



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 6EHB / pdb_00006ehb
Title : OmpU, an outer membrane protein, of Vibrio cholerae
Authors : van den berg, B.; Pathania, M.
Deposited on : 2017-09-13
Resolution : 1.55 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

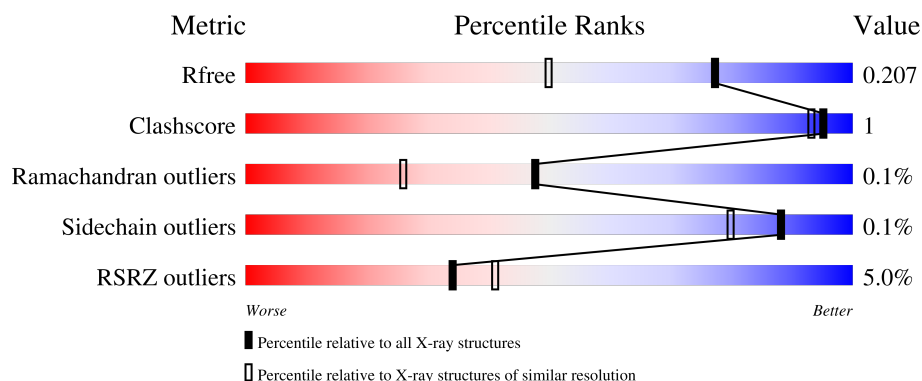
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	320	6% 93% 7% .
1	B	320	5% 89% 10% ..
1	C	320	4% 95% .

2 Entry composition ⓘ

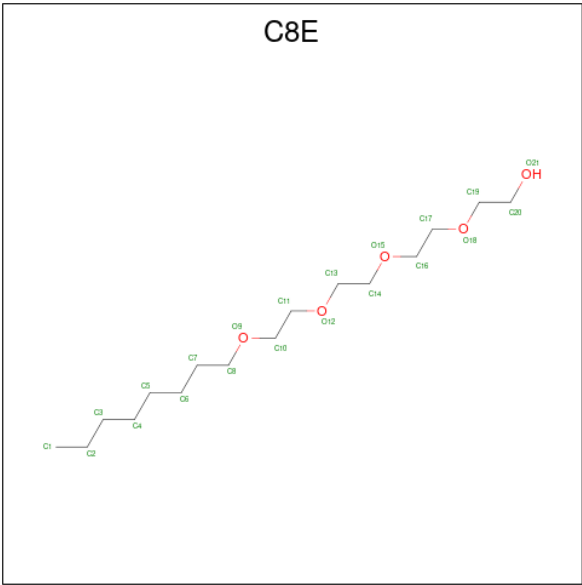
There are 3 unique types of molecules in this entry. The entry contains 8182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Outer membrane protein U.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	1	0
			2434	1518	402	509	5			
1	B	317	Total	C	N	O	S	0	4	0
			2444	1529	401	509	5			
1	C	320	Total	C	N	O	S	0	2	0
			2463	1537	406	515	5			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			6	6		
2	A	1	Total	C	O	0
			12	10	2	
2	A	1	Total	C	O	0
			11	10	1	

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 5 5	0	0
2	A	1	Total C O 9 6 3	0	0
2	A	1	Total C O 10 9 1	0	0
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C O 9 6 3	0	0
2	B	1	Total C O 9 8 1	0	0
2	B	1	Total C O 11 10 1	0	0
2	B	1	Total C O 4 3 1	0	0
2	B	1	Total C O 9 6 3	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C O 7 6 1	0	0
2	C	1	Total C 5 5	0	0
2	C	1	Total C O 14 12 2	0	0
2	C	1	Total C O 10 9 1	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C O 11 10 1	0	0
2	C	1	Total C O 10 9 1	0	0
2	C	1	Total C O 14 9 5	0	0

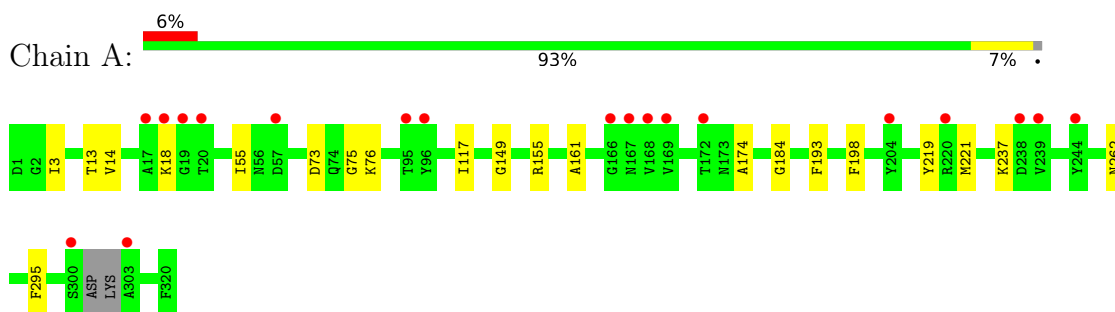
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 213	O 213	0	0
3	B	183	Total 183	O 183	0	0
3	C	243	Total 243	O 243	0	0

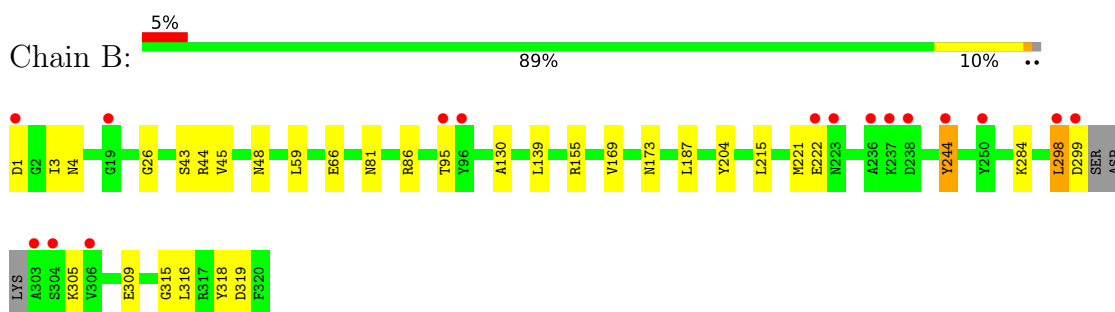
3 Residue-property plots [i](#)

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

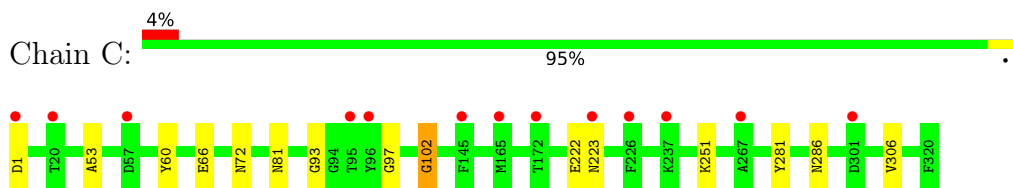
- Molecule 1: Outer membrane protein U



- Molecule 1: Outer membrane protein U



- Molecule 1: Outer membrane protein U



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.72Å 153.84Å 66.17Å 90.00° 102.32° 90.00°	Depositor
Resolution (Å)	49.49 – 1.55 49.49 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.49-1.55) 97.1 (49.49-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.170 , 0.199 0.182 , 0.207	Depositor DCC
R_{free} test set	8445 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8182	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

