wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 04:11 AM EDT

PDB ID	:	5IXM
Title	:	The LPS Transporter LptDE from Yersinia pestis, core complex
Authors	:	Botos, I.; Mayclin, S.J.; McCarthy, J.G.; Buchanan, S.K.
Deposited on	:	2016-03-23
Resolution	:	2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

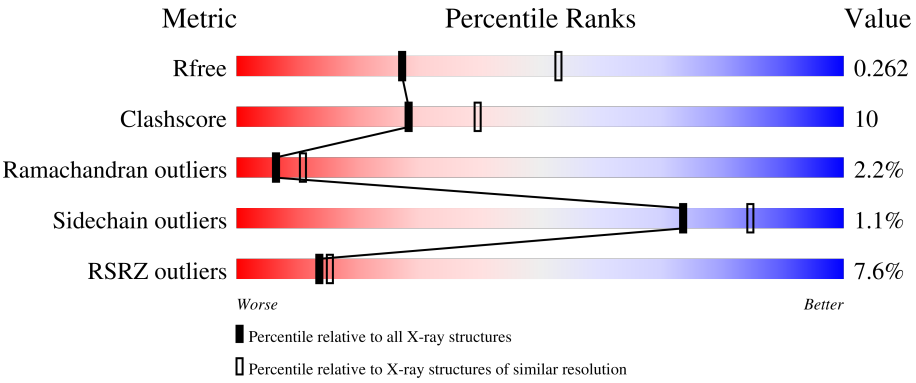
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	577	4% 76% 17% · 6%
1	C	577	5% 75% 18% •• 6%
1	E	577	8% 72% 19% · 7%
1	G	577	5% 74% 18% · 7%
2	B	198	11% 54% 17% · 29%

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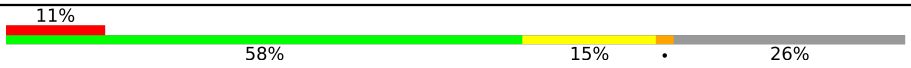
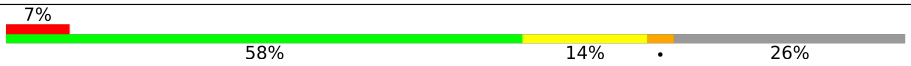
Mol	Chain	Length	Quality of chain
2	D	198	
2	F	198	
2	H	198	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22831 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4349	2765	742	829	13			
1	C	541	Total	C	N	O	S	0	0	0
			4346	2762	742	829	13			
1	E	538	Total	C	N	O	S	0	0	0
			4304	2737	736	818	13			
1	G	539	Total	C	N	O	S	0	0	0
			4329	2753	740	824	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8ZIK3
A	-19	SER	-	expression tag	UNP Q8ZIK3
A	-18	ASN	-	expression tag	UNP Q8ZIK3
A	-17	HIS	-	expression tag	UNP Q8ZIK3
A	-16	HIS	-	expression tag	UNP Q8ZIK3
A	-15	HIS	-	expression tag	UNP Q8ZIK3
A	-14	HIS	-	expression tag	UNP Q8ZIK3
A	-13	HIS	-	expression tag	UNP Q8ZIK3
A	-12	HIS	-	expression tag	UNP Q8ZIK3
A	-11	HIS	-	expression tag	UNP Q8ZIK3
A	-10	HIS	-	expression tag	UNP Q8ZIK3
A	-9	HIS	-	expression tag	UNP Q8ZIK3
A	-8	HIS	-	expression tag	UNP Q8ZIK3
A	-7	GLU	-	expression tag	UNP Q8ZIK3
A	-6	ASN	-	expression tag	UNP Q8ZIK3
A	-5	LEU	-	expression tag	UNP Q8ZIK3
A	-4	TYR	-	expression tag	UNP Q8ZIK3
A	-3	PHE	-	expression tag	UNP Q8ZIK3
A	-2	GLN	-	expression tag	UNP Q8ZIK3
A	-1	SER	-	expression tag	UNP Q8ZIK3
A	0	MET	-	expression tag	UNP Q8ZIK3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP Q8ZIK3
C	-19	SER	-	expression tag	UNP Q8ZIK3
C	-18	ASN	-	expression tag	UNP Q8ZIK3
C	-17	HIS	-	expression tag	UNP Q8ZIK3
C	-16	HIS	-	expression tag	UNP Q8ZIK3
C	-15	HIS	-	expression tag	UNP Q8ZIK3
C	-14	HIS	-	expression tag	UNP Q8ZIK3
C	-13	HIS	-	expression tag	UNP Q8ZIK3
C	-12	HIS	-	expression tag	UNP Q8ZIK3
C	-11	HIS	-	expression tag	UNP Q8ZIK3
C	-10	HIS	-	expression tag	UNP Q8ZIK3
C	-9	HIS	-	expression tag	UNP Q8ZIK3
C	-8	HIS	-	expression tag	UNP Q8ZIK3
C	-7	GLU	-	expression tag	UNP Q8ZIK3
C	-6	ASN	-	expression tag	UNP Q8ZIK3
C	-5	LEU	-	expression tag	UNP Q8ZIK3
C	-4	TYR	-	expression tag	UNP Q8ZIK3
C	-3	PHE	-	expression tag	UNP Q8ZIK3
C	-2	GLN	-	expression tag	UNP Q8ZIK3
C	-1	SER	-	expression tag	UNP Q8ZIK3
C	0	MET	-	expression tag	UNP Q8ZIK3
E	-20	MET	-	initiating methionine	UNP Q8ZIK3
E	-19	SER	-	expression tag	UNP Q8ZIK3
E	-18	ASN	-	expression tag	UNP Q8ZIK3
E	-17	HIS	-	expression tag	UNP Q8ZIK3
E	-16	HIS	-	expression tag	UNP Q8ZIK3
E	-15	HIS	-	expression tag	UNP Q8ZIK3
E	-14	HIS	-	expression tag	UNP Q8ZIK3
E	-13	HIS	-	expression tag	UNP Q8ZIK3
E	-12	HIS	-	expression tag	UNP Q8ZIK3
E	-11	HIS	-	expression tag	UNP Q8ZIK3
E	-10	HIS	-	expression tag	UNP Q8ZIK3
E	-9	HIS	-	expression tag	UNP Q8ZIK3
E	-8	HIS	-	expression tag	UNP Q8ZIK3
E	-7	GLU	-	expression tag	UNP Q8ZIK3
E	-6	ASN	-	expression tag	UNP Q8ZIK3
E	-5	LEU	-	expression tag	UNP Q8ZIK3
E	-4	TYR	-	expression tag	UNP Q8ZIK3
E	-3	PHE	-	expression tag	UNP Q8ZIK3
E	-2	GLN	-	expression tag	UNP Q8ZIK3
E	-1	SER	-	expression tag	UNP Q8ZIK3
E	0	MET	-	expression tag	UNP Q8ZIK3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	MET	-	initiating methionine	UNP Q8ZIK3
G	-19	SER	-	expression tag	UNP Q8ZIK3
G	-18	ASN	-	expression tag	UNP Q8ZIK3
G	-17	HIS	-	expression tag	UNP Q8ZIK3
G	-16	HIS	-	expression tag	UNP Q8ZIK3
G	-15	HIS	-	expression tag	UNP Q8ZIK3
G	-14	HIS	-	expression tag	UNP Q8ZIK3
G	-13	HIS	-	expression tag	UNP Q8ZIK3
G	-12	HIS	-	expression tag	UNP Q8ZIK3
G	-11	HIS	-	expression tag	UNP Q8ZIK3
G	-10	HIS	-	expression tag	UNP Q8ZIK3
G	-9	HIS	-	expression tag	UNP Q8ZIK3
G	-8	HIS	-	expression tag	UNP Q8ZIK3
G	-7	GLU	-	expression tag	UNP Q8ZIK3
G	-6	ASN	-	expression tag	UNP Q8ZIK3
G	-5	LEU	-	expression tag	UNP Q8ZIK3
G	-4	TYR	-	expression tag	UNP Q8ZIK3
G	-3	PHE	-	expression tag	UNP Q8ZIK3
G	-2	GLN	-	expression tag	UNP Q8ZIK3
G	-1	SER	-	expression tag	UNP Q8ZIK3
G	0	MET	-	expression tag	UNP Q8ZIK3

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1107	694	200	212	1			
2	D	146	Total	C	N	O	S	0	0	0
			1133	710	205	217	1			
2	F	145	Total	C	N	O	S	0	0	0
			1128	709	207	211	1			
2	H	147	Total	C	N	O	S	0	0	0
			1154	722	210	220	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP Q7CJV2
B	-3	PRO	-	expression tag	UNP Q7CJV2
B	-2	ASN	-	expression tag	UNP Q7CJV2
B	-1	THR	-	expression tag	UNP Q7CJV2
B	0	SER	-	expression tag	UNP Q7CJV2

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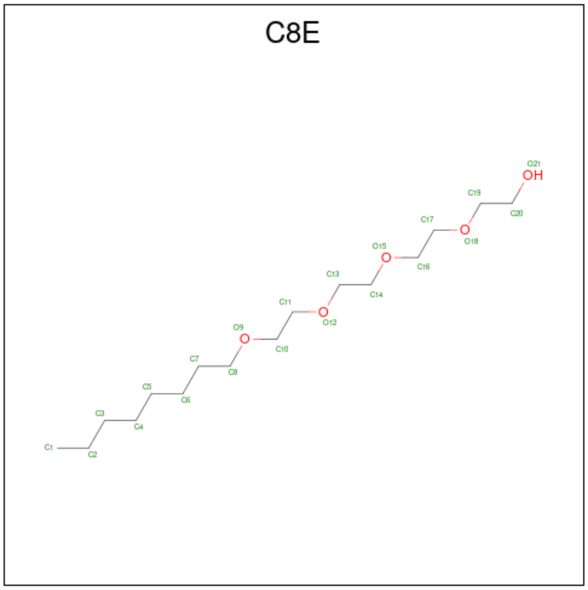
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	HIS	-	expression tag	UNP Q7CJV2
B	189	HIS	-	expression tag	UNP Q7CJV2
B	190	HIS	-	expression tag	UNP Q7CJV2
B	191	HIS	-	expression tag	UNP Q7CJV2
B	192	HIS	-	expression tag	UNP Q7CJV2
B	193	HIS	-	expression tag	UNP Q7CJV2
D	-4	ALA	-	expression tag	UNP Q7CJV2
D	-3	PRO	-	expression tag	UNP Q7CJV2
D	-2	ASN	-	expression tag	UNP Q7CJV2
D	-1	THR	-	expression tag	UNP Q7CJV2
D	0	SER	-	expression tag	UNP Q7CJV2
D	188	HIS	-	expression tag	UNP Q7CJV2
D	189	HIS	-	expression tag	UNP Q7CJV2
D	190	HIS	-	expression tag	UNP Q7CJV2
D	191	HIS	-	expression tag	UNP Q7CJV2
D	192	HIS	-	expression tag	UNP Q7CJV2
D	193	HIS	-	expression tag	UNP Q7CJV2
F	-4	ALA	-	expression tag	UNP Q7CJV2
F	-3	PRO	-	expression tag	UNP Q7CJV2
F	-2	ASN	-	expression tag	UNP Q7CJV2
F	-1	THR	-	expression tag	UNP Q7CJV2
F	0	SER	-	expression tag	UNP Q7CJV2
F	188	HIS	-	expression tag	UNP Q7CJV2
F	189	HIS	-	expression tag	UNP Q7CJV2
F	190	HIS	-	expression tag	UNP Q7CJV2
F	191	HIS	-	expression tag	UNP Q7CJV2
F	192	HIS	-	expression tag	UNP Q7CJV2
F	193	HIS	-	expression tag	UNP Q7CJV2
H	-4	ALA	-	expression tag	UNP Q7CJV2
H	-3	PRO	-	expression tag	UNP Q7CJV2
H	-2	ASN	-	expression tag	UNP Q7CJV2
H	-1	THR	-	expression tag	UNP Q7CJV2
H	0	SER	-	expression tag	UNP Q7CJV2
H	188	HIS	-	expression tag	UNP Q7CJV2
H	189	HIS	-	expression tag	UNP Q7CJV2
H	190	HIS	-	expression tag	UNP Q7CJV2
H	191	HIS	-	expression tag	UNP Q7CJV2
H	192	HIS	-	expression tag	UNP Q7CJV2
H	193	HIS	-	expression tag	UNP Q7CJV2

- 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 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	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 21 16 5	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 21 16 5	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 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0

- Molecule 4 is water.

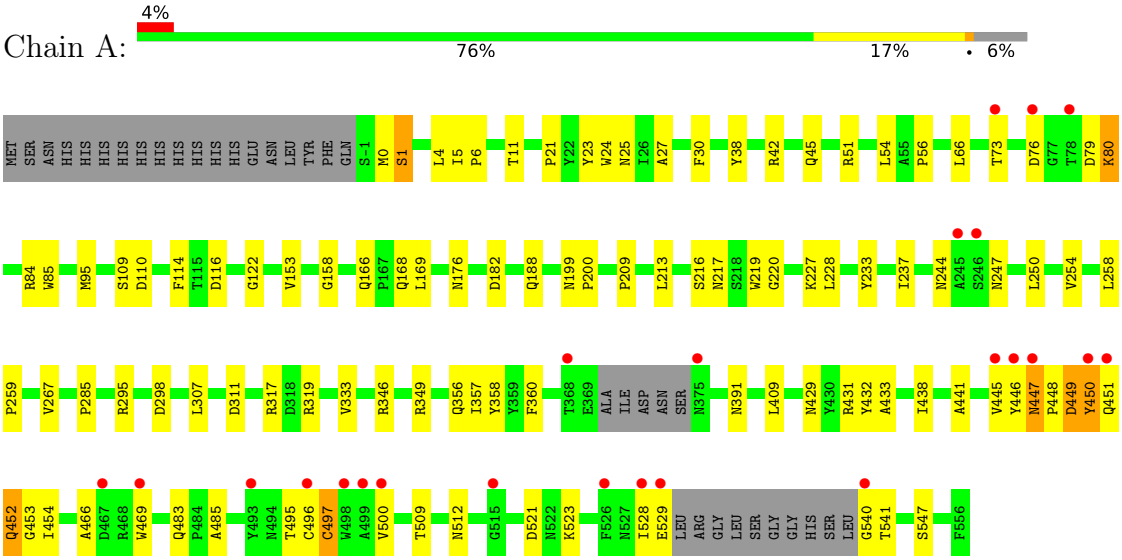
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	148	Total O 148 148	0	0
4	B	38	Total O 38 38	0	0
4	C	125	Total O 125 125	0	0
4	D	27	Total O 27 27	0	0
4	E	75	Total O 75 75	0	0
4	F	16	Total O 16 16	0	0
4	G	92	Total O 92 92	0	0
4	H	19	Total O 19 19	0	0

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.

