



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2022 – 08:12 PM JST

PDB ID : 7VU0
Title : Chitoporin from Escherichia coli
Authors : Suginta, W.; Soysa, H.S.M.
Deposited on : 2021-11-01
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

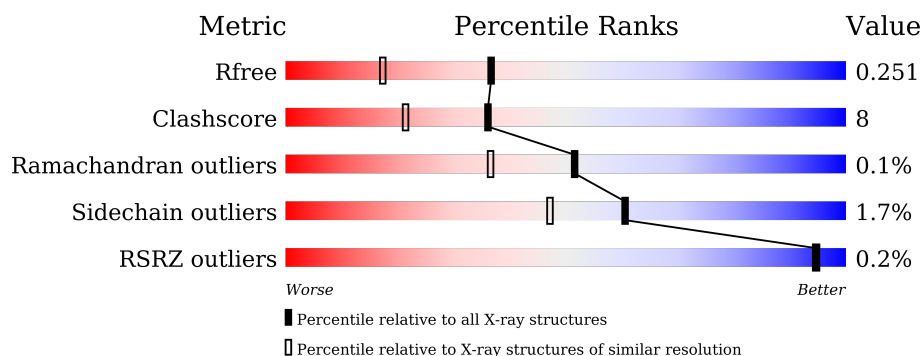
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	442	
1	B	442	

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
3	C8E	A	510	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8852 atoms, of which 629 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.

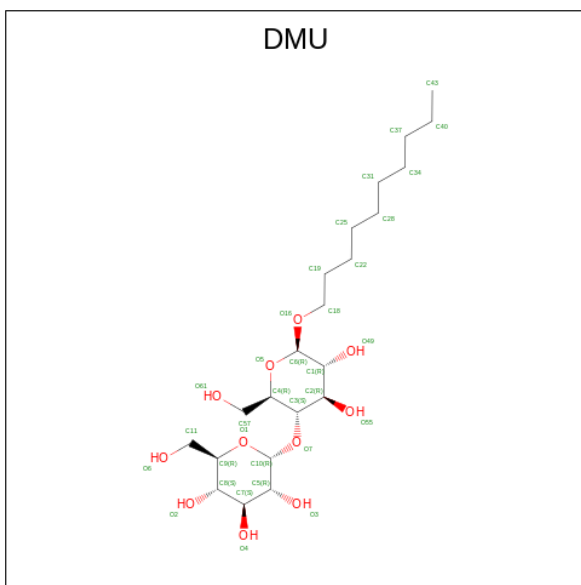
- Molecule 1 is a protein called Chitoporin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	H	N	O	S	0	8	0
			3894	2274	359	570	682	9			
1	B	435	Total	C	H	N	O	S	0	14	0
			3829	2295	270	568	687	9			

There are 12 discrepancies between the modelled and reference sequences:

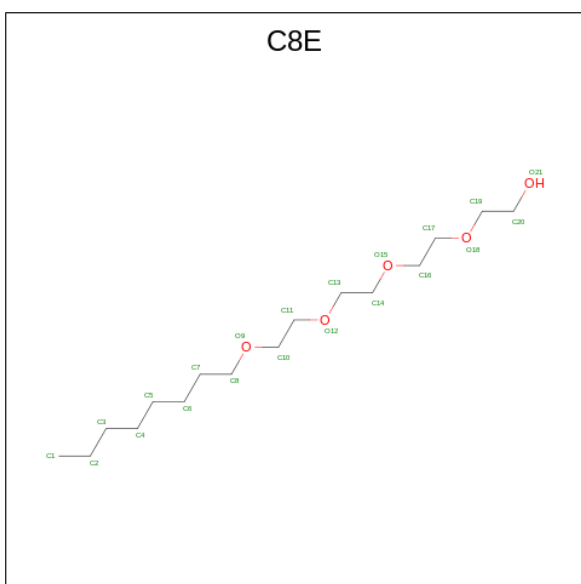
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	HIS	-	expression tag	UNP P75733
A	438	HIS	-	expression tag	UNP P75733
A	439	HIS	-	expression tag	UNP P75733
A	440	HIS	-	expression tag	UNP P75733
A	441	HIS	-	expression tag	UNP P75733
A	442	HIS	-	expression tag	UNP P75733
B	437	HIS	-	expression tag	UNP P75733
B	438	HIS	-	expression tag	UNP P75733
B	439	HIS	-	expression tag	UNP P75733
B	440	HIS	-	expression tag	UNP P75733
B	441	HIS	-	expression tag	UNP P75733
B	442	HIS	-	expression tag	UNP P75733

- Molecule 2 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 29	C 18	O 11	0	0
2	A	1	Total 24	C 13	O 11	0	0
2	B	1	Total 24	C 13	O 11	0	0
2	B	1	Total 29	C 18	O 11	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $\text{C}_{16}\text{H}_{34}\text{O}_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 9 5	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 16 13 3	0	0
3	A	1	Total C O 14 9 5	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C O 8 5 3	0	0
3	A	1	Total C O 14 9 5	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 9 6 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 14 9 5	0	0
3	B	1	Total C O 8 5 3	0	0
3	B	1	Total C O 20 15 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C O 13 9 4	0	0
3	B	1	Total C O 19 15 4	0	0
3	B	1	Total C O 8 5 3	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C O 10 7 3	0	0
3	B	1	Total C O 14 9 5	0	0
3	B	1	Total C O 14 9 5	0	0
3	B	1	Total C 4 4	0	0
3	B	1	Total C 4 4	0	0
3	B	1	Total C 4 4	0	0
3	B	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			15	12	3		
3	B	1	Total	C	O	0	0
			11	7	4		
3	B	1	Total	C	O	0	0
			6	5	1		
3	B	1	Total	C	O	0	0
			12	8	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	B	5	Total	Mg	0	0
			5	5		

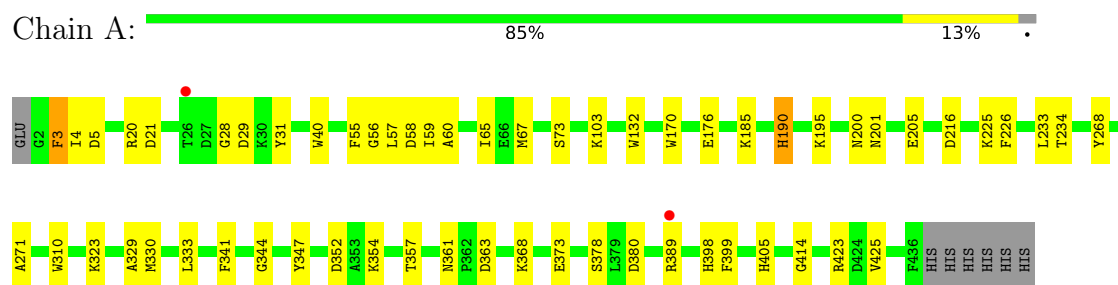
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	304	Total	O	0	0
			304	304		

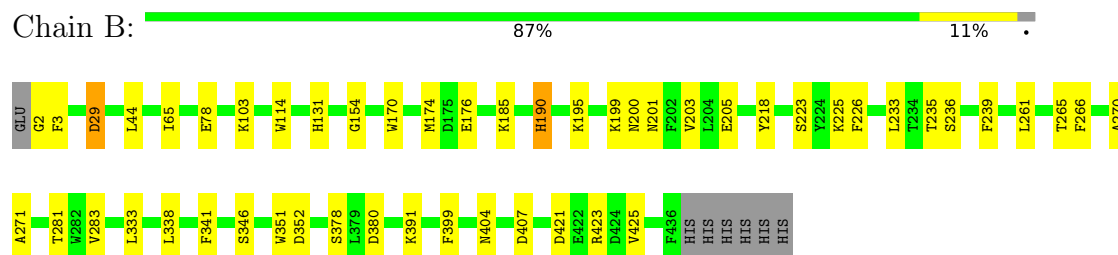
3 Residue-property plots

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: Chitoporin



• Molecule 1: Chitoporin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.08Å 58.86Å 134.71Å 90.00° 110.83° 90.00°	Depositor
Resolution (Å)	63.25 – 1.85 89.80 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (63.25-1.85) 100.0 (89.80-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.253 0.216 , 0.251	Depositor DCC
R_{free} test set	5950 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	1.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 83.26 % 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 2.2694e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMU, 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	0.64	0/3670	0.70	2/4983 (0.0%)
1	B	0.73	0/3713	0.71	0/5043
All	All	0.69	0/7383	0.70	2/10026 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	216	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3535	359	3267	63	0
1	B	3559	270	3303	47	0
2	A	53	0	52	1	0
2	B	53	0	52	0	0
3	A	200	0	254	23	0
3	B	257	0	331	28	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	254	0	0	9	0
5	B	304	0	0	7	0
All	All	8223	629	7259	119	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 (119) 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:391:LYS:HE2	3:B:511:C8E:H41	1.44	0.99
1:B:271:ALA:H	3:B:525:C8E:H132	1.34	0.92
1:A:389:ARG:NH2	5:A:601:HOH:O	2.08	0.87
1:B:65:ILE:HD11	3:B:503:C8E:H131	1.57	0.85
1:B:218:TYR:OH	5:B:601:HOH:O	1.99	0.80
3:A:512:C8E:H161	3:A:522:C8E:C2	2.12	0.79
1:A:330:MET:HE1	5:A:787:HOH:O	1.83	0.78
1:A:333:LEU:HD12	1:A:341:PHE:CD2	2.19	0.78
1:B:185:LYS:NZ	5:B:603:HOH:O	2.18	0.75
1:A:103[A]:LYS:HG3	5:A:749:HOH:O	1.88	0.72
1:A:56:GLY:C	1:A:57[A]:LEU:HD12	2.11	0.70
1:B:114:TRP:CG	3:B:527:C8E:H71	2.28	0.69
1:A:271:ALA:H	3:A:524:C8E:C11	2.06	0.69
1:B:176:GLU:HB3	1:B:185:LYS:HE3	1.73	0.69
1:A:176:GLU:HB3	1:A:185:LYS:HE3	1.75	0.69
1:A:200:ASN:HD21	3:A:509:C8E:H41	1.59	0.68
1:B:200:ASN:HD21	3:B:509:C8E:H52	1.60	0.66
1:A:330:MET:HE2	1:A:330:MET:HA	1.77	0.66
1:A:20:ARG:HH12	3:A:517:C8E:H111	1.60	0.66
1:A:57[B]:LEU:HD22	1:A:58:ASP:N	2.11	0.66
1:B:261[B]:LEU:HD11	1:B:281:THR:HB	1.76	0.66
1:A:271:ALA:H	3:A:524:C8E:H111	1.62	0.65
1:B:200:ASN:HD21	3:B:509:C8E:C5	2.10	0.65
1:B:65:ILE:HD11	3:B:503:C8E:C13	2.27	0.64
1:B:261[B]:LEU:HD13	1:B:283:VAL:CG2	2.27	0.63
1:B:380:ASP:OD2	5:B:602:HOH:O	2.14	0.63
1:A:190:HIS:HE1	3:A:506:C8E:H191	1.63	0.63
1:A:40:TRP:HE1	1:A:67:MET:HE3	1.64	0.62
1:A:352:ASP:O	5:A:602:HOH:O	2.16	0.61
1:B:3:PHE:H	3:B:512:C8E:C19	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:HIS:HE1	3:B:506:C8E:H191	1.66	0.60
1:A:40:TRP:HE1	1:A:67:MET:CE	2.14	0.59
1:A:57[A]:LEU:HD11	3:A:525:C8E:O15	2.03	0.59
1:B:271:ALA:N	3:B:525:C8E:H132	2.13	0.59
1:B:261[B]:LEU:HD13	1:B:283:VAL:HG22	1.84	0.59
1:A:330:MET:CE	5:A:787:HOH:O	2.48	0.59
1:A:57[B]:LEU:HD21	3:A:522:C8E:C7	2.33	0.58
1:A:352:ASP:HB3	5:A:602:HOH:O	2.04	0.57
1:A:361:ASN:OD1	1:A:361:ASN:O	2.21	0.57
1:A:190:HIS:CE1	3:A:506:C8E:H191	2.38	0.57
1:A:323:LYS:NZ	1:A:352:ASP:OD2	2.35	0.57
1:A:310:TRP:HB3	3:A:511:C8E:H42	1.86	0.56
1:A:329:ALA:O	1:A:330:MET:HE2	2.06	0.55
1:B:333:LEU:HD12	1:B:341[B]:PHE:CD2	2.42	0.55
1:B:404:ASN:N	1:B:421:ASP:OD1	2.37	0.55
1:A:40:TRP:CD1	3:A:513:C8E:H202	2.42	0.54
1:B:3:PHE:H	3:B:512:C8E:H191	1.72	0.54
1:B:200:ASN:O	1:B:201:ASN:HB2	2.08	0.54
1:B:200:ASN:ND2	3:B:509:C8E:H52	2.23	0.54
1:A:268:TYR:OH	3:A:524:C8E:H101	2.08	0.53
1:A:330:MET:CE	1:A:344:GLY:HA3	2.38	0.53
1:B:346:SER:OG	1:B:378[A]:SER:OG	2.24	0.53
1:A:330:MET:HE2	1:A:330:MET:CA	2.36	0.53
3:B:506:C8E:H162	3:B:519:C8E:H41	1.89	0.53
1:A:3:PHE:HE2	1:A:57[A]:LEU:HD13	1.74	0.52
1:A:57[B]:LEU:HD11	1:A:59[B]:ILE:HG23	1.91	0.52
1:B:2:GLY:HA3	3:B:512:C8E:H191	1.92	0.52
1:A:170:TRP:HH2	3:A:521:C8E:H162	1.75	0.51
3:B:510:C8E:H61	3:B:523:C8E:H81	1.93	0.51
1:A:57[B]:LEU:HD22	1:A:58:ASP:H	1.75	0.50
1:A:347:TYR:HB2	3:A:505:C8E:H82	1.94	0.49
1:A:399:PHE:HD1	1:A:425:VAL:HG22	1.77	0.49
1:B:103:LYS:HG3	5:B:762:HOH:O	2.12	0.49
1:A:271:ALA:H	3:A:524:C8E:H112	1.77	0.49
1:B:154:GLY:HA2	1:B:199:LYS:HG2	1.96	0.48
1:A:330:MET:HE2	1:A:344:GLY:HA3	1.95	0.48
1:A:373:GLU:O	1:A:405:HIS:HB2	2.14	0.48
1:A:226:PHE:CZ	1:A:233:LEU:HD23	2.48	0.48
1:A:200:ASN:ND2	3:A:509:C8E:H61	2.28	0.47
1:B:3:PHE:H	3:B:512:C8E:H192	1.80	0.47
1:A:354:LYS:HG2	5:A:654:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:CG	5:B:762:HOH:O	2.62	0.47
1:B:236:SER:OG	1:B:265[A]:THR:HG22	2.15	0.47
1:B:239:PHE:CD1	3:B:507:C8E:H162	2.51	0.46
1:A:132:TRP:O	3:A:521:C8E:H131	2.15	0.46
1:A:200:ASN:O	1:A:201:ASN:HB2	2.15	0.46
1:A:57[B]:LEU:HD11	1:A:59[B]:ILE:CG2	2.45	0.46
1:A:21[A]:ASP:OD2	1:A:31:TYR:HB3	2.16	0.46
3:B:528:C8E:H161	5:B:678:HOH:O	2.15	0.45
1:B:170:TRP:CH2	3:B:528:C8E:H141	2.52	0.45
1:B:190:HIS:CE1	3:B:506:C8E:H191	2.48	0.45
1:B:195:LYS:HG3	1:B:205:GLU:HG2	1.97	0.45
1:A:330:MET:CE	1:A:330:MET:CA	2.94	0.45
1:B:154:GLY:HA2	1:B:199:LYS:CG	2.46	0.45
1:B:203[A]:VAL:CG2	1:B:223[A]:SER:HB2	2.46	0.45
3:B:518:C8E:H141	3:B:518:C8E:H171	1.30	0.45
1:A:57[B]:LEU:HD23	3:A:522:C8E:H61	1.98	0.44
1:A:225:LYS:HB3	1:A:234:THR:HG22	1.99	0.44
1:A:414:GLY:N	5:A:605:HOH:O	2.30	0.44
1:A:380:ASP:OD1	1:A:398:HIS:ND1	2.34	0.44
1:A:330:MET:HE3	1:A:330:MET:HB2	1.74	0.44
1:B:131:HIS:HD2	3:B:528:C8E:H142	1.82	0.44
3:A:512:C8E:H191	3:A:512:C8E:H162	1.53	0.43
1:A:60:ALA:HB3	1:A:103[B]:LYS:HB2	1.99	0.43
1:B:131:HIS:CD2	3:B:528:C8E:H142	2.53	0.43
2:A:502:DMU:H40	3:A:503:C8E:H171	1.99	0.43
1:B:226:PHE:CZ	1:B:233:LEU:HD23	2.53	0.43
1:B:78:GLU:OE2	3:B:528:C8E:H162	2.19	0.43
1:A:333:LEU:HD12	1:A:341:PHE:CE2	2.53	0.43
1:A:3:PHE:CD1	1:A:3:PHE:C	2.91	0.43
1:B:44:LEU:HG	3:B:517:C8E:O18	2.19	0.43
1:B:270:ALA:HB1	3:B:525:C8E:H81	2.01	0.43
1:B:399:PHE:HD1	1:B:425:VAL:HG22	1.84	0.43
1:B:235[A]:THR:HG22	1:B:266:PHE:CD1	2.53	0.42
1:B:270:ALA:HA	3:B:525:C8E:H132	2.01	0.42
1:A:28:GLY:O	1:A:29:ASP:OD1	2.38	0.42
1:B:226:PHE:CE1	1:B:233:LEU:HD23	2.54	0.42
1:A:65:ILE:HD11	3:A:503:C8E:H131	2.02	0.42
1:A:170:TRP:CH2	3:A:521:C8E:H162	2.55	0.42
1:A:357:THR:O	1:A:368:LYS:HD2	2.19	0.42
1:B:351:TRP:O	1:B:352:ASP:HB2	2.20	0.41
1:A:3:PHE:HD1	1:A:4:ILE:HG12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HG3	1:A:205:GLU:HG2	2.01	0.41
1:B:338:LEU:HB3	1:B:341[A]:PHE:CD2	2.56	0.41
3:A:521:C8E:H192	5:A:631:HOH:O	2.19	0.41
3:B:528:C8E:H192	5:B:750:HOH:O	2.20	0.41
1:A:378:SER:HA	1:A:399:PHE:O	2.21	0.41
1:A:3:PHE:CE2	1:A:57[A]:LEU:HD13	2.55	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	441/442 (100%)	421 (96%)	20 (4%)	0	100	100
1	B	447/442 (101%)	429 (96%)	17 (4%)	1 (0%)	47	33
All	All	888/884 (100%)	850 (96%)	37 (4%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	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	358/357 (100%)	352 (98%)	6 (2%)	60	47
1	B	364/357 (102%)	358 (98%)	6 (2%)	62	49
All	All	722/714 (101%)	710 (98%)	12 (2%)	60	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	5	ASP
1	A	55	PHE
1	A	73	SER
1	A	190	HIS
1	A	423	ARG
1	B	29	ASP
1	B	174	MET
1	B	190	HIS
1	B	225	LYS
1	B	407	ASP
1	B	423	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	B	361	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 61 ligands modelled in this entry, 8 are monoatomic - leaving 53 for Mogul analysis.

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	DMU	A	501	-	30,30,34	1.62	8 (26%)	41,41,45	1.06	2 (4%)
3	C8E	B	506	-	19,19,20	0.48	0	18,18,19	0.52	0
3	C8E	A	504	-	4,4,20	0.35	0	3,3,19	0.63	0
3	C8E	B	507	-	12,12,20	0.51	0	11,11,19	0.44	0
3	C8E	B	509	-	5,5,20	0.35	0	4,4,19	0.51	0
3	C8E	A	514	-	3,3,20	0.37	0	2,2,19	0.82	0
3	C8E	A	521	-	9,9,20	0.58	0	8,8,19	0.47	0
3	C8E	A	510	-	20,20,20	0.50	0	19,19,19	0.53	0
3	C8E	A	523	-	11,11,20	0.55	0	10,10,19	0.43	0
3	C8E	A	509	-	5,5,20	0.34	0	4,4,19	0.57	0
3	C8E	A	522	-	5,5,20	0.29	0	4,4,19	0.65	0
3	C8E	B	508	-	4,4,20	0.36	0	3,3,19	0.59	0
3	C8E	B	517	-	13,13,20	0.49	0	12,12,19	0.39	0
3	C8E	B	513	-	18,18,20	0.46	0	17,17,19	0.56	0
3	C8E	B	527	-	5,5,20	0.31	0	4,4,19	0.54	0
3	C8E	B	516	-	9,9,20	0.53	0	8,8,19	0.30	0
3	C8E	B	504	-	13,13,20	0.51	0	12,12,19	0.32	0
3	C8E	B	512	-	11,11,20	0.53	0	9,9,19	0.40	0
3	C8E	A	524	-	8,8,20	0.55	0	7,7,19	0.29	0
3	C8E	B	515	-	4,4,20	0.35	0	3,3,19	0.49	0
3	C8E	B	510	-	5,5,20	0.40	0	4,4,19	0.58	0
3	C8E	B	518	-	12,12,20	0.51	0	11,11,19	0.59	0
3	C8E	B	521	-	3,3,20	0.42	0	2,2,19	0.74	0
3	C8E	B	519	-	3,3,20	0.36	0	2,2,19	0.77	0
3	C8E	B	526	-	10,10,20	0.50	0	9,9,19	0.32	0
3	C8E	A	519	-	5,5,20	0.32	0	4,4,19	0.48	0
3	C8E	B	525	4	14,14,20	0.44	0	13,13,19	0.55	0
3	C8E	B	524	4	11,11,20	0.39	0	10,10,19	0.81	0
3	C8E	A	511	-	5,5,20	0.37	0	4,4,19	0.50	0
3	C8E	A	508	-	9,9,20	0.51	0	8,8,19	0.38	0
3	C8E	A	515	-	3,3,20	0.42	0	2,2,19	0.76	0
3	C8E	A	506	-	13,13,20	0.52	0	12,12,19	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	A	518	-	5,5,20	0.36	0	4,4,19	0.57	0
3	C8E	B	520	-	3,3,20	0.36	0	2,2,19	0.75	0
3	C8E	A	505	-	14,14,20	0.39	0	12,12,19	0.79	0
3	C8E	B	523	-	7,7,20	0.49	0	6,6,19	0.48	0
3	C8E	B	503	-	12,12,20	0.55	0	11,11,19	0.65	0
2	DMU	A	502	-	25,25,34	1.61	4 (16%)	36,36,45	1.18	3 (8%)
3	C8E	A	516	-	4,4,20	0.36	0	3,3,19	0.54	0
2	DMU	B	501	-	25,25,34	1.70	7 (28%)	36,36,45	1.15	2 (5%)
3	C8E	B	505	-	7,7,20	0.48	0	6,6,19	0.32	0
3	C8E	A	517	-	3,3,20	0.49	0	2,2,19	0.48	0
3	C8E	B	514	-	7,7,20	0.45	0	6,6,19	0.36	0
3	C8E	A	503	-	13,13,20	0.51	0	12,12,19	0.56	0
3	C8E	A	513	-	13,13,20	0.52	0	12,12,19	0.24	0
3	C8E	A	512	-	7,7,20	0.49	0	6,6,19	0.50	0
3	C8E	A	525	-	7,7,20	0.59	0	6,6,19	0.41	0
3	C8E	B	528	-	11,11,20	0.56	0	10,10,19	0.39	0
3	C8E	B	511	-	5,5,20	0.36	0	4,4,19	0.39	0
3	C8E	A	520	-	4,4,20	0.39	0	3,3,19	0.40	0
3	C8E	A	507	-	6,6,20	0.42	0	5,5,19	0.50	0
2	DMU	B	502	-	30,30,34	1.55	9 (30%)	41,41,45	1.27	3 (7%)
3	C8E	B	522	-	6,6,20	0.50	0	5,5,19	0.45	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	DMU	A	501	-	-	0/15/55/59	0/2/2/2
3	C8E	B	506	-	-	10/17/17/18	-
3	C8E	A	504	-	-	1/2/2/18	-
3	C8E	B	507	-	-	4/10/10/18	-
3	C8E	B	509	-	-	2/3/3/18	-
3	C8E	A	514	-	-	0/1/1/18	-
3	C8E	A	521	-	-	5/7/7/18	-
3	C8E	A	510	-	-	12/18/18/18	-
3	C8E	A	523	-	-	4/9/9/18	-
3	C8E	A	509	-	-	2/3/3/18	-
3	C8E	A	522	-	-	2/3/3/18	-
3	C8E	B	508	-	-	1/2/2/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	517	-	-	7/11/11/18	-
3	C8E	B	513	-	-	10/16/16/18	-
3	C8E	B	527	-	-	2/3/3/18	-
3	C8E	B	516	-	-	4/7/7/18	-
3	C8E	B	504	-	-	8/11/11/18	-
3	C8E	B	512	-	-	3/7/7/18	-
3	C8E	A	524	-	-	3/6/6/18	-
3	C8E	B	515	-	-	2/2/2/18	-
3	C8E	B	510	-	-	2/3/3/18	-
3	C8E	B	518	-	-	7/10/10/18	-
3	C8E	B	521	-	-	0/1/1/18	-
3	C8E	B	519	-	-	0/1/1/18	-
3	C8E	B	526	-	-	6/8/8/18	-
3	C8E	A	519	-	-	2/3/3/18	-
3	C8E	B	525	4	-	9/12/12/18	-
3	C8E	B	524	4	-	2/9/9/18	-
3	C8E	A	511	-	-	1/3/3/18	-
3	C8E	A	508	-	-	4/7/7/18	-
3	C8E	A	515	-	-	0/1/1/18	-
3	C8E	A	506	-	-	7/11/11/18	-
3	C8E	A	518	-	-	2/3/3/18	-
3	C8E	B	520	-	-	0/1/1/18	-
3	C8E	A	505	-	-	6/10/10/18	-
3	C8E	B	523	-	-	2/5/5/18	-
3	C8E	B	503	-	-	5/10/10/18	-
2	DMU	A	502	-	-	2/10/50/59	0/2/2/2
3	C8E	A	516	-	-	2/2/2/18	-
2	DMU	B	501	-	-	1/10/50/59	0/2/2/2
3	C8E	B	505	-	-	3/5/5/18	-
3	C8E	A	517	-	-	1/1/1/18	-
3	C8E	B	514	-	-	4/5/5/18	-
3	C8E	A	503	-	-	9/11/11/18	-
3	C8E	A	513	-	-	6/11/11/18	-
3	C8E	A	512	-	-	4/5/5/18	-
3	C8E	A	525	-	-	2/5/5/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	528	-	-	6/9/9/18	-
3	C8E	B	511	-	-	3/3/3/18	-
3	C8E	A	520	-	-	1/2/2/18	-
3	C8E	A	507	-	-	3/4/4/18	-
2	DMU	B	502	-	-	0/15/55/59	0/2/2/2
3	C8E	B	522	-	-	3/4/4/18	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DMU	O1-C9	4.12	1.54	1.44
2	B	502	DMU	O1-C9	4.05	1.54	1.44
2	B	501	DMU	O1-C9	4.00	1.54	1.44
2	A	502	DMU	O4-C7	3.76	1.51	1.43
2	A	502	DMU	O1-C9	3.71	1.53	1.44
2	B	501	DMU	O4-C7	3.40	1.51	1.43
2	B	501	DMU	C11-C9	-3.16	1.41	1.51
2	A	501	DMU	C11-C9	-3.01	1.41	1.51
2	A	502	DMU	C11-C9	-2.91	1.42	1.51
2	B	501	DMU	C8-C9	2.87	1.59	1.53
2	B	502	DMU	C11-C9	-2.70	1.42	1.51
2	A	501	DMU	C7-C5	-2.54	1.45	1.52
2	A	502	DMU	C8-C9	2.46	1.58	1.53
2	B	502	DMU	O3-C5	2.32	1.48	1.43
2	B	501	DMU	O3-C5	2.31	1.48	1.43
2	A	501	DMU	O5-C6	2.30	1.47	1.41
2	B	502	DMU	C7-C5	-2.22	1.46	1.52
2	B	502	DMU	C8-C7	-2.14	1.46	1.52
2	A	501	DMU	C8-C7	-2.13	1.46	1.52
2	B	502	DMU	O5-C6	2.13	1.47	1.41
2	A	501	DMU	O4-C7	2.12	1.48	1.43
2	B	502	DMU	O55-C2	2.12	1.48	1.43
2	B	501	DMU	O55-C2	2.10	1.47	1.43
2	A	501	DMU	O3-C5	2.09	1.47	1.43
2	B	501	DMU	O5-C6	2.07	1.47	1.41
2	A	501	DMU	O7-C3	2.05	1.49	1.43
2	B	502	DMU	O7-C3	2.03	1.49	1.43
2	B	502	DMU	O4-C7	2.01	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	DMU	O4-C7-C8	-4.21	100.62	110.35
2	A	502	DMU	C6-O5-C4	-3.86	106.11	113.69
2	B	501	DMU	O16-C6-C1	3.37	112.10	108.15
2	A	501	DMU	C11-C9-C8	-3.18	105.55	113.00
2	B	501	DMU	C6-O5-C4	-3.15	107.51	113.69
2	A	502	DMU	O16-C6-C1	2.86	111.50	108.15
2	B	502	DMU	O7-C3-C2	2.47	113.85	107.28
2	B	502	DMU	C10-O7-C3	-2.17	112.60	117.96
2	A	501	DMU	C10-O7-C3	-2.14	112.66	117.96
2	A	502	DMU	O7-C10-O1	-2.14	104.70	110.67

