



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 PM UTC

PDB ID : 7Q3T / pdb_00007q3t
Title : Crystal structure of the OmpK36 D insertion chimera from Klebsiella pneumonia
Authors : Kwong, H.; Beis, K.
Deposited on : 2021-10-28
Resolution : 1.79 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

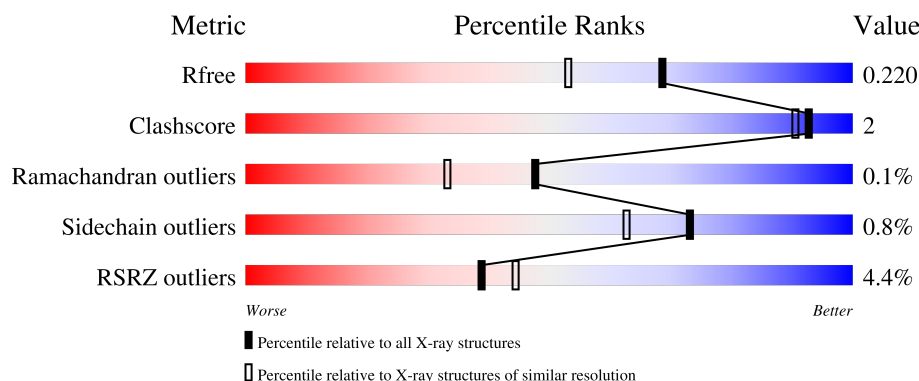
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	346	3% 97% ..
1	B	346	3% 95% 5%
1	C	346	5% 94% 6%
1	D	346	5% 96% .
1	E	346	6% 95% 5%

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Mol	Chain	Length	Quality of chain
1	F	346	4% 97%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17772 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.

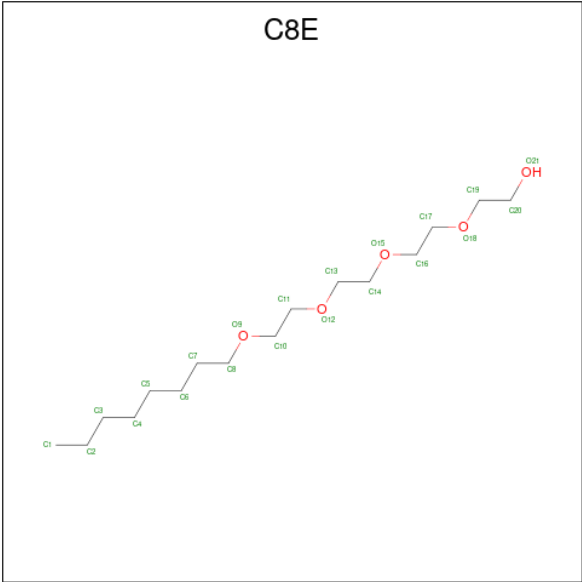
- Molecule 1 is a protein called OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	B	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	C	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	D	346	Total	C	N	O	S	0	1	0
			2711	1700	453	556	2			
1	E	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			
1	F	346	Total	C	N	O	S	0	0	0
			2703	1692	453	556	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP D6QLY0
A	114	ASP	-	insertion	UNP D6QLY0
B	0	GLY	-	expression tag	UNP D6QLY0
B	114	ASP	-	insertion	UNP D6QLY0
C	0	GLY	-	expression tag	UNP D6QLY0
C	114	ASP	-	insertion	UNP D6QLY0
D	0	GLY	-	expression tag	UNP D6QLY0
D	114	ASP	-	insertion	UNP D6QLY0
E	0	GLY	-	expression tag	UNP D6QLY0
E	114	ASP	-	insertion	UNP D6QLY0
F	0	GLY	-	expression tag	UNP D6QLY0
F	114	ASP	-	insertion	UNP D6QLY0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			11	10	1		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			17	14	3		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C		0	0
			8	8			
2	A	1	Total	C	O	0	0
			10	7	3		
2	A	1	Total	C		0	0
			6	6			
2	A	1	Total	C	O	0	0
			10	8	2		
2	A	1	Total	C	O	0	0
			15	12	3		
2	B	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 9 1	0	0
2	B	1	Total C O 14 12 2	0	0
2	B	1	Total C O 9 8 1	0	0
2	B	1	Total C O 16 11 5	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 10 9 1	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 7 4 3	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C O 15 12 3	0	0
2	C	1	Total C O 13 11 2	0	0
2	C	1	Total C O 13 11 2	0	0
2	C	1	Total C O 21 16 5	0	0
2	D	1	Total C O 11 7 4	0	0
2	D	1	Total C O 9 8 1	0	0
2	D	1	Total C O 21 16 5	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 15 12 3	0	0
2	D	1	Total C O 15 10 5	0	0
2	E	1	Total C O 20 15 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 15 12 3	0	0
2	E	1	Total C O 14 11 3	0	0
2	E	1	Total C O 19 15 4	0	0
2	F	1	Total C O 9 6 3	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C O 10 9 1	0	0
2	F	1	Total C O 9 8 1	0	0
2	F	1	Total C O 10 9 1	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C O 11 10 1	0	0
2	F	1	Total C O 13 11 2	0	0
2	F	1	Total C O 17 14 3	0	0