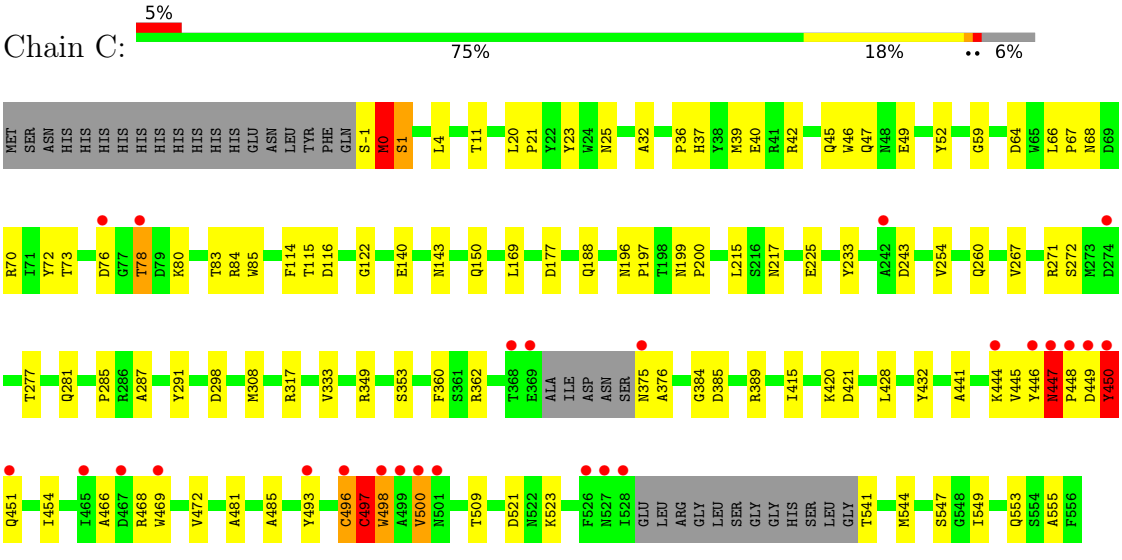
• Molecule 1: LPS-assembly protein LptD

Chain A:



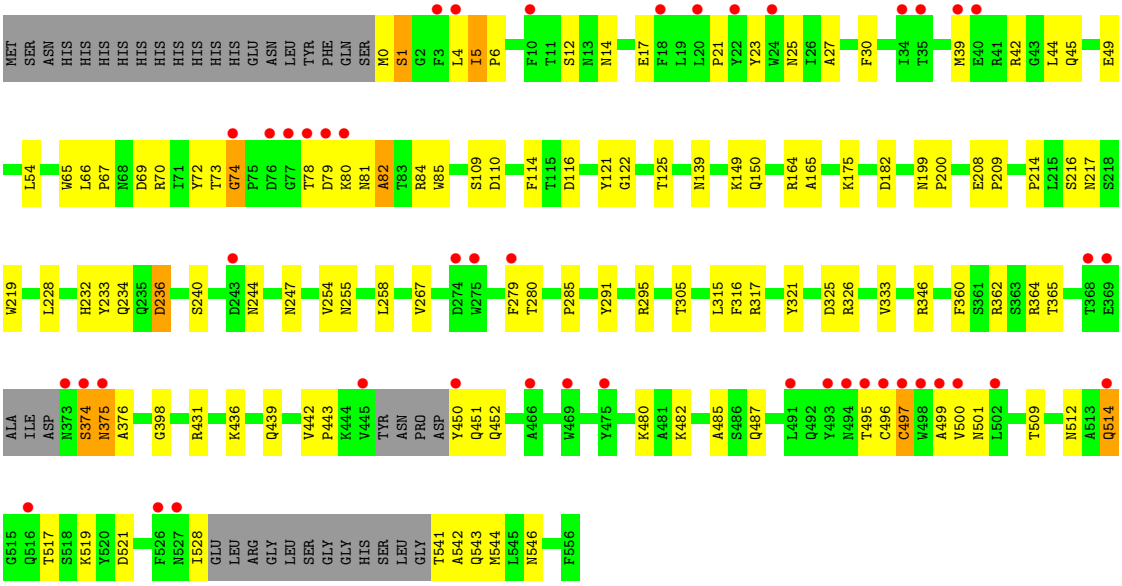
• Molecule 1: LPS-assembly protein LptD

Chain C:



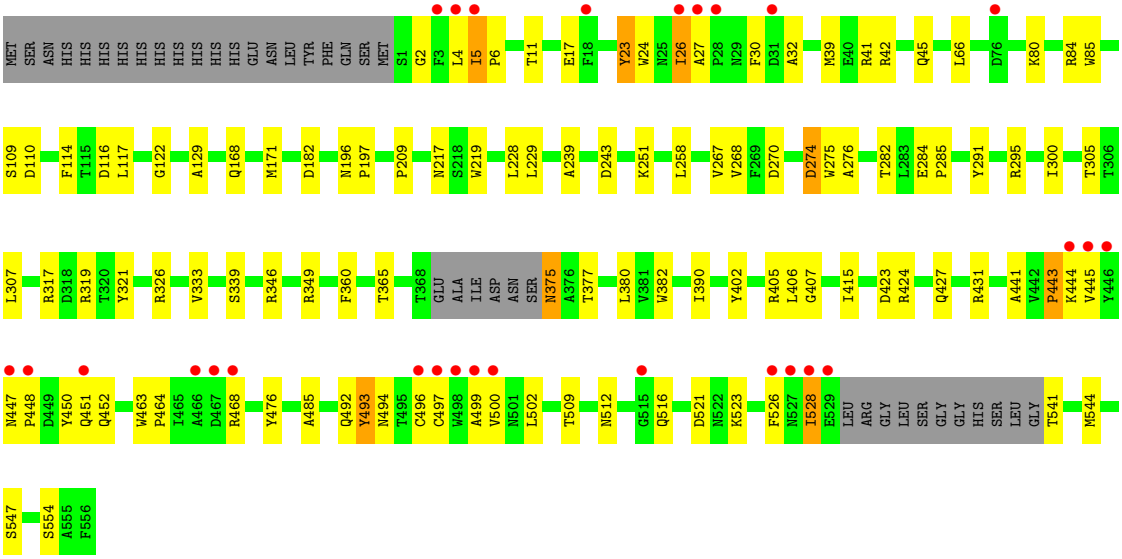
• Molecule 1: LPS-assembly protein LptD

Chain E:



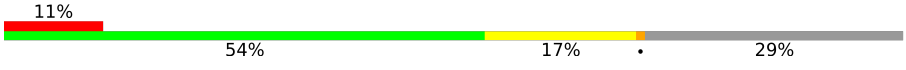
• Molecule 1: LPS-assembly protein LptD

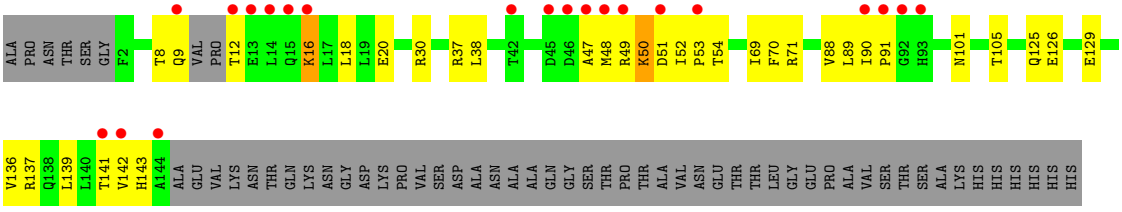
Chain G:



• Molecule 2: LPS-assembly lipoprotein LptE

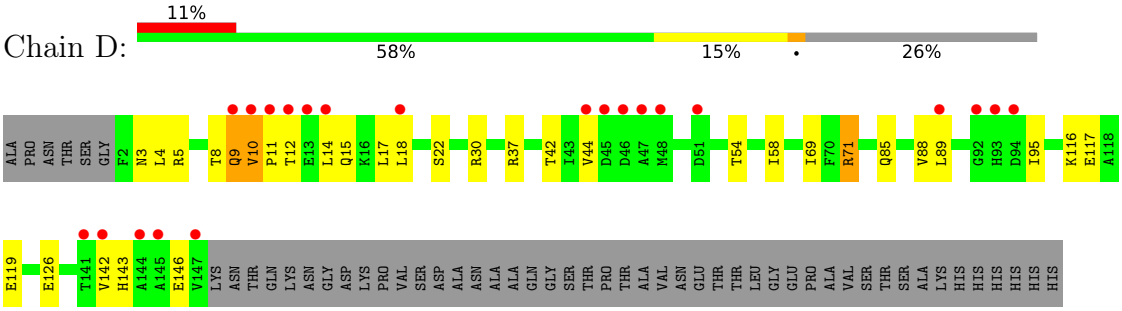
Chain B:





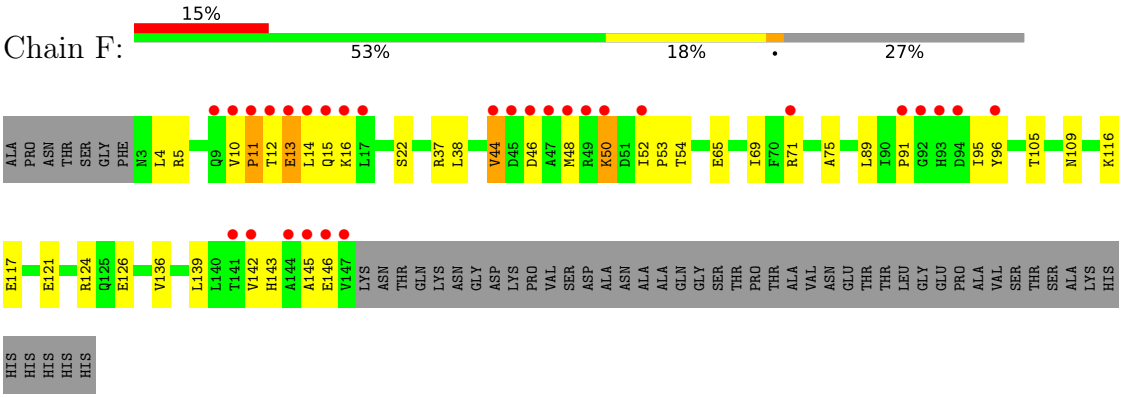
• Molecule 2: LPS-assembly lipoprotein LptE

Chain D:



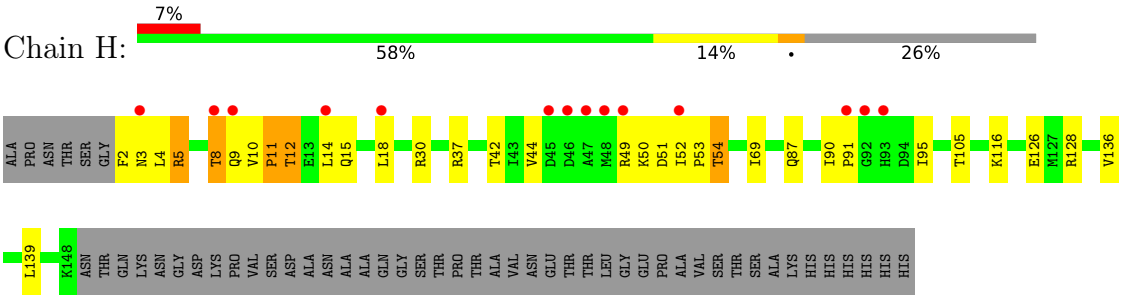
- Molecule 2: LPS-assembly lipoprotein LptE

Chain F:



- Molecule 2: LPS-assembly lipoprotein LptE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.89Å 176.35Å 143.85Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	40.13 – 2.75 49.33 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.13-2.75) 94.3 (49.33-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.261 0.216 , 0.262	Depositor DCC
R_{free} test set	5392 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22831	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.26	0/4471	0.50	0/6091
1	C	0.27	0/4468	0.50	1/6087 (0.0%)
1	E	0.27	0/4423	0.52	0/6024
1	G	0.28	1/4451 (0.0%)	0.50	0/6065
2	B	0.28	0/1121	0.57	0/1523
2	D	0.29	0/1148	0.58	0/1564
2	F	0.29	0/1143	0.54	0/1555
2	H	0.26	0/1169	0.55	0/1589
All	All	0.27	1/22394 (0.0%)	0.52	1/30498 (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	C	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	493	TYR	CD1-CE1	-5.17	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	447	ASN	N-CA-C	6.49	128.52	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	78	THR	Peptide
1	E	374	SER	Peptide

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	4349	0	4105	80	1
1	C	4346	0	4108	79	1
1	E	4304	0	4065	91	0
1	G	4329	0	4092	83	0
2	B	1107	0	1111	29	0
2	D	1133	0	1139	32	0
2	F	1128	0	1149	30	0
2	H	1154	0	1172	29	0
3	A	105	0	170	13	0
3	C	189	0	306	13	0
3	E	84	0	136	2	0
3	G	63	0	102	5	0
4	A	148	0	0	18	1
4	B	38	0	0	9	0
4	C	125	0	0	17	1
4	D	27	0	0	4	0
4	E	75	0	0	27	2
4	F	16	0	0	5	0
4	G	92	0	0	20	2
4	H	19	0	0	5	0
All	All	22831	0	21655	429	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 10.

