Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:15 AM BST

PDB ID	:	4GEY
Title	:	High pH structure of Pseudomonas putida OprB
Authors	:	van den Berg, B.
Deposited on	:	2012-08-02
Resolution	:	2.70 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

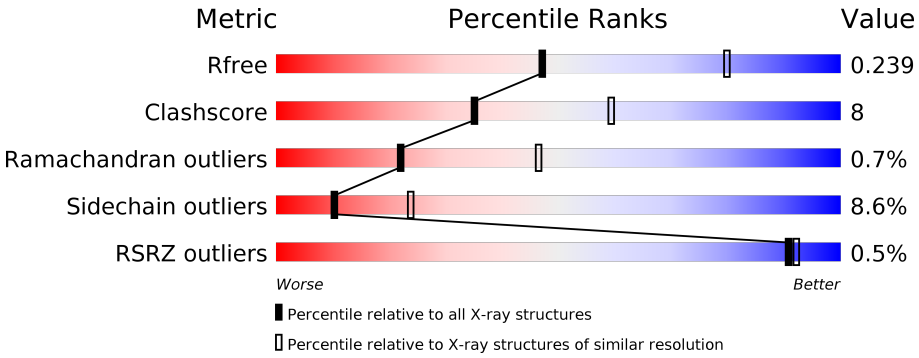
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	76% 16%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3597 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.

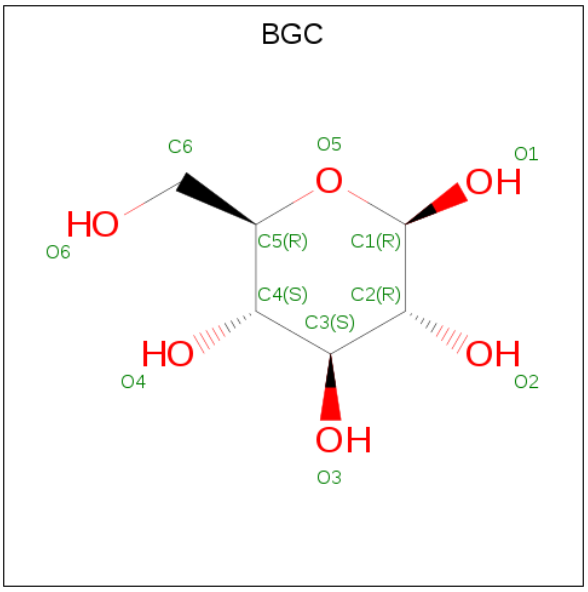
- Molecule 1 is a protein called Porin B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	420	3309	2104	570	629	2	4	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

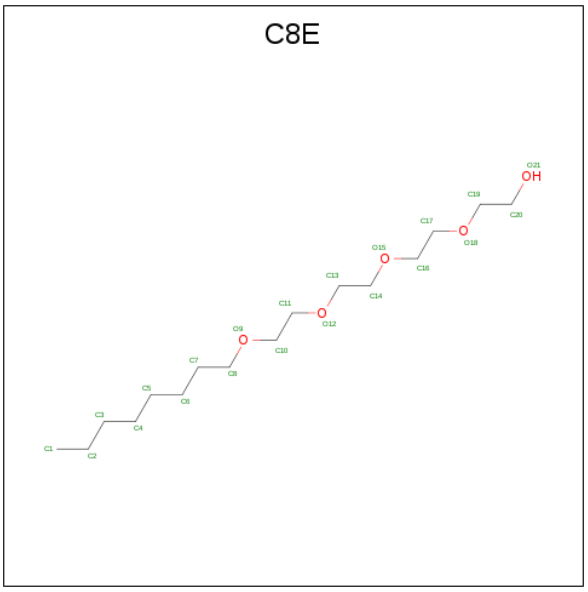
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP E4R6F8
A	-13	ASN	-	expression tag	UNP E4R6F8
A	-12	VAL	-	expression tag	UNP E4R6F8
A	-11	ARG	-	expression tag	UNP E4R6F8
A	-10	LEU	-	expression tag	UNP E4R6F8
A	-9	GLN	-	expression tag	UNP E4R6F8
A	-8	HIS	-	expression tag	UNP E4R6F8
A	-7	HIS	-	expression tag	UNP E4R6F8
A	-6	HIS	-	expression tag	UNP E4R6F8
A	-5	HIS	-	expression tag	UNP E4R6F8
A	-4	HIS	-	expression tag	UNP E4R6F8
A	-3	HIS	-	expression tag	UNP E4R6F8
A	-2	HIS	-	expression tag	UNP E4R6F8
A	-1	LEU	-	expression tag	UNP E4R6F8
A	0	GLU	-	expression tag	UNP E4R6F8
A	220	MSE	LEU	engineered mutation	UNP E4R6F8
A	222	MSE	VAL	engineered mutation	UNP E4R6F8

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	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 12 10 2	0	0
3	A	1	Total C O 21 16 5	0	0

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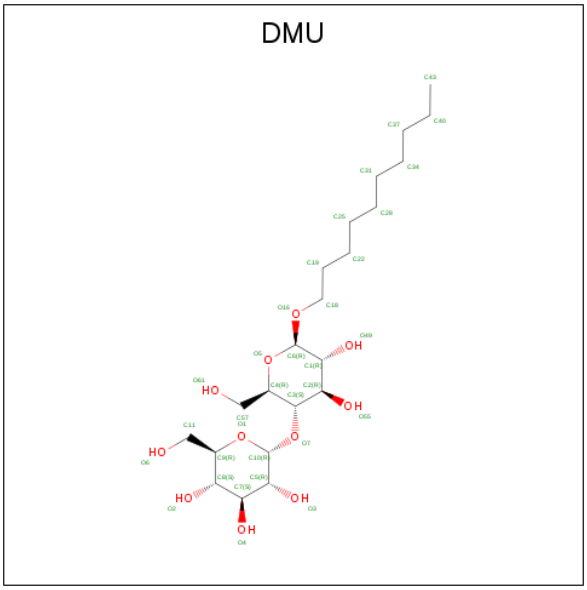
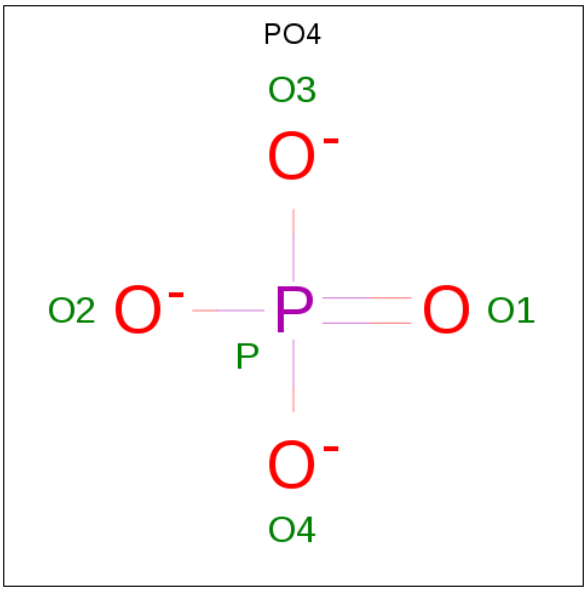
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 15 10 5	0	0
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 13 11 2	0	0
3	A	1	Total C O 9 6 3	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 30 19 11	0	0
4	A	1	Total C O 31 20 11	0	0
4	A	1	Total C O 30 19 11	0	0
4	A	1	Total C O 29 18 11	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

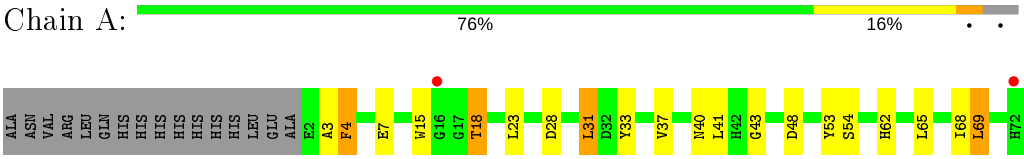
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	47	Total O 47 47	0	0

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: Porin B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.34Å 88.34Å 177.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 2.70 42.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.98-2.70) 96.8 (42.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.239 0.193 , 0.239	Depositor DCC
R_{free} test set	2007 reflections (8.85%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BGC, C8E, DMU

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	0.41	0/3398	0.58	0/4609

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	3309	0	3085	54	0
2	A	12	0	12	4	0
3	A	104	0	156	7	0
4	A	120	0	132	2	0
5	A	5	0	0	0	0
6	A	47	0	0	0	0
All	All	3597	0	3385	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (57) 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:185:THR:HG22	1:A:187:ALA:H	1.46	0.80
1:A:33:TYR:OH	1:A:53:TYR:OH	2.02	0.78
1:A:170:ASN:HB2	2:A:501:BGC:H6C1	1.66	0.77
1:A:106:GLU:O	2:A:501:BGC:O2	1.99	0.77
1:A:115:ARG:NH2	1:A:201:ASN:O	2.19	0.75
1:A:68:ILE:HG22	1:A:69:LEU:HD13	1.71	0.73
1:A:302:THR:HG23	1:A:304:HIS:NE2	2.08	0.68
1:A:395:LEU:HD12	3:A:503:C8E:H62	1.75	0.68
1:A:131:ASP:HB3	1:A:181:LYS:HB3	1.75	0.67
1:A:41:LEU:HD11	1:A:413:ALA:HB2	1.78	0.65
1:A:110:ARG:O	1:A:115:ARG:NH1	2.29	0.65
1:A:83:ARG:HH12	2:A:501:BGC:H2	1.63	0.63
1:A:382:GLY:HA2	1:A:392:ARG:HB3	1.82	0.62
1:A:28:ASP:HB3	1:A:62:HIS:HB3	1.84	0.59
1:A:65:LEU:HD22	1:A:69:LEU:HD22	1.84	0.58
1:A:260:GLN:HG2	1:A:267:PHE:CE2	2.40	0.57
1:A:48:ASP:OD1	1:A:92:ARG:NH1	2.39	0.56
1:A:223:GLU:OE2	1:A:238:ARG:HD3	2.06	0.55
1:A:302:THR:HG22	1:A:314:TYR:HB3	1.89	0.55
1:A:108:TRP:O	2:A:501:BGC:O2	2.23	0.55
1:A:79:ALA:HB3	1:A:118:GLN:HB2	1.89	0.54
1:A:15:TRP:O	1:A:18:THR:HG23	2.09	0.53
1:A:185:THR:CG2	1:A:187:ALA:H	2.20	0.53
1:A:302:THR:HB	1:A:314:TYR:HD1	1.73	0.53
1:A:379:LEU:HG	3:A:503:C8E:H82	1.90	0.53
1:A:37:VAL:HG22	1:A:53:TYR:HD1	1.74	0.53
1:A:94:SER:HB3	1:A:99:GLY:HA2	1.92	0.51
3:A:507:C8E:H72	4:A:513:DMU:H15	1.91	0.51
1:A:282:GLN:HB3	3:A:509:C8E:H192	1.93	0.51
1:A:240:GLY:HA3	1:A:277:TRP:CE2	2.47	0.50
1:A:161:GLY:HA2	1:A:168:TRP:CD1	2.47	0.50
3:A:507:C8E:H62	3:A:508:C8E:H71	1.94	0.49
1:A:222:MSE:HE2	3:A:502:C8E:H61	1.96	0.48
1:A:131:ASP:OD1	1:A:179:ARG:NH2	2.45	0.47
1:A:392:ARG:HA	1:A:393:PRO:HD2	1.82	0.46
1:A:136:ARG:HA	1:A:175:GLN:O	2.16	0.46
1:A:185:THR:HG22	1:A:187:ALA:N	2.25	0.46
1:A:225:VAL:HG22	1:A:238:ARG:HG2	1.98	0.45
1:A:48:ASP:O	1:A:92:ARG:HD2	2.17	0.45
1:A:161:GLY:HA3	1:A:170:ASN:HD21	1.82	0.44
1:A:31:LEU:HD13	1:A:421:PHE:CD2	2.52	0.44
1:A:362:TYR:HA	1:A:367:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:N	1:A:88:LEU:HD11	2.33	0.43
1:A:273:LYS:NZ	1:A:309:ASN:OD1	2.52	0.42
1:A:240:GLY:HA3	1:A:277:TRP:CZ2	2.54	0.42
1:A:74:ALA:HA	1:A:122:LYS:O	2.19	0.42
1:A:352:LEU:O	1:A:356:GLN:HG2	2.20	0.42
1:A:43:GLY:HA3	1:A:409:ASN:O	2.20	0.41
1:A:302:THR:CG2	1:A:314:TYR:HB3	2.49	0.41
1:A:388:TRP:CE3	1:A:389:LEU:HB2	2.55	0.41
1:A:161:GLY:HA3	1:A:170:ASN:ND2	2.35	0.41
1:A:73:ASP:N	1:A:73:ASP:OD1	2.54	0.41
1:A:136:ARG:HB3	1:A:174:SER:HB2	2.03	0.40
4:A:513:DMU:H30	4:A:513:DMU:H35	2.03	0.40
1:A:393:PRO:HB2	3:A:503:C8E:H52	2.04	0.40
1:A:88:LEU:HD13	1:A:93:ILE:HD11	2.04	0.40
1:A:399:LYS:HE3	1:A:400:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	418/436 (96%)	398 (95%)	17 (4%)	3 (1%)	22 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	4	PHE
1	A	73	ASP