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	1.53	8/2479 (0.3%)	1.23	4/3346 (0.1%)
1	B	1.54	15/2499 (0.6%)	1.24	6/3374 (0.2%)
1	C	1.48	7/2510 (0.3%)	1.22	3/3389 (0.1%)
All	All	1.51	30/7488 (0.4%)	1.23	13/10109 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	VAL	CA-C	7.28	1.59	1.52
1	B	45	VAL	N-CA	-6.52	1.38	1.46
1	A	149	GLY	N-CA	6.43	1.54	1.45
1	B	221	MET	CA-C	-6.27	1.45	1.52
1	B	59	LEU	N-CA	6.22	1.53	1.46
1	A	13	THR	C-O	-6.21	1.16	1.24
1	B	86	ARG	CZ-NH1	-6.10	1.24	1.32
1	A	295	PHE	CA-C	-6.07	1.45	1.52
1	B	215	LEU	CA-C	-6.06	1.45	1.52
1	B	66	GLU	CA-C	-6.03	1.45	1.52
1	B	26	GLY	C-N	-5.98	1.26	1.33
1	C	72	ASN	CA-CB	-5.91	1.47	1.53
1	B	44	ARG	CA-C	-5.88	1.45	1.52
1	B	318	TYR	N-CA	-5.88	1.39	1.46
1	C	93	GLY	N-CA	-5.67	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ASN	CG-ND2	5.54	1.44	1.33
1	C	53	ALA	CA-CB	-5.53	1.45	1.53
1	B	284	LYS	N-CA	-5.36	1.40	1.45
1	B	315	GLY	CA-C	-5.35	1.47	1.51
1	A	198	PHE	CA-C	-5.33	1.46	1.52
1	C	60	TYR	CA-C	5.33	1.59	1.52
1	A	55	ILE	CA-CB	-5.30	1.49	1.55
1	C	1	ASP	C-O	5.23	1.34	1.23
1	A	184	GLY	CA-C	-5.19	1.45	1.51
1	B	319	ASP	N-CA	5.17	1.52	1.46
1	C	66	GLU	CA-C	-5.16	1.46	1.52
1	B	284	LYS	CA-C	5.13	1.57	1.52
1	A	117	ILE	N-CA	-5.10	1.40	1.46
1	C	97	GLY	N-CA	5.10	1.52	1.45
1	A	14	VAL	C-O	-5.04	1.19	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	ASN	N-CA-C	6.84	120.93	112.59
1	A	155	ARG	CG-CD-NE	-5.77	99.31	112.00
1	A	149	GLY	O-C-N	-5.74	119.19	123.61
1	B	155	ARG	CG-CD-NE	-5.72	99.42	112.00
1	C	306	VAL	O-C-N	5.63	127.63	121.83
1	B	48	ASN	N-CA-C	5.53	117.80	109.23
1	C	102	GLY	N-CA-C	-5.52	105.22	111.85
1	A	75	GLY	N-CA-C	5.51	122.93	115.32
1	B	43	SER	CA-C-O	-5.45	115.77	121.55
1	B	130	ALA	N-CA-C	5.34	117.51	111.11
1	B	298	LEU	N-CA-C	5.33	116.77	111.07
1	B	244	TYR	N-CA-C	5.17	117.25	109.23
1	A	262	ASN	CB-CG-ND2	5.05	123.98	116.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	102	GLY	Mainchain
1	C	81	ASN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2434	0	2267	7	0
1	B	2444	0	2285	8	3
1	C	2463	0	2293	3	0
2	A	61	0	87	1	0
2	B	55	0	76	1	0
2	C	86	0	140	3	2
3	A	213	0	0	1	0
3	B	183	0	0	2	1
3	C	243	0	0	0	1
All	All	8182	0	7148	18	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (18) 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:C:281:TYR:HB2	2:C:409:C8E:H131	1.80	0.64
1:B:316:LEU:HB2	2:B:401:C8E:H11	1.82	0.59
1:B:139:LEU:HD11	2:C:404:C8E:H61	1.88	0.56
1:A:193:PHE:HB3	2:A:403:C8E:H31	1.91	0.52
1:B:187:LEU:HD12	1:B:204[A]:TYR:CZ	2.45	0.52
1:A:219:TYR:CE2	1:A:221:MET:HE2	2.44	0.52
1:B:95:THR:OG1	3:B:501:HOH:O	2.19	0.51
1:B:1:ASP:HB3	1:B:4:ASN:O	2.10	0.51
1:B:3:ILE:HD11	3:B:569:HOH:O	2.11	0.50
1:B:298:LEU:O	1:B:299:ASP:C	2.54	0.50
1:C:222:GLU:O	1:C:223:ASN:HB2	2.11	0.50
1:A:3:ILE:HD11	3:A:627:HOH:O	2.12	0.49
1:A:219:TYR:CD2	1:A:221:MET:HE2	2.48	0.48
1:A:161:ALA:HB1	1:A:174:ALA:CB	2.47	0.45
1:C:251:LYS:HE2	2:C:401:C8E:H13	1.98	0.45
1:B:305:LYS:O	1:B:309:GLU:HG2	2.18	0.43
1:A:161:ALA:HB1	1:A:174:ALA:HB2	2.01	0.42
1:A:73:ASP:HB3	1:A:76:LYS:O	2.20	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:TYR:OH	2:C:405:C8E:O9[1_656]	1.95	0.25
1:B:173:ASN:ND2	1:B:222:GLU:OE2[1_554]	2.01	0.19
3:B:674:HOH:O	3:C:727:HOH:O[1_655]	2.06	0.14
1:B:244:TYR:OH	2:C:405:C8E:C8[1_656]	2.08	0.12

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	315/320 (98%)	300 (95%)	14 (4%)	1 (0%)	36	18
1	B	317/320 (99%)	305 (96%)	12 (4%)	0	100	100
1	C	320/320 (100%)	306 (96%)	14 (4%)	0	100	100
All	All	952/960 (99%)	911 (96%)	40 (4%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LYS

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	243/244 (100%)	242 (100%)	1 (0%)	84	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	245/244 (100%)	245 (100%)	0	100	100
1	C	246/244 (101%)	246 (100%)	0	100	100
All	All	734/732 (100%)	733 (100%)	1 (0%)	88	80

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	74	GLN
1	A	254	GLN
1	B	40	GLN
1	B	173	ASN
1	B	210	GLN
1	B	211	ASN
1	B	254	GLN
1	B	274	ASN
1	C	4	ASN
1	C	5	GLN
1	C	74	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	C8E	A	404	-	4,4,20	0.50	0	3,3,19	1.35	0
2	C8E	C	403	-	4,4,20	0.18	0	3,3,19	0.56	0
2	C8E	A	407	-	7,7,20	0.57	0	6,6,19	0.79	0
2	C8E	C	404	-	13,13,20	0.62	0	12,12,19	0.72	0
2	C8E	A	402	-	11,11,20	0.43	0	10,10,19	0.38	0
2	C8E	B	401	-	7,7,20	0.23	0	6,6,19	0.59	0
2	C8E	A	405	-	8,8,20	0.55	0	7,7,19	0.77	0
2	C8E	C	402	-	6,6,20	0.59	0	5,5,19	0.58	0
2	C8E	C	407	-	10,10,20	0.70	0	9,9,19	1.00	1 (11%)
2	C8E	C	409	-	13,13,20	0.76	0	12,12,19	1.13	1 (8%)
2	C8E	A	401	-	5,5,20	0.36	0	4,4,19	0.56	0
2	C8E	B	406	-	3,3,20	0.49	0	2,2,19	1.38	0
2	C8E	C	401	-	7,7,20	0.49	0	6,6,19	0.93	0
2	C8E	B	403	-	8,8,20	0.69	0	7,7,19	0.71	0
2	C8E	A	406	-	9,9,20	0.58	0	8,8,19	0.80	0
2	C8E	B	402	-	4,4,20	0.15	0	3,3,19	0.46	0
2	C8E	B	407	-	8,8,20	0.61	0	7,7,19	0.69	0
2	C8E	C	406	-	6,6,20	0.31	0	5,5,19	0.34	0
2	C8E	C	408	-	9,9,20	0.65	0	8,8,19	0.97	0
2	C8E	B	405	-	10,10,20	0.61	0	9,9,19	0.35	0
2	C8E	C	405	-	9,9,20	0.51	0	8,8,19	0.74	0
2	C8E	A	403	-	10,10,20	0.56	0	9,9,19	0.72	0
2	C8E	B	404	-	8,8,20	0.48	0	7,7,19	0.59	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	C8E	A	404	-	-	2/2/2/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	C	403	-	-	1/2/2/18	-
2	C8E	A	407	-	-	0/5/5/18	-
2	C8E	C	404	-	-	4/11/11/18	-
2	C8E	A	402	-	-	2/9/9/18	-
2	C8E	B	401	-	-	1/5/5/18	-
2	C8E	A	405	-	-	4/6/6/18	-
2	C8E	C	402	-	-	0/4/4/18	-
2	C8E	C	407	-	-	3/8/8/18	-
2	C8E	C	409	-	-	4/11/11/18	-
2	C8E	A	401	-	-	0/3/3/18	-
2	C8E	B	406	-	-	0/0/1/18	-
2	C8E	C	401	-	-	3/5/5/18	-
2	C8E	B	403	-	-	4/6/6/18	-
2	C8E	A	406	-	-	1/7/7/18	-
2	C8E	B	402	-	-	0/2/2/18	-
2	C8E	B	407	-	-	2/6/6/18	-
2	C8E	C	406	-	-	2/4/4/18	-
2	C8E	C	408	-	-	6/7/7/18	-
2	C8E	B	405	-	-	0/8/8/18	-
2	C8E	C	405	-	-	0/7/7/18	-
2	C8E	A	403	-	-	2/8/8/18	-
2	C8E	B	404	-	-	0/6/6/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	407	C8E	C10-O9-C8	2.38	121.41	113.06
2	C	409	C8E	C13-O12-C11	2.30	123.34	113.26