The worst 5 of 429 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:A:298:ASP:OD1	4:A:701:HOH:O	1.82	0.95
2:F:13:GLU:HG3	2:F:14:LEU:HG	1.51	0.93
2:B:12:THR:N	4:B:202:HOH:O	2.01	0.93
1:A:168:GLN:NE2	4:A:704:HOH:O	2.00	0.92
1:G:443:PRO:O	1:G:445:VAL:N	2.04	0.91

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:846:HOH:O	4:C:823:HOH:O[2_746]	1.86	0.34
4:E:774:HOH:O	4:G:778:HOH:O[2_657]	2.12	0.08
4:E:774:HOH:O	4:G:780:HOH:O[2_657]	2.15	0.05
1:A:38:TYR:OH	1:C:40:GLU:OE2[2_846]	2.19	0.01

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	537/577 (93%)	490 (91%)	36 (7%)	11 (2%)	7 13
1	C	535/577 (93%)	491 (92%)	33 (6%)	11 (2%)	7 12
1	E	530/577 (92%)	483 (91%)	33 (6%)	14 (3%)	5 8
1	G	533/577 (92%)	488 (92%)	38 (7%)	7 (1%)	12 21
2	B	137/198 (69%)	123 (90%)	9 (7%)	5 (4%)	3 5
2	D	144/198 (73%)	134 (93%)	7 (5%)	3 (2%)	7 12
2	F	143/198 (72%)	131 (92%)	6 (4%)	6 (4%)	3 3
2	H	145/198 (73%)	135 (93%)	7 (5%)	3 (2%)	7 12
All	All	2704/3100 (87%)	2475 (92%)	169 (6%)	60 (2%)	6 11

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	80	LYS
1	A	445	VAL
1	A	447	ASN
1	A	496	CYS

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	454/487 (93%)	452 (100%)	2 (0%)	91	94
1	C	456/487 (94%)	449 (98%)	7 (2%)	65	79
1	E	449/487 (92%)	444 (99%)	5 (1%)	73	84
1	G	453/487 (93%)	447 (99%)	6 (1%)	69	82
2	B	121/169 (72%)	121 (100%)	0	100	100
2	D	123/169 (73%)	122 (99%)	1 (1%)	81	89
2	F	122/169 (72%)	120 (98%)	2 (2%)	62	78
2	H	127/169 (75%)	125 (98%)	2 (2%)	62	78
All	All	2305/2624 (88%)	2280 (99%)	25 (1%)	73	84

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	517	THR
1	G	5	ILE
2	H	54	THR
2	F	50	LYS
1	G	23	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	501	ASN

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Mol	Chain	Res	Type
1	G	427	GLN
1	G	501	ASN
1	G	492	GLN
1	E	168	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	E	602	-	20,20,20	0.39	0	19,19,19	0.31	0
3	C8E	G	602	-	20,20,20	0.39	0	19,19,19	0.32	0
3	C8E	C	602	-	20,20,20	0.37	0	19,19,19	0.38	0
3	C8E	C	606	-	20,20,20	0.38	0	19,19,19	0.39	0
3	C8E	C	608	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	601	-	20,20,20	0.38	0	19,19,19	0.33	0
3	C8E	E	604	-	20,20,20	0.41	0	19,19,19	0.35	0
3	C8E	E	601	-	20,20,20	0.35	0	19,19,19	0.59	0
3	C8E	A	605	-	20,20,20	0.36	0	19,19,19	0.52	0
3	C8E	E	603	-	20,20,20	0.38	0	19,19,19	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	C8E	C	609	-	20,20,20	0.39	0	19,19,19	0.38	0
3	C8E	C	603	-	20,20,20	0.39	0	19,19,19	0.37	0
3	C8E	A	604	-	20,20,20	0.37	0	19,19,19	0.47	0
3	C8E	G	601	-	20,20,20	0.37	0	19,19,19	0.43	0
3	C8E	C	604	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	607	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	C	605	-	20,20,20	0.40	0	19,19,19	0.33	0
3	C8E	A	603	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	A	601	-	20,20,20	0.40	0	19,19,19	0.32	0
3	C8E	G	603	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	A	602	-	20,20,20	0.38	0	19,19,19	0.36	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	E	602	-	-	11/18/18/18	-
3	C8E	G	602	-	-	13/18/18/18	-
3	C8E	C	602	-	-	16/18/18/18	-
3	C8E	C	606	-	-	13/18/18/18	-
3	C8E	C	608	-	-	14/18/18/18	-
3	C8E	C	601	-	-	12/18/18/18	-
3	C8E	E	604	-	-	12/18/18/18	-
3	C8E	E	601	-	-	10/18/18/18	-
3	C8E	A	605	-	-	11/18/18/18	-
3	C8E	E	603	-	-	14/18/18/18	-
3	C8E	C	609	-	-	14/18/18/18	-
3	C8E	C	603	-	-	10/18/18/18	-
3	C8E	A	604	-	-	14/18/18/18	-
3	C8E	G	601	-	-	13/18/18/18	-
3	C8E	C	604	-	-	10/18/18/18	-
3	C8E	C	607	-	-	11/18/18/18	-
3	C8E	C	605	-	-	10/18/18/18	-
3	C8E	A	603	-	-	10/18/18/18	-
3	C8E	A	601	-	-	13/18/18/18	-
3	C8E	G	603	-	-	13/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	602	-	-	15/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 259 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	C8E	O18-C19-C20-O21
3	C	602	C8E	C2-C3-C4-C5
3	C	604	C8E	C2-C3-C4-C5
3	A	603	C8E	C3-C4-C5-C6
3	C	608	C8E	O12-C13-C14-O15

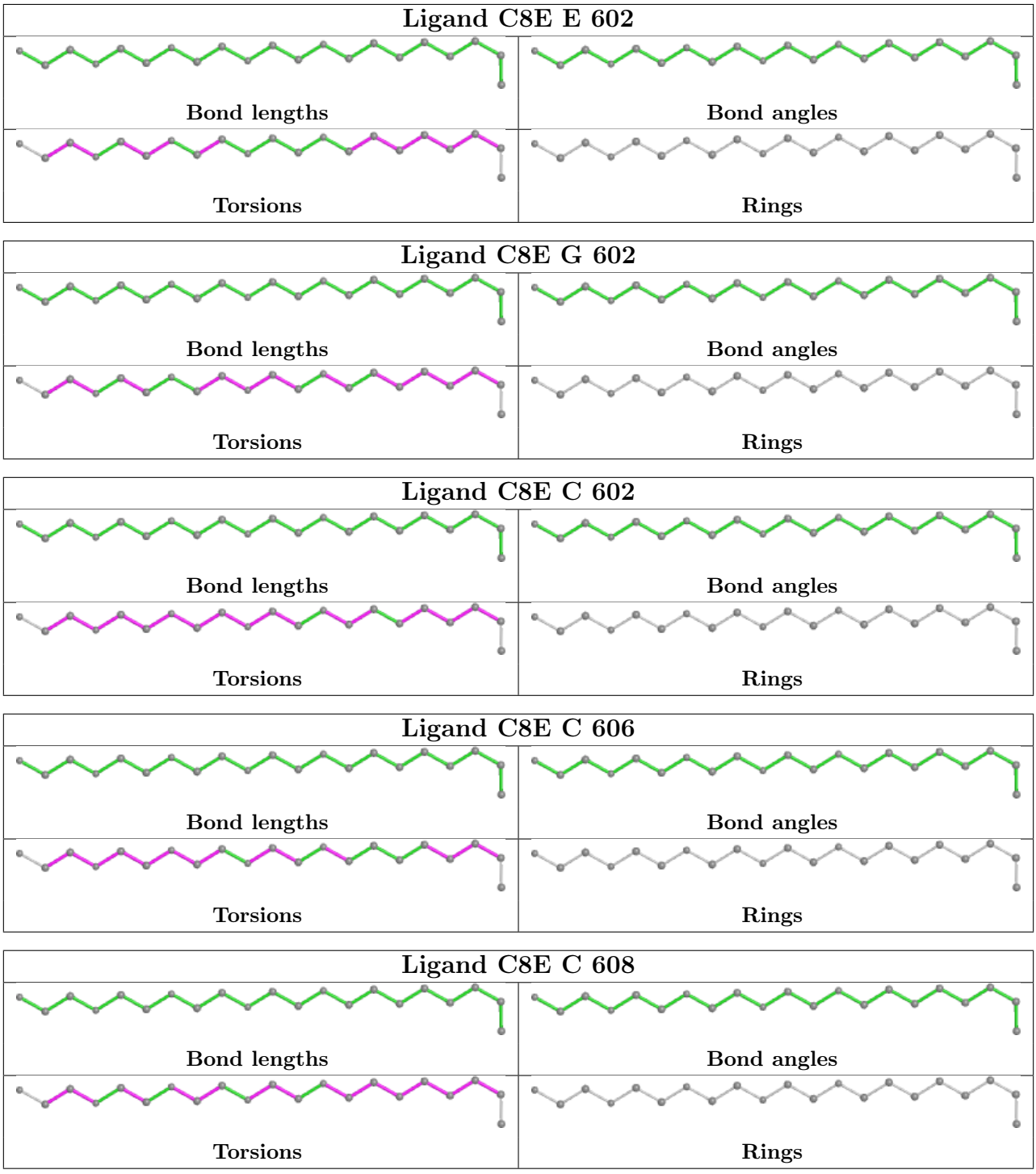
There are no ring outliers.

15 monomers are involved in 32 short contacts:

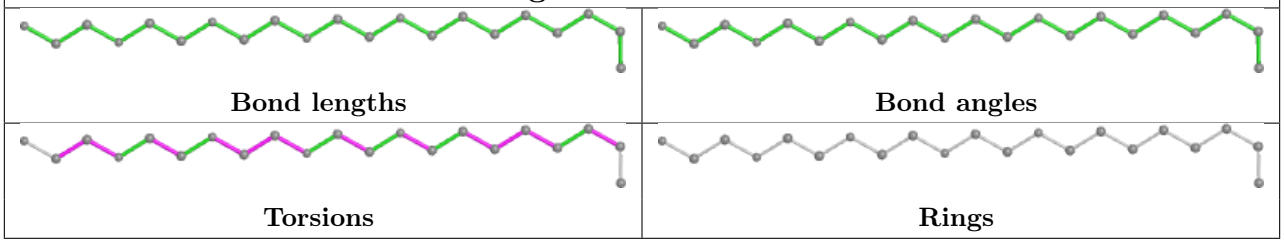
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	C8E	2	0
3	C	602	C8E	5	0
3	C	601	C8E	4	0
3	A	605	C8E	1	0
3	E	603	C8E	2	0
3	C	603	C8E	1	0
3	A	604	C8E	2	0
3	G	601	C8E	2	0
3	C	604	C8E	1	0
3	C	607	C8E	1	0
3	C	605	C8E	1	0
3	A	603	C8E	2	0
3	A	601	C8E	4	0
3	G	603	C8E	1	0
3	A	602	C8E	4	0

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

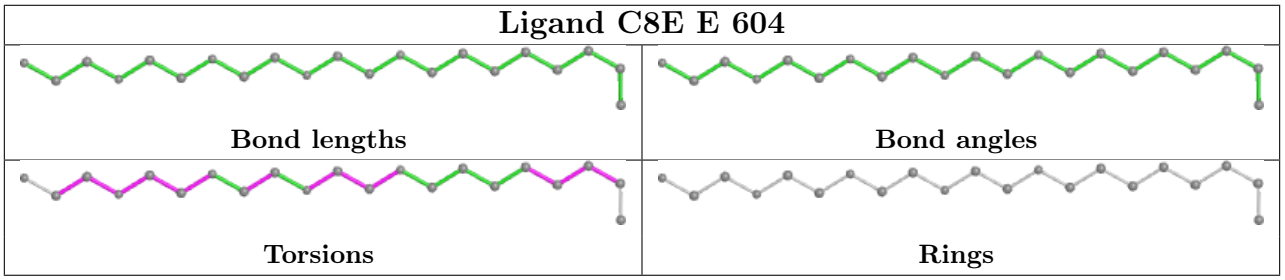
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



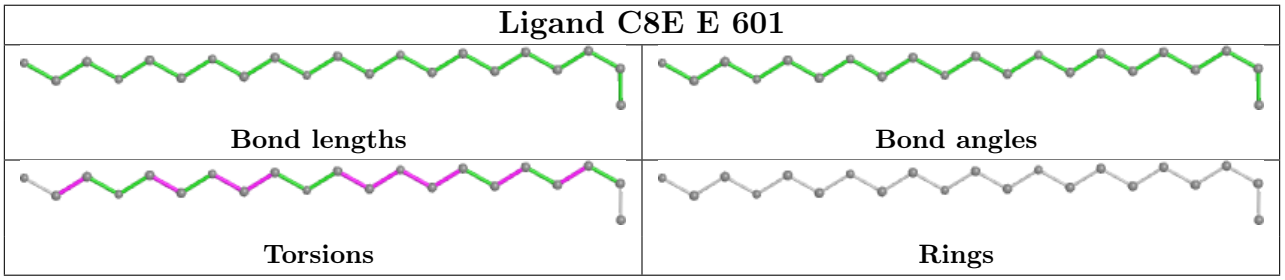
Ligand C8E C 601



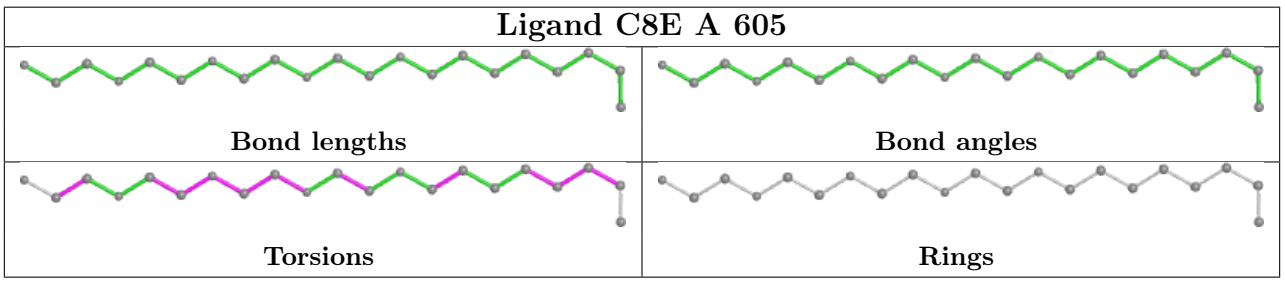
Ligand C8E E 604



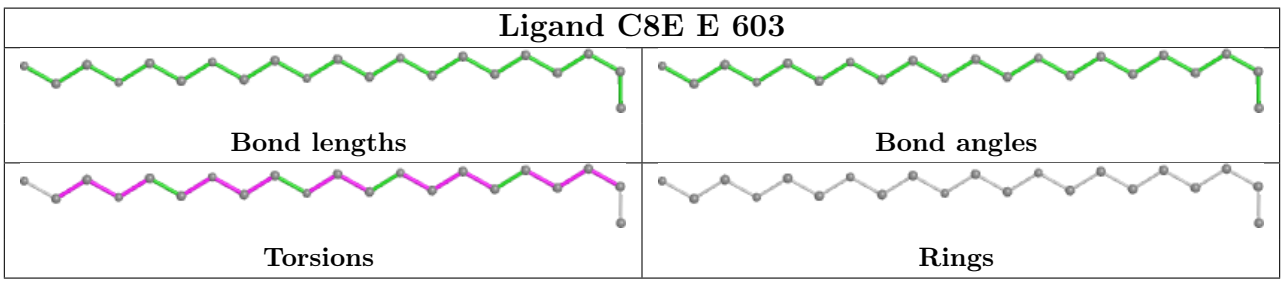
Ligand C8E E 601



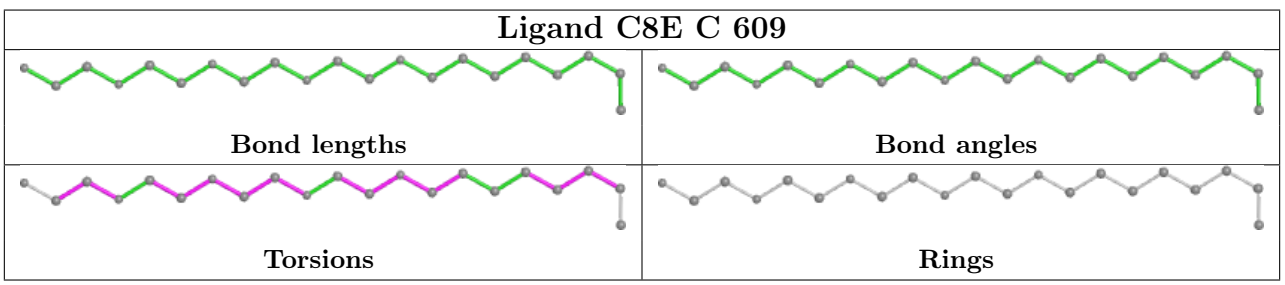
Ligand C8E A 605



Ligand C8E E 603



Ligand C8E C 609



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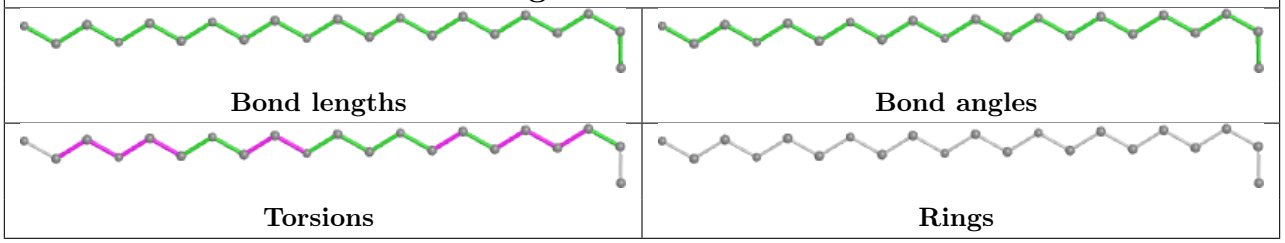

