



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:44 am BST

PDB ID : 3PGU
Title : Phe3Glu mutant of EcFadL
Authors : Lepore, B.W.; Indic, M.; Pham, H.; Hearn, E.; Patel, D.; van den Berg, B.
Deposited on : 2010-11-02
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

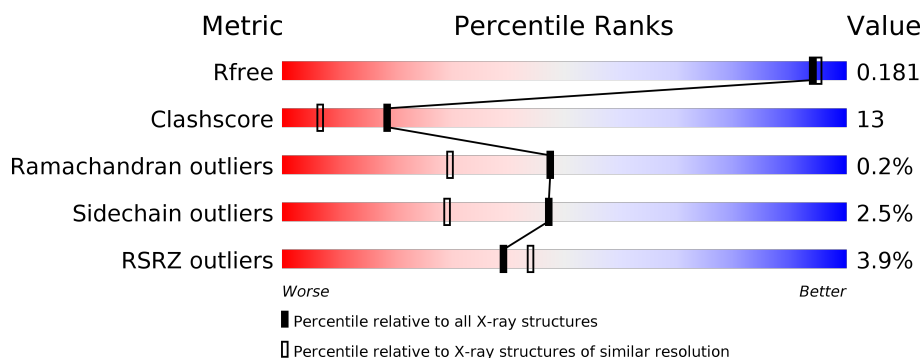
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	427	<div> <div>4%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	446	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3945 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.

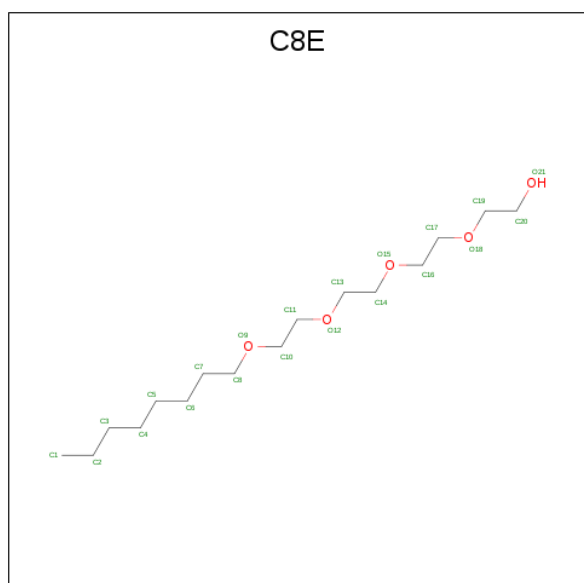
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	32	0
			3412	2152	595	657	8			

There are 7 discrepancies between the modelled and reference sequences:

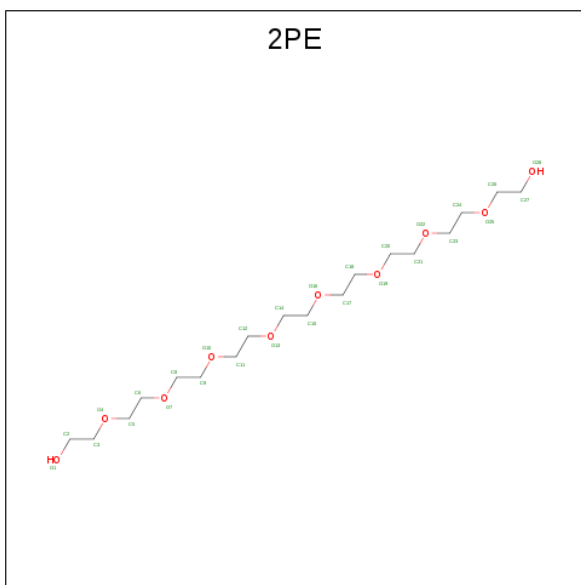
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLU	PHE	ENGINEERED MUTATION	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			8	5	3		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			15	10	5		
2	A	1	Total	C	O	0	0
			8	5	3		
2	A	1	Total	C	O	0	0
			16	11	5		
2	A	1	Total	C	O	0	0
			16	11	5		
2	A	1	Total	C	O	0	0
			16	11	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			15	10	5		

- Molecule 3 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 28	C 18	O 10	0	0
3	A	1	Total 28	C 18	O 10	0	0
3	A	1	Total 28	C 18	O 10	0	0

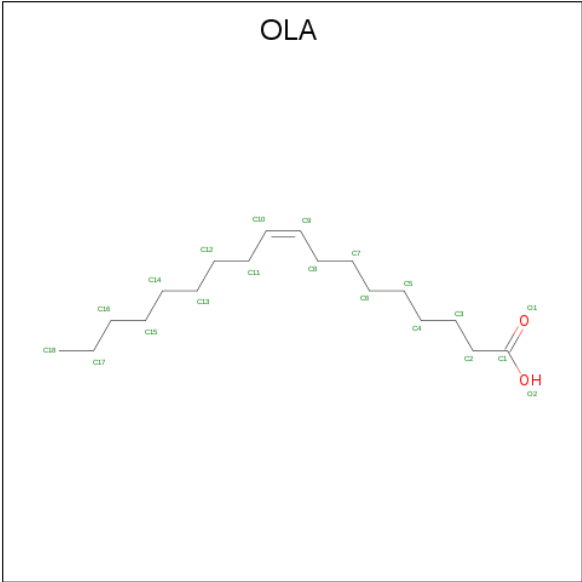
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ni 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	11	2		

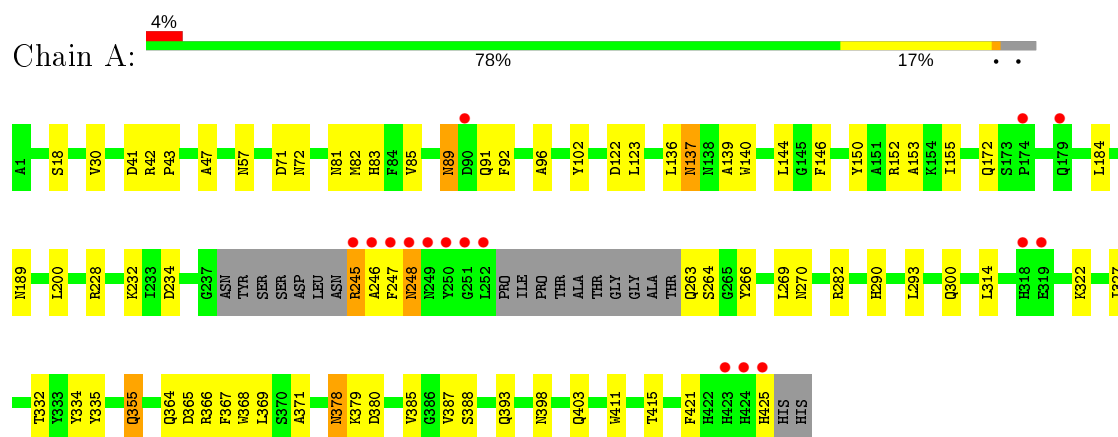
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	246	Total	O	0	0
			246	246		

3 Residue-property plots [i](#)

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

- Molecule 1: Long-chain fatty acid transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 65.20Å 280.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 – 1.70 43.79 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.51-1.70) 94.4 (43.79-1.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_572)	Depositor
R, R_{free}	0.168 , 0.180 0.182 , 0.181	Depositor DCC
R_{free} test set	2504 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3945	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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: C8E, OLA, 2PE, NA, NI

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	0.35	0/3503	0.57	0/4759

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 [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	3412	0	3184	92	0
2	A	186	0	251	12	0
3	A	84	0	114	10	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	13	0	16	0	0
7	A	246	0	0	3	0
All	All	3945	0	3565	96	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 13.