- Molecule 3 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Li 2 2	0	0
3	B	2	Total Li 2 2	0	0
3	C	2	Total Li 2 2	0	0
3	D	2	Total Li 2 2	0	0
3	E	2	Total Li 2 2	0	0
3	F	2	Total Li 2 2	0	0

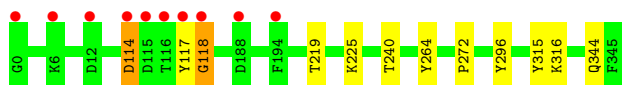
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total 177	O 177	0	0
4	B	148	Total 148	O 148	0	0
4	C	148	Total 148	O 148	0	0
4	D	162	Total 162	O 162	0	0
4	E	153	Total 153	O 153	0	0
4	F	153	Total 153	O 153	0	0

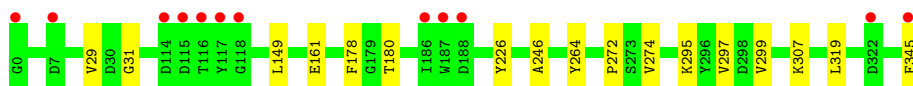
3 Residue-property plots [i](#)

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.

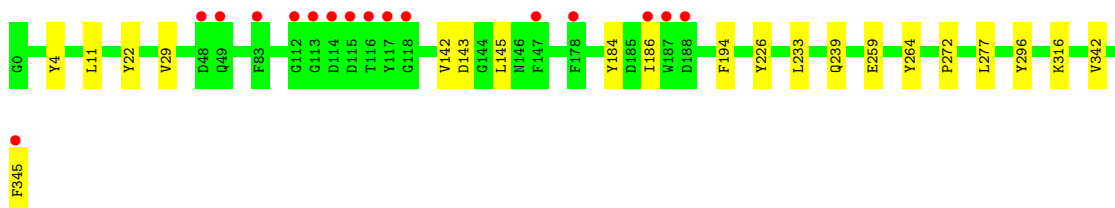
- Molecule 1: OmpK36



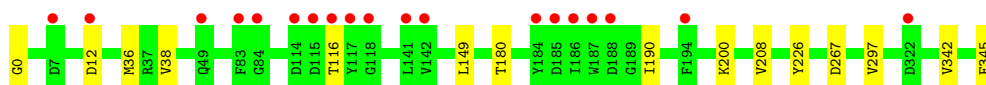
- Molecule 1: OmpK36



- Molecule 1: OmpK36



- Molecule 1: OmpK36

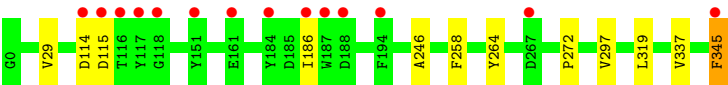


- Molecule 1: OmpK36





● Molecule 1: OmpK36



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.02Å 73.61Å 158.66Å 91.04° 97.26° 103.16°	Depositor
Resolution (Å)	78.60 – 1.79 78.60 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.4 (78.60-1.79) 97.4 (78.60-1.79)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.78Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.185 , 0.213 0.190 , 0.220	Depositor DCC
R_{free} test set	11110 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17772	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LI, 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	0.69	0/2763	0.93	0/3741
1	B	0.70	0/2763	0.91	3/3741 (0.1%)
1	C	0.67	0/2763	0.91	3/3741 (0.1%)
1	D	0.67	0/2775	0.91	3/3757 (0.1%)
1	E	0.69	0/2763	0.90	1/3741 (0.0%)
1	F	0.67	0/2763	0.90	4/3741 (0.1%)
All	All	0.68	0/16590	0.91	14/22462 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	345	PHE	CA-CB-CG	7.33	121.13	113.80
1	B	345	PHE	CA-CB-CG	6.30	120.10	113.80
1	F	246	ALA	N-CA-C	-5.80	101.53	109.71
1	C	186	ILE	N-CA-C	-5.75	105.24	110.82
1	E	345	PHE	CA-CB-CG	5.75	119.55	113.80
1	D	342	VAL	N-CA-C	5.73	116.37	108.12
1	F	115	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	345	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	342	VAL	N-CA-C	5.25	115.45	108.11
1	B	31	GLY	N-CA-C	5.19	119.63	112.52
1	B	246	ALA	N-CA-C	-5.11	104.21	110.65
1	D	208	VAL	N-CA-CB	5.10	114.43	110.45
1	D	345	PHE	CA-CB-CG	5.07	118.87	113.80
1	F	114	ASP	N-CA-C	5.05	117.21	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2703	0	2481	6	0
1	B	2703	0	2481	10	0
1	C	2703	0	2481	9	0
1	D	2711	0	2490	9	0
1	E	2703	0	2481	10	0
1	F	2703	0	2481	4	0
2	A	162	0	259	2	0
2	B	119	0	192	5	0
2	C	68	0	112	2	0
2	D	82	0	127	5	0
2	E	68	0	104	7	0
2	F	94	0	157	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	177	0	0	0	0
4	B	148	0	0	0	0
4	C	148	0	0	0	0
4	D	162	0	0	0	0
4	E	153	0	0	0	0
4	F	153	0	0	0	0