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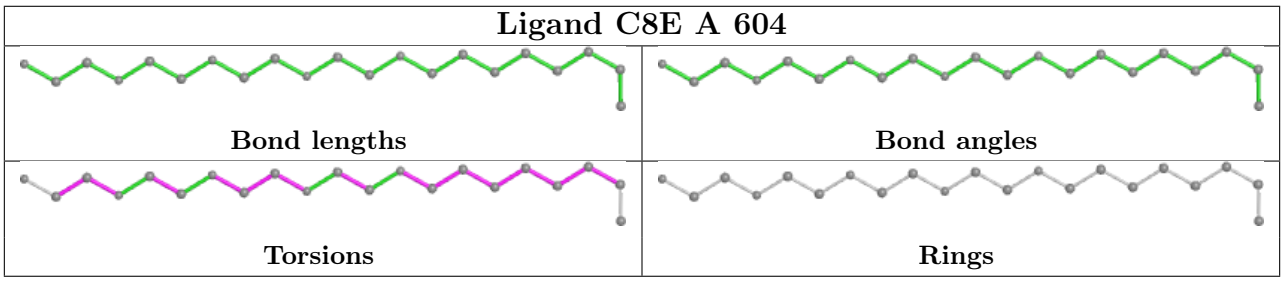

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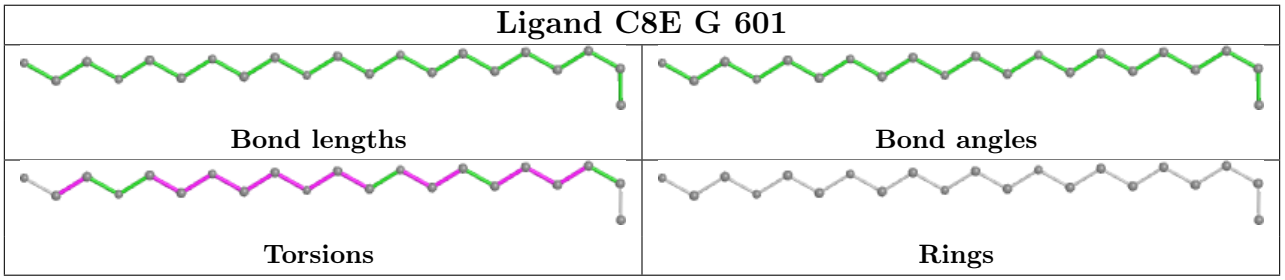

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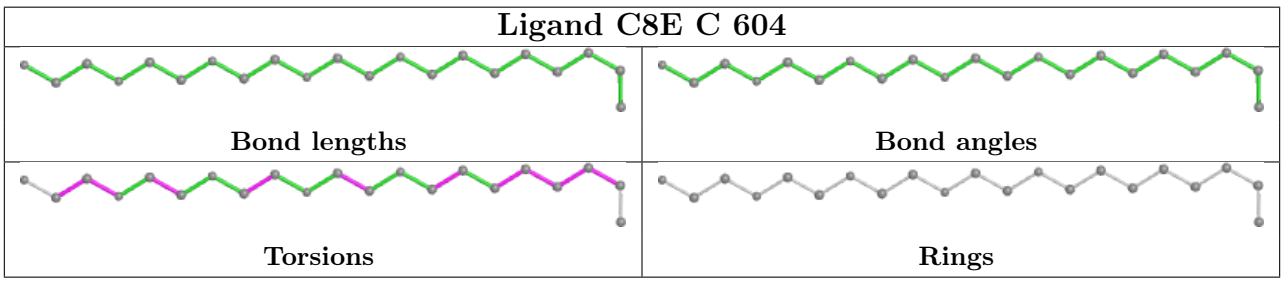

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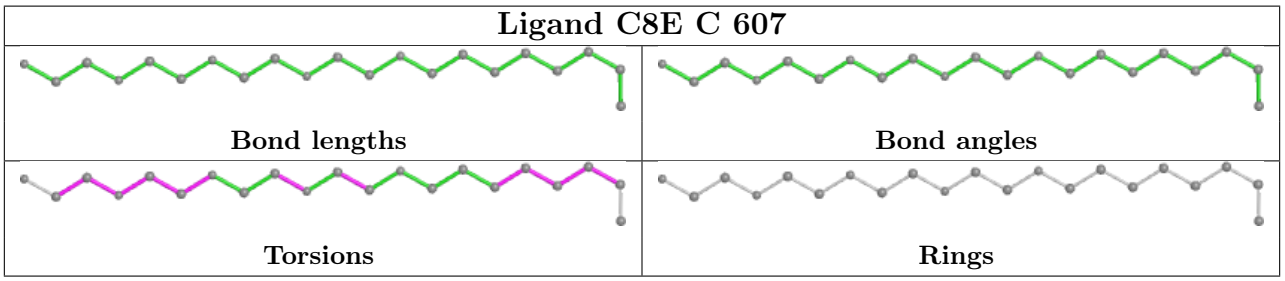

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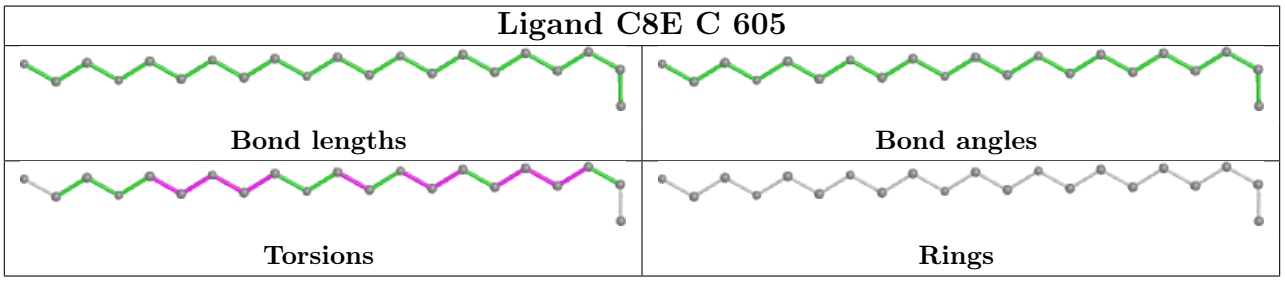
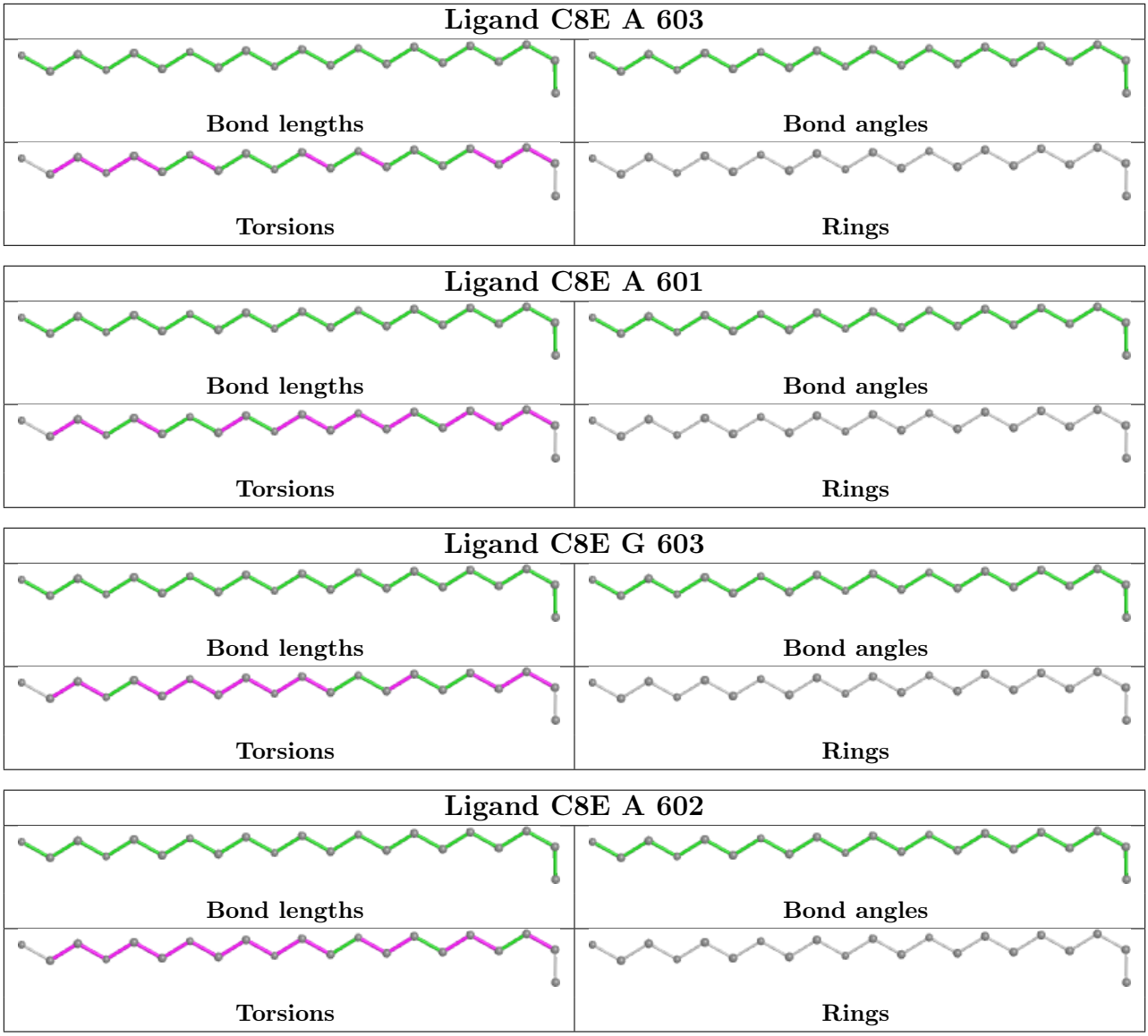




5.7 Other polymers

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	543/577 (94%)	0.06	24 (4%)	34	37	13, 32, 84, 131	0
1	C	541/577 (93%)	0.07	26 (4%)	30	34	11, 33, 89, 128	0
1	E	538/577 (93%)	0.50	45 (8%)	11	12	21, 53, 110, 166	0
1	G	539/577 (93%)	0.20	28 (5%)	27	31	18, 44, 97, 140	0
2	B	141/198 (71%)	0.55	21 (14%)	2	2	14, 36, 102, 127	0
2	D	146/198 (73%)	0.59	22 (15%)	2	2	13, 38, 106, 123	0
2	F	145/198 (73%)	0.84	29 (20%)	1	1	28, 54, 117, 145	0
2	H	147/198 (74%)	0.40	14 (9%)	8	8	19, 45, 101, 124	0
All	All	2740/3100 (88%)	0.29	209 (7%)	13	15	11, 41, 103, 166	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	500	VAL	9.1
2	F	11	PRO	8.5
1	A	446	TYR	7.9
2	B	142	VAL	6.5
2	F	14	LEU	6.4

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

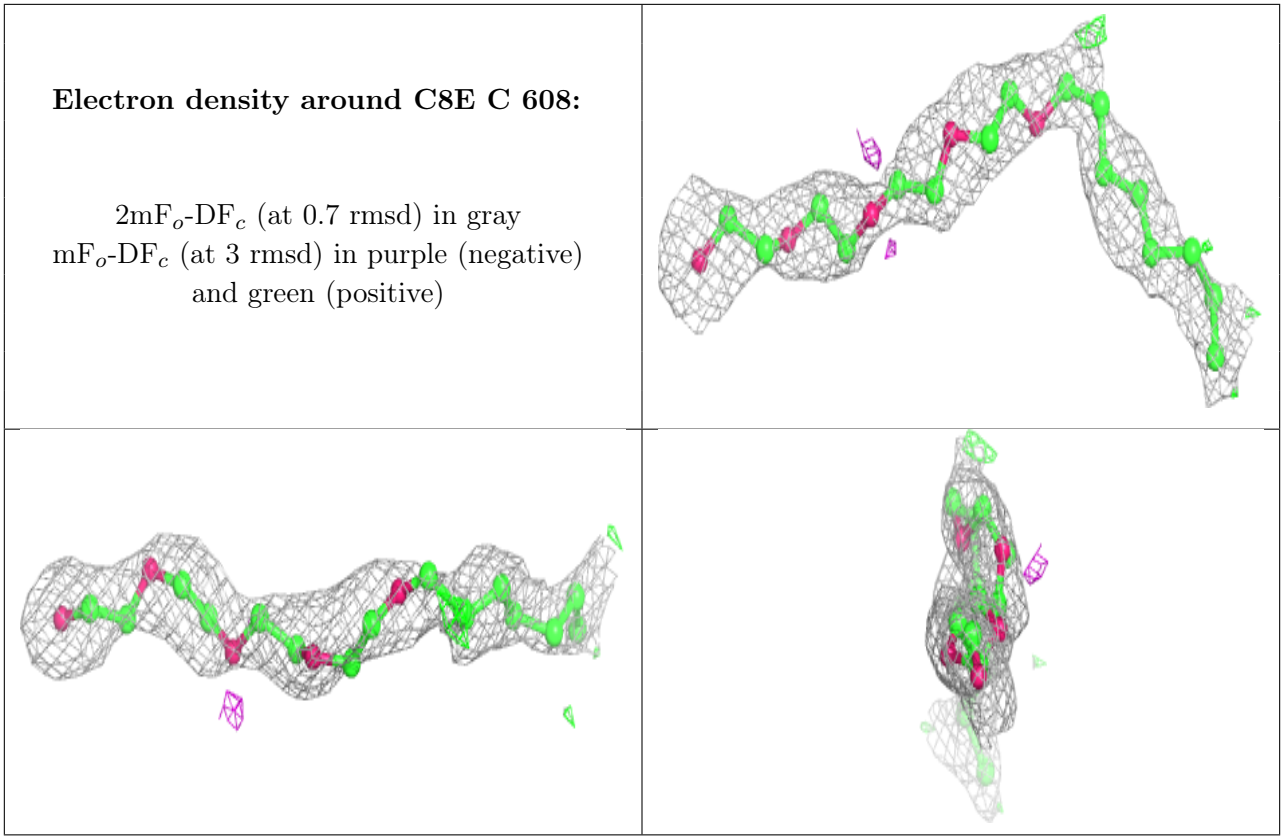
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C	608	21/21	0.82	0.30	31,56,78,86	0
3	C8E	C	604	21/21	0.83	0.41	46,65,83,90	0
3	C8E	E	604	21/21	0.84	0.32	38,63,85,93	0
3	C8E	E	603	21/21	0.85	0.30	20,47,69,75	0
3	C8E	A	601	21/21	0.85	0.28	24,38,60,74	0
3	C8E	A	603	21/21	0.86	0.36	31,65,88,99	0
3	C8E	C	605	21/21	0.87	0.23	38,52,71,88	0
3	C8E	G	603	21/21	0.87	0.43	33,76,105,109	0
3	C8E	C	602	21/21	0.88	0.25	30,47,60,73	0
3	C8E	C	607	21/21	0.88	0.29	26,54,74,94	0
3	C8E	C	609	21/21	0.89	0.24	21,60,103,110	0
3	C8E	G	602	21/21	0.89	0.31	35,55,115,123	0
3	C8E	A	602	21/21	0.89	0.23	28,44,65,72	0
3	C8E	A	605	21/21	0.90	0.31	31,57,109,114	0
3	C8E	E	602	21/21	0.90	0.33	24,42,69,82	0
3	C8E	C	606	21/21	0.90	0.26	22,48,69,71	0
3	C8E	E	601	21/21	0.92	0.24	33,48,86,89	0
3	C8E	C	601	21/21	0.92	0.27	29,44,80,96	0
3	C8E	G	601	21/21	0.93	0.22	21,48,62,73	0
3	C8E	C	603	21/21	0.94	0.23	25,47,71,74	0
3	C8E	A	604	21/21	0.95	0.20	22,34,46,49	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.