All (96) 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:247:PHE:HB3	1:A:248:ASN:HB2	1.43	1.01
1:A:43[B]:PRO:HG2	1:A:421:PHE:HB2	1.47	0.95
1:A:146:PHE:HB3	2:A:433:C8E:H52	1.52	0.92
1:A:355:GLN:HE21	1:A:355:GLN:H	1.18	0.87
1:A:245:ARG:HA	1:A:247:PHE:H	1.39	0.85
1:A:367:PHE:CE2	1:A:369:LEU:HD21	2.13	0.84
1:A:282[A]:ARG:HH22	2:A:446:C8E:H162	1.43	0.83
1:A:378:ASN:HD22	1:A:380:ASP:H	1.26	0.83
1:A:123[A]:LEU:HD21	1:A:269:LEU:HD21	1.59	0.82
1:A:102:TYR:HE2	1:A:123[A]:LEU:CD2	2.03	0.71
1:A:293:LEU:HD13	1:A:327[A]:ILE:HD11	1.72	0.71
1:A:247:PHE:CB	1:A:248:ASN:HB2	2.21	0.70
1:A:364:GLN:HE21	1:A:366:ARG:HE	1.38	0.70
1:A:152[B]:ARG:HH11	1:A:152[B]:ARG:HG2	1.59	0.68
1:A:245:ARG:HA	1:A:247:PHE:N	2.10	0.67
1:A:355:GLN:NE2	1:A:355:GLN:H	1.92	0.67
1:A:30:VAL:HG21	1:A:85[B]:VAL:HG11	1.77	0.67
1:A:322:LYS:HE2	7:A:676:HOH:O	1.94	0.66
1:A:415[B]:THR:HG23	3:A:437:2PE:H171	1.78	0.65
1:A:247:PHE:N	1:A:248:ASN:HB3	2.13	0.64
1:A:89:ASN:ND2	1:A:91:GLN:H	1.95	0.64
1:A:245:ARG:CA	1:A:246:ALA:HB3	2.28	0.64
1:A:150:TYR:CE2	1:A:152[B]:ARG:HD2	2.35	0.62
1:A:378:ASN:ND2	1:A:380:ASP:H	1.95	0.61
1:A:57:ASN:ND2	1:A:72:ASN:H	2.00	0.60
3:A:436:2PE:H111	3:A:438:2PE:H112	1.82	0.60
1:A:89:ASN:HD22	1:A:91:GLN:H	1.50	0.59
1:A:245:ARG:HA	1:A:246:ALA:HB3	1.85	0.59
1:A:89:ASN:C	1:A:89:ASN:HD22	2.06	0.58
1:A:155:ILE:HD12	1:A:200[B]:LEU:HD23	1.85	0.58
1:A:245:ARG:HB3	1:A:248:ASN:ND2	2.20	0.57
1:A:355:GLN:N	1:A:355:GLN:HE21	1.97	0.57
1:A:385:VAL:HG13	3:A:437:2PE:H151	1.86	0.56
1:A:245:ARG:N	1:A:246:ALA:HB3	2.19	0.56
1:A:398[A]:ASN:ND2	1:A:403:GLN:HG2	2.20	0.56
1:A:137:ASN:ND2	1:A:140:TRP:H	2.04	0.56
1:A:371:ALA:HB1	3:A:437:2PE:H31	1.88	0.55
1:A:152[B]:ARG:NH1	1:A:152[B]:ARG:HG2	2.21	0.55
1:A:385:VAL:HG12	3:A:437:2PE:H111	1.89	0.54
1:A:335:TYR:O	2:A:446:C8E:H72	2.08	0.53
1:A:270:ASN:H	1:A:300:GLN:NE2	2.08	0.52
1:A:102:TYR:HE2	1:A:123[A]:LEU:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:HB2	1:A:82[B]:MET:HG3	1.91	0.52
1:A:364:GLN:NE2	1:A:366:ARG:HE	2.06	0.51
1:A:150:TYR:CE2	1:A:152[A]:ARG:HD3	2.45	0.51
1:A:282[B]:ARG:NH2	1:A:334:TYR:CZ	2.78	0.51
1:A:245:ARG:CA	1:A:247:PHE:H	2.19	0.50
1:A:57:ASN:HD22	1:A:72:ASN:H	1.59	0.50
1:A:415[B]:THR:HG23	3:A:437:2PE:C17	2.42	0.50
1:A:137:ASN:C	1:A:137:ASN:HD22	2.15	0.49
1:A:137:ASN:ND2	1:A:139:ALA:H	2.10	0.49
1:A:232:LYS:NZ	1:A:270:ASN:HD21	2.10	0.48
1:A:123[A]:LEU:HD21	1:A:269:LEU:CD2	2.39	0.48
1:A:137:ASN:HD22	1:A:139:ALA:H	1.61	0.48
2:A:433:C8E:O18	2:A:433:C8E:H141	2.13	0.48
1:A:379:LYS:HG2	1:A:379:LYS:O	2.12	0.48
1:A:387:VAL:HB	3:A:437:2PE:H112	1.96	0.48
2:A:447:C8E:H21	2:A:447:C8E:H52	1.47	0.47
1:A:290:HIS:HE1	1:A:332:THR:OG1	1.96	0.47
1:A:41:ASP:OD2	1:A:42[B]:ARG:HG3	2.14	0.47
1:A:18:SER:OG	1:A:290:HIS:HD2	1.98	0.47
1:A:385:VAL:HG12	3:A:437:2PE:H91	1.96	0.47
1:A:247:PHE:N	1:A:248:ASN:CB	2.77	0.46
1:A:282[B]:ARG:NH2	7:A:567:HOH:O	2.48	0.46
1:A:364:GLN:HE22	1:A:366:ARG:HH21	1.64	0.46
1:A:172:GLN:NE2	2:A:447:C8E:H32	2.30	0.46
1:A:228[B]:ARG:HG3	1:A:228[B]:ARG:O	2.16	0.46
1:A:96:ALA:HB1	2:A:429:C8E:H202	1.98	0.46
1:A:200[B]:LEU:HD12	1:A:264:SER:O	2.16	0.46
1:A:367:PHE:CE2	1:A:369:LEU:CD2	2.94	0.46
1:A:102:TYR:HE2	1:A:123[A]:LEU:HD23	1.79	0.45
1:A:293:LEU:HD13	1:A:327[A]:ILE:CD1	2.46	0.45
1:A:367:PHE:HE2	1:A:369:LEU:HD21	1.74	0.45
1:A:146:PHE:CD2	2:A:433:C8E:H71	2.52	0.45
1:A:102:TYR:CE2	1:A:123[A]:LEU:HD21	2.52	0.45
1:A:266:TYR:CD2	1:A:314[A]:LEU:HD23	2.52	0.45
1:A:378:ASN:HD22	1:A:378:ASN:C	2.20	0.44
1:A:144:LEU:HB3	2:A:444:C8E:H161	2.00	0.44
1:A:247:PHE:CA	1:A:248:ASN:CB	2.95	0.43
1:A:152[B]:ARG:N	1:A:152[B]:ARG:HD3	2.34	0.43
1:A:365:ASP:H	1:A:393:GLN:HE21	1.65	0.42
1:A:189:ASN:OD1	2:A:447:C8E:H131	2.19	0.42
1:A:136:LEU:HD21	3:A:438:2PE:H271	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:443:C8E:H171	2:A:443:C8E:H141	1.37	0.42
1:A:411:TRP:CZ3	2:A:431:C8E:H192	2.55	0.42
1:A:89:ASN:ND2	1:A:92:PHE:H	2.17	0.41
1:A:368:TRP:HE3	1:A:388[A]:SER:HG	1.66	0.41
1:A:57:ASN:HD22	1:A:71:ASP:HA	1.85	0.41
1:A:30:VAL:CG2	1:A:85[B]:VAL:HG11	2.47	0.41
1:A:83:HIS:CD2	7:A:673:HOH:O	2.73	0.41
1:A:369:LEU:N	1:A:369:LEU:HD22	2.36	0.41
1:A:81:ASN:HD22	1:A:83:HIS:CE1	2.39	0.41
1:A:122:ASP:O	1:A:153[A]:ALA:HA	2.21	0.40
1:A:385:VAL:CG1	3:A:437:2PE:H111	2.51	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	434/427 (102%)	425 (98%)	8 (2%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	ASN

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	350/337 (104%)	342 (98%)	8 (2%)	50	33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	137	ASN
1	A	184	LEU
1	A	234	ASP
1	A	245	ARG
1	A	355	GLN
1	A	378	ASN
1	A	425	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	81	ASN
1	A	83	HIS
1	A	89	ASN
1	A	127	ASN
1	A	129	ASN
1	A	137	ASN
1	A	138	ASN
1	A	147	ASN
1	A	169	GLN
1	A	172	GLN
1	A	182	GLN
1	A	263	GLN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	378	ASN
1	A	393	GLN
1	A	416	ASN
1	A	425	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
3	2PE	A	438	-	27,27,27	0.68	0	26,26,26	1.56	0
2	C8E	A	431	-	9,9,20	0.41	0	8,8,19	0.29	0
3	2PE	A	437	-	27,27,27	0.68	0	26,26,26	1.57	0
2	C8E	A	433	-	20,20,20	0.38	0	19,19,19	0.36	0
2	C8E	A	429	-	7,7,20	0.38	0	6,6,19	0.36	0
2	C8E	A	439	-	7,7,20	0.38	0	6,6,19	0.24	0
2	C8E	A	449	-	14,14,20	0.44	0	13,13,19	0.27	0
2	C8E	A	447	-	20,20,20	0.38	0	19,19,19	0.36	0
3	2PE	A	436	-	27,27,27	0.67	0	26,26,26	1.56	0
2	C8E	A	430	-	9,9,20	0.41	0	8,8,19	0.25	0
2	C8E	A	443	-	15,15,20	0.42	0	14,14,19	0.26	0
2	C8E	A	444	-	15,15,20	0.42	0	14,14,19	0.27	0
2	C8E	A	434	-	9,9,20	0.40	0	8,8,19	0.33	0
2	C8E	A	428	-	9,9,20	0.39	0	8,8,19	0.23	0
2	C8E	A	435	-	14,14,20	0.46	0	13,13,19	0.30	0
2	C8E	A	446	-	15,15,20	0.42	0	14,14,19	0.29	0
2	C8E	A	432	-	9,9,20	0.40	0	8,8,19	0.29	0
6	OLA	A	448	-	9,12,19	1.01	1 (11%)	8,12,19	0.93	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	2PE	A	438	-	-	14/25/25/25	-
2	C8E	A	431	-	-	5/7/7/18	-
3	2PE	A	437	-	-	14/25/25/25	-
2	C8E	A	433	-	-	13/18/18/18	-
2	C8E	A	429	-	-	4/5/5/18	-
2	C8E	A	439	-	-	4/5/5/18	-
2	C8E	A	449	-	-	9/12/12/18	-
2	C8E	A	447	-	-	14/18/18/18	-
3	2PE	A	436	-	-	13/25/25/25	-
2	C8E	A	430	-	-	4/7/7/18	-
2	C8E	A	443	-	-	9/13/13/18	-
2	C8E	A	444	-	-	9/13/13/18	-
2	C8E	A	434	-	-	5/7/7/18	-
2	C8E	A	428	-	-	4/7/7/18	-
2	C8E	A	435	-	-	10/12/12/18	-
2	C8E	A	446	-	-	7/13/13/18	-
2	C8E	A	432	-	-	6/7/7/18	-
6	OLA	A	448	-	-	2/8/10/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	448	OLA	C4-C3	-2.58	1.37	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	443	C8E	C17-C16-O15-C14
3	A	436	2PE	O22-C23-C24-O25
2	A	447	C8E	O12-C13-C14-O15
3	A	438	2PE	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
3	A	438	2PE	O22-C23-C24-O25
2	A	443	C8E	O15-C16-C17-O18
3	A	437	2PE	O7-C8-C9-O10
3	A	438	2PE	O4-C5-C6-O7
3	A	437	2PE	O13-C14-C15-O16
3	A	436	2PE	O19-C20-C21-O22
2	A	435	C8E	O12-C13-C14-O15
2	A	449	C8E	O15-C16-C17-O18
3	A	438	2PE	C11-C12-O13-C14
3	A	436	2PE	O7-C8-C9-O10
3	A	438	2PE	O13-C14-C15-O16
2	A	446	C8E	O18-C19-C20-O21
2	A	443	C8E	C6-C7-C8-O9
2	A	447	C8E	C2-C3-C4-C5
2	A	433	C8E	O12-C13-C14-O15
2	A	446	C8E	C6-C7-C8-O9
3	A	438	2PE	C2-C3-O4-C5
2	A	444	C8E	C6-C7-C8-O9
3	A	437	2PE	O4-C5-C6-O7
3	A	437	2PE	C6-C5-O4-C3
3	A	437	2PE	O19-C20-C21-O22
2	A	449	C8E	O18-C19-C20-O21
2	A	428	C8E	O12-C13-C14-O15
3	A	437	2PE	O1-C2-C3-O4
2	A	439	C8E	O12-C13-C14-O15
2	A	430	C8E	O18-C19-C20-O21
2	A	432	C8E	C17-C16-O15-C14
2	A	433	C8E	C6-C7-C8-O9
2	A	443	C8E	O18-C19-C20-O21
2	A	431	C8E	O18-C19-C20-O21
2	A	432	C8E	O18-C19-C20-O21
2	A	433	C8E	O18-C19-C20-O21
2	A	430	C8E	O12-C13-C14-O15
2	A	434	C8E	O12-C13-C14-O15
2	A	434	C8E	O18-C19-C20-O21
3	A	436	2PE	O13-C14-C15-O16
2	A	447	C8E	C3-C4-C5-C6
2	A	433	C8E	C2-C3-C4-C5
2	A	429	C8E	C17-C16-O15-C14
2	A	429	C8E	O18-C19-C20-O21
2	A	447	C8E	O9-C10-C11-O12
2	A	444	C8E	O15-C16-C17-O18

