Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 07:00 pm GMT

PDB ID	:	4D5B
Title	:	Crystal structure of CymA from Klebsiella oxytoca
Authors	:	van den Berg, B.; Bhamidimarri, S.P.; Kleinekathoefer, U.; Winterhalter, M.
Deposited on	:	2014-11-03
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

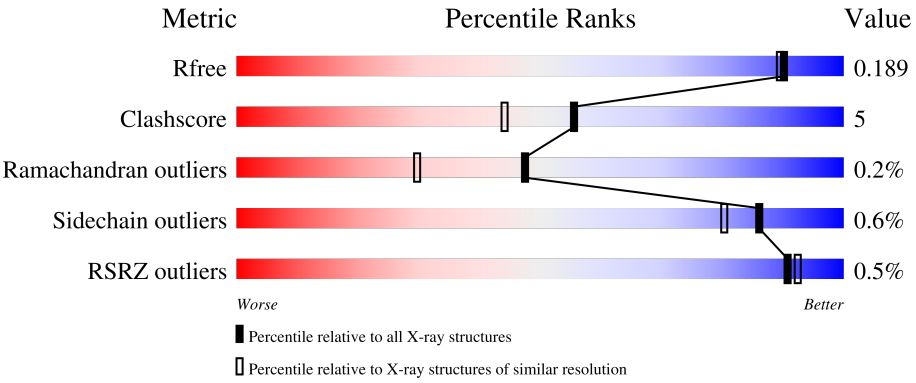
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	339	% 84% 8% 8%
1	B	339	83% 8% 9%
2	C	6	100%
2	D	6	33% 67%
2	E	6	33% 67%

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Mol	Chain	Length	Quality of chain
2	F	6	17% 67% 17%

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	GLC	D	1	X	-	-	-
2	GLC	D	3	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6657 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 CYMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	30	9	0
			2645	1689	441	513	2			
1	B	309	Total	C	N	O	S	12	6	0
			2597	1656	433	506	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q48391
A	-13	ASN	-	expression tag	UNP Q48391
A	-12	VAL	-	expression tag	UNP Q48391
A	-11	ARG	-	expression tag	UNP Q48391
A	-10	LEU	-	expression tag	UNP Q48391
A	-9	GLN	-	expression tag	UNP Q48391
A	-8	HIS	-	expression tag	UNP Q48391
A	-7	HIS	-	expression tag	UNP Q48391
A	-6	HIS	-	expression tag	UNP Q48391
A	-5	HIS	-	expression tag	UNP Q48391
A	-4	HIS	-	expression tag	UNP Q48391
A	-3	HIS	-	expression tag	UNP Q48391
A	-2	HIS	-	expression tag	UNP Q48391
A	-1	LEU	-	expression tag	UNP Q48391
A	0	GLU	-	expression tag	UNP Q48391
B	-14	ALA	-	expression tag	UNP Q48391
B	-13	ASN	-	expression tag	UNP Q48391
B	-12	VAL	-	expression tag	UNP Q48391
B	-11	ARG	-	expression tag	UNP Q48391
B	-10	LEU	-	expression tag	UNP Q48391
B	-9	GLN	-	expression tag	UNP Q48391
B	-8	HIS	-	expression tag	UNP Q48391
B	-7	HIS	-	expression tag	UNP Q48391
B	-6	HIS	-	expression tag	UNP Q48391
B	-5	HIS	-	expression tag	UNP Q48391

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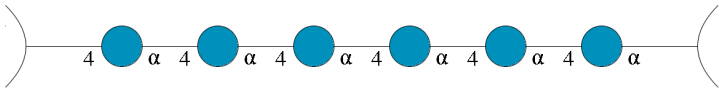
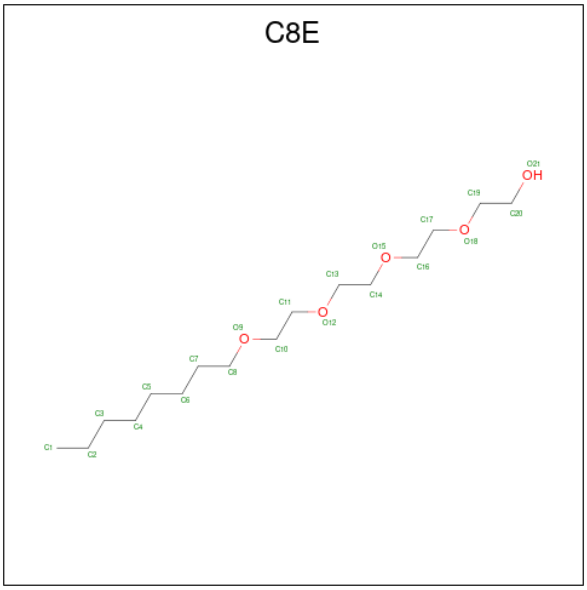
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q48391
B	-3	HIS	-	expression tag	UNP Q48391
B	-2	HIS	-	expression tag	UNP Q48391
B	-1	LEU	-	expression tag	UNP Q48391
B	0	GLU	-	expression tag	UNP Q48391

- Molecule 2 is an oligosaccharide called Cyclohexakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	6	Total C O 66 36 30	0	0	0
2	D	6	Total C O 66 36 30	0	0	0
2	E	6	Total C O 66 36 30	0	0	0
2	F	6	Total C O 66 36 30	0	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 8 5 3	0	0
3	A	1	Total C O 19 14 5	0	0
3	A	1	Total C O 17 12 5	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C O 16 11 5	0	0
3	A	1	Total C O 12 9 3	0	0
3	A	1	Total C O 11 10 1	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 13 9 4	0	0
3	A	1	Total C O 9 8 1	0	0
3	B	1	Total C O 21 16 5	0	0
3	B	1	Total C O 16 12 4	0	0
3	B	1	Total C O 12 10 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 9 6 3	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 13 9 4	0	0
3	B	1	Total C O 9 6 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 19 16 3	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 7 6 1	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 13 10 3	3	0

- Molecule 4 is water.

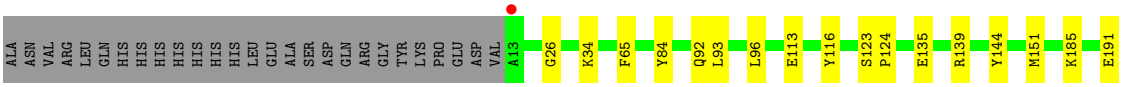
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	423	Total O 423 423	0	0
4	B	362	Total O 362 362	0	0

3 Residue-property plots (i)

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

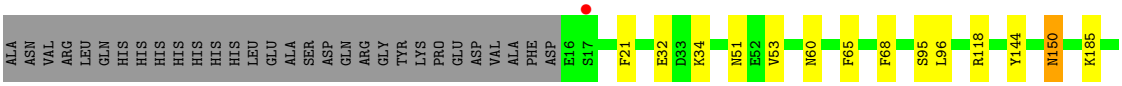
• Molecule 1: CYMA

Chain A:



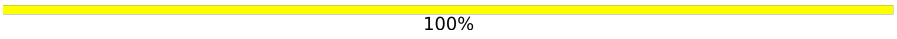
• Molecule 1: CYMA

Chain B:



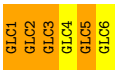
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain C:



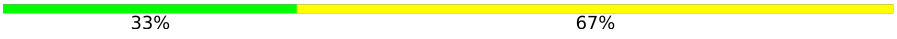
• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

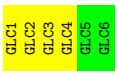
Chain D:



• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

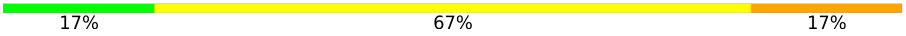
Chain E:





• Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.56Å 77.40Å 110.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.05 – 1.70 47.10 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.05-1.70) 96.1 (47.10-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.167 , 0.190 0.174 , 0.189	Depositor DCC
R_{free} test set	1999 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6657	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% 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: C8E, GLC

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	0.39	0/2734	0.52	0/3689
1	B	0.37	0/2685	0.53	0/3620
All	All	0.38	0/5419	0.53	0/7309

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2645	0	2488	24	0
1	B	2597	0	2436	27	0
2	C	66	0	54	0	0
2	D	66	0	54	6	0
2	E	66	0	54	0	0
2	F	66	0	54	1	0
3	A	169	0	236	13	0
3	B	197	0	290	15	0
4	A	423	0	0	8	4
4	B	362	0	0	5	4
All	All	6657	0	5666	58	4

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 (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:OE2	4:B:2323:HOH:O	1.93	0.86
1:A:139:ARG:NH2	2:D:3:GLC:H62	1.97	0.80
1:B:51:ASN:HD21	3:B:1334:C8E:H102	1.48	0.79
1:A:34:LYS:HD2	4:A:2026:HOH:O	1.87	0.75
1:B:316:PHE:HB2	3:B:1333:C8E:H71	1.72	0.72
1:B:118:ARG:NH1	4:B:2169:HOH:O	2.24	0.70
1:B:144:TYR:HE2	3:B:1340:C8E:H52	1.60	0.67
1:A:295:GLU:OE2	4:A:2373:HOH:O	2.14	0.65
1:A:135:GLU:OE2	4:A:2203:HOH:O	2.14	0.65
1:B:288:TYR:CE1	3:B:1332:C8E:H112	2.32	0.64
1:A:139:ARG:HH22	2:D:3:GLC:H62	1.61	0.63
1:A:198:TYR:HB2	3:A:1330:C8E:H171	1.81	0.63
3:A:1327:C8E:H142	1:B:53:VAL:HB	1.82	0.62
4:B:2142:HOH:O	2:F:3:GLC:H62	2.04	0.56
1:B:278:ILE:HG22	3:B:1329:C8E:H82	1.89	0.54
1:B:150:ASN:ND2	4:B:2189:HOH:O	2.40	0.53
1:A:144:TYR:HE2	3:A:1332:C8E:H102	1.73	0.52
1:A:92:GLN:HE21	3:A:1331:C8E:H171	1.75	0.52
1:B:51:ASN:ND2	3:B:1334:C8E:H102	2.22	0.52
1:A:275:GLU:OE1	4:A:2353:HOH:O	2.18	0.51
1:B:288:TYR:CZ	3:B:1332:C8E:H112	2.46	0.50
1:A:185:LYS:NZ	3:A:1334:C8E:H161	2.27	0.50
4:A:2183:HOH:O	1:B:324:PHE:OXT	2.18	0.50
1:A:116:TYR:HB2	3:A:1331:C8E:H172	1.94	0.49
4:A:2149:HOH:O	2:D:2:GLC:H61	2.12	0.49
1:A:65:PHE:HZ	1:A:96:LEU:HD22	1.78	0.49
1:B:323:ARG:NH2	4:B:2314:HOH:O	2.45	0.49
1:A:191:GLU:HB3	1:A:228:GLN:HG2	1.95	0.48
1:A:151:MET:HG2	1:A:185:LYS:HG3	1.96	0.48
3:A:1331:C8E:H112	1:B:21:PHE:HB2	1.94	0.48
1:B:32[A]:GLU:OE2	1:B:34:LYS:HD2	2.14	0.48
1:B:51:ASN:ND2	3:B:1334:C8E:H71	2.27	0.48
1:A:26:GLY:HA2	3:A:1327:C8E:H101	1.95	0.48
1:B:268:ARG:HB3	3:B:1343:C8E:H42	1.95	0.47
1:A:319:GLN:OE1	2:D:5:GLC:H2	2.14	0.47
1:B:185:LYS:HD2	3:B:1338:C8E:H161	1.96	0.47
1:B:190:TRP:CH2	3:B:1339:C8E:H41	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PHE:HB3	1:B:95:SER:HB3	1.98	0.46
1:A:93:LEU:HD11	1:A:113:GLU:HG2	1.98	0.45
3:A:1328:C8E:H171	3:A:1328:C8E:H142	1.76	0.44
4:A:2150:HOH:O	2:D:2:GLC:H61	2.17	0.44
1:A:316:PHE:CD2	3:A:1336:C8E:H71	2.53	0.44
3:A:1327:C8E:H102	3:A:1327:C8E:H132	1.69	0.44
1:A:286:ALA:HB1	3:A:1328:C8E:H191	1.99	0.43
1:B:237:LEU:HD23	3:B:1339:C8E:H51	2.01	0.42
1:A:84:TYR:CE1	1:A:124:PRO:HD3	2.55	0.42
1:B:231:PHE:HB2	1:B:234:ALA:HB3	2.00	0.42
3:A:1331:C8E:H202	3:A:1331:C8E:H102	2.02	0.42
3:B:1327:C8E:H31	3:B:1331:C8E:H51	2.01	0.42
1:B:65:PHE:HZ	1:B:96:LEU:HD22	1.84	0.41
1:B:225:PRO:HD2	1:B:241:VAL:O	2.19	0.41
1:A:123:SER:HB2	1:A:124:PRO:HD2	2.03	0.41
1:A:139:ARG:HH22	2:D:3:GLC:C6	2.31	0.41
1:B:21:PHE:CE2	1:B:60:ASN:HB2	2.55	0.41
1:A:240:ARG:NH2	4:A:2308:HOH:O	2.54	0.41
1:B:185:LYS:HD3	3:B:1338:C8E:H201	2.02	0.41
1:B:282:TRP:CD1	3:B:1329:C8E:H71	2.56	0.41

All (4) 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)
4:A:2088:HOH:O	4:B:2201:HOH:O[2_765]	1.93	0.27
4:A:2210:HOH:O	4:B:2327:HOH:O[4_555]	2.00	0.20
4:A:2086:HOH:O	4:B:2166:HOH:O[4_555]	2.09	0.11
4:A:2144:HOH:O	4:B:2069:HOH:O[2_755]	2.10	0.10

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	319/339 (94%)	315 (99%)	3 (1%)	1 (0%)	41 24
1	B	313/339 (92%)	309 (99%)	4 (1%)	0	100 100
All	All	632/678 (93%)	624 (99%)	7 (1%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ALA

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	280/295 (95%)	279 (100%)	1 (0%)	91 87
1	B	274/295 (93%)	272 (99%)	2 (1%)	84 77
All	All	554/590 (94%)	551 (100%)	3 (0%)	86 83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	B	150	ASN
1	B	319	GLN

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

Mol	Chain	Res	Type
1	B	51	ASN

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)

24 monosaccharides 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	GLC	C	1	2	11,11,12	0.37	0	15,15,17	1.80	3 (20%)
2	GLC	C	2	2	11,11,12	0.58	0	15,15,17	0.97	1 (6%)
2	GLC	C	3	2	11,11,12	0.55	0	15,15,17	1.65	1 (6%)
2	GLC	C	4	2	11,11,12	0.40	0	15,15,17	0.92	1 (6%)
2	GLC	C	5	2	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
2	GLC	C	6	2	11,11,12	0.64	0	15,15,17	0.99	1 (6%)
2	GLC	D	1	2	11,11,12	0.42	0	15,15,17	2.31	3 (20%)
2	GLC	D	2	2	11,11,12	0.53	0	15,15,17	2.17	6 (40%)
2	GLC	D	3	2	11,11,12	0.47	0	15,15,17	2.77	6 (40%)
2	GLC	D	4	2	11,11,12	0.33	0	15,15,17	0.90	1 (6%)
2	GLC	D	5	2	11,11,12	0.47	0	15,15,17	1.45	4 (26%)
2	GLC	D	6	2	11,11,12	0.73	0	15,15,17	1.95	4 (26%)
2	GLC	E	1	2	11,11,12	0.40	0	15,15,17	1.53	3 (20%)
2	GLC	E	2	2	11,11,12	0.46	0	15,15,17	1.79	4 (26%)
2	GLC	E	3	2	11,11,12	0.41	0	15,15,17	1.78	2 (13%)
2	GLC	E	4	2	11,11,12	0.28	0	15,15,17	0.86	1 (6%)
2	GLC	E	5	2	11,11,12	0.57	0	15,15,17	0.97	0
2	GLC	E	6	2	11,11,12	0.59	0	15,15,17	0.90	0
2	GLC	F	1	2	11,11,12	0.49	0	15,15,17	1.76	3 (20%)
2	GLC	F	2	2	11,11,12	0.56	0	15,15,17	2.11	4 (26%)
2	GLC	F	3	2	11,11,12	0.56	0	15,15,17	1.94	3 (20%)
2	GLC	F	4	2	11,11,12	0.43	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	F	5	2	11,11,12	0.56	0	15,15,17	1.26	2 (13%)
2	GLC	F	6	2	11,11,12	0.58	0	15,15,17	0.99	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	GLC	C	1	2	-	0/2/19/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	2/2/4/5	1/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	1/1/4/5	1/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	1/2/19/22	0/1/1/1
2	GLC	D	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/19/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/19/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	0/2/19/22	0/1/1/1
2	GLC	F	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	GLC	C1-O5-C5	6.36	120.81	112.19
2	D	1	GLC	C1-O5-C5	6.22	120.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	GLC	C1-O5-C5	5.85	120.11	112.19
2	C	1	GLC	C1-O5-C5	5.30	119.38	112.19
2	D	3	GLC	O5-C5-C6	5.17	115.31	107.20
2	C	3	GLC	C1-O5-C5	5.03	119.01	112.19
2	D	2	GLC	C1-O5-C5	4.99	118.95	112.19
2	F	3	GLC	C1-O5-C5	4.87	118.80	112.19
2	E	3	GLC	C1-O5-C5	4.73	118.60	112.19
2	E	2	GLC	C1-O5-C5	4.68	118.53	112.19
2	D	1	GLC	O5-C5-C6	4.59	114.40	107.20
2	D	6	GLC	C3-C4-C5	4.04	117.44	110.24
2	F	1	GLC	C1-O5-C5	4.03	117.65	112.19
2	E	1	GLC	C1-O5-C5	3.95	117.54	112.19
2	D	3	GLC	C1-C2-C3	3.94	114.51	109.67
2	F	1	GLC	C3-C4-C5	3.62	116.70	110.24
2	F	3	GLC	C3-C4-C5	3.61	116.68	110.24
2	F	2	GLC	C3-C4-C5	3.33	116.19	110.24
2	D	6	GLC	C2-C3-C4	3.31	116.62	110.89
2	E	2	GLC	O5-C5-C4	3.25	118.73	110.83
2	E	1	GLC	O5-C5-C6	3.25	112.29	107.20
2	D	2	GLC	O4-C4-C3	-3.21	102.93	110.35
2	D	2	GLC	O5-C5-C4	3.21	118.63	110.83
2	D	1	GLC	C1-C2-C3	3.16	113.55	109.67
2	D	6	GLC	C1-C2-C3	3.05	113.42	109.67
2	F	5	GLC	C1-O5-C5	3.05	116.32	112.19
2	D	2	GLC	C3-C4-C5	3.00	115.59	110.24
2	F	2	GLC	O5-C5-C4	2.99	118.11	110.83
2	D	5	GLC	C1-O5-C5	2.86	116.07	112.19
2	D	3	GLC	C3-C4-C5	2.85	115.33	110.24
2	C	1	GLC	O4-C4-C3	-2.80	103.89	110.35
2	D	3	GLC	O5-C1-C2	2.70	114.94	110.77
2	D	6	GLC	O4-C4-C5	-2.70	102.60	109.30
2	C	5	GLC	C1-O5-C5	2.68	115.82	112.19
2	F	1	GLC	O5-C5-C6	2.62	111.30	107.20
2	E	4	GLC	O4-C4-C3	-2.48	104.61	110.35
2	F	3	GLC	C2-C3-C4	2.40	115.05	110.89
2	D	2	GLC	C1-C2-C3	2.39	112.60	109.67
2	C	4	GLC	O4-C4-C3	-2.36	104.90	110.35
2	F	4	GLC	O4-C4-C3	-2.33	104.95	110.35
2	E	2	GLC	O4-C4-C3	-2.19	105.28	110.35
2	F	2	GLC	O4-C4-C3	-2.19	105.30	110.35
2	E	1	GLC	O4-C4-C3	-2.16	105.34	110.35
2	C	1	GLC	O6-C6-C5	-2.16	103.90	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C1-O5-C5	2.13	115.08	112.19
2	D	5	GLC	C3-C4-C5	2.13	114.03	110.24
2	E	2	GLC	O6-C6-C5	-2.13	104.00	111.29
2	D	2	GLC	C2-C3-C4	2.12	114.57	110.89
2	F	5	GLC	O5-C5-C4	2.06	115.85	110.83
2	D	3	GLC	C6-C5-C4	2.04	117.78	113.00
2	E	3	GLC	O3-C3-C2	2.03	113.88	109.99
2	D	4	GLC	O4-C4-C3	-2.03	105.66	110.35
2	C	6	GLC	O2-C2-C1	2.02	113.28	109.15
2	D	5	GLC	C1-C2-C3	2.02	112.15	109.67
2	D	5	GLC	O3-C3-C2	-2.01	106.14	109.99

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1	GLC	C2
2	D	1	GLC	C3
2	D	3	GLC	C2

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	5	GLC	C4-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	GLC	1	0

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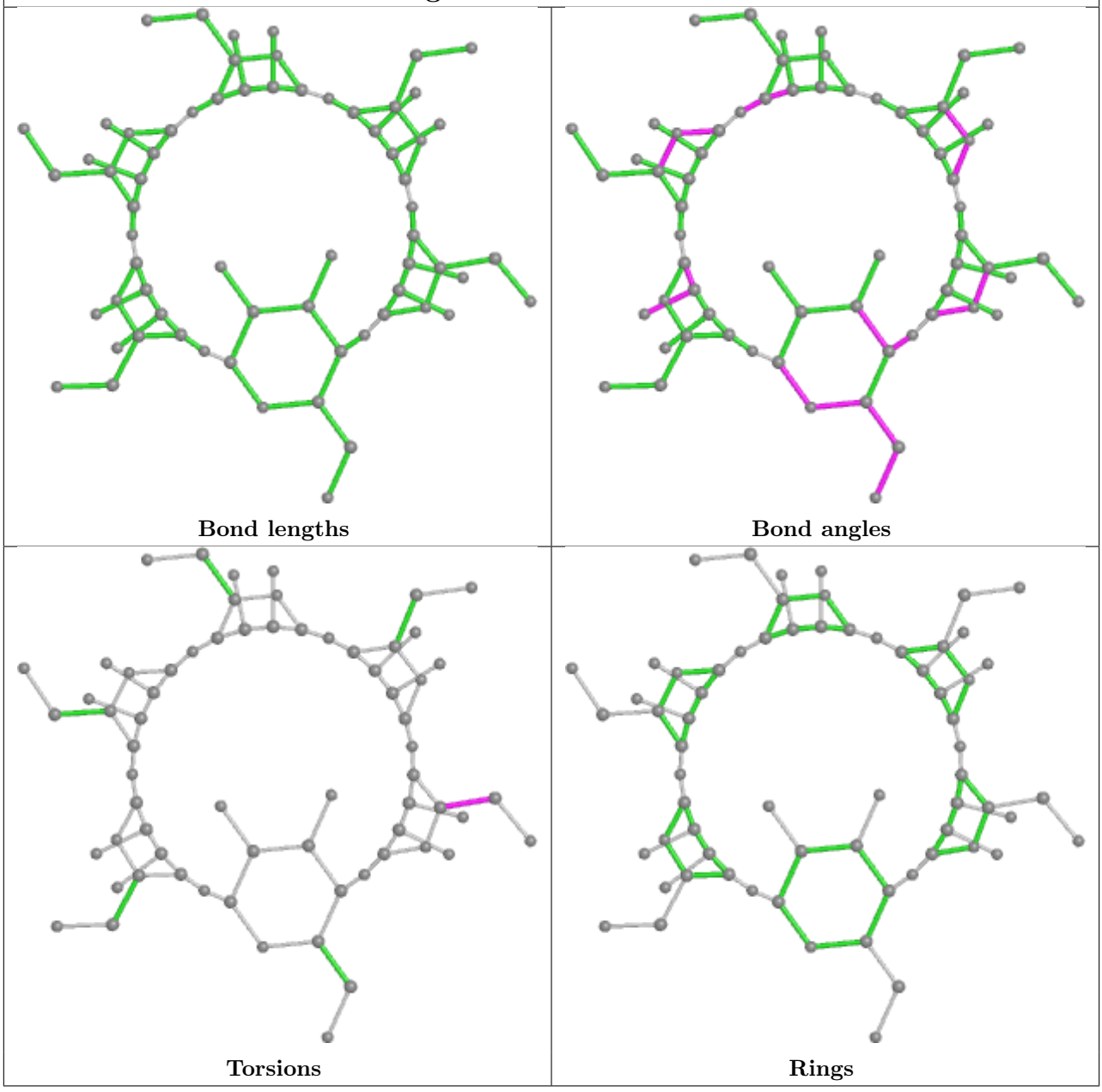
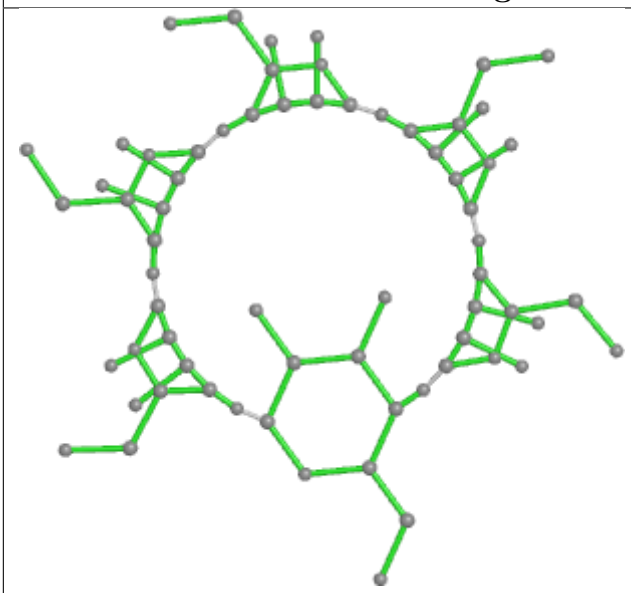
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	2	0
2	D	3	GLC	3	0
2	D	5	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