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	337/352 (96%)	308 (91%)	29 (9%)	10 24

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	7	GLU
1	A	18	THR
1	A	23	LEU
1	A	31	LEU
1	A	54	SER
1	A	69	LEU
1	A	73	ASP
1	A	82	GLU
1	A	84	SER
1	A	88	LEU
1	A	97	ARG
1	A	113	THR
1	A	153	LEU
1	A	156	CYS
1	A	168	TRP
1	A	179	ARG
1	A	185	THR
1	A	260	GLN
1	A	265	GLU
1	A	302	THR
1	A	314	TYR
1	A	316	GLN
1	A	320	VAL
1	A	352	LEU
1	A	353	LEU
1	A	389	LEU
1	A	395	LEU
1	A	399	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

14 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	507	-	9,9,20	0.29	0	8,8,19	0.44	0
4	DMU	A	512	-	31,31,34	2.29	10 (32%)	42,42,45	1.69	7 (16%)
3	C8E	A	508	-	12,12,20	0.47	0	11,11,19	0.38	0
3	C8E	A	503	-	20,20,20	0.46	0	19,19,19	0.40	0
3	C8E	A	509	-	8,8,20	0.46	0	7,7,19	0.36	0
3	C8E	A	504	-	11,11,20	0.48	0	10,10,19	0.23	0
4	DMU	A	510	-	31,31,34	2.37	11 (35%)	42,42,45	1.54	5 (11%)
5	PO4	A	514	-	4,4,4	0.86	0	6,6,6	0.47	0
4	DMU	A	511	-	32,32,34	2.22	11 (34%)	43,43,45	1.94	9 (20%)
4	DMU	A	513	-	30,30,34	2.36	11 (36%)	41,41,45	1.67	7 (17%)
2	BGC	A	501	-	12,12,12	2.65	5 (41%)	17,17,17	1.13	2 (11%)
3	C8E	A	506	-	11,11,20	0.33	0	10,10,19	0.40	0
3	C8E	A	502	-	11,11,20	0.31	0	10,10,19	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	C8E	A	505	-	14,14,20	0.47	0	13,13,19	0.35	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	507	-	-	5/7/7/18	-
4	DMU	A	512	-	-	4/16/56/59	0/2/2/2
3	C8E	A	508	-	-	6/10/10/18	-
3	C8E	A	503	-	-	13/18/18/18	-
3	C8E	A	509	-	-	3/6/6/18	-
3	C8E	A	504	-	-	7/9/9/18	-
4	DMU	A	510	-	-	4/16/56/59	0/2/2/2
4	DMU	A	511	-	-	7/17/57/59	0/2/2/2
4	DMU	A	513	-	-	6/15/55/59	0/2/2/2
2	BGC	A	501	-	-	2/2/22/22	0/1/1/1
3	C8E	A	506	-	-	3/9/9/18	-
3	C8E	A	502	-	-	6/9/9/18	-
3	C8E	A	505	-	-	5/12/12/18	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	511	DMU	C11-C9	-5.80	1.32	1.51
4	A	510	DMU	C11-C9	-5.67	1.32	1.51
4	A	513	DMU	C11-C9	-5.63	1.33	1.51
4	A	512	DMU	C11-C9	-5.61	1.33	1.51
4	A	513	DMU	C57-C4	-4.79	1.35	1.51
4	A	510	DMU	C57-C4	-4.78	1.35	1.51
4	A	513	DMU	O1-C9	4.74	1.55	1.44
4	A	511	DMU	C57-C4	-4.74	1.35	1.51
2	A	501	BGC	C3-C2	-4.72	1.40	1.52
4	A	512	DMU	C57-C4	-4.69	1.36	1.51
2	A	501	BGC	C6-C5	-4.67	1.36	1.51
4	A	510	DMU	O5-C4	4.66	1.55	1.44
4	A	512	DMU	O5-C4	4.48	1.55	1.44
4	A	511	DMU	O5-C4	4.35	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	DMU	O1-C9	4.31	1.54	1.44
4	A	512	DMU	O1-C9	4.20	1.54	1.44
4	A	513	DMU	O5-C4	4.17	1.54	1.44
4	A	511	DMU	O1-C9	4.01	1.54	1.44
4	A	510	DMU	C7-C5	-3.78	1.42	1.52
2	A	501	BGC	O5-C5	3.59	1.53	1.44
4	A	511	DMU	C7-C5	-3.54	1.43	1.52
4	A	510	DMU	C2-C1	-3.51	1.43	1.52
4	A	513	DMU	C7-C5	-3.49	1.43	1.52
4	A	512	DMU	C7-C5	-3.42	1.43	1.52
2	A	501	BGC	C1-C2	-3.25	1.44	1.52
4	A	512	DMU	C2-C1	-3.22	1.44	1.52
4	A	513	DMU	C2-C1	-3.00	1.44	1.52
4	A	511	DMU	C2-C1	-2.83	1.45	1.52
4	A	511	DMU	O49-C1	2.73	1.49	1.43
4	A	510	DMU	C6-C1	-2.68	1.44	1.52
4	A	513	DMU	C6-C1	-2.63	1.44	1.52
4	A	513	DMU	O49-C1	2.63	1.49	1.43
4	A	512	DMU	C6-C1	-2.43	1.45	1.52
4	A	513	DMU	C8-C9	2.41	1.58	1.53
4	A	512	DMU	O49-C1	2.40	1.48	1.43
4	A	510	DMU	O49-C1	2.29	1.48	1.43
4	A	510	DMU	O3-C5	2.27	1.48	1.43
2	A	501	BGC	C4-C3	-2.26	1.46	1.52
4	A	511	DMU	O16-C6	2.25	1.44	1.40
4	A	512	DMU	O3-C5	2.17	1.48	1.43
4	A	513	DMU	O3-C5	2.15	1.48	1.43
4	A	513	DMU	C10-C5	-2.10	1.46	1.52
4	A	511	DMU	O55-C2	2.06	1.47	1.43
4	A	510	DMU	O16-C6	2.05	1.43	1.40
4	A	511	DMU	C6-C1	-2.05	1.46	1.52
4	A	512	DMU	C8-C9	2.04	1.57	1.53
4	A	510	DMU	C10-C5	-2.03	1.46	1.52
4	A	511	DMU	C8-C7	-2.01	1.47	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	511	DMU	C10-O1-C9	5.48	124.44	113.69
4	A	510	DMU	C10-O1-C9	5.33	124.14	113.69
4	A	512	DMU	C18-O16-C6	5.14	122.36	113.84
4	A	511	DMU	C1-C2-C3	5.09	121.31	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	512	DMU	C10-O1-C9	4.90	123.31	113.69
4	A	513	DMU	C10-O1-C9	4.71	122.93	113.69
4	A	513	DMU	C18-O16-C6	4.30	120.97	113.84
4	A	511	DMU	C6-C1-C2	4.11	118.55	110.00
4	A	513	DMU	C7-C8-C9	3.89	117.18	110.24
4	A	511	DMU	C10-C5-C7	3.77	117.84	110.00
4	A	510	DMU	C18-O16-C6	3.49	119.62	113.84
4	A	513	DMU	C1-C2-C3	3.35	117.33	109.68
4	A	511	DMU	O16-C6-C1	3.11	113.15	108.30
4	A	510	DMU	O1-C10-C5	3.04	116.79	110.35
4	A	511	DMU	C18-O16-C6	2.84	118.56	113.84
4	A	511	DMU	O1-C10-C5	2.74	116.16	110.35
4	A	512	DMU	C1-C2-C3	2.70	115.85	109.68
4	A	512	DMU	C7-C8-C9	2.65	114.96	110.24
4	A	510	DMU	O16-C18-C19	2.51	118.36	109.56
2	A	501	BGC	O6-C6-C5	2.47	119.75	111.29
4	A	511	DMU	O16-C18-C19	2.36	117.83	109.56
4	A	513	DMU	C6-O5-C4	2.33	118.27	113.69
4	A	513	DMU	C8-C7-C5	2.29	114.82	110.82
4	A	512	DMU	O16-C18-C19	2.25	117.47	109.56
4	A	510	DMU	C6-O5-C4	2.17	117.94	113.69
4	A	513	DMU	C6-C1-C2	2.15	114.47	110.00
4	A	511	DMU	O7-C10-C5	2.07	113.47	108.10
4	A	512	DMU	O7-C10-C5	2.06	113.44	108.10
4	A	512	DMU	O1-C10-C5	2.06	114.70	110.35
2	A	501	BGC	O5-C5-C4	-2.02	106.02	109.69