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Mol	Chain	Res	Type	Atoms
3	A	438	2PE	O16-C17-C18-O19
2	A	447	C8E	C16-C17-O18-C19
2	A	433	C8E	C4-C5-C6-C7
3	A	438	2PE	O19-C20-C21-O22
2	A	447	C8E	C4-C5-C6-C7
2	A	449	C8E	O12-C13-C14-O15
2	A	447	C8E	C5-C6-C7-C8
2	A	447	C8E	O18-C19-C20-O21
2	A	431	C8E	O12-C13-C14-O15
2	A	435	C8E	O18-C19-C20-O21
2	A	432	C8E	O12-C13-C14-O15
3	A	436	2PE	O4-C5-C6-O7
2	A	444	C8E	O12-C13-C14-O15
2	A	435	C8E	C16-C17-O18-C19
2	A	433	C8E	C16-C17-O18-C19
3	A	438	2PE	O25-C26-C27-O28
2	A	446	C8E	O12-C13-C14-O15
3	A	436	2PE	O1-C2-C3-O4
2	A	428	C8E	O15-C16-C17-O18
2	A	433	C8E	C1-C2-C3-C4
2	A	447	C8E	C1-C2-C3-C4
2	A	429	C8E	O15-C16-C17-O18
2	A	447	C8E	O15-C16-C17-O18
2	A	443	C8E	O12-C13-C14-O15
3	A	436	2PE	O10-C11-C12-O13
2	A	447	C8E	C6-C7-C8-O9
6	A	448	OLA	C4-C5-C6-C7
2	A	444	C8E	C20-C19-O18-C17
3	A	438	2PE	O1-C2-C3-O4
3	A	438	2PE	C14-C15-O16-C17
3	A	438	2PE	C18-C17-O16-C15
3	A	437	2PE	C15-C14-O13-C12
2	A	428	C8E	C13-C14-O15-C16
2	A	435	C8E	C17-C16-O15-C14
2	A	432	C8E	C13-C14-O15-C16
3	A	436	2PE	C21-C20-O19-C18
2	A	447	C8E	C20-C19-O18-C17
2	A	435	C8E	C20-C19-O18-C17
2	A	444	C8E	C13-C14-O15-C16
2	A	443	C8E	C20-C19-O18-C17
2	A	433	C8E	C20-C19-O18-C17
3	A	436	2PE	C18-C17-O16-C15

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Mol	Chain	Res	Type	Atoms
2	A	449	C8E	C20-C19-O18-C17
2	A	447	C8E	C7-C8-O9-C10
2	A	433	C8E	C14-C13-O12-C11
2	A	429	C8E	C20-C19-O18-C17
2	A	439	C8E	C10-C11-O12-C13
2	A	444	C8E	C14-C13-O12-C11
3	A	437	2PE	C9-C8-O7-C6
2	A	449	C8E	C13-C14-O15-C16
2	A	434	C8E	C17-C16-O15-C14
2	A	444	C8E	C17-C16-O15-C14
6	A	448	OLA	C5-C6-C7-C8
2	A	430	C8E	C13-C14-O15-C16
2	A	444	C8E	C7-C8-O9-C10
2	A	449	C8E	C14-C13-O12-C11
2	A	447	C8E	C14-C13-O12-C11
2	A	435	C8E	C13-C14-O15-C16
2	A	433	C8E	C13-C14-O15-C16
2	A	435	C8E	C10-C11-O12-C13
3	A	436	2PE	C11-C12-O13-C14
2	A	431	C8E	C20-C19-O18-C17
2	A	449	C8E	O9-C10-C11-O12
2	A	435	C8E	C7-C8-O9-C10
3	A	436	2PE	C24-C23-O22-C21
3	A	437	2PE	C5-C6-O7-C8
2	A	432	C8E	C20-C19-O18-C17
2	A	431	C8E	C16-C17-O18-C19
3	A	436	2PE	C8-C9-O10-C11
2	A	446	C8E	C20-C19-O18-C17
3	A	437	2PE	O25-C26-C27-O28
2	A	449	C8E	C10-C11-O12-C13
2	A	433	C8E	C11-C10-O9-C8
2	A	443	C8E	C7-C8-O9-C10
2	A	433	C8E	C7-C8-O9-C10
2	A	444	C8E	O9-C10-C11-O12
2	A	449	C8E	C7-C8-O9-C10
2	A	431	C8E	C13-C14-O15-C16
2	A	446	C8E	C17-C16-O15-C14
2	A	435	C8E	C11-C10-O9-C8
2	A	430	C8E	O15-C16-C17-O18
3	A	438	2PE	C8-C9-O10-C11
2	A	439	C8E	O9-C10-C11-O12
2	A	428	C8E	C17-C16-O15-C14

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Mol	Chain	Res	Type	Atoms
3	A	437	2PE	O10-C11-C12-O13
3	A	437	2PE	C12-C11-O10-C9
3	A	436	2PE	C12-C11-O10-C9
2	A	434	C8E	C20-C19-O18-C17
2	A	446	C8E	C7-C8-O9-C10
3	A	438	2PE	C27-C26-O25-C24
3	A	437	2PE	C20-C21-O22-C23
2	A	433	C8E	C17-C16-O15-C14
2	A	443	C8E	O9-C10-C11-O12
2	A	443	C8E	C13-C14-O15-C16
2	A	439	C8E	C14-C13-O12-C11
2	A	434	C8E	O15-C16-C17-O18
2	A	446	C8E	C10-C11-O12-C13
2	A	432	C8E	O15-C16-C17-O18
3	A	437	2PE	C14-C15-O16-C17
2	A	435	C8E	O15-C16-C17-O18

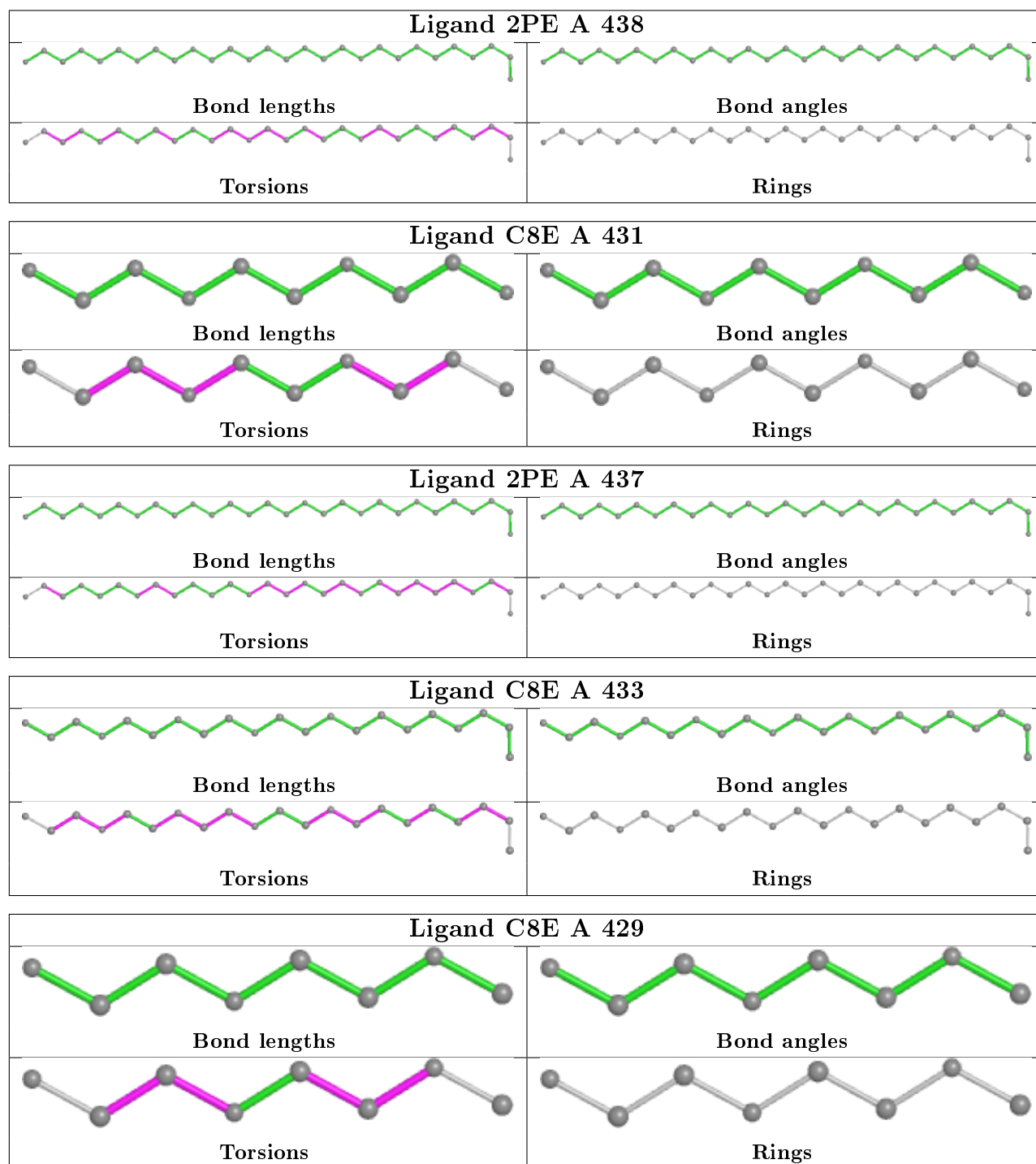
There are no ring outliers.