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	C8E	O9-C10-C11-O12
2	A	406	C8E	C6-C7-C8-O9
2	A	405	C8E	O15-C16-C17-O18
2	B	407	C8E	O15-C16-C17-O18

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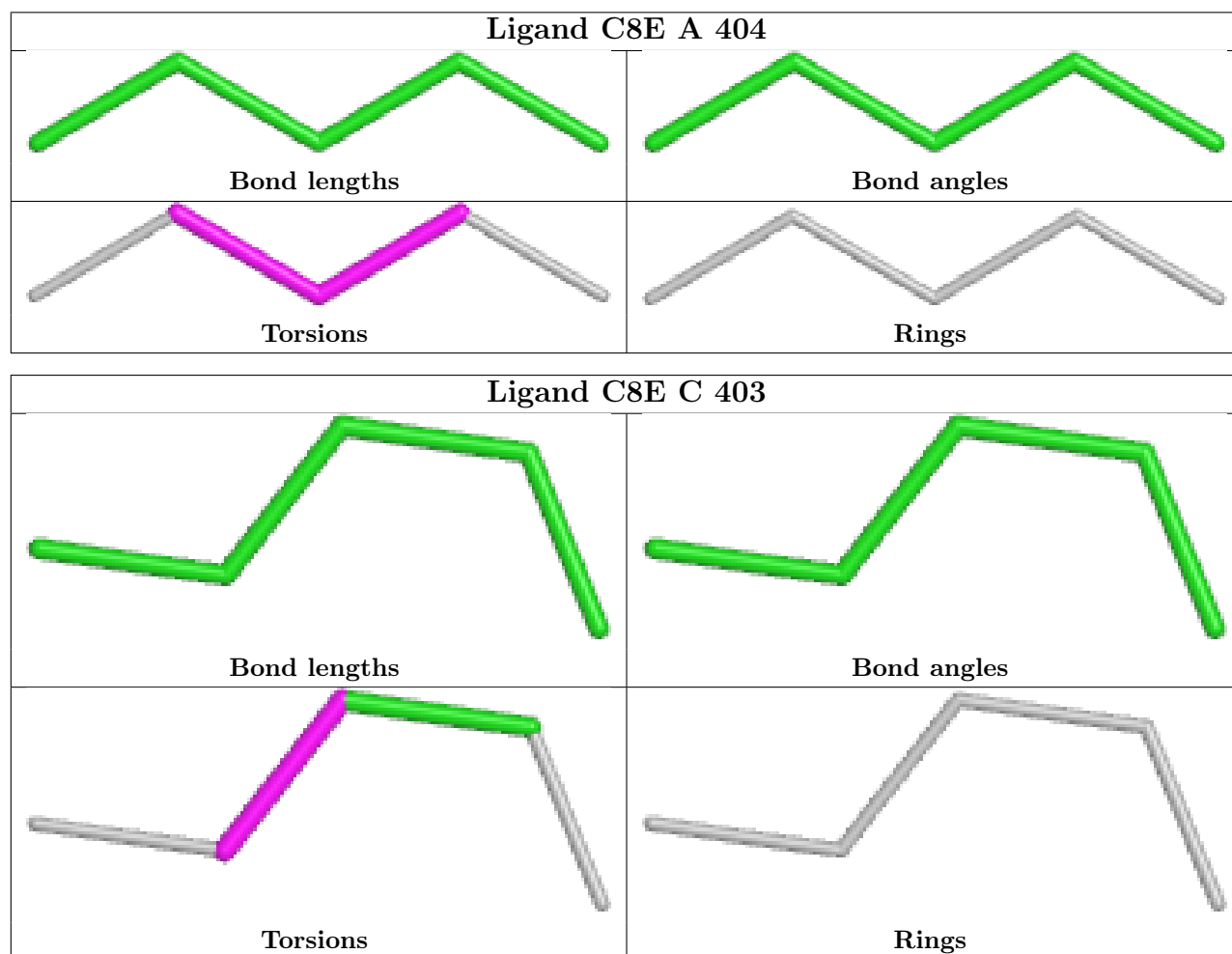
Mol	Chain	Res	Type	Atoms
2	C	404	C8E	C6-C7-C8-O9
2	C	407	C8E	C6-C7-C8-O9
2	C	408	C8E	C6-C7-C8-O9
2	C	404	C8E	C5-C6-C7-C8
2	C	408	C8E	C4-C5-C6-C7
2	C	401	C8E	C3-C4-C5-C6
2	C	404	C8E	C4-C5-C6-C7
2	B	403	C8E	O12-C13-C14-O15
2	B	401	C8E	C1-C2-C3-C4
2	C	409	C8E	O9-C10-C11-O12
2	C	401	C8E	C5-C6-C7-C8
2	A	403	C8E	C2-C3-C4-C5
2	C	408	C8E	C1-C2-C3-C4
2	C	408	C8E	C3-C4-C5-C6
2	C	409	C8E	O12-C13-C14-O15
2	A	404	C8E	C3-C4-C5-C6
2	C	406	C8E	C1-C2-C3-C4
2	C	403	C8E	C2-C3-C4-C5
2	C	408	C8E	C2-C3-C4-C5
2	C	407	C8E	C11-C10-O9-C8
2	B	407	C8E	O18-C19-C20-O21
2	B	403	C8E	C14-C13-O12-C11
2	A	405	C8E	C16-C17-O18-C19
2	B	403	C8E	C11-C10-O9-C8
2	A	405	C8E	O18-C19-C20-O21
2	C	409	C8E	C14-C13-O12-C11
2	B	403	C8E	O9-C10-C11-O12
2	C	401	C8E	C1-C2-C3-C4
2	C	406	C8E	C3-C4-C5-C6
2	C	409	C8E	O15-C16-C17-O18
2	C	407	C8E	C2-C3-C4-C5
2	A	404	C8E	C2-C3-C4-C5
2	C	408	C8E	C5-C6-C7-C8
2	A	403	C8E	C6-C7-C8-O9
2	A	405	C8E	C13-C14-O15-C16
2	C	404	C8E	O9-C10-C11-O12
2	A	402	C8E	C10-C11-O12-C13