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	C8E	C17-C16-O15-C14
3	A	512	C8E	C16-C17-O18-C19
3	B	518	C8E	C17-C16-O15-C14
3	B	506	C8E	O18-C19-C20-O21
3	B	513	C8E	C7-C8-O9-C10
3	B	504	C8E	O15-C16-C17-O18
3	B	513	C8E	O12-C13-C14-O15
3	A	506	C8E	O12-C13-C14-O15
3	A	508	C8E	O12-C13-C14-O15
3	A	513	C8E	O12-C13-C14-O15
3	B	528	C8E	O15-C16-C17-O18
3	A	503	C8E	O12-C13-C14-O15
3	A	524	C8E	O12-C13-C14-O15
3	B	507	C8E	O12-C13-C14-O15
3	B	516	C8E	O12-C13-C14-O15
3	B	525	C8E	O9-C10-C11-O12
3	B	506	C8E	O12-C13-C14-O15
3	B	517	C8E	O12-C13-C14-O15
3	B	526	C8E	O12-C13-C14-O15
3	A	512	C8E	O18-C19-C20-O21
3	B	507	C8E	O9-C10-C11-O12
3	B	517	C8E	O18-C19-C20-O21
3	B	518	C8E	O18-C19-C20-O21
3	B	525	C8E	O12-C13-C14-O15
3	A	521	C8E	O15-C16-C17-O18
3	A	510	C8E	O12-C13-C14-O15
3	B	506	C8E	C6-C7-C8-O9
3	B	528	C8E	C20-C19-O18-C17

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Mol	Chain	Res	Type	Atoms
3	A	503	C8E	O18-C19-C20-O21
3	A	506	C8E	O18-C19-C20-O21
3	A	521	C8E	O12-C13-C14-O15
3	B	505	C8E	O18-C19-C20-O21
3	B	522	C8E	O15-C16-C17-O18
3	B	522	C8E	O18-C19-C20-O21
2	A	502	DMU	C1-C6-O16-C18
3	B	524	C8E	C2-C3-C4-C5
3	B	525	C8E	C4-C5-C6-C7
3	B	525	C8E	C3-C4-C5-C6
3	A	504	C8E	C3-C4-C5-C6
3	B	504	C8E	O12-C13-C14-O15
3	A	505	C8E	O15-C16-C17-O18
3	B	507	C8E	O18-C19-C20-O21
3	B	513	C8E	C4-C5-C6-C7
3	B	514	C8E	O12-C13-C14-O15
3	A	517	C8E	O9-C10-C11-O12
3	A	505	C8E	C7-C8-O9-C10
3	A	520	C8E	C3-C4-C5-C6
3	B	510	C8E	C4-C5-C6-C7
2	A	502	DMU	O5-C6-O16-C18
3	A	506	C8E	O9-C10-C11-O12
3	B	527	C8E	C5-C6-C7-C8
3	B	523	C8E	C6-C7-C8-O9
3	A	509	C8E	C3-C4-C5-C6
3	B	513	C8E	C6-C7-C8-O9
3	B	518	C8E	O15-C16-C17-O18
3	B	505	C8E	C16-C17-O18-C19
3	B	504	C8E	O18-C19-C20-O21
3	A	522	C8E	C2-C3-C4-C5
3	B	511	C8E	C2-C3-C4-C5
3	B	512	C8E	O18-C19-C20-O21
3	B	528	C8E	O18-C19-C20-O21
3	A	519	C8E	C2-C3-C4-C5
3	B	515	C8E	C2-C3-C4-C5
3	A	510	C8E	C17-C16-O15-C14
3	B	513	C8E	C3-C4-C5-C6
3	A	510	C8E	C7-C8-O9-C10
3	A	511	C8E	C4-C5-C6-C7
3	A	510	C8E	C6-C7-C8-O9
3	B	503	C8E	O12-C13-C14-O15
3	A	509	C8E	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	511	C8E	C3-C4-C5-C6
3	A	519	C8E	C4-C5-C6-C7
3	A	508	C8E	O15-C16-C17-O18
3	A	523	C8E	C10-C11-O12-C13
3	B	515	C8E	C3-C4-C5-C6
3	A	512	C8E	C17-C16-O15-C14
3	B	526	C8E	C17-C16-O15-C14
3	A	516	C8E	C3-C4-C5-C6
3	A	516	C8E	C2-C3-C4-C5
3	A	524	C8E	C14-C13-O12-C11
3	A	510	C8E	O18-C19-C20-O21
3	B	524	C8E	C7-C8-O9-C10
3	A	506	C8E	C13-C14-O15-C16
3	B	516	C8E	C13-C14-O15-C16
3	A	506	C8E	C16-C17-O18-C19
3	B	514	C8E	C10-C11-O12-C13
3	A	503	C8E	C20-C19-O18-C17
3	A	521	C8E	C13-C14-O15-C16
3	B	528	C8E	C16-C17-O18-C19
3	A	505	C8E	C17-C16-O15-C14
3	A	512	C8E	C20-C19-O18-C17
3	B	506	C8E	C13-C14-O15-C16
3	B	517	C8E	C13-C14-O15-C16
3	A	513	C8E	C13-C14-O15-C16
3	A	503	C8E	C13-C14-O15-C16
3	B	506	C8E	C20-C19-O18-C17
3	B	506	C8E	C10-C11-O12-C13
3	A	510	C8E	C10-C11-O12-C13
3	A	508	C8E	C10-C11-O12-C13
3	B	503	C8E	C16-C17-O18-C19
3	A	507	C8E	O18-C19-C20-O21
3	A	521	C8E	C16-C17-O18-C19
3	B	506	C8E	C17-C16-O15-C14
3	B	506	C8E	C7-C8-O9-C10
3	B	513	C8E	C16-C17-O18-C19
3	B	517	C8E	C10-C11-O12-C13
3	B	525	C8E	C10-C11-O12-C13
3	A	507	C8E	C16-C17-O18-C19
3	B	504	C8E	C13-C14-O15-C16
3	B	509	C8E	C2-C3-C4-C5
3	B	504	C8E	C10-C11-O12-C13
3	A	523	C8E	C20-C19-O18-C17

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Mol	Chain	Res	Type	Atoms
3	B	512	C8E	C20-C19-O18-C17
3	B	514	C8E	C11-C10-O9-C8
3	A	503	C8E	C16-C17-O18-C19
3	A	513	C8E	C14-C13-O12-C11
3	B	526	C8E	C10-C11-O12-C13
3	A	523	C8E	O15-C16-C17-O18
3	B	525	C8E	C6-C7-C8-O9
3	B	523	C8E	C7-C8-O9-C10
3	B	525	C8E	C7-C8-O9-C10
3	A	524	C8E	O9-C10-C11-O12
3	A	510	C8E	C11-C10-O9-C8
3	B	503	C8E	C10-C11-O12-C13
3	A	523	C8E	O12-C13-C14-O15
3	B	518	C8E	C20-C19-O18-C17
3	A	506	C8E	C17-C16-O15-C14
3	A	505	C8E	C3-C4-C5-C6
3	A	513	C8E	C16-C17-O18-C19
3	B	517	C8E	C20-C19-O18-C17
3	A	525	C8E	O15-C16-C17-O18
3	B	518	C8E	C13-C14-O15-C16
3	B	508	C8E	C4-C5-C6-C7
3	A	503	C8E	C10-C11-O12-C13
3	A	525	C8E	C20-C19-O18-C17
3	A	503	C8E	O9-C10-C11-O12
3	A	513	C8E	C20-C19-O18-C17
3	A	510	C8E	C3-C4-C5-C6
3	B	516	C8E	C17-C16-O15-C14
3	B	506	C8E	C2-C3-C4-C5
3	A	505	C8E	C2-C3-C4-C5
3	B	507	C8E	O15-C16-C17-O18
3	B	517	C8E	O15-C16-C17-O18
3	B	522	C8E	C20-C19-O18-C17
3	A	522	C8E	C4-C5-C6-C7
3	B	526	C8E	C11-C10-O9-C8
3	B	511	C8E	C4-C5-C6-C7
3	A	513	C8E	O15-C16-C17-O18
3	B	509	C8E	C4-C5-C6-C7
3	B	526	C8E	O9-C10-C11-O12
3	B	512	C8E	O9-C10-C11-O12
3	B	504	C8E	C16-C17-O18-C19
3	B	528	C8E	C17-C16-O15-C14
3	A	521	C8E	C20-C19-O18-C17

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Mol	Chain	Res	Type	Atoms
3	B	525	C8E	C2-C3-C4-C5
3	A	510	C8E	C20-C19-O18-C17
3	B	513	C8E	C1-C2-C3-C4
2	B	501	DMU	O6-C11-C9-O1
3	A	518	C8E	C4-C5-C6-C7
3	B	510	C8E	C3-C4-C5-C6
3	B	527	C8E	C6-C7-C8-O9
3	A	505	C8E	C13-C14-O15-C16
3	B	518	C8E	C10-C11-O12-C13
3	B	506	C8E	O9-C10-C11-O12
3	B	517	C8E	C17-C16-O15-C14
3	B	518	C8E	O9-C10-C11-O12
3	B	526	C8E	O15-C16-C17-O18
3	B	504	C8E	O9-C10-C11-O12
3	B	505	C8E	O15-C16-C17-O18
3	A	510	C8E	C4-C5-C6-C7
3	B	516	C8E	O9-C10-C11-O12
3	B	528	C8E	C14-C13-O12-C11
3	A	503	C8E	O15-C16-C17-O18
3	B	503	C8E	O15-C16-C17-O18
3	A	518	C8E	C2-C3-C4-C5
3	B	525	C8E	C11-C10-O9-C8
3	B	513	C8E	O9-C10-C11-O12
3	A	508	C8E	C14-C13-O12-C11
3	A	510	C8E	O9-C10-C11-O12
3	B	513	C8E	O15-C16-C17-O18
3	B	514	C8E	O9-C10-C11-O12
3	B	513	C8E	C10-C11-O12-C13
3	A	506	C8E	O15-C16-C17-O18
3	B	504	C8E	C20-C19-O18-C17
3	A	510	C8E	O15-C16-C17-O18
3	A	503	C8E	C11-C10-O9-C8
3	A	507	C8E	C20-C19-O18-C17

There are no ring outliers.

27 monomers are involved in 51 short contacts:

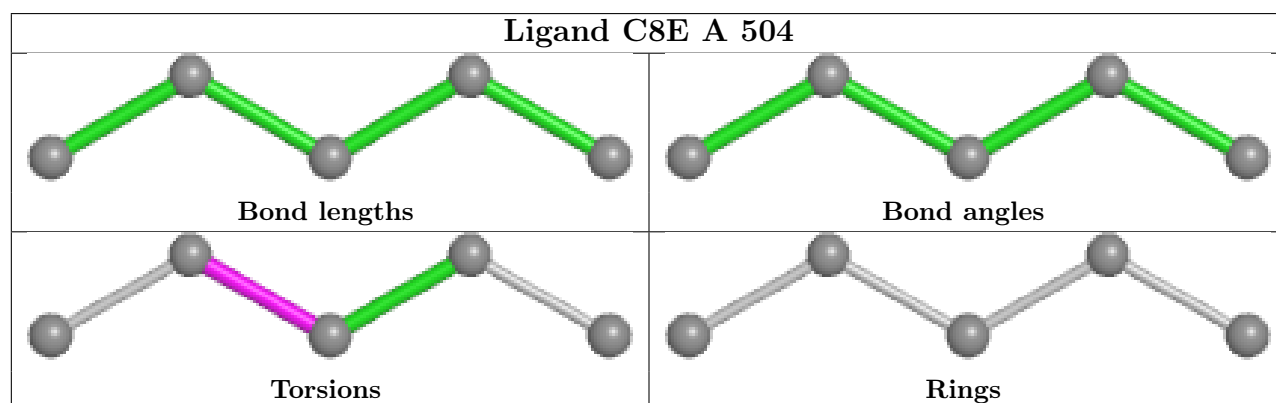
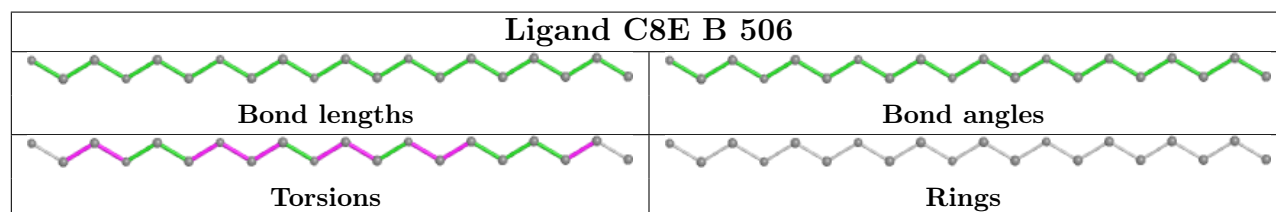
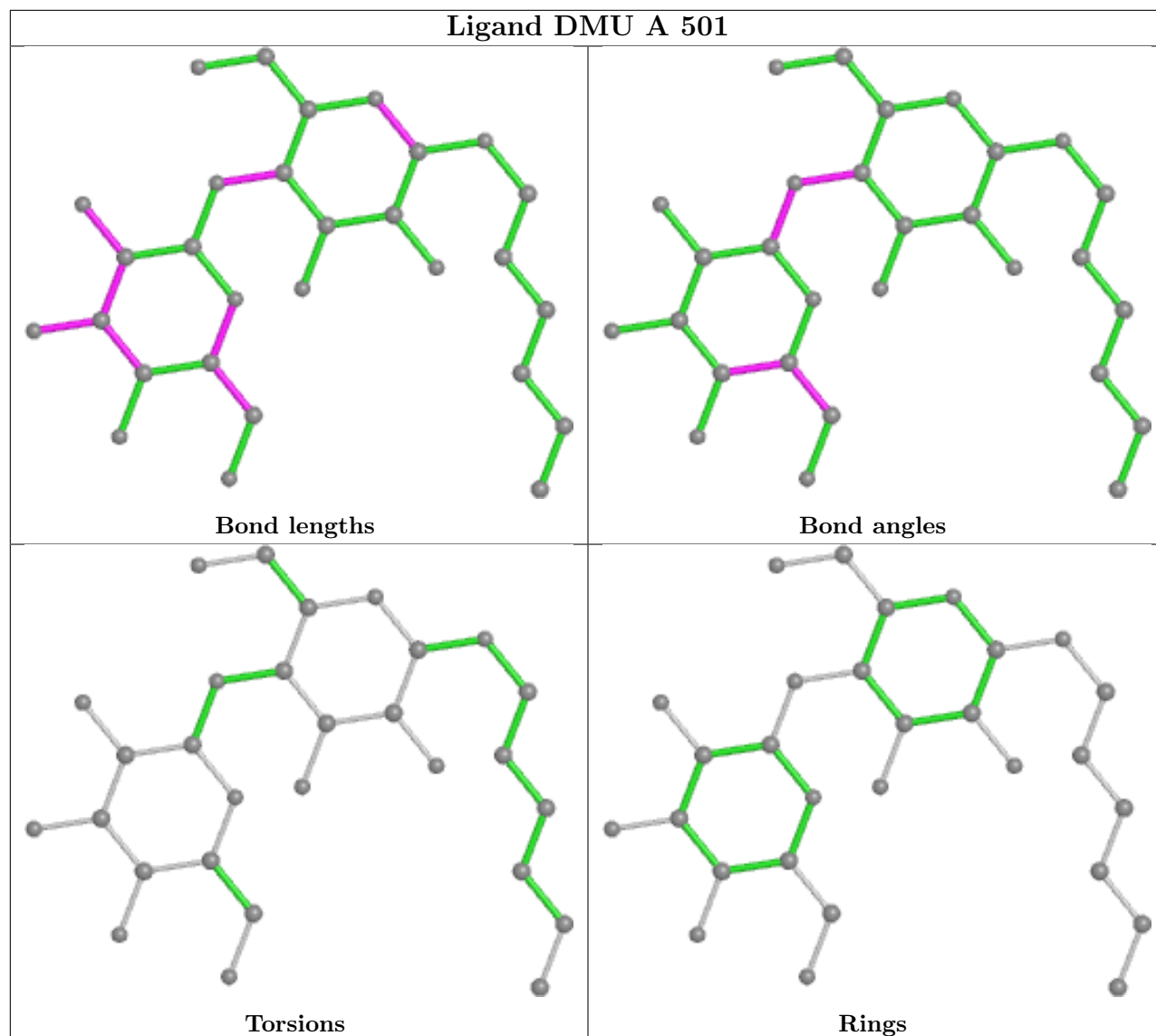
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	506	C8E	3	0
3	B	507	C8E	1	0
3	B	509	C8E	3	0
3	A	521	C8E	4	0