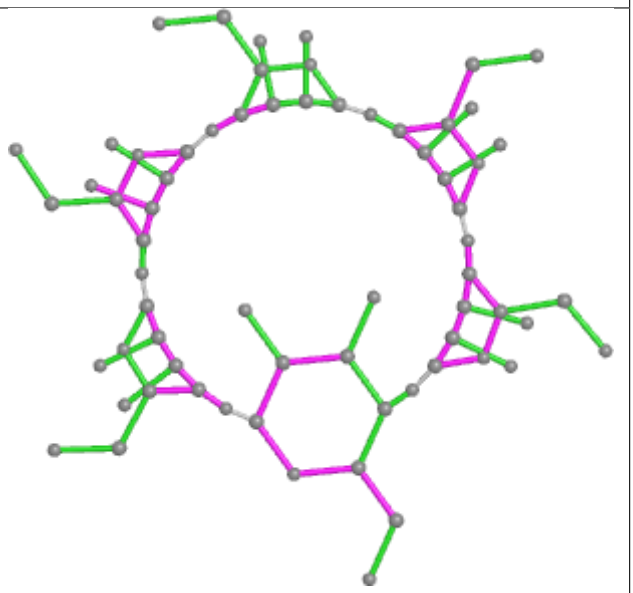
Oligosaccharide Chain C



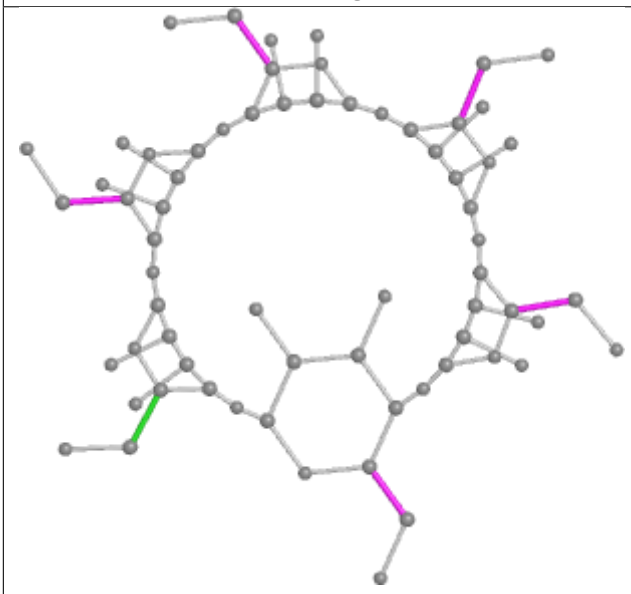
Oligosaccharide Chain D



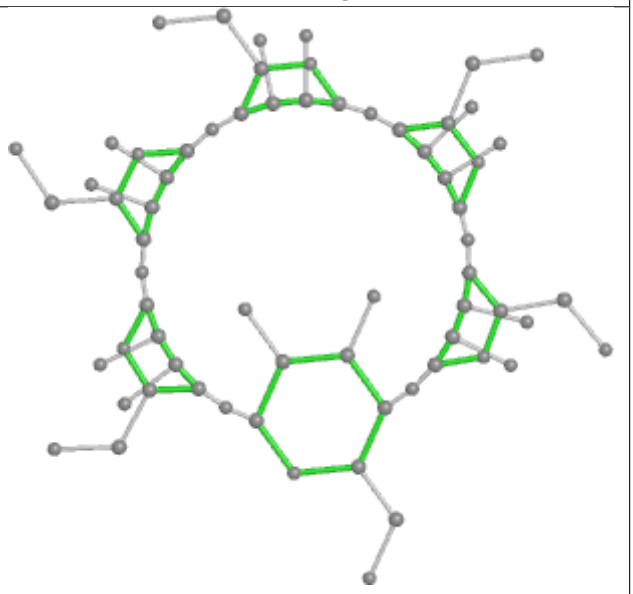
Bond lengths



Bond angles

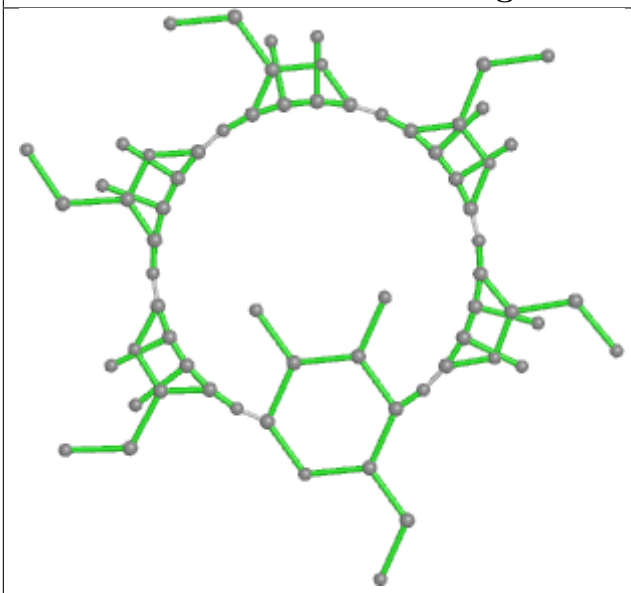


Torsions

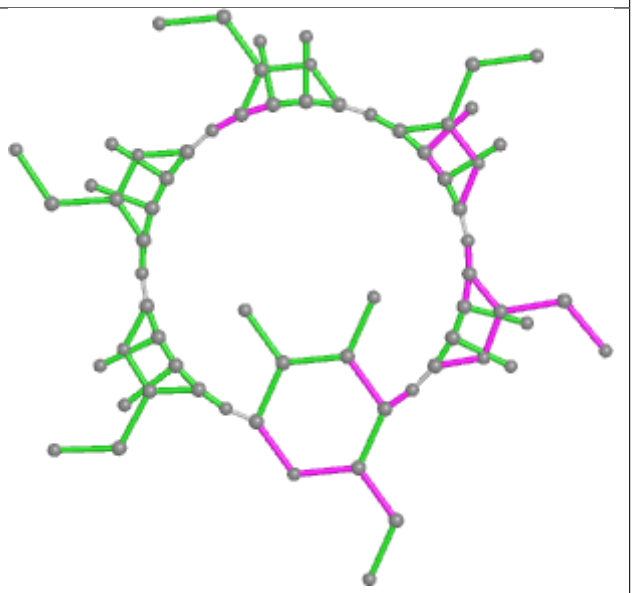


Rings

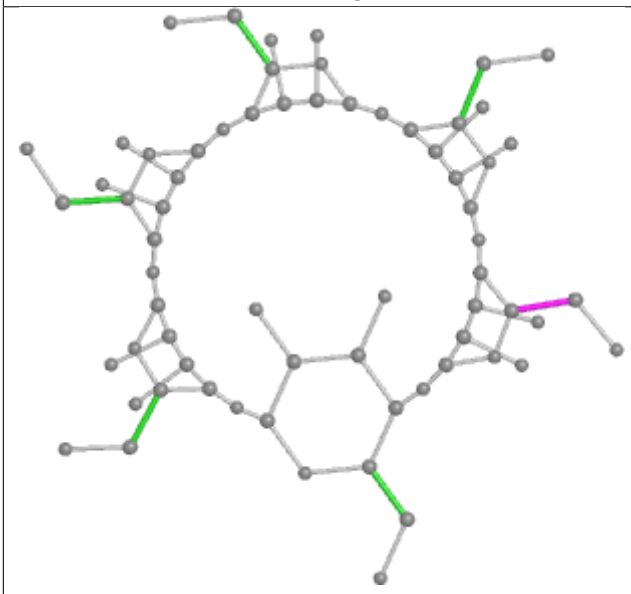
Oligosaccharide Chain E



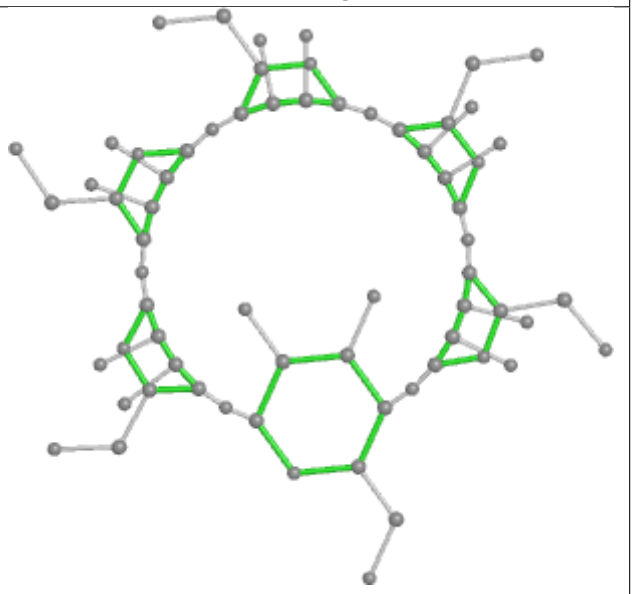
Bond lengths



Bond angles

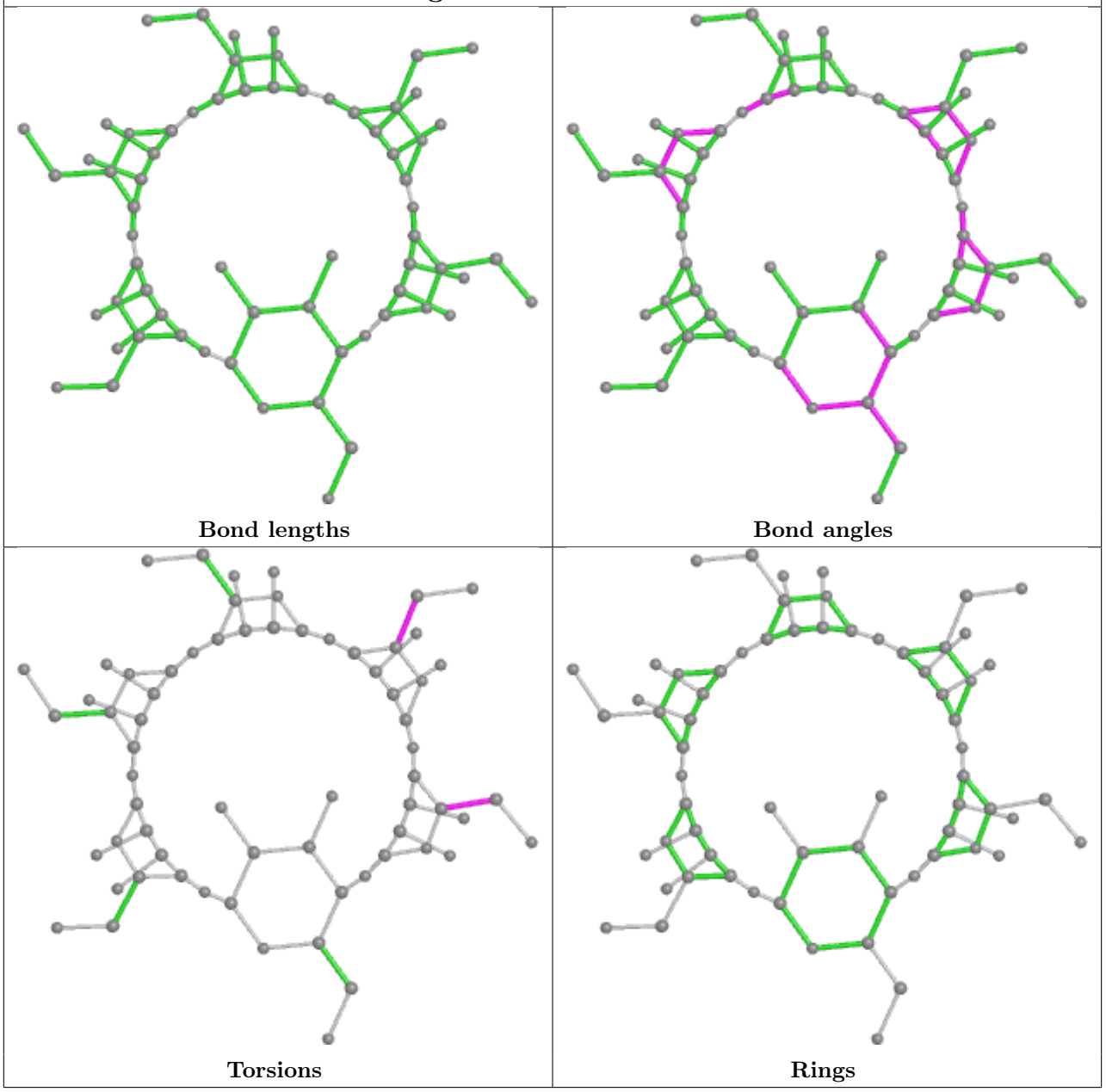


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

30 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	$\#\|Z\|>2$
3	C8E	A	1328	-	18,18,20	0.37	0	17,17,19	0.49	0
3	C8E	B	1332	-	8,8,20	0.45	0	7,7,19	0.43	0
3	C8E	B	1339	-	6,6,20	0.27	0	5,5,19	0.45	0
3	C8E	A	1337	-	20,20,20	0.44	0	19,19,19	0.35	0
3	C8E	B	1328	-	15,15,20	0.36	0	14,14,19	0.36	0
3	C8E	A	1338	-	12,12,20	0.46	0	11,11,19	0.18	0
3	C8E	B	1338	-	12,12,20	0.42	0	11,11,19	0.25	0
3	C8E	A	1339	-	8,8,20	0.26	0	7,7,19	0.48	0
3	C8E	B	1327	-	20,20,20	0.38	0	19,19,19	0.42	0
3	C8E	A	1332	-	11,11,20	0.44	0	10,10,19	0.37	0
3	C8E	B	1330	-	7,7,20	0.50	0	6,6,19	0.21	0
3	C8E	A	1327	-	7,7,20	0.36	0	6,6,19	0.24	0
3	C8E	A	1336	-	9,9,20	0.25	0	8,8,19	0.61	0
3	C8E	B	1342	-	6,6,20	0.25	0	5,5,19	0.51	0
3	C8E	B	1334	-	12,12,20	0.43	0	11,11,19	0.19	0
3	C8E	B	1336	-	6,6,20	0.25	0	5,5,19	0.41	0
3	C8E	B	1341	-	7,7,20	0.25	0	6,6,19	0.54	0
3	C8E	B	1331	-	13,13,20	0.38	0	12,12,19	0.43	0
3	C8E	B	1337	-	16,16,20	0.41	0	13,13,19	0.38	0
3	C8E	A	1329	-	15,15,20	0.35	0	13,13,19	0.35	0
3	C8E	A	1335	-	6,6,20	0.24	0	5,5,19	0.46	0
3	C8E	B	1335	-	8,8,20	0.47	0	7,7,19	0.57	0
3	C8E	B	1343	-	12,12,20	0.38	0	11,11,19	0.25	0
3	C8E	B	1333	-	13,13,20	0.38	0	12,12,19	0.57	0
3	C8E	B	1329	-	11,11,20	0.29	0	10,10,19	0.52	0
3	C8E	B	1340	-	6,6,20	0.25	0	5,5,19	0.40	0
3	C8E	A	1333	-	10,10,20	0.35	0	9,9,19	0.52	0
3	C8E	A	1331	-	15,15,20	0.43	0	14,14,19	0.39	0
3	C8E	A	1334	-	9,9,20	0.41	0	8,8,19	0.24	0
3	C8E	A	1330	-	14,14,20	0.34	0	12,12,19	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	1328	-	-	11/16/16/18	-
3	C8E	B	1332	-	-	4/6/6/18	-
3	C8E	B	1339	-	-	2/4/4/18	-
3	C8E	A	1337	-	-	8/18/18/18	-
3	C8E	B	1328	-	-	7/13/13/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	1338	-	-	6/10/10/18	-
3	C8E	B	1338	-	-	4/10/10/18	-
3	C8E	A	1339	-	-	6/6/6/18	-
3	C8E	B	1327	-	-	10/18/18/18	-
3	C8E	A	1332	-	-	3/9/9/18	-
3	C8E	B	1330	-	-	3/5/5/18	-
3	C8E	A	1327	-	-	4/5/5/18	-
3	C8E	A	1336	-	-	3/7/7/18	-
3	C8E	B	1342	-	-	2/4/4/18	-
3	C8E	B	1334	-	-	6/10/10/18	-
3	C8E	B	1336	-	-	2/4/4/18	-
3	C8E	B	1341	-	-	1/5/5/18	-
3	C8E	B	1331	-	-	6/11/11/18	-
3	C8E	B	1337	-	-	5/10/10/18	-
3	C8E	A	1329	-	-	6/11/11/18	-
3	C8E	A	1335	-	-	0/4/4/18	-
3	C8E	B	1335	-	-	4/6/6/18	-
3	C8E	B	1343	-	-	7/10/10/18	-
3	C8E	B	1333	-	-	6/11/11/18	-
3	C8E	B	1329	-	-	6/9/9/18	-
3	C8E	B	1340	-	-	3/4/4/18	-
3	C8E	A	1333	-	-	7/8/8/18	-
3	C8E	A	1331	-	-	6/13/13/18	-
3	C8E	A	1334	-	-	6/7/7/18	-
3	C8E	A	1330	-	-	9/10/10/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1335	C8E	C14-C13-O12-C11
3	B	1327	C8E	O12-C13-C14-O15
3	A	1328	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	B	1333	C8E	C3-C4-C5-C6
3	A	1338	C8E	O12-C13-C14-O15
3	B	1331	C8E	O9-C10-C11-O12
3	B	1332	C8E	O9-C10-C11-O12
3	A	1328	C8E	O18-C19-C20-O21
3	A	1334	C8E	O9-C10-C11-O12
3	B	1335	C8E	O9-C10-C11-O12
3	B	1338	C8E	O9-C10-C11-O12
3	B	1343	C8E	O12-C13-C14-O15
3	B	1328	C8E	O9-C10-C11-O12
3	A	1328	C8E	C6-C7-C8-O9
3	B	1331	C8E	C6-C7-C8-O9
3	A	1329	C8E	O15-C16-C17-O18
3	B	1328	C8E	C6-C7-C8-O9
3	A	1328	C8E	C3-C4-C5-C6
3	B	1327	C8E	O18-C19-C20-O21
3	B	1332	C8E	O12-C13-C14-O15
3	B	1327	C8E	C2-C3-C4-C5
3	A	1333	C8E	C2-C3-C4-C5
3	A	1339	C8E	C2-C3-C4-C5
3	B	1333	C8E	C4-C5-C6-C7
3	B	1340	C8E	C4-C5-C6-C7
3	B	1343	C8E	C4-C5-C6-C7
3	A	1334	C8E	O15-C16-C17-O18
3	A	1336	C8E	C3-C4-C5-C6
3	B	1339	C8E	C2-C3-C4-C5
3	A	1330	C8E	C7-C8-O9-C10
3	A	1336	C8E	C7-C8-O9-C10
3	A	1337	C8E	C6-C7-C8-O9
3	A	1333	C8E	C3-C4-C5-C6
3	A	1329	C8E	C17-C16-O15-C14
3	A	1333	C8E	C6-C7-C8-O9
3	A	1327	C8E	O9-C10-C11-O12
3	A	1327	C8E	O12-C13-C14-O15
3	B	1342	C8E	C3-C4-C5-C6
3	A	1339	C8E	C3-C4-C5-C6
3	B	1329	C8E	C4-C5-C6-C7
3	A	1339	C8E	C4-C5-C6-C7
3	A	1330	C8E	O18-C19-C20-O21
3	A	1331	C8E	O18-C19-C20-O21
3	A	1337	C8E	O18-C19-C20-O21
3	B	1327	C8E	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	1328	C8E	C4-C5-C6-C7
3	B	1331	C8E	C2-C3-C4-C5
3	B	1329	C8E	C1-C2-C3-C4
3	B	1343	C8E	C6-C7-C8-O9
3	B	1340	C8E	C6-C7-C8-O9
3	A	1333	C8E	C1-C2-C3-C4
3	A	1330	C8E	O15-C16-C17-O18
3	B	1331	C8E	C14-C13-O12-C11
3	B	1328	C8E	C16-C17-O18-C19
3	B	1329	C8E	C3-C4-C5-C6
3	A	1337	C8E	O12-C13-C14-O15
3	B	1332	C8E	C7-C8-O9-C10
3	A	1338	C8E	C20-C19-O18-C17
3	B	1336	C8E	C3-C4-C5-C6
3	B	1342	C8E	C4-C5-C6-C7
3	B	1335	C8E	C17-C16-O15-C14
3	A	1327	C8E	C13-C14-O15-C16
3	B	1341	C8E	C4-C5-C6-C7
3	B	1338	C8E	O15-C16-C17-O18
3	B	1333	C8E	C6-C7-C8-O9
3	A	1329	C8E	C6-C7-C8-O9
3	B	1327	C8E	C11-C10-O9-C8
3	A	1329	C8E	O18-C19-C20-O21
3	B	1327	C8E	C16-C17-O18-C19
3	B	1327	C8E	C13-C14-O15-C16
3	B	1338	C8E	C20-C19-O18-C17
3	B	1327	C8E	C20-C19-O18-C17
3	A	1330	C8E	C6-C7-C8-O9
3	A	1328	C8E	C10-C11-O12-C13
3	B	1337	C8E	C13-C14-O15-C16
3	A	1339	C8E	C5-C6-C7-C8
3	B	1337	C8E	C14-C13-O12-C11
3	A	1337	C8E	C14-C13-O12-C11
3	A	1338	C8E	C14-C13-O12-C11
3	B	1343	C8E	C14-C13-O12-C11
3	B	1328	C8E	C17-C16-O15-C14
3	B	1343	C8E	C10-C11-O12-C13
3	A	1339	C8E	C6-C7-C8-O9
3	A	1328	C8E	C17-C16-O15-C14
3	B	1335	C8E	C13-C14-O15-C16
3	A	1330	C8E	C16-C17-O18-C19
3	B	1337	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	1329	C8E	C5-C6-C7-C8
3	B	1329	C8E	O9-C10-C11-O12
3	B	1329	C8E	C7-C8-O9-C10
3	A	1331	C8E	C20-C19-O18-C17
3	A	1327	C8E	C10-C11-O12-C13
3	B	1334	C8E	C10-C11-O12-C13
3	A	1329	C8E	C7-C8-O9-C10
3	A	1331	C8E	C7-C8-O9-C10
3	B	1343	C8E	C7-C8-O9-C10
3	A	1330	C8E	C17-C16-O15-C14
3	B	1331	C8E	C10-C11-O12-C13
3	A	1332	C8E	C11-C10-O9-C8
3	B	1334	C8E	O12-C13-C14-O15
3	A	1337	C8E	C16-C17-O18-C19
3	A	1336	C8E	C1-C2-C3-C4
3	B	1331	C8E	C7-C8-O9-C10
3	A	1331	C8E	C14-C13-O12-C11
3	A	1334	C8E	C17-C16-O15-C14
3	A	1337	C8E	C7-C8-O9-C10
3	B	1333	C8E	C7-C8-O9-C10
3	A	1334	C8E	C13-C14-O15-C16
3	B	1328	C8E	C10-C11-O12-C13
3	A	1334	C8E	C14-C13-O12-C11
3	A	1333	C8E	C7-C8-O9-C10
3	B	1339	C8E	C3-C4-C5-C6
3	A	1331	C8E	C17-C16-O15-C14
3	B	1327	C8E	C10-C11-O12-C13
3	A	1337	C8E	C3-C4-C5-C6
3	B	1337	C8E	C3-C4-C5-C6
3	A	1337	C8E	C17-C16-O15-C14
3	B	1338	C8E	C16-C17-O18-C19
3	A	1330	C8E	C4-C5-C6-C7
3	A	1330	C8E	C3-C4-C5-C6
3	B	1332	C8E	C14-C13-O12-C11
3	A	1333	C8E	C11-C10-O9-C8
3	B	1329	C8E	C6-C7-C8-O9
3	B	1330	C8E	C14-C13-O12-C11
3	B	1343	C8E	O9-C10-C11-O12
3	B	1337	C8E	C10-C11-O12-C13
3	A	1334	C8E	C10-C11-O12-C13
3	A	1330	C8E	C20-C19-O18-C17
3	B	1334	C8E	C14-C13-O12-C11

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Mol	Chain	Res	Type	Atoms
3	A	1339	C8E	C1-C2-C3-C4
3	B	1334	C8E	C7-C8-O9-C10
3	B	1333	C8E	O9-C10-C11-O12
3	A	1332	C8E	O12-C13-C14-O15
3	B	1334	C8E	O9-C10-C11-O12
3	B	1340	C8E	C5-C6-C7-C8
3	A	1328	C8E	C7-C8-O9-C10
3	A	1328	C8E	C20-C19-O18-C17
3	B	1336	C8E	C4-C5-C6-C7
3	B	1334	C8E	C6-C7-C8-O9
3	B	1330	C8E	C11-C10-O9-C8
3	B	1330	C8E	C7-C8-O9-C10
3	A	1338	C8E	C11-C10-O9-C8
3	A	1332	C8E	C17-C16-O15-C14
3	A	1333	C8E	C4-C5-C6-C7
3	A	1338	C8E	O15-C16-C17-O18
3	A	1331	C8E	C10-C11-O12-C13
3	B	1333	C8E	C14-C13-O12-C11
3	B	1328	C8E	O15-C16-C17-O18
3	B	1328	C8E	O12-C13-C14-O15
3	A	1328	C8E	O15-C16-C17-O18
3	B	1327	C8E	O15-C16-C17-O18
3	A	1328	C8E	O9-C10-C11-O12
3	A	1338	C8E	O9-C10-C11-O12

There are no ring outliers.