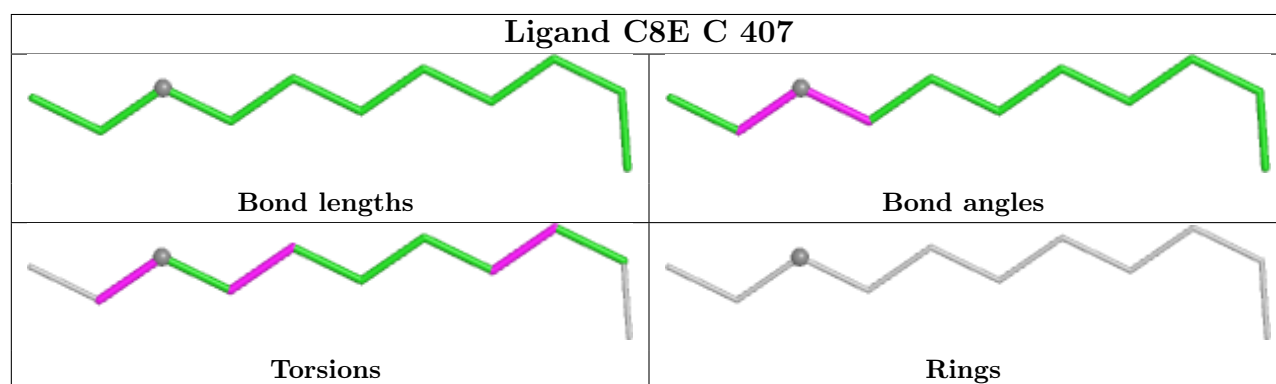
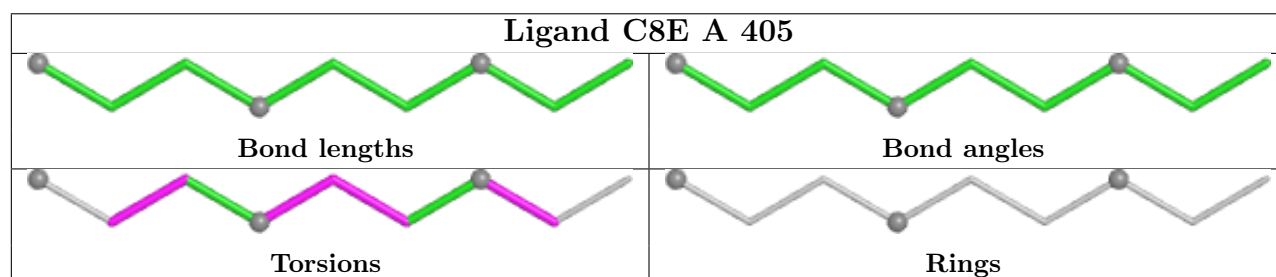
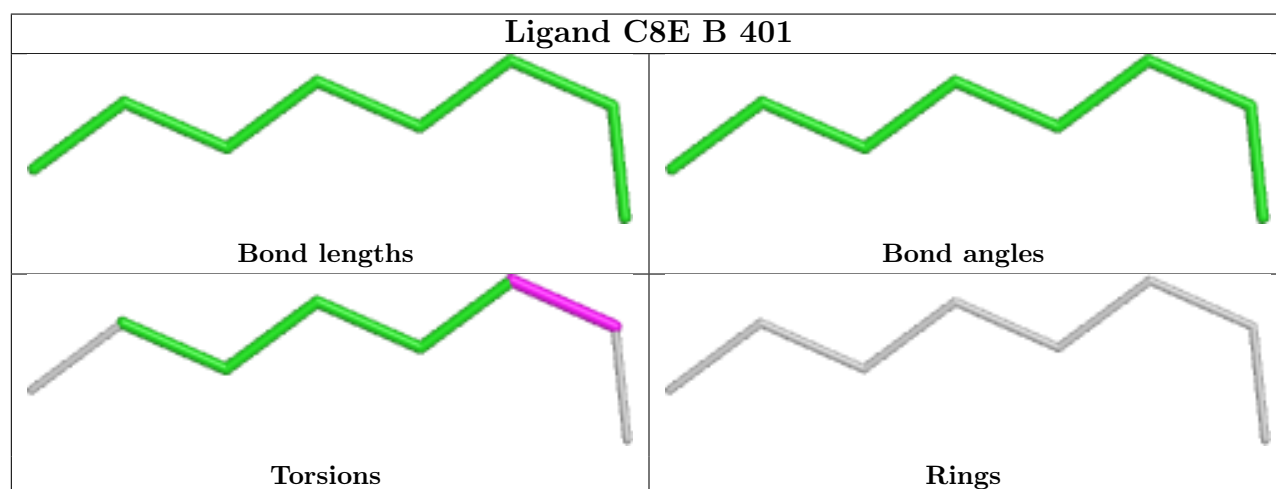
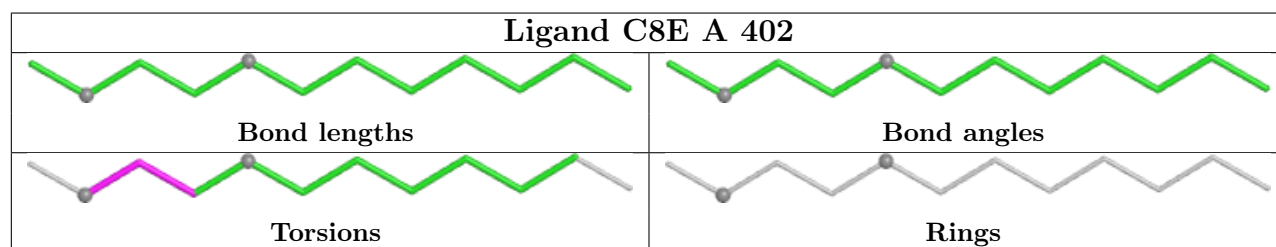
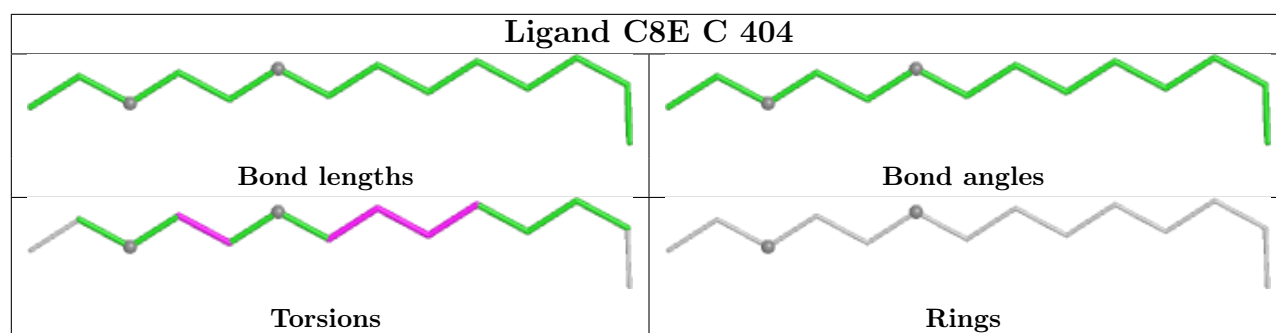
There are no ring outliers.

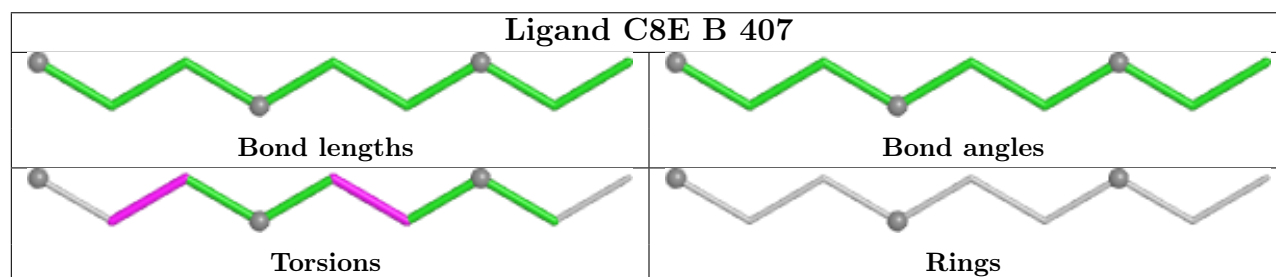
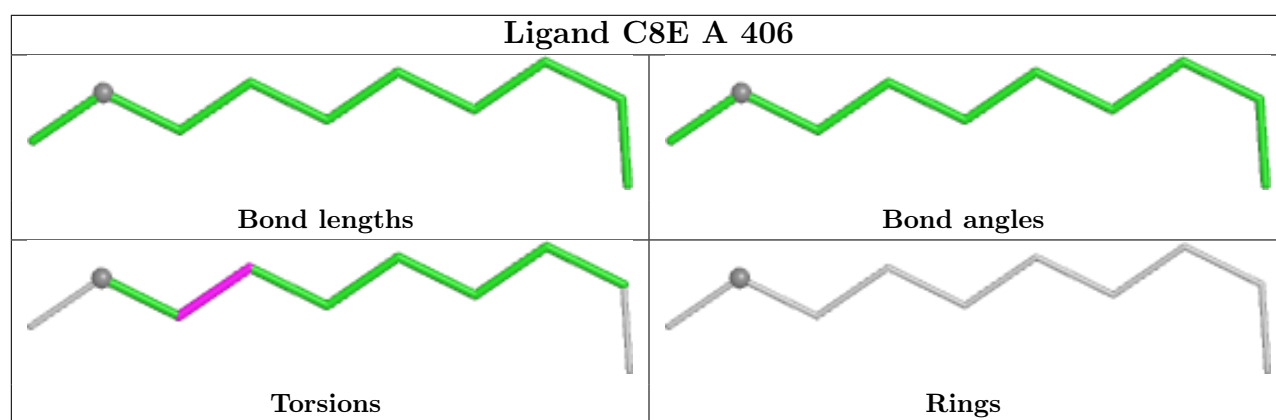
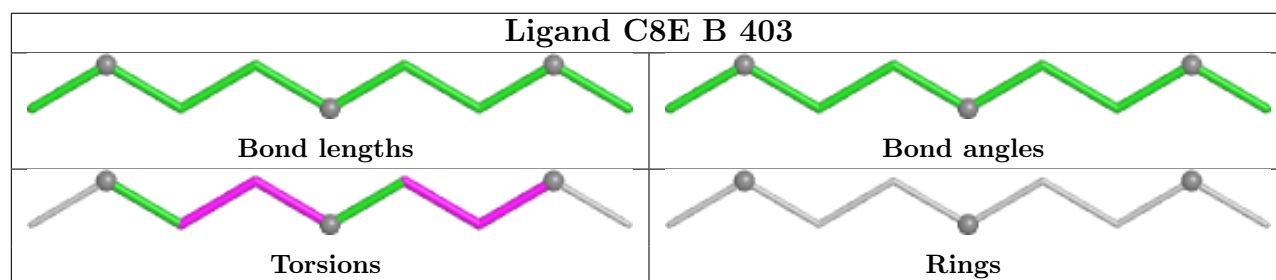
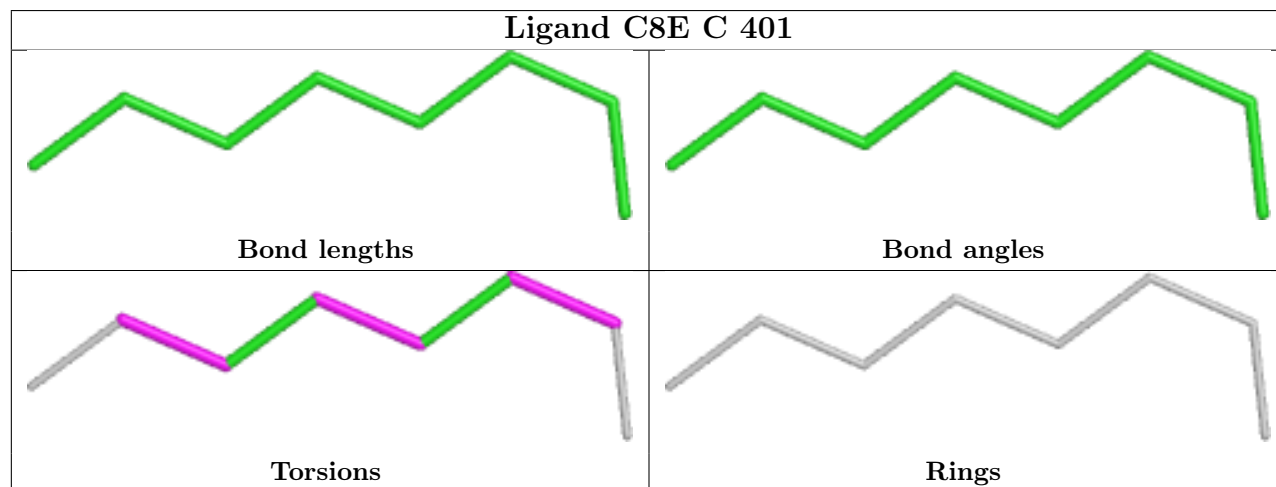
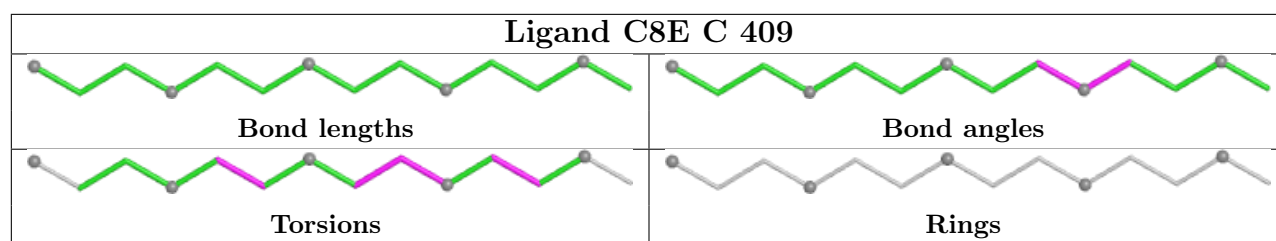
6 monomers are involved in 7 short contacts:

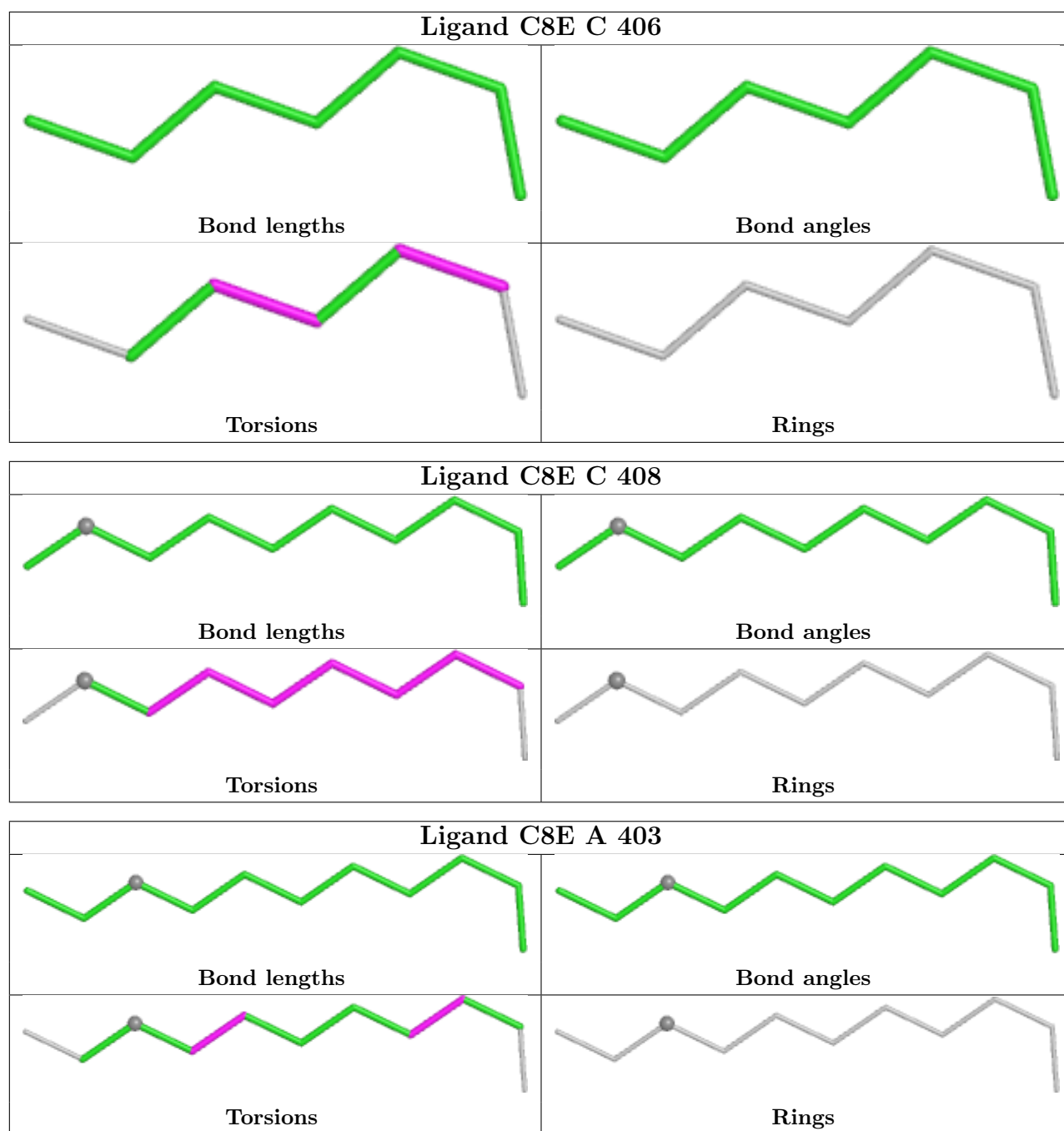
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	C8E	1	0
2	B	401	C8E	1	0
2	C	409	C8E	1	0
2	C	401	C8E	1	0
2	C	405	C8E	0	2
2	A	403	C8E	1	0

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.