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	DMU	C1-C6-O16-C18
4	A	511	DMU	O5-C6-O16-C18
4	A	511	DMU	O1-C10-O7-C3
4	A	510	DMU	O1-C10-O7-C3
4	A	511	DMU	O5-C4-C57-O61
3	A	504	C8E	O12-C13-C14-O15
4	A	511	DMU	C3-C4-C57-O61
3	A	504	C8E	O15-C16-C17-O18
3	A	504	C8E	O18-C19-C20-O21
4	A	511	DMU	O16-C18-C19-C22
3	A	502	C8E	C6-C7-C8-O9

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Mol	Chain	Res	Type	Atoms
3	A	503	C8E	O12-C13-C14-O15
3	A	505	C8E	O12-C13-C14-O15
3	A	502	C8E	C4-C5-C6-C7
3	A	507	C8E	C2-C3-C4-C5
3	A	503	C8E	C2-C3-C4-C5
4	A	513	DMU	C19-C22-C25-C28
3	A	506	C8E	C3-C4-C5-C6
3	A	505	C8E	O18-C19-C20-O21
3	A	509	C8E	O15-C16-C17-O18
3	A	502	C8E	C2-C3-C4-C5
3	A	503	C8E	C3-C4-C5-C6
3	A	507	C8E	C6-C7-C8-O9
3	A	508	C8E	C4-C5-C6-C7
3	A	503	C8E	C6-C7-C8-O9
3	A	507	C8E	C4-C5-C6-C7
3	A	502	C8E	C3-C4-C5-C6
3	A	508	C8E	C3-C4-C5-C6
3	A	506	C8E	C5-C6-C7-C8
4	A	513	DMU	O1-C10-O7-C3
4	A	512	DMU	C18-C19-C22-C25
3	A	503	C8E	O18-C19-C20-O21
3	A	507	C8E	C3-C4-C5-C6
3	A	508	C8E	C6-C7-C8-O9
3	A	503	C8E	C1-C2-C3-C4
4	A	510	DMU	O6-C11-C9-O1
4	A	513	DMU	O6-C11-C9-O1
3	A	502	C8E	C1-C2-C3-C4
4	A	512	DMU	O16-C18-C19-C22
4	A	510	DMU	O16-C18-C19-C22
3	A	508	C8E	C2-C3-C4-C5
3	A	504	C8E	C13-C14-O15-C16
3	A	503	C8E	C17-C16-O15-C14
3	A	503	C8E	C16-C17-O18-C19
4	A	512	DMU	C25-C28-C31-C34
3	A	503	C8E	C4-C5-C6-C7
3	A	503	C8E	C13-C14-O15-C16
3	A	504	C8E	C14-C13-O12-C11
3	A	502	C8E	O9-C10-C11-O12
4	A	510	DMU	C19-C22-C25-C28
3	A	503	C8E	C7-C8-O9-C10
3	A	509	C8E	C16-C17-O18-C19
4	A	513	DMU	C5-C10-O7-C3

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Mol	Chain	Res	Type	Atoms
3	A	508	C8E	C7-C8-O9-C10
2	A	501	BGC	C4-C5-C6-O6
2	A	501	BGC	O5-C5-C6-O6
4	A	511	DMU	C28-C31-C34-C37
3	A	504	C8E	C10-C11-O12-C13
4	A	513	DMU	C1-C6-O16-C18
3	A	505	C8E	C7-C8-O9-C10
3	A	506	C8E	C2-C3-C4-C5
4	A	513	DMU	O5-C6-O16-C18
3	A	507	C8E	C7-C8-O9-C10
3	A	509	C8E	O18-C19-C20-O21
3	A	503	C8E	O15-C16-C17-O18
3	A	505	C8E	C13-C14-O15-C16
3	A	503	C8E	C10-C11-O12-C13
4	A	512	DMU	C19-C22-C25-C28
3	A	504	C8E	C20-C19-O18-C17
3	A	505	C8E	O9-C10-C11-O12
3	A	508	C8E	O9-C10-C11-O12

There are no ring outliers.

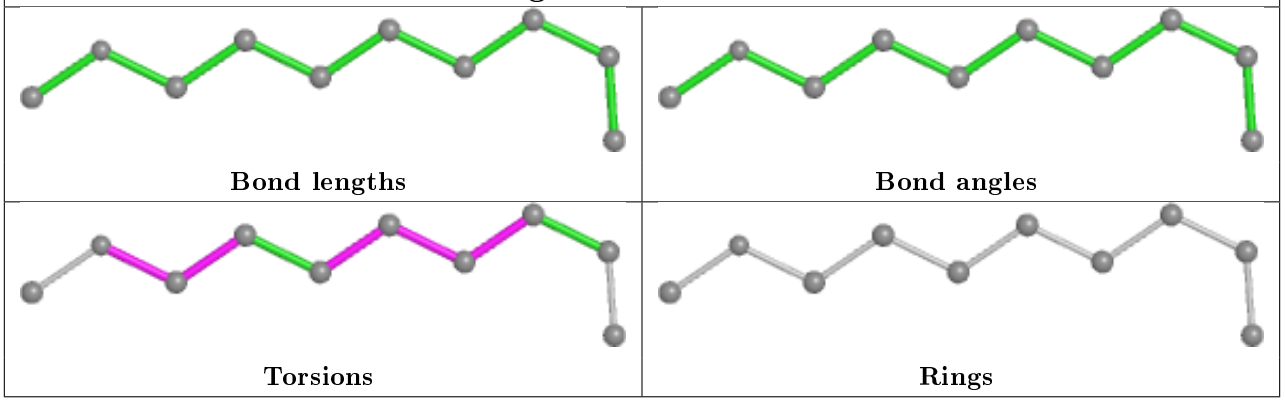
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	C8E	2	0
3	A	508	C8E	1	0
3	A	503	C8E	3	0
3	A	509	C8E	1	0
4	A	513	DMU	2	0
2	A	501	BGC	4	0
3	A	502	C8E	1	0

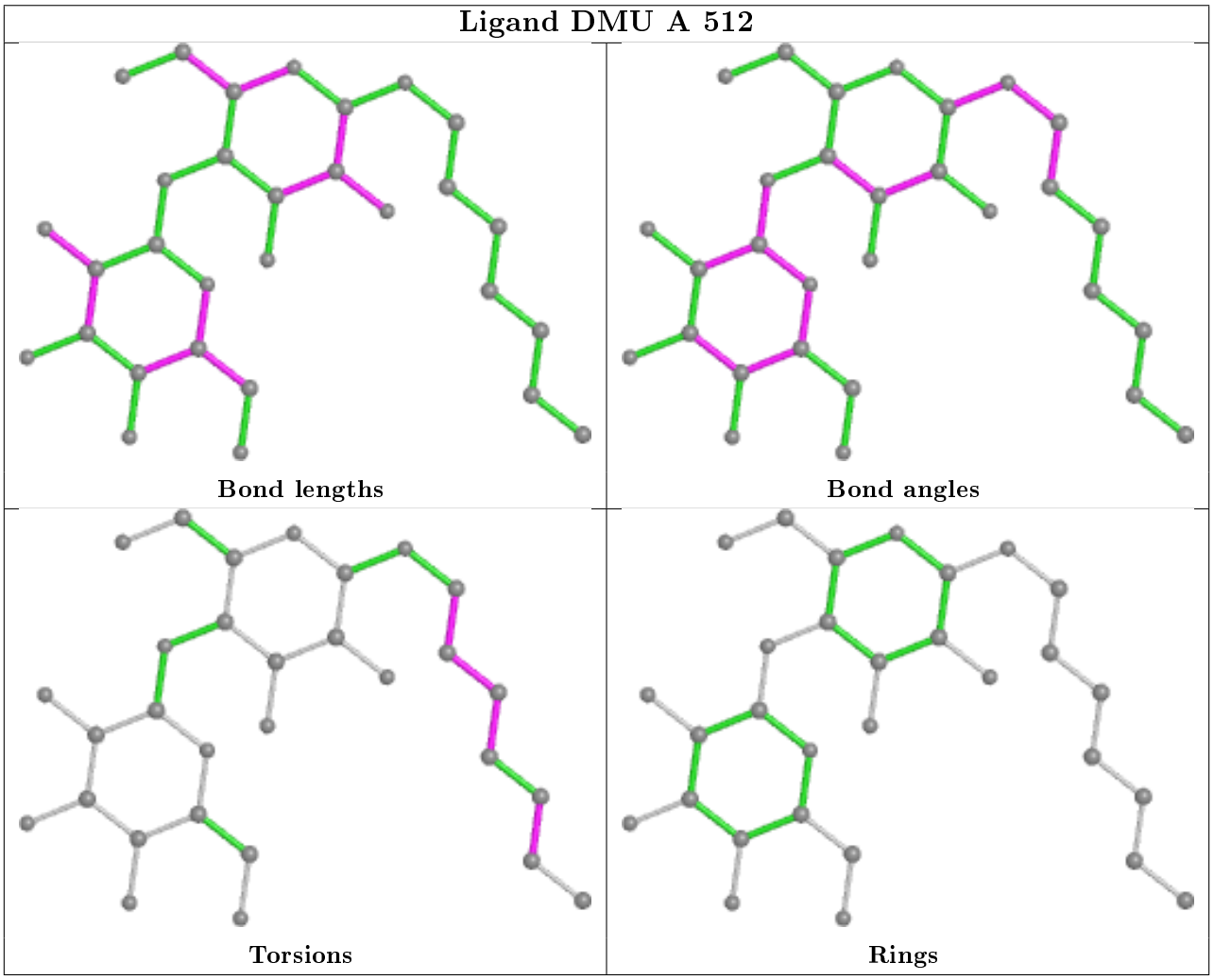
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