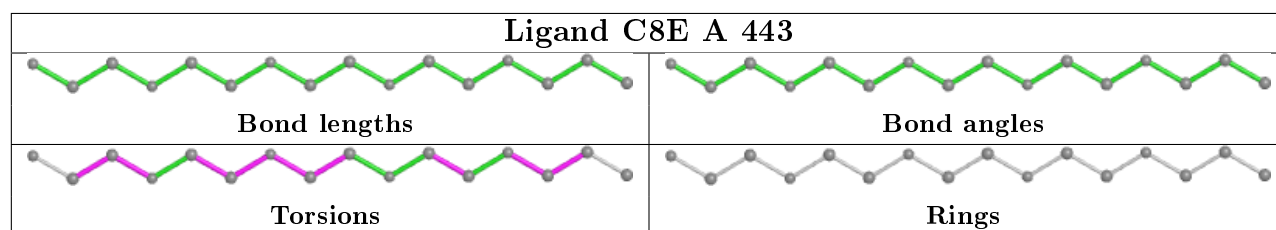
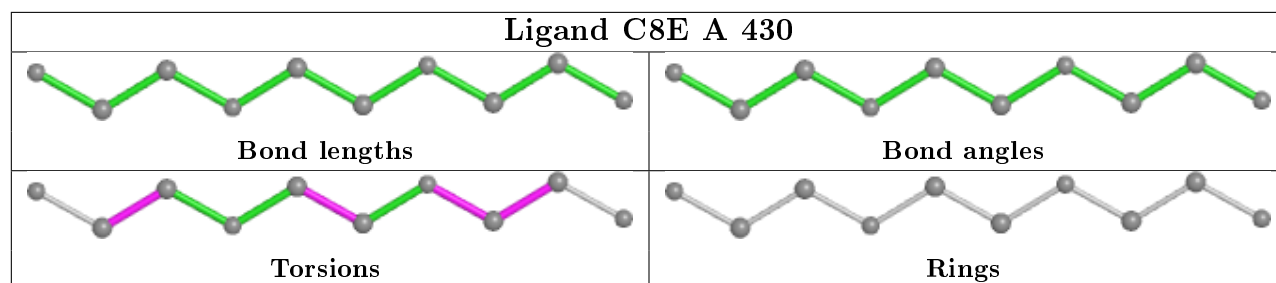
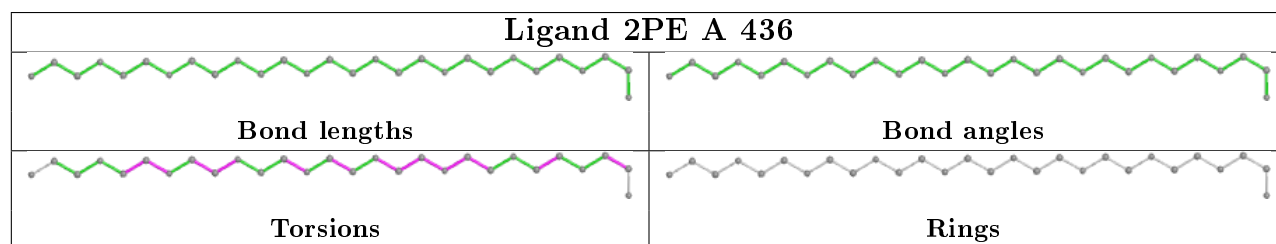
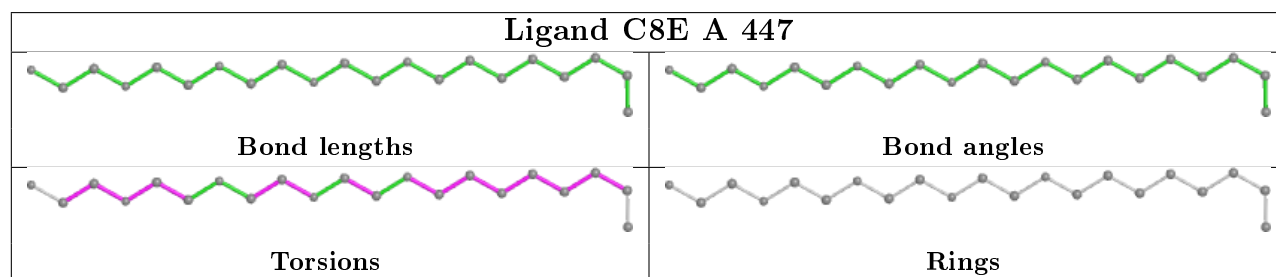
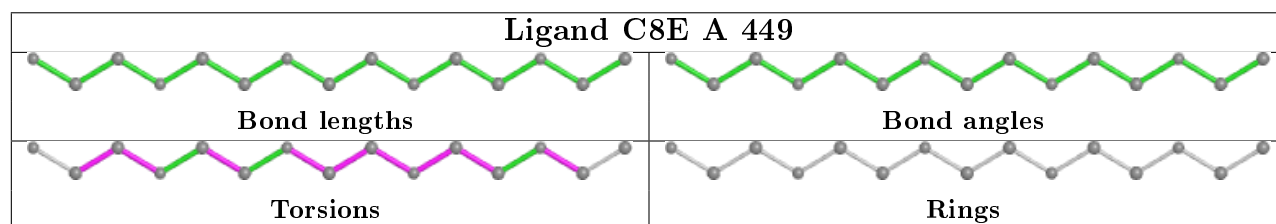
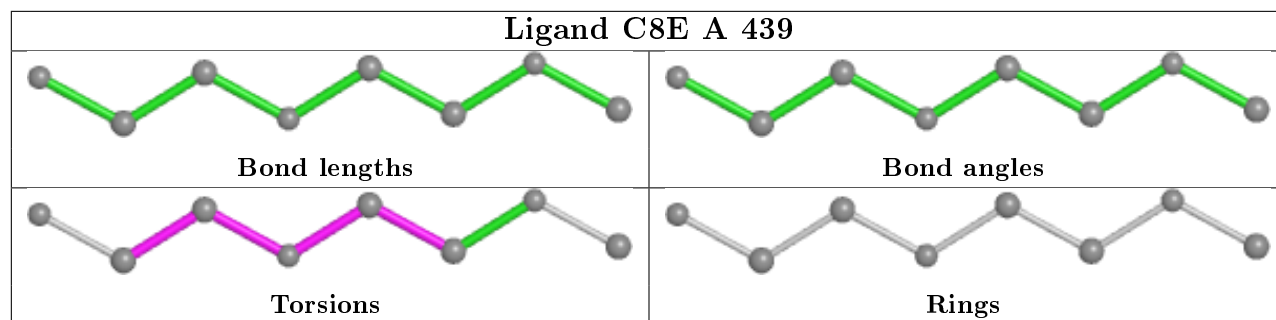
10 monomers are involved in 22 short contacts:

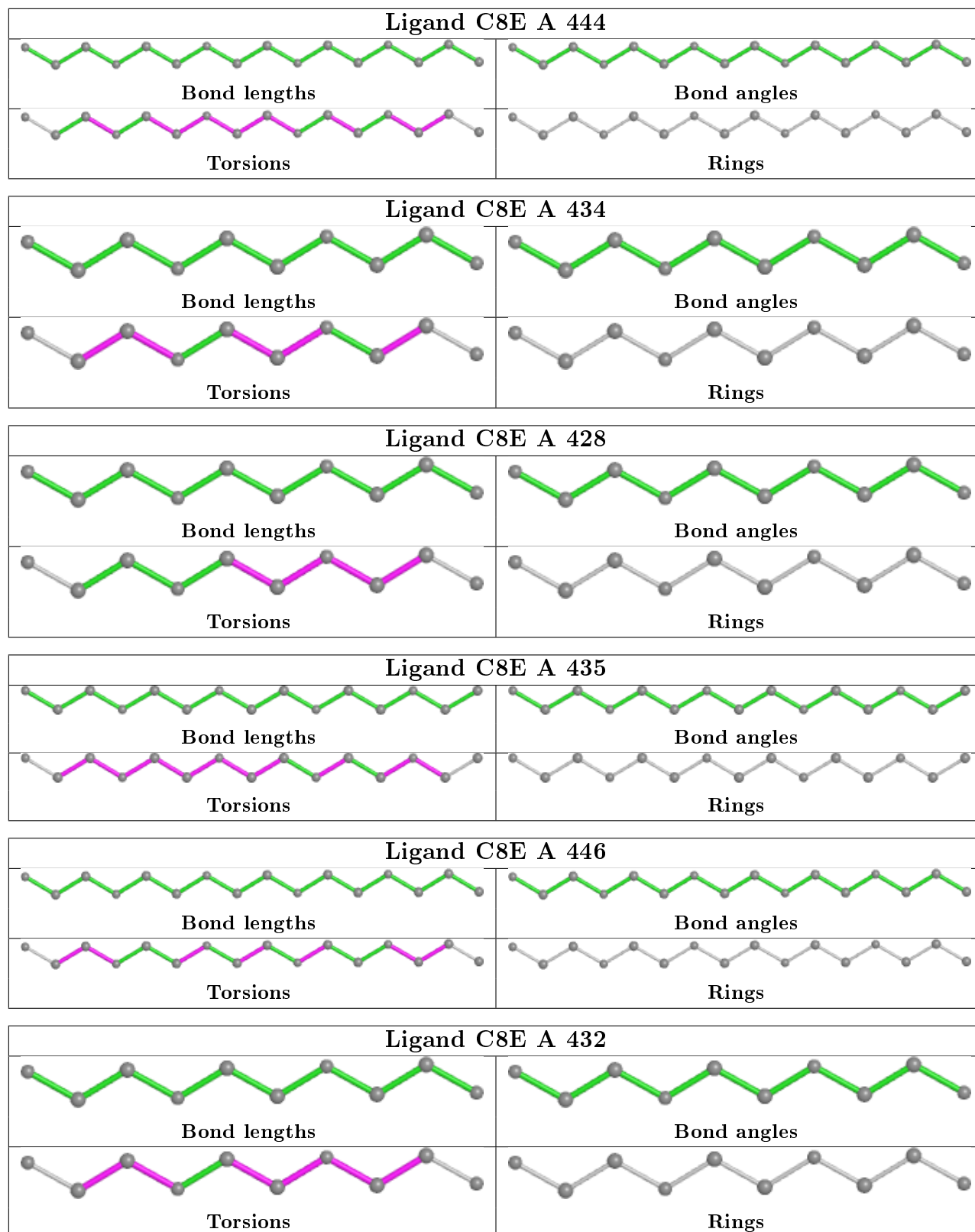
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	438	2PE	2	0
2	A	431	C8E	1	0
3	A	437	2PE	8	0
2	A	433	C8E	3	0
2	A	429	C8E	1	0
2	A	447	C8E	3	0
3	A	436	2PE	1	0
2	A	443	C8E	1	0
2	A	444	C8E	1	0
2	A	446	C8E	2	0

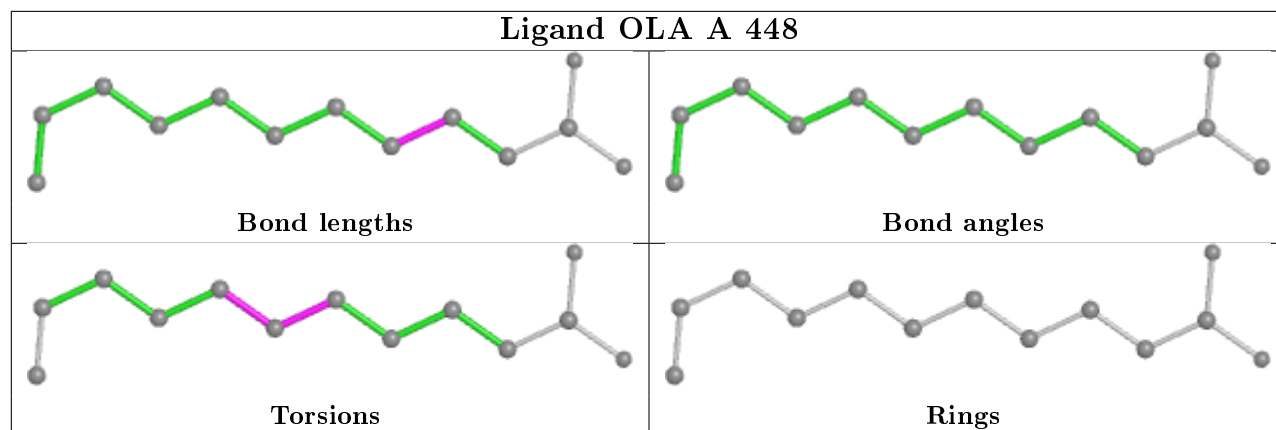
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	408/427 (95%)	0.07	16 (3%)	39 44	9, 15, 34, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	HIS	9.6
1	A	247	PHE	7.1
1	A	252	LEU	6.1
1	A	250	TYR	5.7
1	A	249	ASN	5.3
1	A	424	HIS	5.2
1	A	246	ALA	5.2
1	A	248	ASN	3.7
1	A	245	ARG	3.7
1	A	319	GLU	3.1
1	A	251	GLY	2.7
1	A	423	HIS	2.6
1	A	174	PRO	2.6
1	A	318	HIS	2.5
1	A	90	ASP	2.3
1	A	179	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

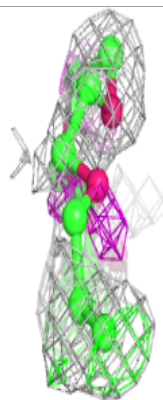
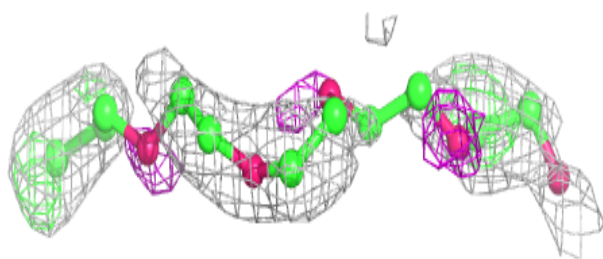
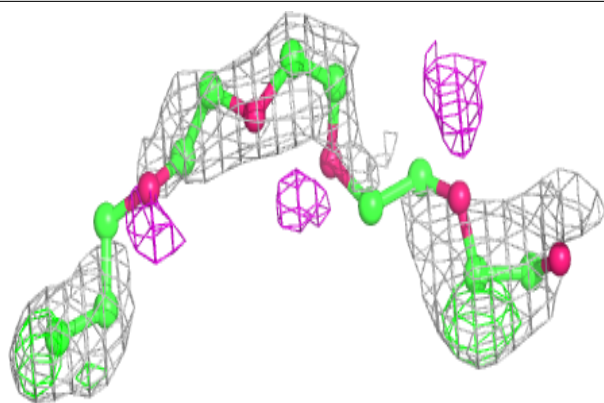
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C8E	A	444	16/21	0.36	0.36	40,70,80,80	0
2	C8E	A	446	16/21	0.42	0.43	73,83,86,87	0
2	C8E	A	447	21/21	0.44	0.38	62,69,71,71	21
2	C8E	A	433	21/21	0.54	0.24	30,49,69,70	0
2	C8E	A	443	16/21	0.61	0.35	47,74,82,82	0
2	C8E	A	439	8/21	0.63	0.16	56,58,65,66	0
2	C8E	A	431	10/21	0.72	0.23	64,70,75,75	0
3	2PE	A	437	28/28	0.73	0.17	53,60,72,75	0
3	2PE	A	438	28/28	0.73	0.18	40,58,68,71	0
2	C8E	A	435	15/21	0.74	0.17	56,65,74,75	0
2	C8E	A	434	10/21	0.74	0.23	48,53,58,61	0
2	C8E	A	428	10/21	0.76	0.19	32,56,59,64	0
5	NA	A	445	1/1	0.77	0.14	32,32,32,32	0
2	C8E	A	429	8/21	0.78	0.24	49,50,59,59	0
5	NA	A	442	1/1	0.79	0.10	48,48,48,48	0
3	2PE	A	436	28/28	0.79	0.16	35,50,64,65	0
2	C8E	A	430	10/21	0.79	0.16	42,49,54,55	0
2	C8E	A	449	15/21	0.79	0.17	30,51,66,67	0
2	C8E	A	432	10/21	0.79	0.28	57,60,67,70	0
6	OLA	A	448	13/20	0.92	0.13	20,26,42,42	0
4	NI	A	440	1/1	0.98	0.36	20,20,20,20	0
4	NI	A	441	1/1	0.99	0.33	19,19,19,19	0

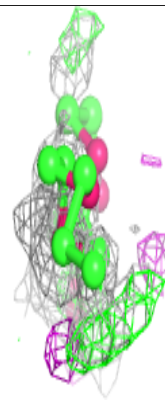
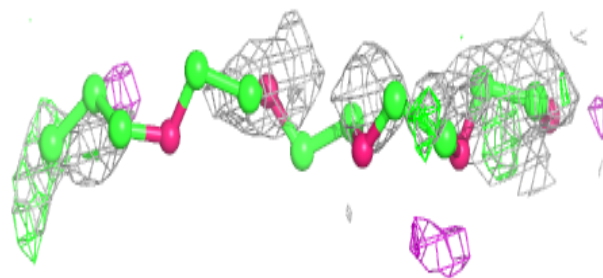
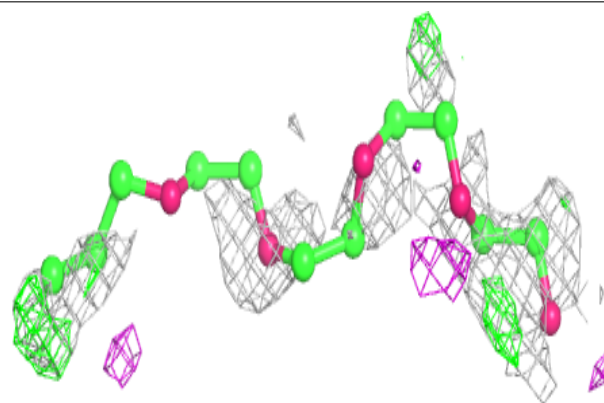
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E A 444:

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

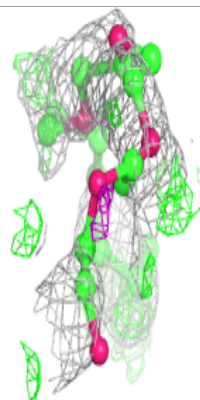
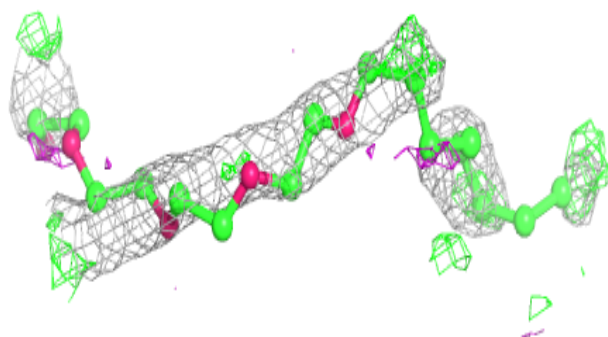
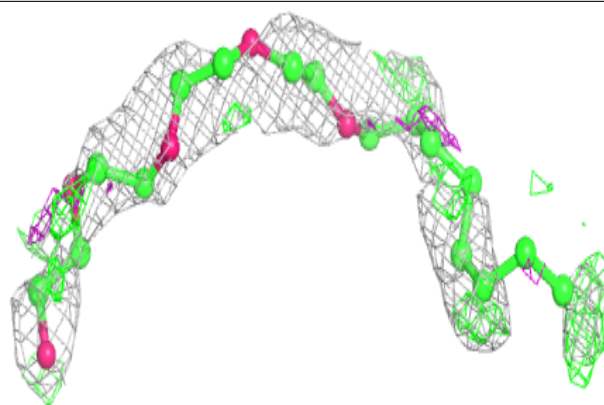
**Electron density around C8E A 446:**

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

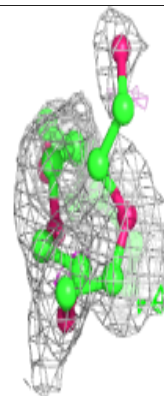
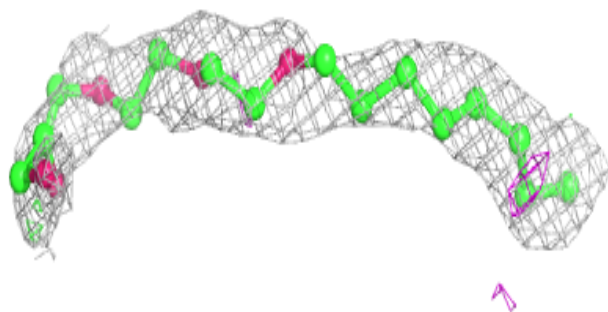
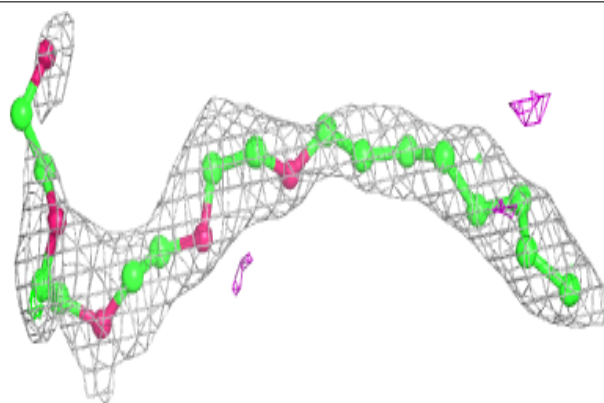


Electron density around C8E A 447:

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

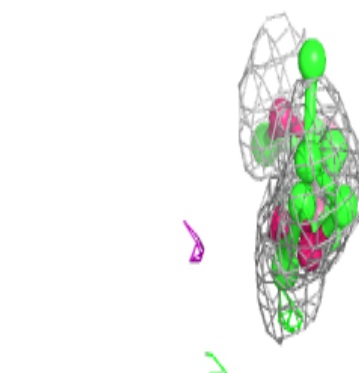
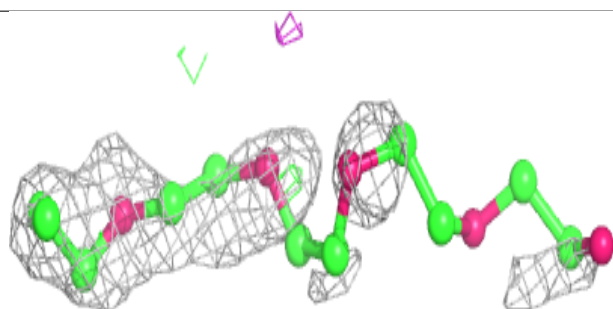
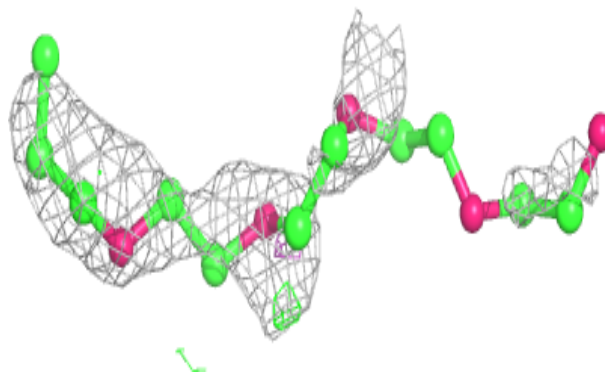
**Electron density around C8E A 433:**

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

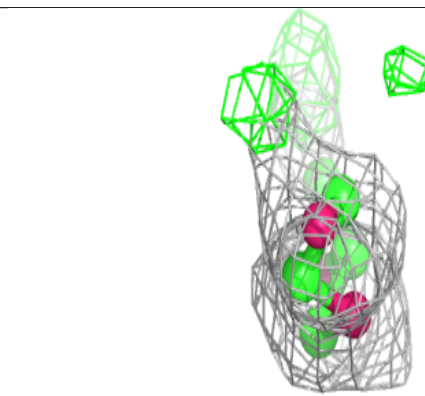
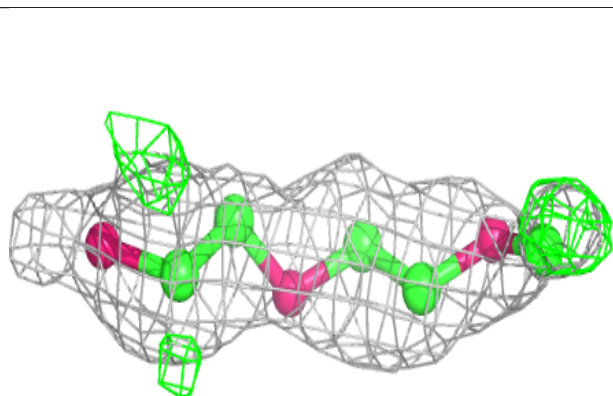
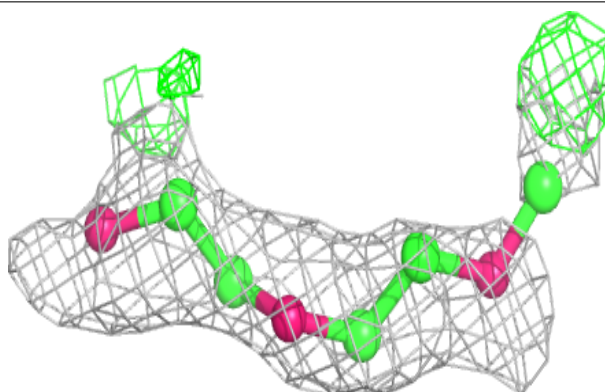


Electron density around C8E A 443:

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

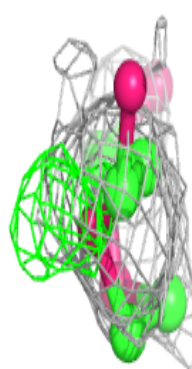
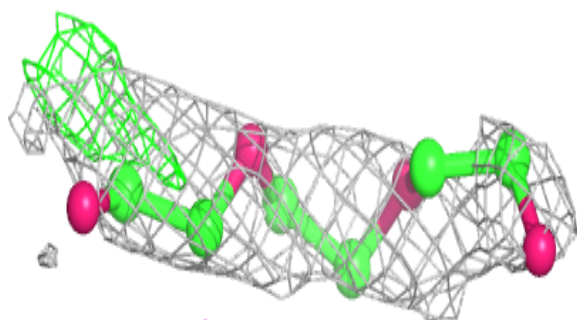
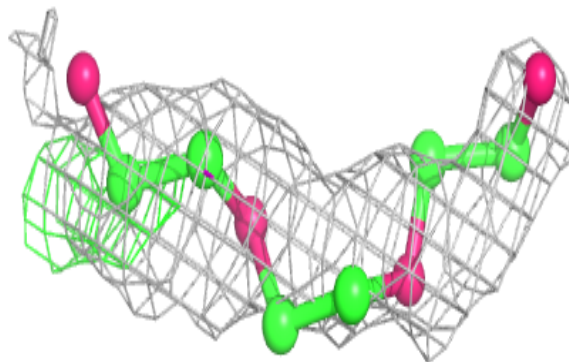
**Electron density around C8E A 439:**