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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	318/320 (99%)	0.16	19 (5%)	27 33	11, 20, 40, 65	1 (0%)
1	B	317/320 (99%)	0.35	16 (5%)	34 41	13, 22, 40, 72	4 (1%)
1	C	320/320 (100%)	0.02	13 (4%)	41 49	10, 18, 37, 57	2 (0%)
All	All	955/960 (99%)	0.18	48 (5%)	34 41	10, 20, 40, 72	7 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	ALA	6.4
1	B	1	ASP	4.3
1	A	303	ALA	4.1
1	A	244	TYR	4.0
1	A	96	TYR	3.6
1	A	19	GLY	3.5
1	A	18	LYS	3.5
1	C	165	MET	3.3
1	B	299	ASP	3.3
1	B	304	SER	3.3
1	C	96	TYR	3.1
1	A	20	THR	3.1
1	B	244	TYR	3.0
1	C	267	ALA	3.0
1	A	204	TYR	2.9
1	C	172	THR	2.8
1	A	167	ASN	2.8
1	C	145	PHE	2.8
1	B	222	GLU	2.8
1	C	226	PHE	2.7
1	A	169	VAL	2.7
1	A	239	VAL	2.6
1	A	168	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	237	LYS	2.6
1	A	95	THR	2.5
1	A	17	ALA	2.4
1	C	301	ASP	2.4
1	A	220	ARG	2.3
1	B	237	LYS	2.3
1	B	238	ASP	2.3
1	B	236	ALA	2.3
1	B	95	THR	2.3
1	A	172	THR	2.2
1	A	57	ASP	2.2
1	C	95	THR	2.2
1	A	300	SER	2.2
1	B	223	ASN	2.2
1	C	1	ASP	2.2
1	B	96	TYR	2.1
1	B	250	TYR	2.1
1	C	223	ASN	2.1
1	B	298	LEU	2.1
1	A	238	ASP	2.1
1	B	19	GLY	2.1
1	C	57	ASP	2.1
1	A	166	GLY	2.0
1	C	20	THR	2.0
1	B	306[A]	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

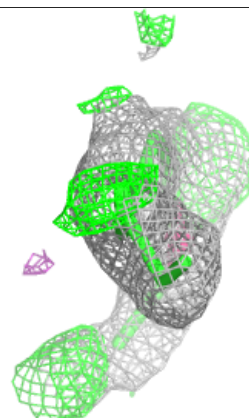
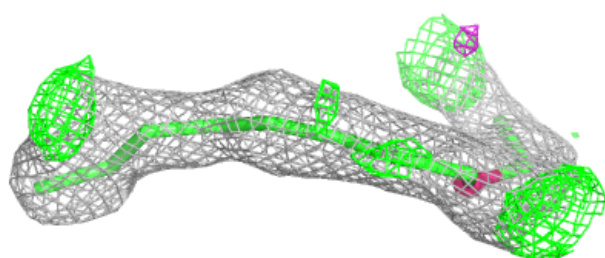
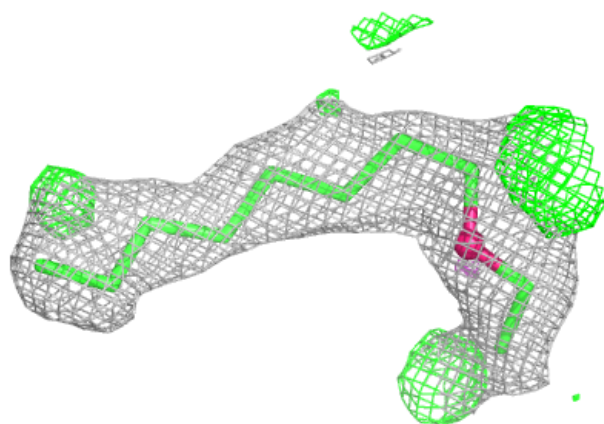
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	C	407	11/21	0.75	0.22	39,46,54,57	0
2	C8E	B	405	11/21	0.77	0.36	51,88,123,124	0
2	C8E	B	403	9/21	0.79	0.21	46,51,54,54	0
2	C8E	A	406	10/21	0.80	0.23	46,50,52,52	0
2	C8E	A	405	9/21	0.80	0.19	44,51,63,63	0
2	C8E	C	408	10/21	0.81	0.22	42,47,49,50	0
2	C8E	A	404	5/21	0.83	0.23	33,37,40,41	0
2	C8E	B	407	9/21	0.83	0.18	44,50,54,55	0
2	C8E	A	407	8/21	0.84	0.18	36,40,42,47	0
2	C8E	C	404	14/21	0.85	0.17	26,47,53,56	0
2	C8E	C	405	10/21	0.85	0.33	179,219,243,247	0
2	C8E	C	401	8/21	0.86	0.21	33,43,46,47	0
2	C8E	C	403	5/21	0.86	0.21	41,42,44,46	0
2	C8E	B	404	9/21	0.86	0.15	35,44,54,57	0
2	C8E	C	406	7/21	0.87	0.18	44,47,48,48	0
2	C8E	B	406	4/21	0.87	0.19	38,45,45,45	0
2	C8E	B	402	5/21	0.87	0.19	33,34,38,40	0
2	C8E	A	403	11/21	0.88	0.14	26,30,34,36	0
2	C8E	C	409	14/21	0.88	0.15	38,42,50,52	0
2	C8E	B	401	8/21	0.89	0.17	29,31,40,44	0
2	C8E	A	402	12/21	0.91	0.13	30,39,51,53	0
2	C8E	C	402	7/21	0.92	0.10	26,27,32,34	0
2	C8E	A	401	6/21	0.92	0.10	22,24,27,35	0

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

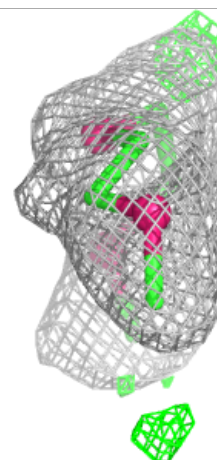
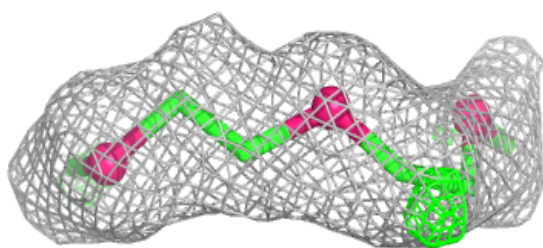
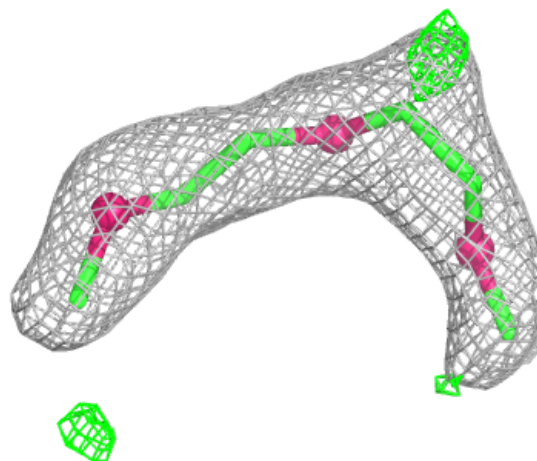
Electron density around C8E C 407:

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



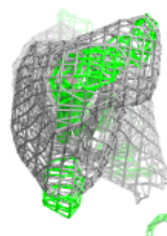
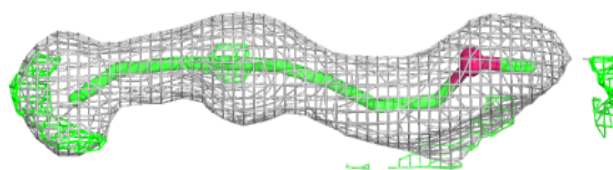
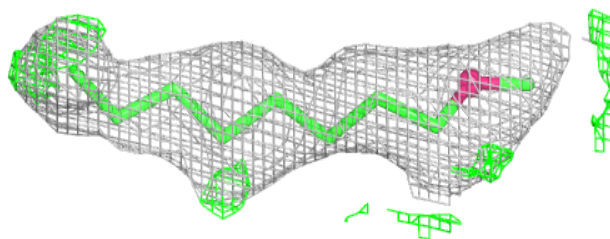
Electron density around C8E B 403:

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and green (positive)

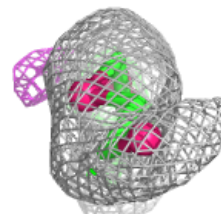
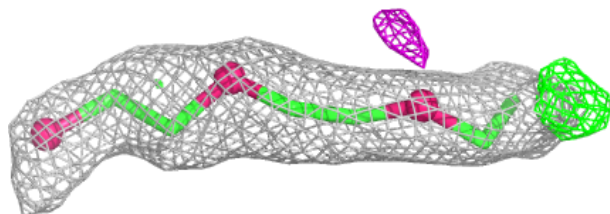
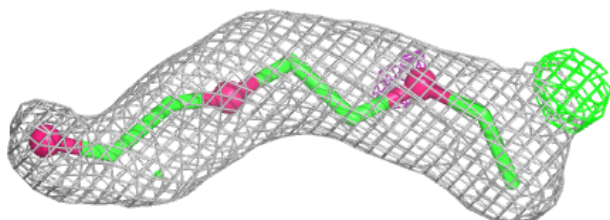


Electron density around C8E A 406:

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and green (positive)