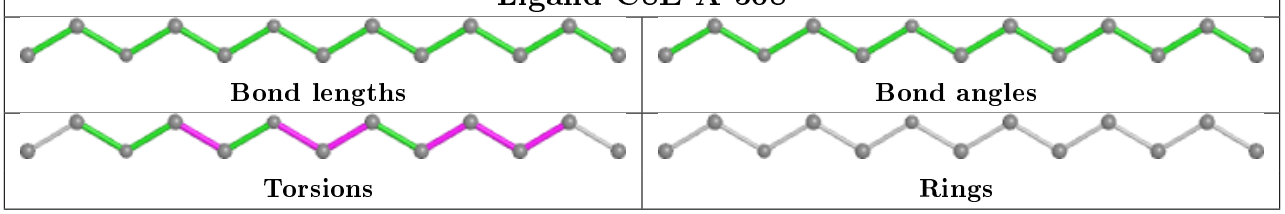
Ligand C8E A 507

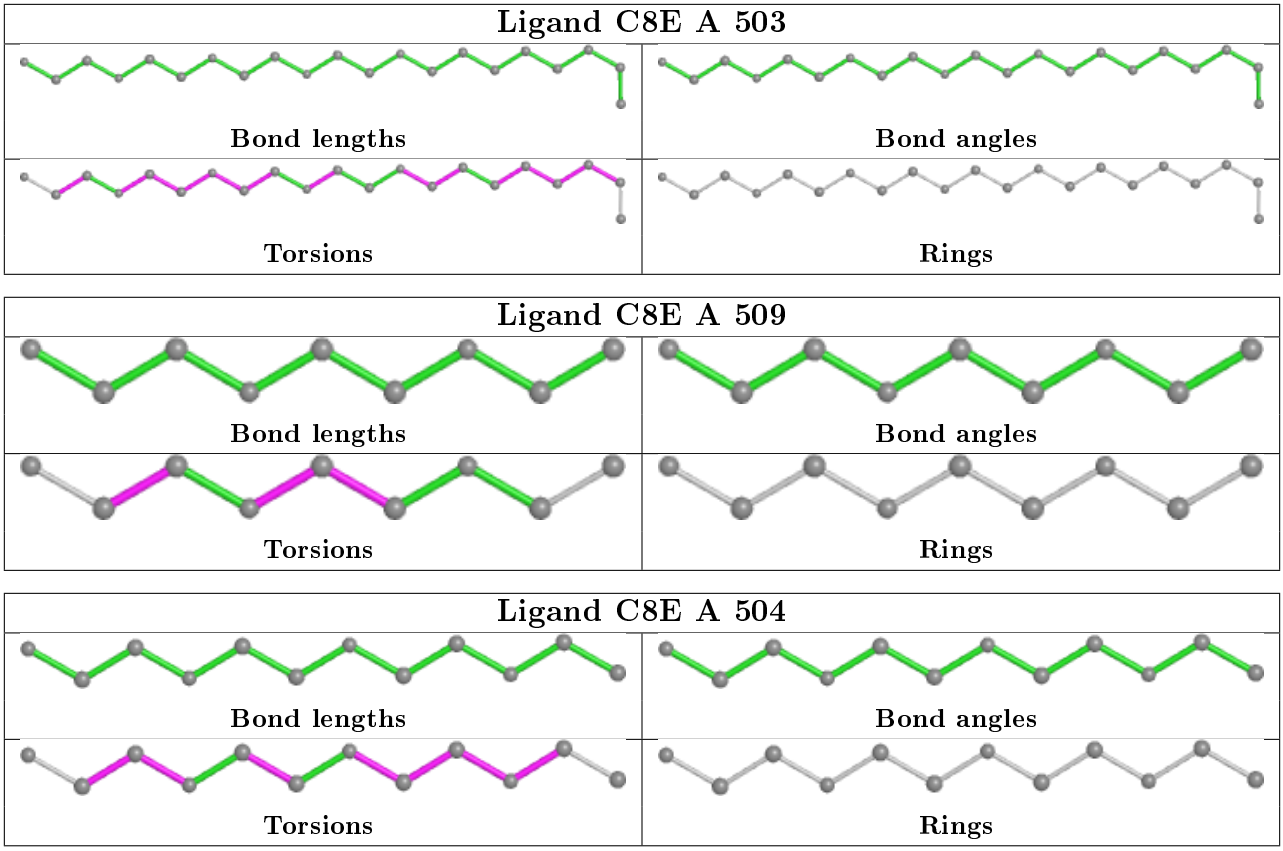


Ligand DMU A 512

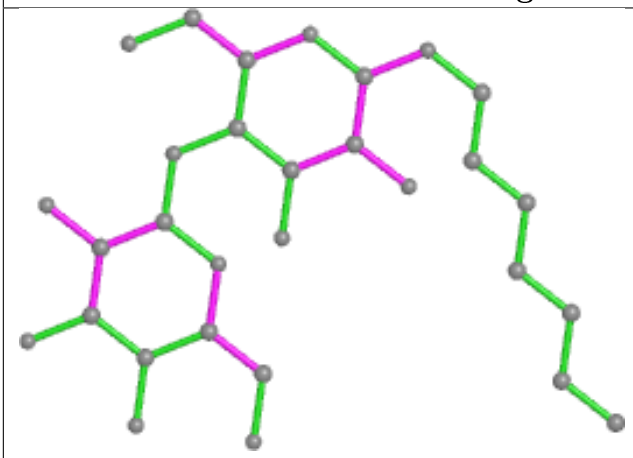


Ligand C8E A 508

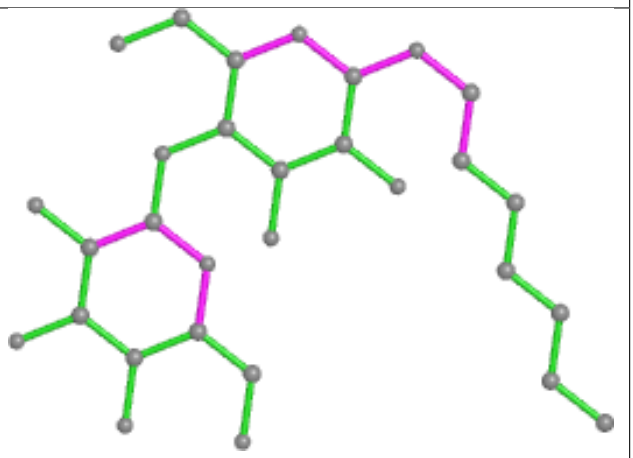



Ligand C8E A 503
Bond lengths
Bond angles
Torsions
Rings
Ligand C8E A 509
Bond lengths
Bond angles
Torsions
Rings
Ligand C8E A 504
Bond lengths
Bond angles
Torsions
Rings

