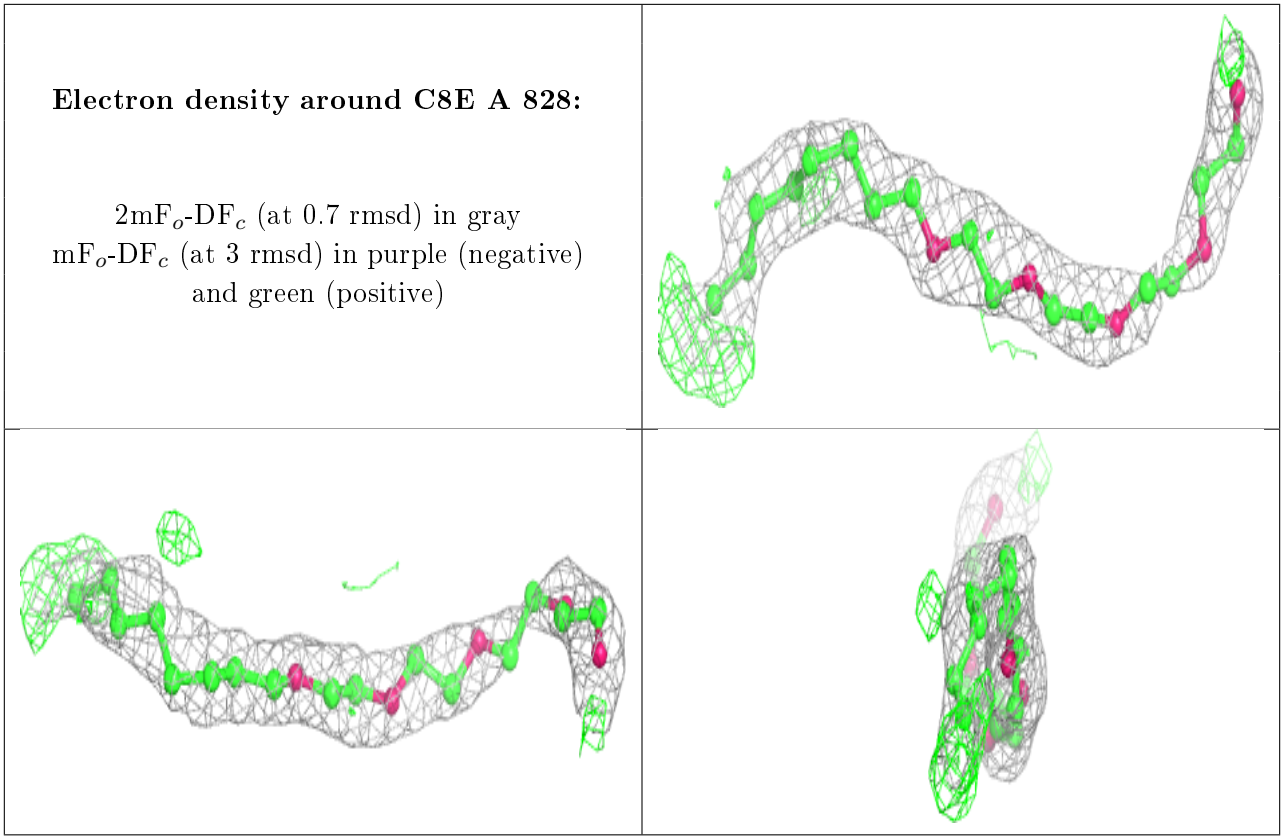
Electron density around C8E C 834:

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



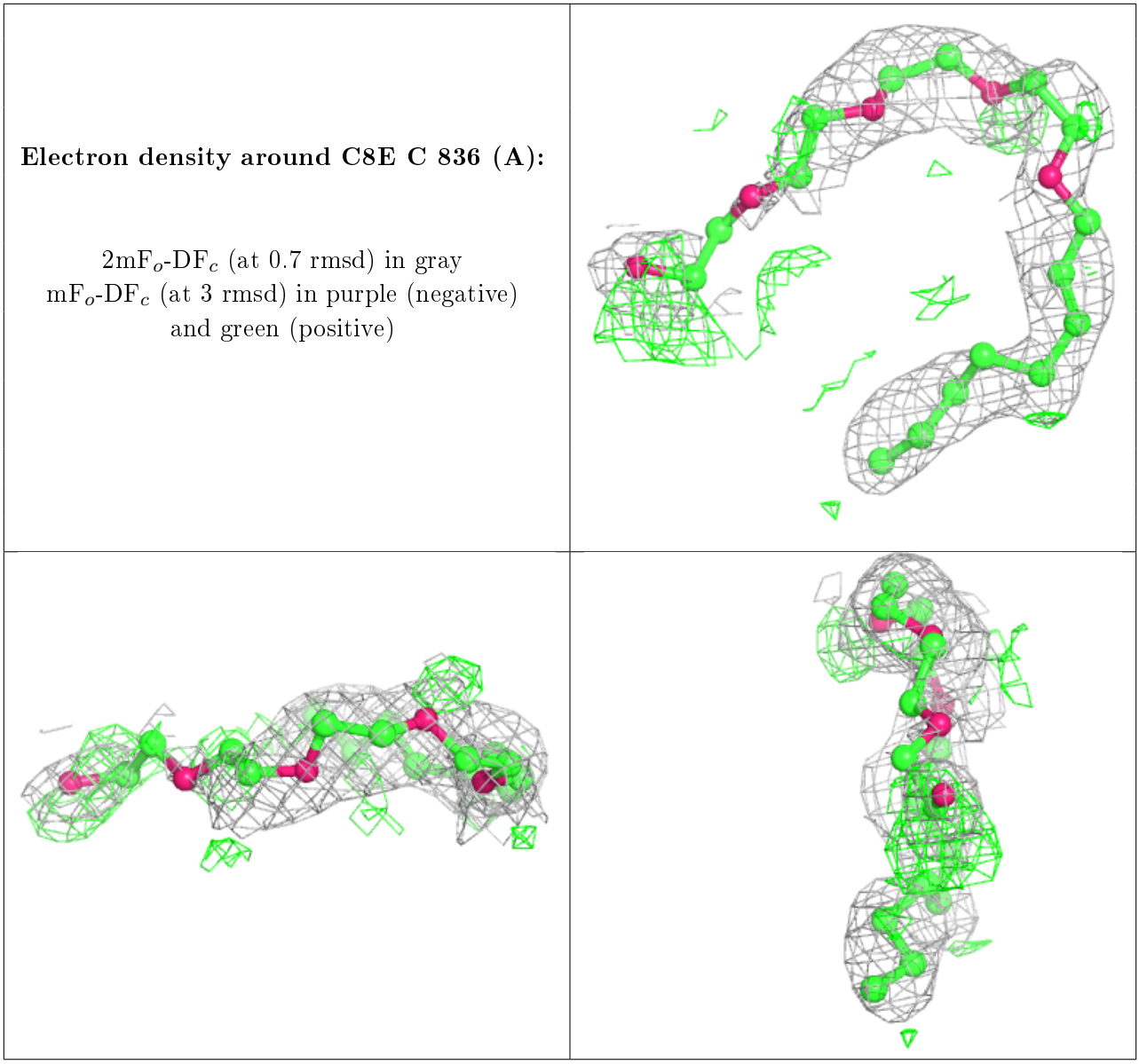
Electron density around C8E A 828:

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



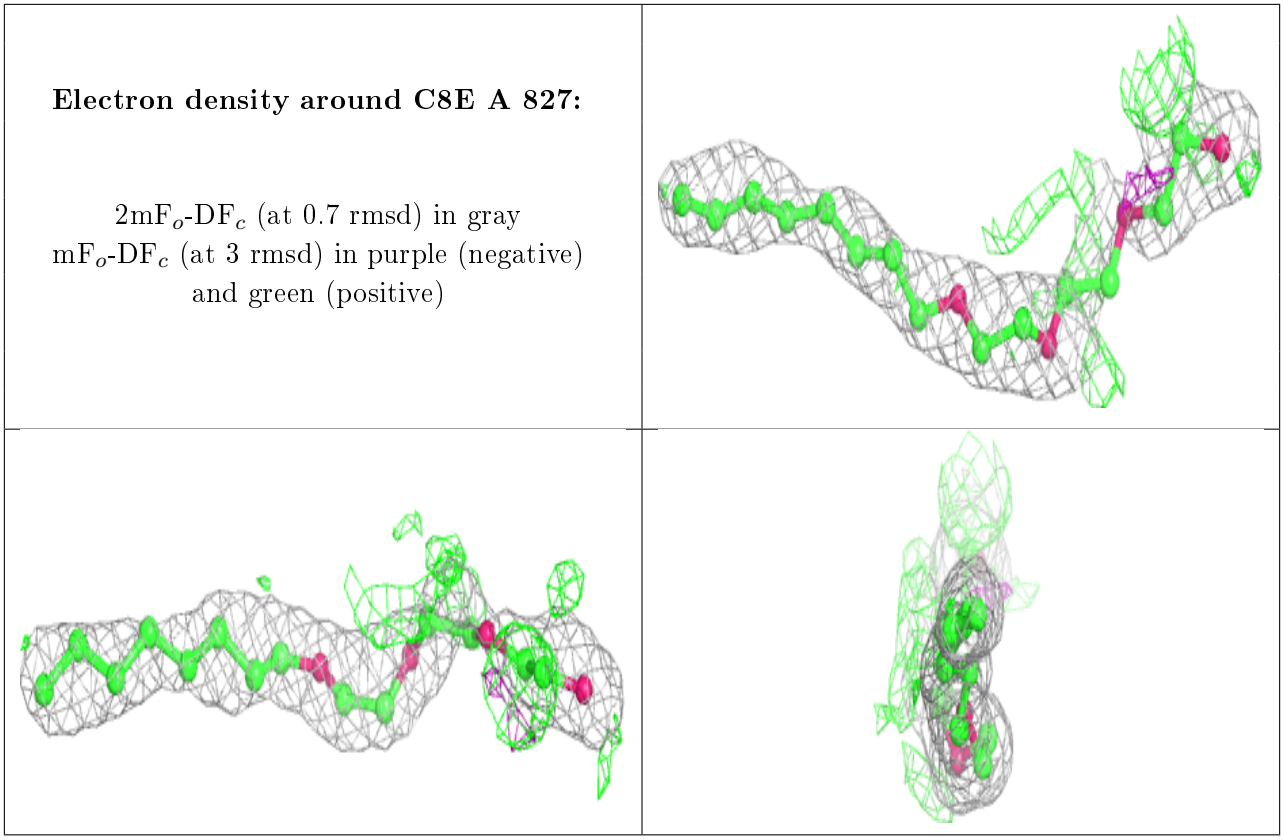
Electron density around C8E C 836 (A):