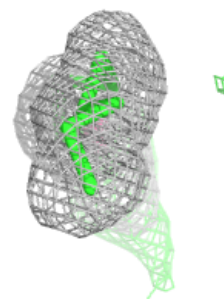
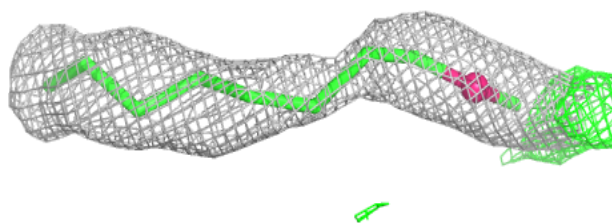
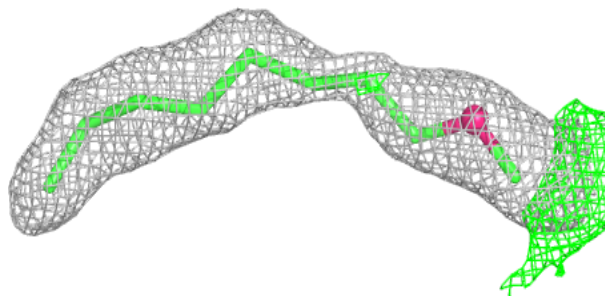
**Electron density around C8E A 405:**

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and green (positive)

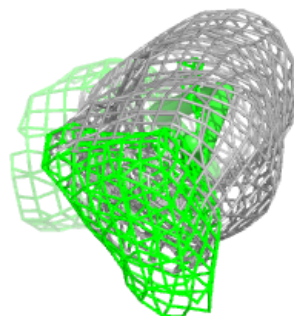
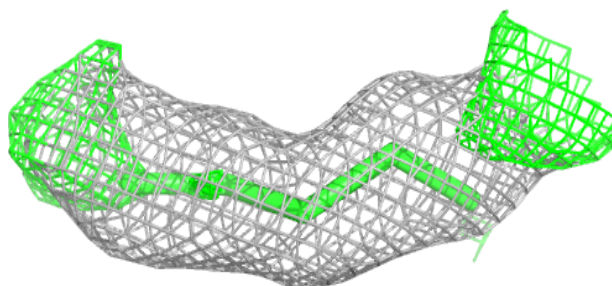
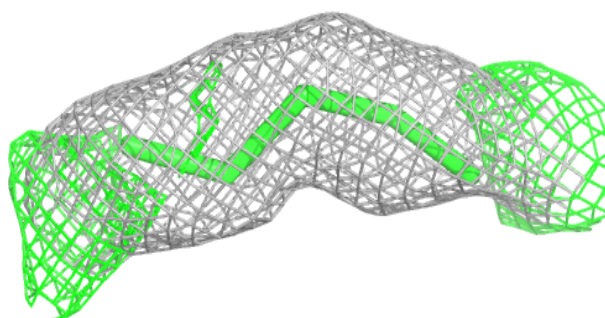


Electron density around C8E C 408:

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and green (positive)

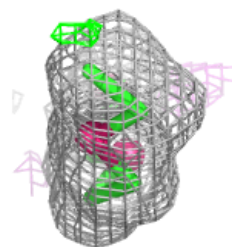
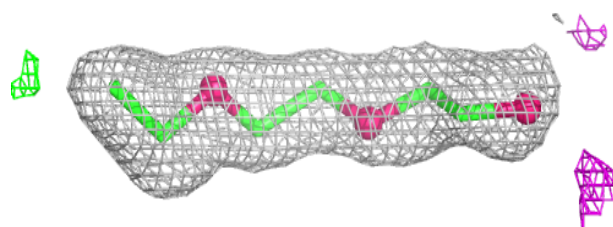
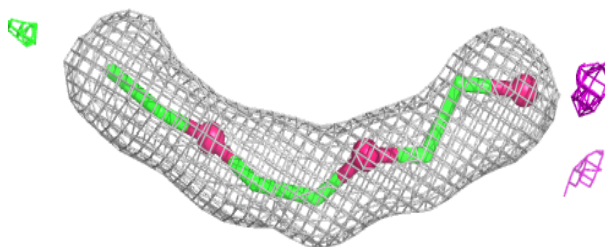
**Electron density around C8E A 404:**

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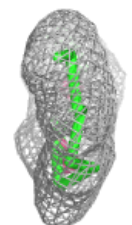
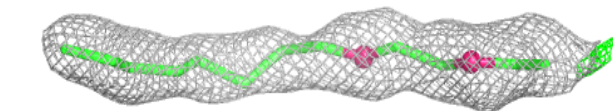
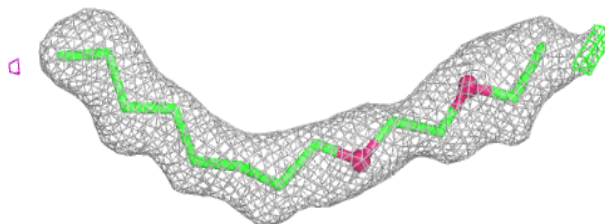


Electron density around C8E B 407:

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

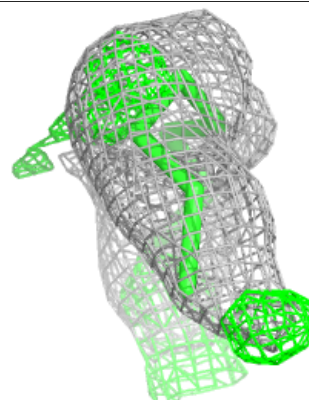
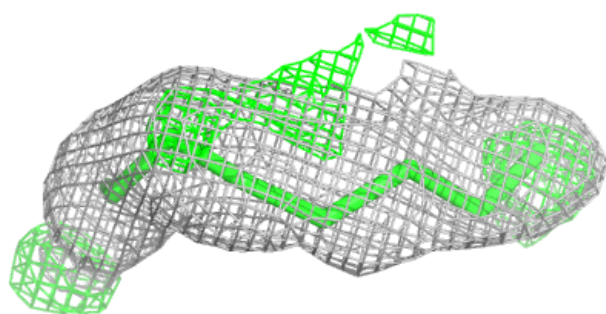
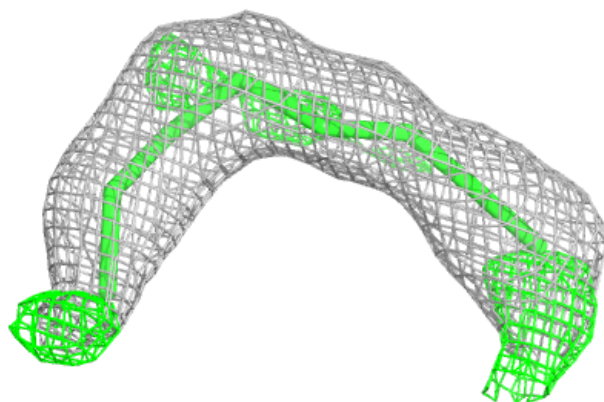
**Electron density around C8E C 404:**

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

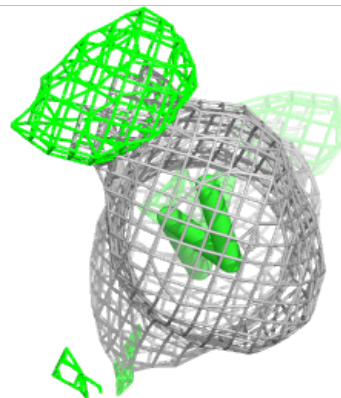
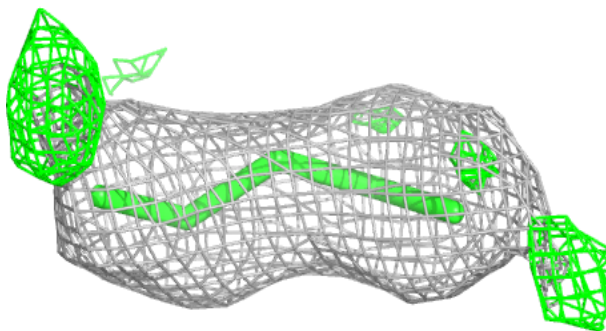
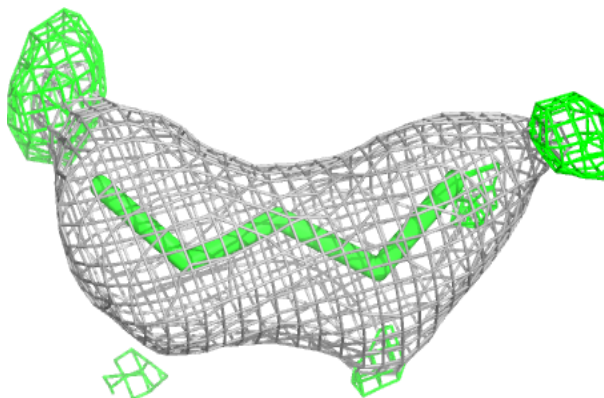