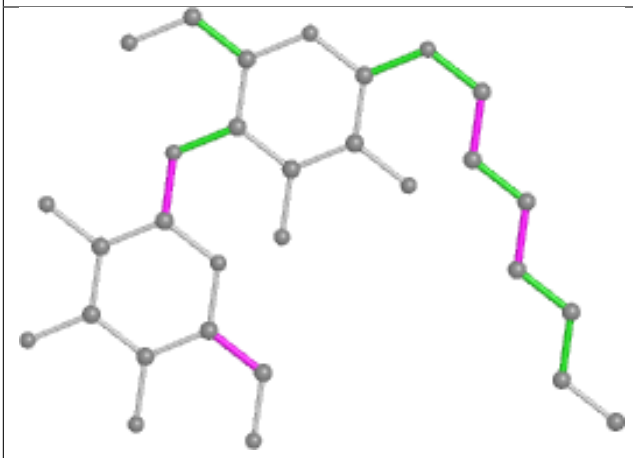
Ligand DMU A 510



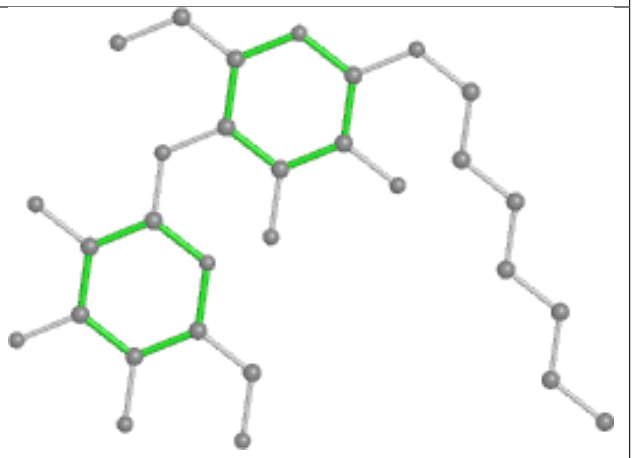
Bond lengths



Bond angles

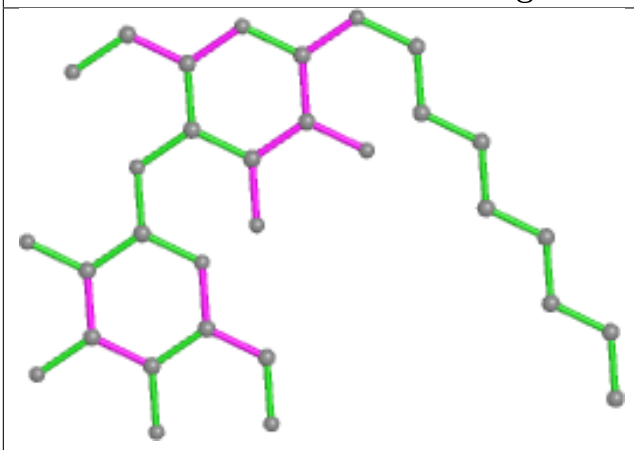


Torsions

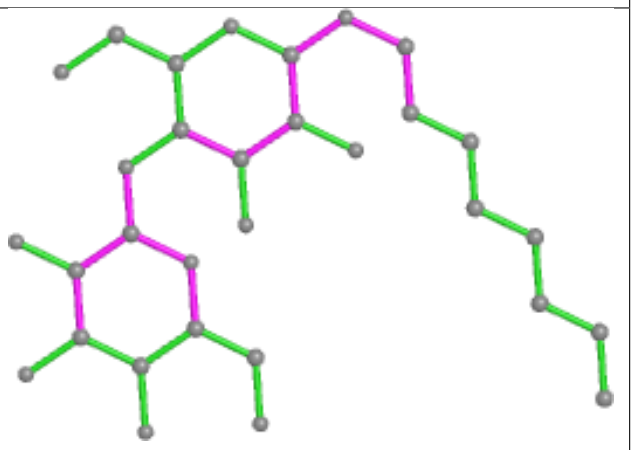


Rings

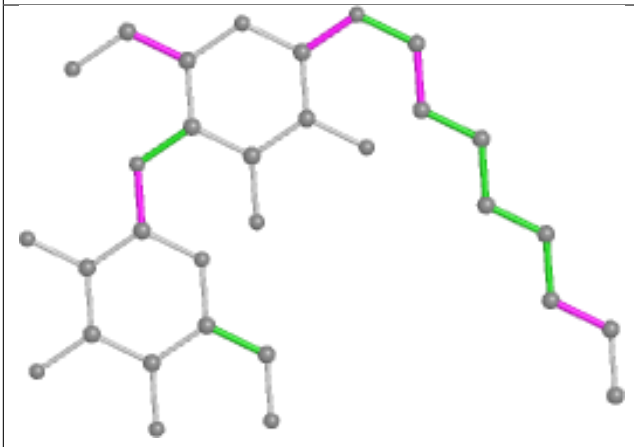
Ligand DMU A 511



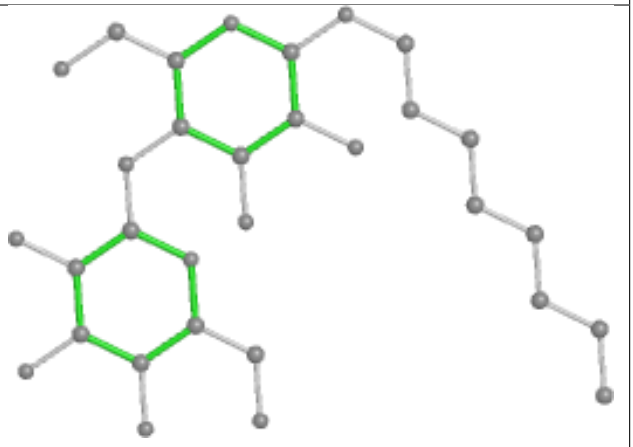
Bond lengths



Bond angles

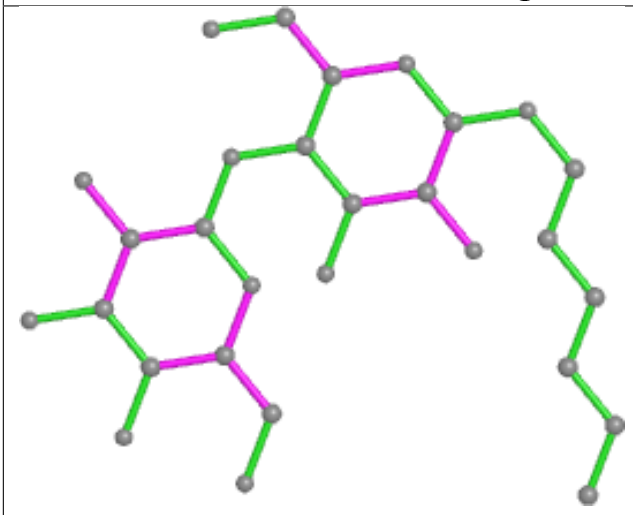


Torsions

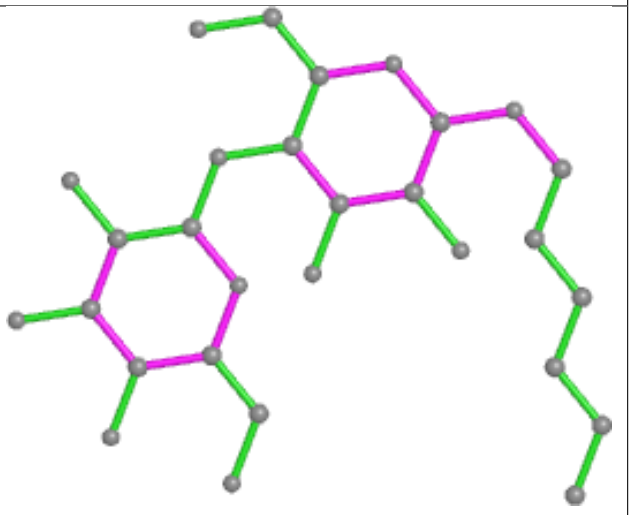


Rings

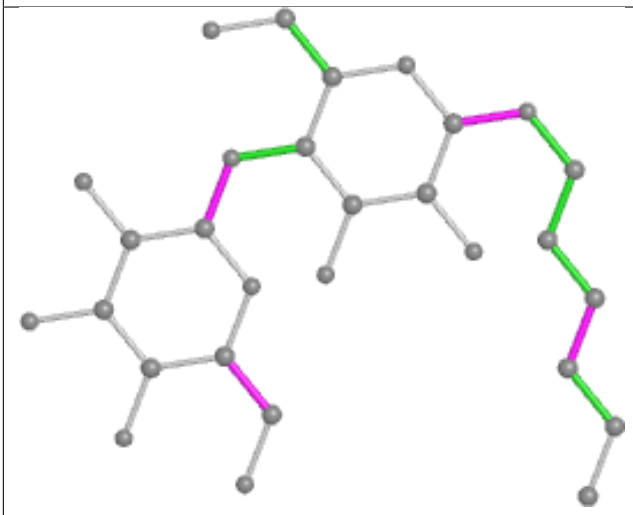
Ligand DMU A 513



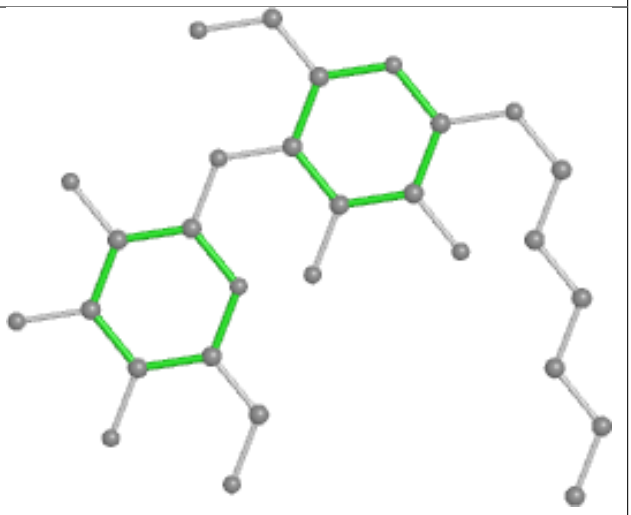
Bond lengths



Bond angles

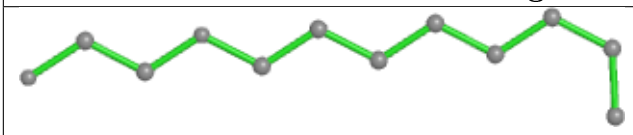


Torsions

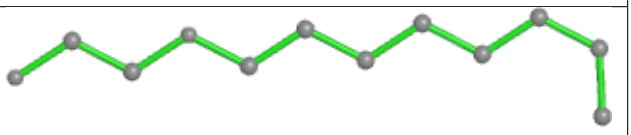


Rings

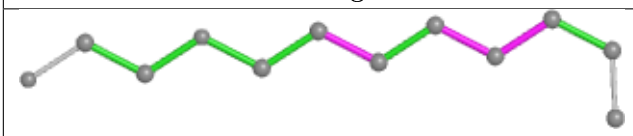
Ligand C8E A 506



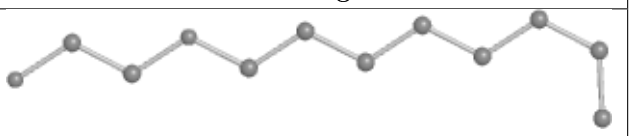
Bond lengths



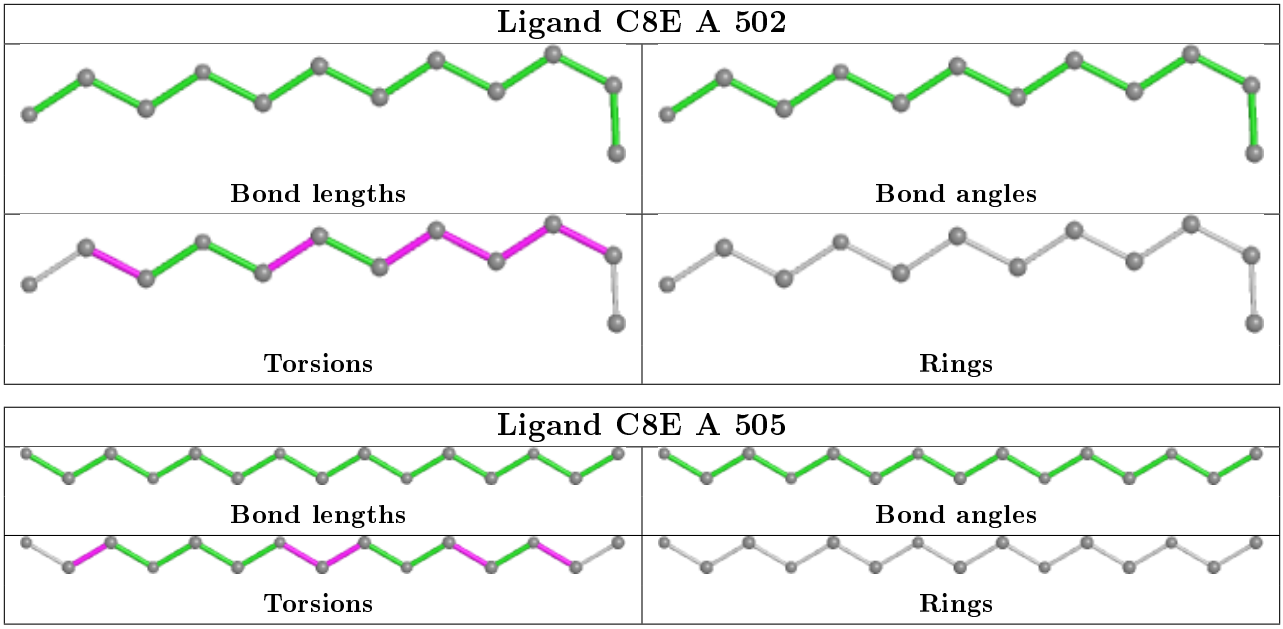
Bond angles



Torsions



Rings



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	416/436 (95%)	-0.43	2 (0%) 91 92	22, 35, 55, 65	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	HIS	2.4
1	A	16	GLY	2.1

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

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	503	21/21	0.70	0.30	50,67,79,80	0
3	C8E	A	504	12/21	0.72	0.36	66,76,87,88	0
3	C8E	A	508	13/21	0.75	0.24	40,70,73,73	0
3	C8E	A	509	9/21	0.84	0.28	47,50,69,70	0
5	PO4	A	514	5/5	0.84	0.26	106,108,110,111	0