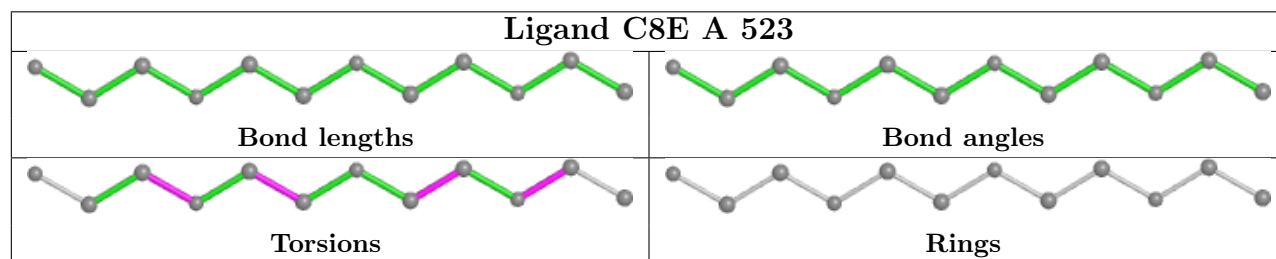
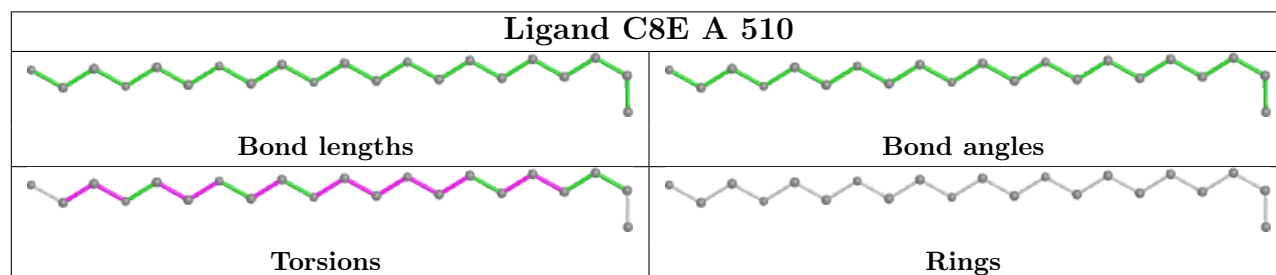
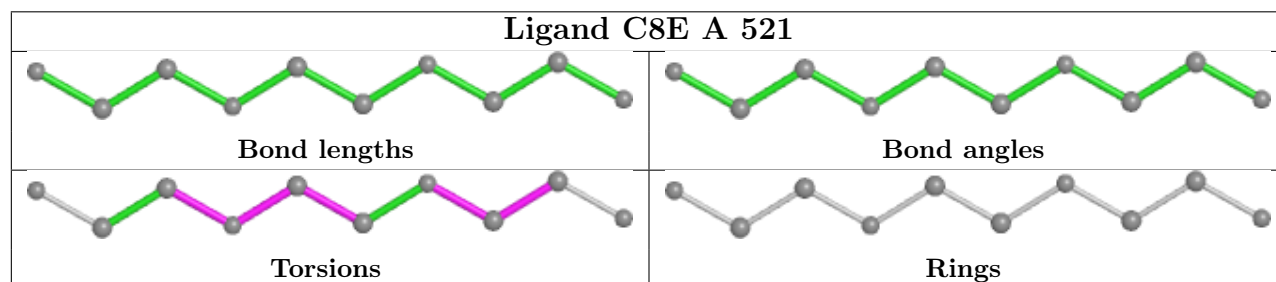
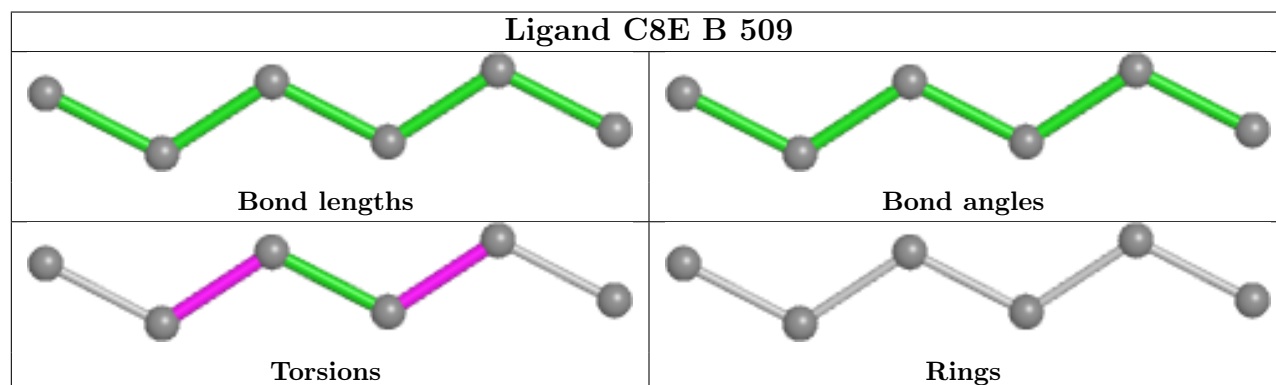
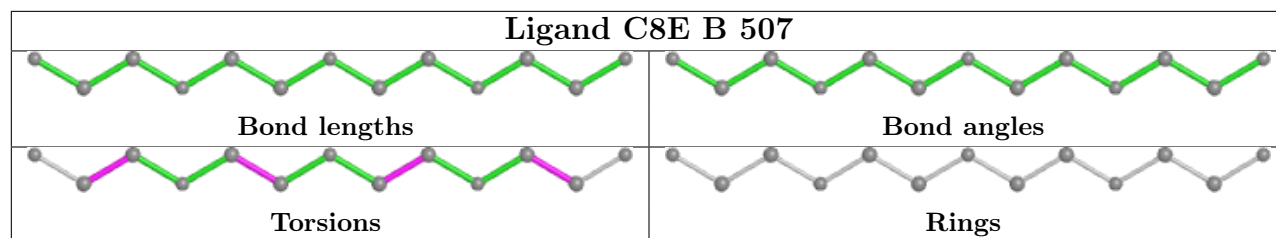
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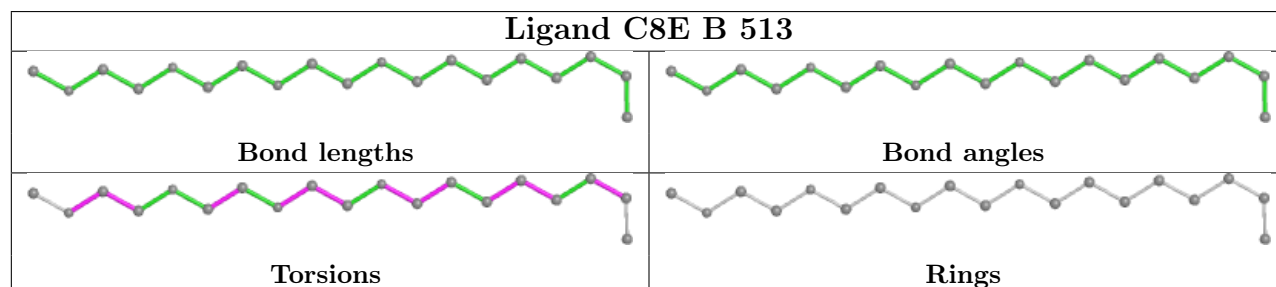
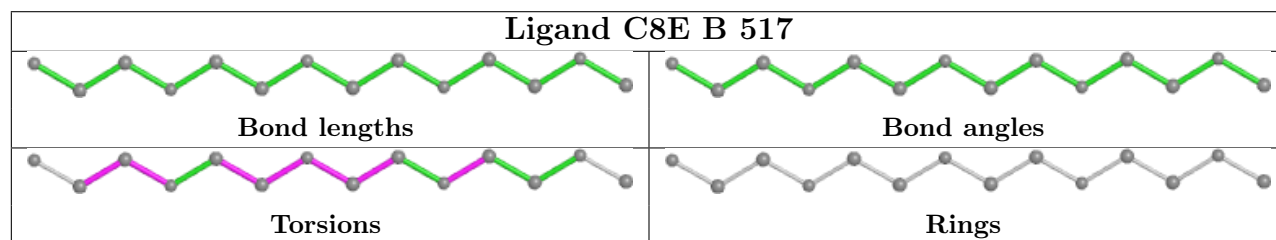
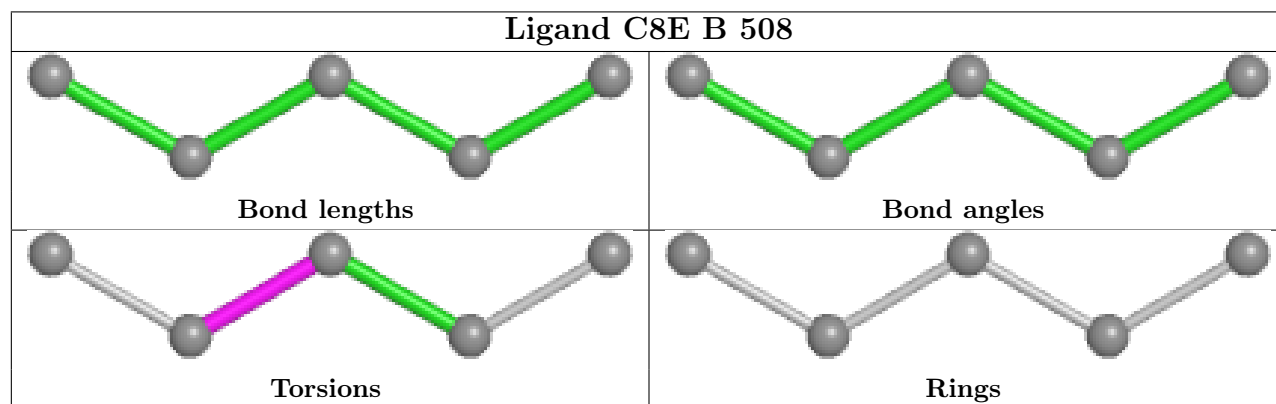
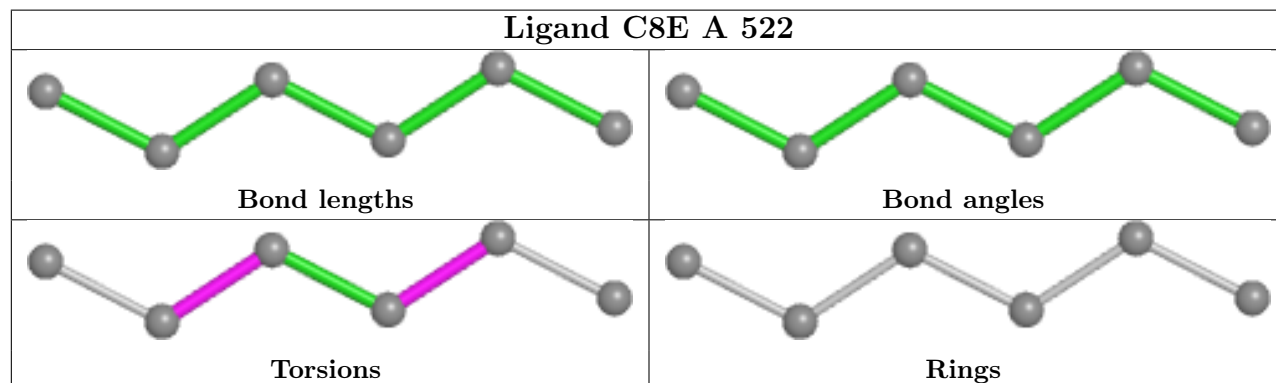
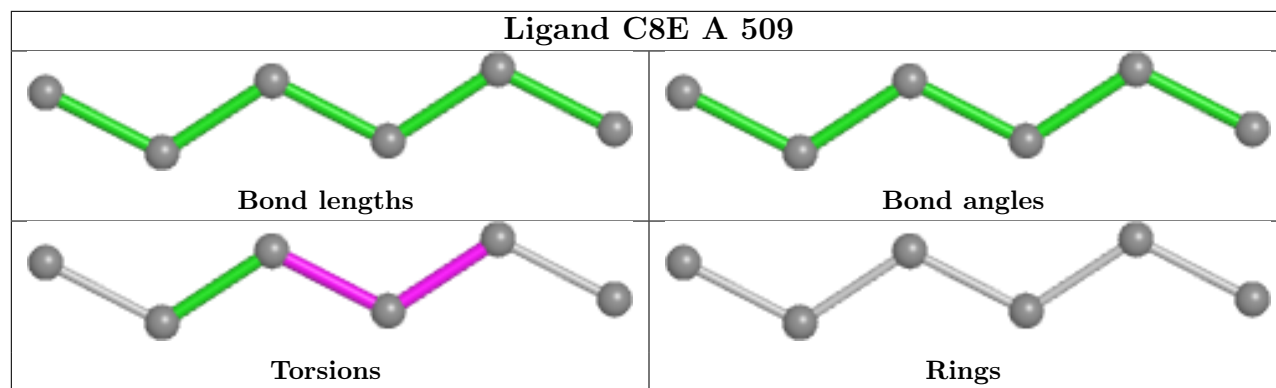
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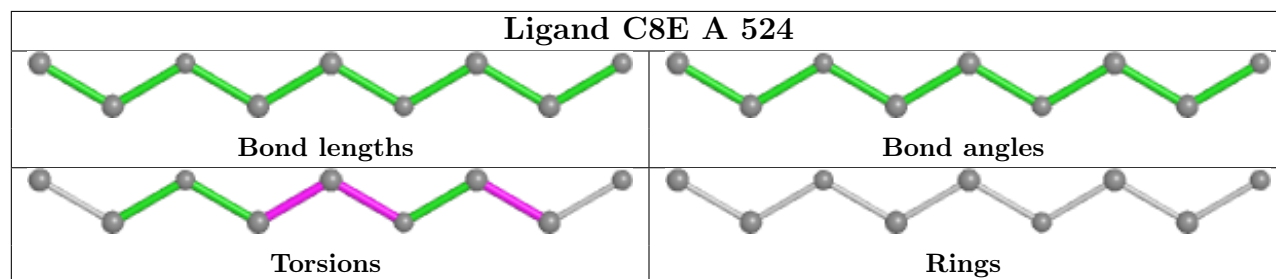
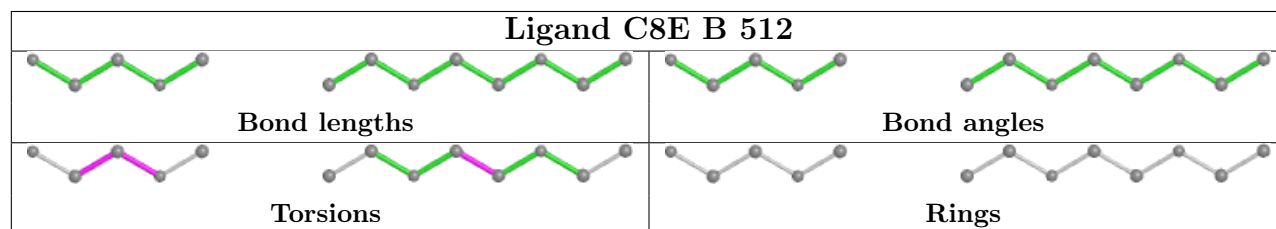
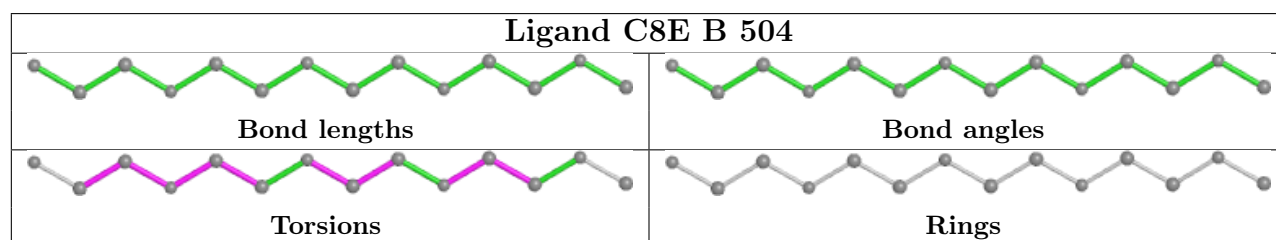
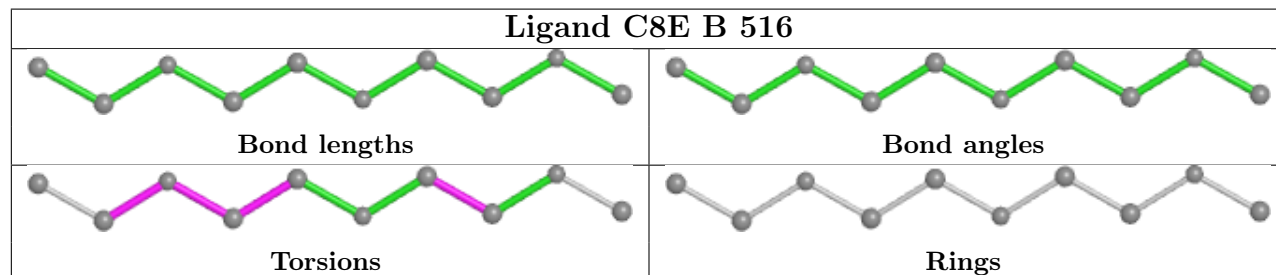
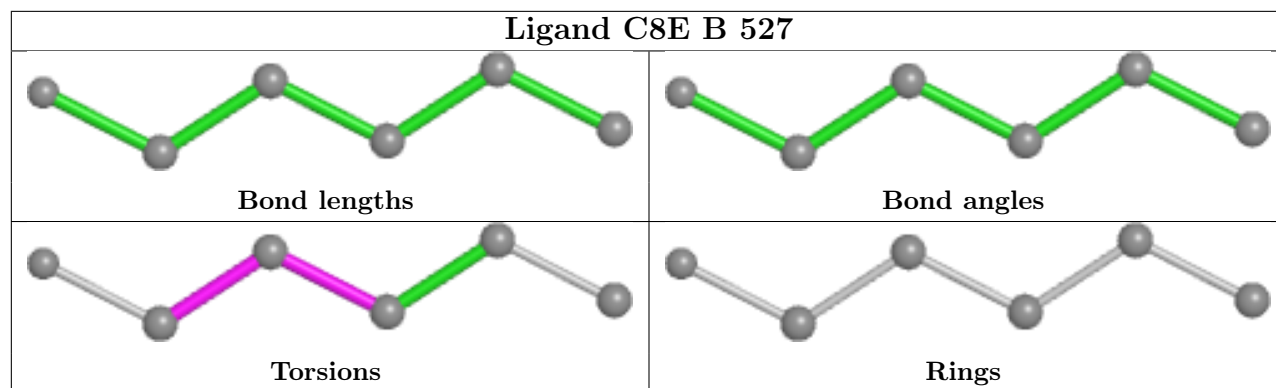
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	C8E	2	0
3	A	522	C8E	3	0
3	B	517	C8E	1	0
3	B	527	C8E	1	0
3	B	512	C8E	4	0
3	A	524	C8E	4	0
3	B	510	C8E	1	0
3	B	518	C8E	1	0
3	B	519	C8E	1	0
3	B	525	C8E	4	0
3	A	511	C8E	1	0
3	A	506	C8E	2	0
3	A	505	C8E	1	0
3	B	523	C8E	1	0
3	B	503	C8E	2	0
2	A	502	DMU	1	0
3	A	517	C8E	1	0
3	A	503	C8E	2	0
3	A	513	C8E	1	0
3	A	512	C8E	2	0
3	A	525	C8E	1	0
3	B	528	C8E	6	0
3	B	511	C8E	1	0

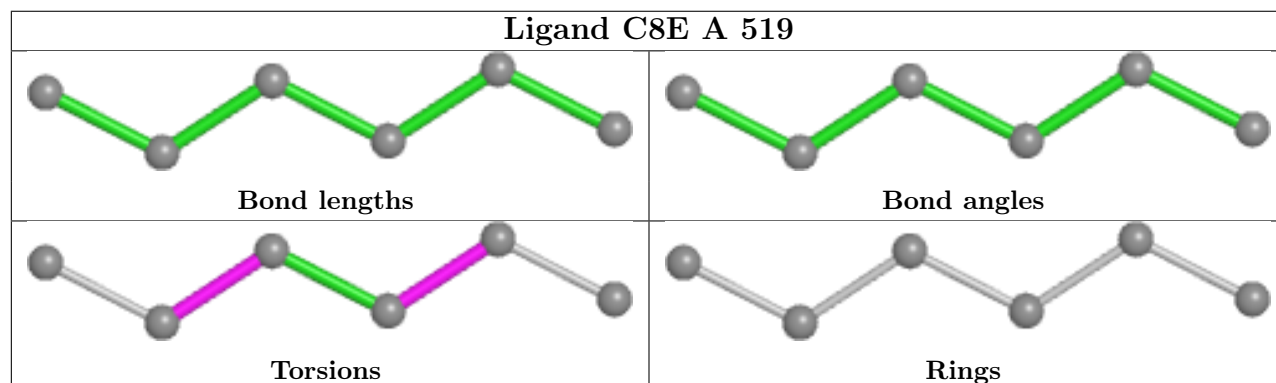
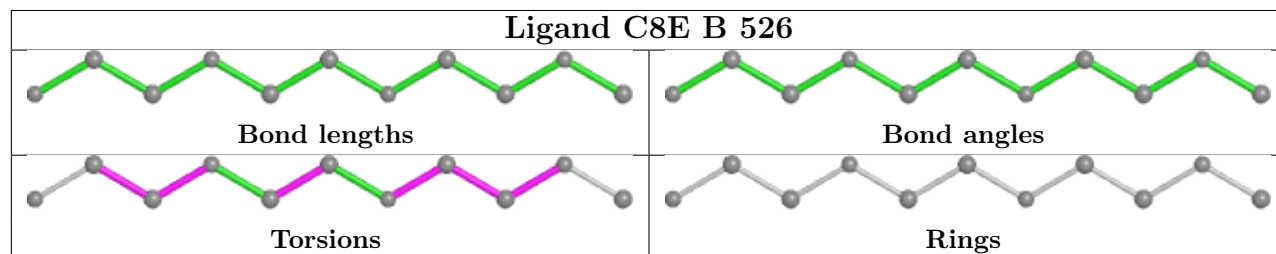
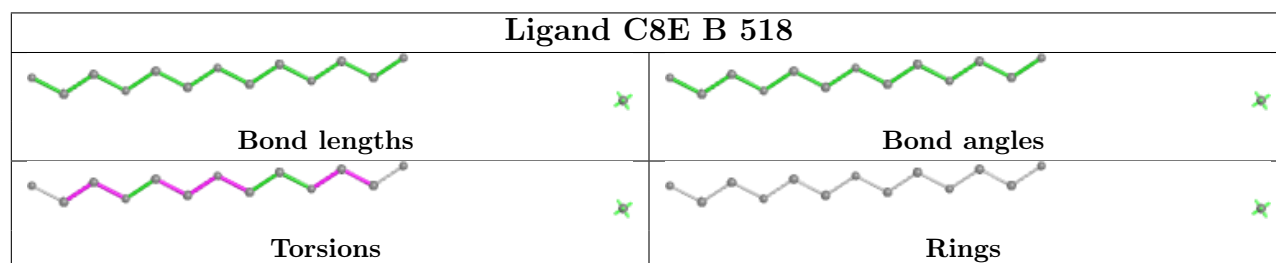
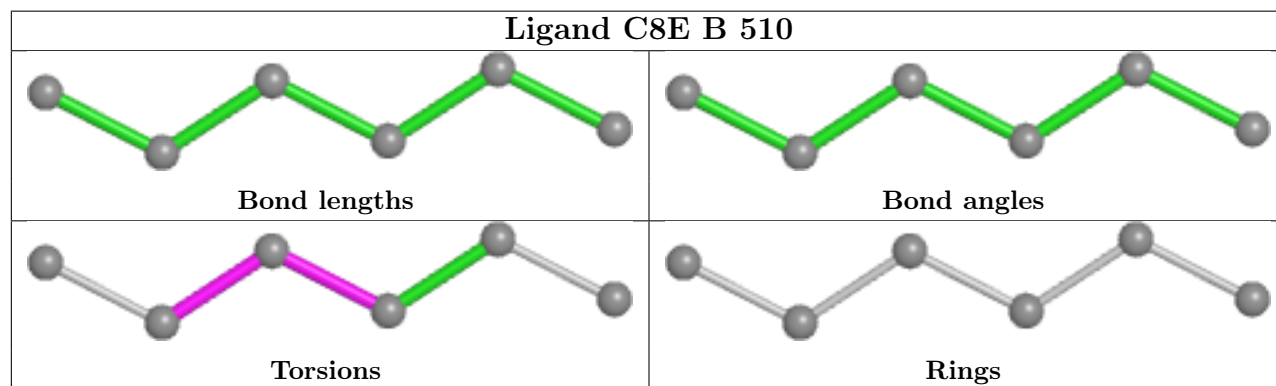
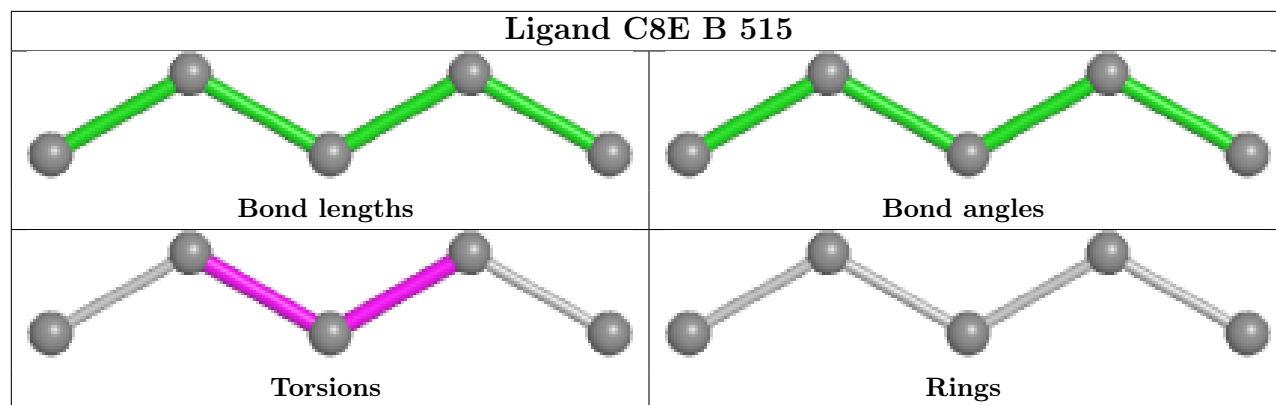
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