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

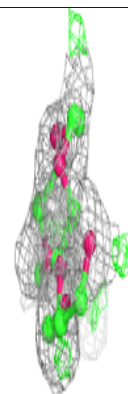
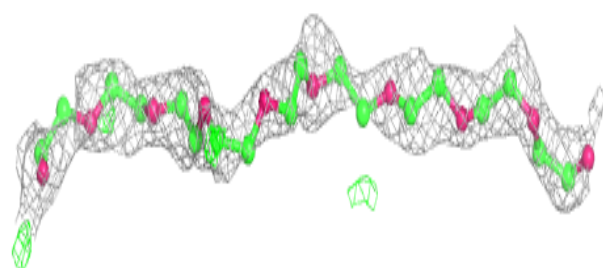
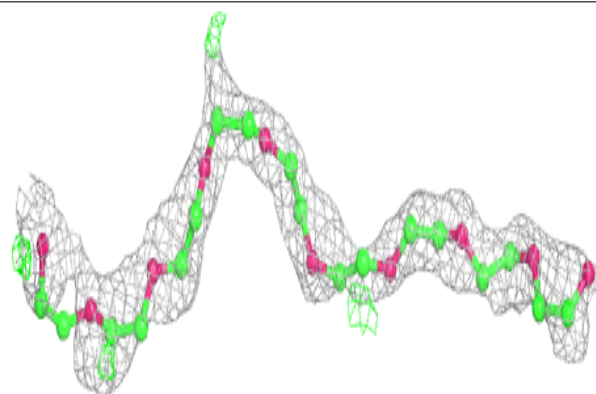


Electron density around C8E A 431:

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

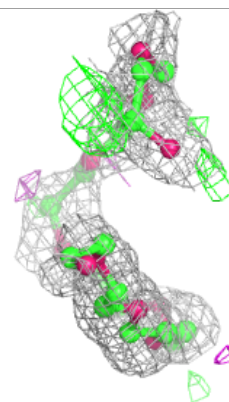
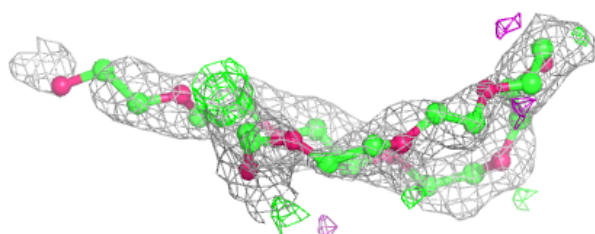
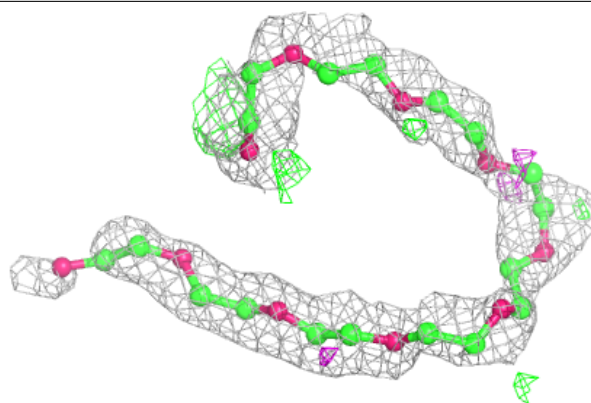
**Electron density around 2PE A 437:**

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

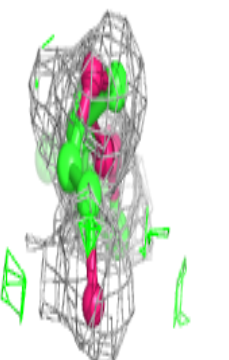
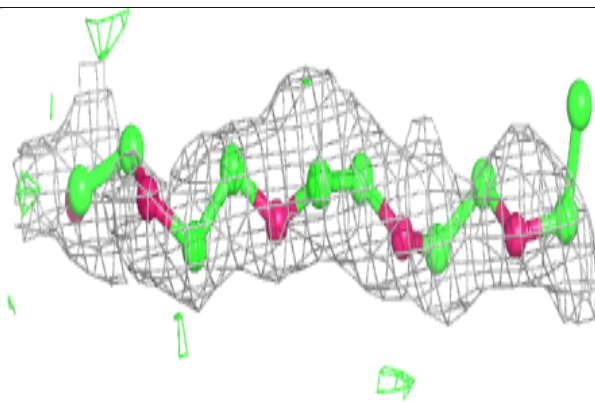
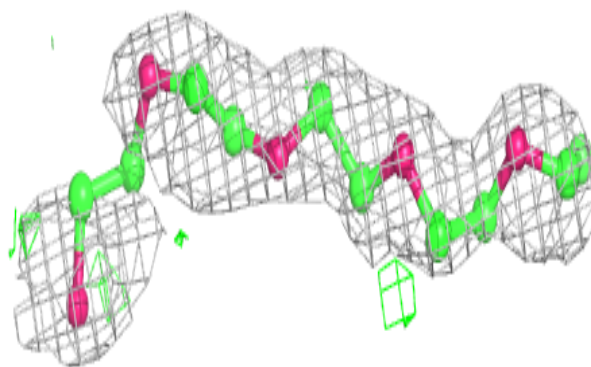


Electron density around 2PE A 438:

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

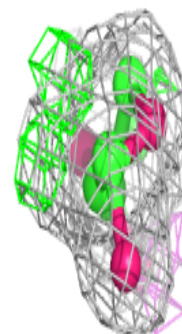
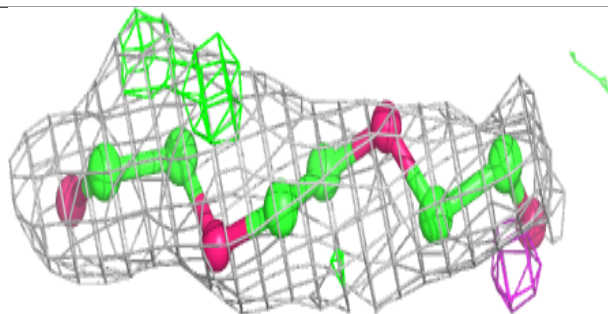
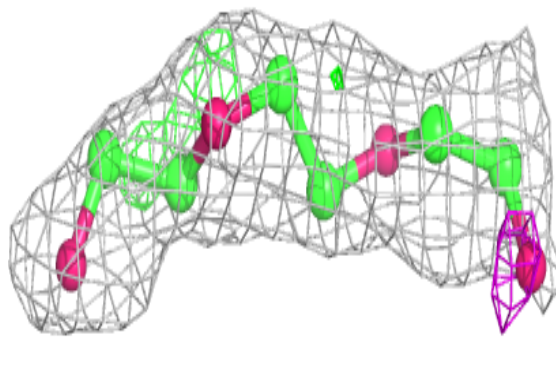
**Electron density around C8E A 435:**

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

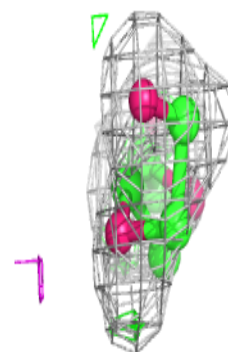
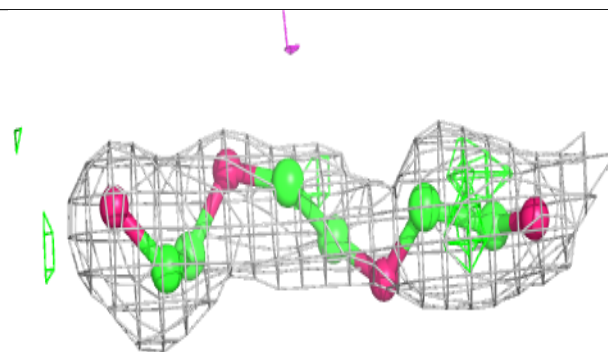
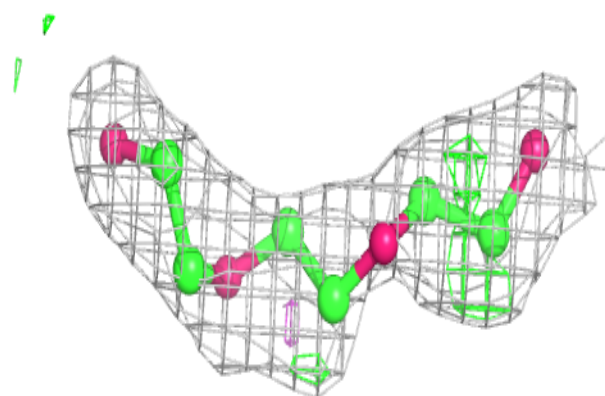


Electron density around C8E A 434:

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

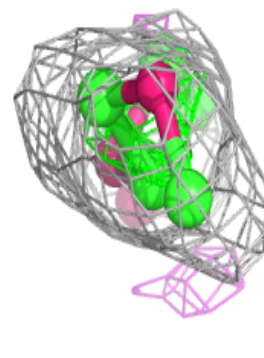
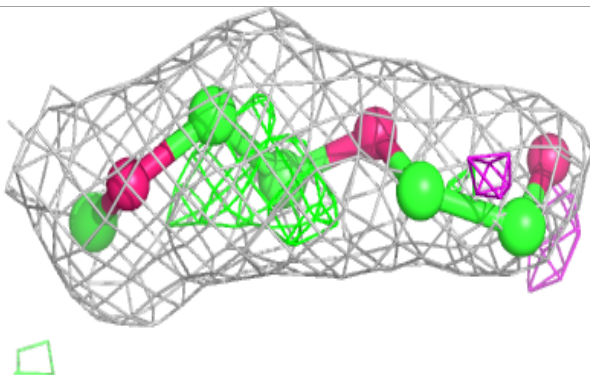
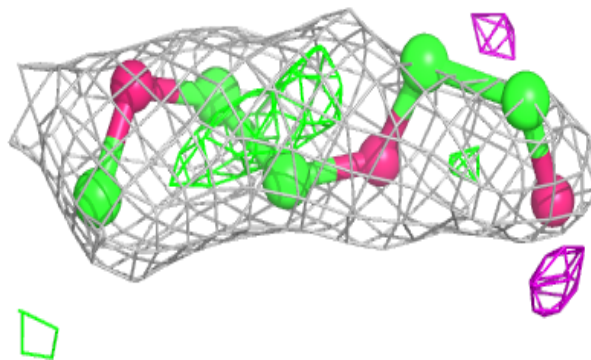
**Electron density around C8E A 428:**