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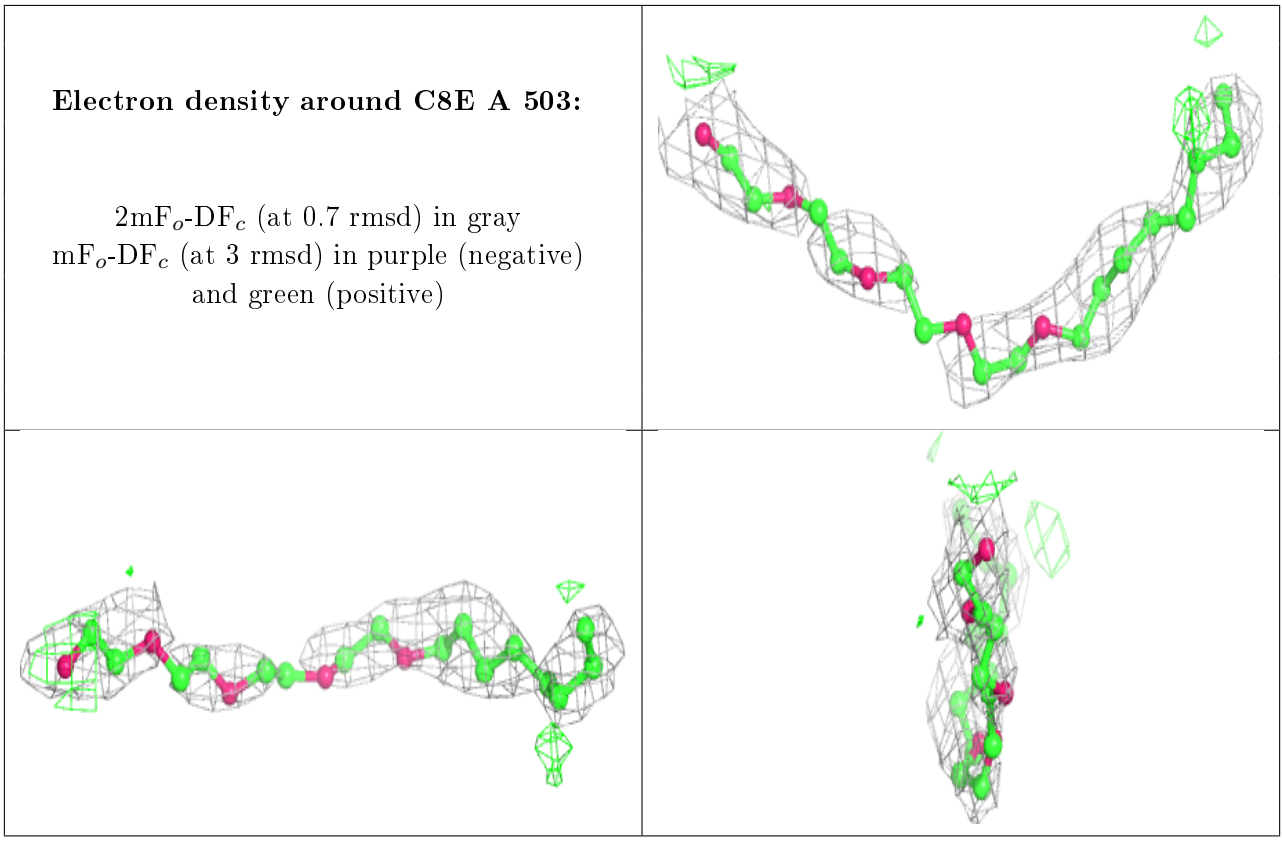
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	A	501	12/12	0.84	0.37	48,55,61,71	12
3	C8E	A	505	15/21	0.84	0.26	50,62,89,90	0
4	DMU	A	513	29/33	0.88	0.23	43,69,110,113	0
3	C8E	A	506	12/21	0.89	0.30	54,60,67,72	0
3	C8E	A	507	10/21	0.89	0.26	44,51,59,63	0
4	DMU	A	511	31/33	0.91	0.17	31,53,64,69	0
4	DMU	A	512	30/33	0.92	0.26	38,66,91,95	0
4	DMU	A	510	30/33	0.92	0.28	43,57,85,92	0
3	C8E	A	502	12/21	0.95	0.18	34,43,52,55	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.

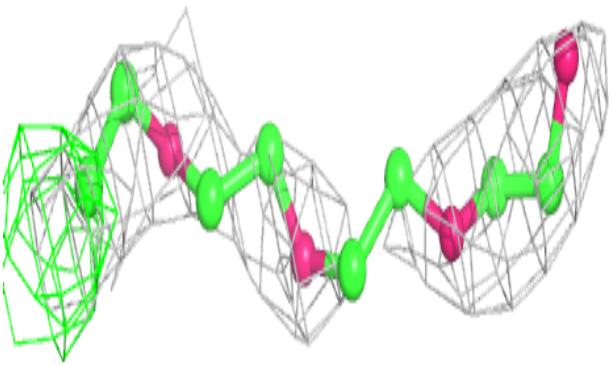
Electron density around C8E A 503:

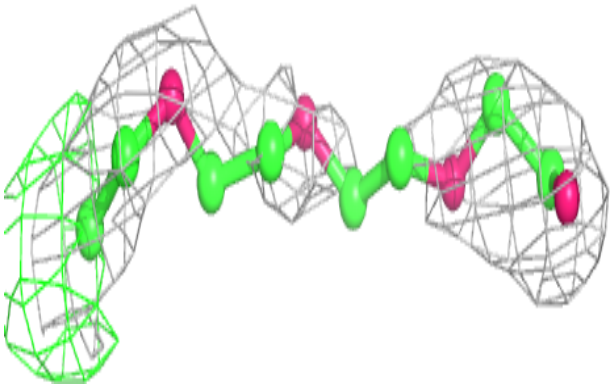
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

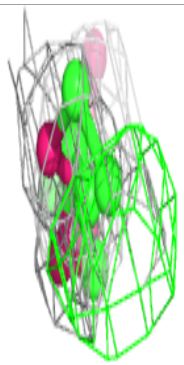


Electron density around C8E A 504:

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

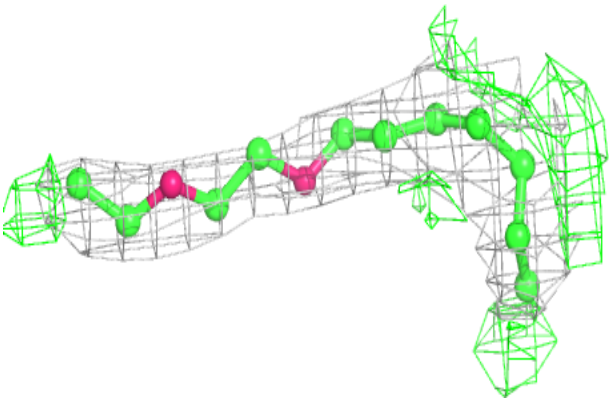


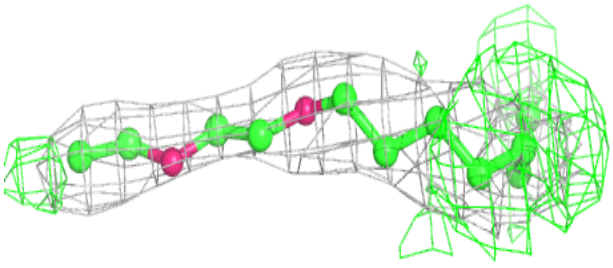


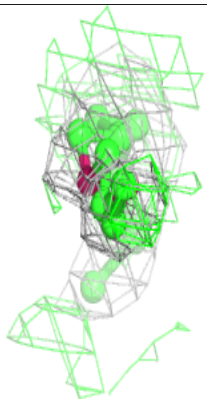


Electron density around C8E A 508:

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

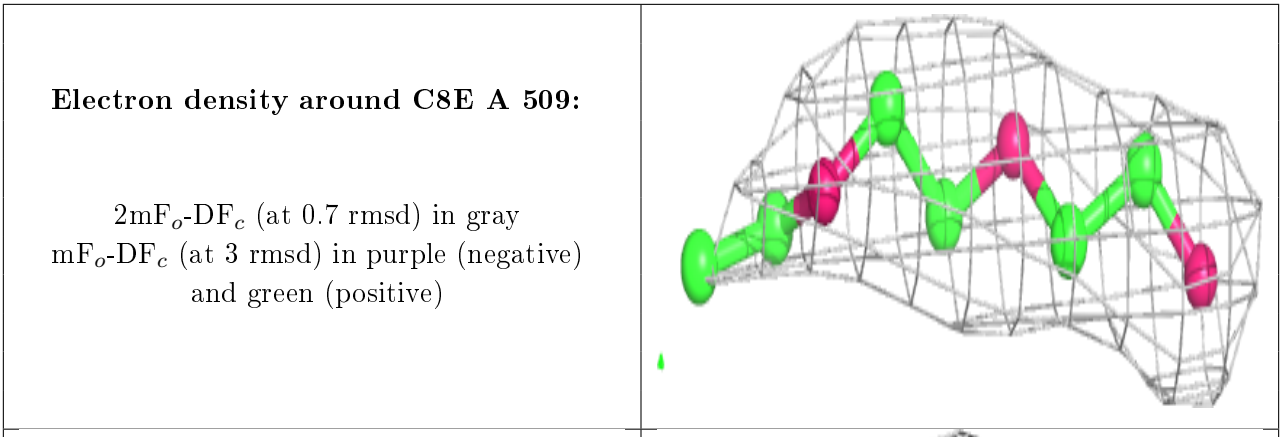






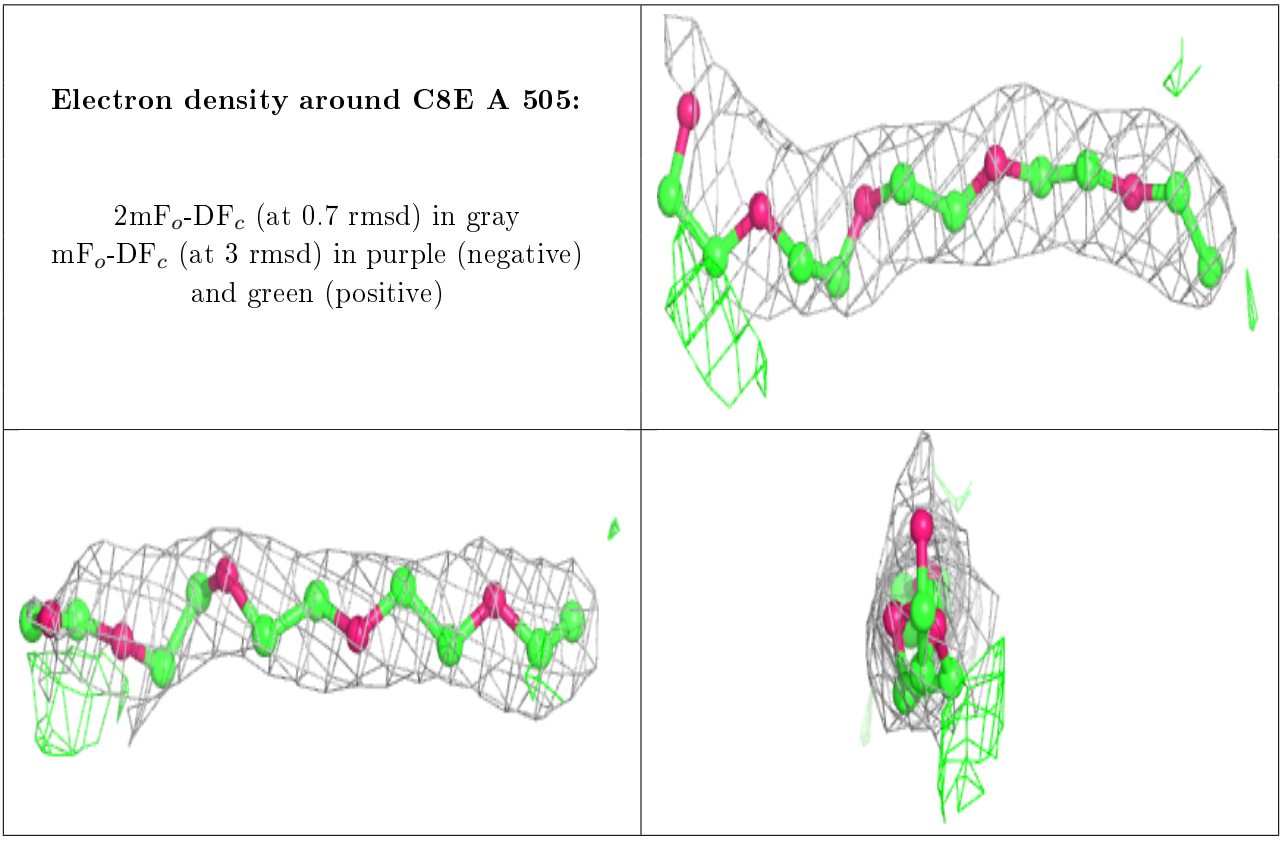
Electron density around C8E A 509:

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



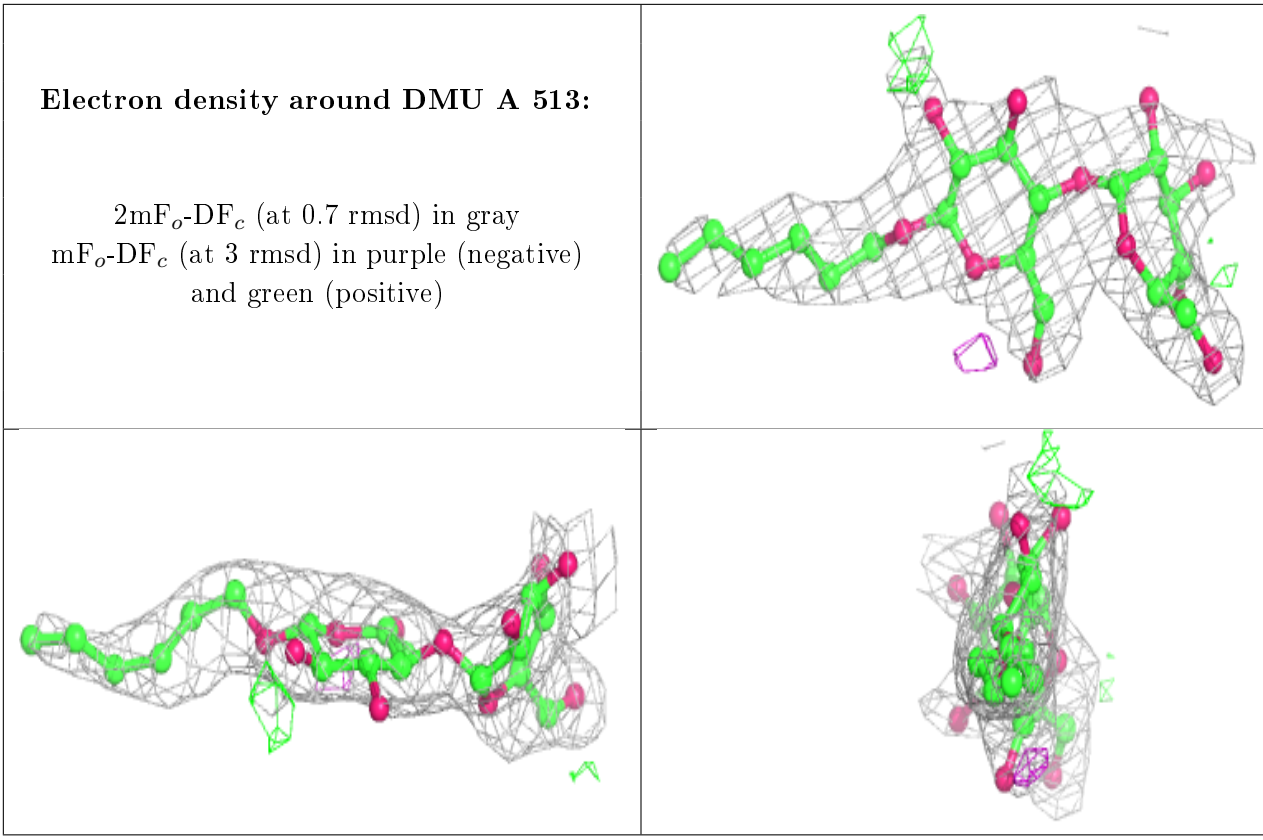
Electron density around C8E A 505:

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



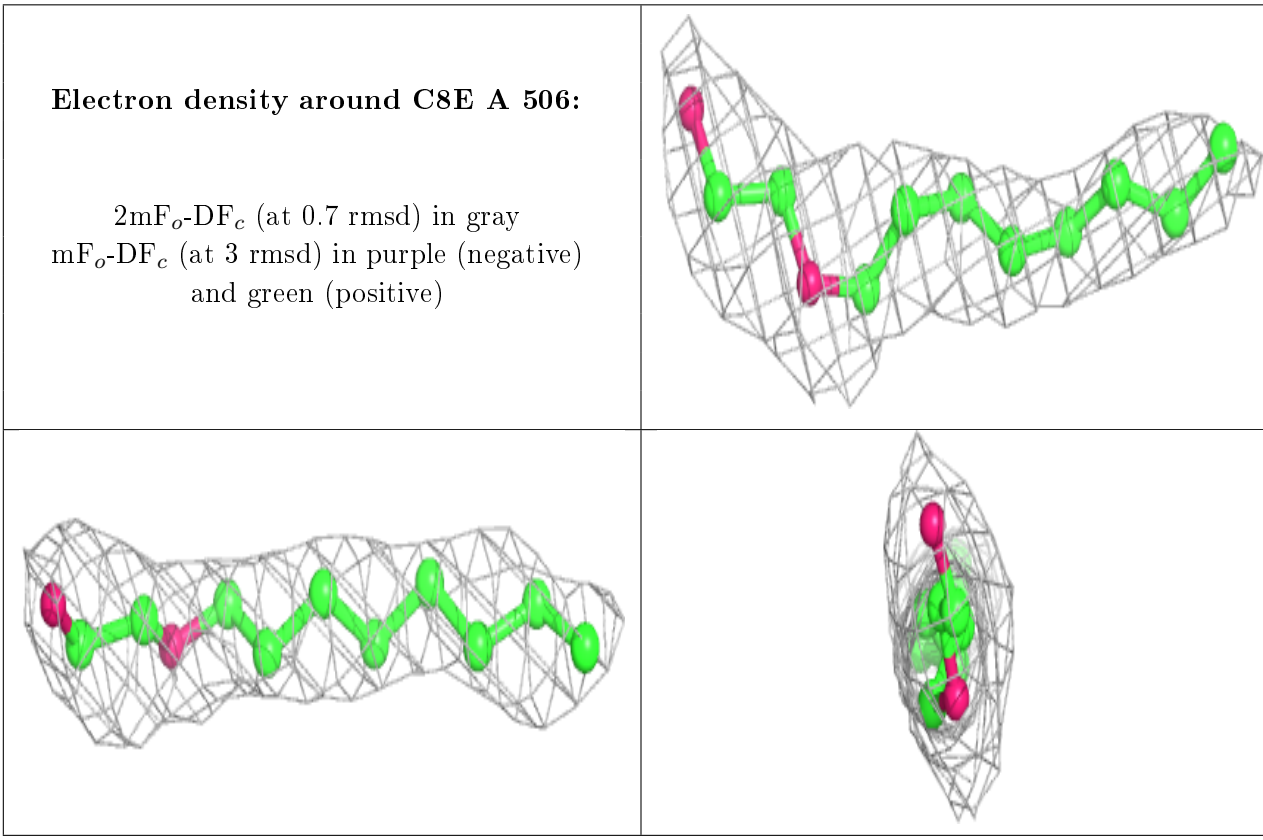
Electron density around DMU A 513:

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



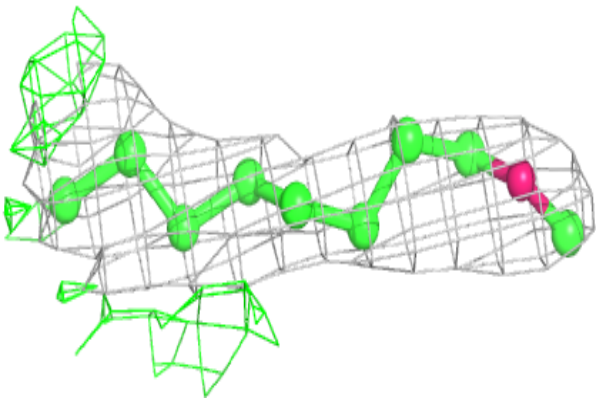
Electron density around C8E A 506:

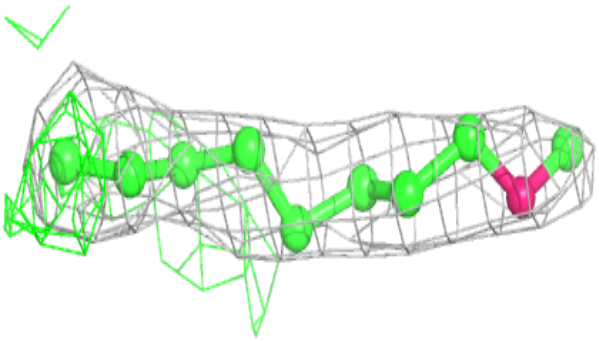
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

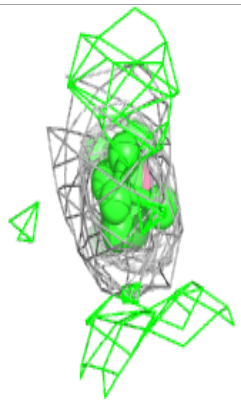


Electron density around C8E A 507:

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

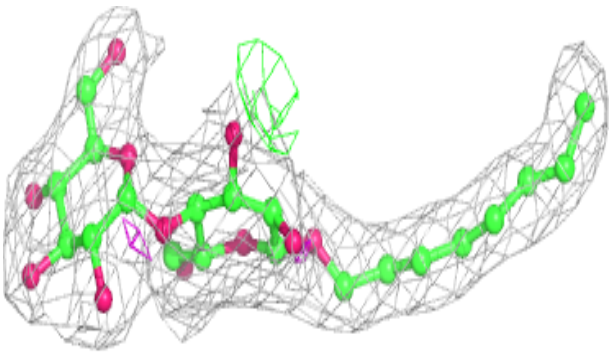


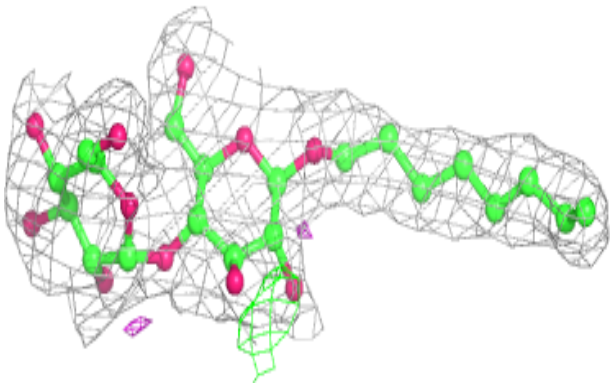


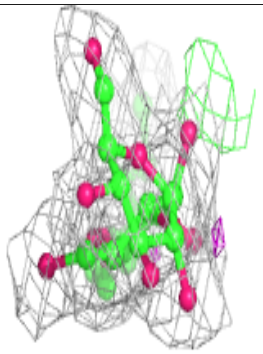


Electron density around DMU A 511:

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

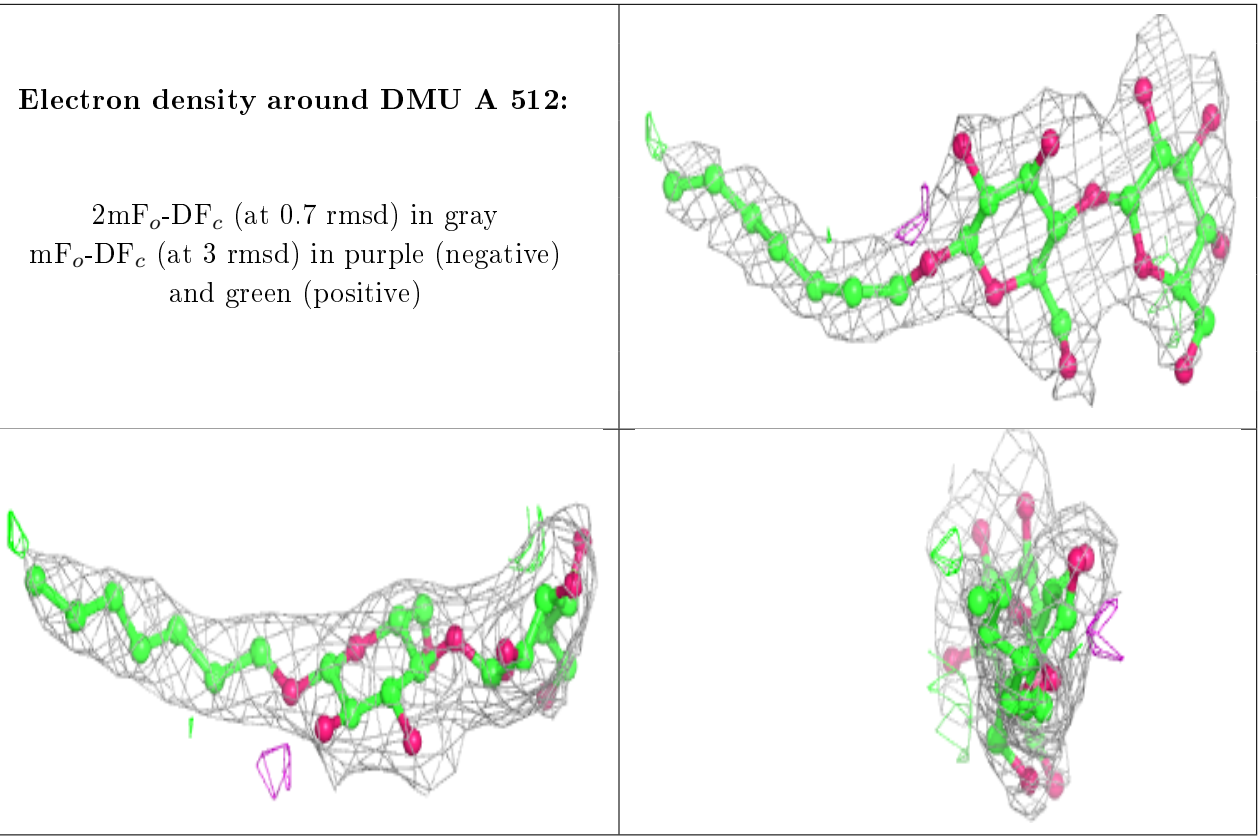






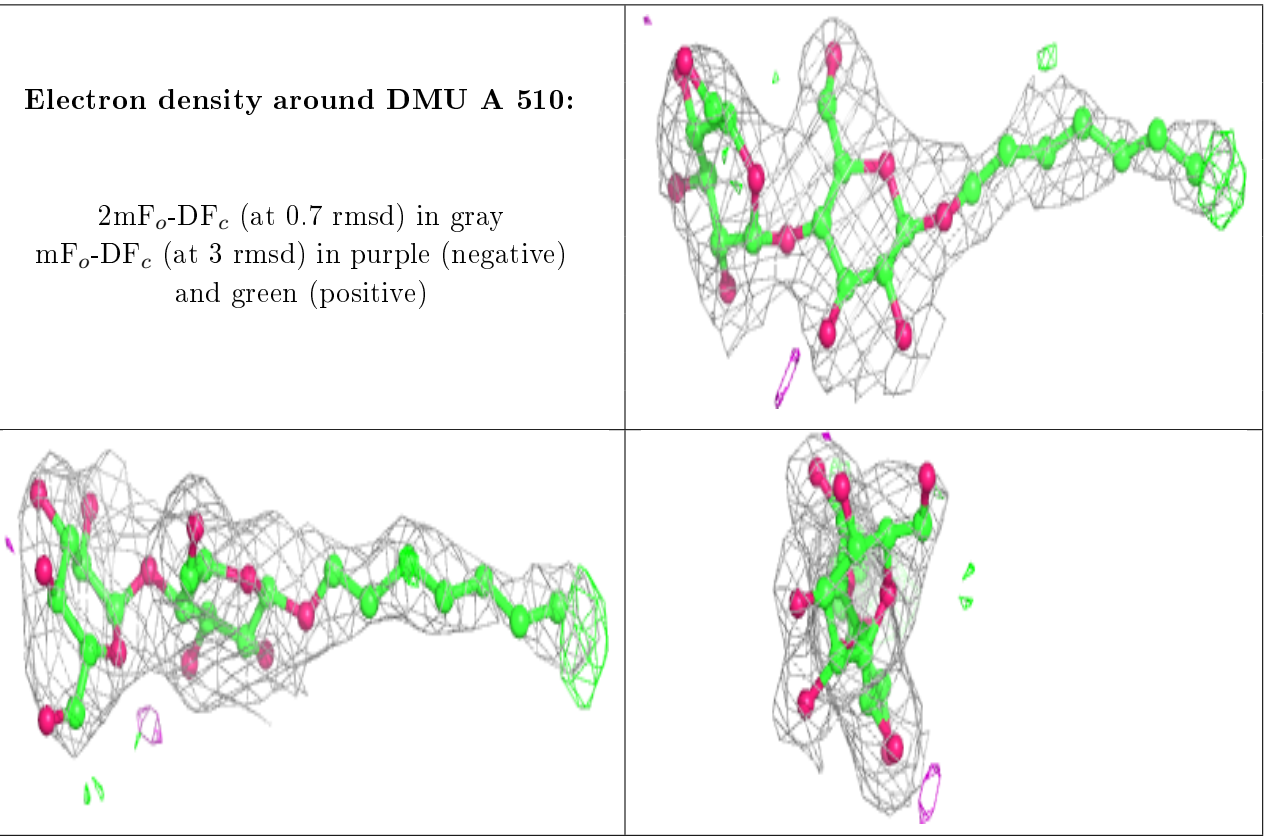
Electron density around DMU A 512:

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



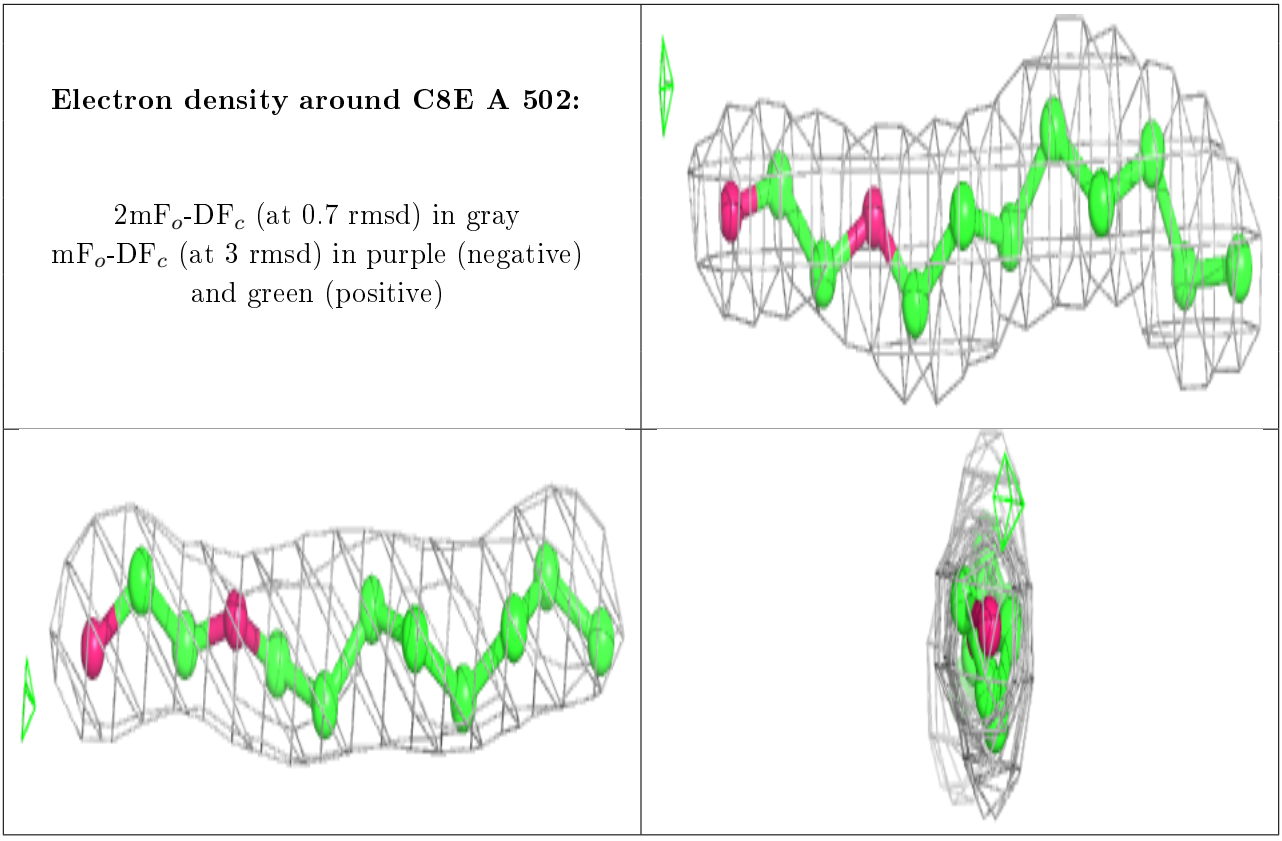
Electron density around DMU A 510:

$2mF_o$-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 502:

$2mF_o$-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.