All	All	17772	0	15846	50	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 2.

All (50) 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:E:180:THR:HG23	2:E:401:C8E:H52	1.73	0.71
1:E:194:PHE:HB3	2:E:401:C8E:H71	1.74	0.68
1:A:117:TYR:O	1:A:118:GLY:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:TYR:HD2	2:E:406:C8E:H141	1.65	0.60
1:B:178:PHE:CZ	1:B:180:THR:HG23	2.38	0.59
1:F:258:PHE:HE1	2:F:408:C8E:H32	1.69	0.56
1:D:200:LYS:HE3	2:D:508:C8E:H131	1.88	0.55
1:C:194:PHE:HB3	2:C:407:C8E:H101	1.89	0.55
1:D:149:LEU:HD23	1:D:180:THR:HG22	1.89	0.54
1:D:200:LYS:HZ1	2:D:508:C8E:H131	1.71	0.54
1:E:4:TYR:HB3	1:E:11:LEU:HB2	1.89	0.54
1:A:114:ASP:HB3	1:A:118:GLY:HA2	1.90	0.54
2:A:505:C8E:H111	2:A:506:C8E:H131	1.89	0.54
1:E:210:ALA:HB1	1:E:286:ARG:HD2	1.89	0.54
1:B:226:TYR:HB2	2:B:401:C8E:H22	1.92	0.52
1:B:149:LEU:HD23	1:B:180:THR:HG22	1.90	0.52
1:A:264:TYR:O	1:A:272:PRO:HD2	2.10	0.52
2:E:401:C8E:H132	2:E:401:C8E:H172	1.93	0.51
1:D:200:LYS:CE	2:D:508:C8E:H131	2.41	0.49
1:A:315:TYR:HB2	2:A:501:C8E:H172	1.94	0.49
1:B:297:VAL:HG11	2:B:410:C8E:H61	1.94	0.48
2:C:407:C8E:H112	1:E:184:TYR:CE1	2.49	0.48
1:A:296:TYR:CD1	1:A:316:LYS:HG3	2.49	0.47
1:C:142:VAL:HG21	2:E:401:C8E:H102	1.95	0.47
1:F:337:VAL:HG21	2:F:406:C8E:H72	1.96	0.46
1:D:200:LYS:NZ	2:D:508:C8E:H131	2.29	0.46
1:A:219:THR:HG22	1:A:240:THR:HG22	1.97	0.46
1:F:264:TYR:O	1:F:272:PRO:HD2	2.15	0.45
1:F:297:VAL:HG23	1:F:319:LEU:HD11	1.99	0.45
1:E:220:TYR:HB3	2:E:401:C8E:H101	1.99	0.45
1:E:298:ASP:OD2	1:E:314:ASP:OD1	2.35	0.45
1:E:264:TYR:O	1:E:272:PRO:HD2	2.17	0.45
1:B:274:VAL:HG13	2:B:403:C8E:H42	1.99	0.44
1:C:264:TYR:O	1:C:272:PRO:HD2	2.17	0.44
1:C:145:LEU:HD13	1:C:184:TYR:HB3	2.00	0.44
1:D:297:VAL:HG11	2:D:506:C8E:H41	1.99	0.44
1:C:22:TYR:HD2	1:C:29:VAL:HG13	1.83	0.44
1:E:239:GLN:HB2	2:E:401:C8E:H171	2.00	0.44
1:C:226:TYR:HB3	1:C:233:LEU:HB2	1.98	0.43
1:D:36:MET:HE1	1:D:38:VAL:HB	2.00	0.43
1:B:178:PHE:CZ	1:B:180:THR:CG2	3.01	0.43
1:C:296:TYR:CD1	1:C:316:LYS:HG3	2.53	0.43
1:C:259:GLU:HG2	1:C:277:LEU:HG	2.00	0.42
1:D:0:GLY:HA3	1:D:12:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HG21	2:B:410:C8E:H52	2.01	0.42
1:C:4:TYR:HB3	1:C:11:LEU:HB2	2.02	0.42
1:B:272:PRO:HB3	2:B:411:C8E:H31	2.02	0.42
1:B:264:TYR:O	1:B:272:PRO:HD2	2.19	0.41
1:B:295:LYS:HG2	1:B:319:LEU:HB2	2.03	0.41
1:D:190:ILE:HG12	1:D:226:TYR:HD1	1.84	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	344/346 (99%)	325 (94%)	17 (5%)	2 (1%)	21	9
1	B	344/346 (99%)	327 (95%)	17 (5%)	0	100	100
1	C	344/346 (99%)	328 (95%)	16 (5%)	0	100	100
1	D	345/346 (100%)	326 (94%)	19 (6%)	0	100	100
1	E	344/346 (99%)	324 (94%)	20 (6%)	0	100	100
1	F	344/346 (99%)	326 (95%)	18 (5%)	0	100	100
All	All	2065/2076 (100%)	1956 (95%)	107 (5%)	2 (0%)	48	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	114	ASP