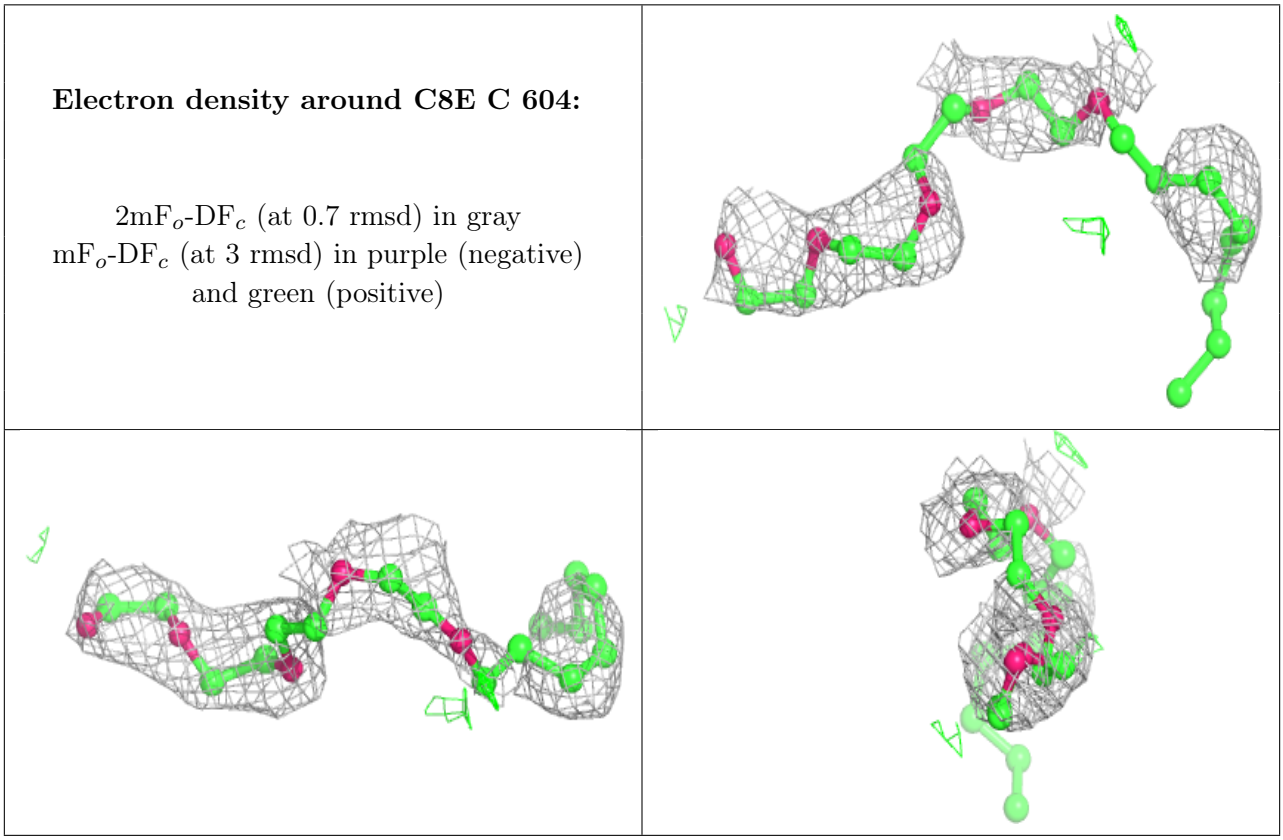
Electron density around C8E C 608:

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



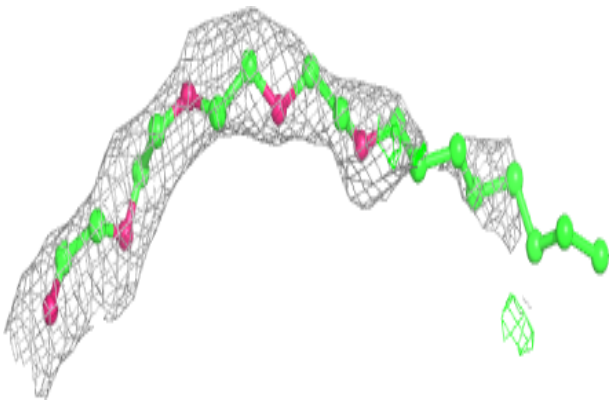
Electron density around C8E C 604:

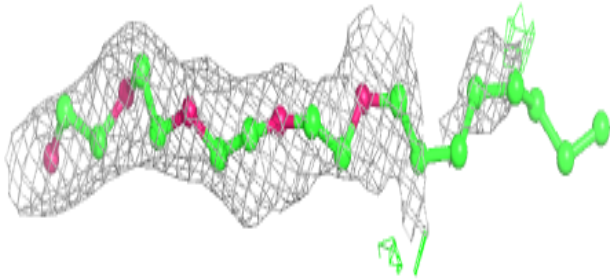
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

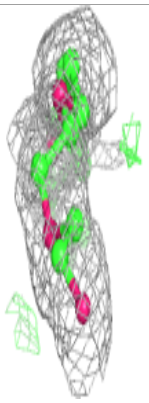


Electron density around C8E E 604:

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

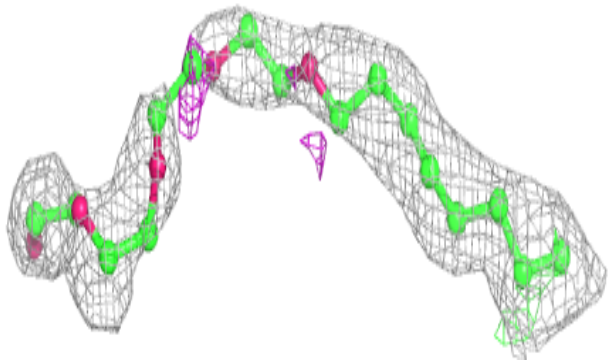


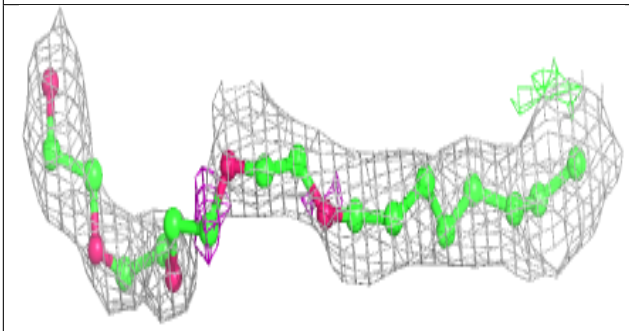


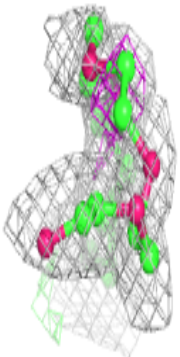


Electron density around C8E E 603:

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

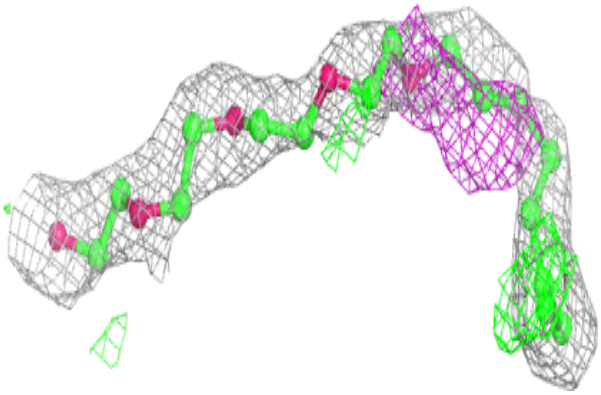


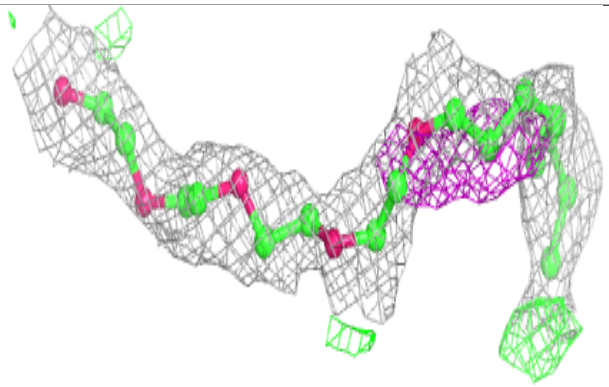


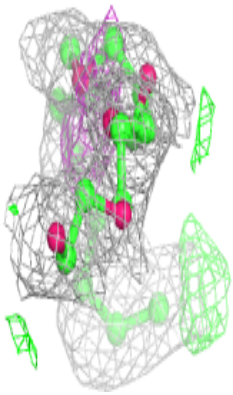


Electron density around C8E A 601:

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

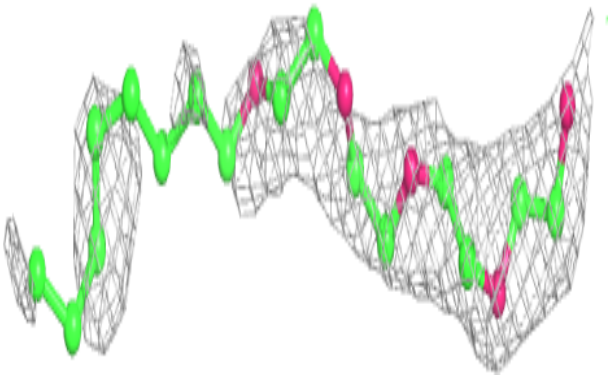


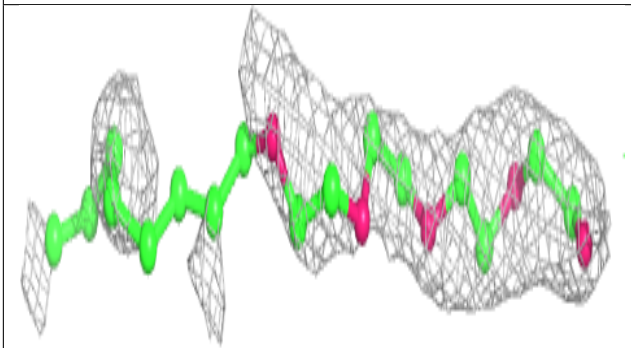


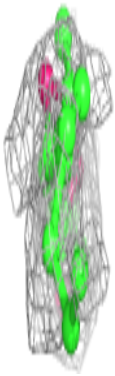


Electron density around C8E A 603:

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

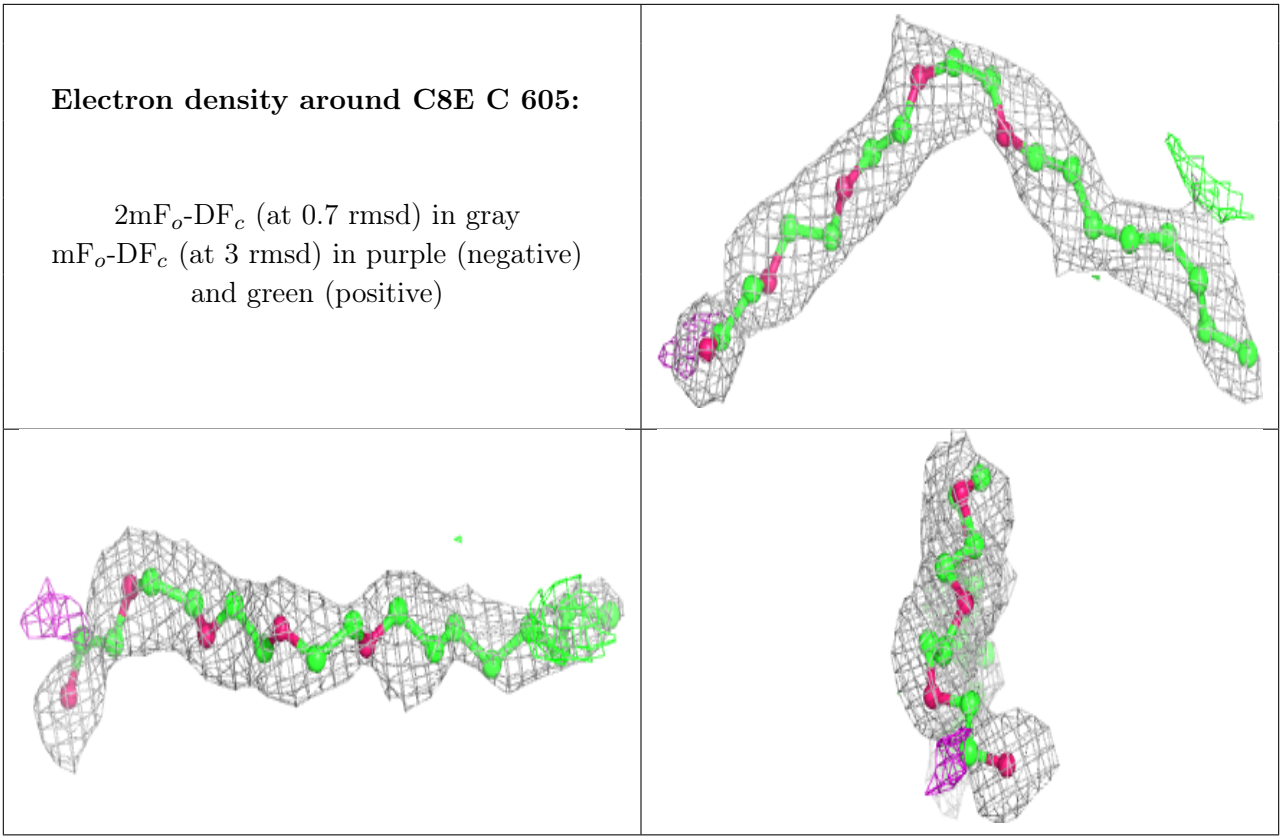






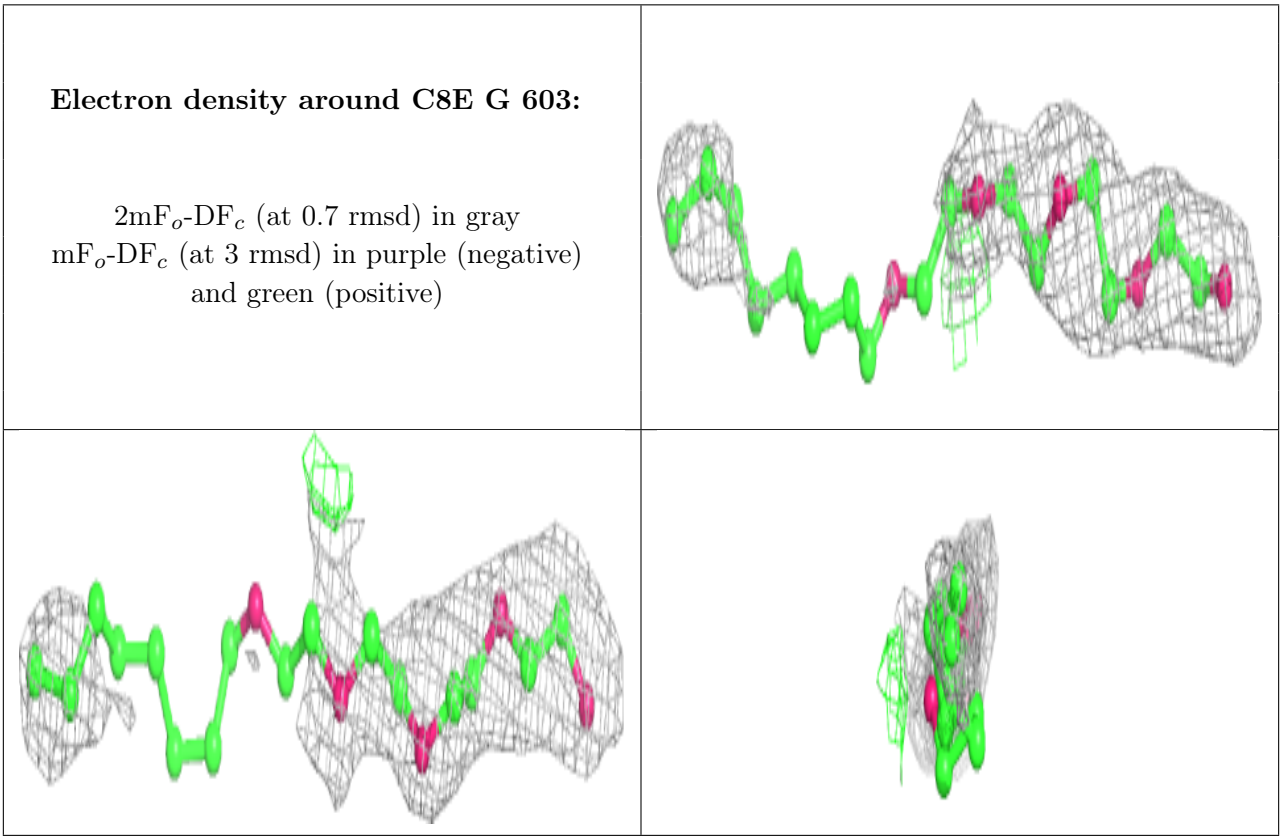
Electron density around C8E C 605:

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



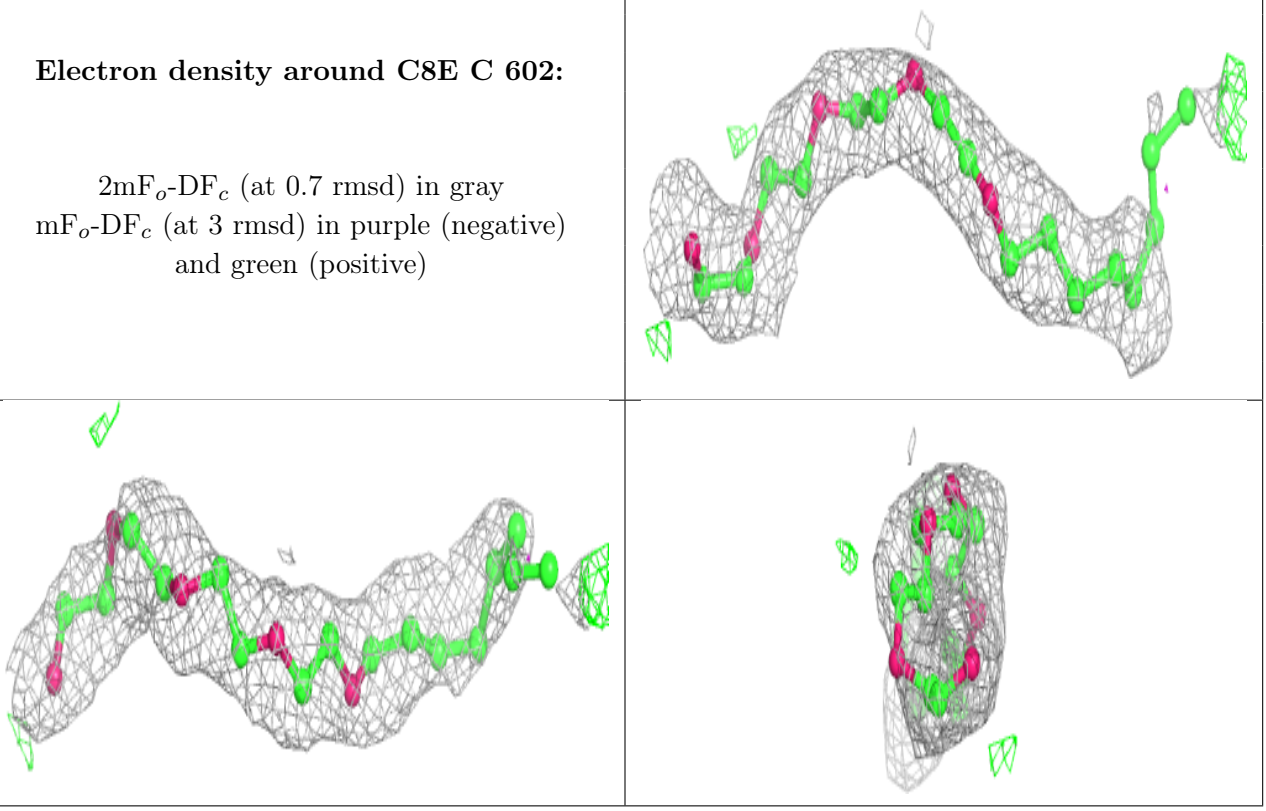
Electron density around C8E G 603:

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



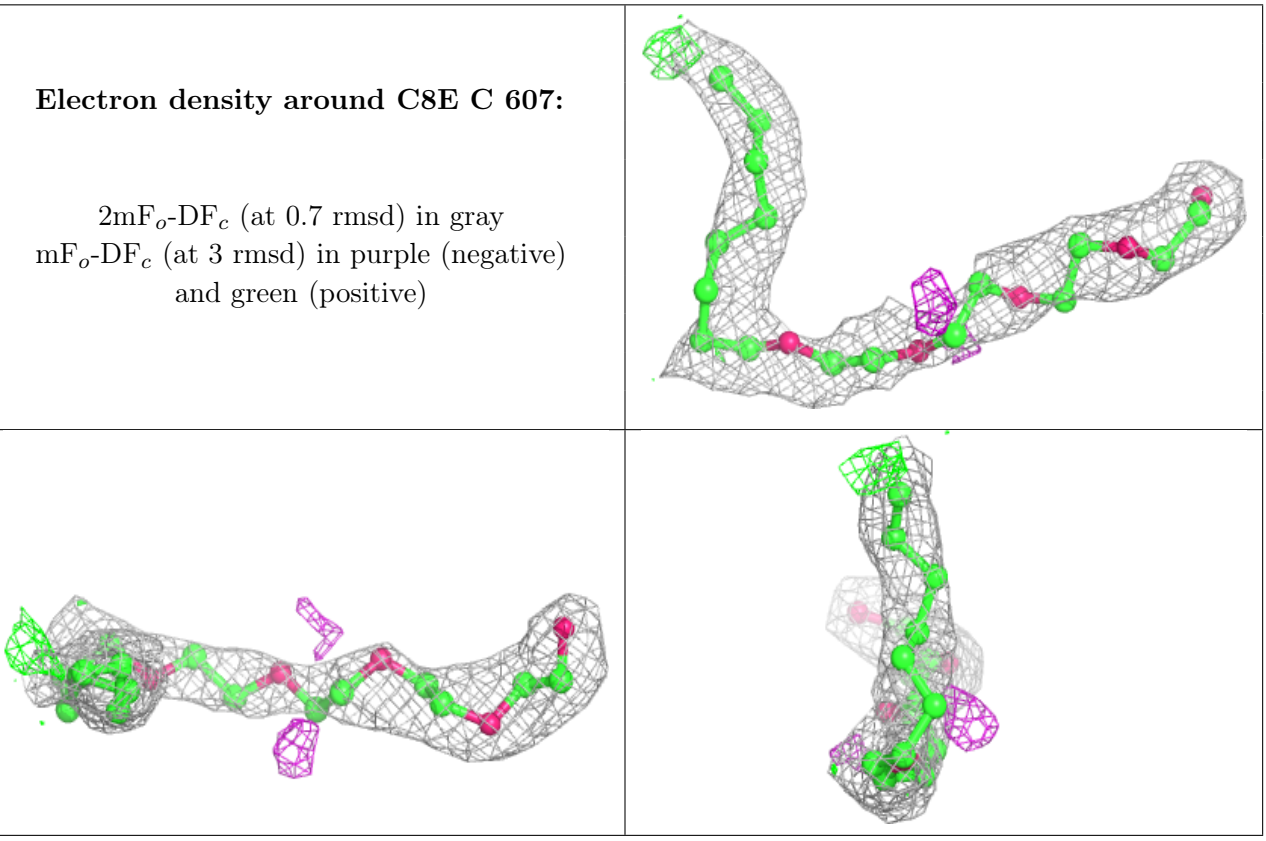
Electron density around C8E C 602:

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



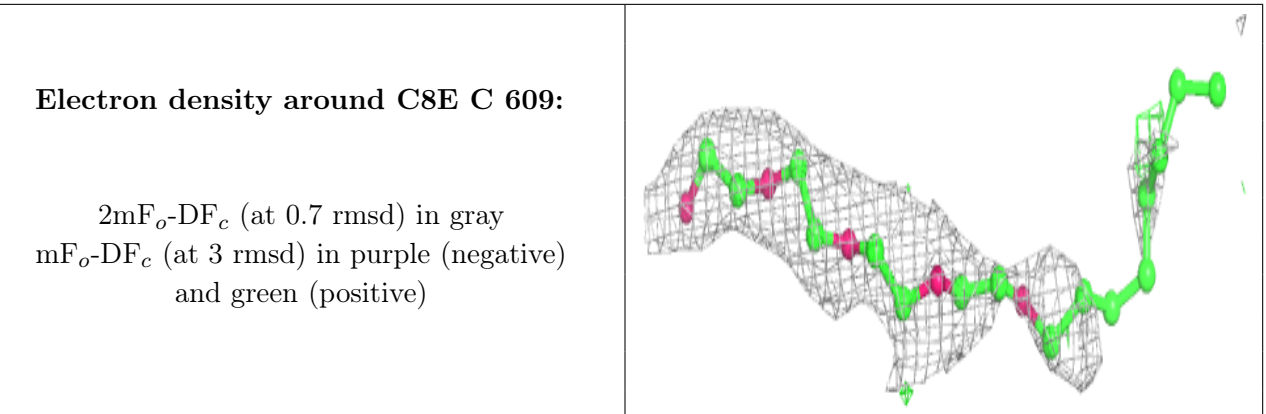
Electron density around C8E C 607:

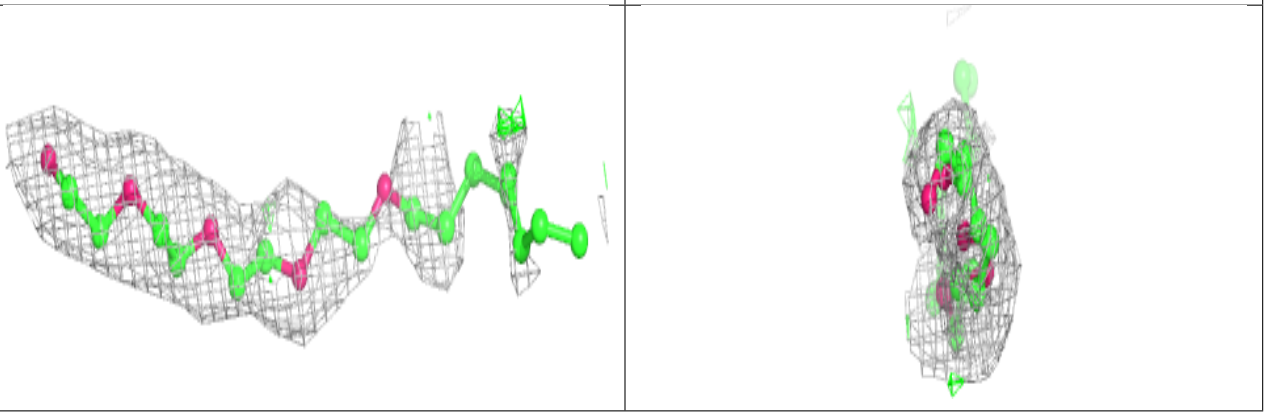
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around C8E C 609:

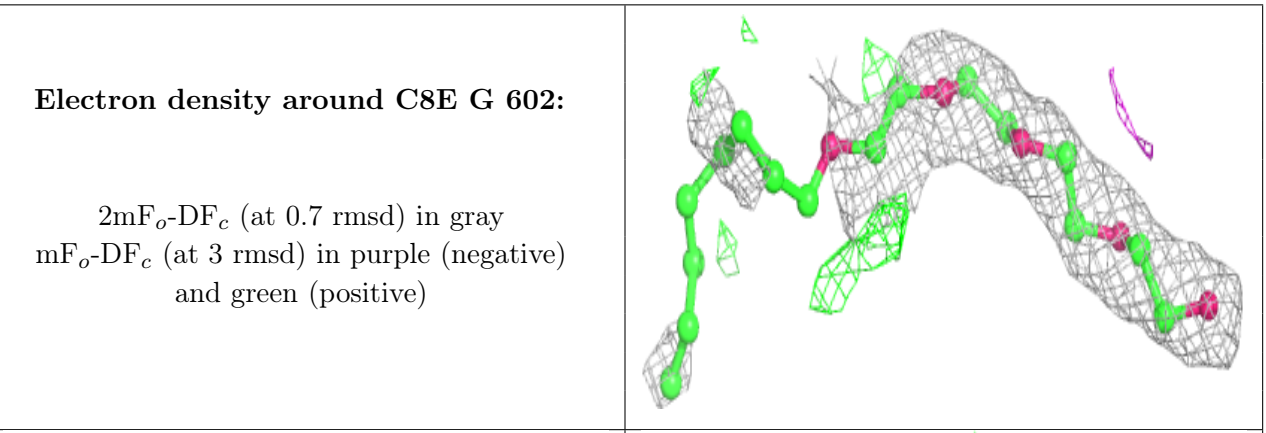
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