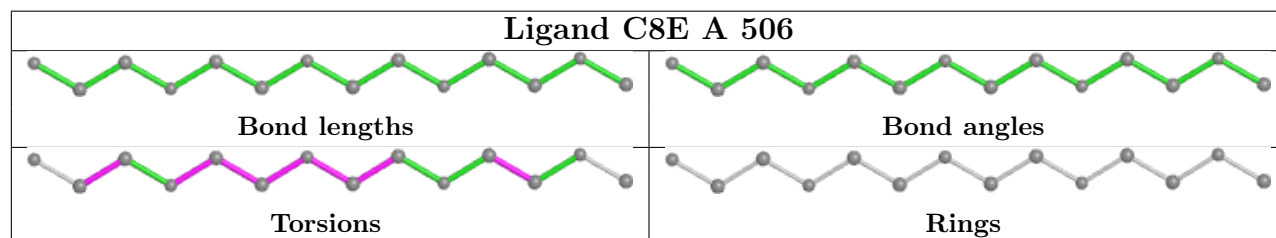
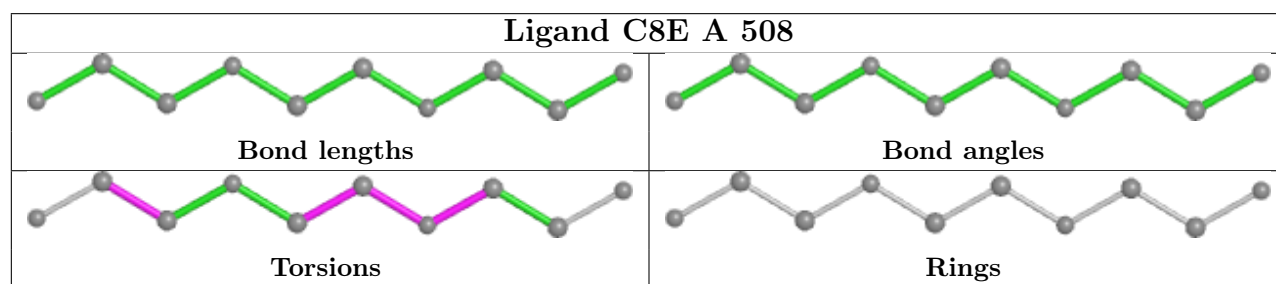
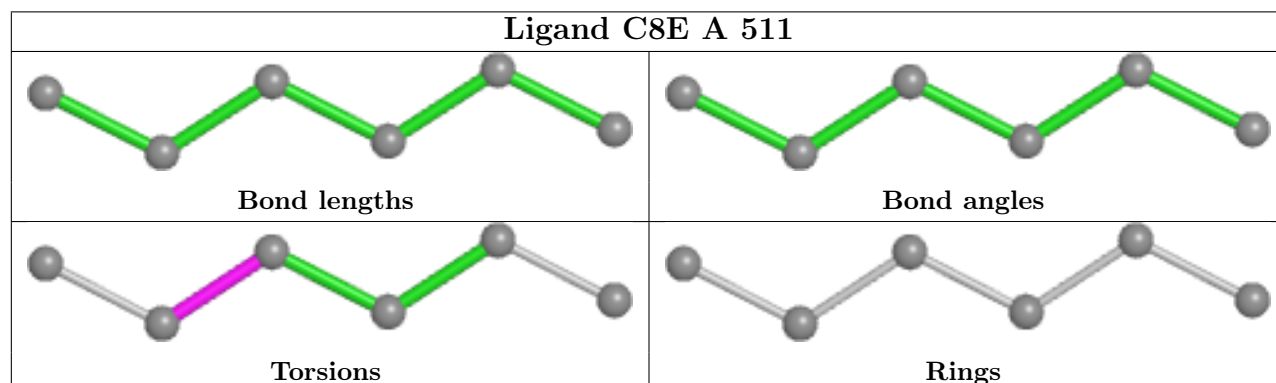
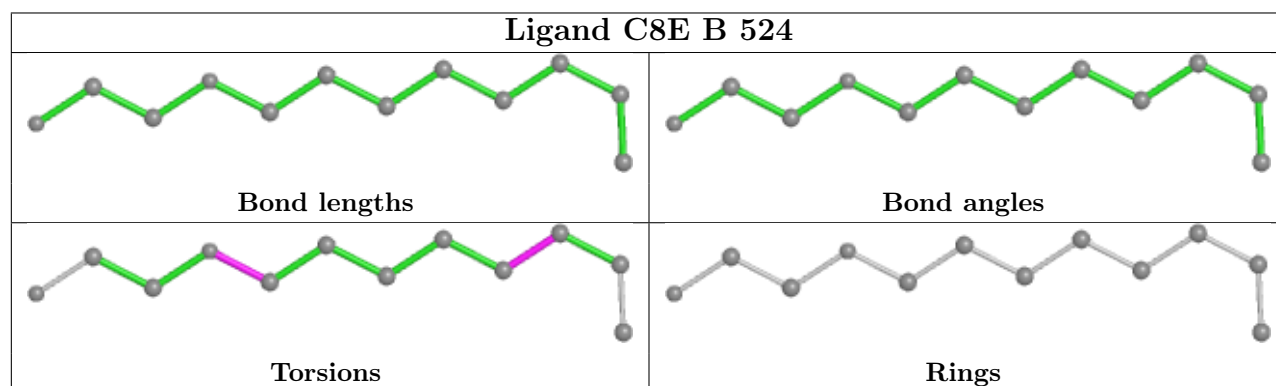
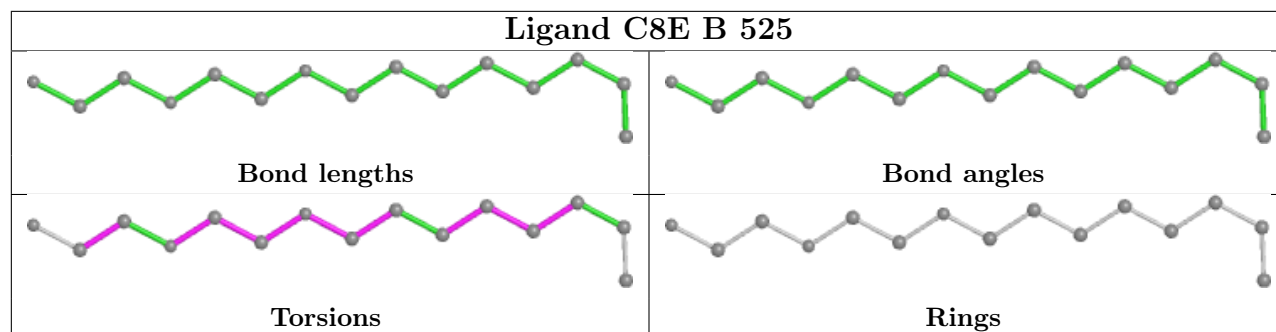


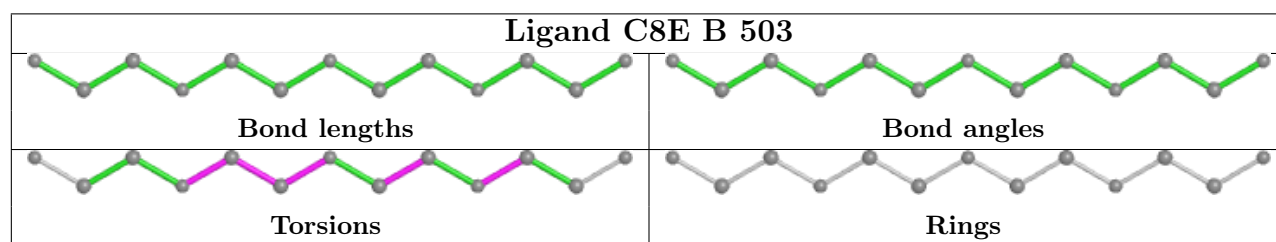
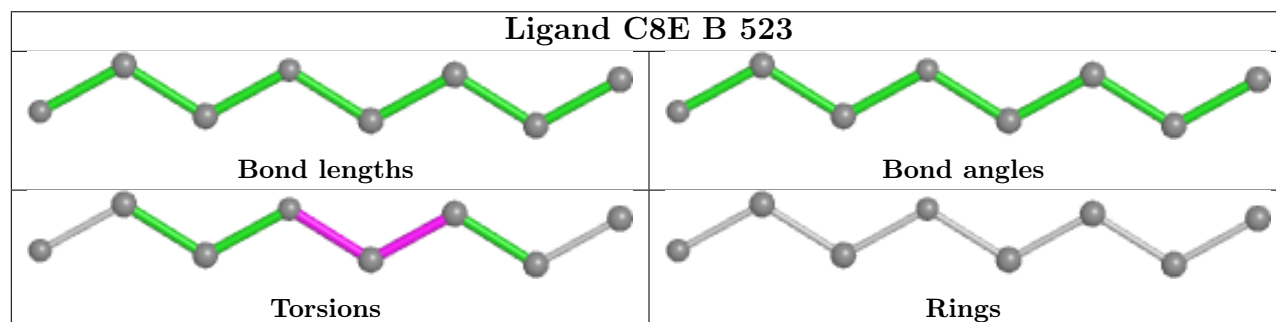
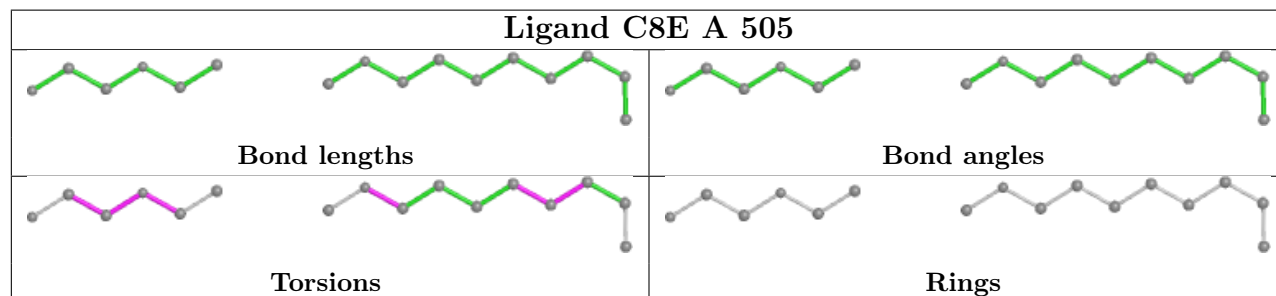
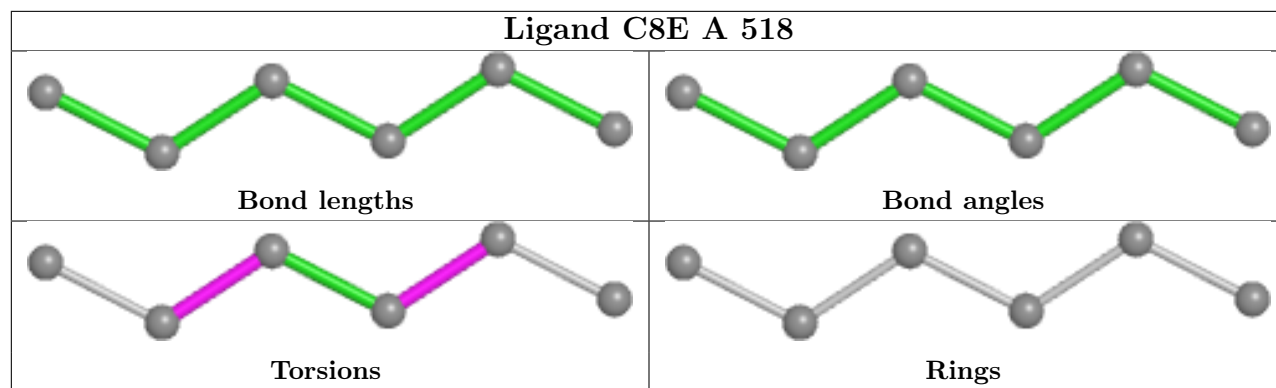