17 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1328	C8E	2	0
3	B	1332	C8E	2	0
3	B	1339	C8E	2	0
3	B	1338	C8E	2	0
3	B	1327	C8E	1	0
3	A	1332	C8E	1	0
3	A	1327	C8E	3	0
3	A	1336	C8E	1	0
3	B	1334	C8E	3	0
3	B	1331	C8E	1	0
3	B	1343	C8E	1	0
3	B	1333	C8E	1	0
3	B	1329	C8E	2	0

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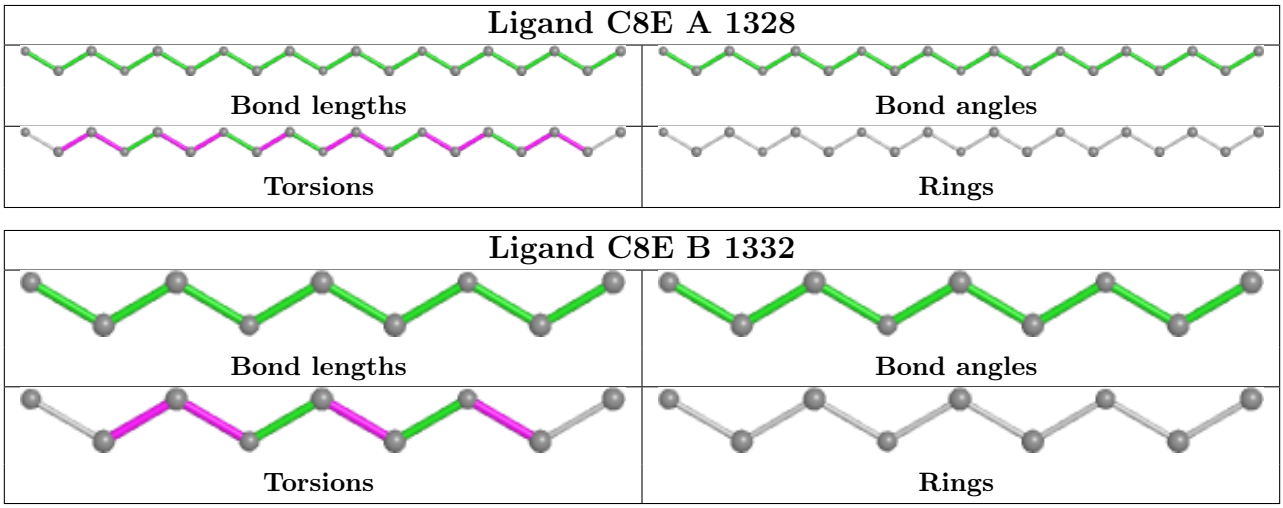
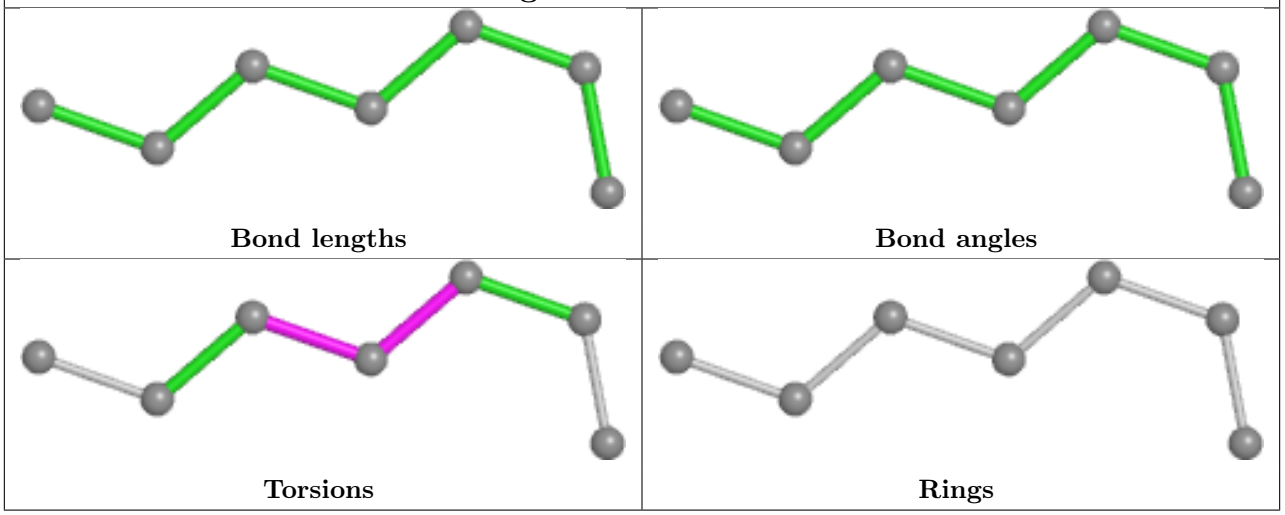
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1340	C8E	1	0
3	A	1331	C8E	4	0
3	A	1334	C8E	1	0
3	A	1330	C8E	1	0

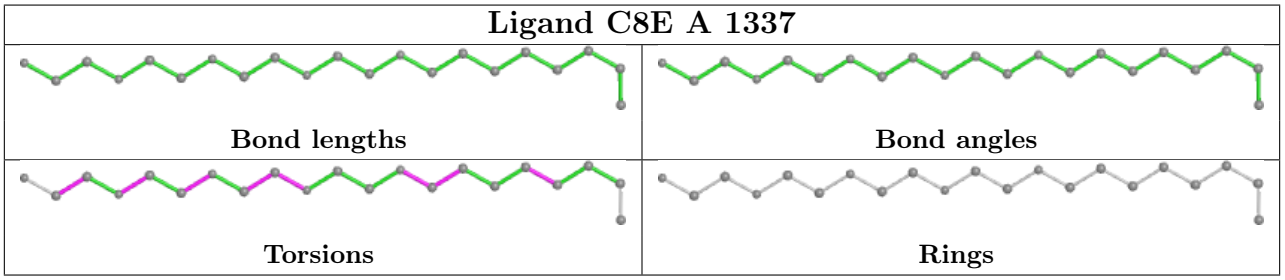
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



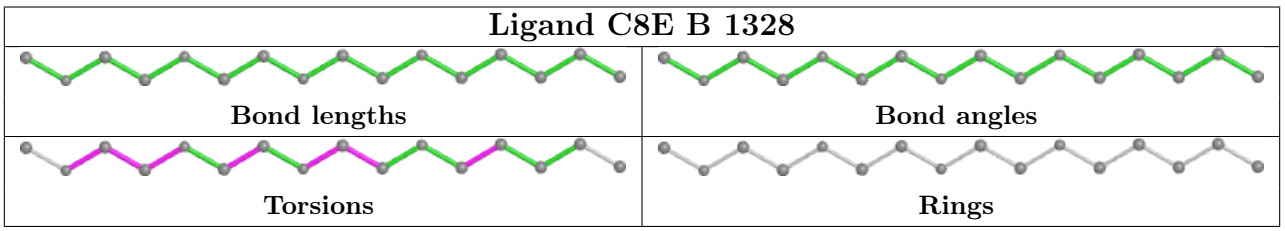
Ligand C8E B 1339



Ligand C8E A 1337



Ligand C8E B 1328



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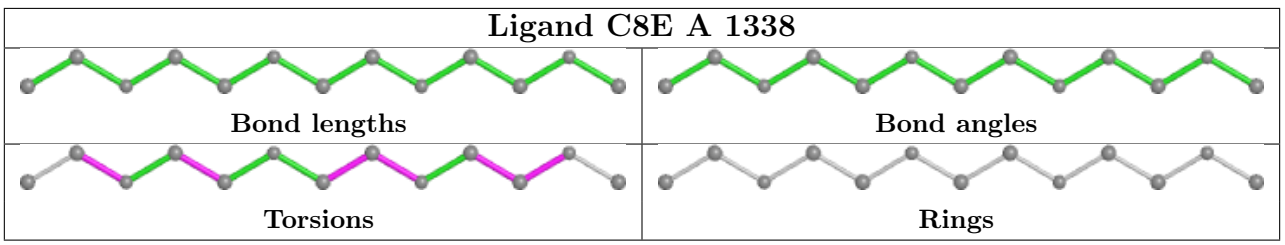

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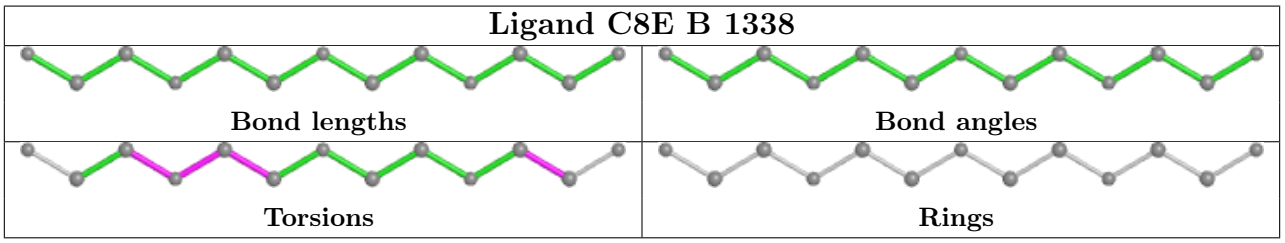
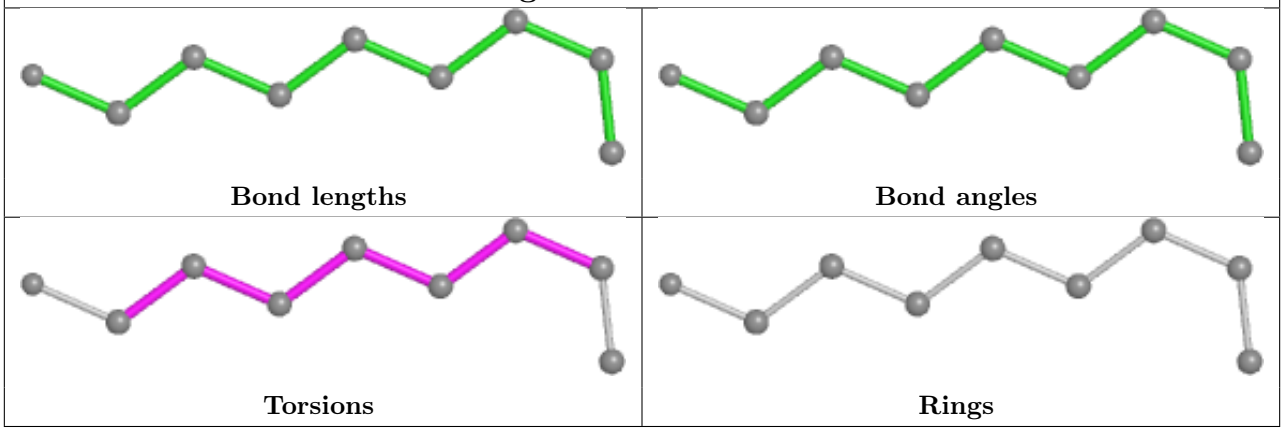


Ligand C8E A 1339



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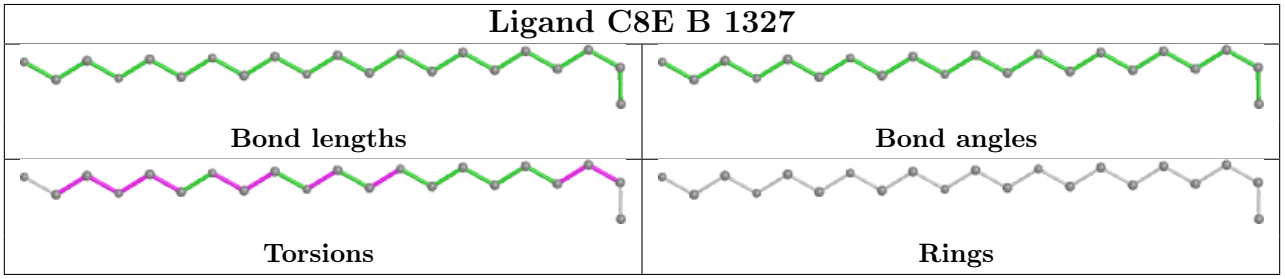
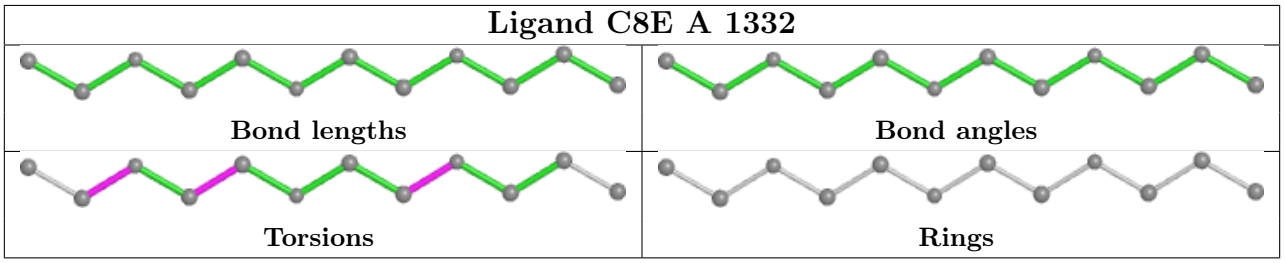
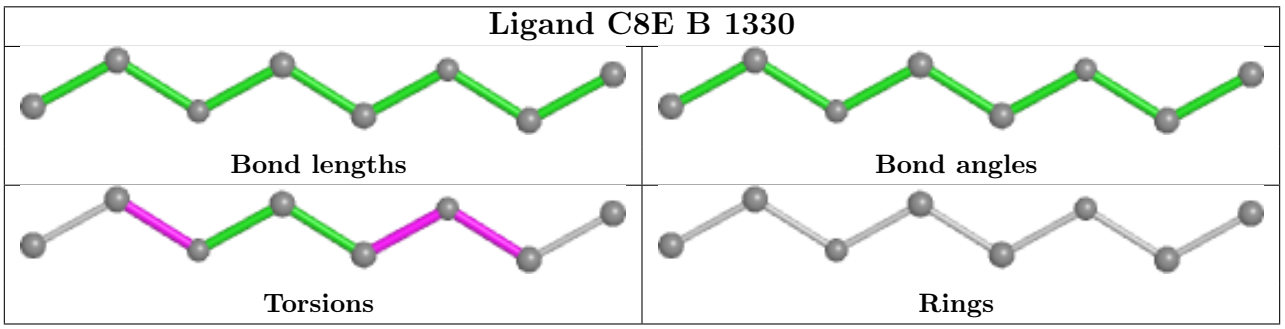


Ligand C8E A 1332



Ligand C8E B 1330



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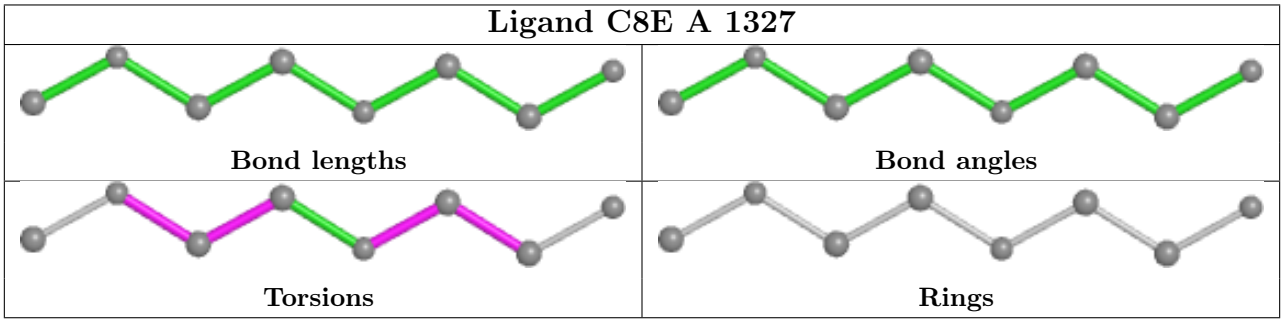
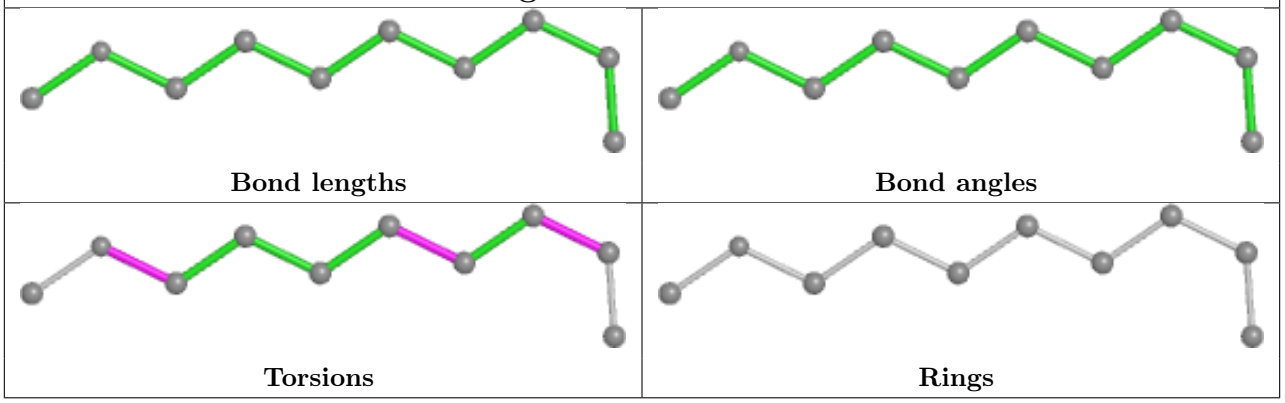
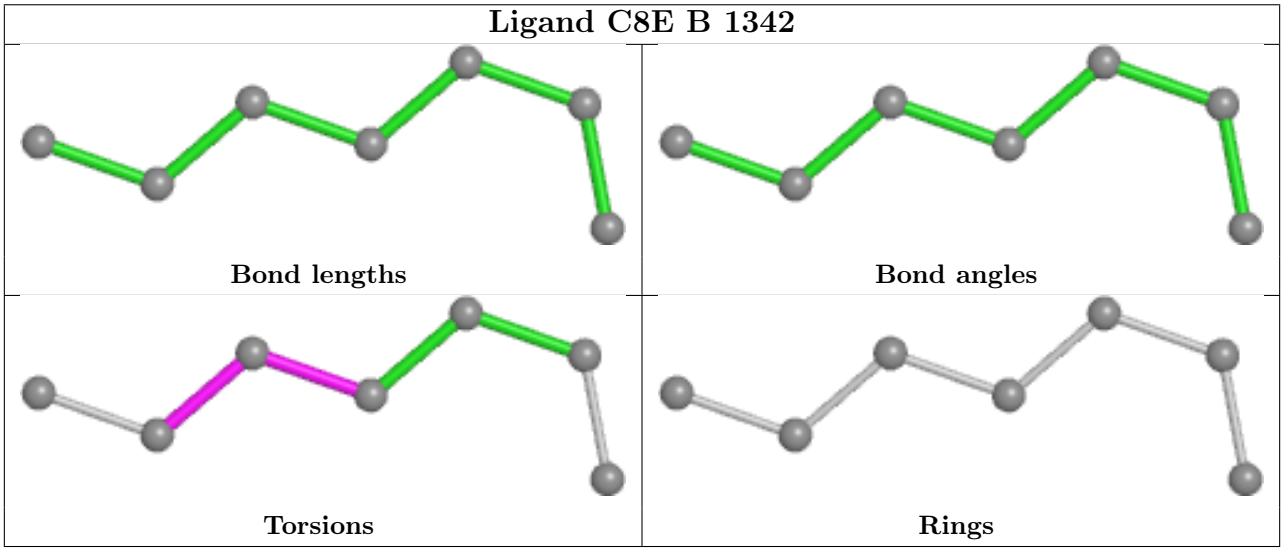