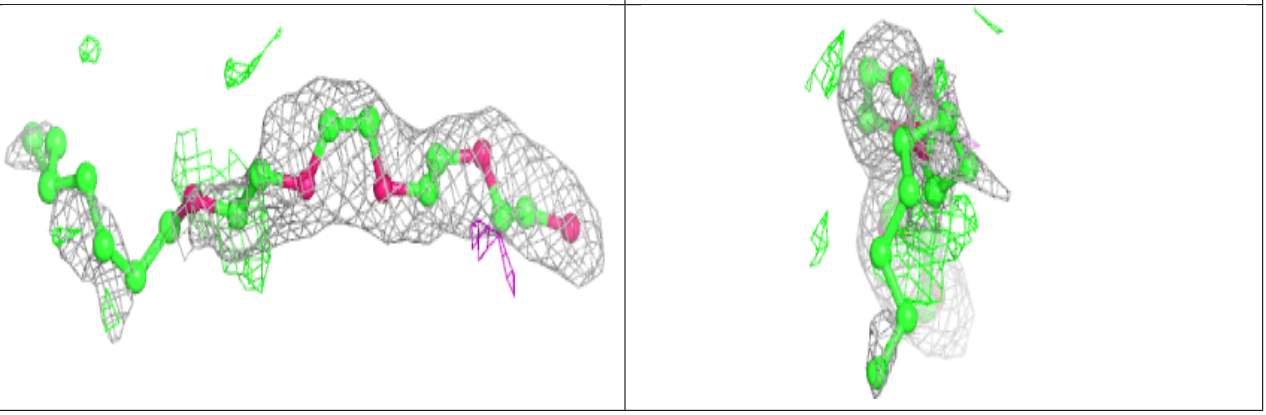




Electron density around C8E G 602:

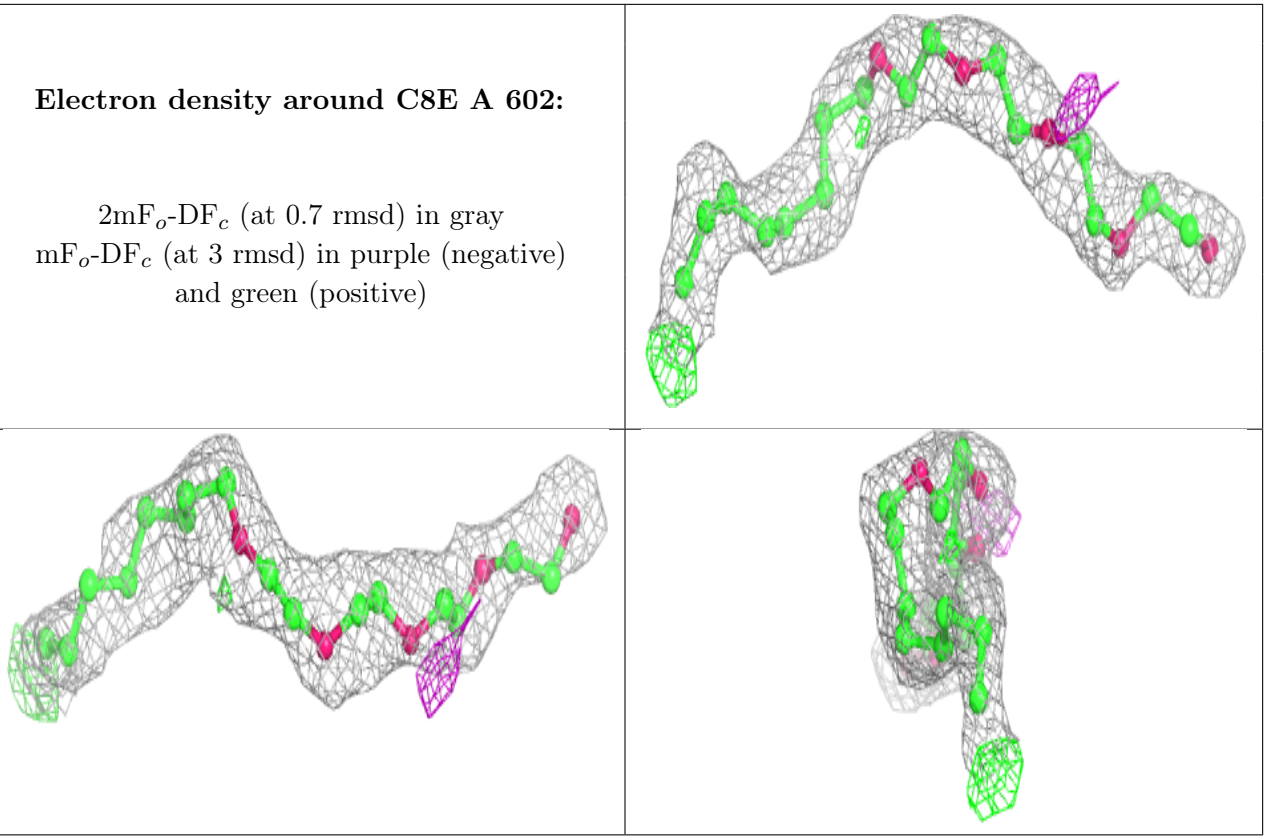
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





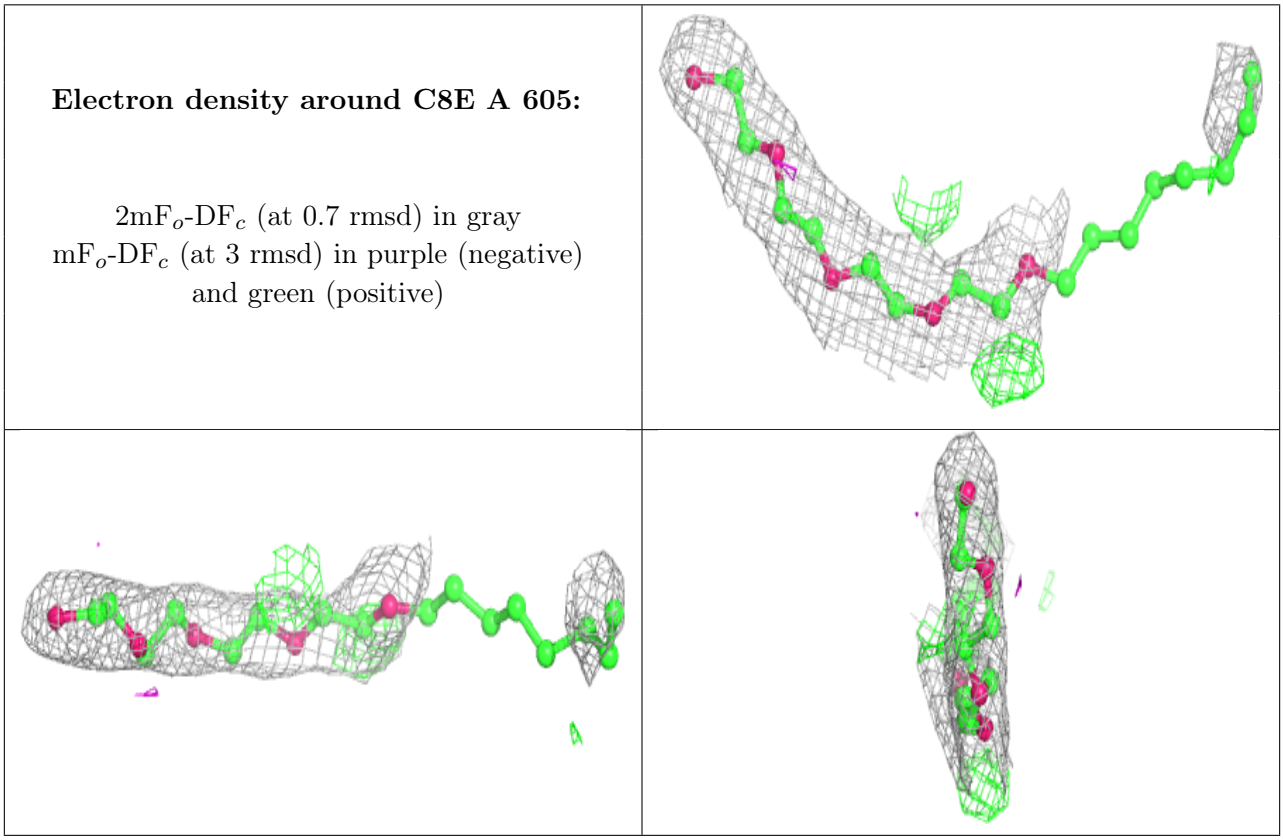
Electron density around C8E A 602:

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



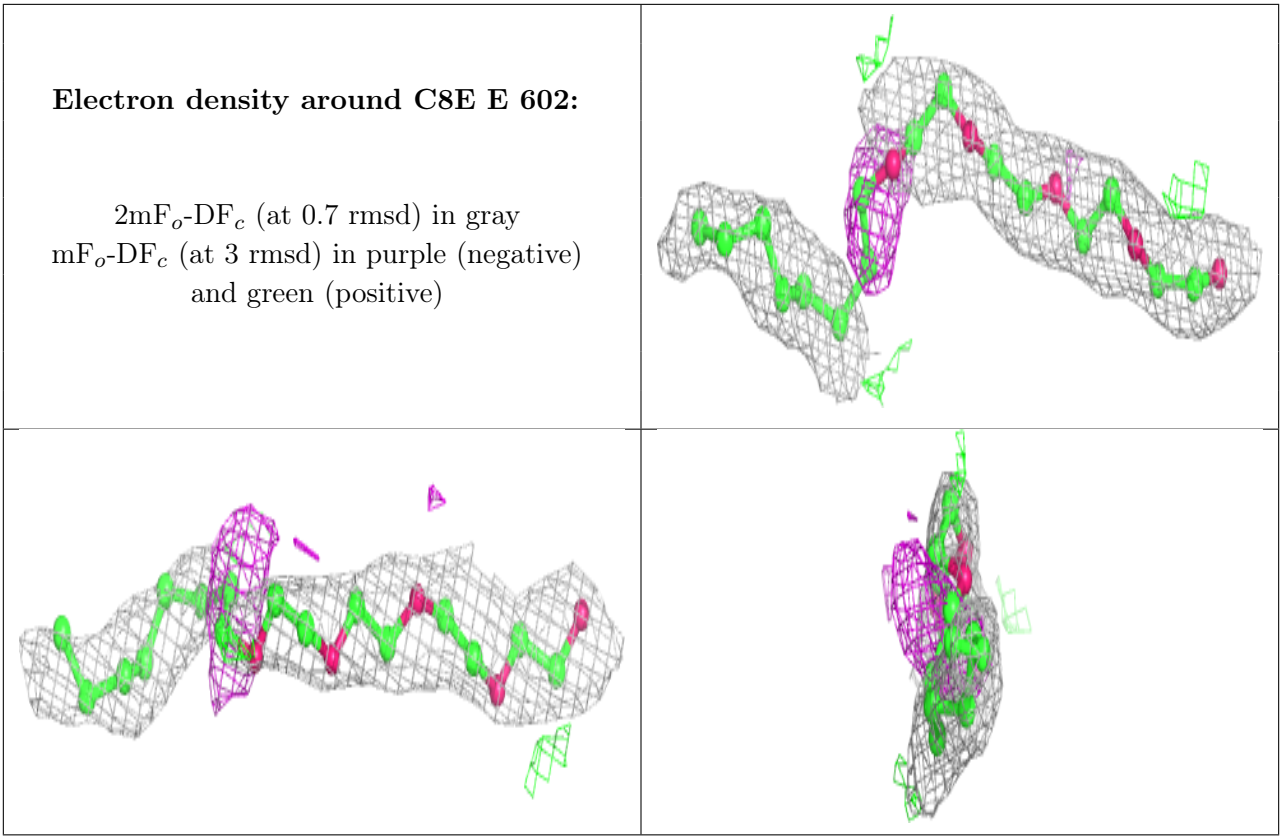
Electron density around C8E A 605:

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



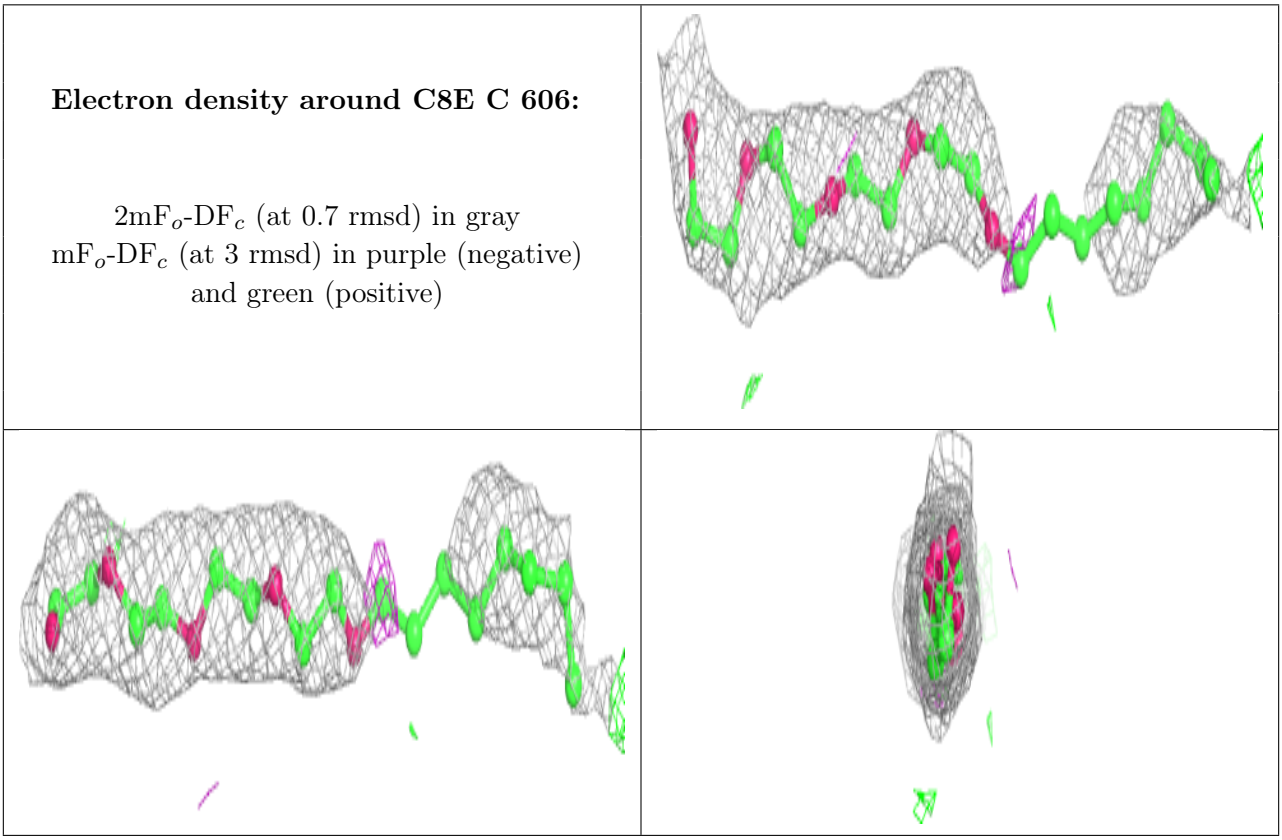
Electron density around C8E E 602:

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



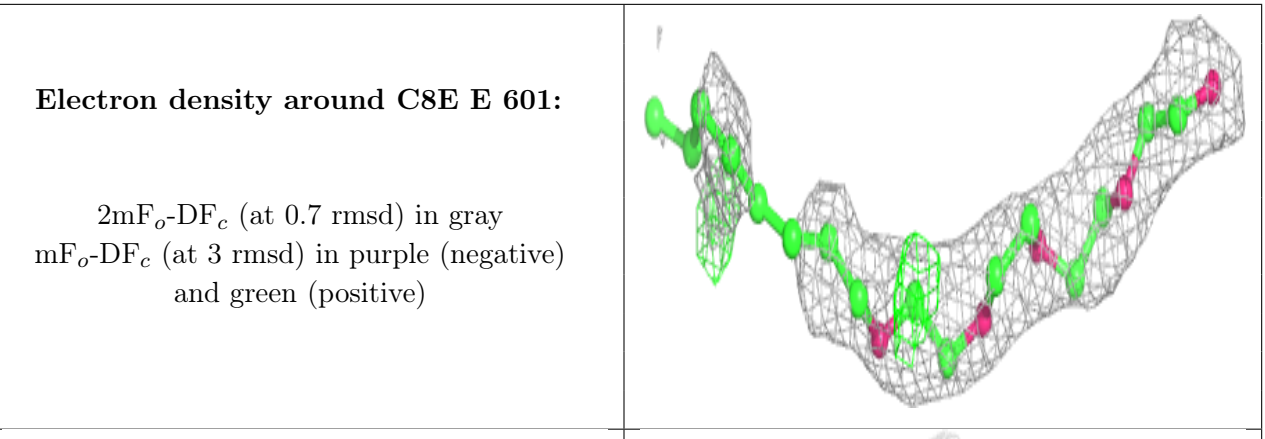
Electron density around C8E C 606:

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



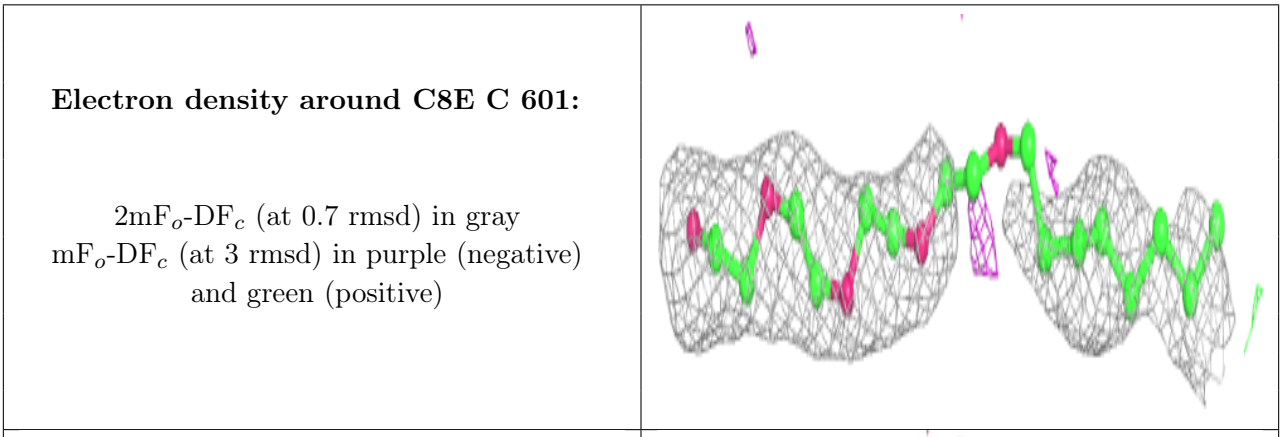
Electron density around C8E E 601:

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



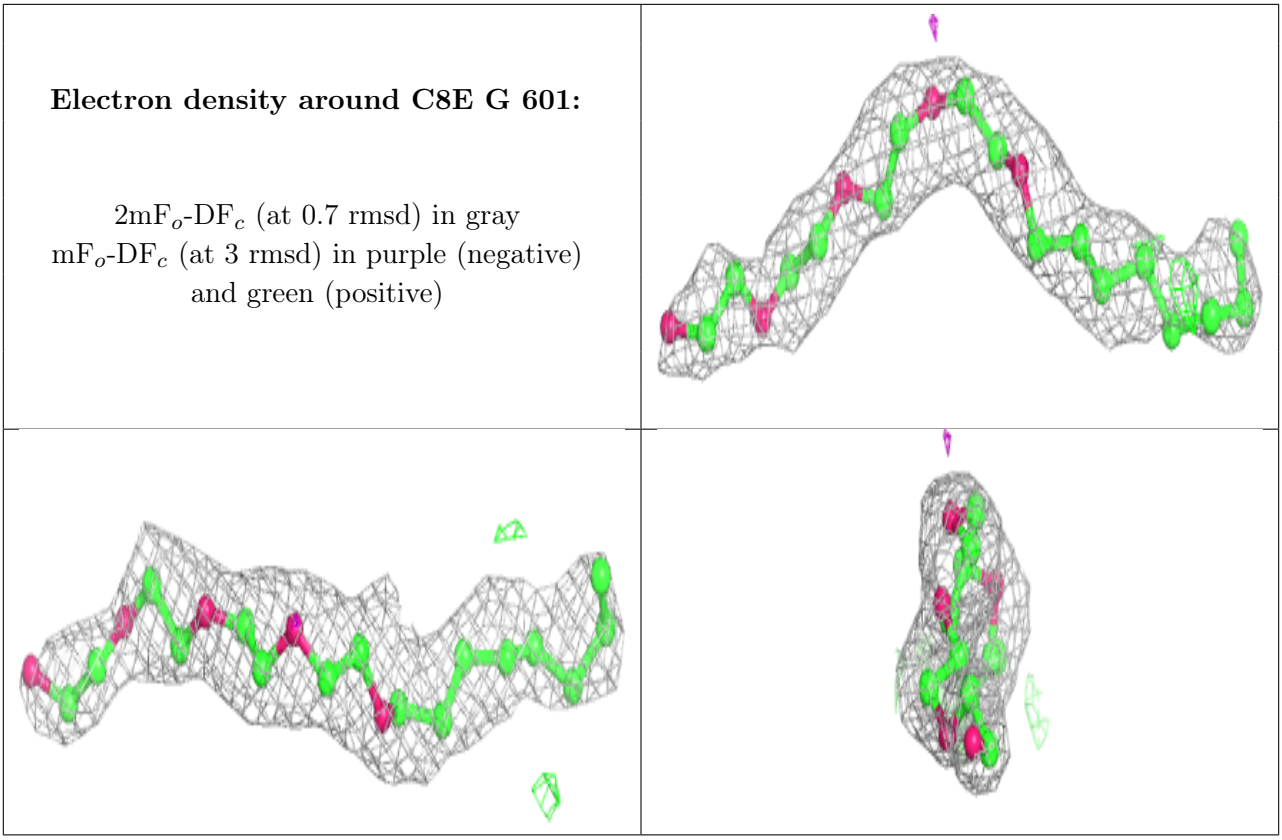
Electron density around C8E C 601:

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



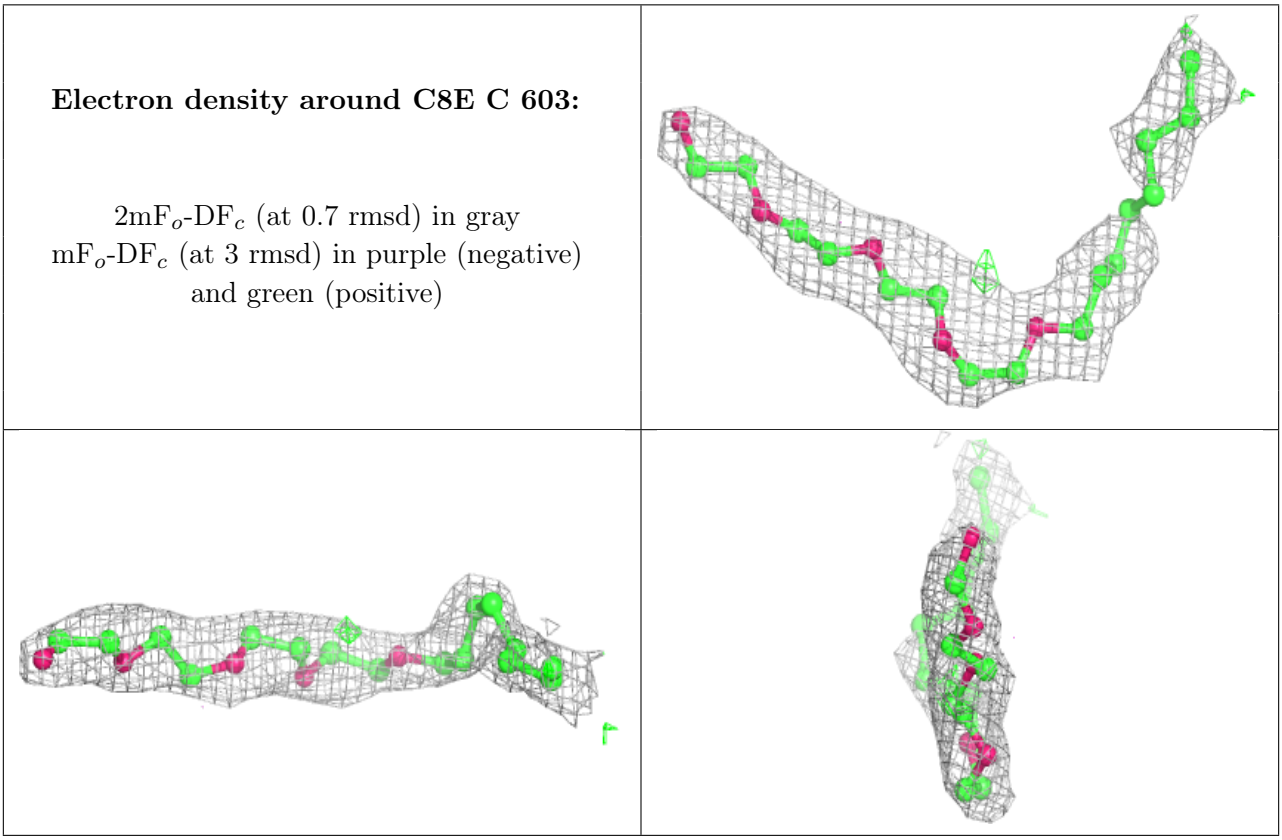
Electron density around C8E G 601:

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



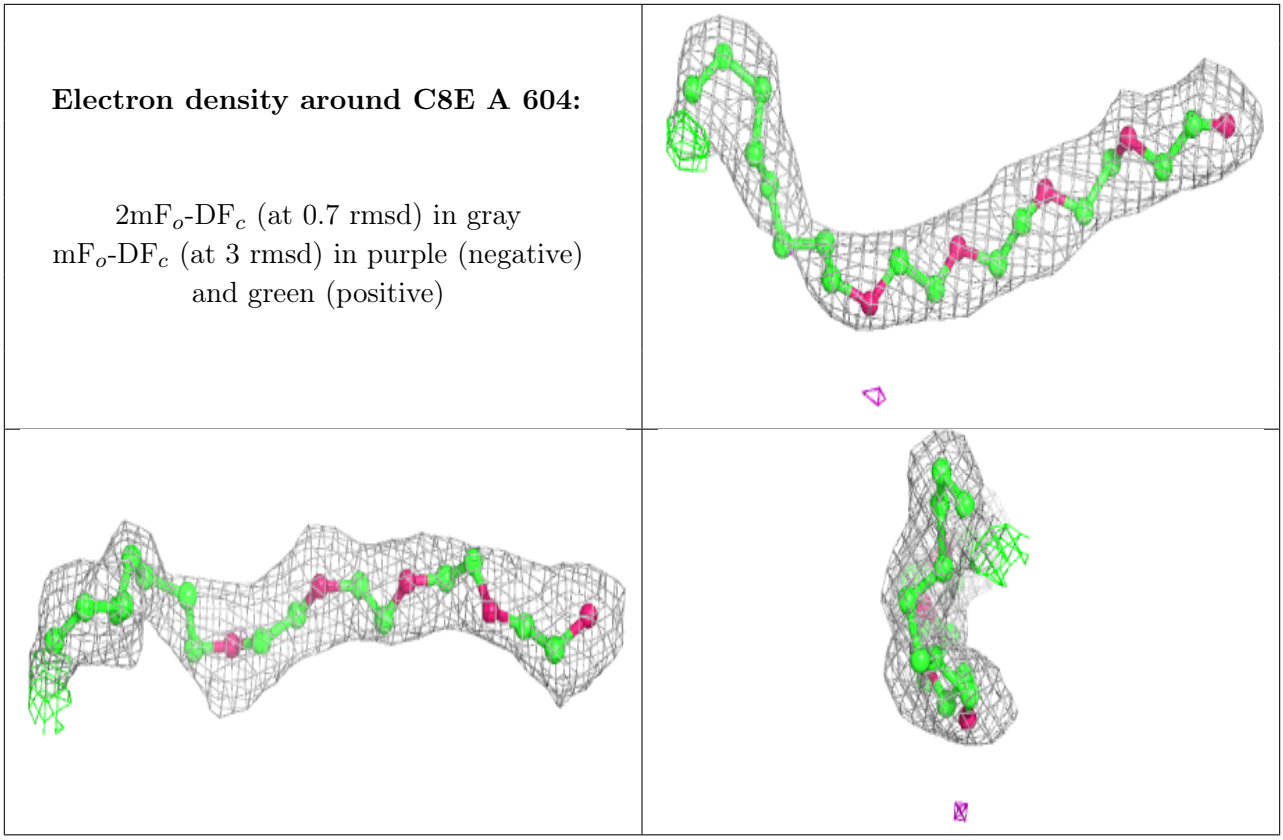
Electron density around C8E C 603:

$2mF_o$-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 604:

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



6.5 Other polymers (i)

There are no such residues in this entry.