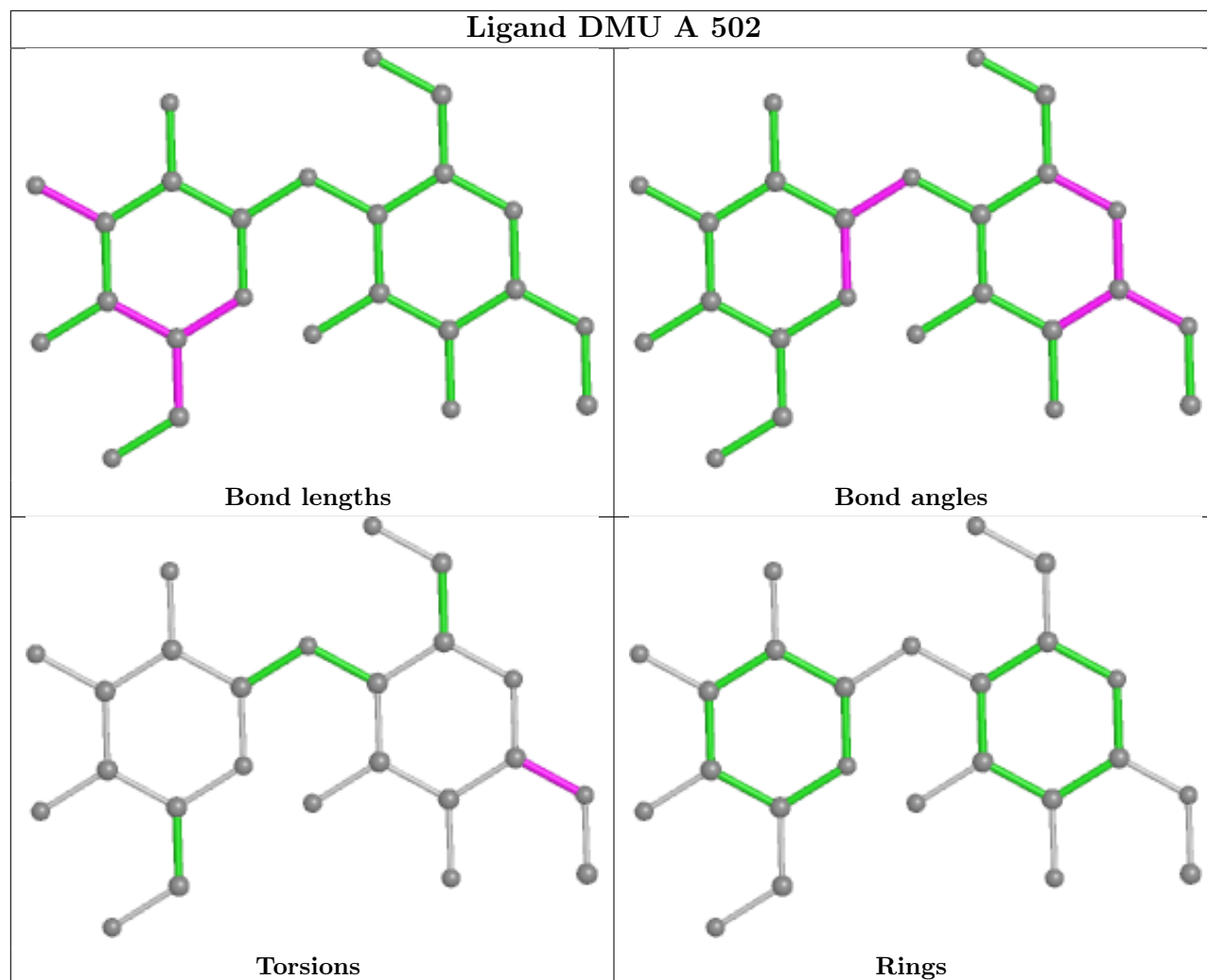




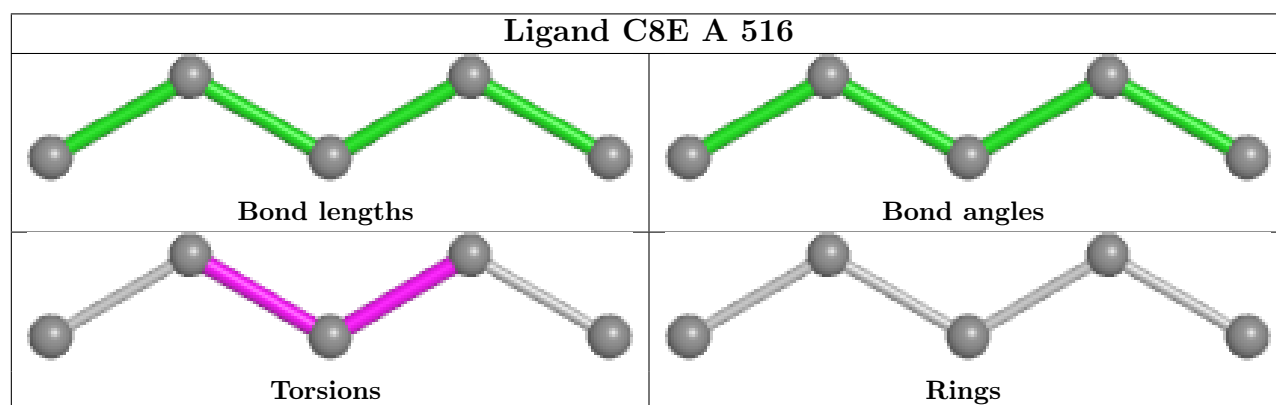


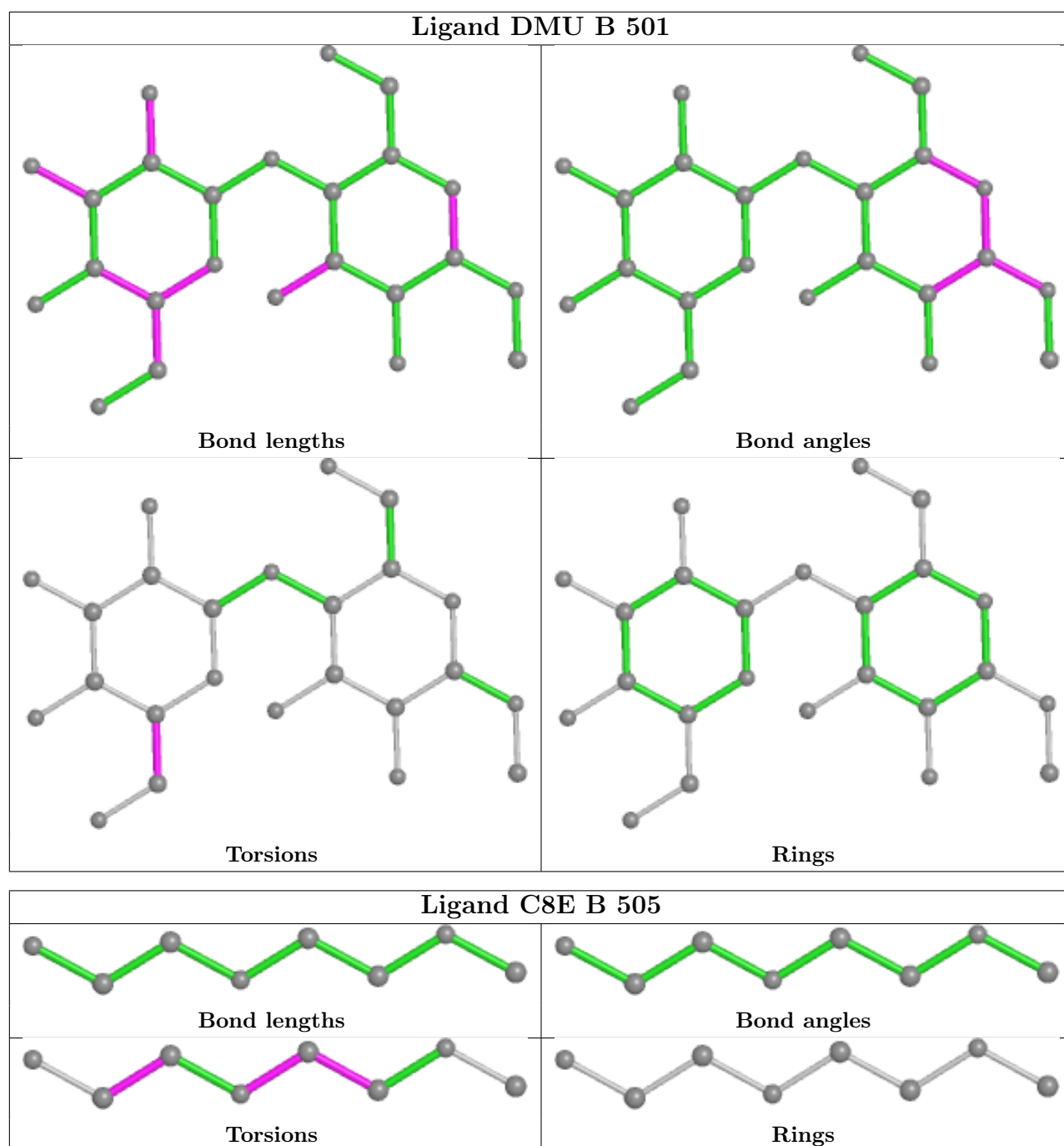


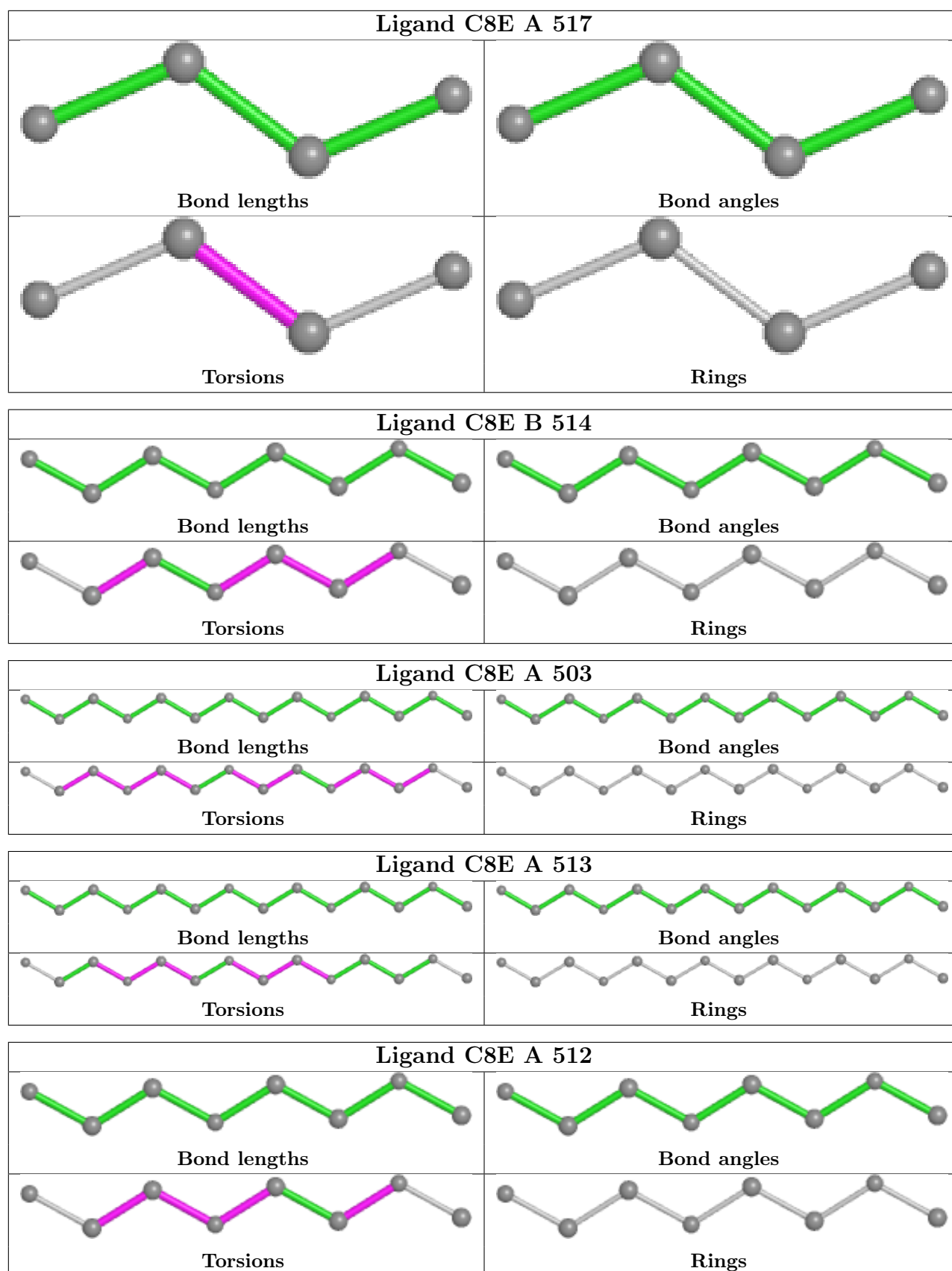
Ligand DMU A 502

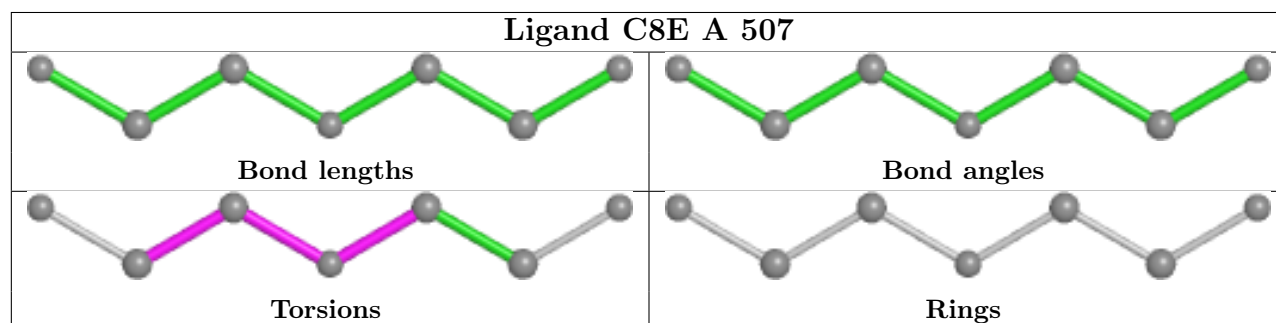
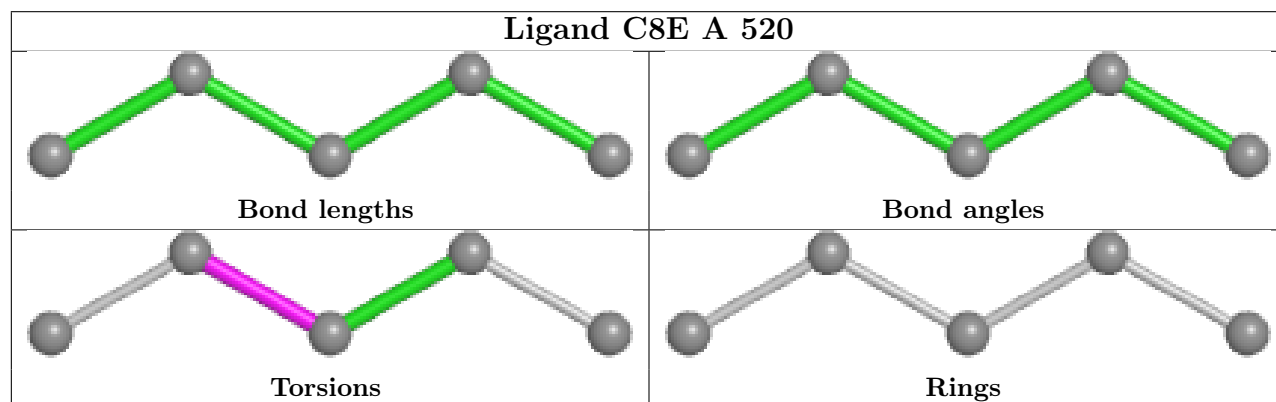
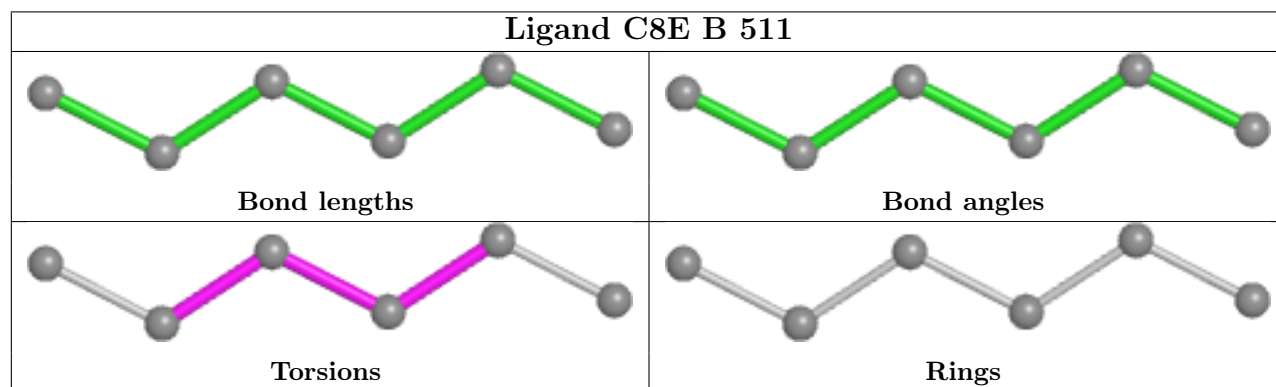
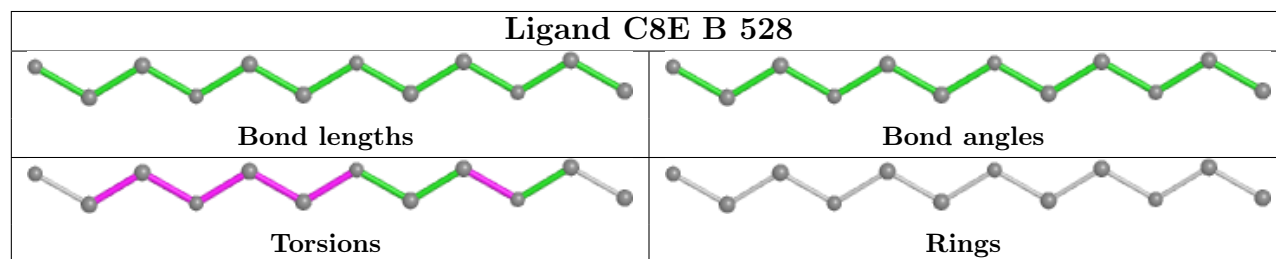
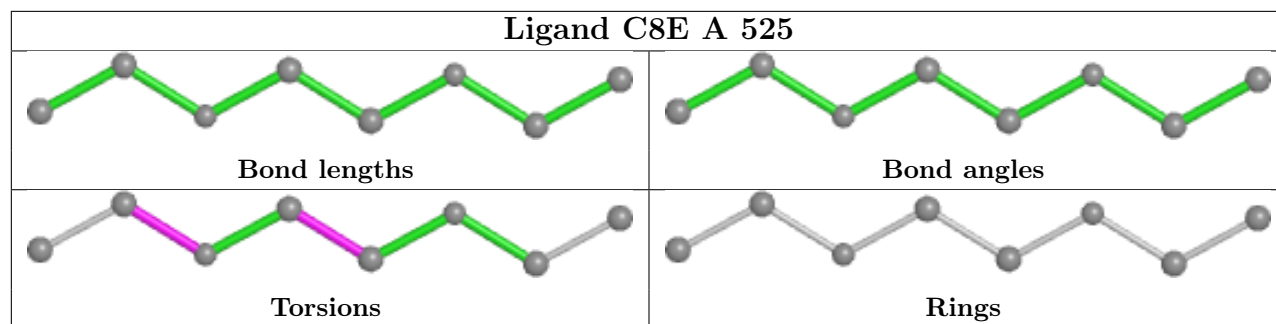


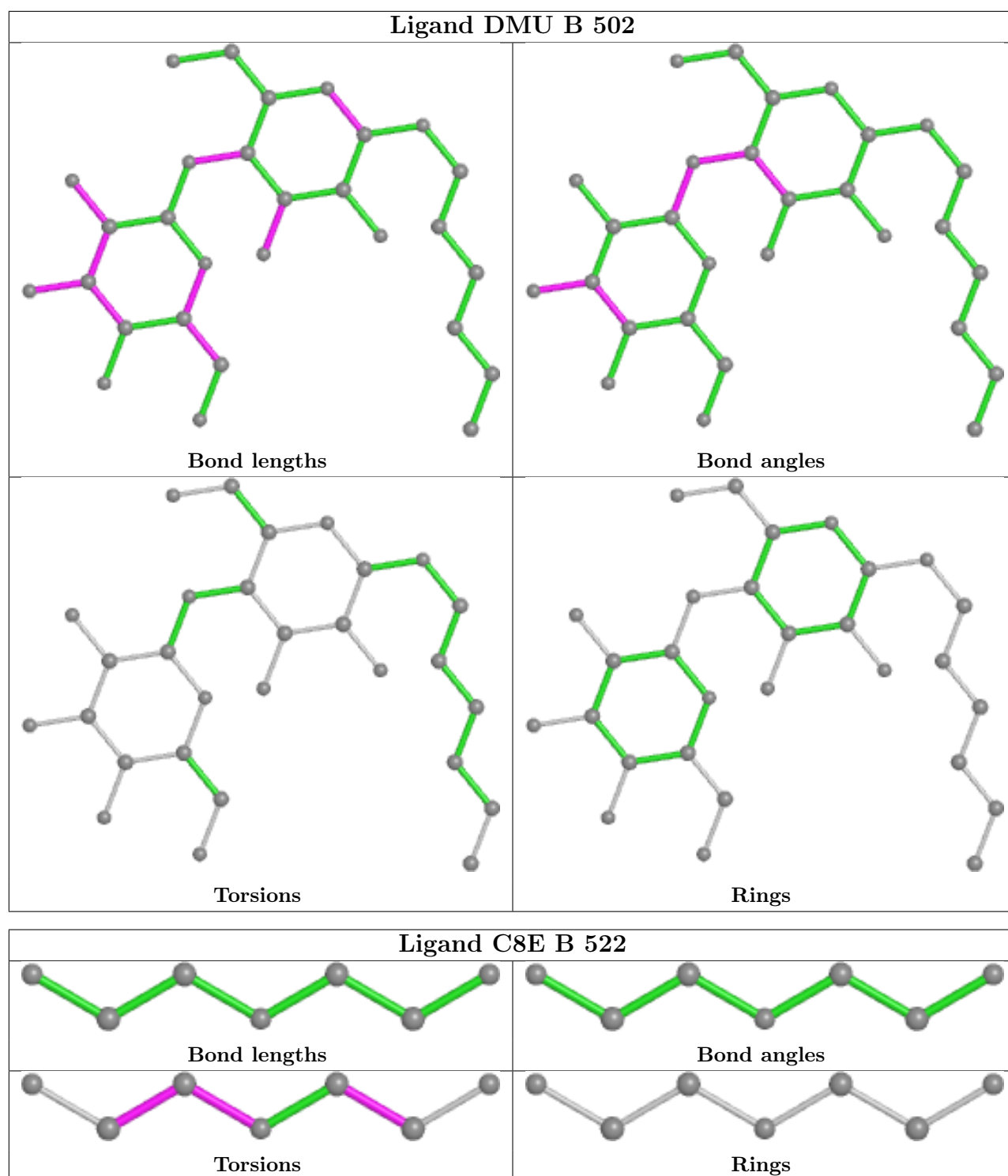
Ligand C8E A 516











5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	435/442 (98%)	-0.30	2 (0%) 91 91	16, 29, 56, 132	0
1	B	435/442 (98%)	-0.41	0 100 100	15, 26, 45, 120	0
All	All	870/884 (98%)	-0.35	2 (0%) 95 94	15, 27, 52, 132	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	ARG	2.9
1	A	26	THR	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C8E	B	513	19/21	0.60	0.35	37,52,63,65	0
3	C8E	B	523	8/21	0.62	0.34	44,50,61,62	0
3	C8E	A	510	21/21	0.64	0.42	40,60,73,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C8E	A	525	8/21	0.64	0.21	54,59,67,69	0
3	C8E	B	517	14/21	0.65	0.34	34,60,76,79	0
3	C8E	A	511	6/21	0.65	0.15	36,40,43,44	0
3	C8E	A	509	6/21	0.69	0.14	41,49,51,51	0
3	C8E	A	516	5/21	0.70	0.15	39,47,47,48	0
3	C8E	B	527	6/21	0.71	0.20	60,74,76,78	0
3	C8E	B	506	20/21	0.72	0.33	37,53,61,62	0
3	C8E	B	511	6/21	0.72	0.16	42,52,54,59	0
3	C8E	A	513	14/21	0.72	0.38	53,68,73,80	0
3	C8E	A	512	8/21	0.73	0.24	48,54,57,59	0
3	C8E	A	524	9/21	0.74	0.17	48,59,64,69	0
3	C8E	B	507	13/21	0.75	0.29	49,53,58,59	0
3	C8E	B	521	4/21	0.75	0.28	54,55,57,58	0
3	C8E	B	504	14/21	0.75	0.36	51,64,70,71	0
3	C8E	B	525	15/21	0.75	0.18	40,59,75,76	0
3	C8E	A	506	14/21	0.75	0.24	35,56,64,65	0
3	C8E	B	505	8/21	0.76	0.28	53,57,64,65	0
3	C8E	B	515	5/21	0.77	0.35	48,48,52,53	0
3	C8E	B	524	12/21	0.77	0.16	36,46,64,64	0
3	C8E	B	512	13/21	0.77	0.13	41,53,58,64	0
3	C8E	A	520	5/21	0.77	0.20	41,42,47,47	0
3	C8E	A	521	10/21	0.78	0.27	29,40,49,50	0
3	C8E	B	509	6/21	0.78	0.12	39,45,47,48	0
3	C8E	A	518	6/21	0.78	0.15	42,43,45,46	0
3	C8E	A	505	16/21	0.78	0.20	46,52,58,59	0
3	C8E	A	503	14/21	0.79	0.32	33,55,75,82	0
3	C8E	A	523	12/21	0.79	0.20	37,48,54,55	0
3	C8E	B	503	13/21	0.79	0.27	33,44,62,69	0
3	C8E	A	504	5/21	0.80	0.15	47,47,49,54	0
3	C8E	B	510	6/21	0.80	0.12	37,38,41,43	0
3	C8E	B	516	10/21	0.80	0.27	52,56,59,63	0
3	C8E	B	514	8/21	0.81	0.28	36,45,52,54	0
3	C8E	B	508	5/21	0.81	0.15	32,35,37,40	0
3	C8E	B	526	11/21	0.81	0.25	45,56,61,65	0
3	C8E	A	522	6/21	0.81	0.26	48,49,50,50	0
3	C8E	A	508	10/21	0.82	0.24	44,52,64,73	0
3	C8E	B	518	14/21	0.82	0.24	37,51,61,63	0
3	C8E	B	522	7/21	0.84	0.17	39,53,57,60	0
3	C8E	A	519	6/21	0.84	0.15	37,40,43,47	0
3	C8E	A	507	7/21	0.85	0.28	37,41,50,51	0
3	C8E	A	514	4/21	0.87	0.23	30,30,34,36	0
4	MG	B	532	1/1	0.87	0.07	45,45,45,45	0

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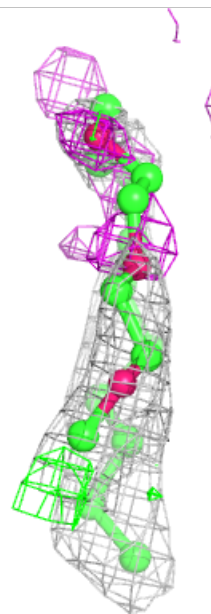
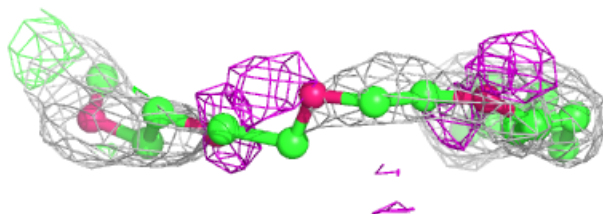
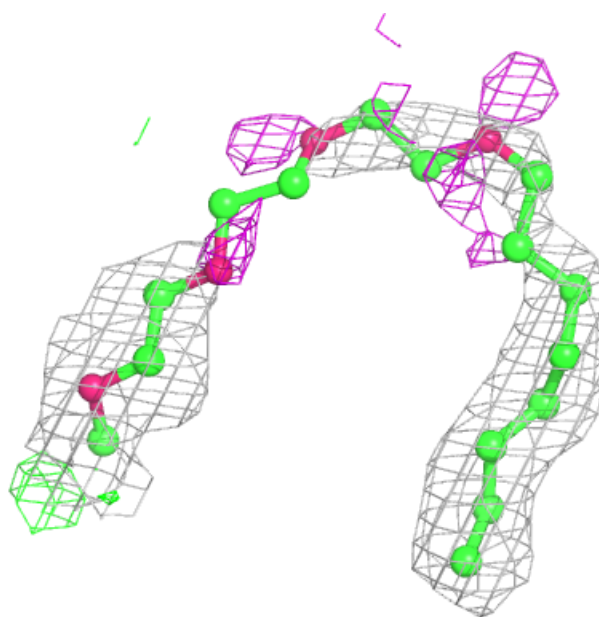
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C8E	A	517	4/21	0.88	0.19	34,34,39,43	0
3	C8E	B	528	12/21	0.89	0.26	43,63,89,90	0
4	MG	B	529	1/1	0.91	0.13	30,30,30,30	0
4	MG	B	533	1/1	0.91	0.07	49,49,49,49	0
3	C8E	B	519	4/21	0.93	0.12	26,32,33,46	0
4	MG	A	528	1/1	0.94	0.09	30,30,30,30	0
4	MG	B	531	1/1	0.94	0.17	35,35,35,35	0
4	MG	A	527	1/1	0.95	0.17	37,37,37,37	0
2	DMU	B	501	24/33	0.95	0.09	19,29,38,44	0
2	DMU	A	502	24/33	0.95	0.08	23,31,42,48	0
3	C8E	A	515	4/21	0.96	0.09	31,32,37,38	0
3	C8E	B	520	4/21	0.96	0.14	27,31,35,36	0
2	DMU	A	501	29/33	0.96	0.08	19,25,36,42	0
2	DMU	B	502	29/33	0.96	0.09	17,23,30,36	0
4	MG	B	530	1/1	0.98	0.07	28,28,28,28	0
4	MG	A	526	1/1	0.98	0.03	46,46,46,46	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.

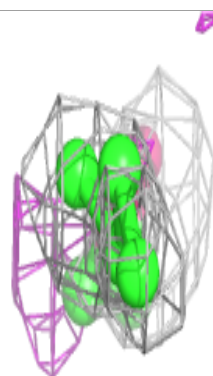
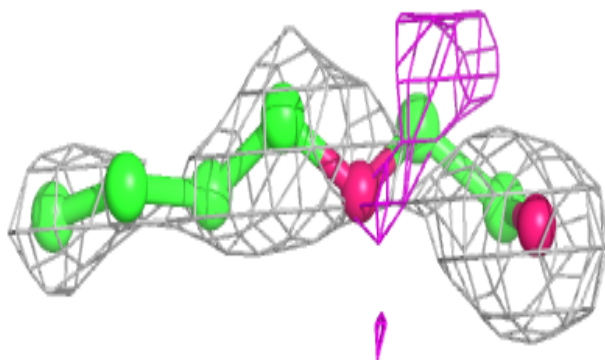
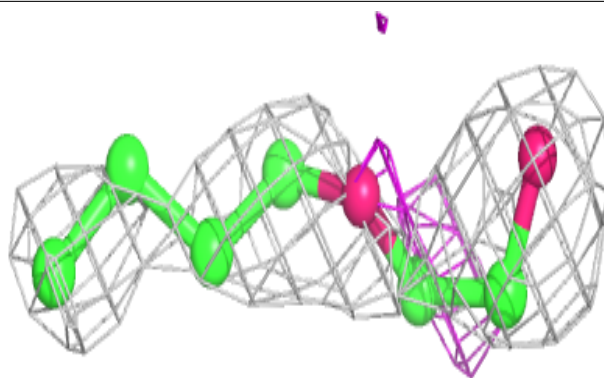
Electron density around C8E B 513:

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



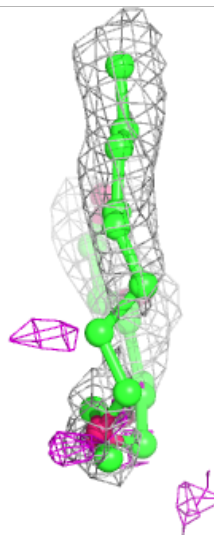
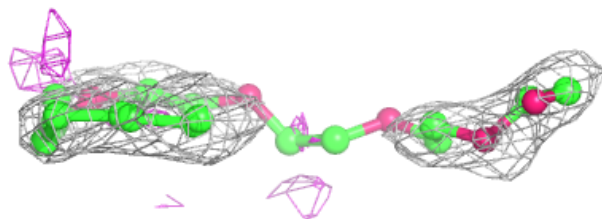
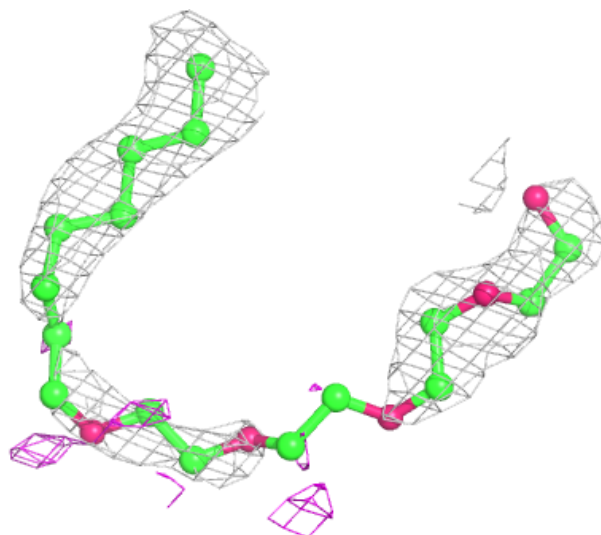
Electron density around C8E B 523:

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



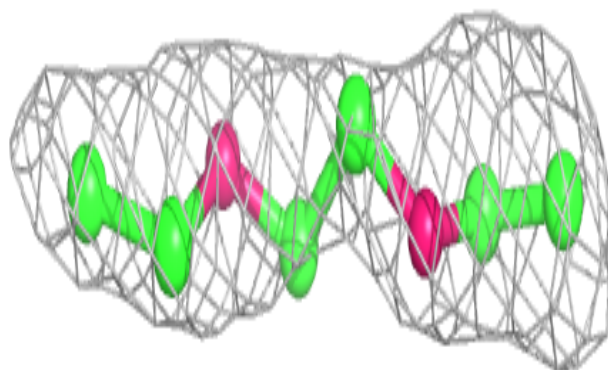
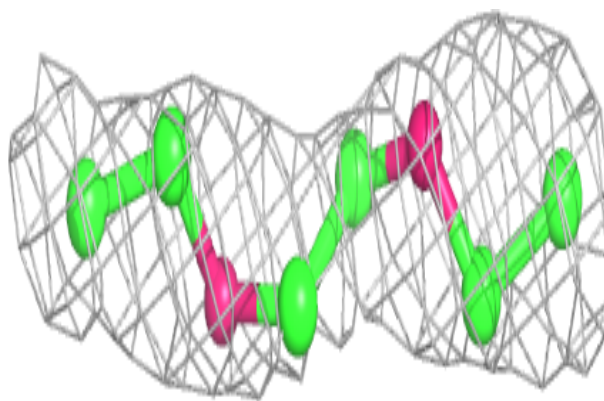
Electron density around C8E A 510:

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

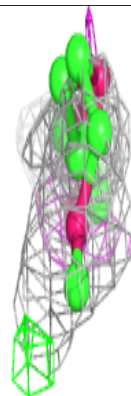
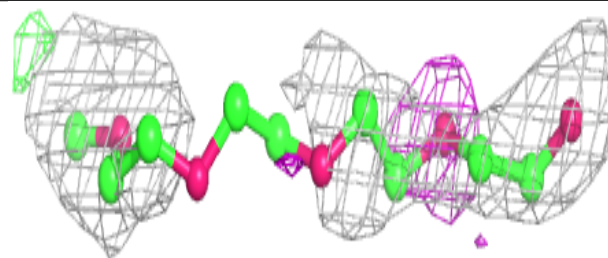
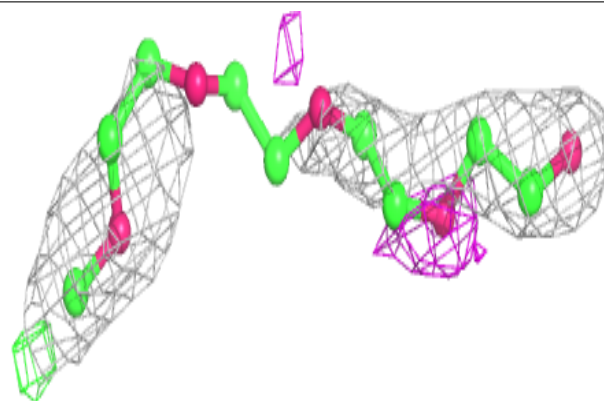


Electron density around C8E A 525:

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

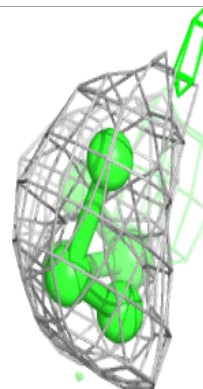
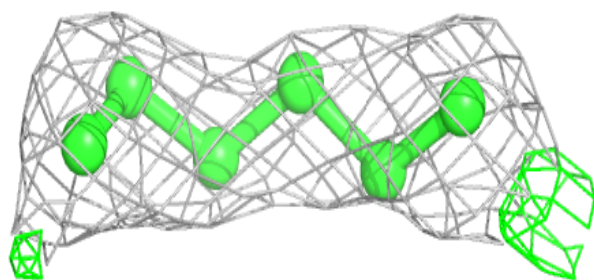
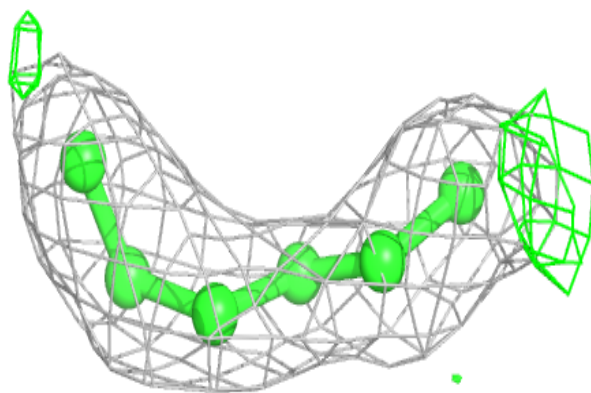
**Electron density around C8E B 517:**

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

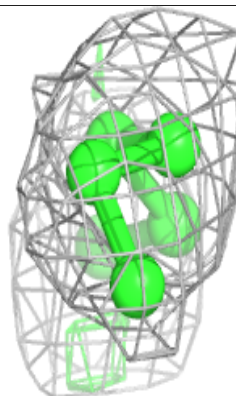
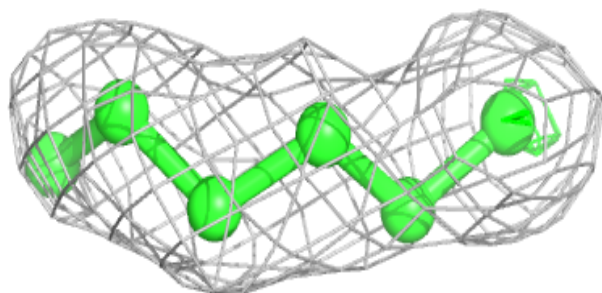
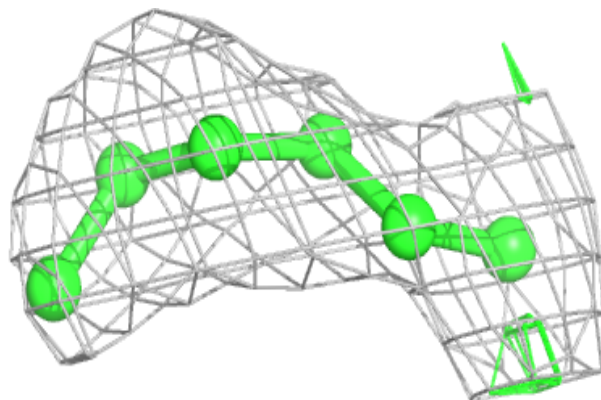


Electron density around C8E A 511:

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

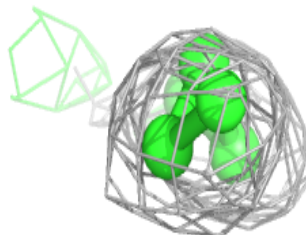
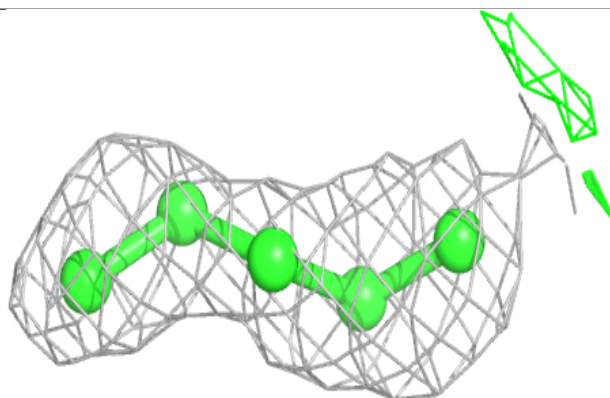
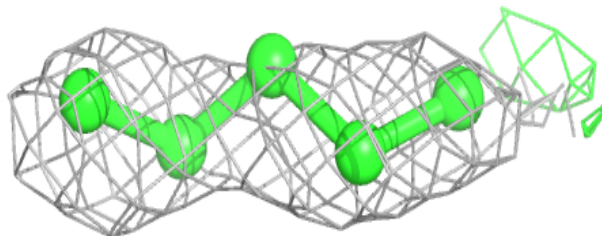
**Electron density around C8E A 509:**

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

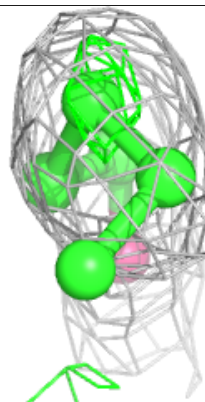
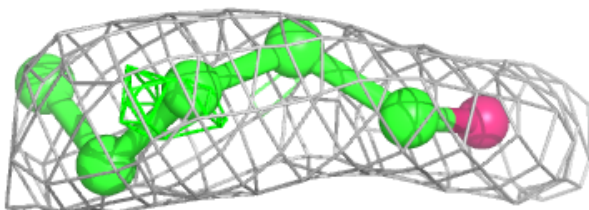
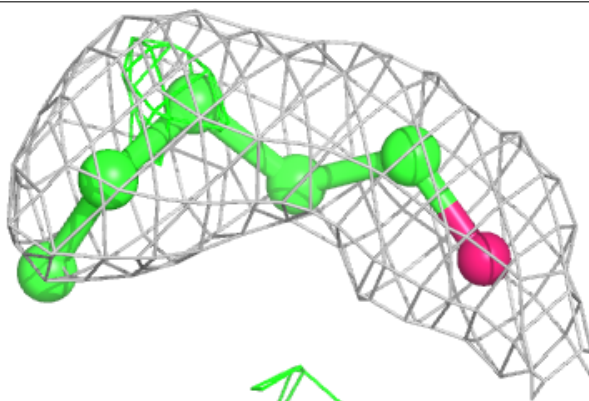


Electron density around C8E A 516:

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

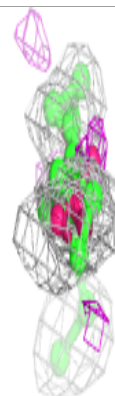
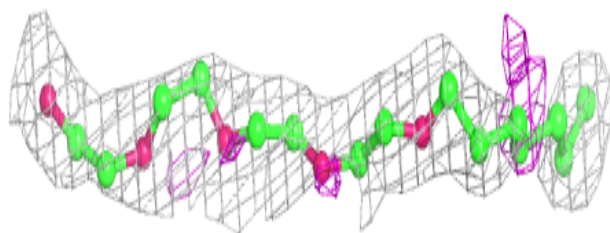
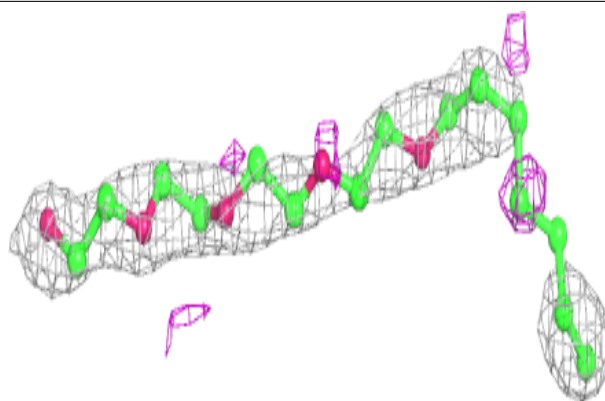
**Electron density around C8E B 527:**

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

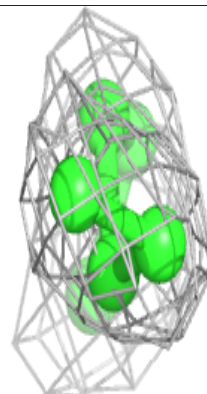
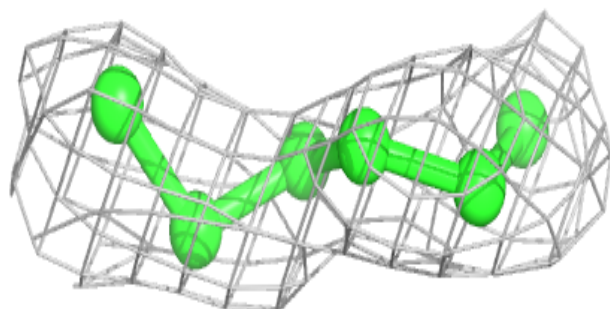
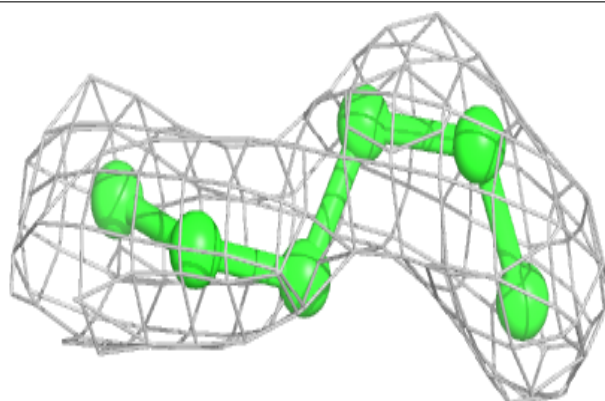


Electron density around C8E B 506:

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

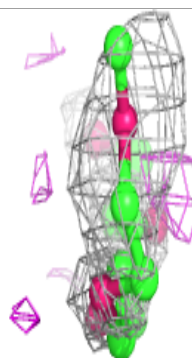
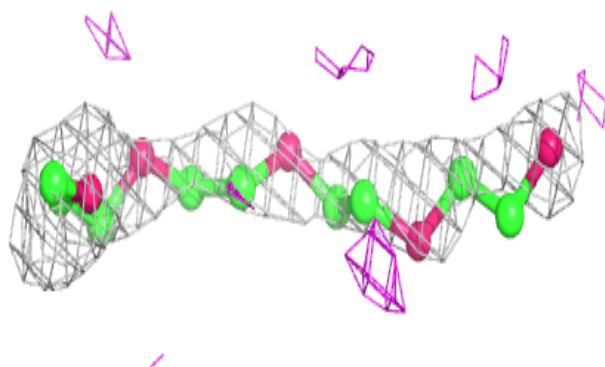
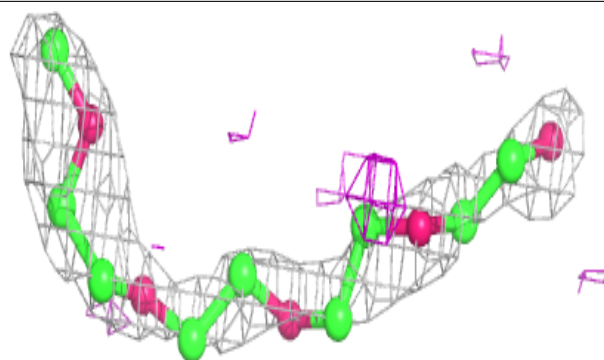
**Electron density around C8E B 511:**

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

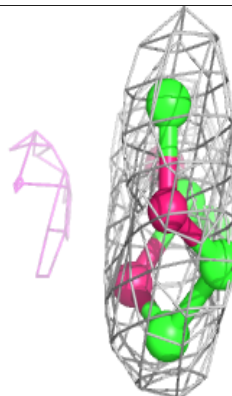
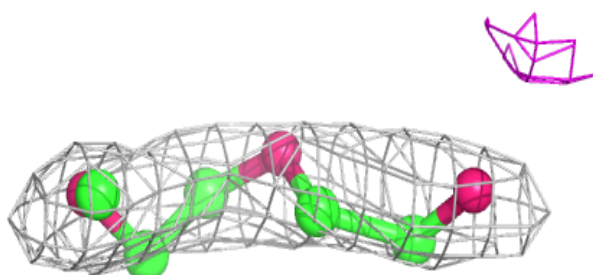
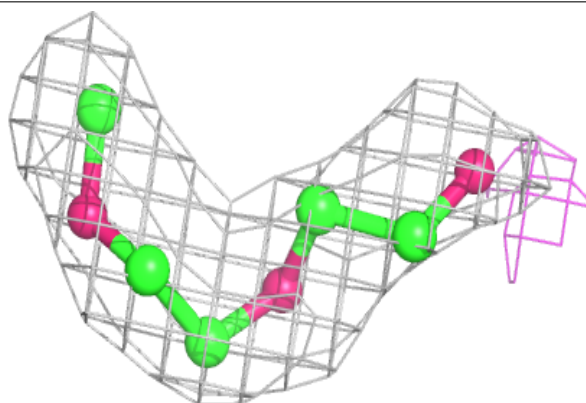


Electron density around C8E A 513:

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

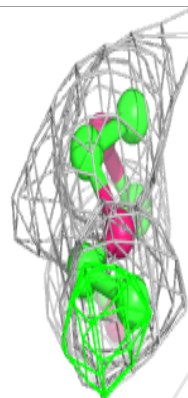
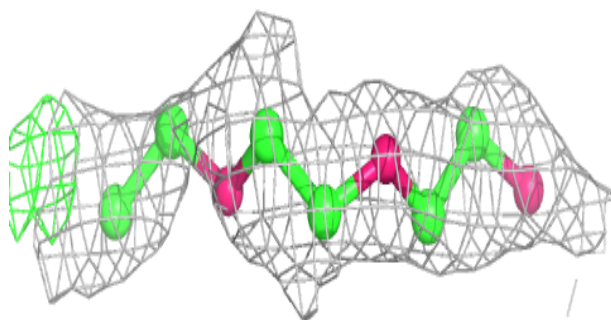
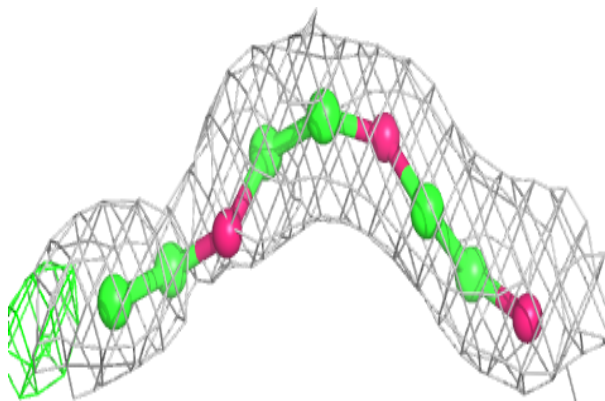
**Electron density around C8E A 512:**

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

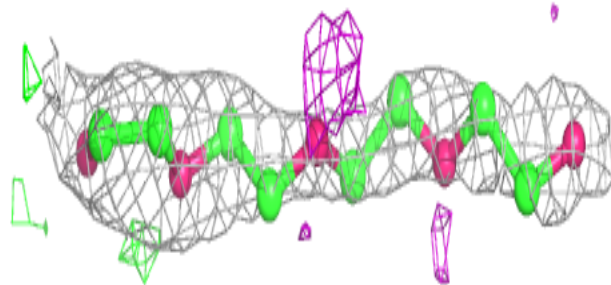
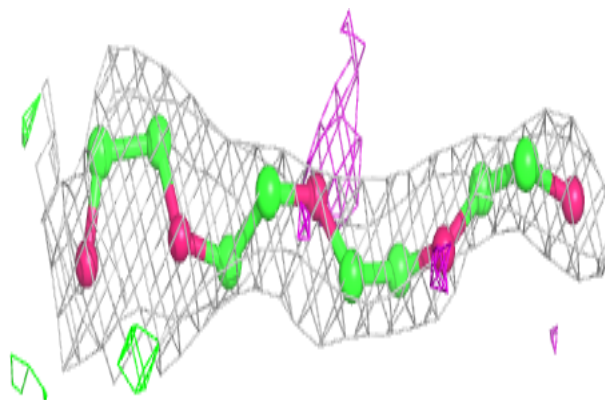


Electron density around C8E A 524:

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and green (positive)

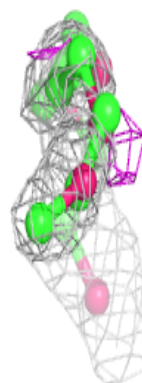
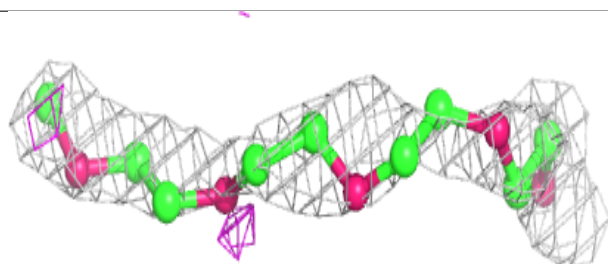
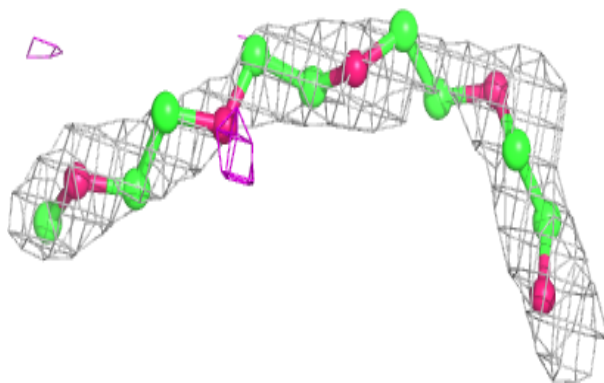
**Electron density around C8E B 507:**

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

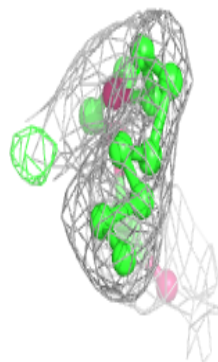
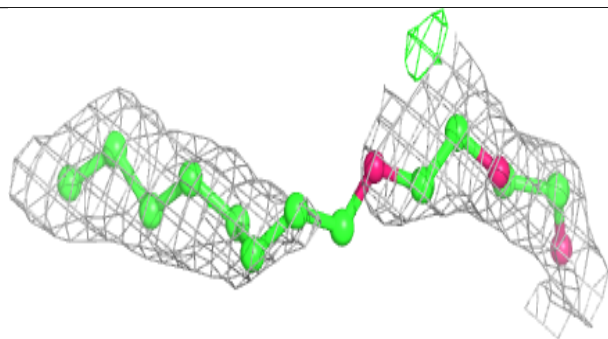
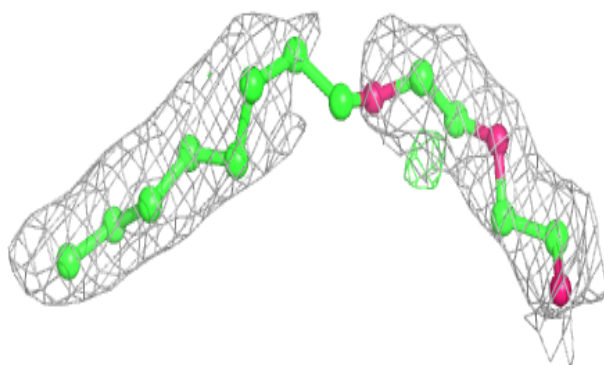


Electron density around C8E B 504:

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and green (positive)

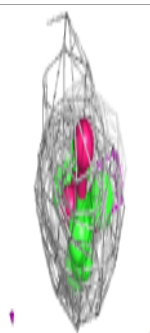
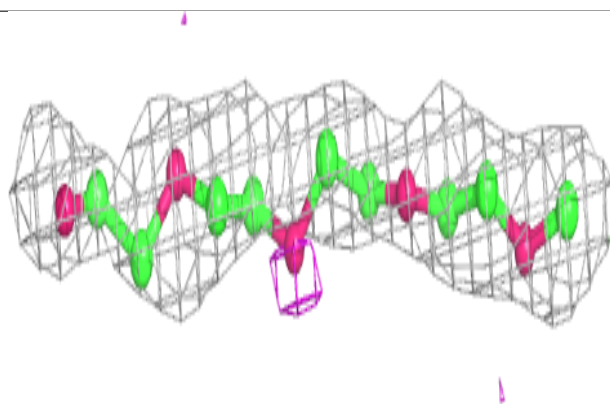
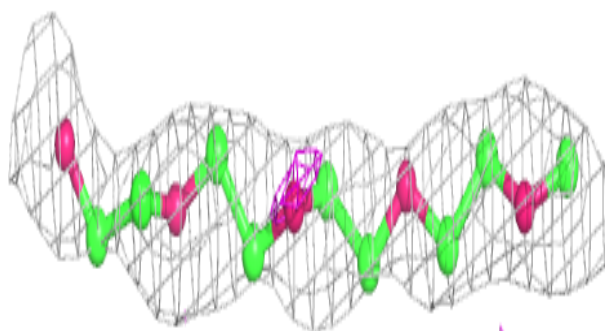
**Electron density around C8E B 525:**

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

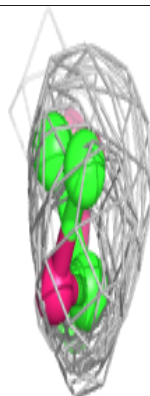
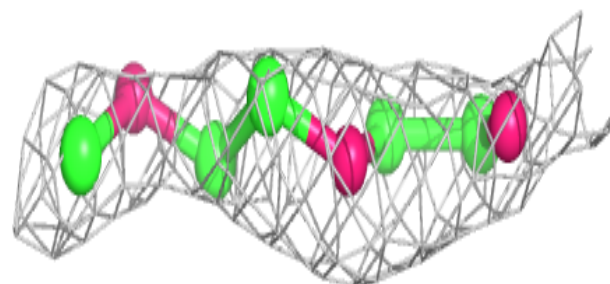
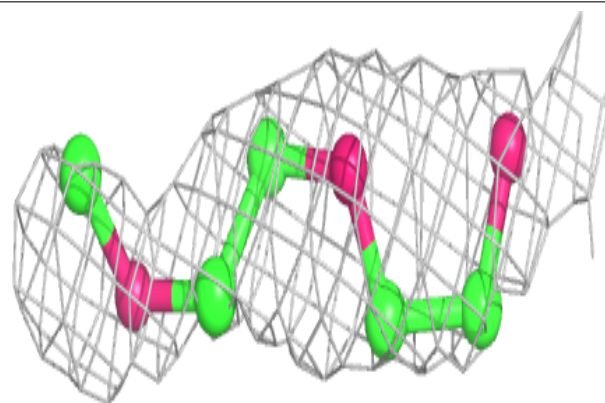


Electron density around C8E A 506:

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and green (positive)

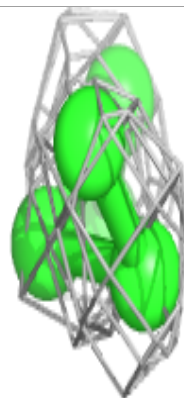
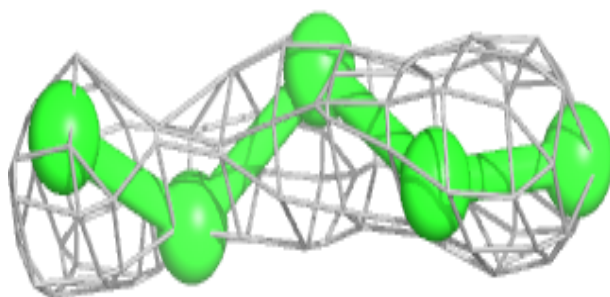
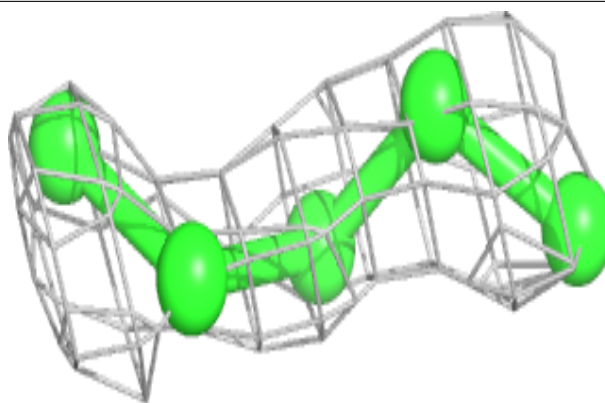
**Electron density around C8E B 505:**