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



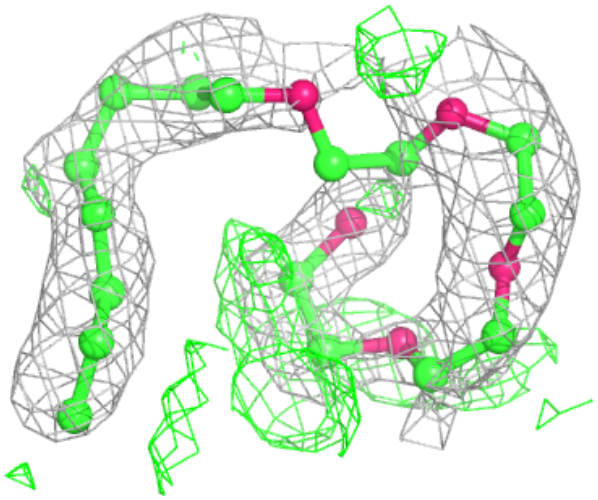
Electron density around C8E A 827:

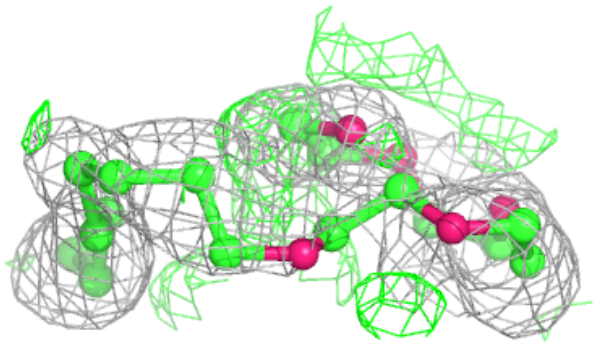
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

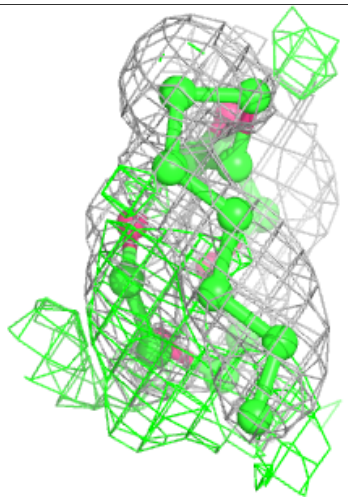


Electron density around C8E C 836 (B):

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

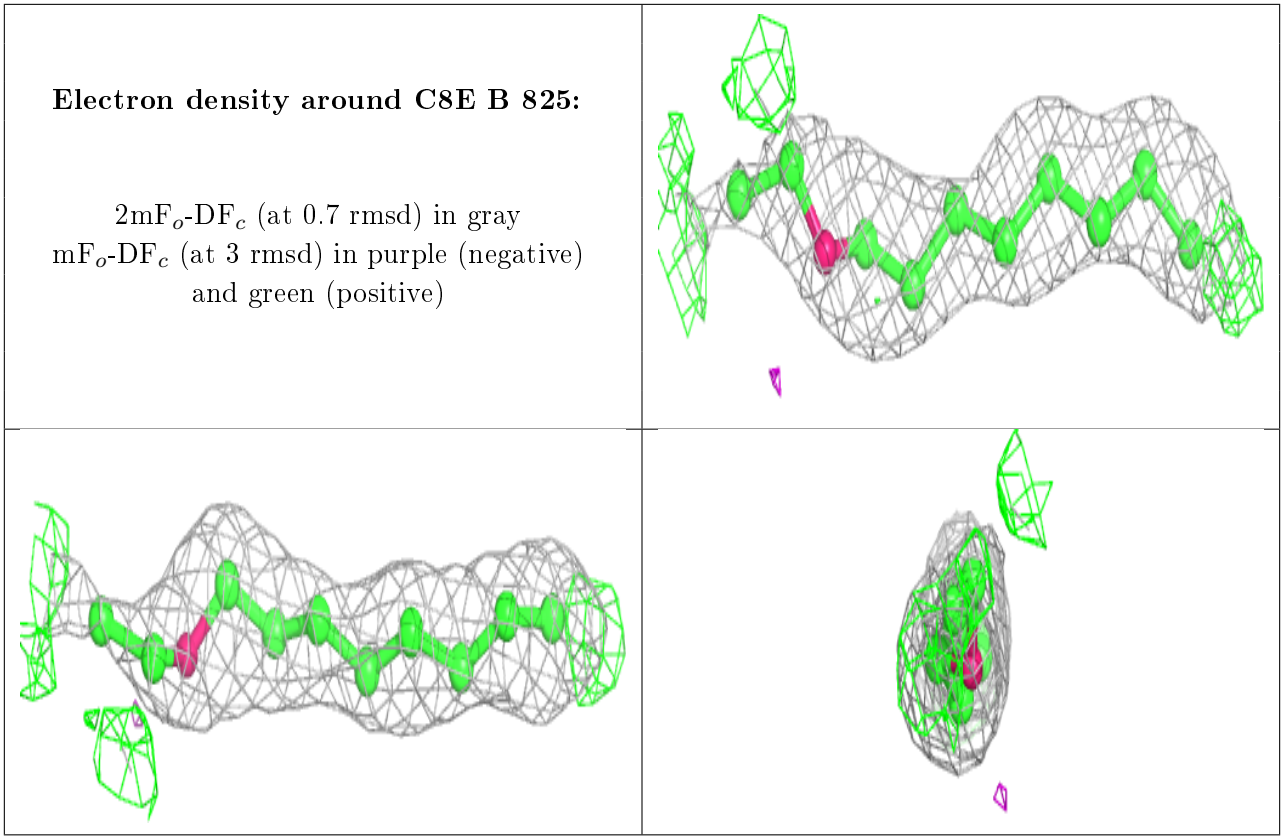






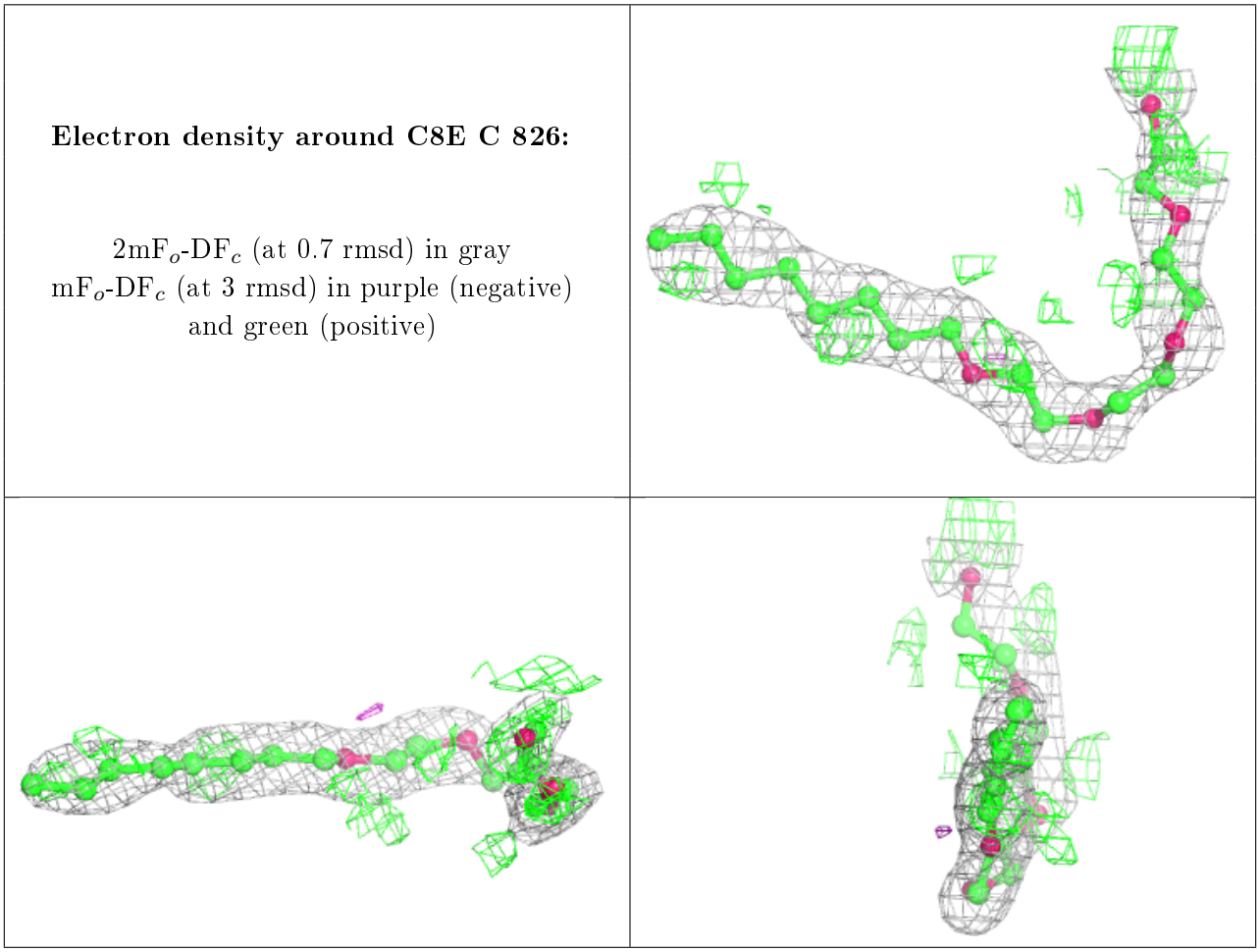
Electron density around C8E B 825:

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



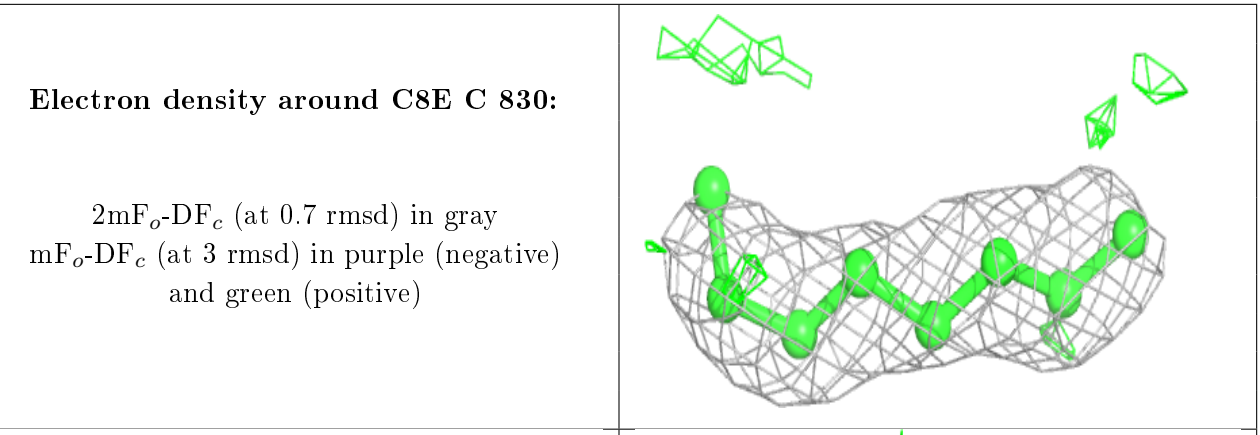
Electron density around C8E C 826:

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



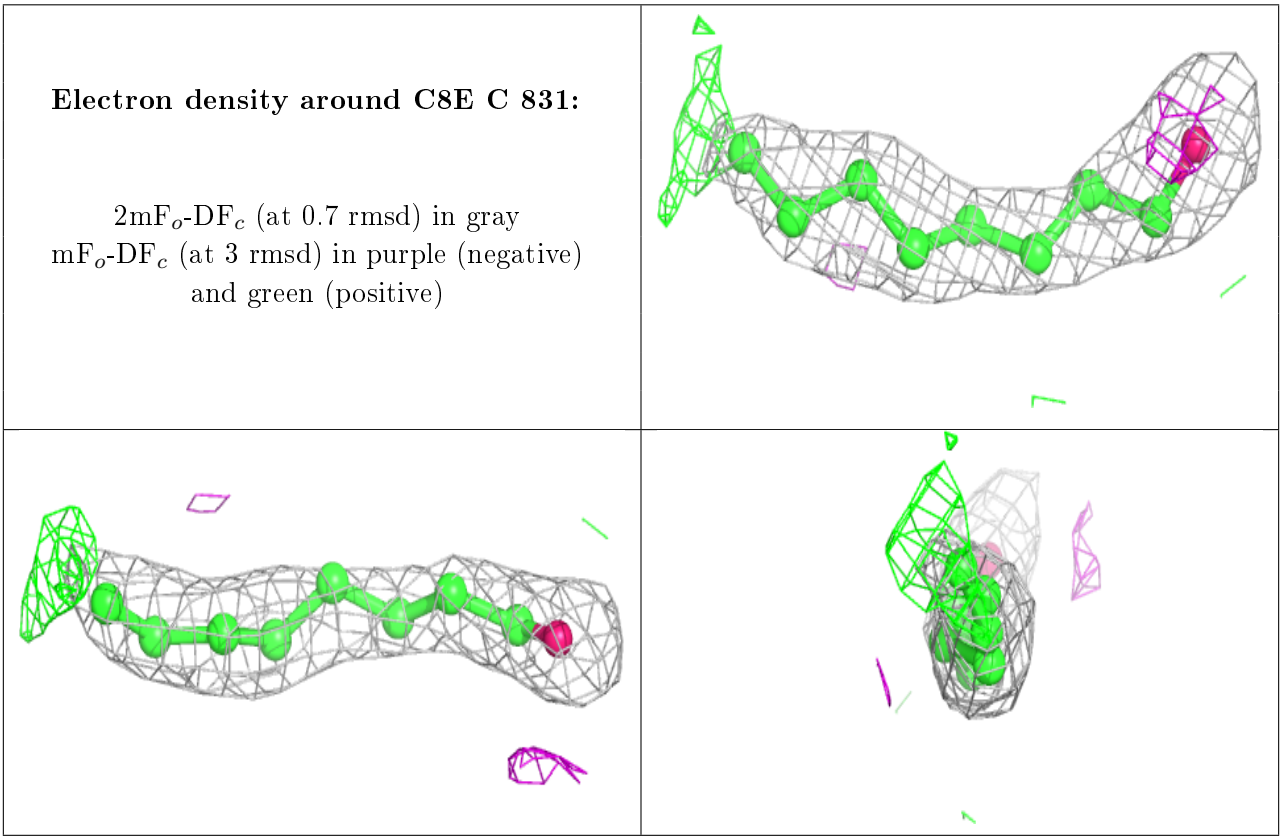
Electron density around C8E C 830:

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



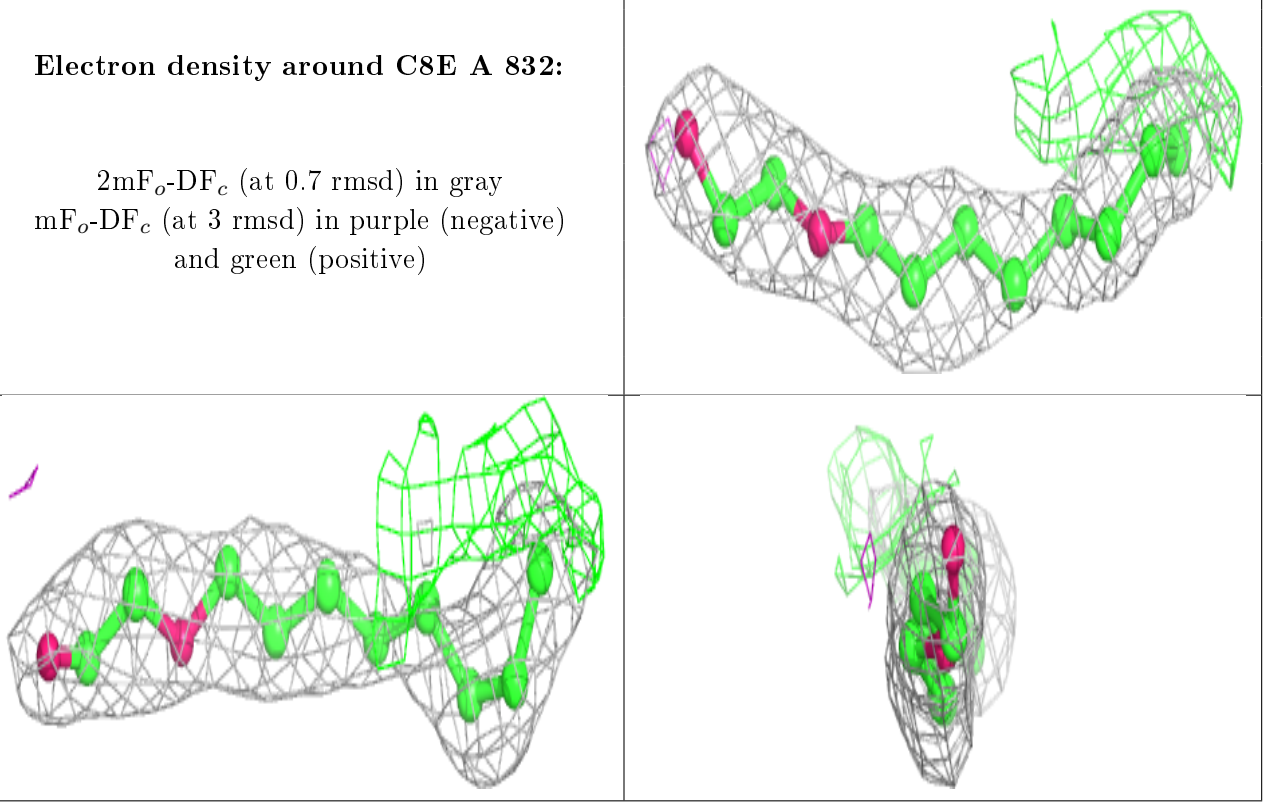
Electron density around C8E C 831:

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



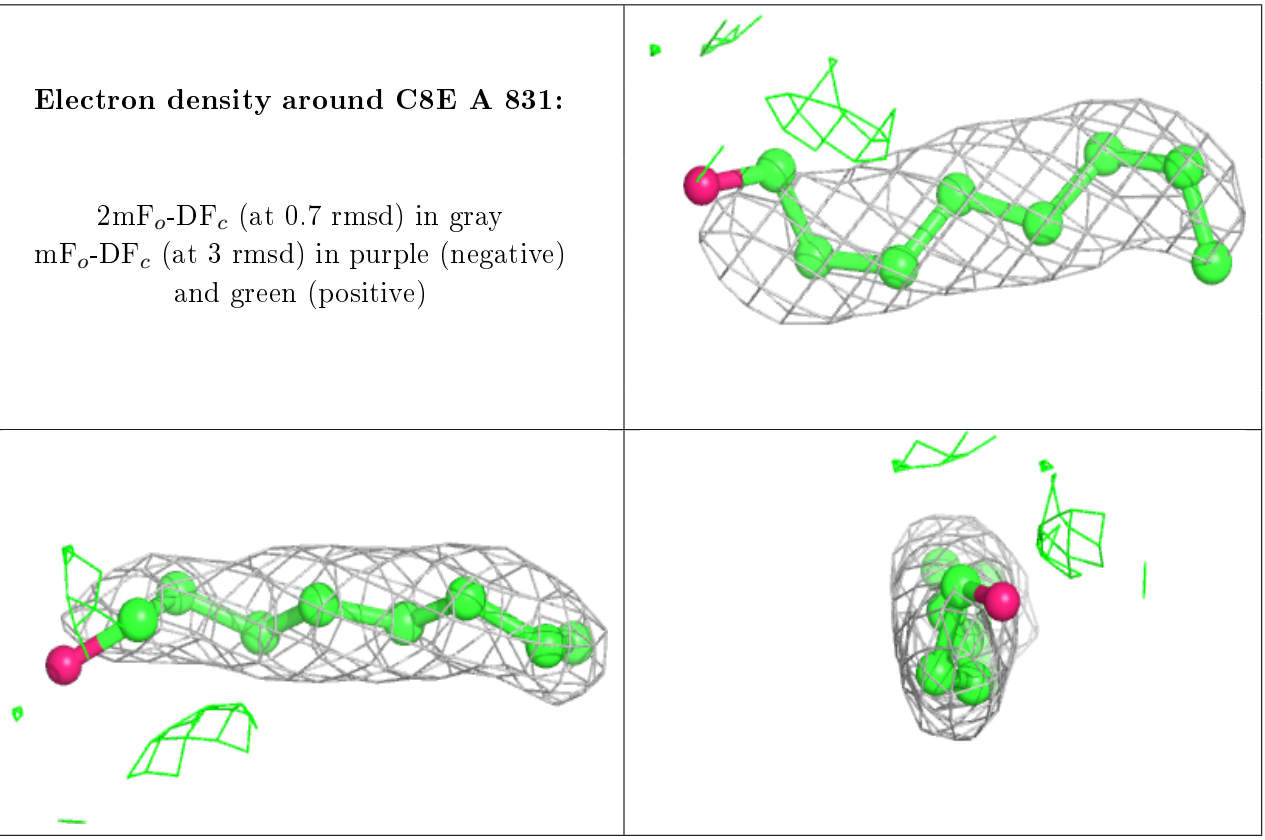
Electron density around C8E A 832:

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



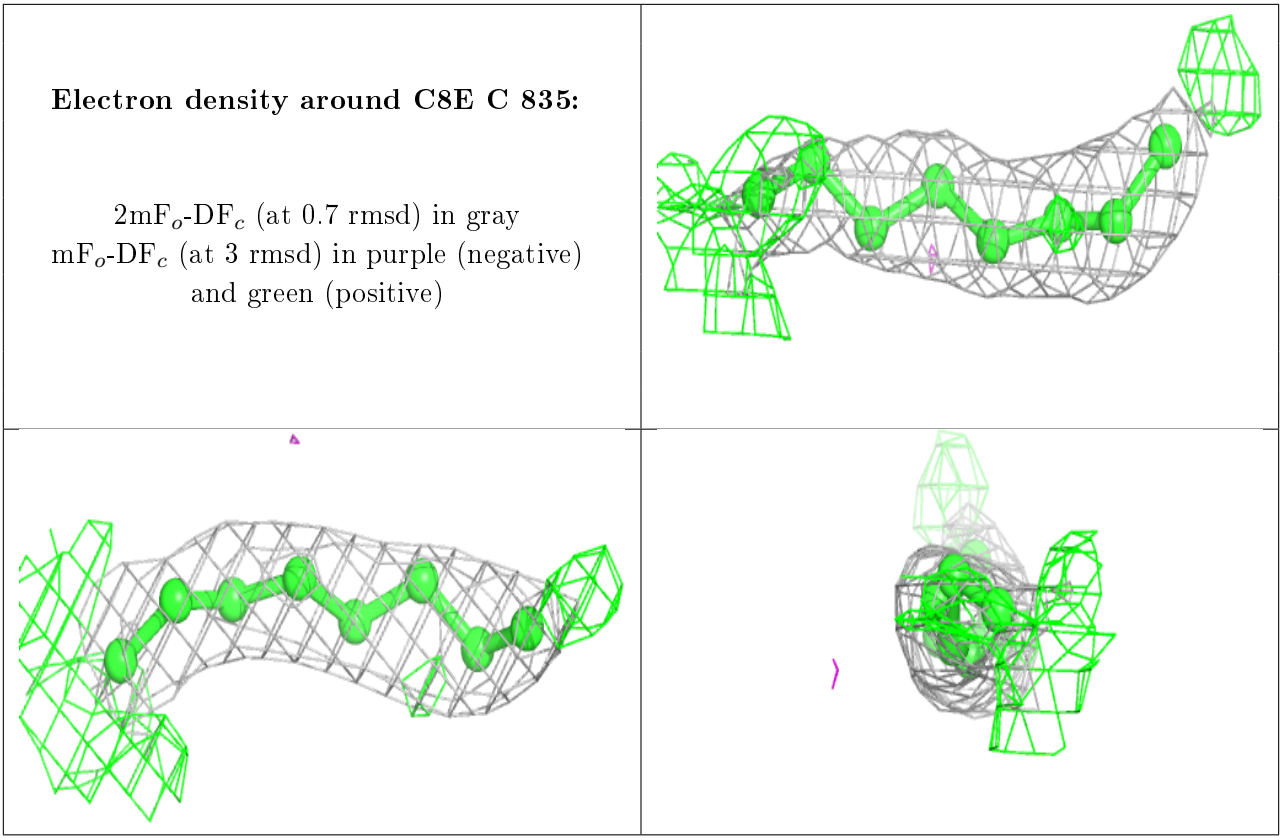
Electron density around C8E A 831:

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



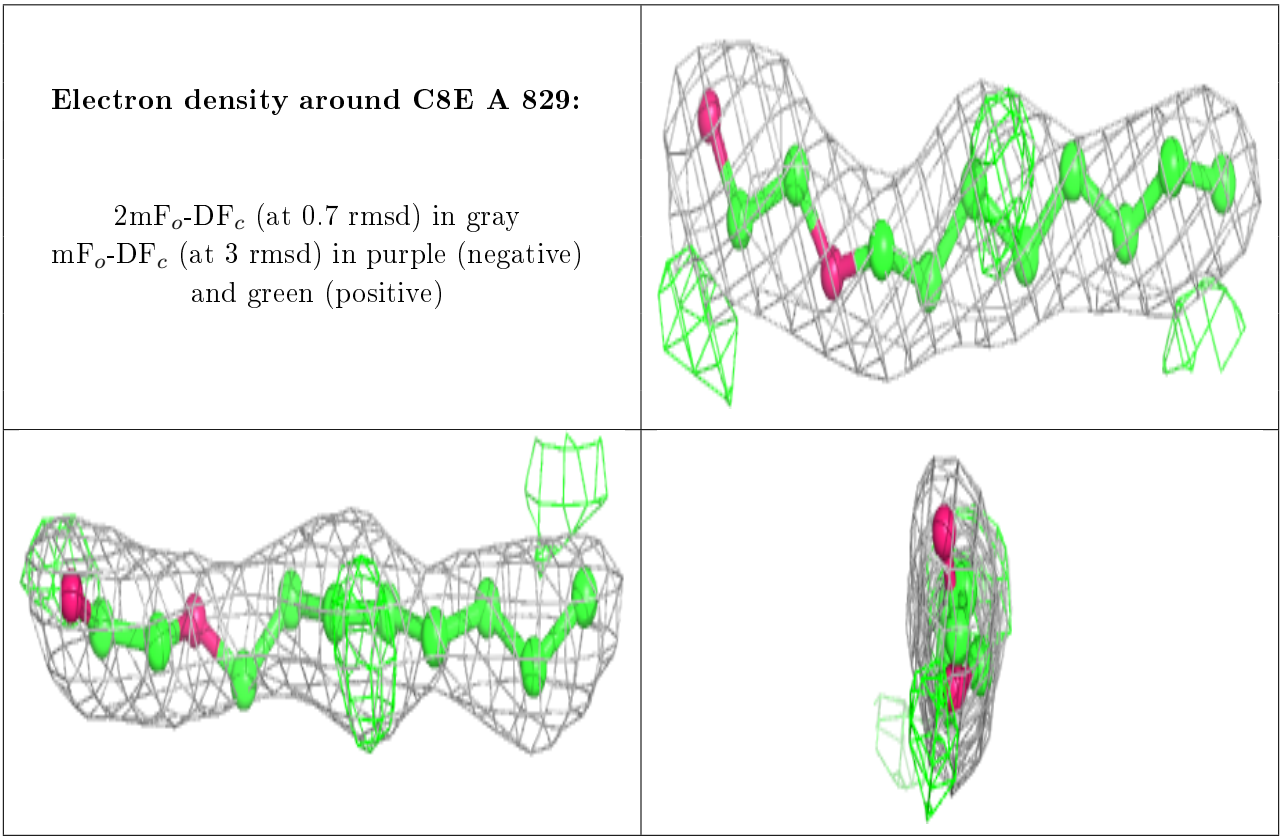
Electron density around C8E C 835:

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



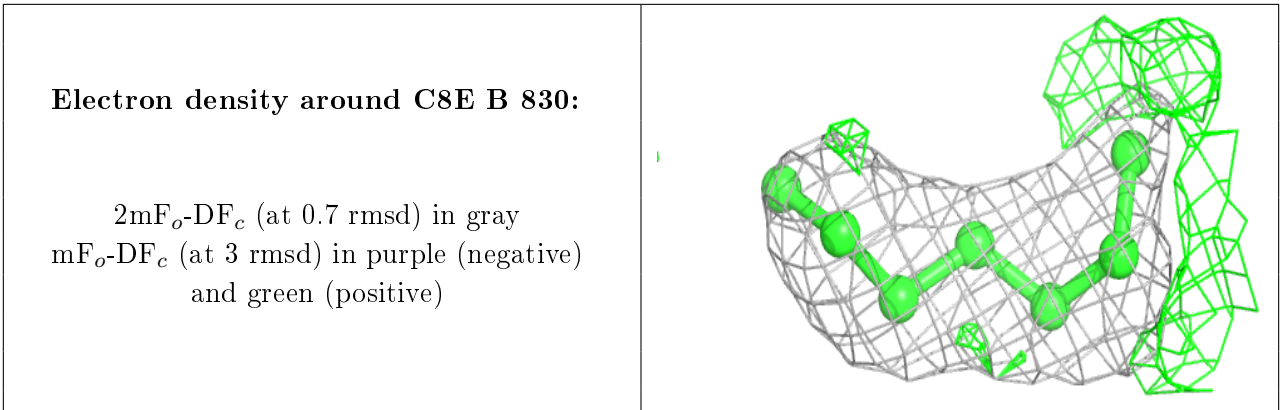
Electron density around C8E A 829:

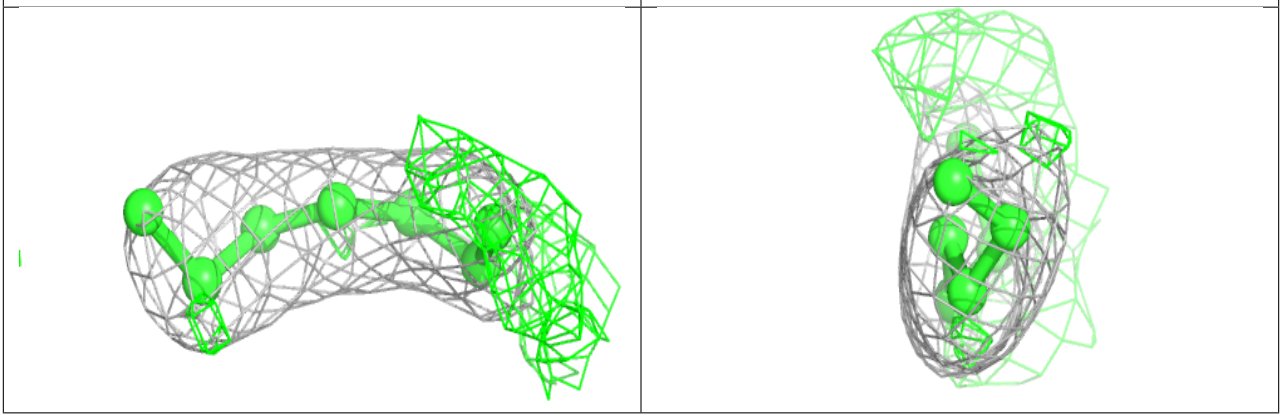
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around C8E B 830:

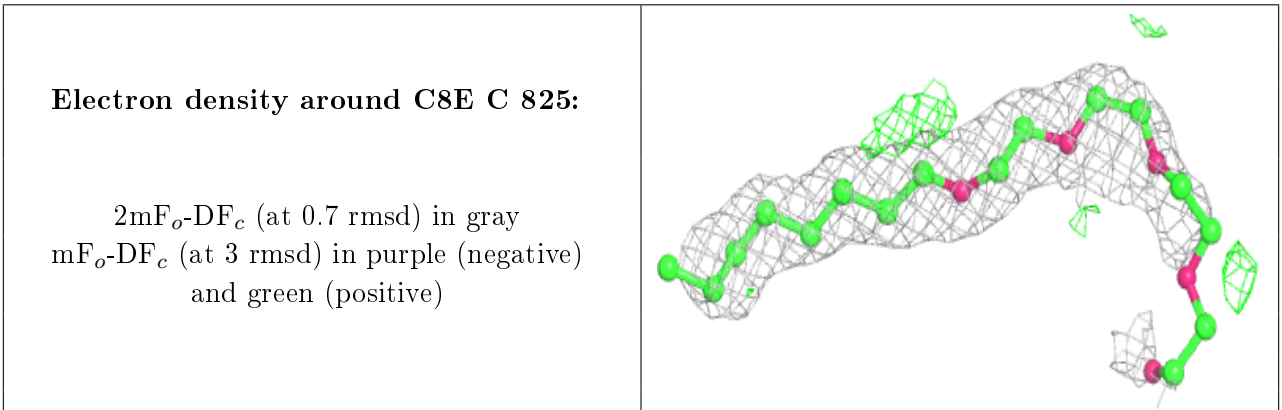
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