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

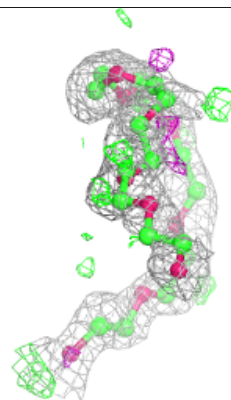
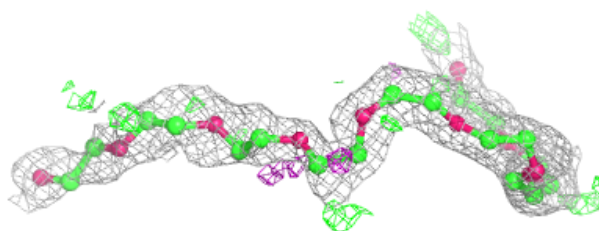
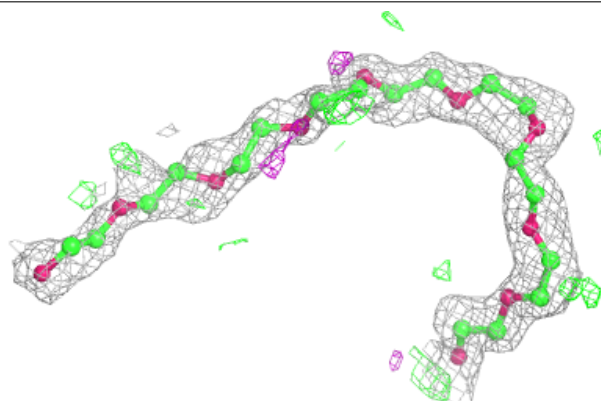


Electron density around C8E A 429:

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

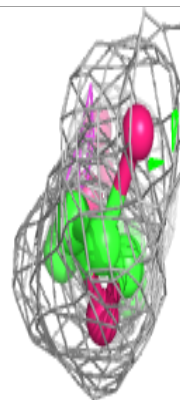
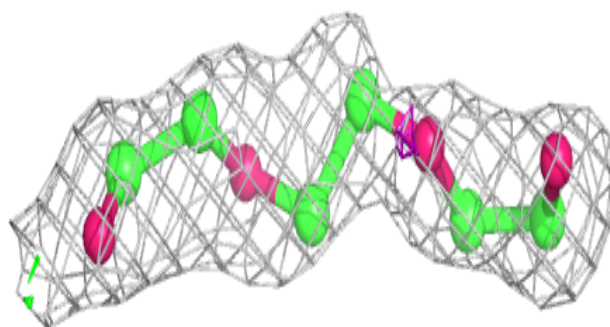
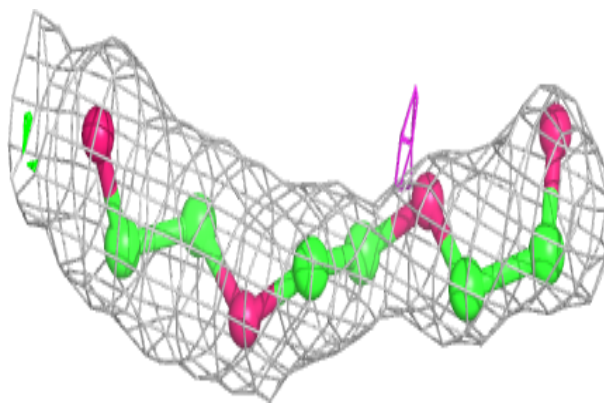
**Electron density around 2PE A 436:**

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

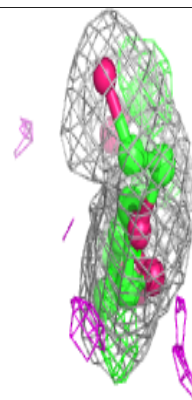
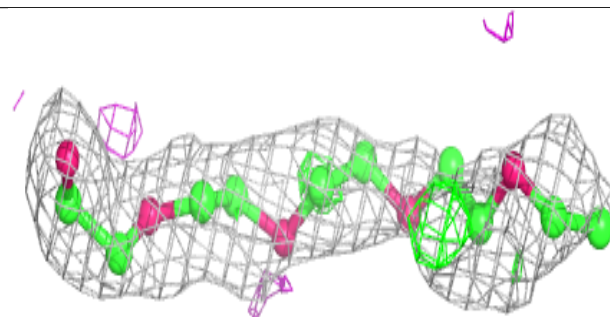
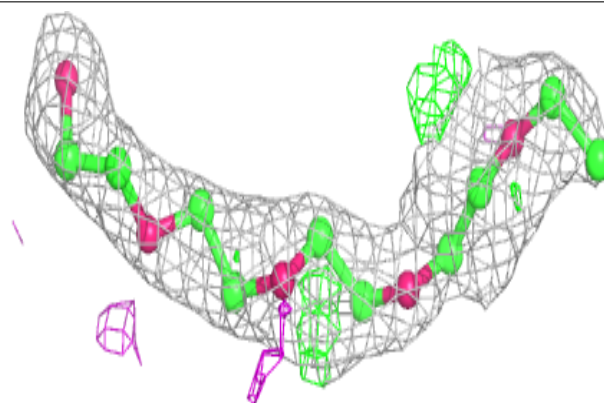


Electron density around C8E A 430:

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

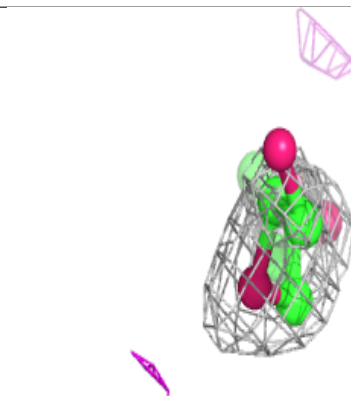
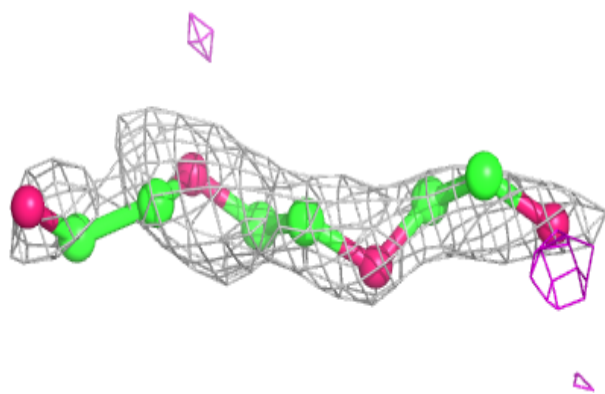
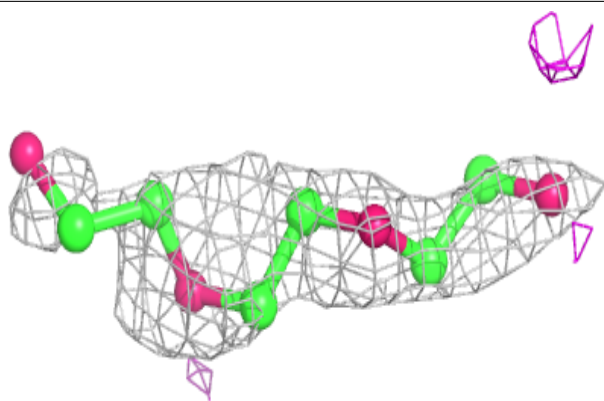
**Electron density around C8E A 449:**

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

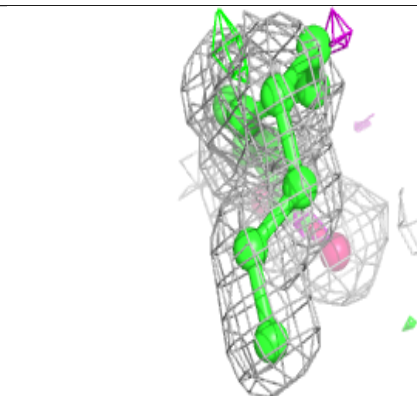
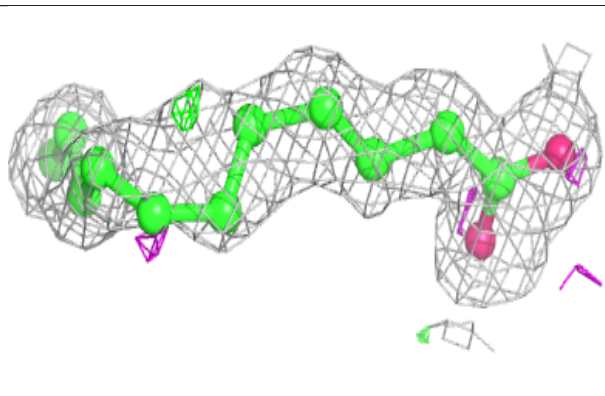
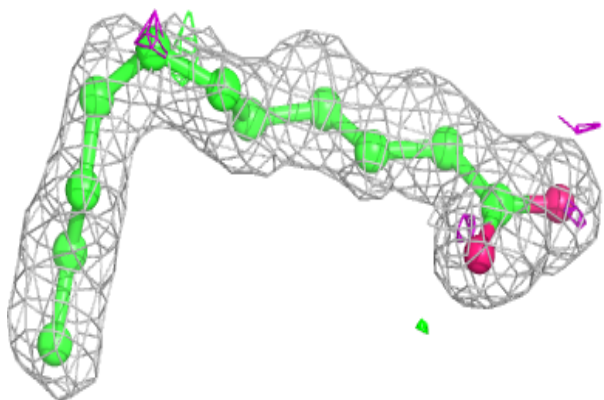


Electron density around C8E A 432:

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

**Electron density around OLA A 448:**

$2mF_o-DF_c$ (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.