5.3.2 Protein sidechains ⓘ

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	277/277 (100%)	275 (99%)	2 (1%)	76	66
1	B	277/277 (100%)	274 (99%)	3 (1%)	65	51
1	C	277/277 (100%)	275 (99%)	2 (1%)	76	66
1	D	278/277 (100%)	276 (99%)	2 (1%)	76	66
1	E	277/277 (100%)	276 (100%)	1 (0%)	84	78
1	F	277/277 (100%)	274 (99%)	3 (1%)	65	51
All	All	1663/1662 (100%)	1650 (99%)	13 (1%)	73	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	LYS
1	A	344	GLN
1	B	29	VAL
1	B	161	GLU
1	B	307	LYS
1	C	143	ASP
1	C	239	GLN
1	D	116	THR
1	D	267	ASP
1	E	29	VAL
1	F	29	VAL
1	F	186	ILE
1	F	345	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	55	GLN
1	A	121	ASN
1	A	216	ASN

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	55	GLN
1	B	71	GLN
1	B	152	GLN
1	B	278	GLN
1	C	71	GLN
1	C	124	GLN
1	C	239	GLN
1	C	256	GLN
1	C	278	GLN
1	D	55	GLN
1	D	71	GLN
1	D	229	ASN
1	E	71	GLN
1	E	152	GLN
1	E	216	ASN
1	E	308	ASN
1	F	71	GLN
1	F	124	GLN
1	F	229	ASN
1	F	344	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 [i](#)