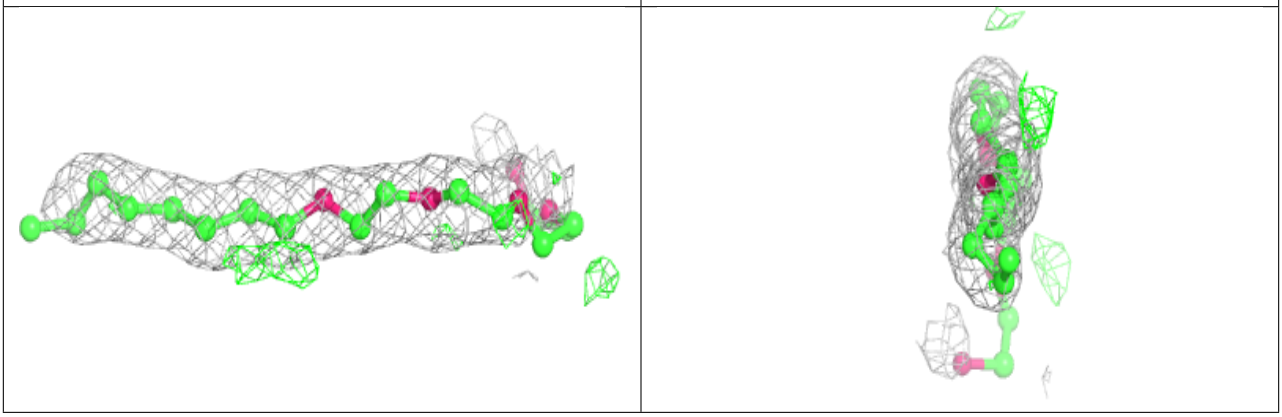




Electron density around C8E C 825:

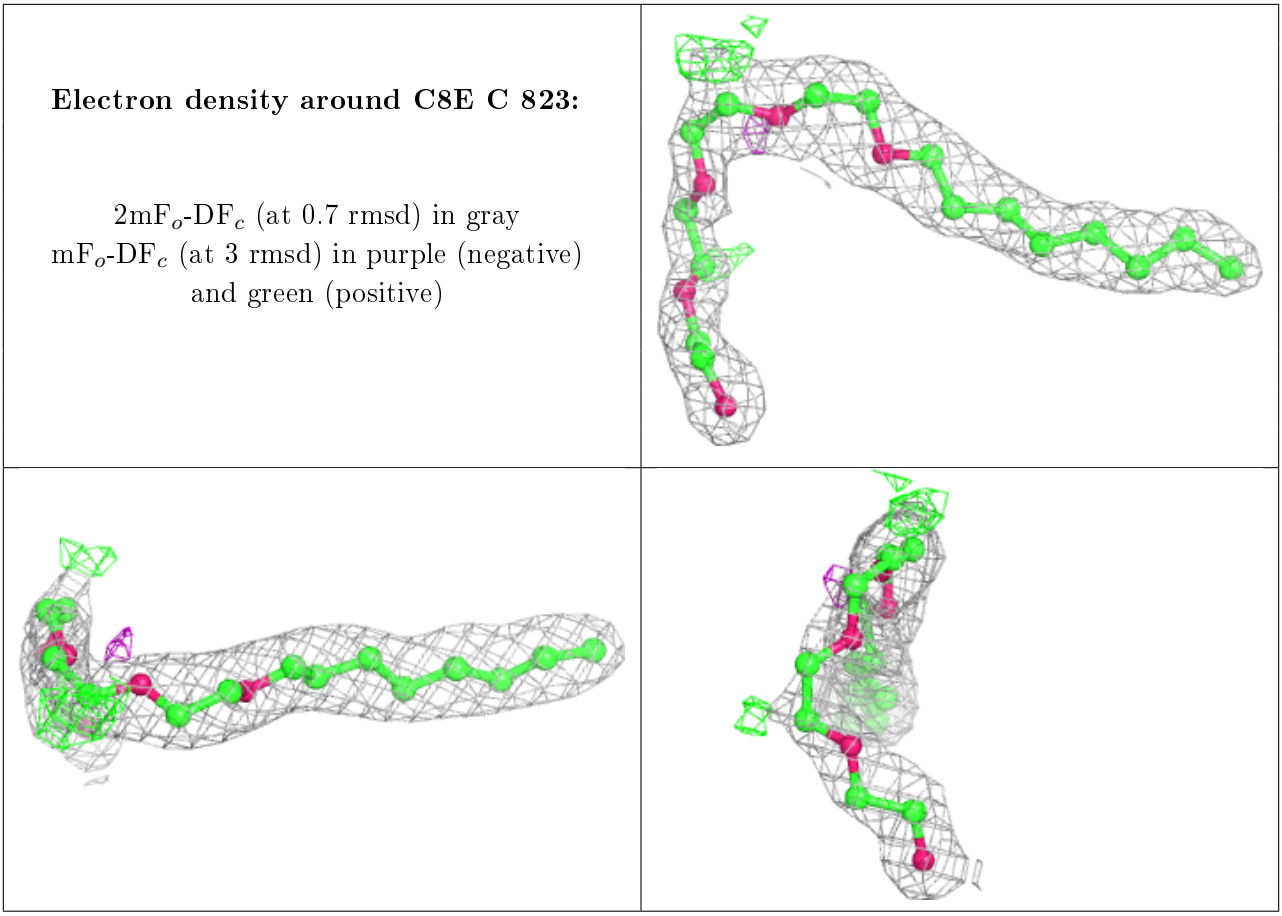
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





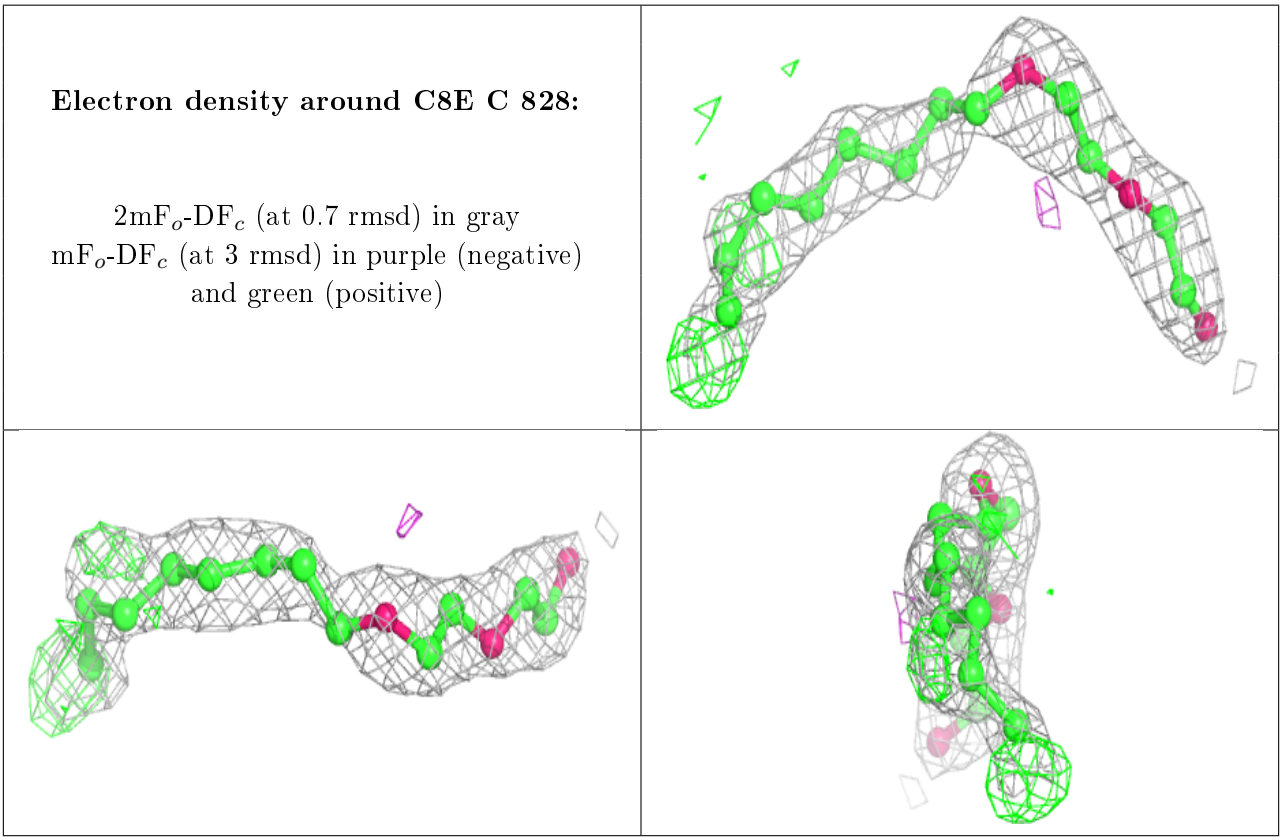
Electron density around C8E C 823:

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



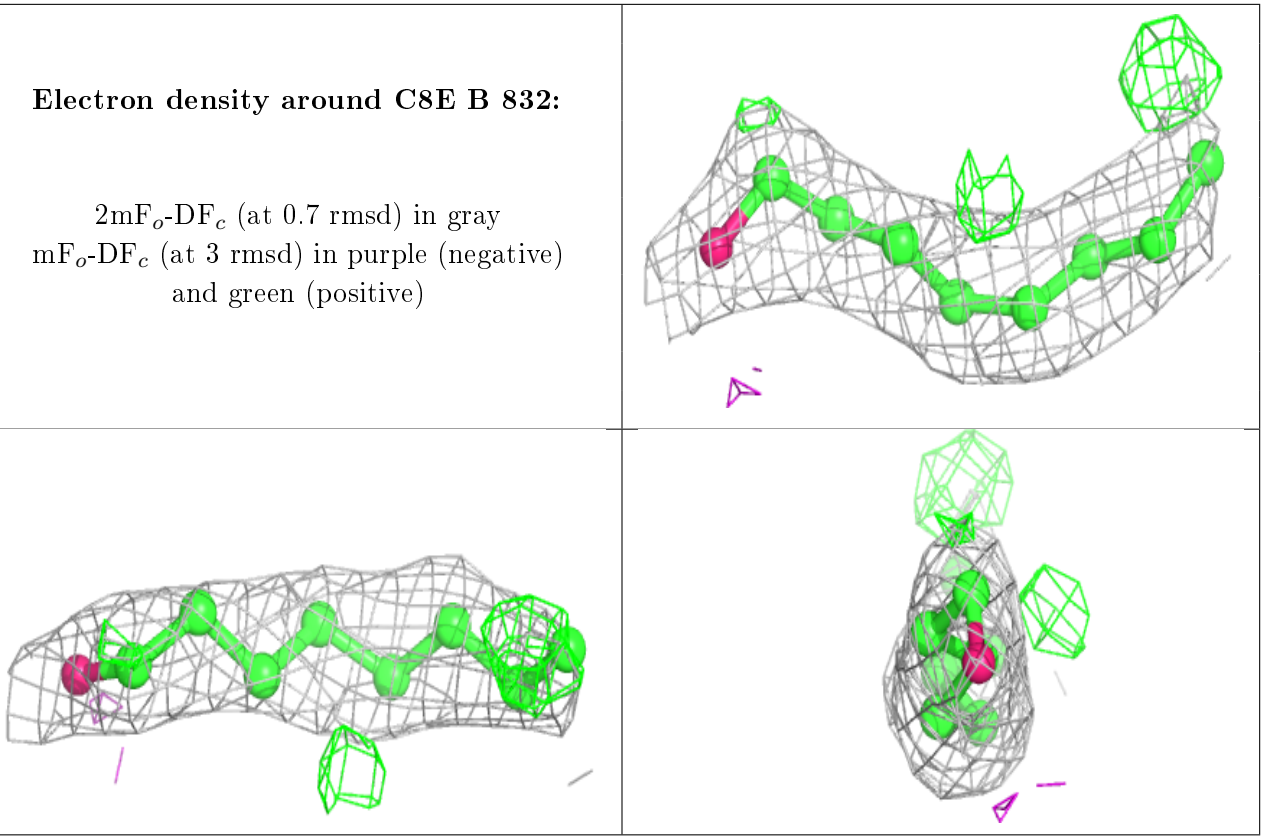
Electron density around C8E C 828:

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



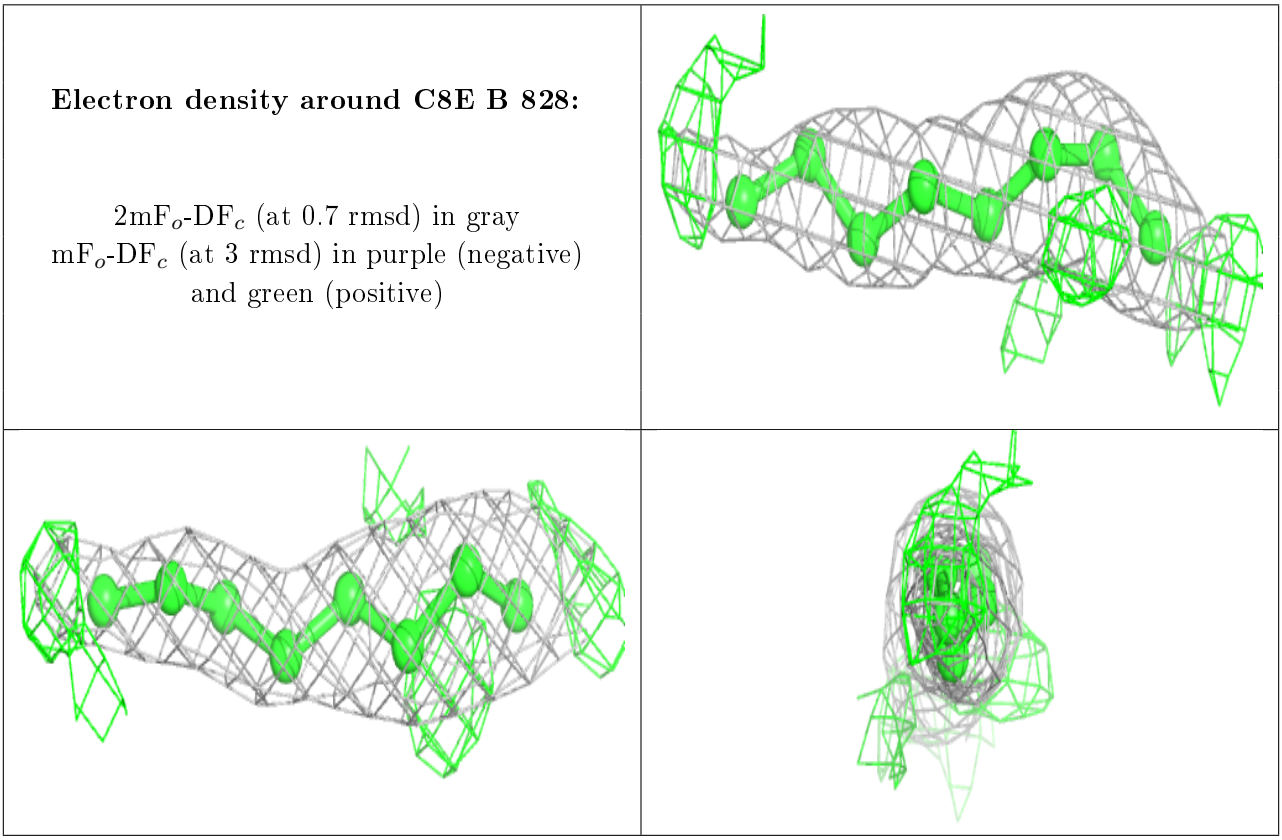
Electron density around C8E B 832:

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



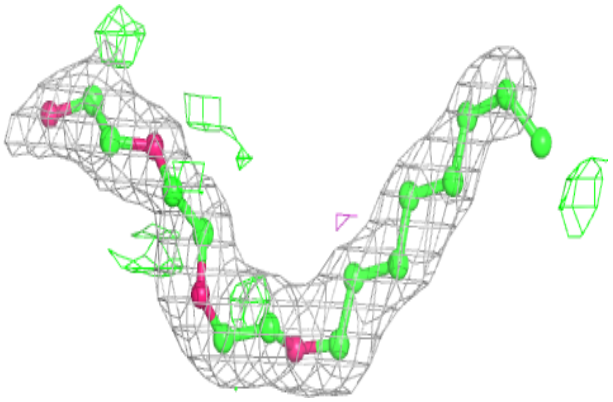
Electron density around C8E B 828:

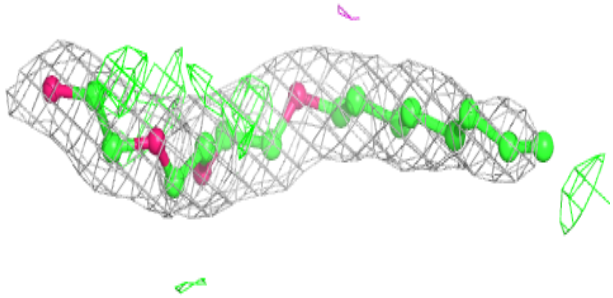
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

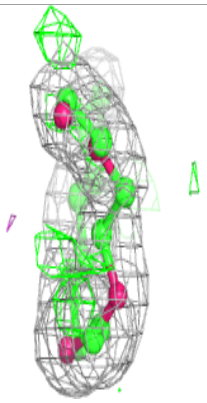


Electron density around C8E C 824:

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

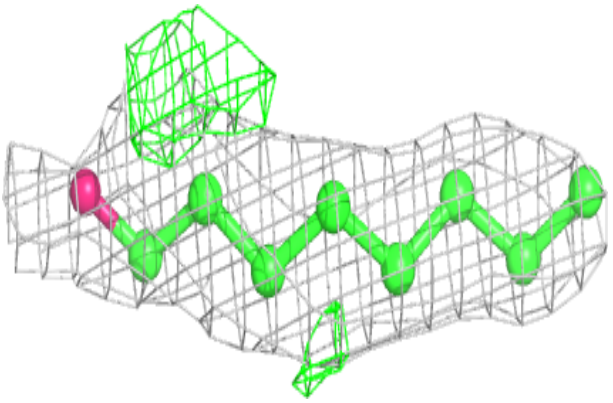


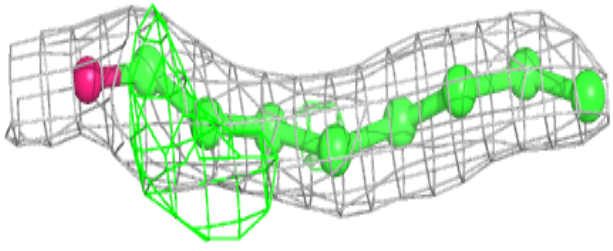


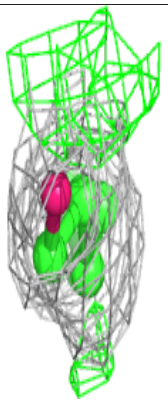


Electron density around C8E B 827:

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

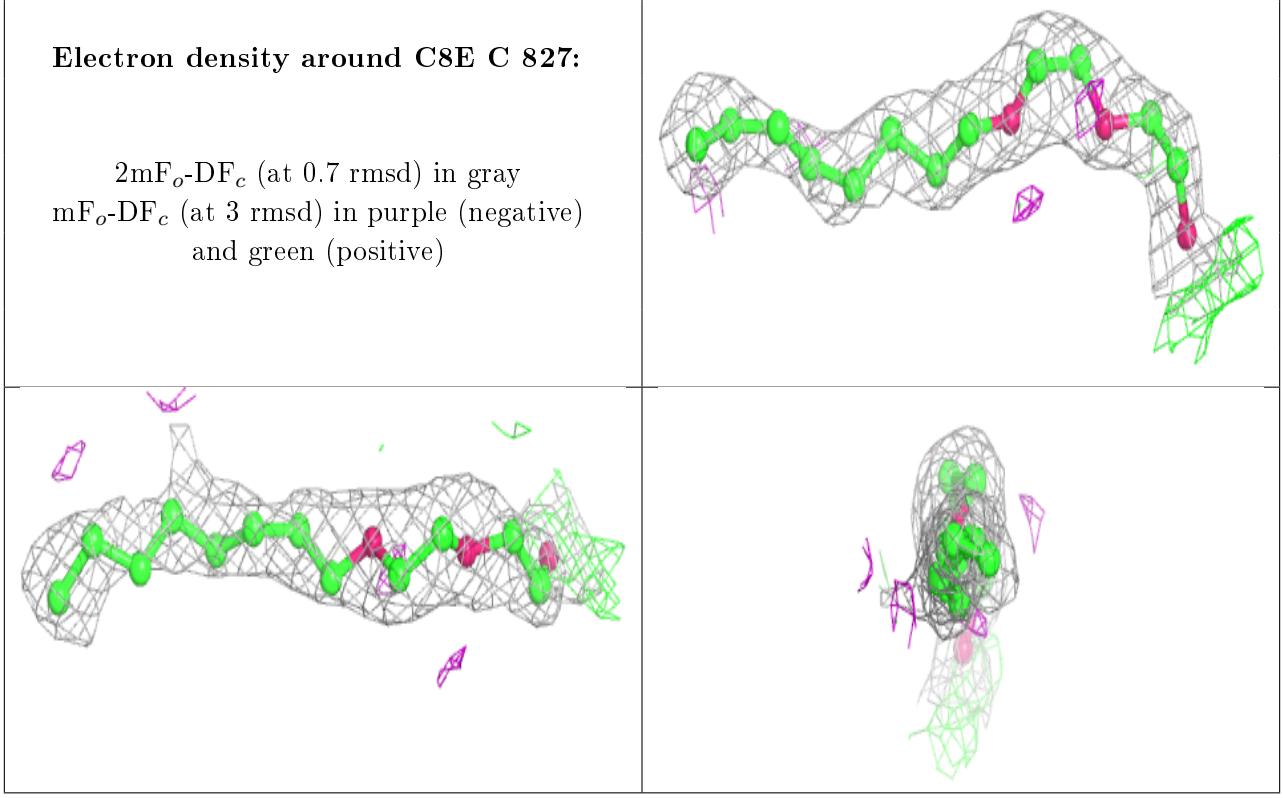






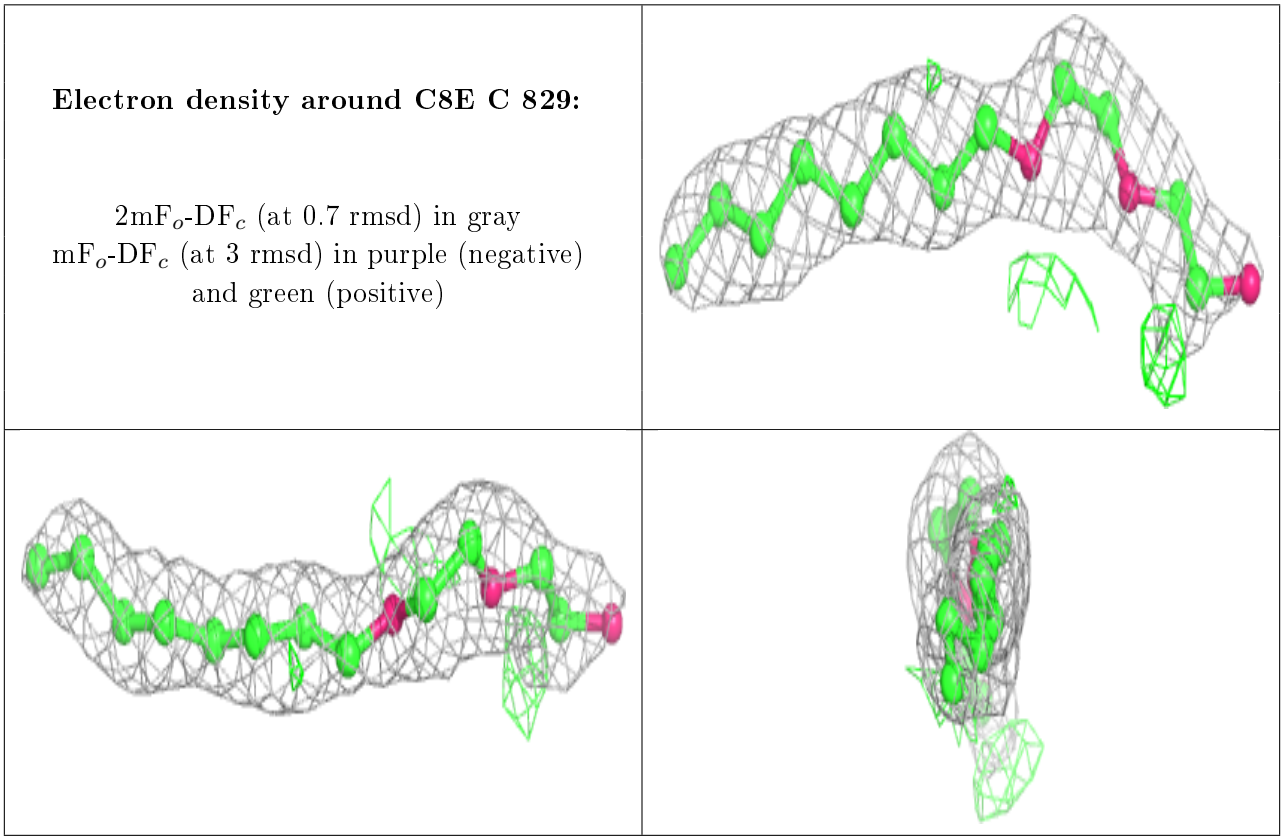
Electron density around C8E C 827:

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



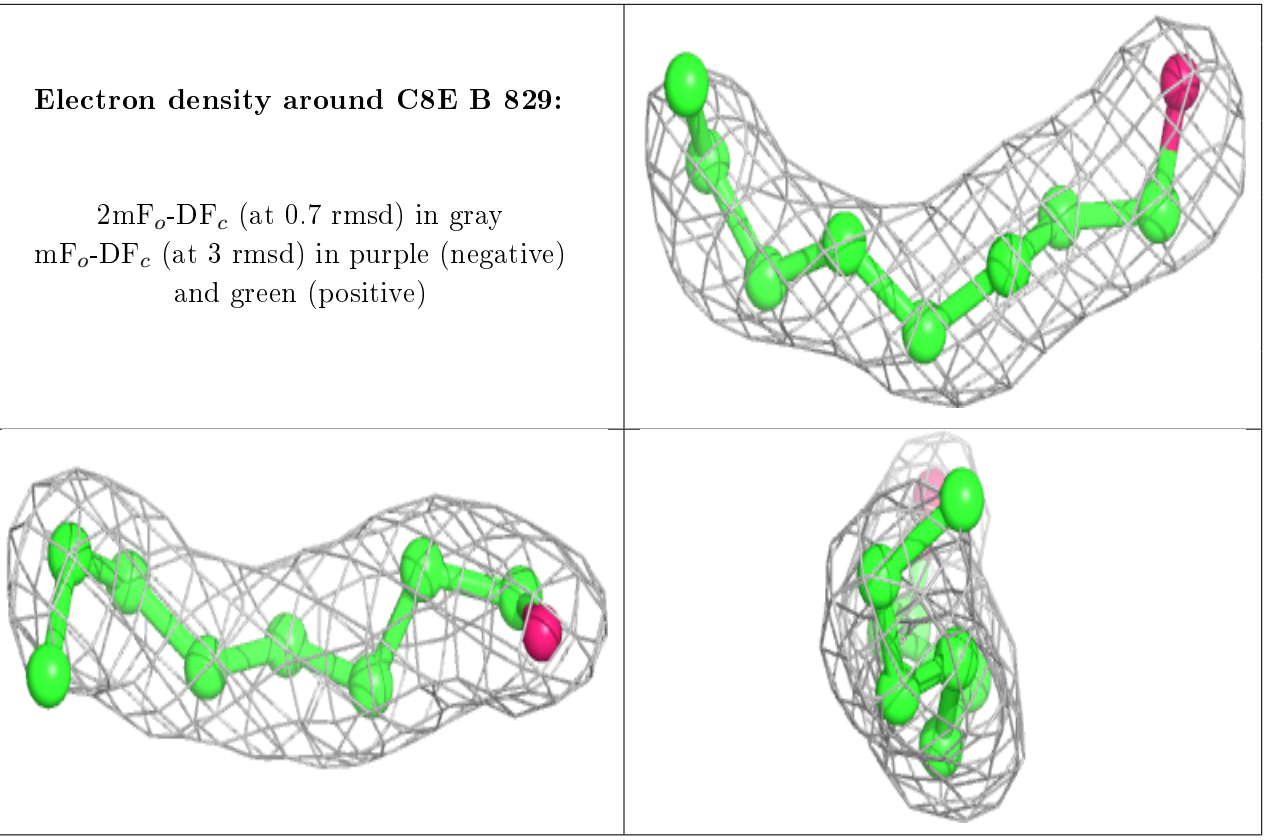
Electron density around C8E C 829:

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



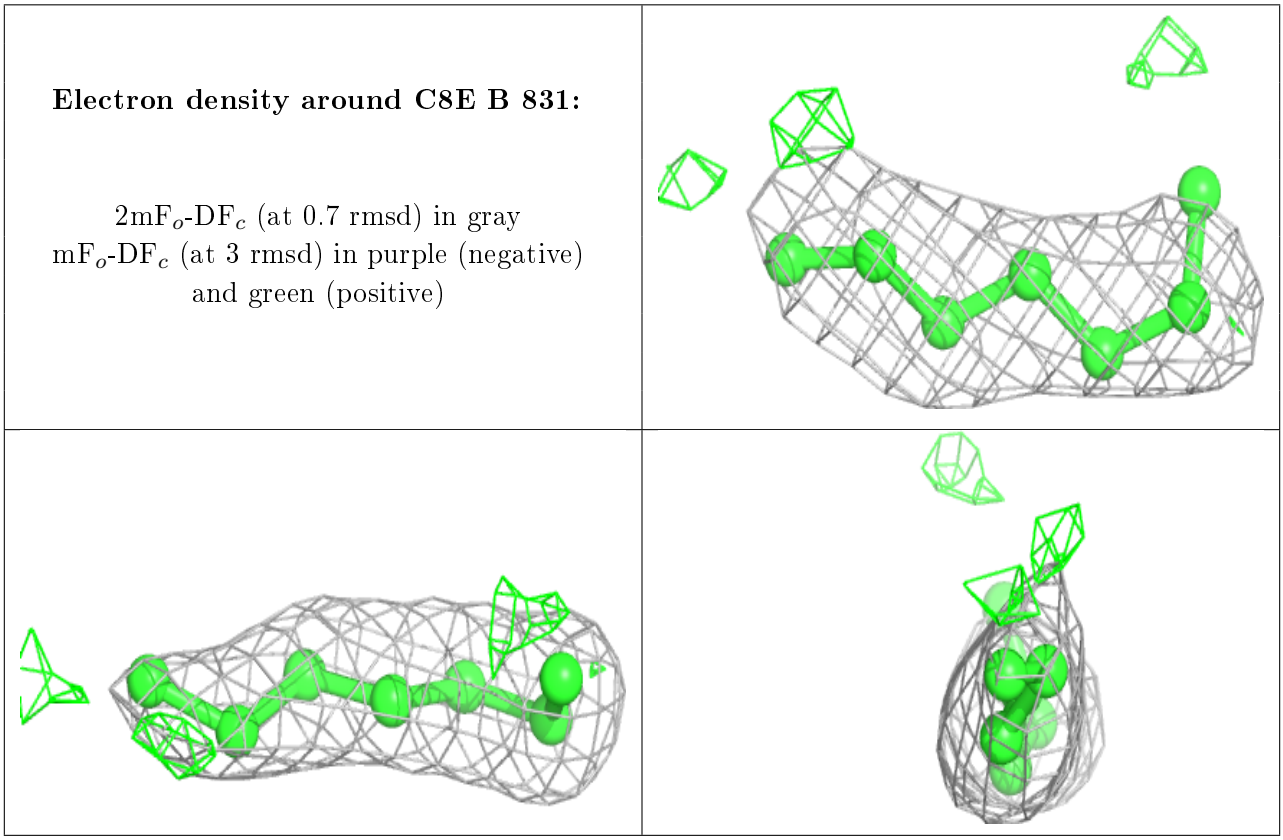
Electron density around C8E B 829:

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



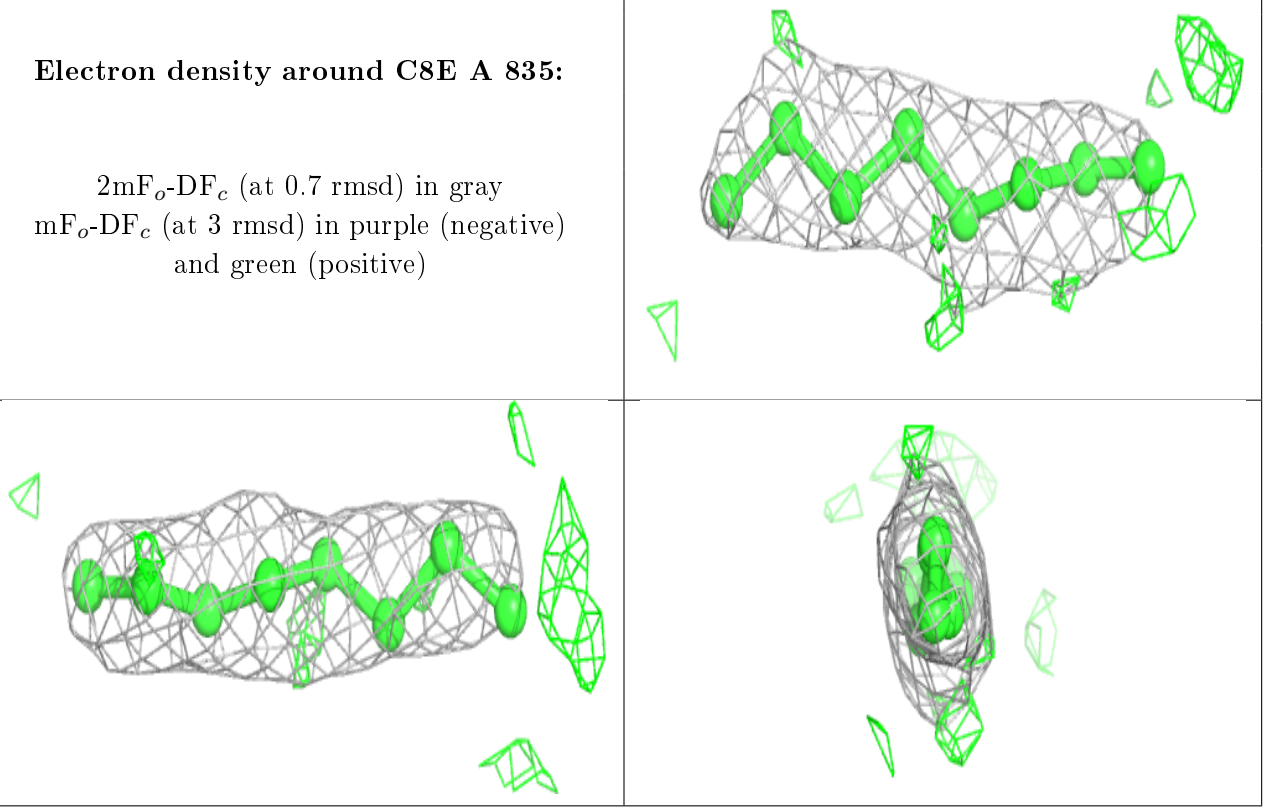
Electron density around C8E B 831:

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



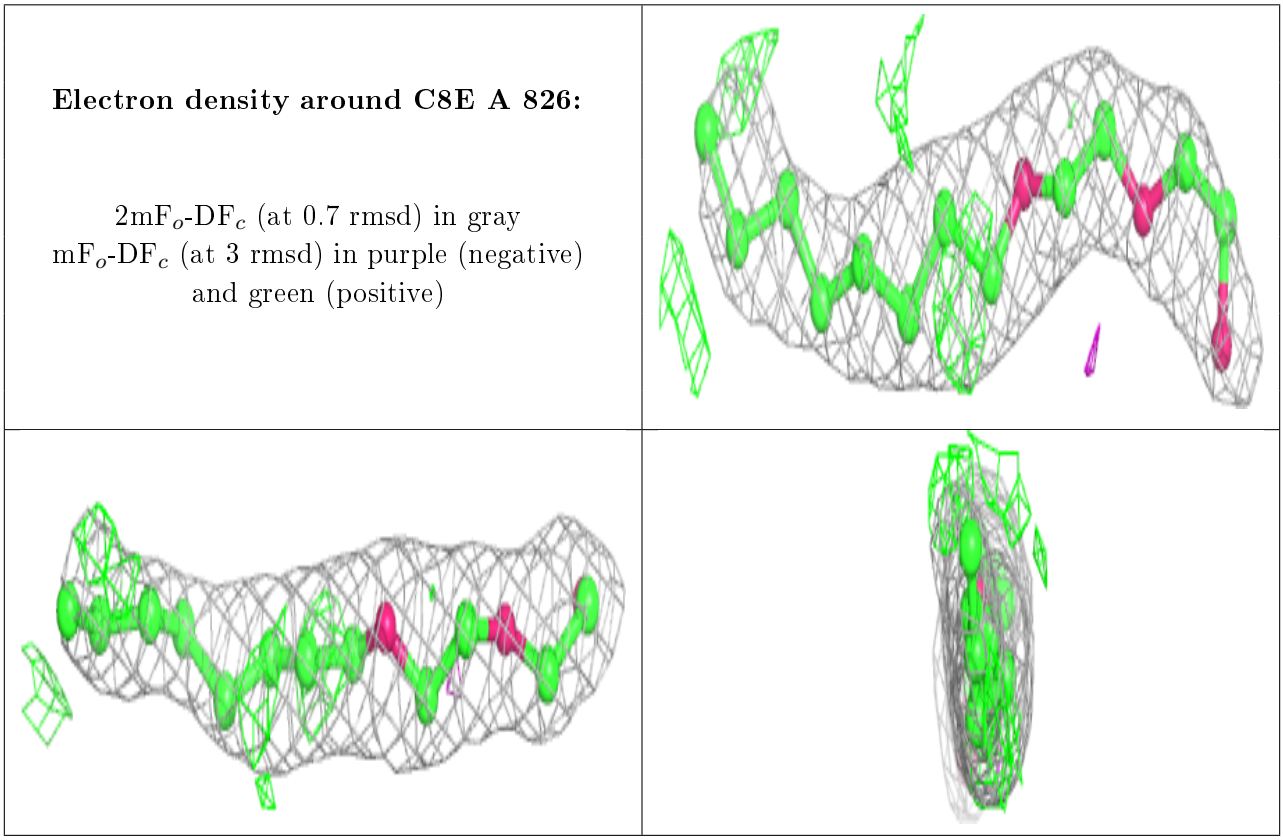
Electron density around C8E A 835:

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



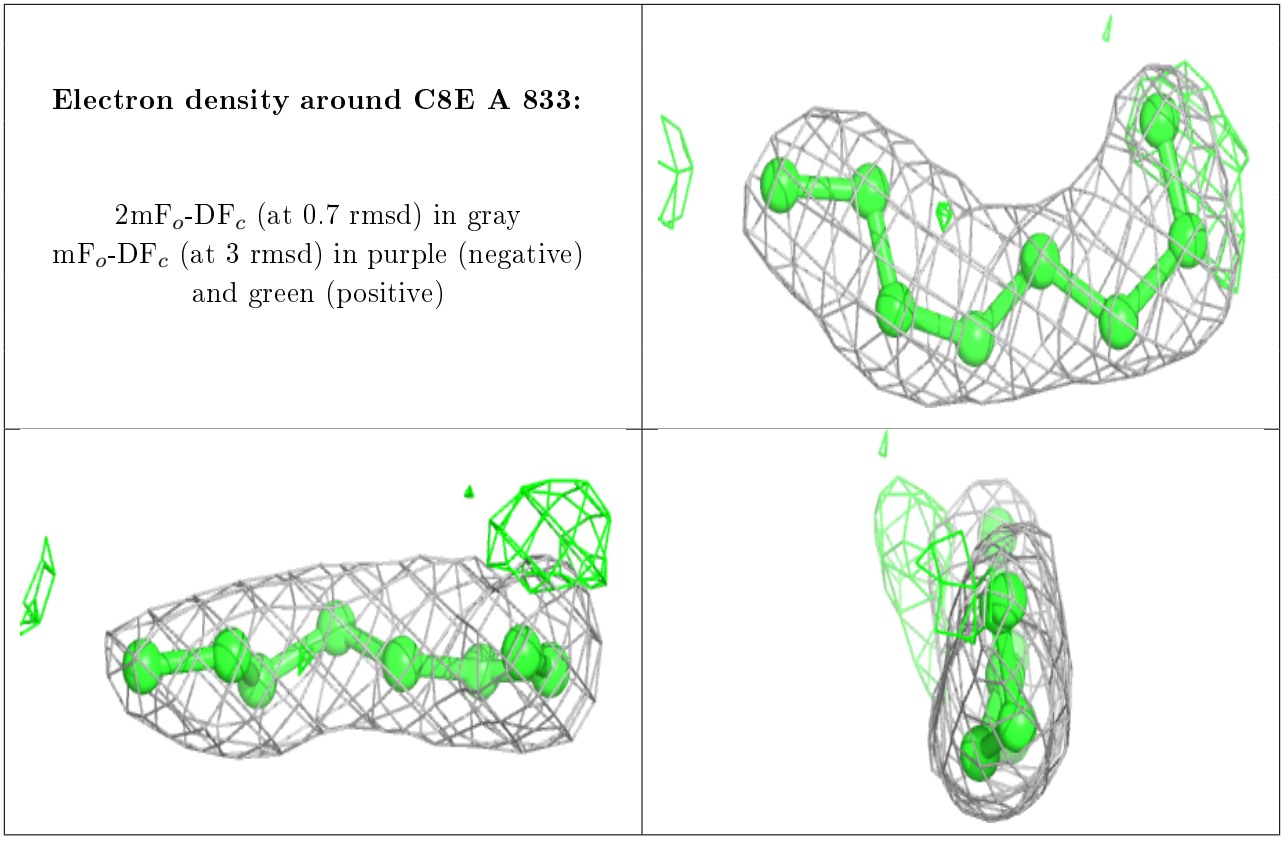
Electron density around C8E A 826:

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



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)



6.5 Other polymers

There are no such residues in this entry.