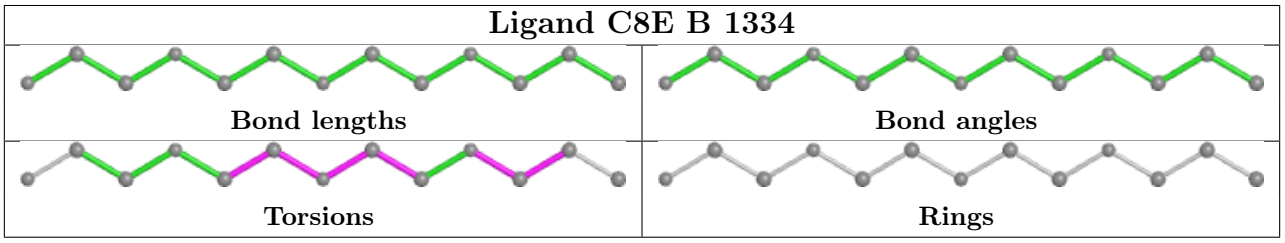
Ligand C8E A 1336



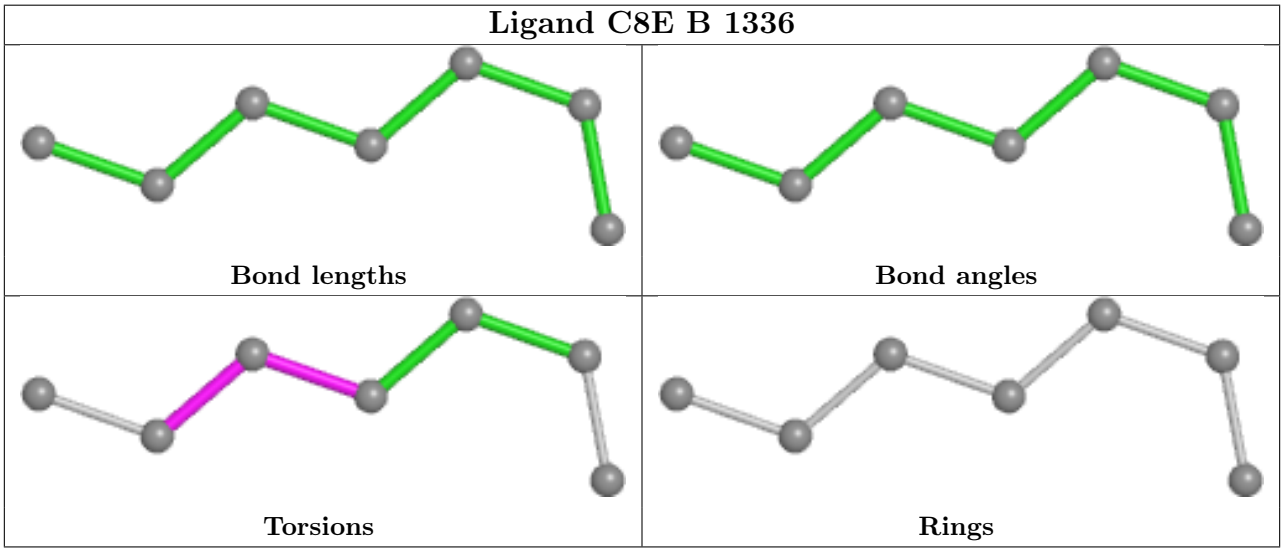
Ligand C8E B 1342



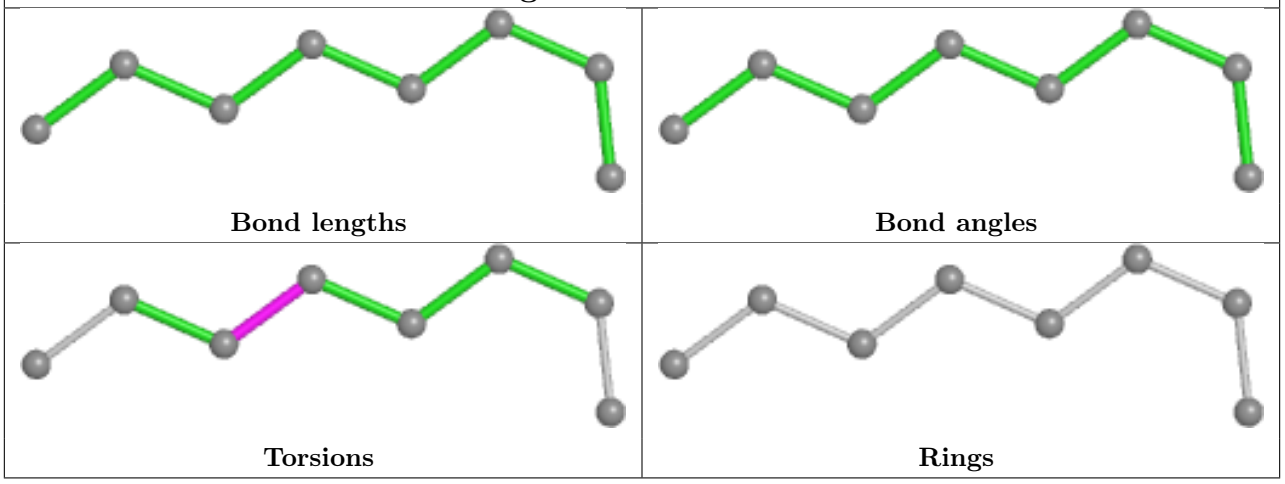
Ligand C8E B 1334



Ligand C8E B 1336



Ligand C8E B 1341



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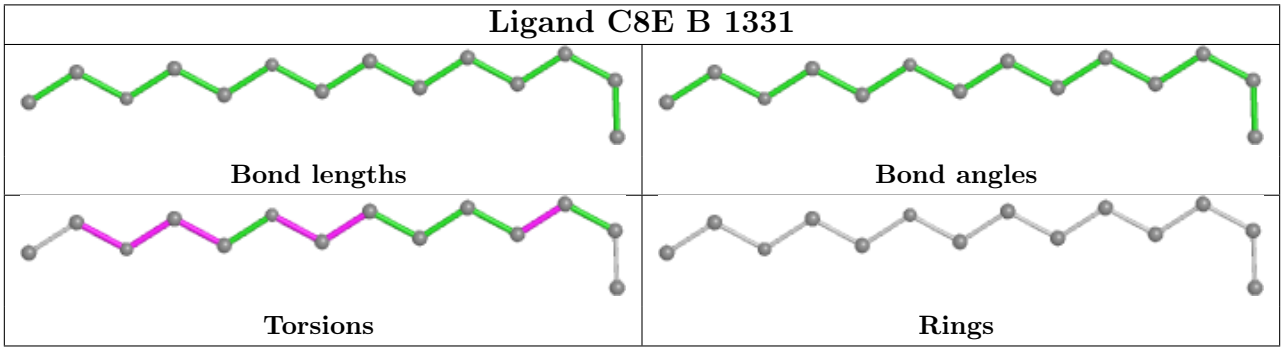

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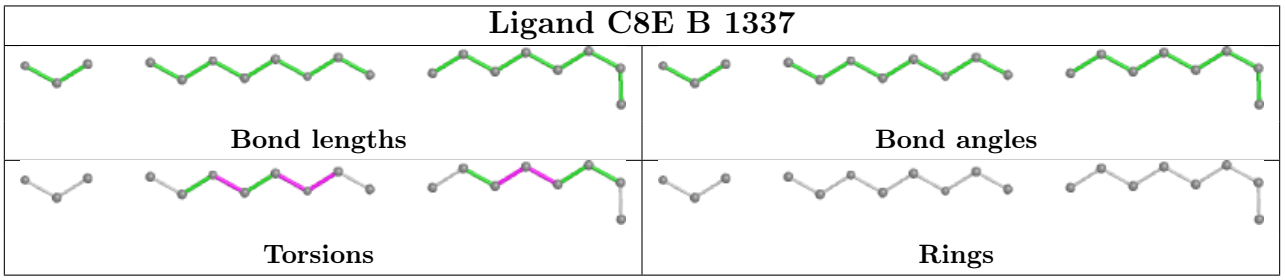

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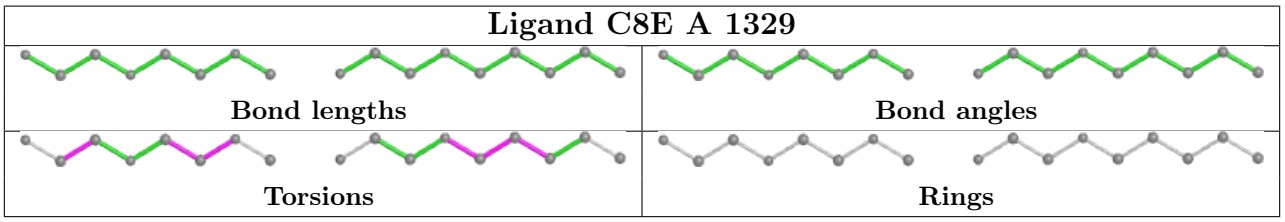

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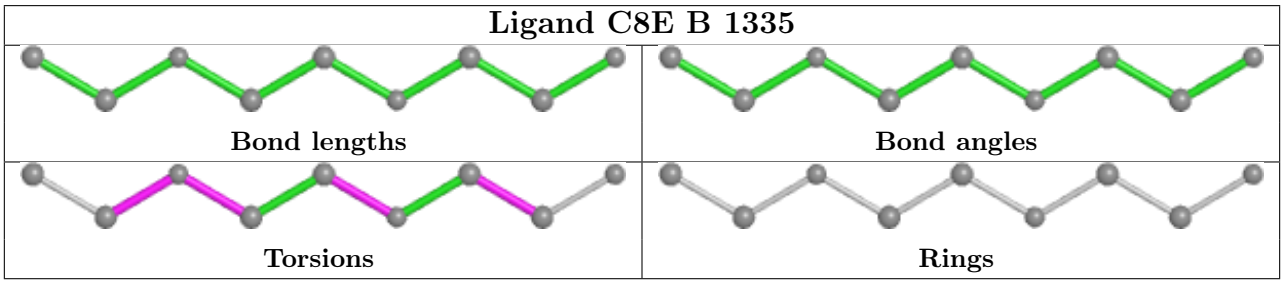

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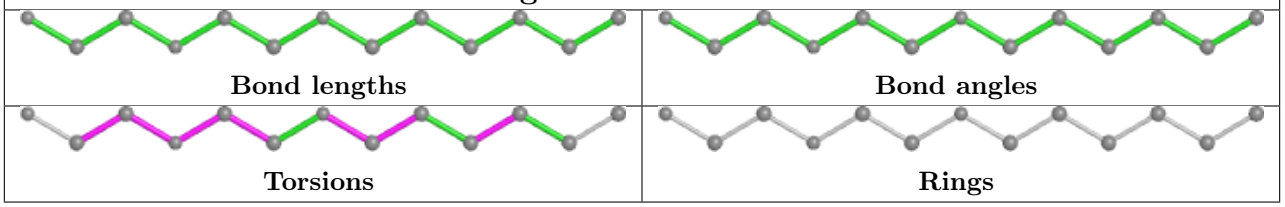

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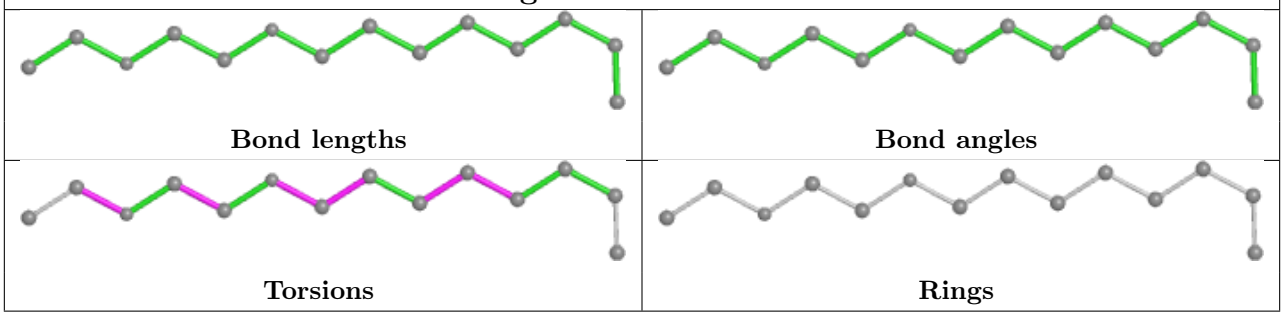

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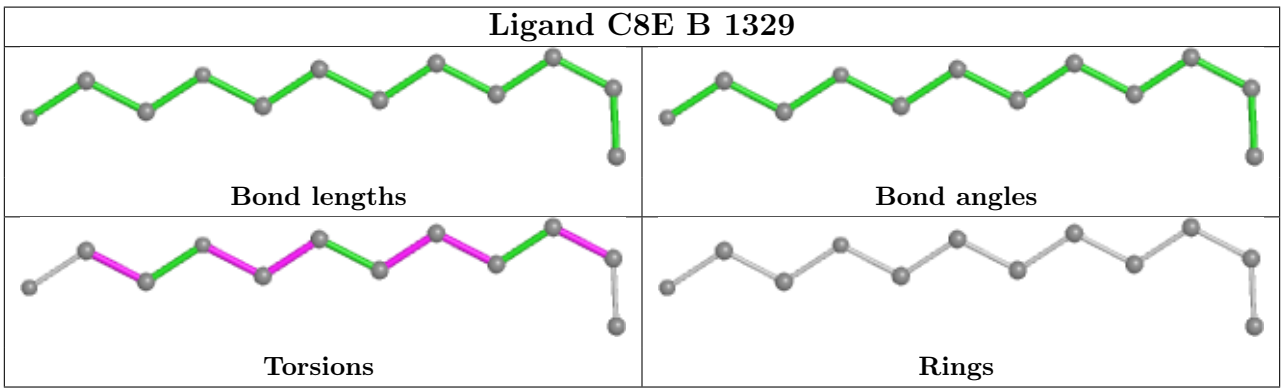

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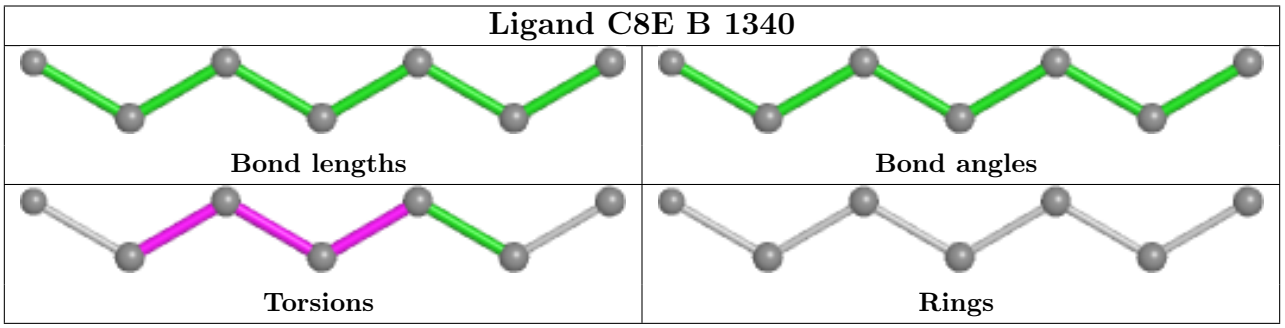
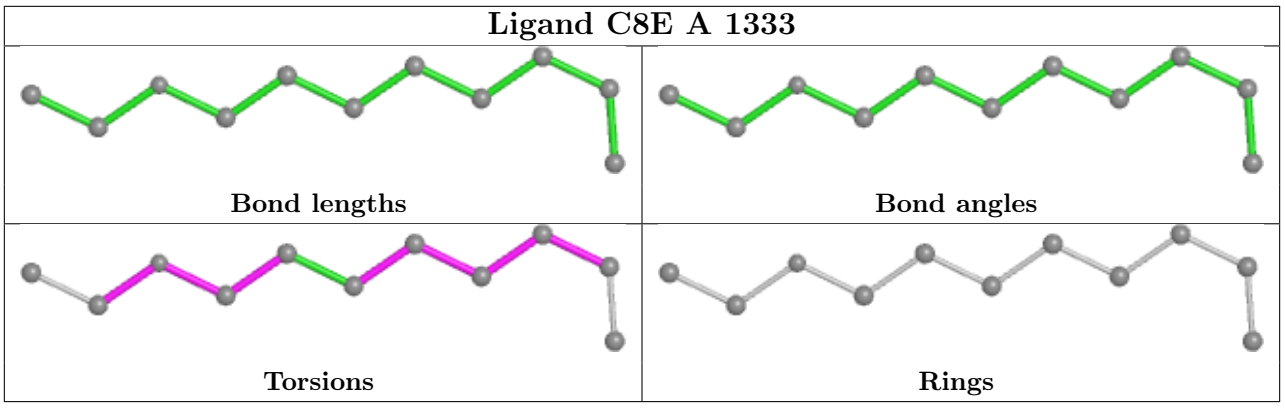
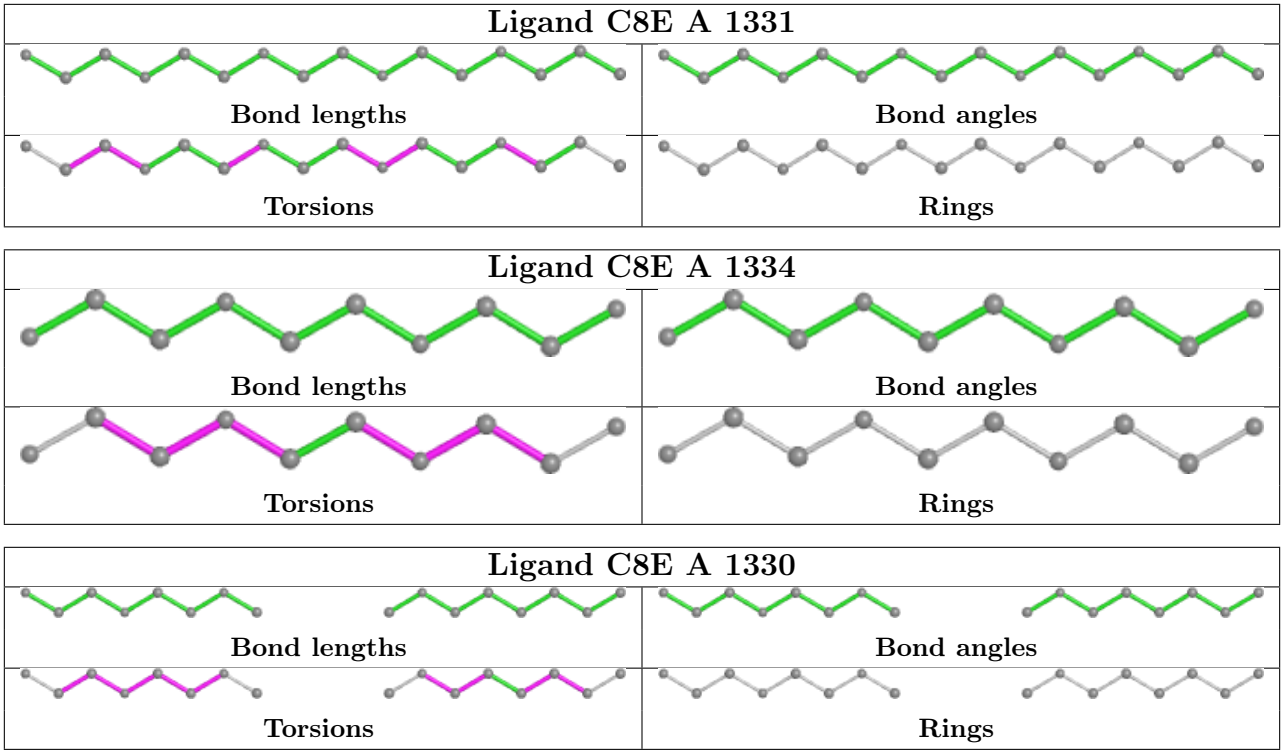


Ligand C8E A 1333





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	312/339 (92%)	-0.26	2 (0%)	89	91	16, 23, 41, 66	8 (2%)
1	B	309/339 (91%)	-0.21	1 (0%)	94	94	16, 26, 42, 62	4 (1%)
All	All	621/678 (91%)	-0.24	3 (0%)	91	92	16, 24, 42, 66	12 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	2.7
1	A	233	ASP	2.3
1	B	17	SER	2.2

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

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

6.3 Carbohydrates

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
2	GLC	D	1	11/12	0.58	0.24	65,74,78,78	0
2	GLC	D	3	11/12	0.74	0.21	62,72,80,84	0
2	GLC	D	4	11/12	0.77	0.13	43,53,62,63	0
2	GLC	D	2	11/12	0.83	0.14	61,70,79,82	0
2	GLC	D	6	11/12	0.83	0.15	35,45,61,71	0
2	GLC	F	5	11/12	0.88	0.12	32,36,39,39	0

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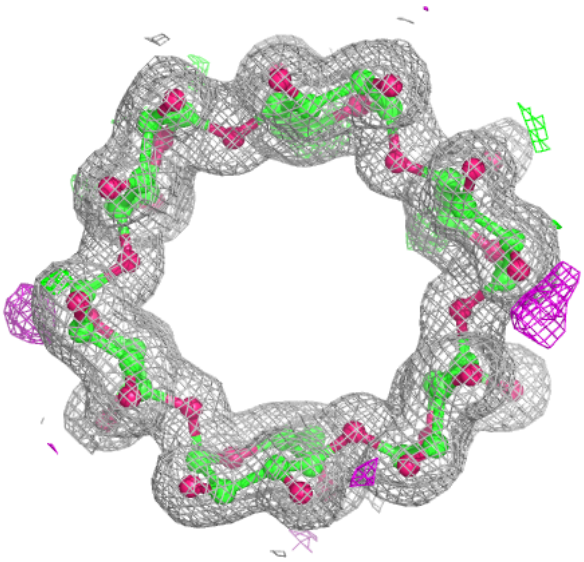
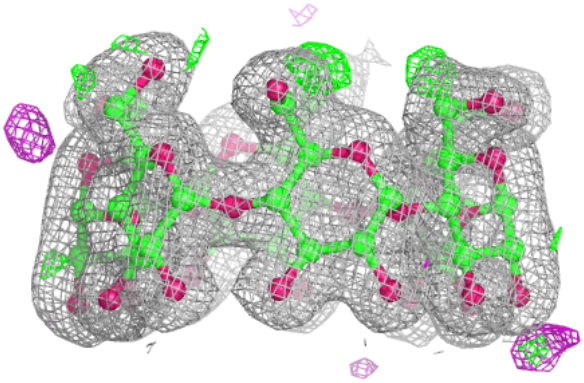
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	F	2	11/12	0.89	0.12	38,41,69,79	0
2	GLC	F	3	11/12	0.89	0.11	36,39,52,64	0
2	GLC	D	5	11/12	0.89	0.11	32,39,48,52	0
2	GLC	F	4	11/12	0.90	0.13	34,39,44,45	0
2	GLC	F	1	11/12	0.92	0.10	28,32,43,52	0
2	GLC	E	6	11/12	0.93	0.11	25,27,35,36	0
2	GLC	E	3	11/12	0.93	0.10	29,35,40,45	0
2	GLC	C	2	11/12	0.94	0.08	23,27,30,31	0
2	GLC	F	6	11/12	0.94	0.08	23,29,32,40	0
2	GLC	E	4	11/12	0.95	0.08	29,32,36,39	0
2	GLC	E	5	11/12	0.95	0.09	26,30,31,36	0
2	GLC	E	1	11/12	0.95	0.12	20,26,33,40	0
2	GLC	C	3	11/12	0.96	0.07	22,24,32,33	0
2	GLC	E	2	11/12	0.96	0.09	26,30,40,44	0
2	GLC	C	5	11/12	0.96	0.07	18,20,28,34	0
2	GLC	C	4	11/12	0.97	0.06	19,21,26,27	0
2	GLC	C	1	11/12	0.97	0.06	20,23,29,30	0
2	GLC	C	6	11/12	0.98	0.06	17,20,25,28	0

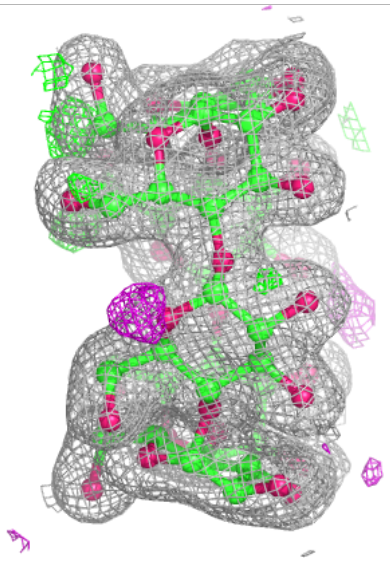
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