Electron density around C8E C 401:

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and green (positive)

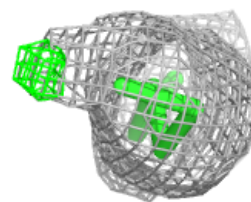
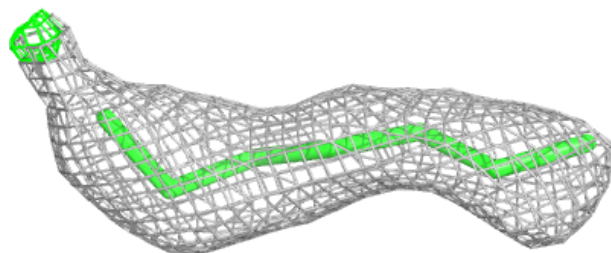
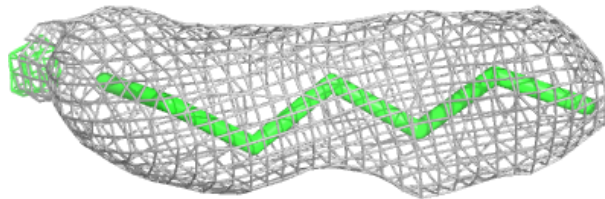
**Electron density around C8E C 403:**

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

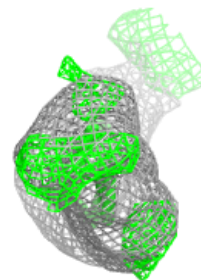
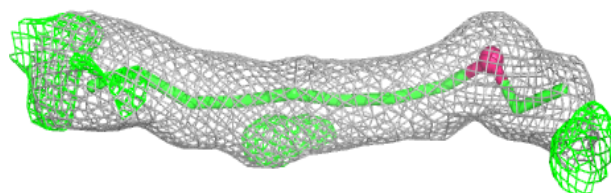
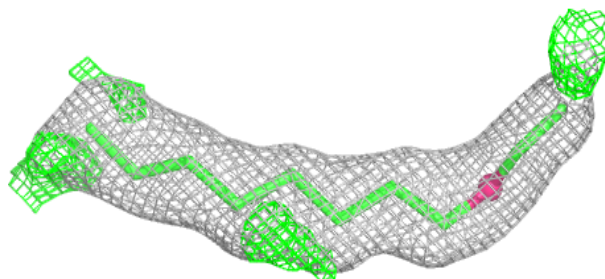


Electron density around C8E C 406:

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

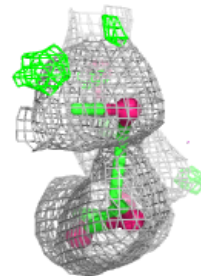
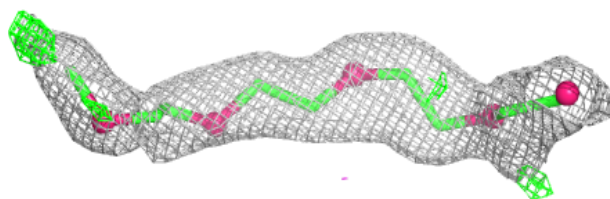
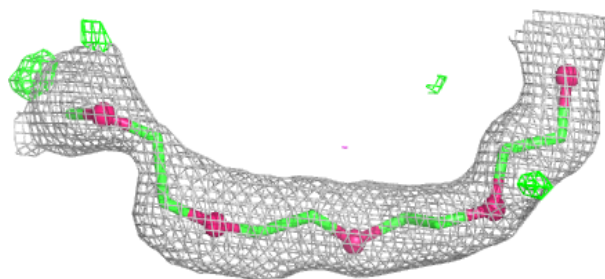
**Electron density around C8E A 403:**

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

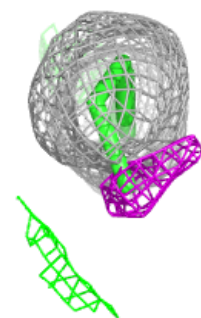
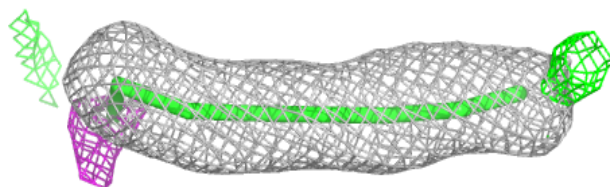
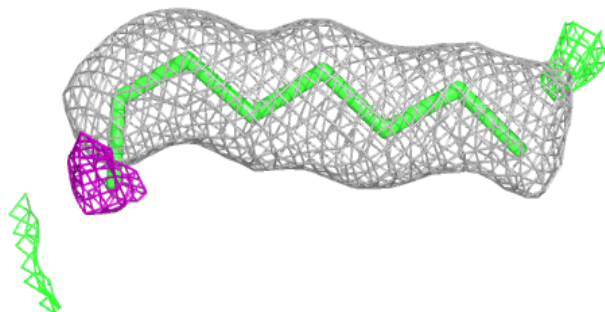


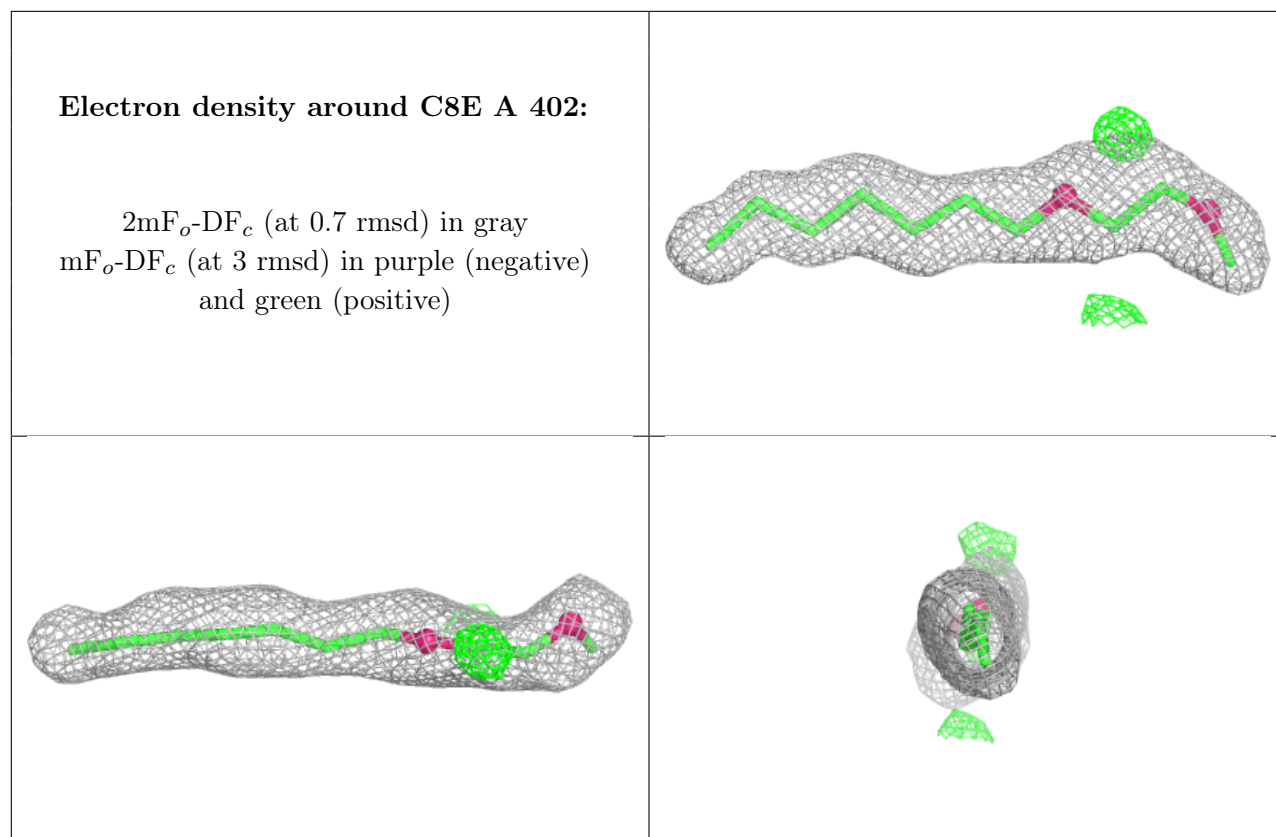
Electron density around C8E C 409:

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

**Electron density around C8E B 401:**

$2mF_o-DF_c$ (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.