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

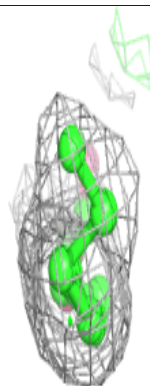
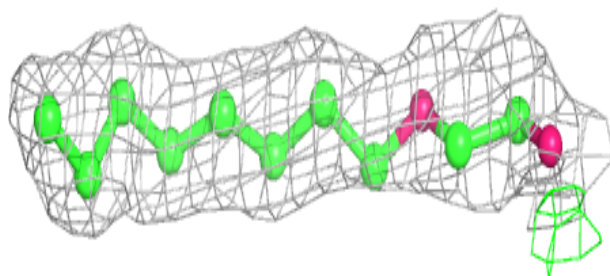
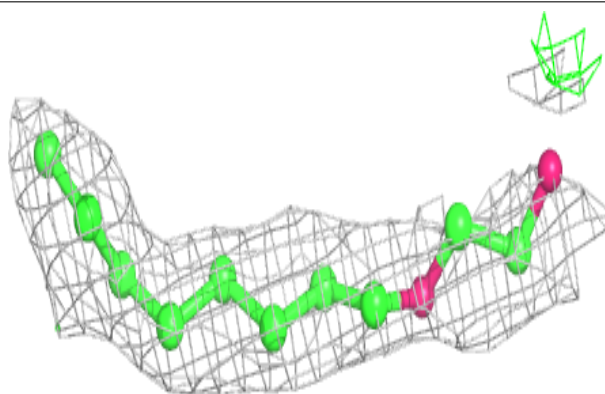


Electron density around C8E B 515:

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and green (positive)

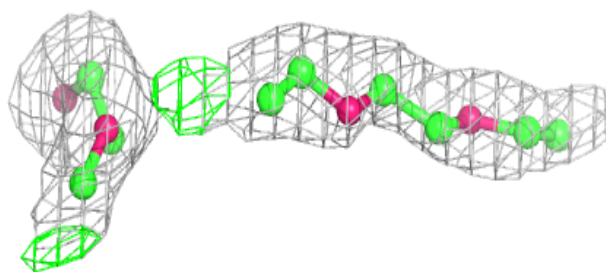
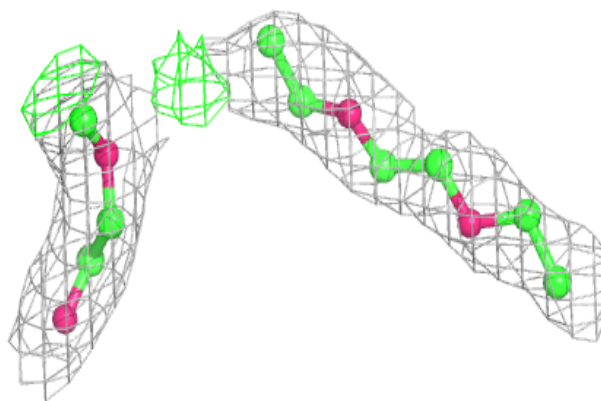
**Electron density around C8E B 524:**

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

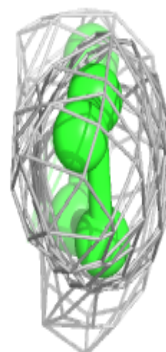
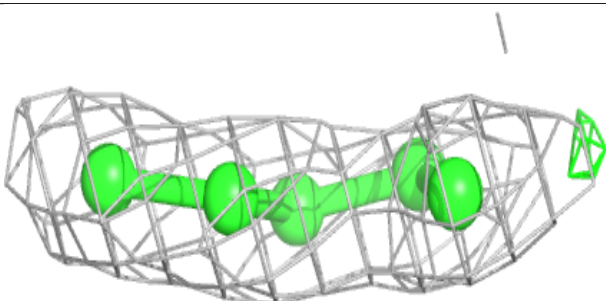
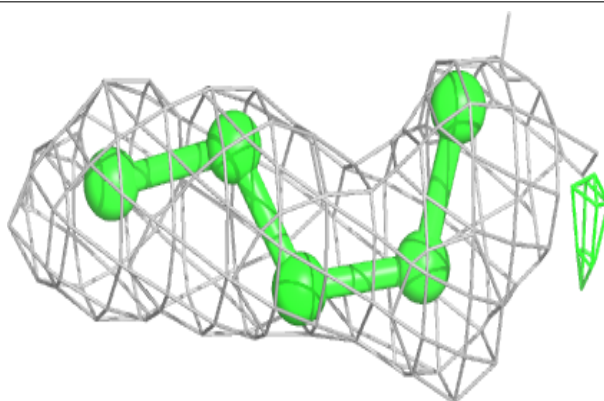


Electron density around C8E B 512:

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

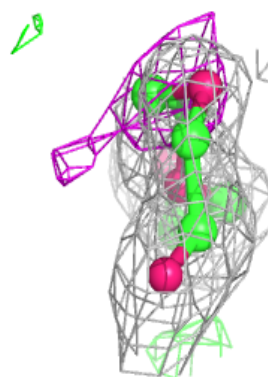
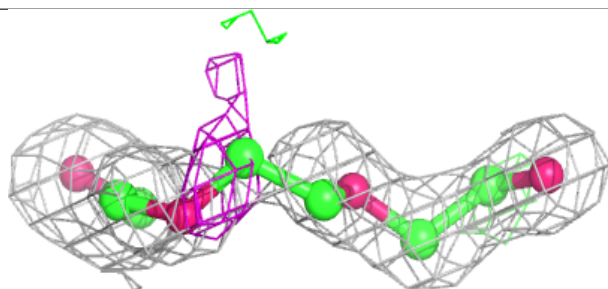
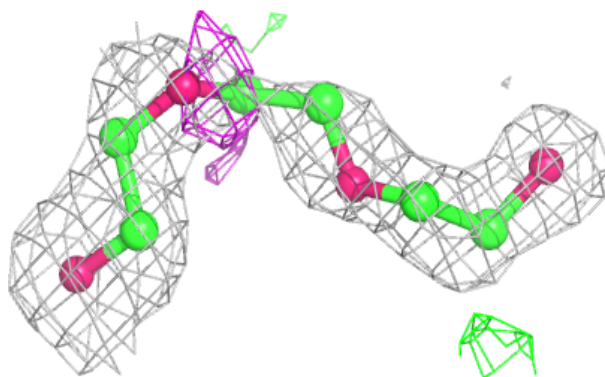
**Electron density around C8E A 520:**

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

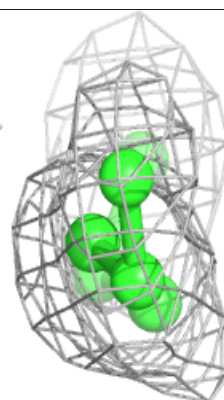
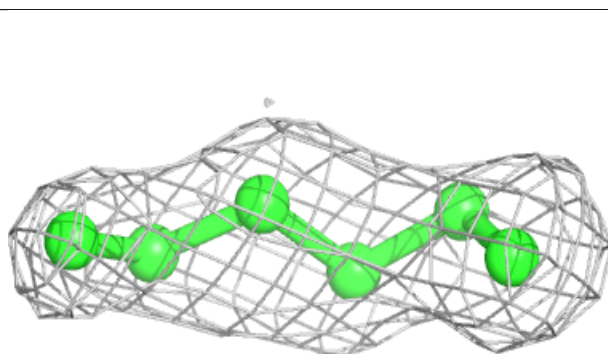
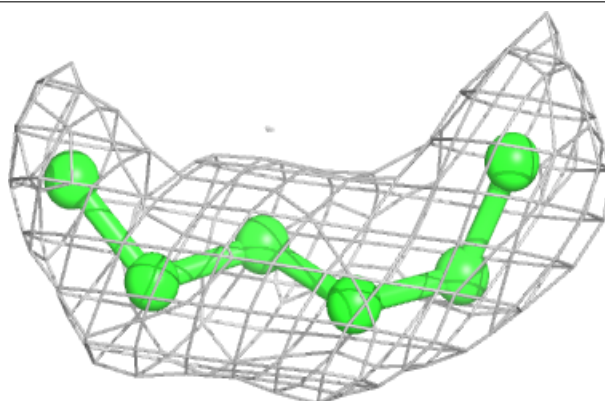


Electron density around C8E A 521:

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

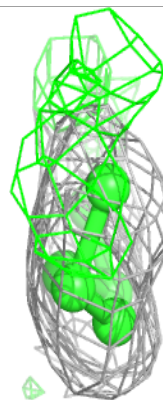
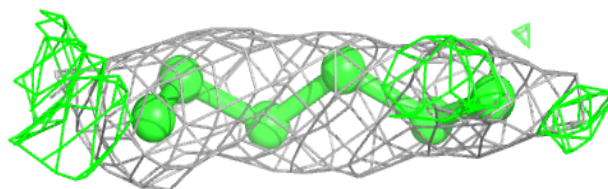
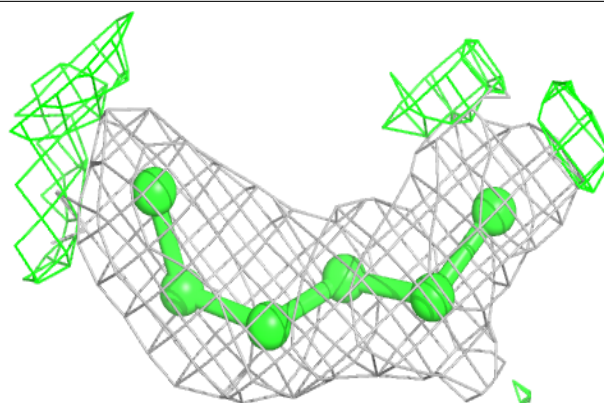
**Electron density around C8E B 509:**

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

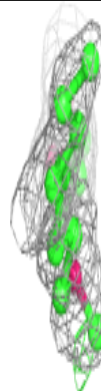
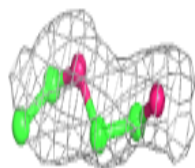
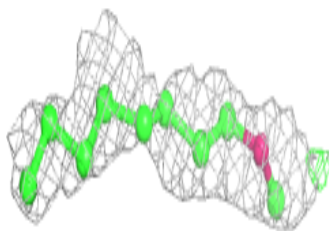
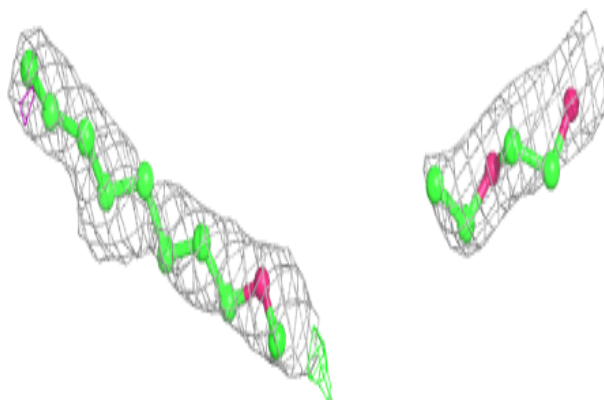


Electron density around C8E A 518:

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

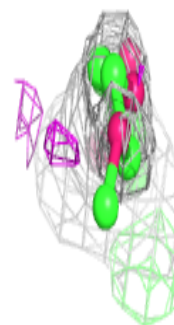
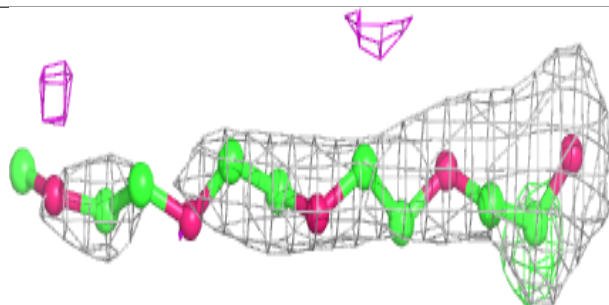
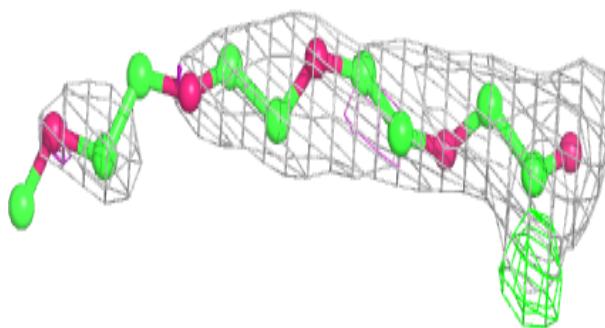
**Electron density around C8E A 505:**

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

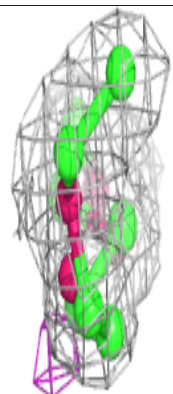
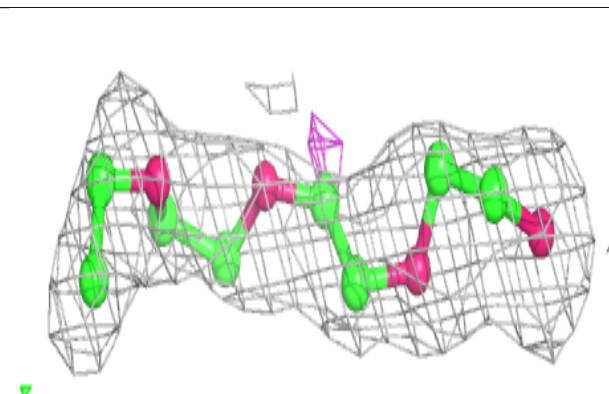
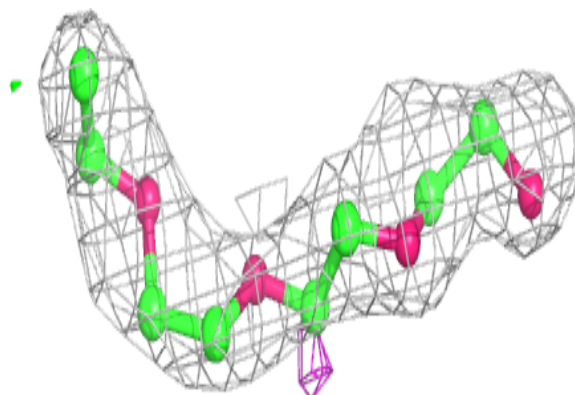


Electron density around C8E A 503:

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

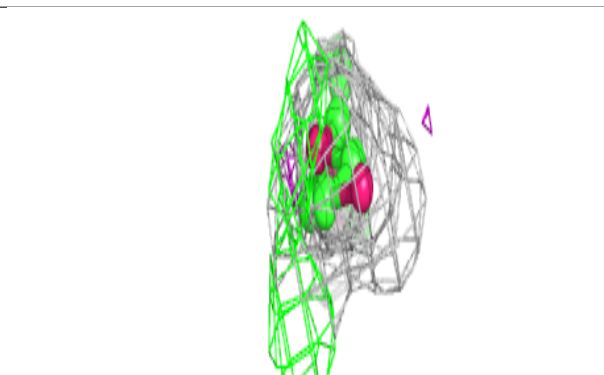
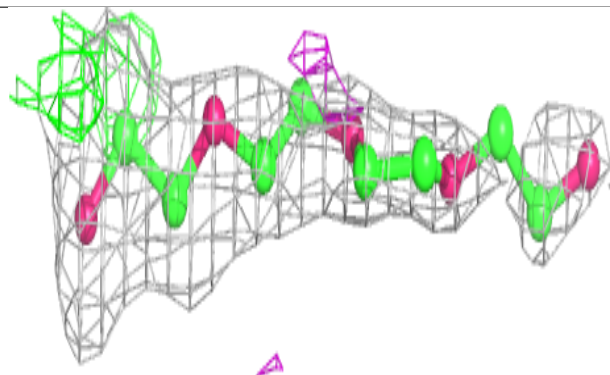
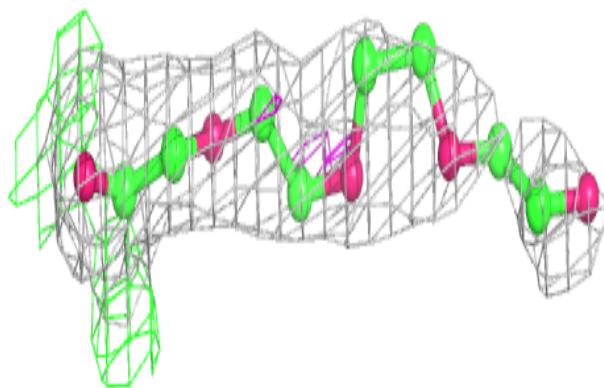
**Electron density around C8E A 523:**

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

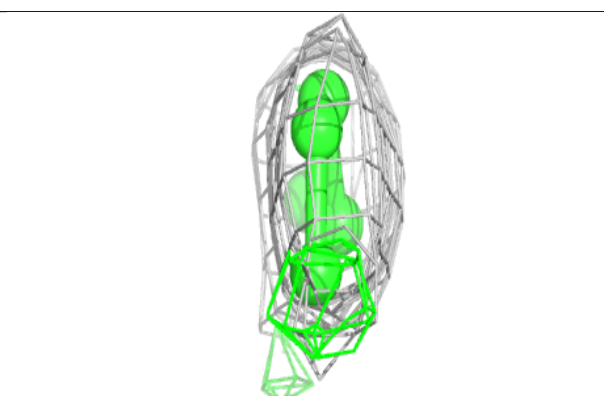
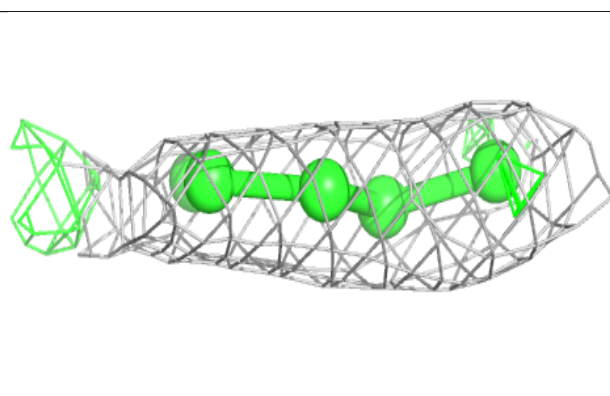
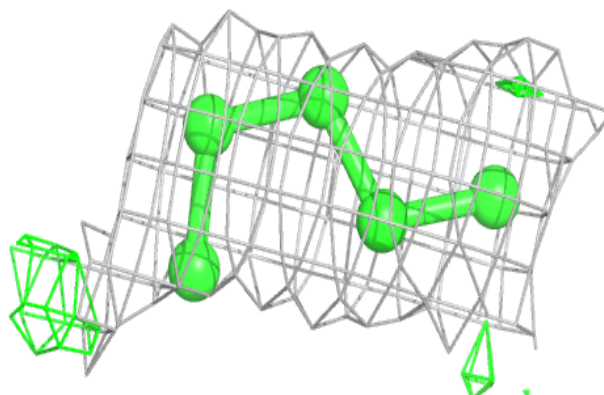


Electron density around C8E B 503:

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

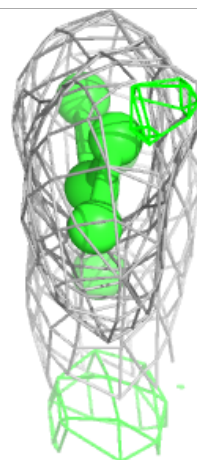
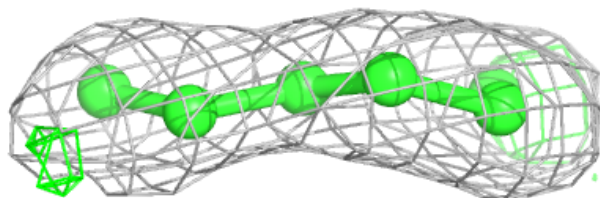
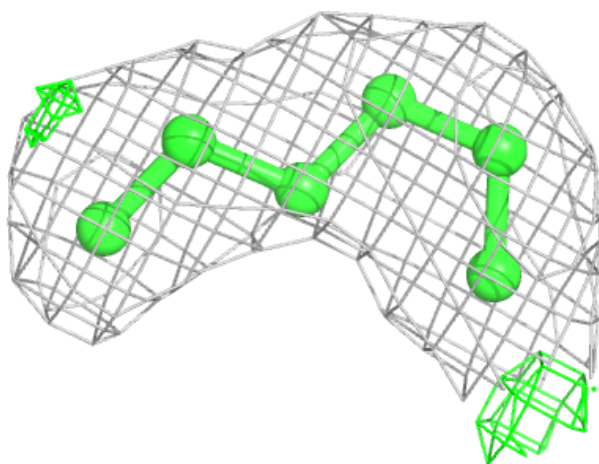
**Electron density around C8E A 504:**

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



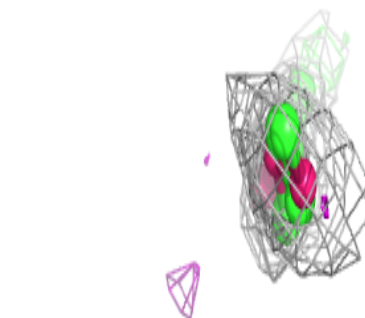
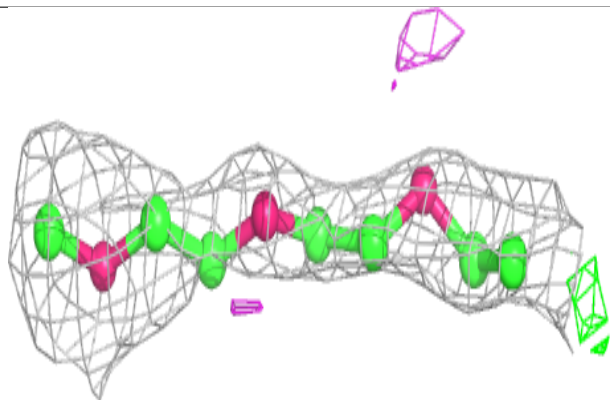
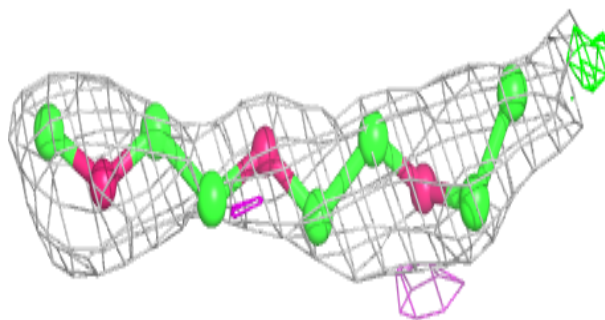
Electron density around C8E B 510:

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

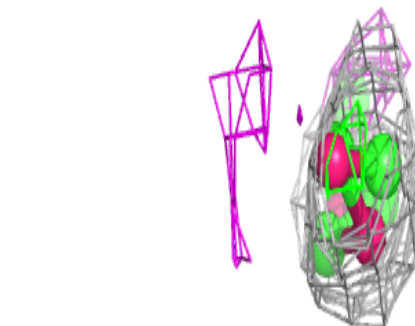
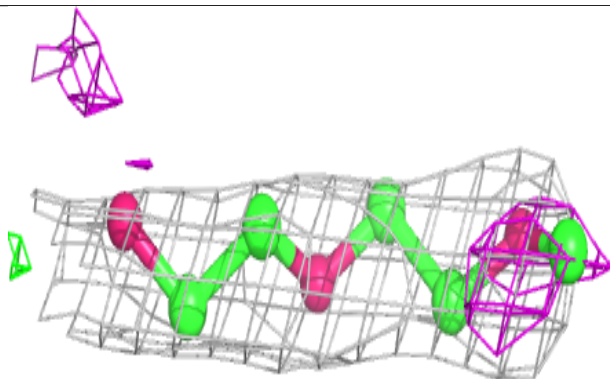
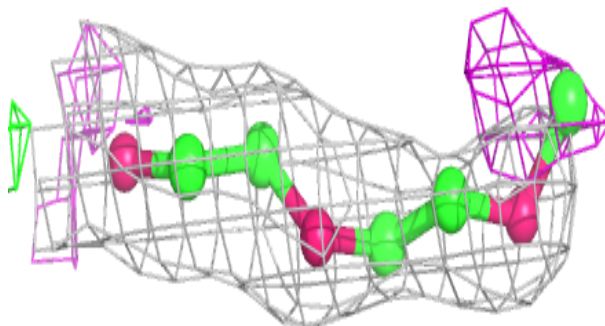


Electron density around C8E B 516:

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

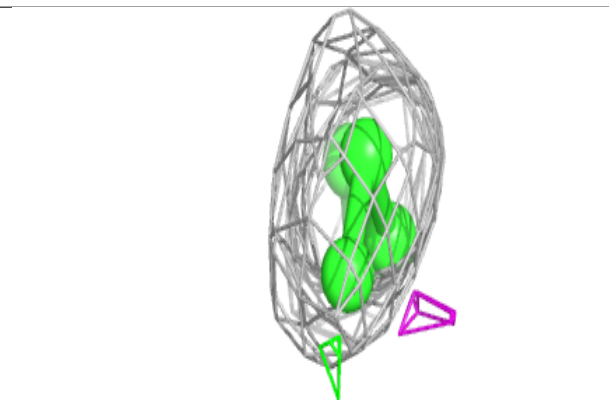
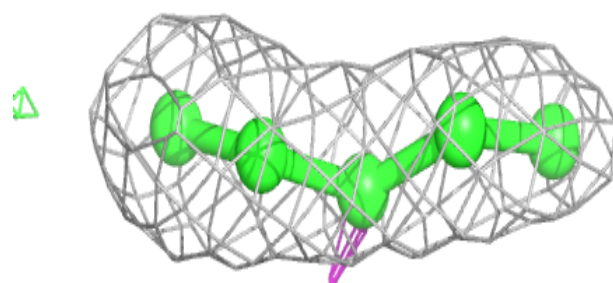
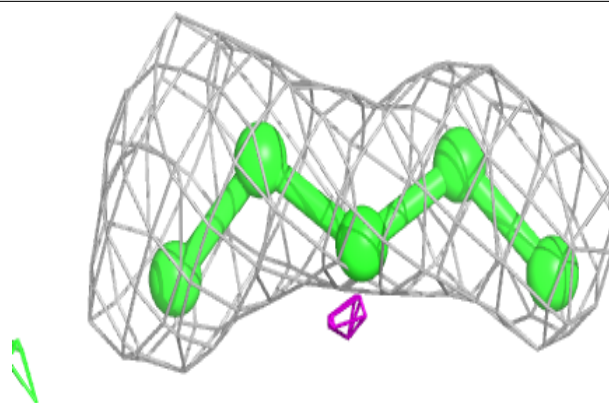
**Electron density around C8E B 514:**

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

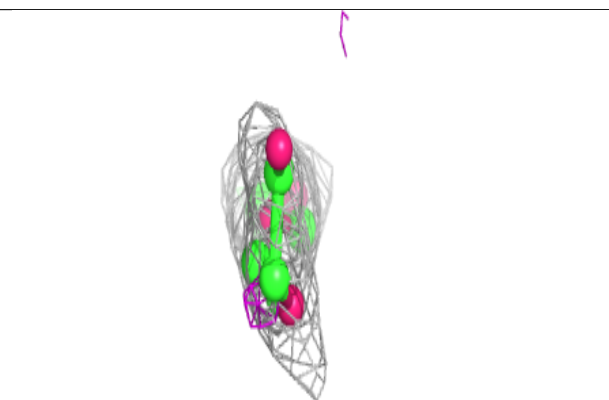
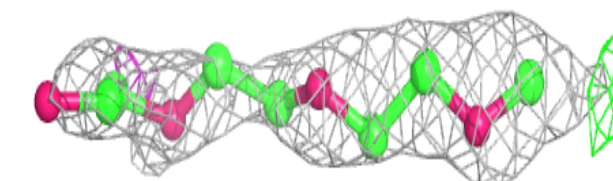
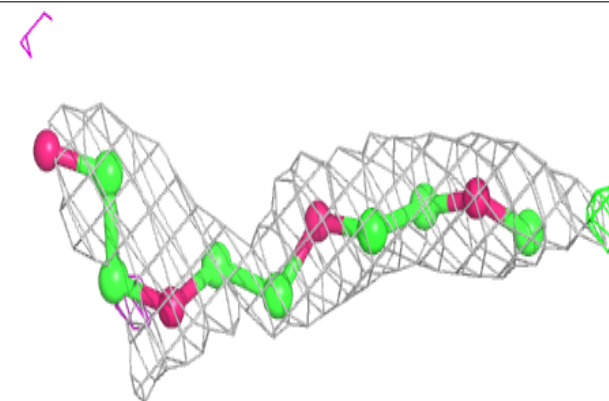


Electron density around C8E B 508:

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

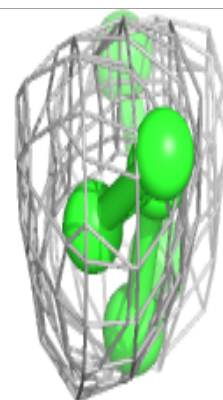
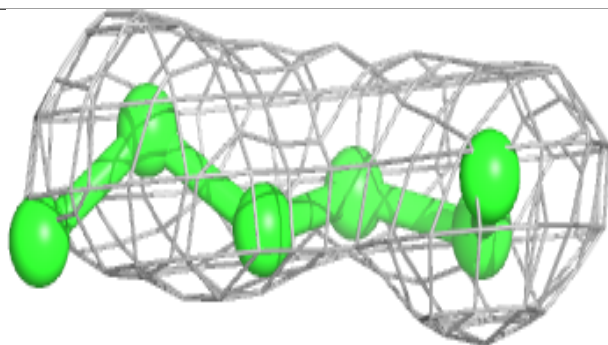
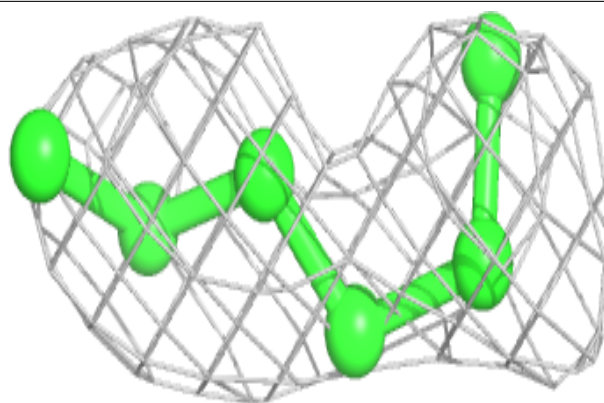
**Electron density around C8E B 526:**

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

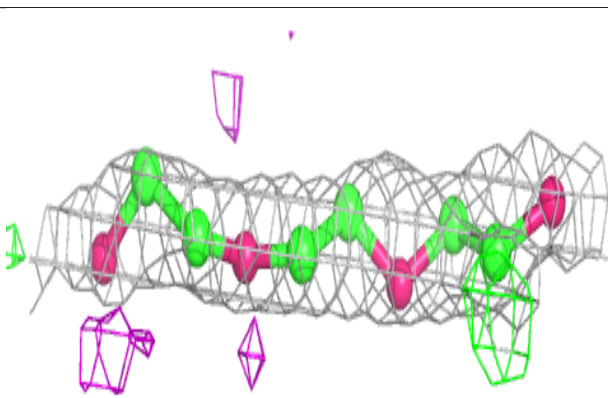
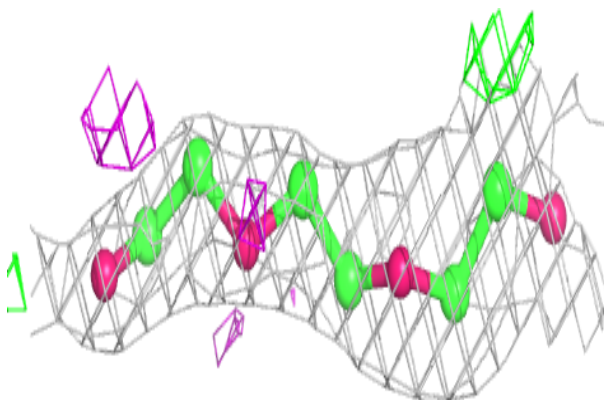


Electron density around C8E A 522:

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

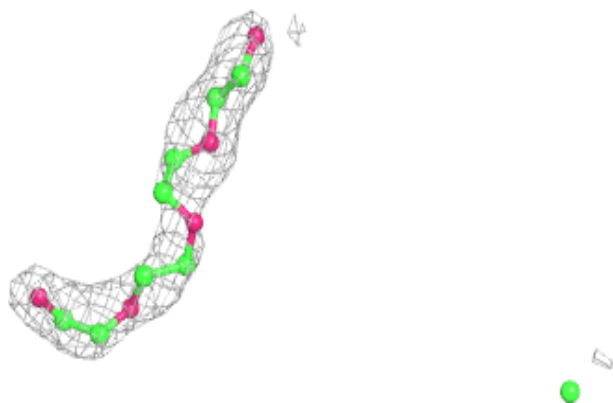
**Electron density around C8E A 508:**

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

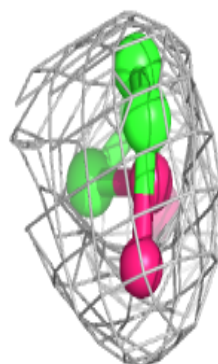
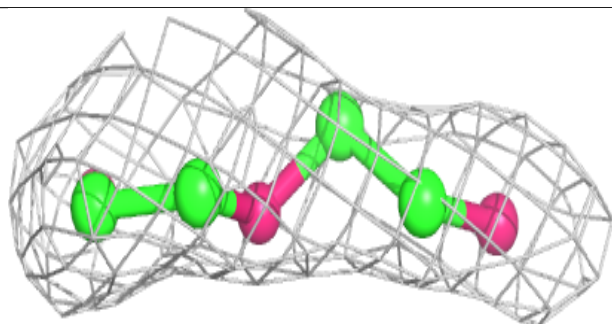
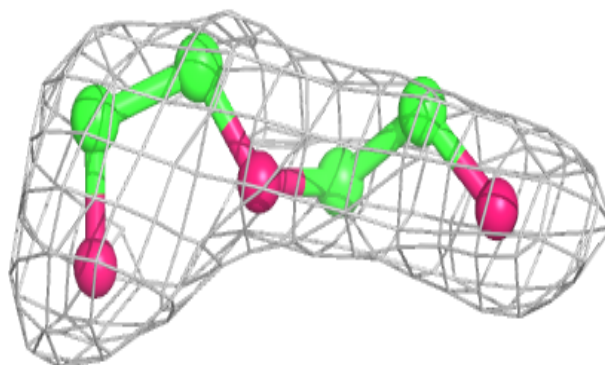


Electron density around C8E B 518:

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

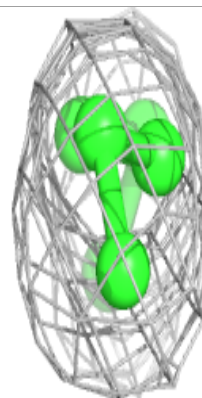
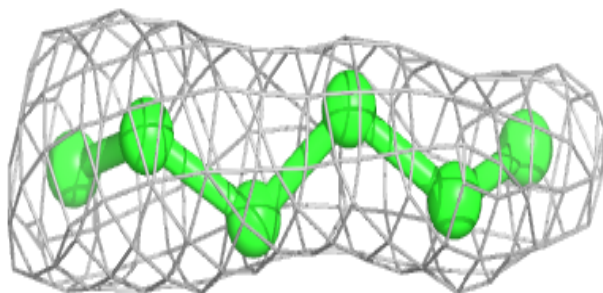
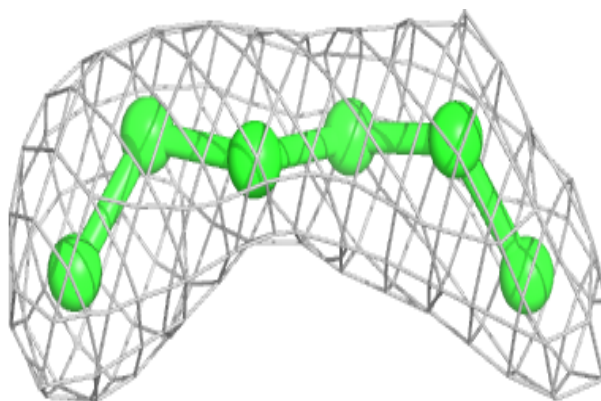
**Electron density around C8E B 522:**

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

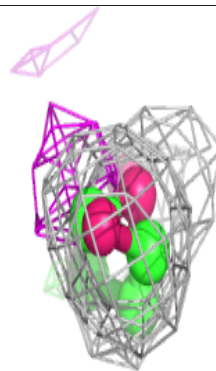
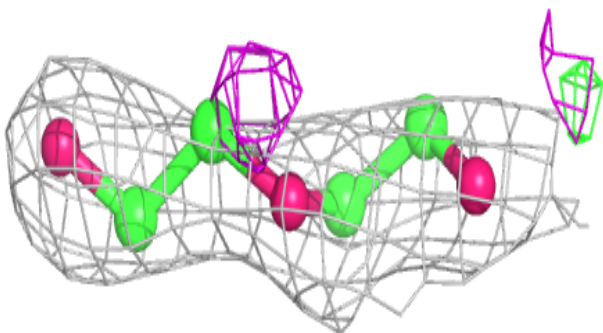
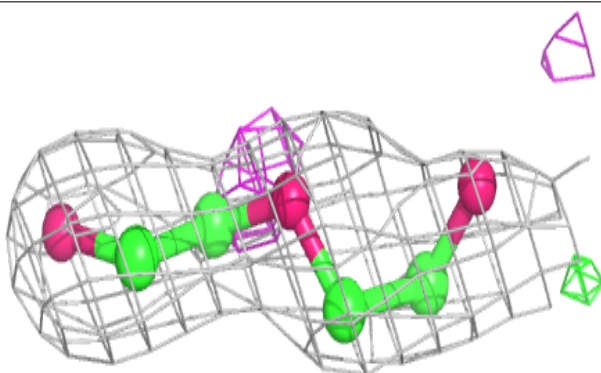


Electron density around C8E A 519:

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

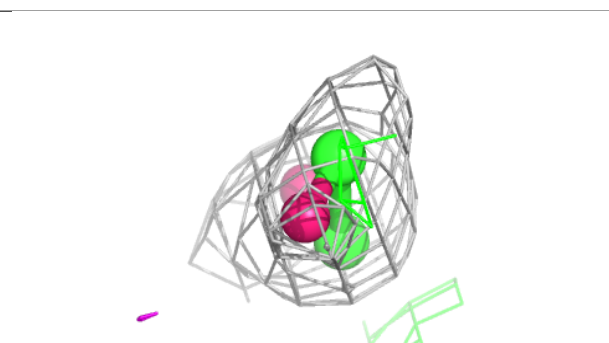
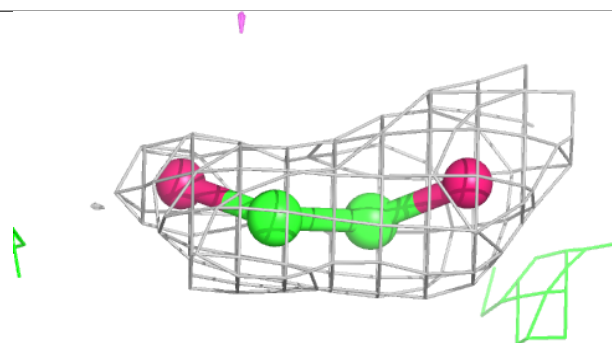
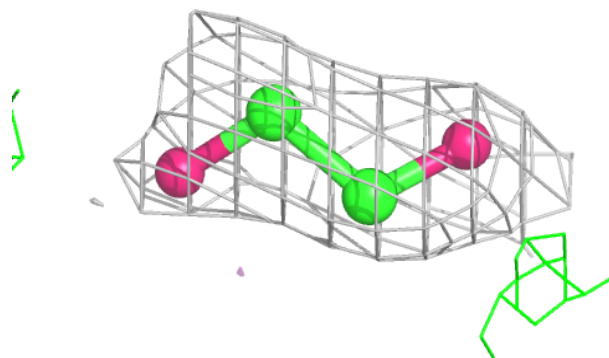
**Electron density around C8E A 507:**

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

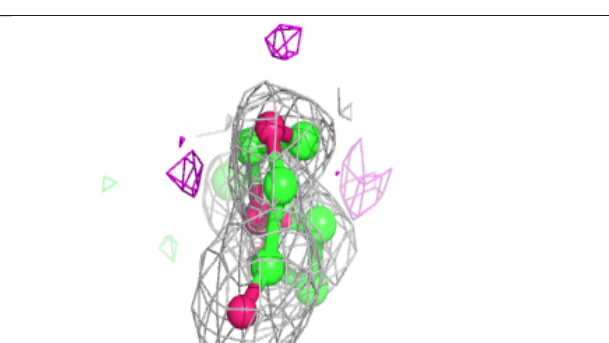
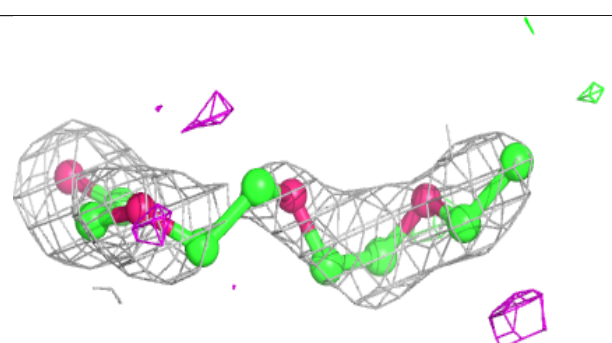
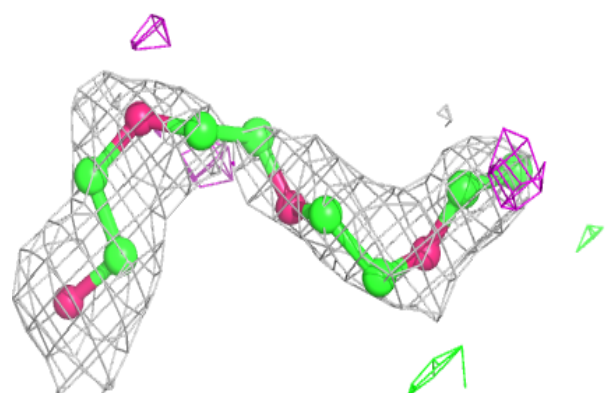


Electron density around C8E A 517:

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

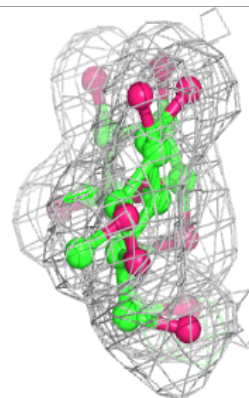
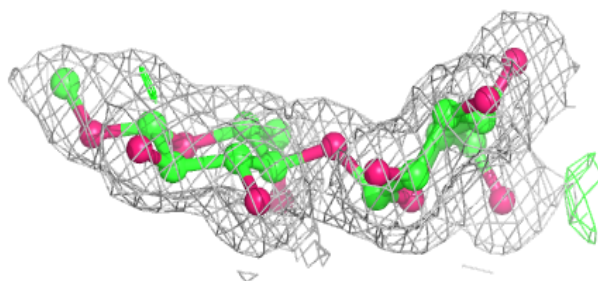
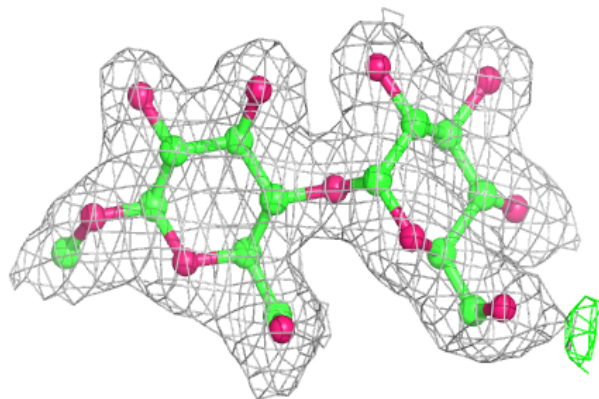
**Electron density around C8E B 528:**

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

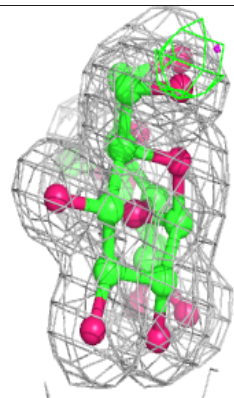
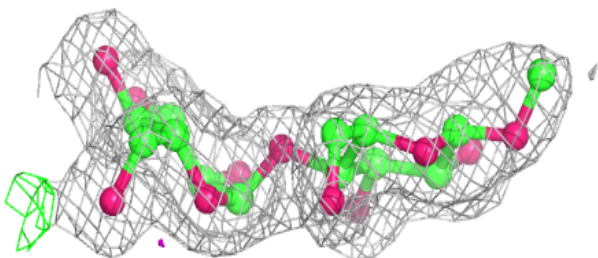
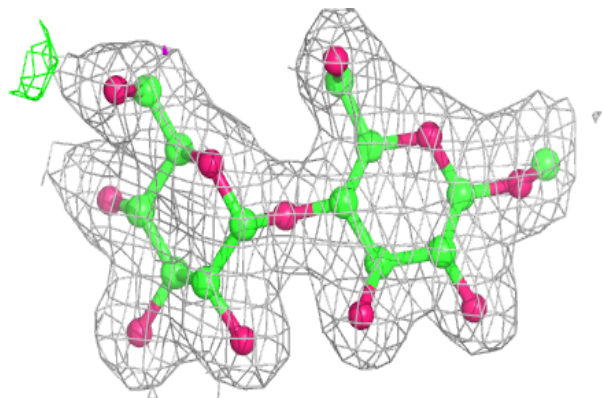


Electron density around DMU B 501:

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

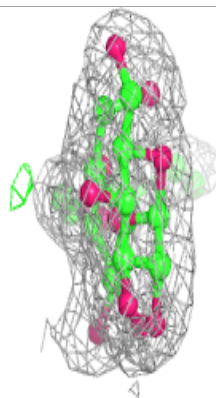
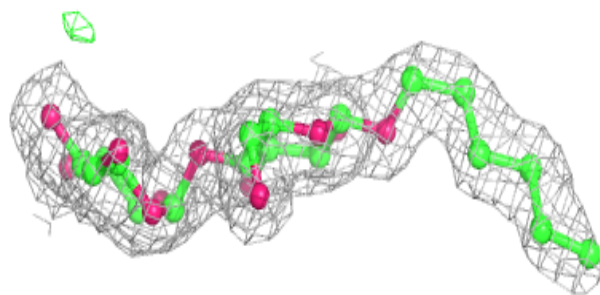
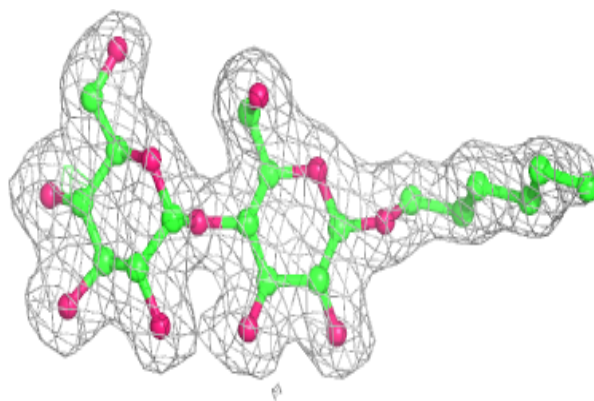
**Electron density around DMU A 502:**

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

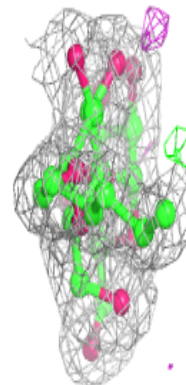
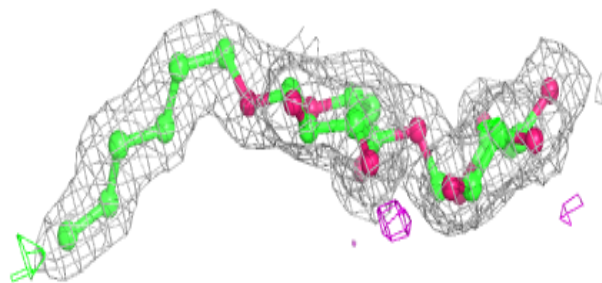
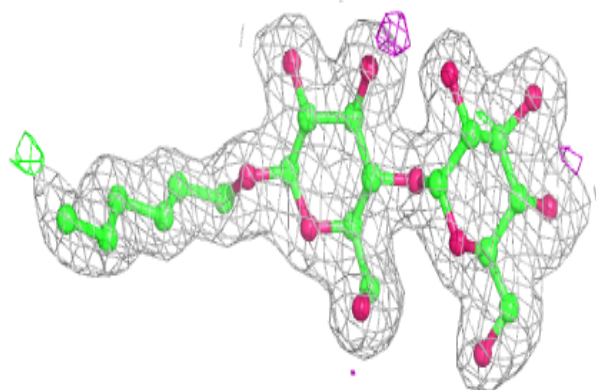


Electron density around DMU A 501:

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

**Electron density around DMU B 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 [i](#)

There are no such residues in this entry.