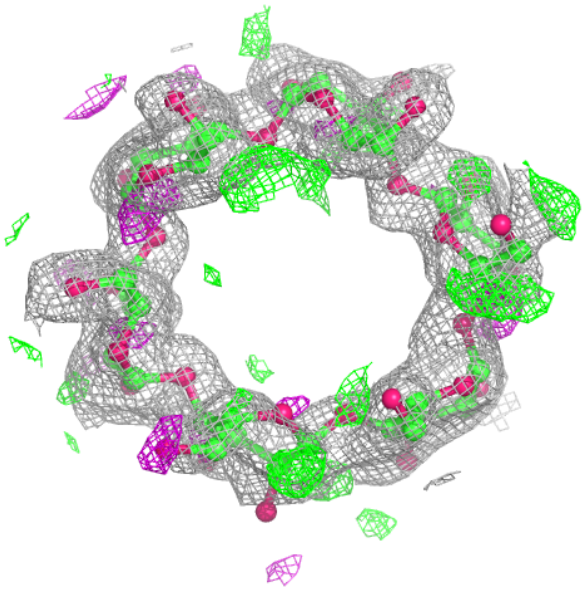


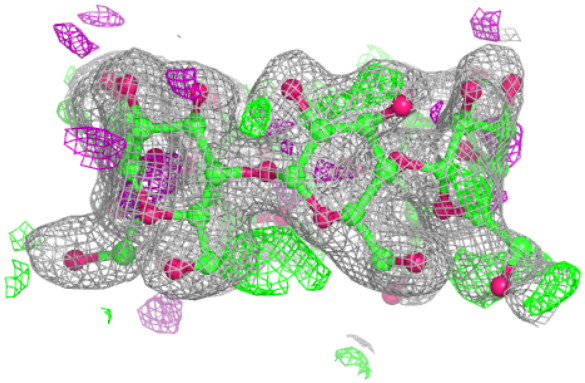


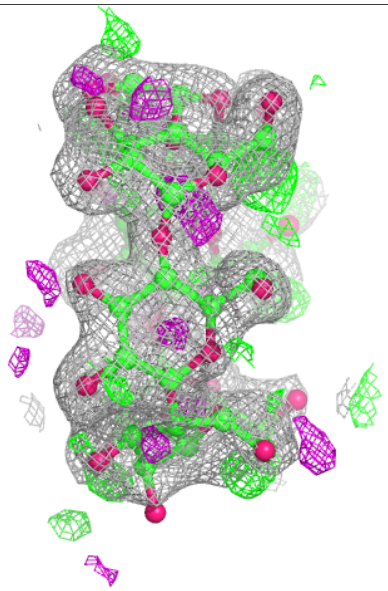


Electron density around Chain D:

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

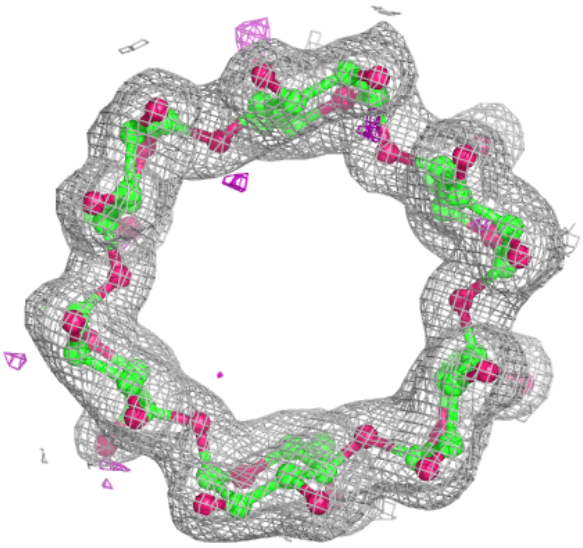


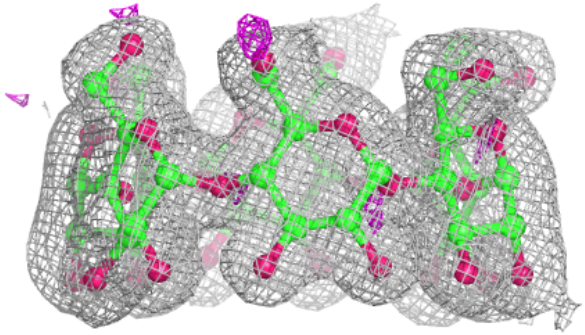


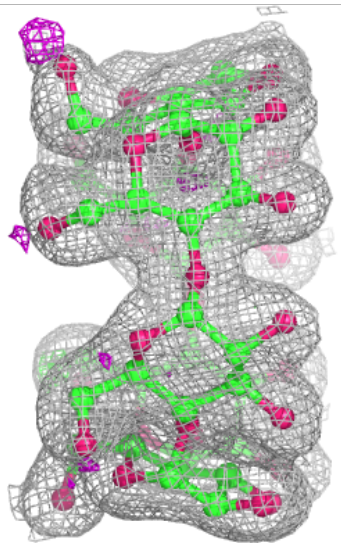


Electron density around Chain E:

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

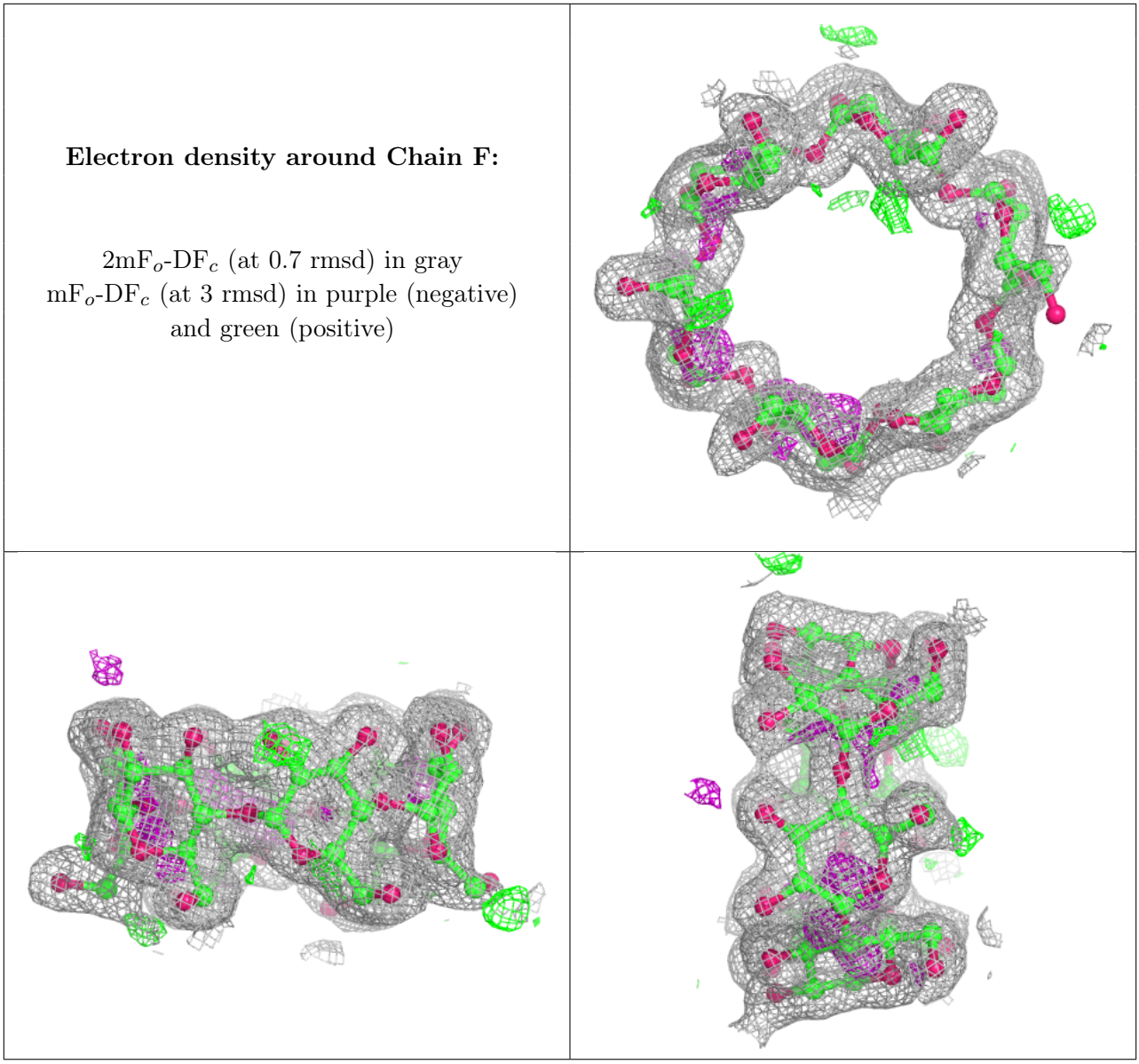






Electron density around Chain F:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1337	21/21	0.58	0.25	38,54,67,77	0
3	C8E	B	1335	9/21	0.64	0.22	54,73,79,80	0
3	C8E	A	1334	10/21	0.67	0.13	62,67,69,72	0
3	C8E	B	1340	7/21	0.69	0.19	51,55,57,58	0
3	C8E	A	1339	9/21	0.70	0.21	57,65,77,77	0

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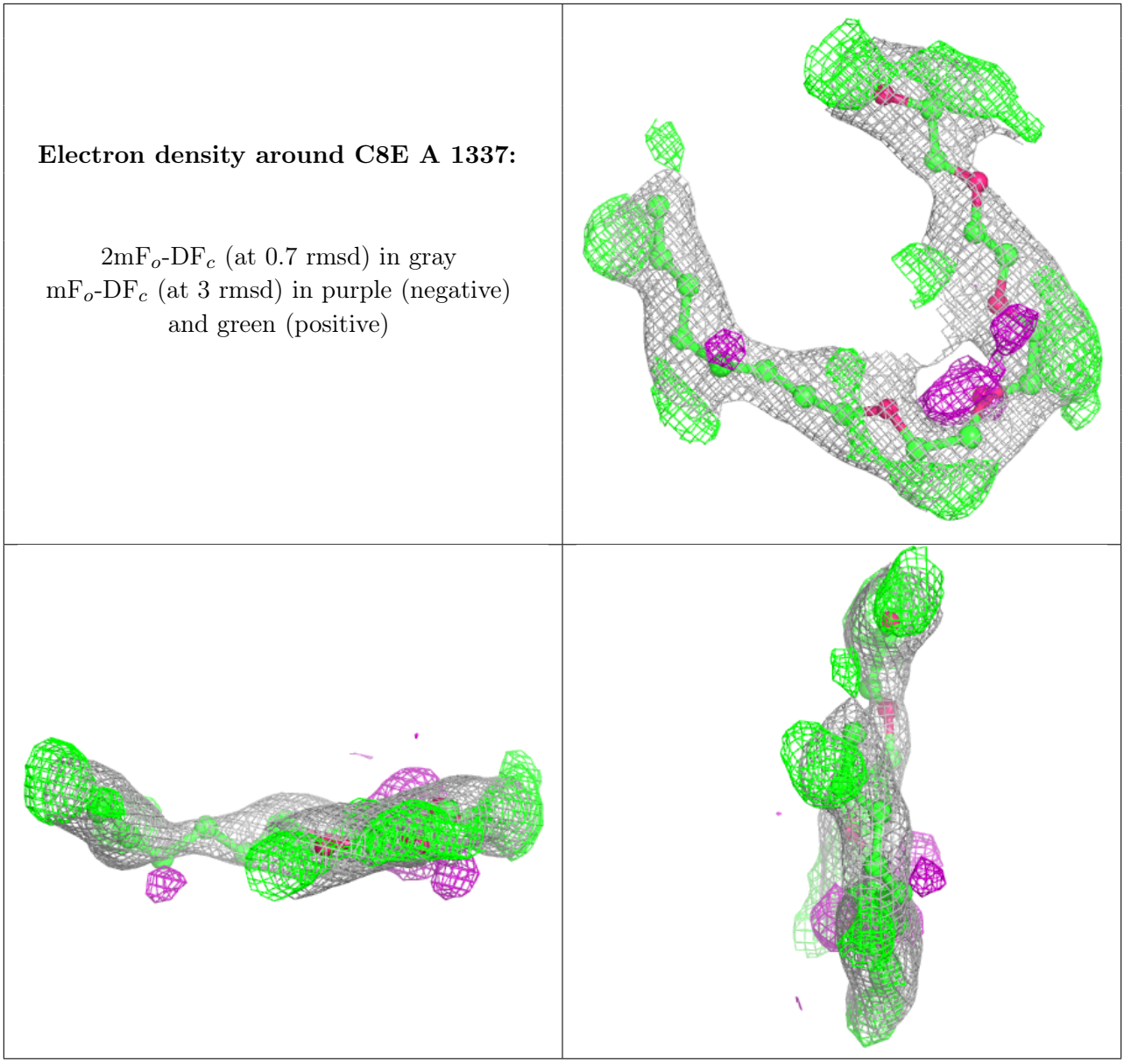
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C8E	B	1331	14/21	0.71	0.21	45,52,66,66	0
3	C8E	B	1332	9/21	0.72	0.19	52,61,69,69	0
3	C8E	A	1332	12/21	0.74	0.18	41,60,67,68	0
3	C8E	B	1334	13/21	0.74	0.19	47,51,66,69	0
3	C8E	B	1343	13/21	0.74	0.15	45,48,53,60	3
3	C8E	A	1336	10/21	0.77	0.21	48,55,66,67	0
3	C8E	B	1339	7/21	0.79	0.19	32,48,51,52	0
3	C8E	A	1333	11/21	0.79	0.12	51,55,60,63	0
3	C8E	B	1338	13/21	0.79	0.23	54,61,75,76	0
3	C8E	B	1327	21/21	0.80	0.20	41,52,64,68	0
3	C8E	B	1337	19/21	0.80	0.16	34,45,64,65	0
3	C8E	A	1338	13/21	0.81	0.22	38,66,73,75	0
3	C8E	A	1330	16/21	0.81	0.20	33,49,69,71	0
3	C8E	B	1333	14/21	0.82	0.16	29,46,56,59	0
3	C8E	A	1327	8/21	0.84	0.16	37,51,59,68	0
3	C8E	B	1342	7/21	0.84	0.25	52,53,57,58	0
3	C8E	B	1329	12/21	0.84	0.25	39,47,59,60	0
3	C8E	A	1328	19/21	0.87	0.22	39,56,72,75	0
3	C8E	B	1336	7/21	0.87	0.12	38,40,43,45	0
3	C8E	A	1329	17/21	0.88	0.15	41,58,66,69	0
3	C8E	A	1331	16/21	0.89	0.13	28,38,49,59	0
3	C8E	B	1341	8/21	0.89	0.12	42,43,48,49	0
3	C8E	B	1328	16/21	0.90	0.14	31,46,59,61	0
3	C8E	B	1330	8/21	0.91	0.18	33,41,49,51	0
3	C8E	A	1335	7/21	0.92	0.12	31,33,37,42	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.

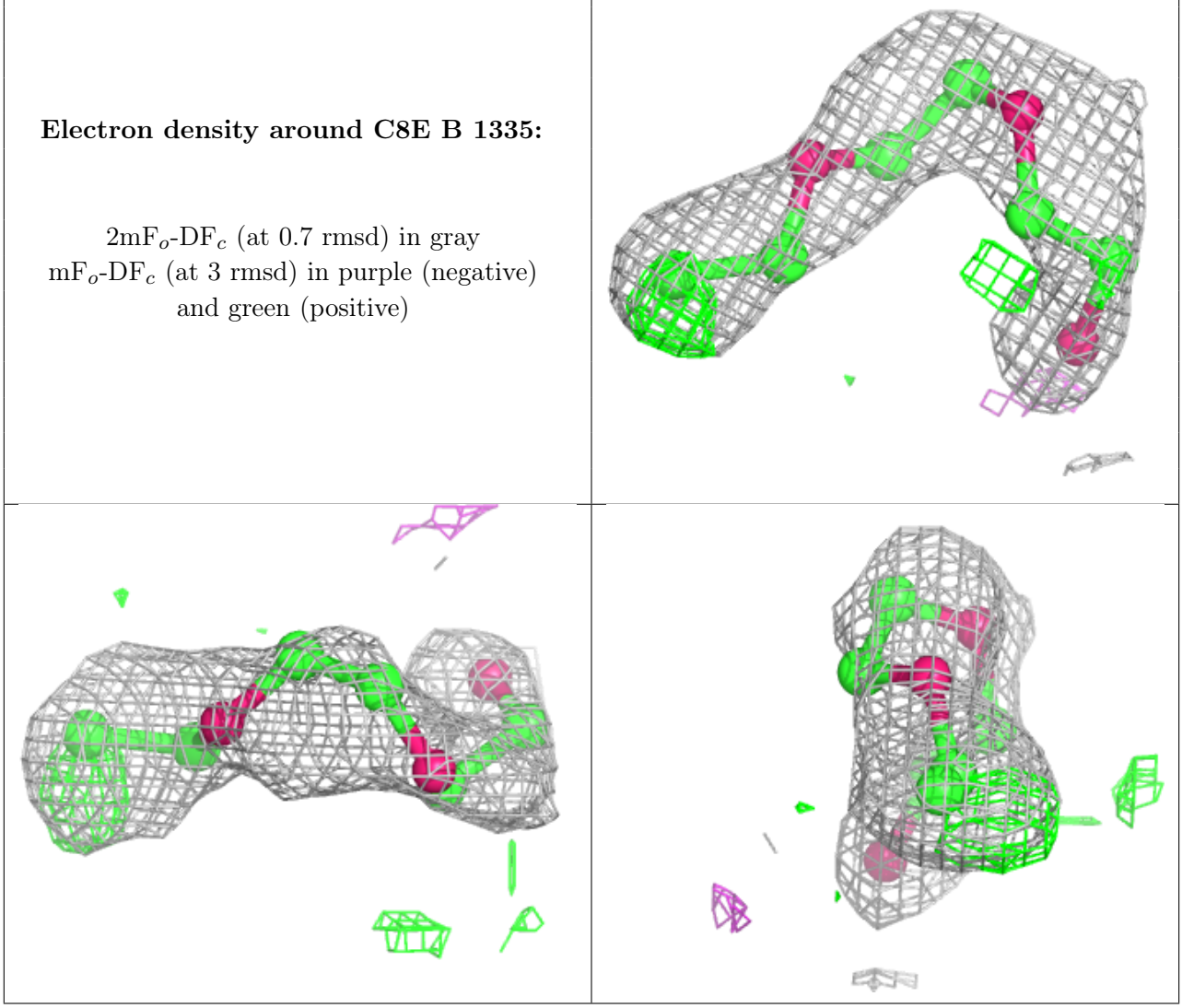
Electron density around C8E A 1337:

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



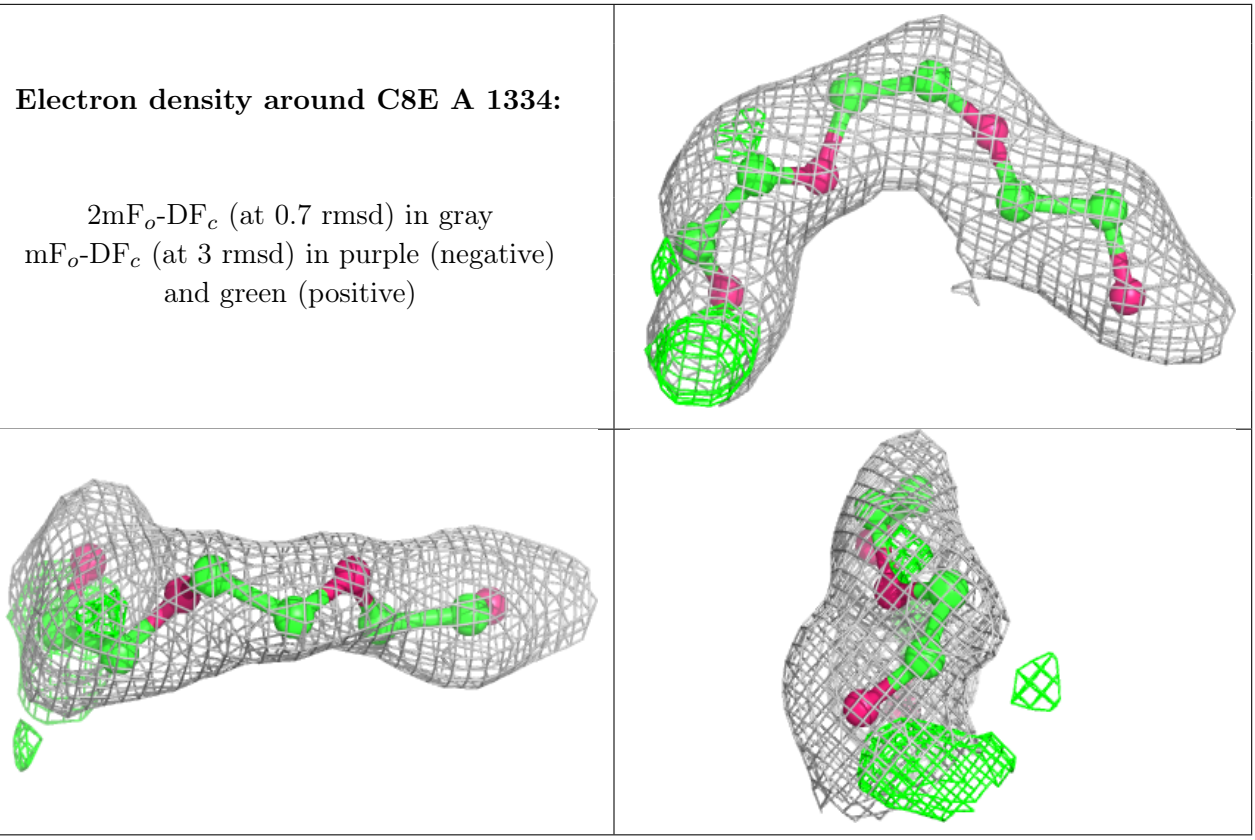
Electron density around C8E B 1335:

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



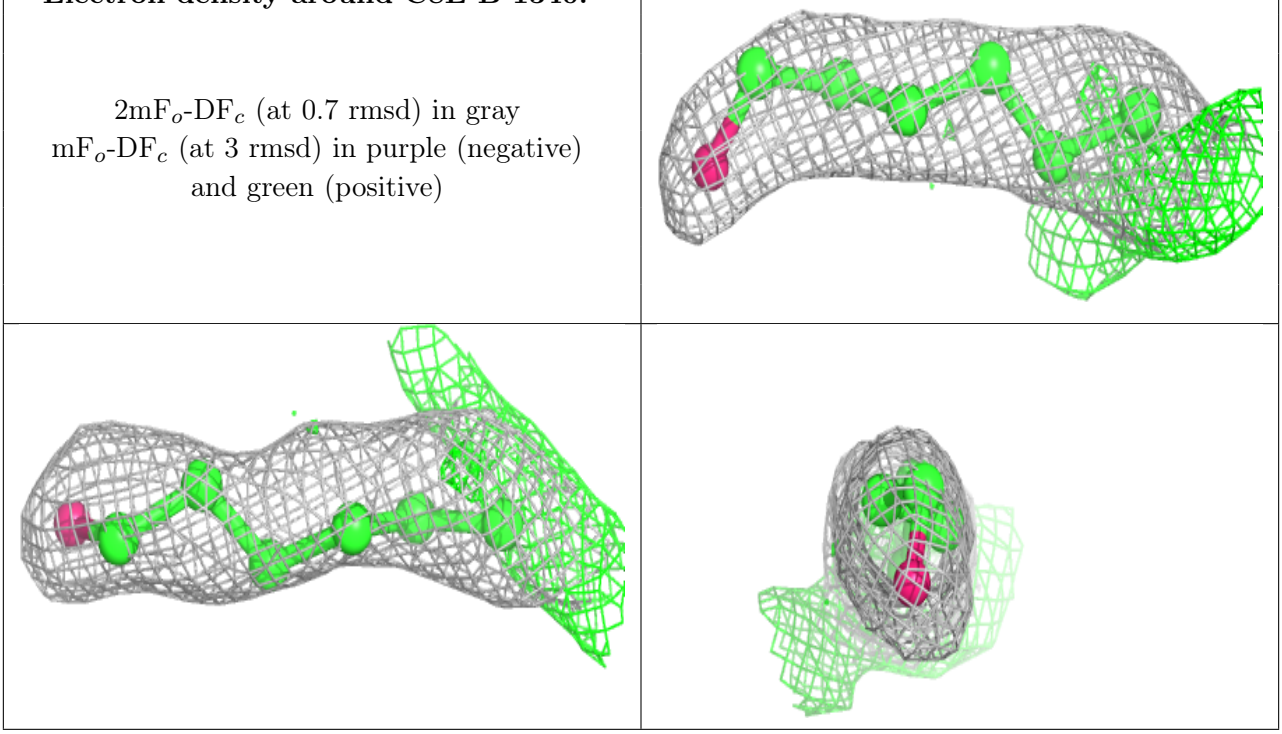
Electron density around C8E A 1334:

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



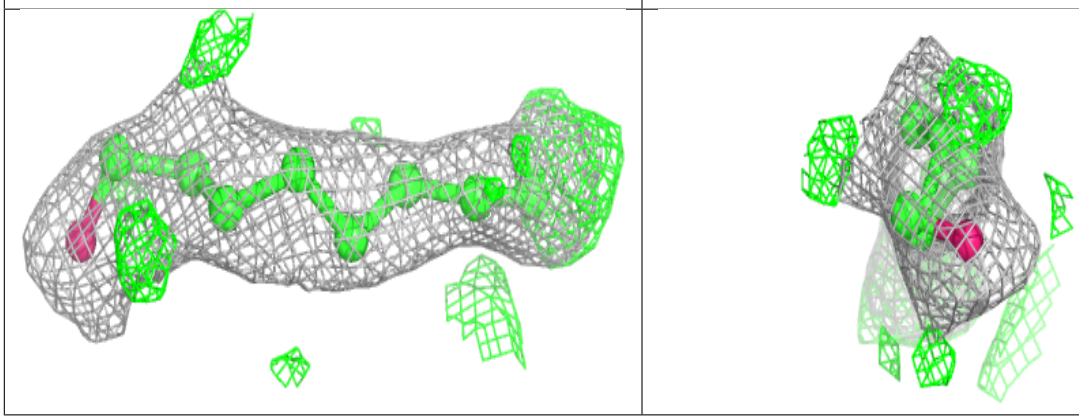
Electron density around C8E B 1340:

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



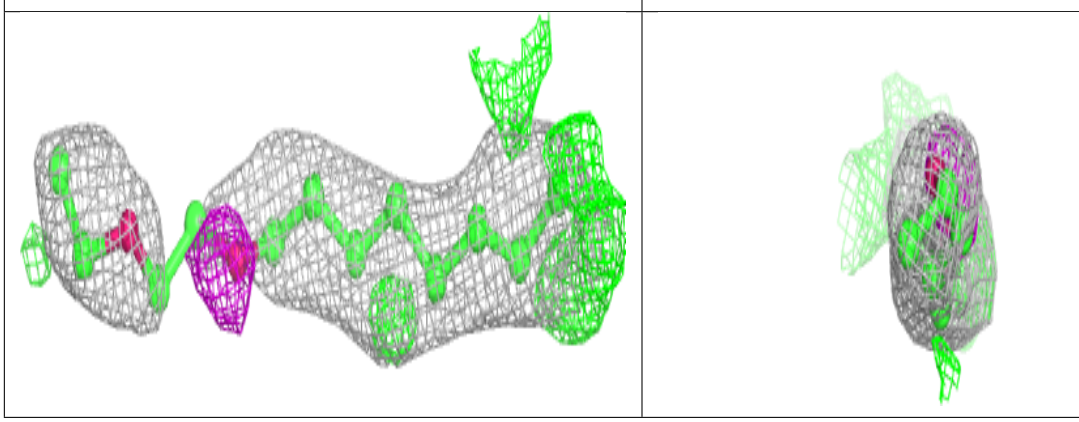
Electron density around C8E A 1339:

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



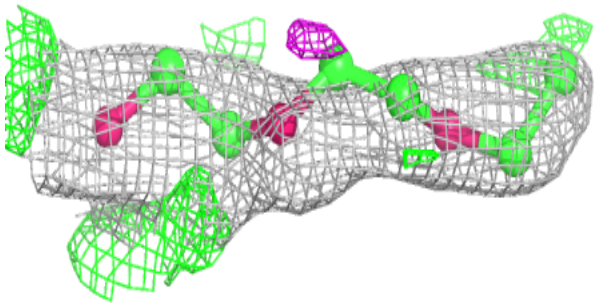
Electron density around C8E B 1331:

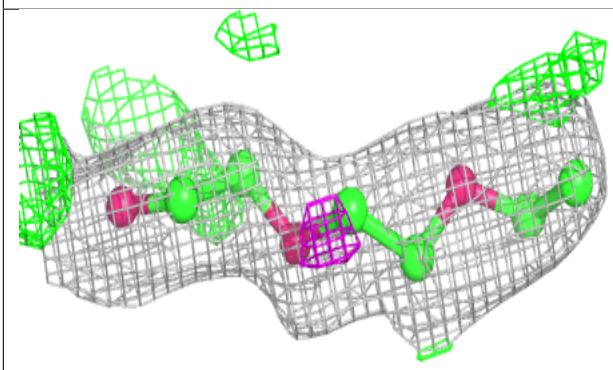
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

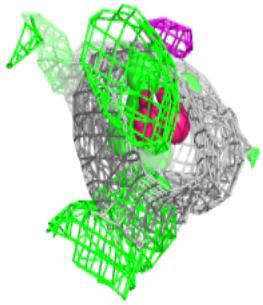


Electron density around C8E B 1332:

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

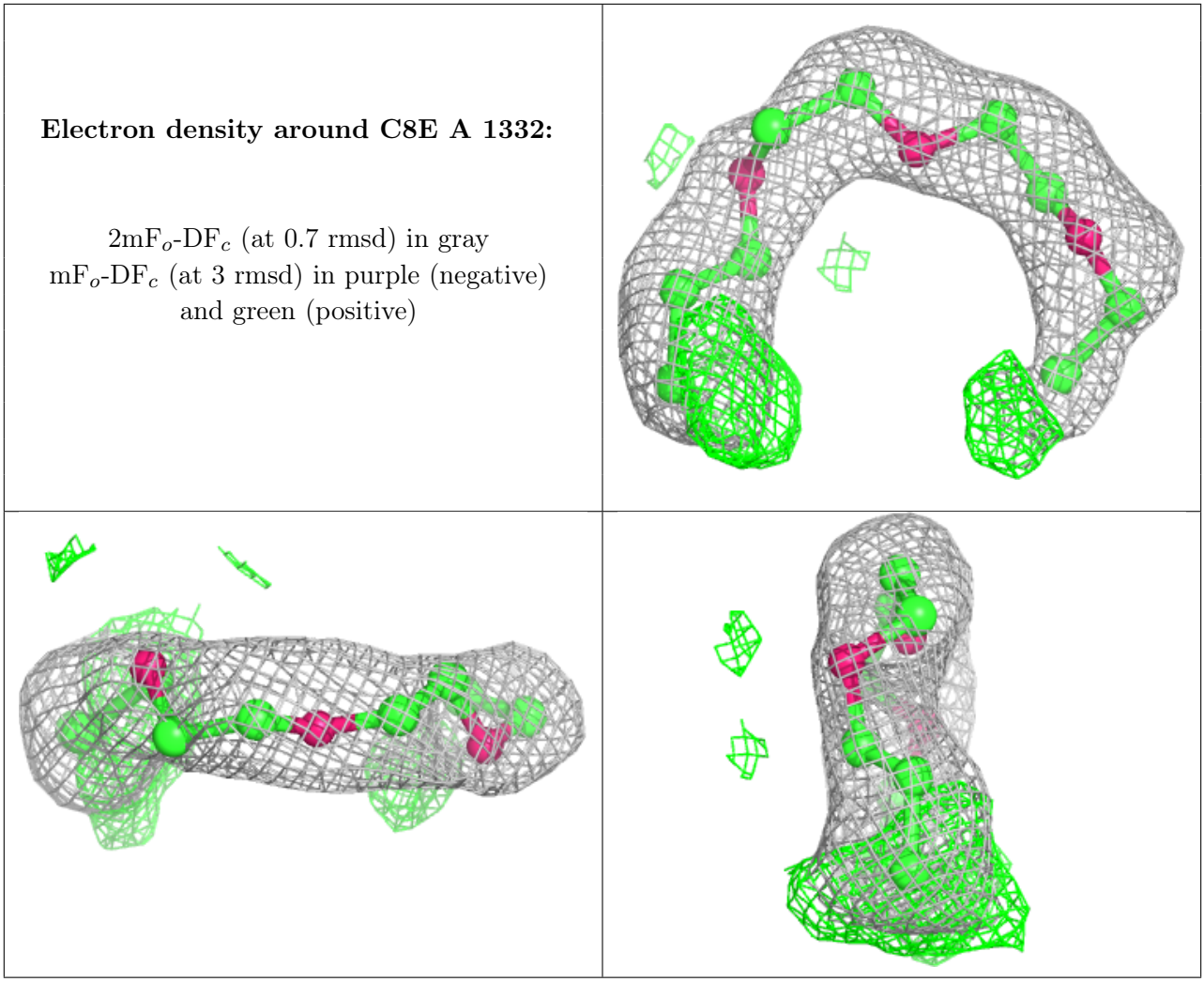






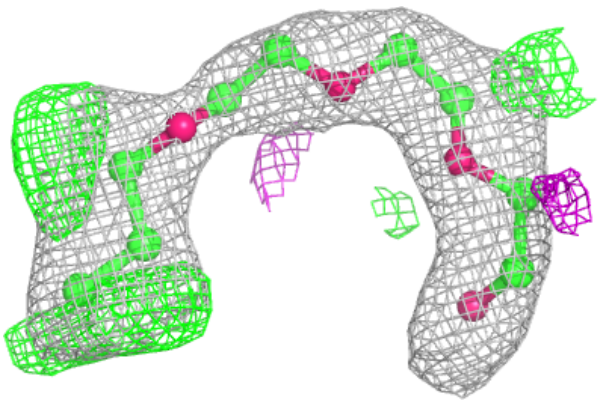
Electron density around C8E A 1332:

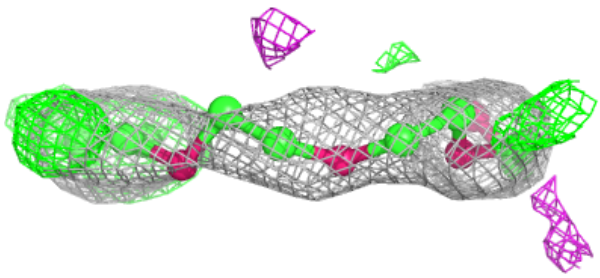
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

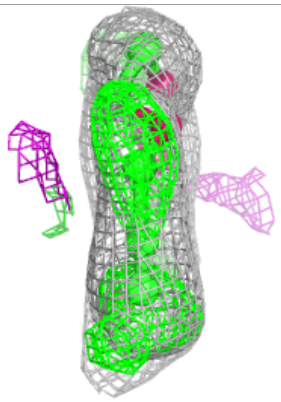


Electron density around C8E B 1334:

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

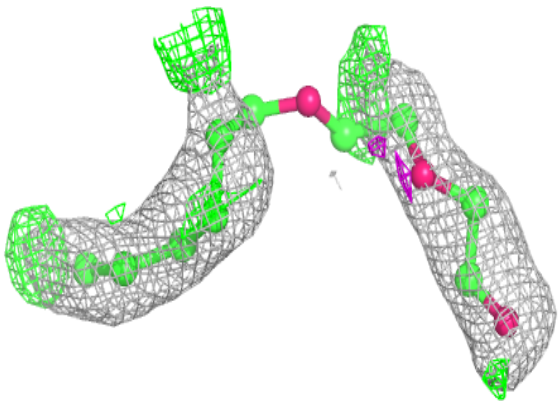


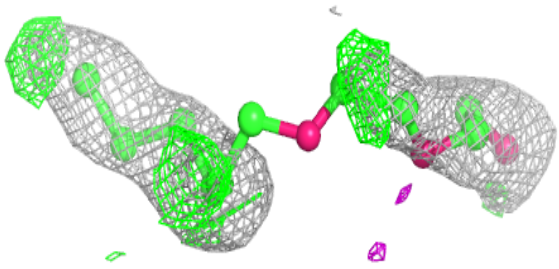


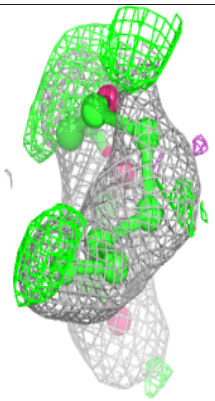


Electron density around C8E B 1343:

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

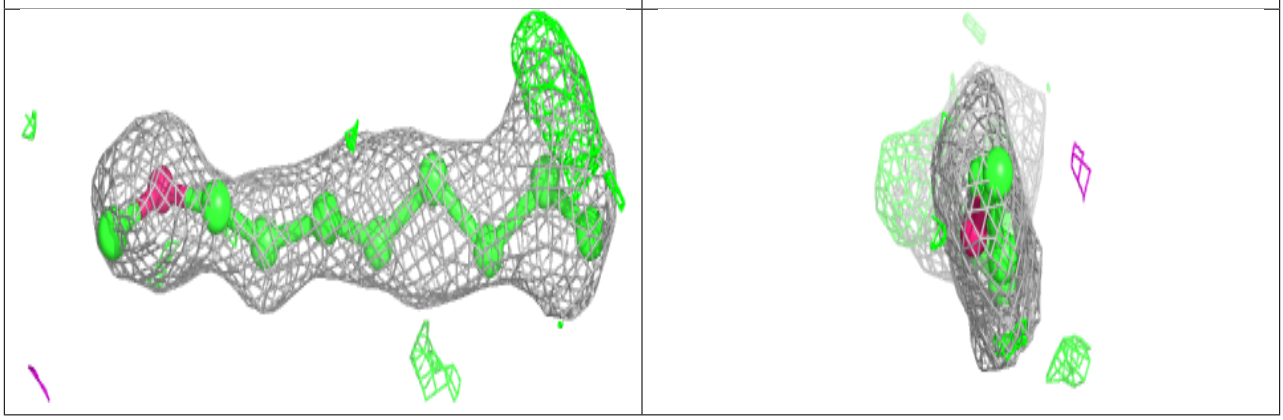






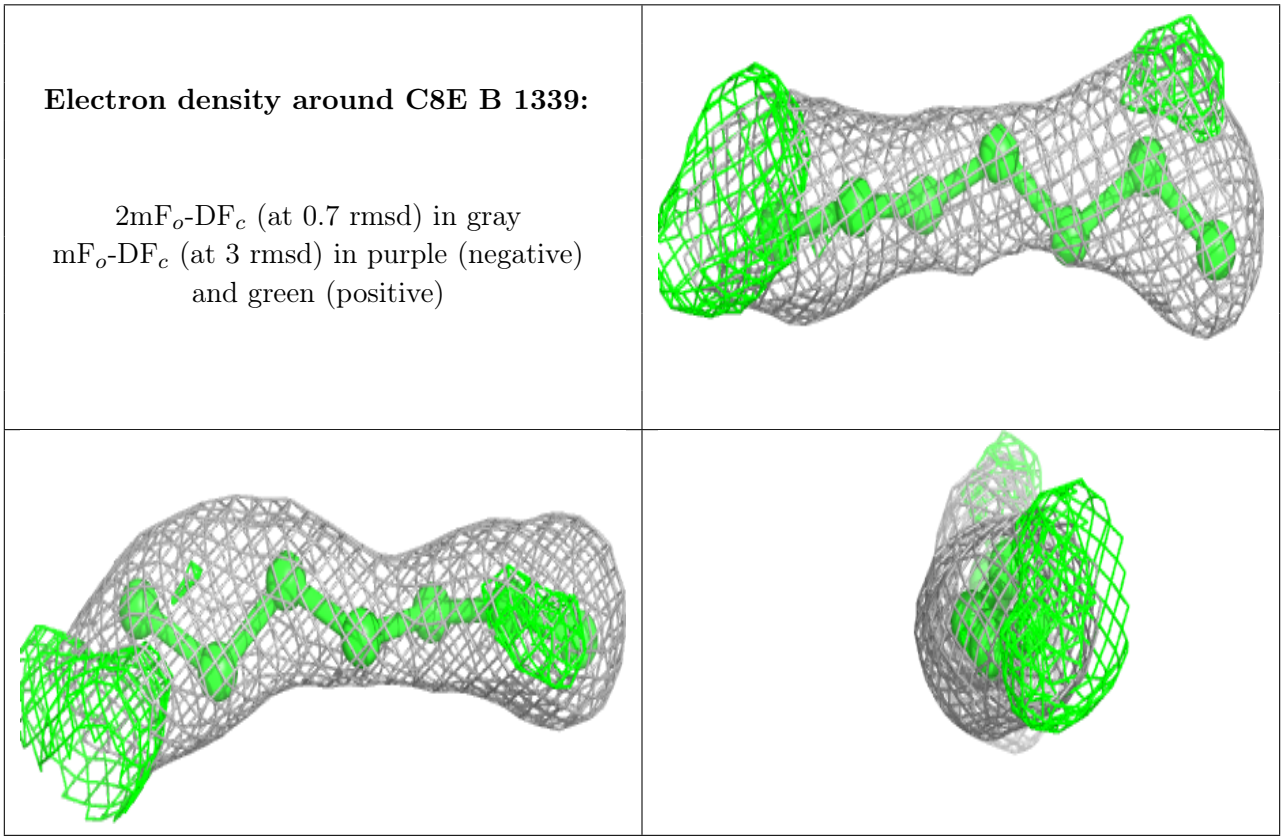
Electron density around C8E A 1336:

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



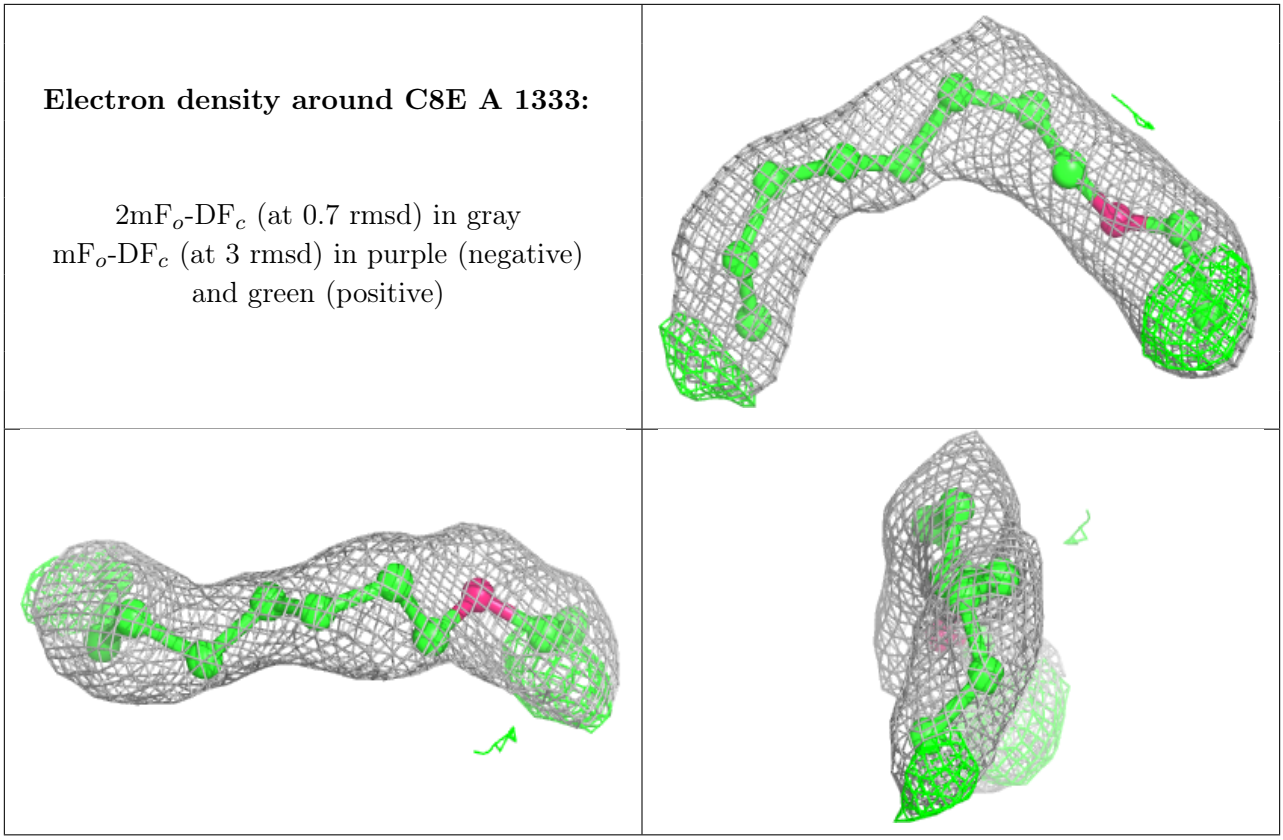
Electron density around C8E B 1339:

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



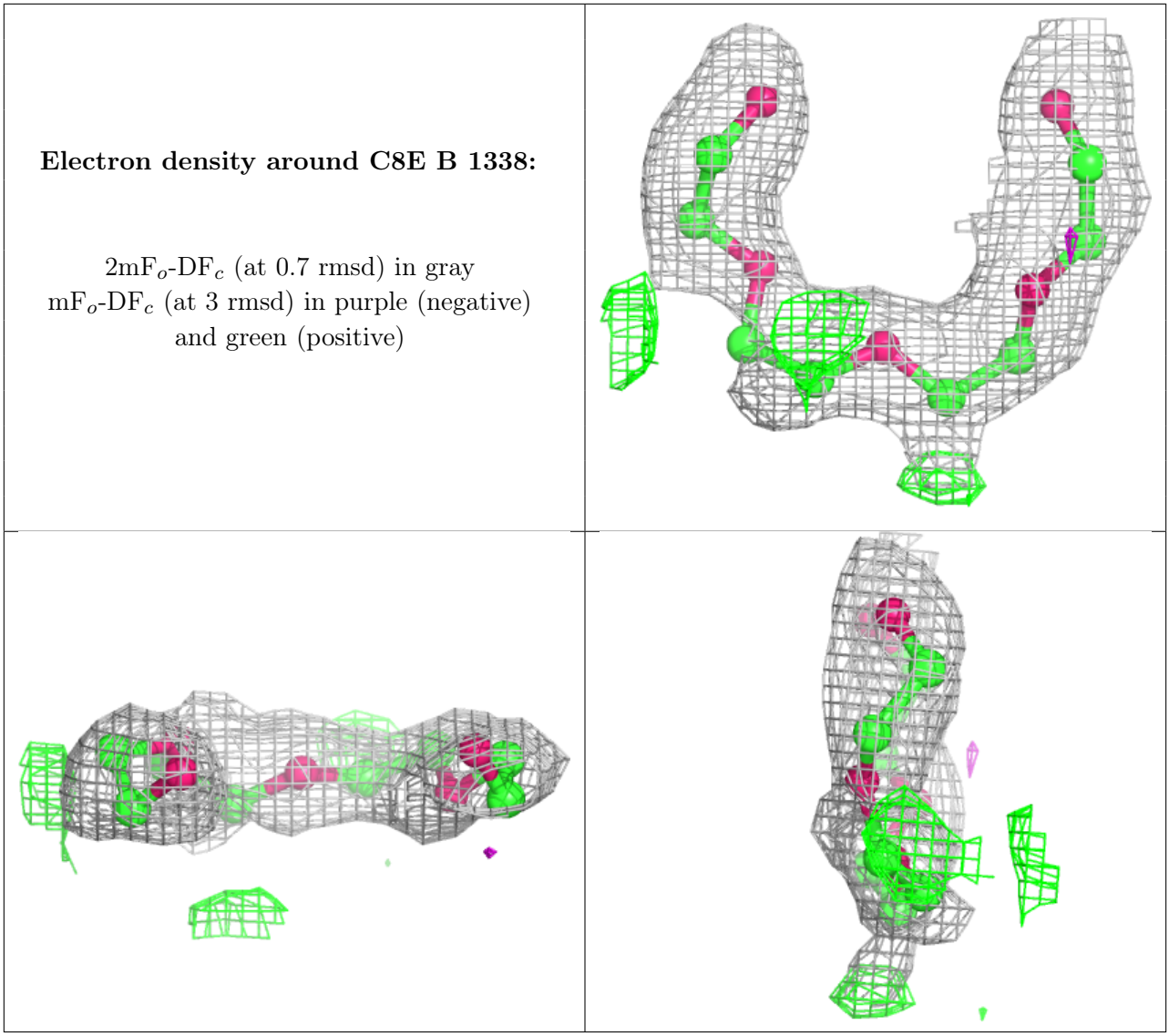
Electron density around C8E A 1333:

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



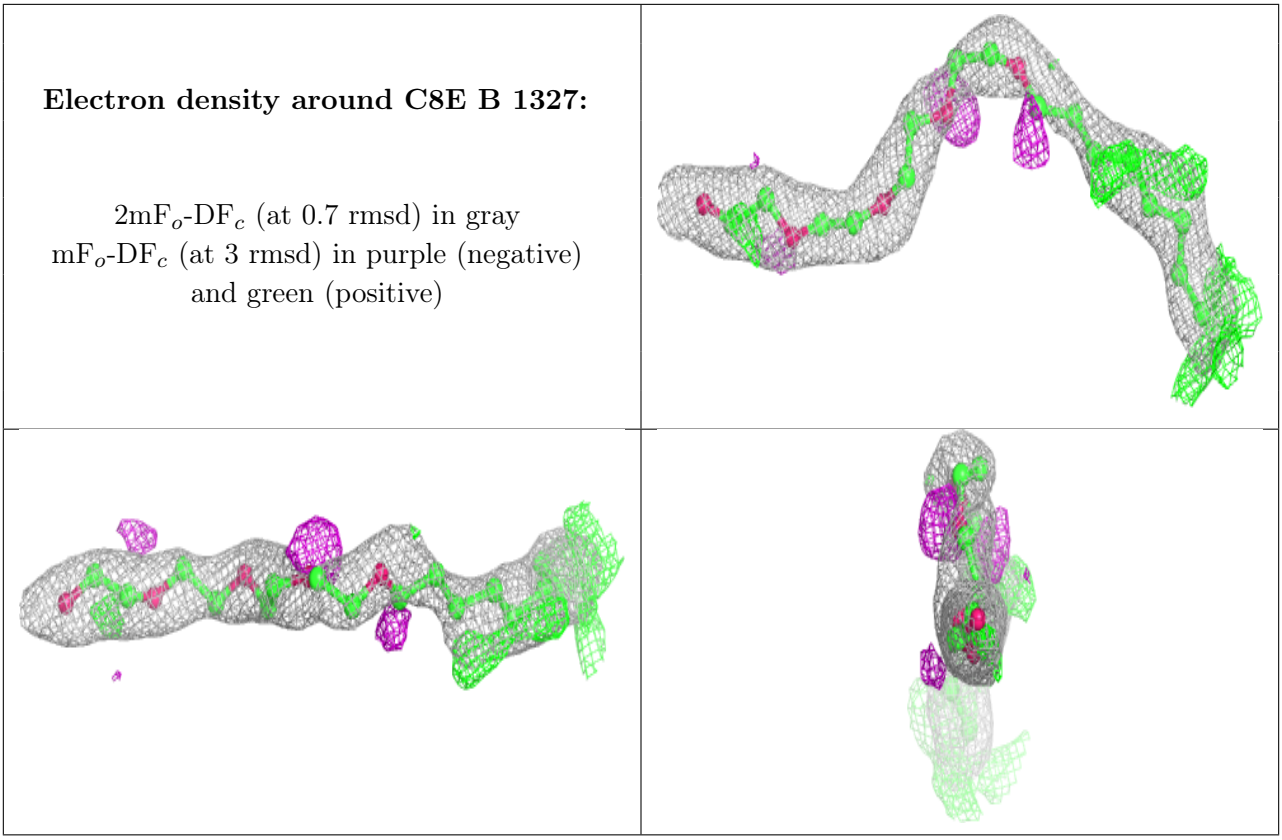
Electron density around C8E B 1338:

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



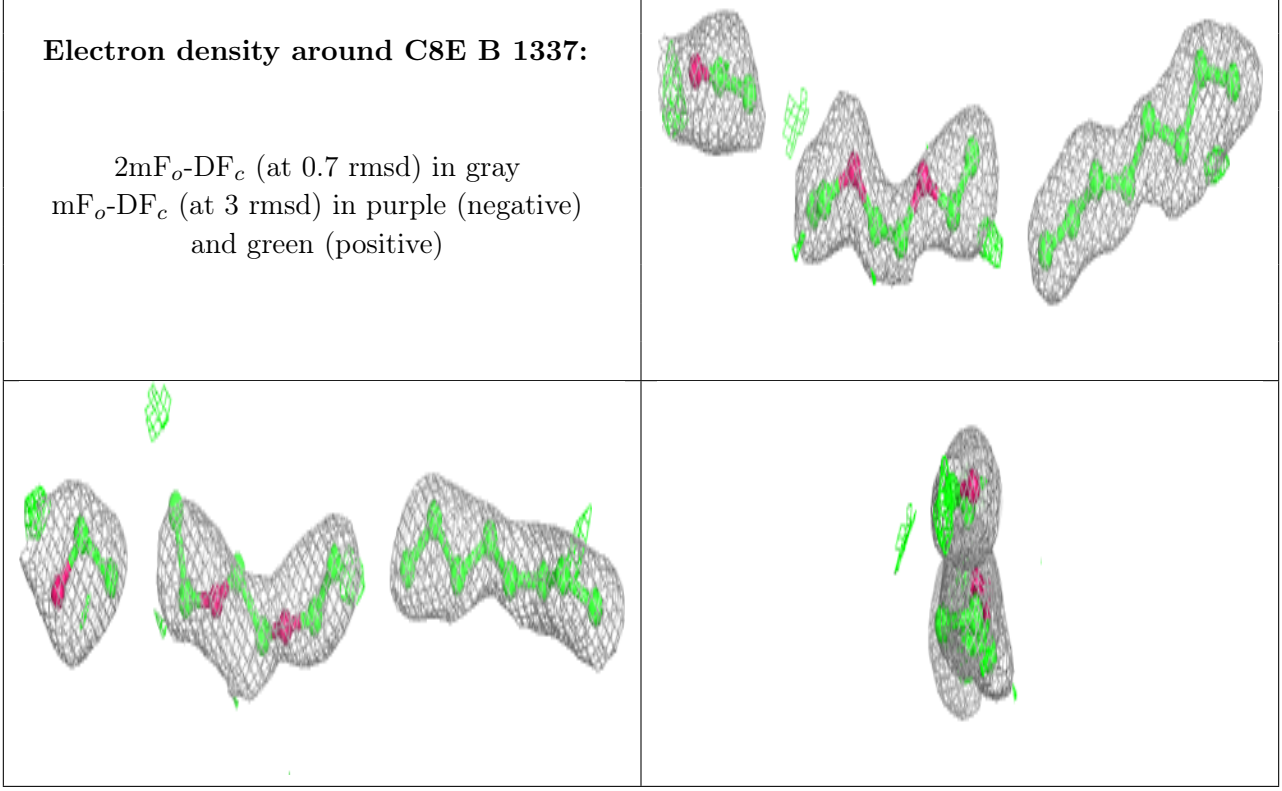
Electron density around C8E B 1327:

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



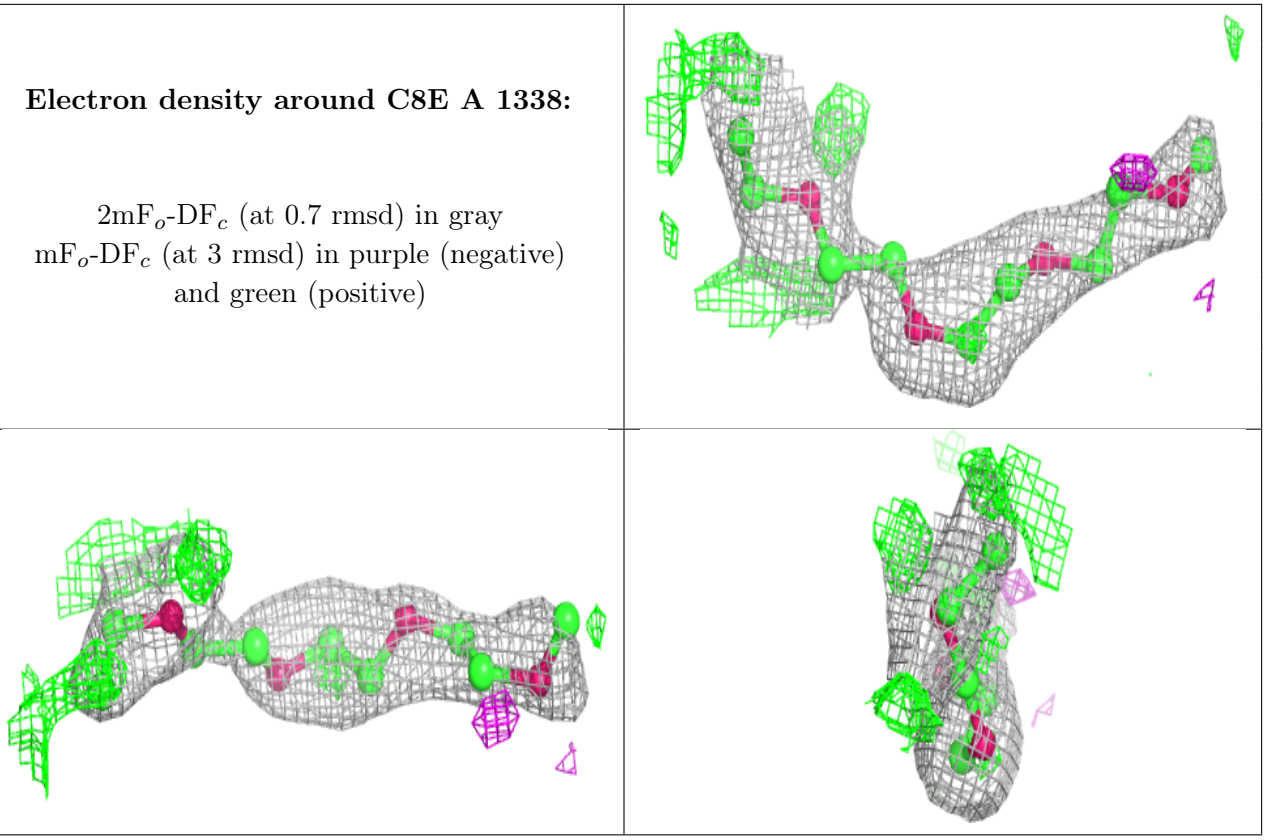
Electron density around C8E B 1337:

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



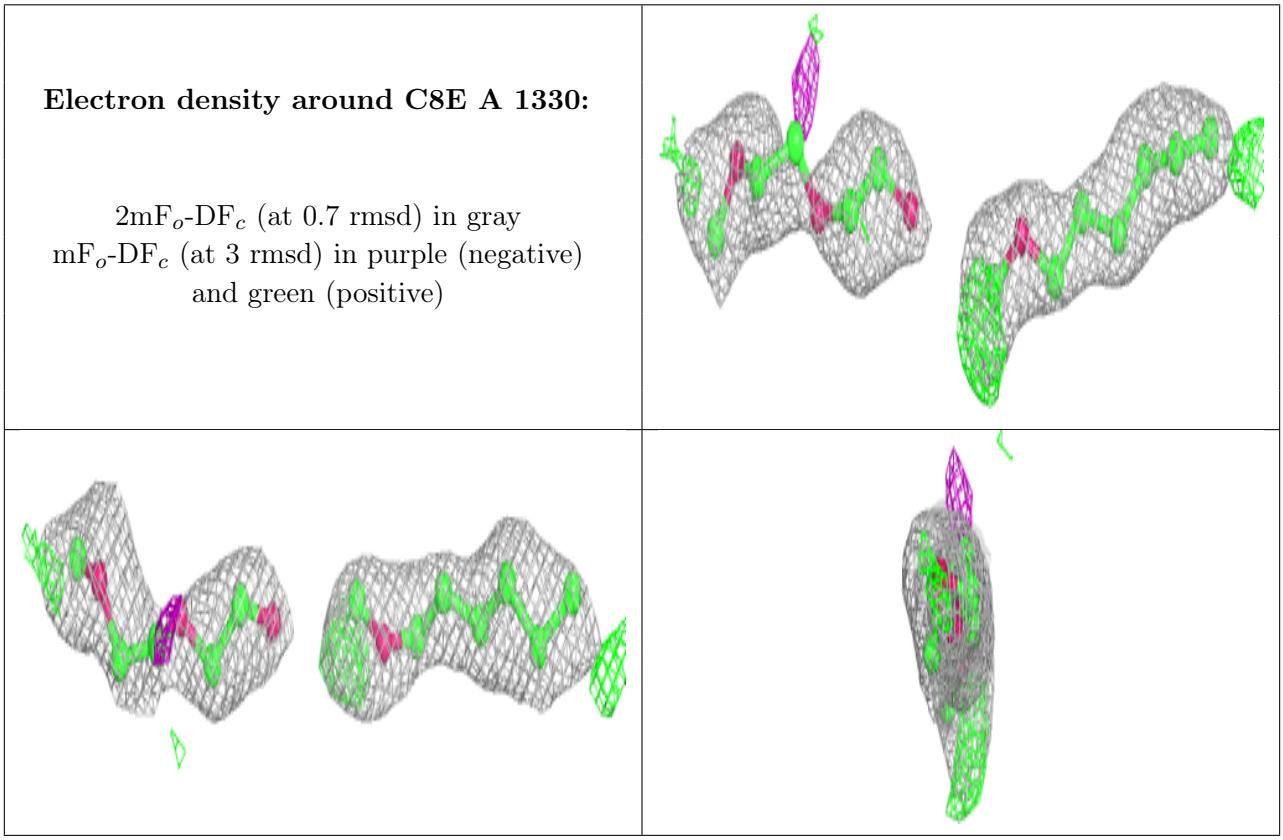
Electron density around C8E A 1338:

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



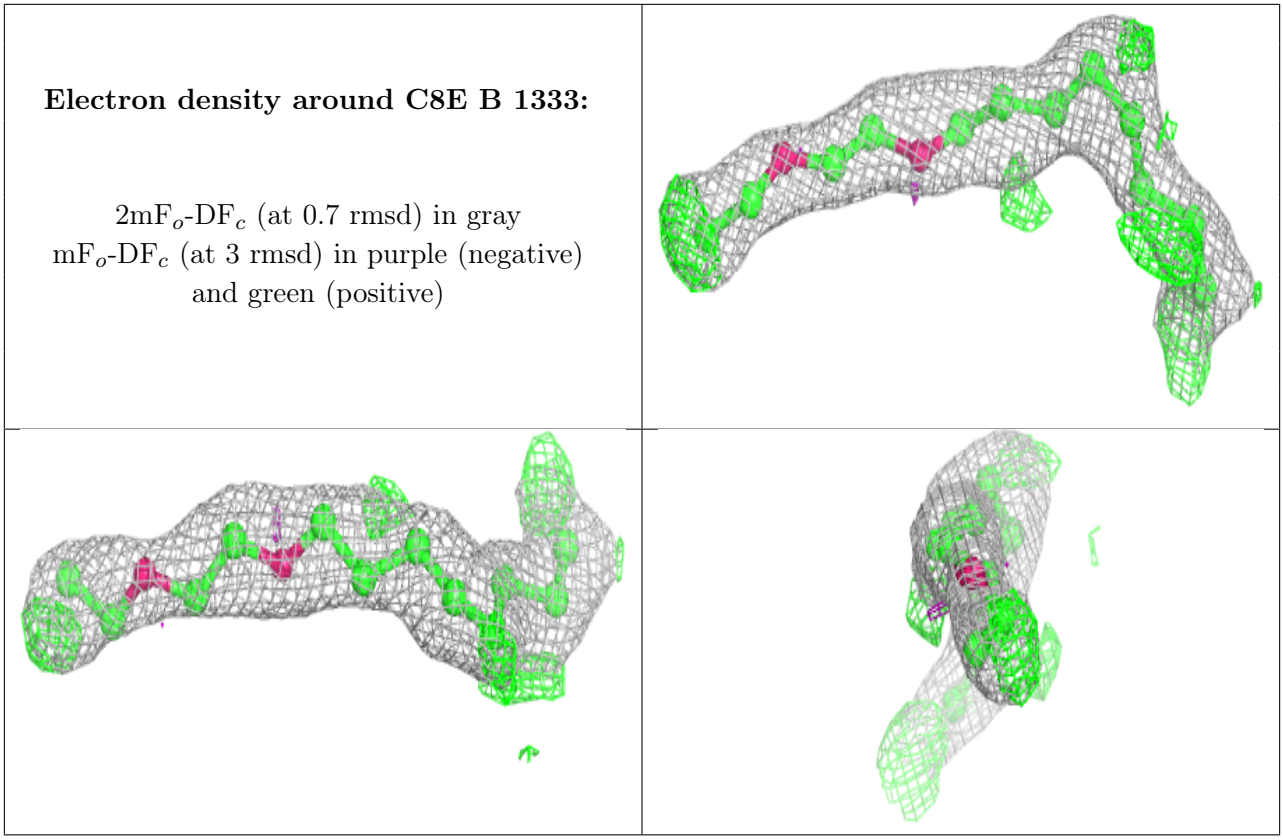
Electron density around C8E A 1330:

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



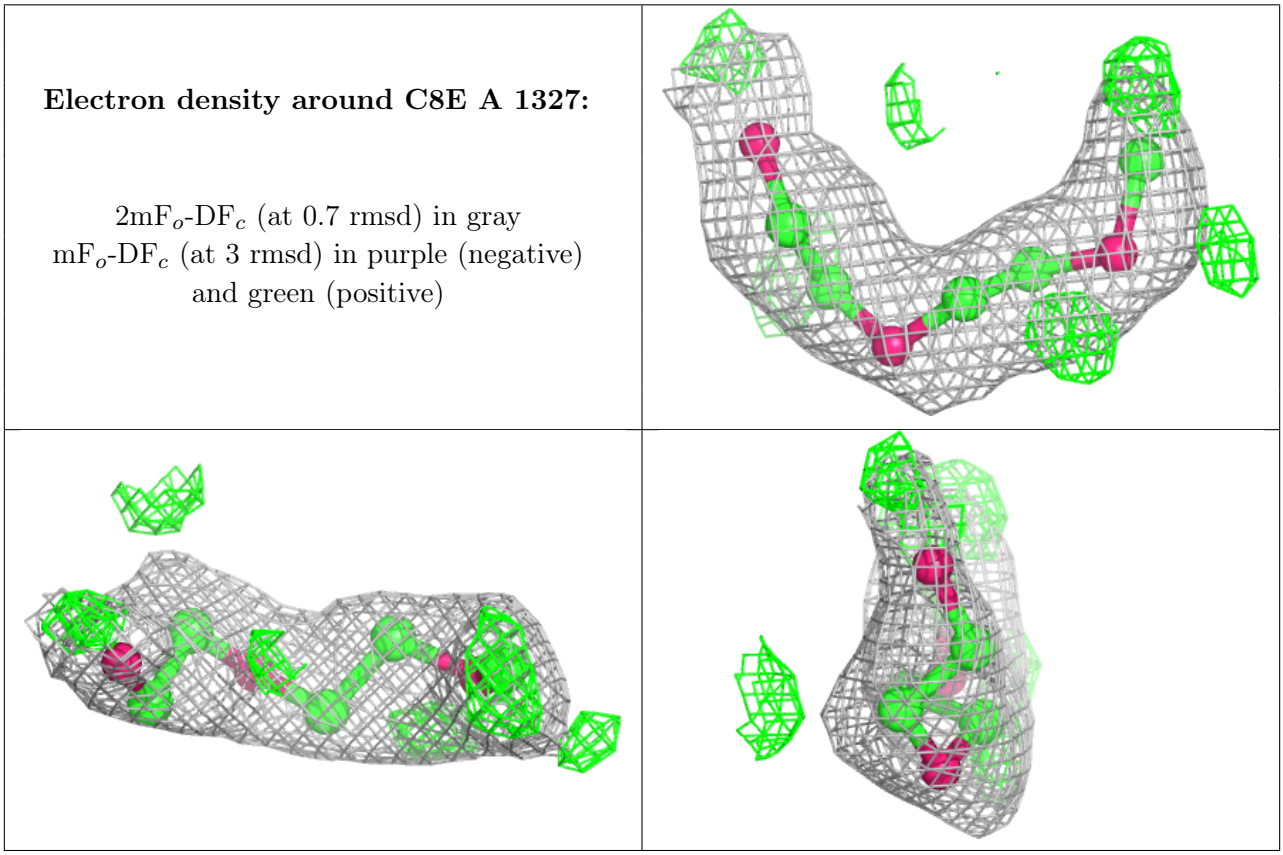
Electron density around C8E B 1333:

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



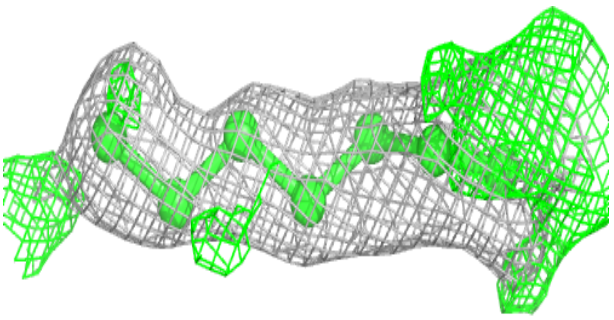
Electron density around C8E A 1327:

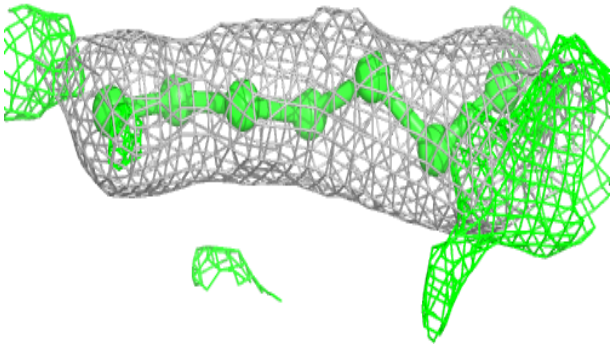
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

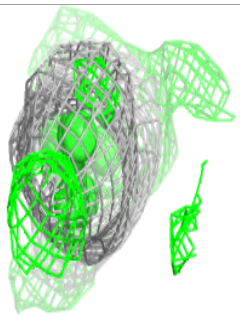


Electron density around C8E B 1342:

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

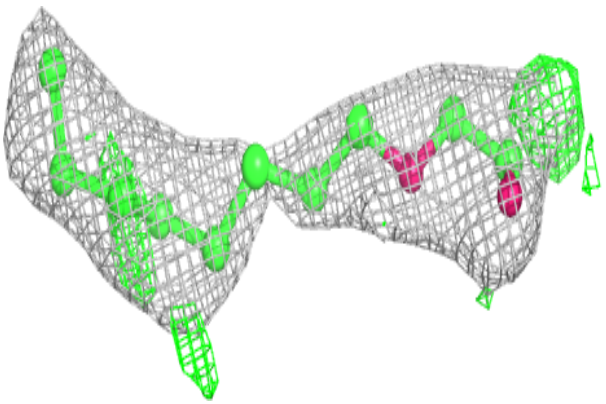


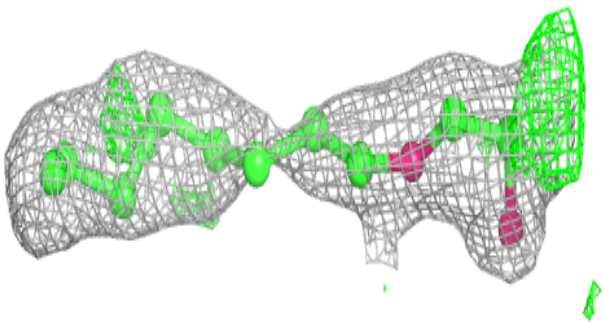


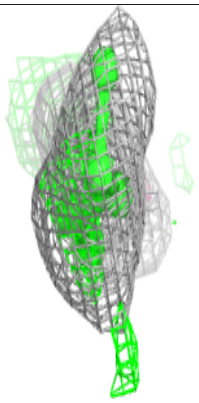


Electron density around C8E B 1329:

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

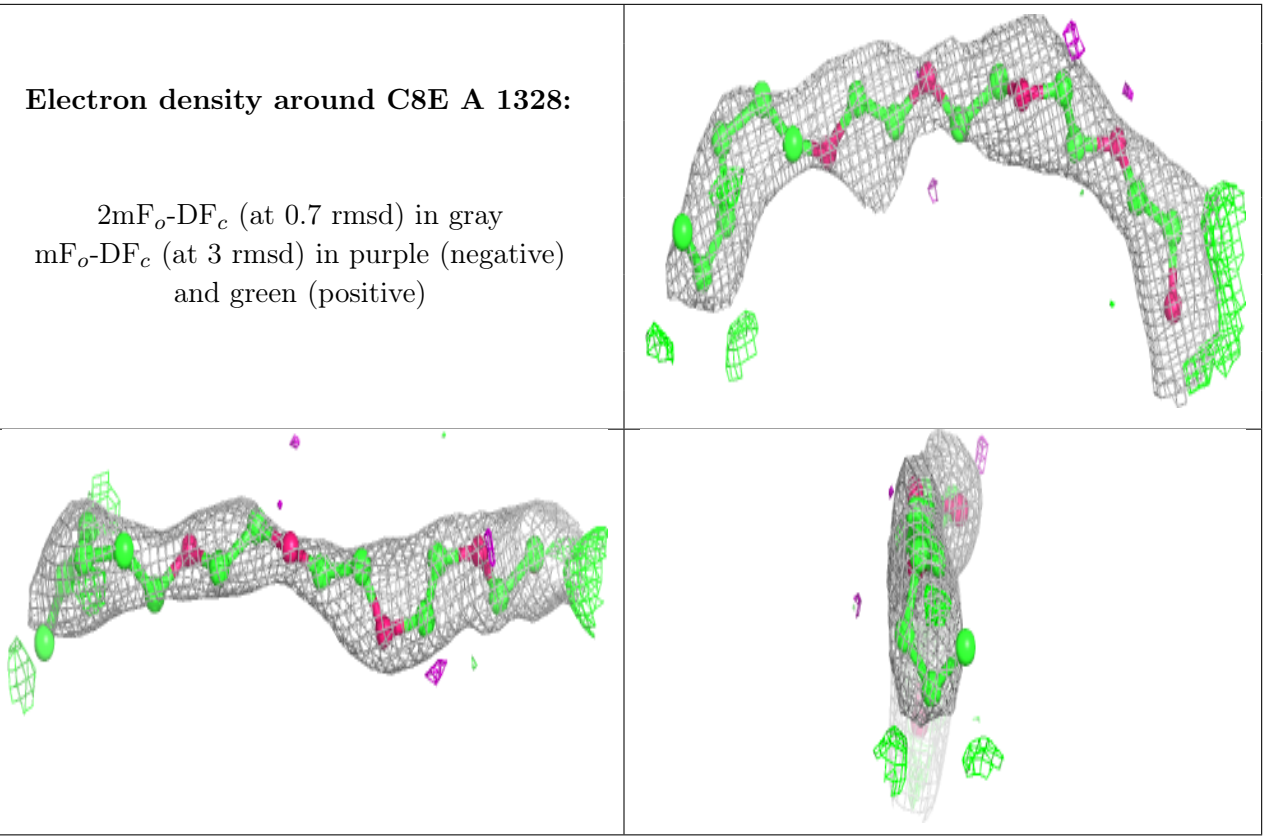






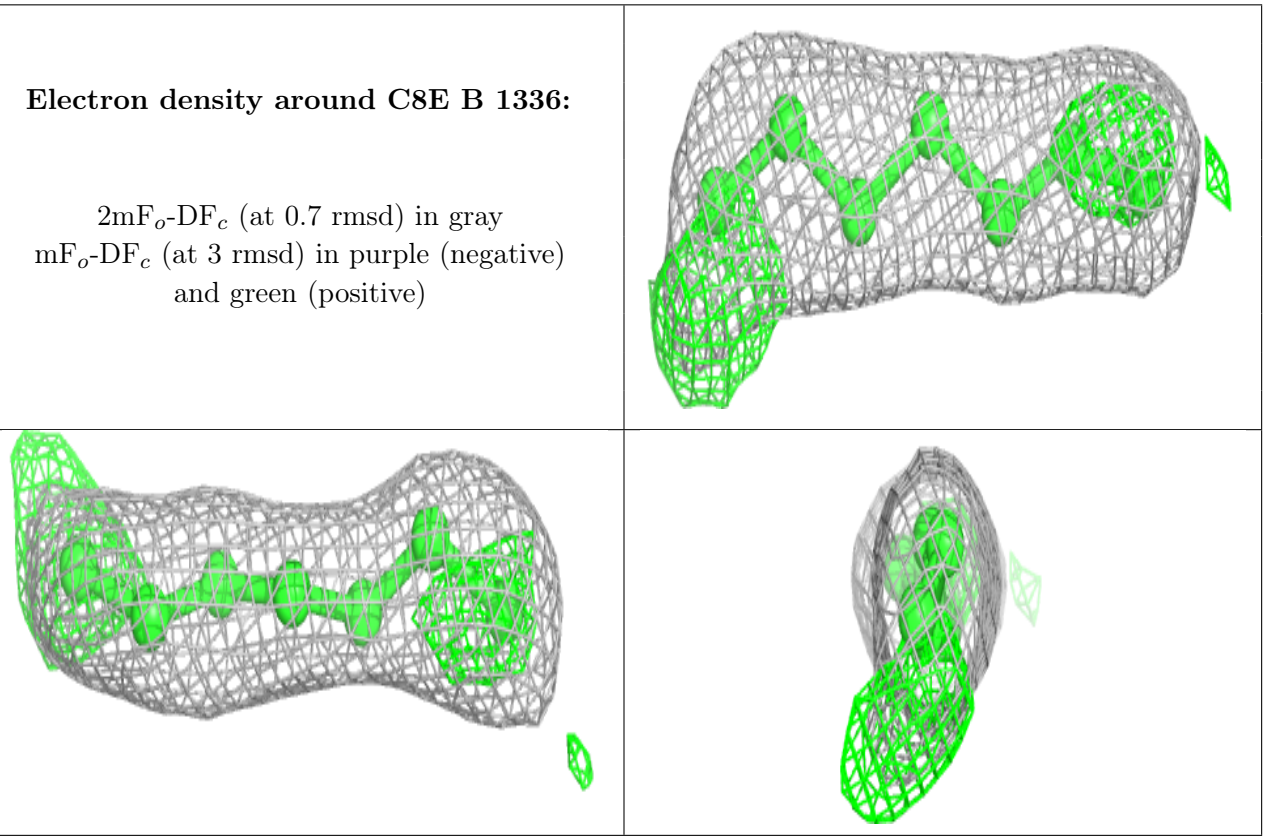
Electron density around C8E A 1328:

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



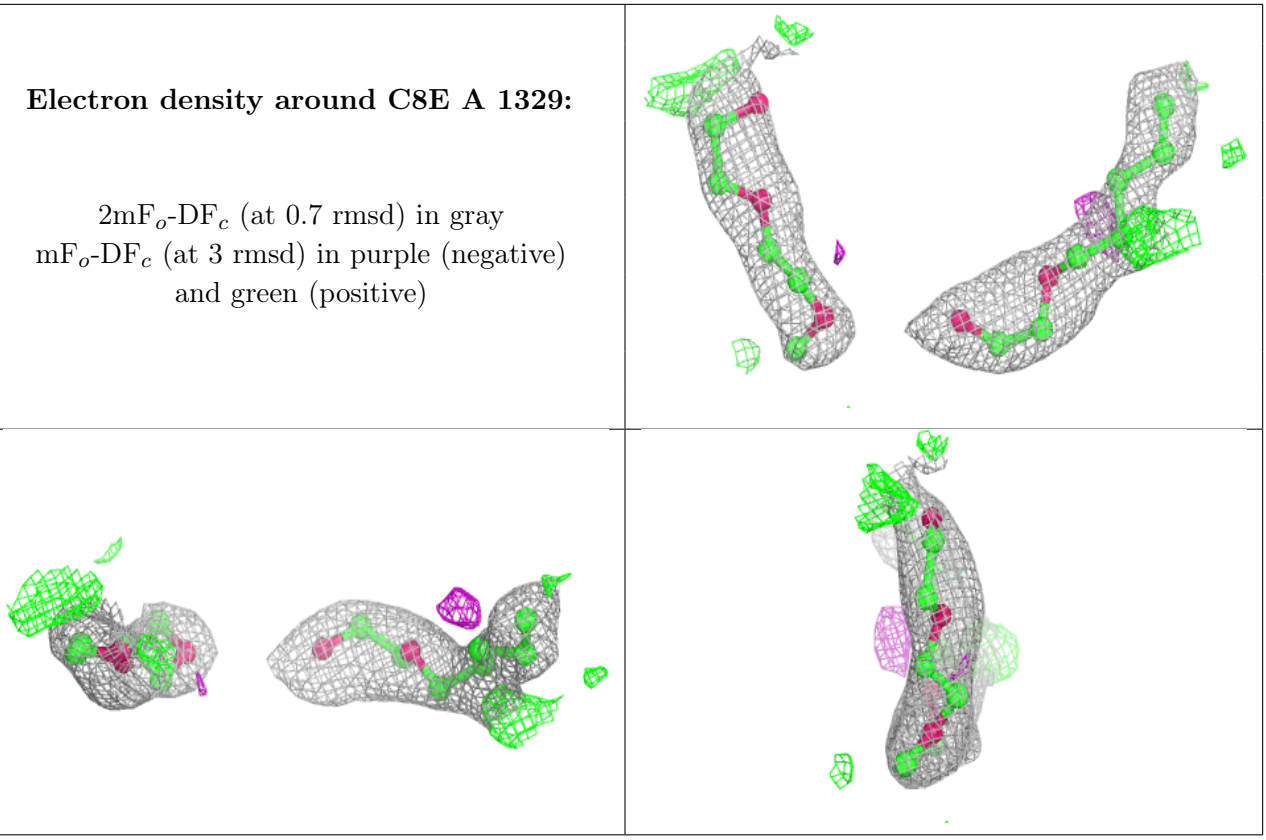
Electron density around C8E B 1336:

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



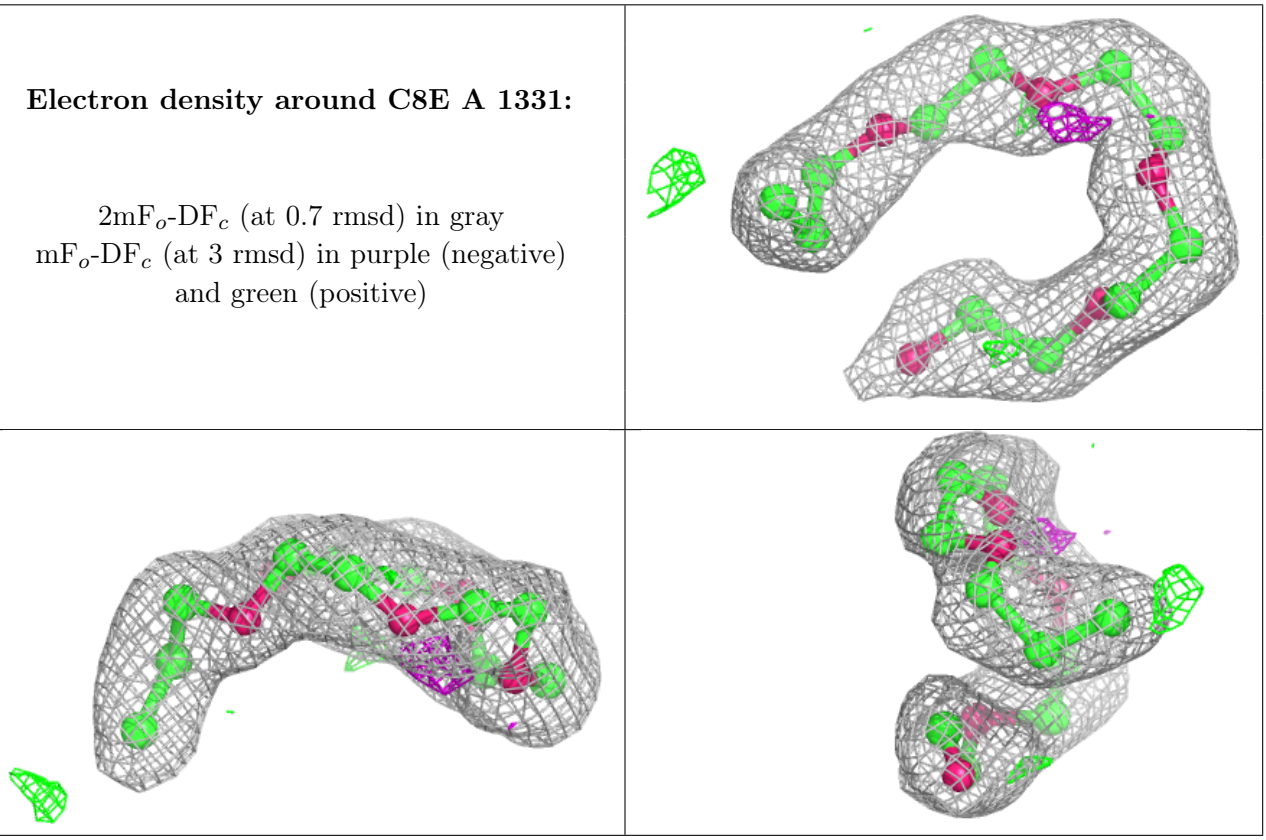
Electron density around C8E A 1329:

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



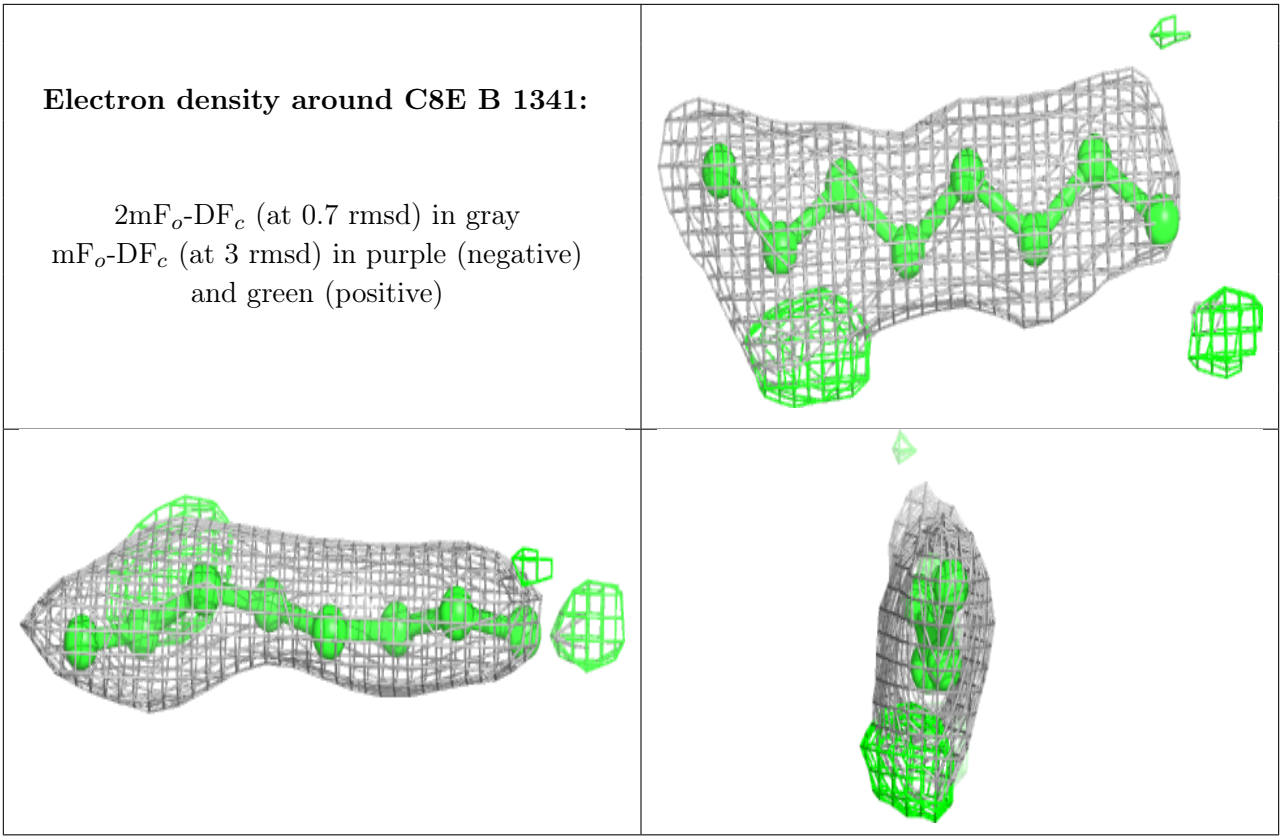
Electron density around C8E A 1331:

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



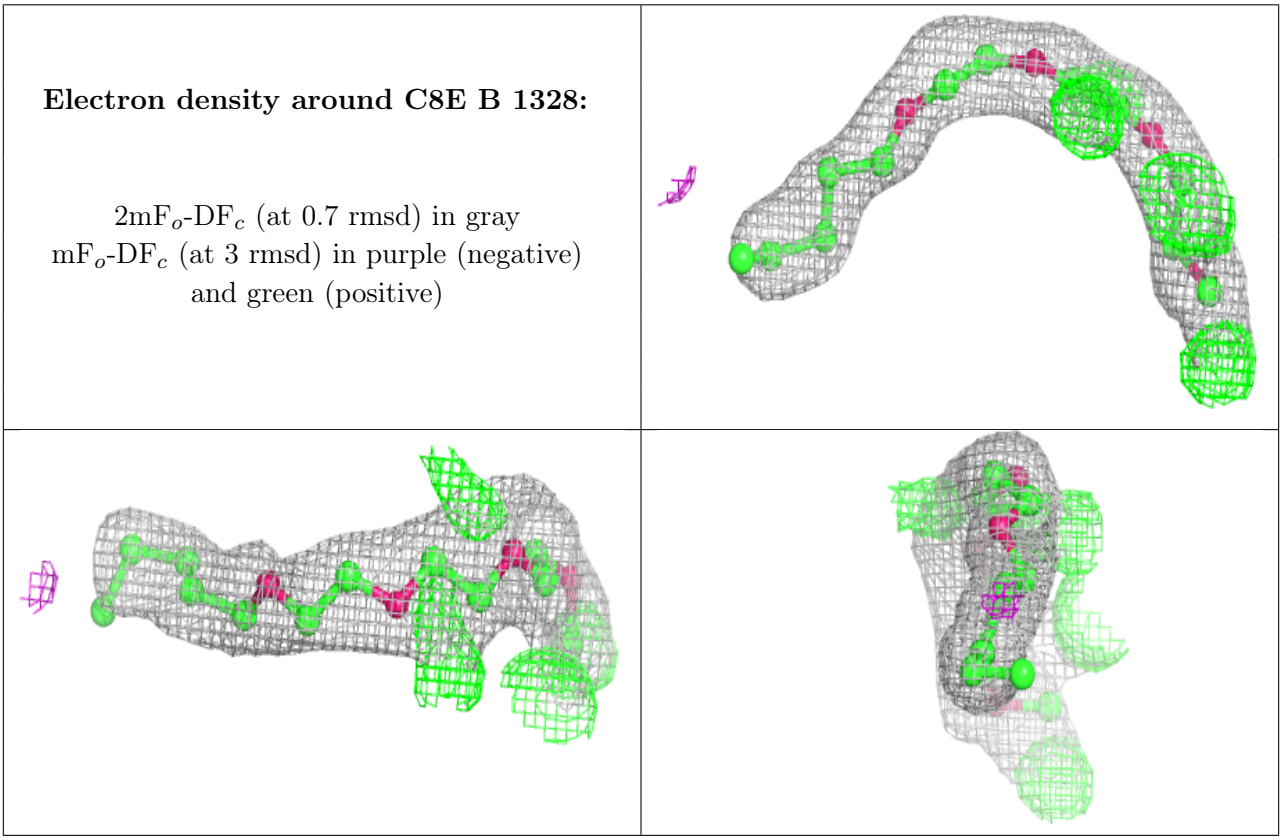
Electron density around C8E B 1341:

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



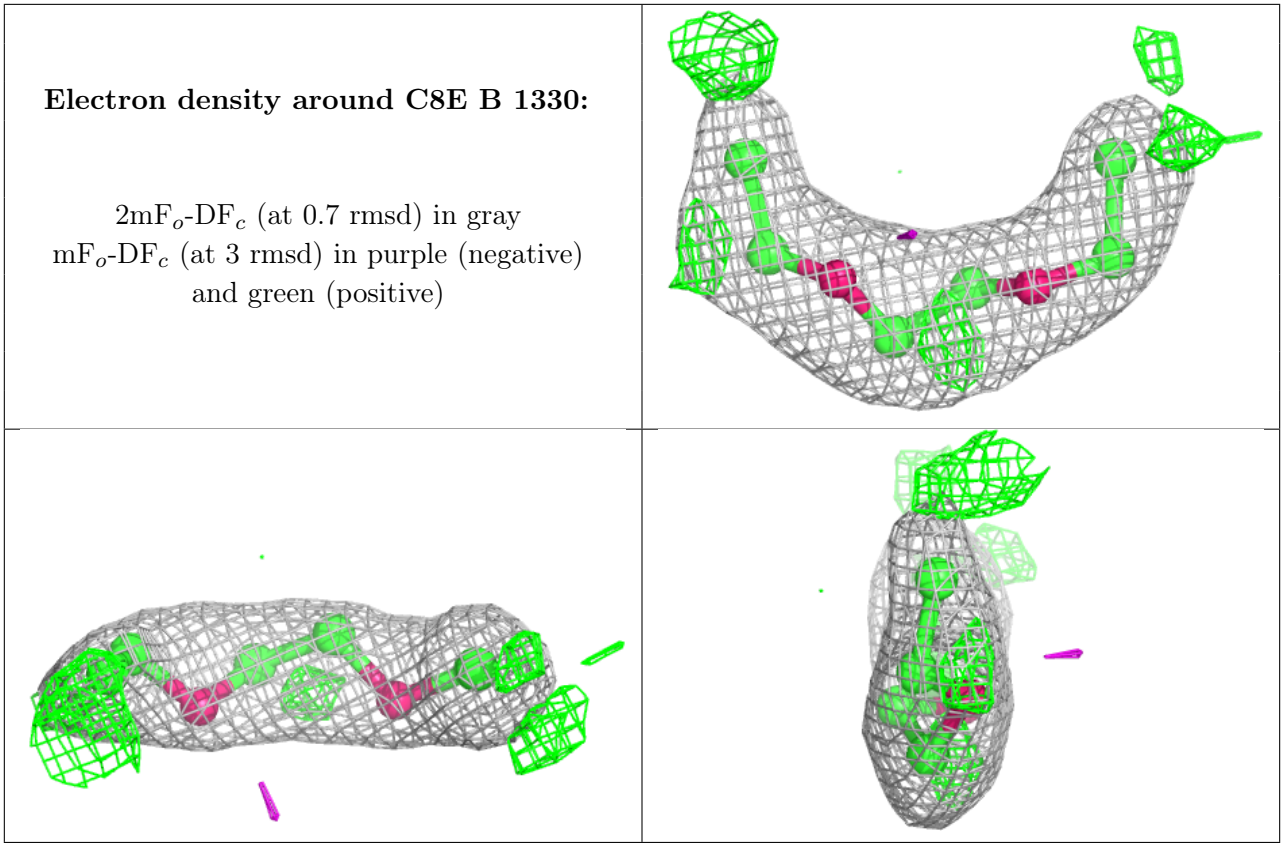
Electron density around C8E B 1328:

$2mF_o$-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 1330:

$2mF_o$-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.