Of 59 ligands modelled in this entry, 12 are monoatomic - leaving 47 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	C8E	B	409	-	9,9,20	0.29	0	8,8,19	0.51	0
2	C8E	B	412	-	6,6,20	0.46	0	5,5,19	0.27	0
2	C8E	E	406	-	18,18,20	0.38	0	17,17,19	0.43	0
2	C8E	C	403	-	5,5,20	0.26	0	4,4,19	0.41	0
2	C8E	A	513	-	5,5,20	0.20	0	4,4,19	0.51	0
2	C8E	E	403	-	12,12,20	0.27	0	10,10,19	0.55	0
2	C8E	A	506	-	11,11,20	0.43	0	10,10,19	0.37	0
2	C8E	A	515	-	14,14,20	0.35	0	13,13,19	0.45	0
2	C8E	F	409	-	10,10,20	0.37	0	9,9,19	0.46	0
2	C8E	F	405	-	9,9,20	0.37	0	8,8,19	0.56	0
2	C8E	C	407	-	20,20,20	0.37	0	19,19,19	0.42	0
2	C8E	B	408	-	7,7,20	0.25	0	6,6,19	0.53	0
2	C8E	A	509	-	8,8,20	0.22	0	7,7,19	0.57	0
2	C8E	F	411	-	16,16,20	0.45	0	15,15,19	0.35	0
2	C8E	C	404	-	14,14,20	0.38	0	13,13,19	0.44	0
2	C8E	B	404	-	8,8,20	0.25	0	7,7,19	0.56	0
2	C8E	C	405	-	12,12,20	0.35	0	11,11,19	0.48	0
2	C8E	B	405	-	15,15,20	0.47	0	14,14,19	0.23	0
2	C8E	E	402	-	14,14,20	0.38	0	13,13,19	0.43	0
2	C8E	B	403	-	13,13,20	0.36	0	12,12,19	0.46	0
2	C8E	A	511	-	7,7,20	0.26	0	6,6,19	0.44	0
2	C8E	F	410	-	12,12,20	0.38	0	11,11,19	0.41	0
2	C8E	A	507	-	16,16,20	0.48	0	15,15,19	0.41	0
2	C8E	E	401	-	19,19,20	0.49	0	18,18,19	0.59	0
2	C8E	B	402	-	9,9,20	0.39	0	8,8,19	0.48	0
2	C8E	C	406	-	12,12,20	0.44	0	11,11,19	0.41	0
2	C8E	D	501	-	10,10,20	0.45	0	9,9,19	0.29	0
2	C8E	F	403	-	8,8,20	0.46	0	7,7,19	0.29	0
2	C8E	F	407	-	9,9,20	0.35	0	8,8,19	0.41	0
2	C8E	D	506	-	10,10,20	0.35	0	9,9,19	0.53	0
2	C8E	A	508	-	8,8,20	0.22	0	7,7,19	0.56	0
2	C8E	F	404	-	6,6,20	0.29	0	5,5,19	0.38	0
2	C8E	A	514	-	9,9,20	0.48	0	8,8,19	0.23	0
2	C8E	B	411	-	11,11,20	0.31	0	10,10,19	0.49	0
2	C8E	F	406	-	8,8,20	0.24	0	7,7,19	0.49	0
2	C8E	D	508	-	14,14,20	0.45	0	13,13,19	0.50	0
2	C8E	B	410	-	11,11,20	0.35	0	10,10,19	0.51	0
2	C8E	D	505	-	20,20,20	0.43	0	19,19,19	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C8E	B	401	-	20,20,20	0.38	0	19,19,19	0.46	0
2	C8E	A	502	-	10,10,20	0.36	0	9,9,19	0.62	0
2	C8E	A	510	-	12,12,20	0.39	0	11,11,19	0.46	0
2	C8E	D	507	-	14,14,20	0.34	0	13,13,19	0.59	0
2	C8E	F	408	-	7,7,20	0.22	0	6,6,19	0.69	0
2	C8E	D	502	-	8,8,20	0.22	0	7,7,19	0.53	0
2	C8E	A	501	-	20,20,20	0.53	0	19,19,19	0.43	0
2	C8E	A	512	-	9,9,20	0.47	0	8,8,19	0.23	0
2	C8E	A	505	-	20,20,20	0.41	0	19,19,19	0.41	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	B	409	-	-	2/7/7/18	-
2	C8E	B	412	-	-	2/4/4/18	-
2	C8E	E	406	-	-	6/16/16/18	-
2	C8E	C	403	-	-	1/3/3/18	-
2	C8E	A	513	-	-	0/3/3/18	-
2	C8E	E	403	-	-	1/8/8/18	-
2	C8E	A	506	-	-	6/9/9/18	-
2	C8E	A	515	-	-	5/12/12/18	-
2	C8E	F	409	-	-	2/8/8/18	-
2	C8E	F	405	-	-	3/7/7/18	-
2	C8E	C	407	-	-	6/18/18/18	-
2	C8E	B	408	-	-	4/5/5/18	-
2	C8E	A	509	-	-	3/6/6/18	-
2	C8E	F	411	-	-	6/14/14/18	-
2	C8E	C	404	-	-	6/12/12/18	-
2	C8E	B	404	-	-	1/6/6/18	-
2	C8E	C	405	-	-	3/10/10/18	-
2	C8E	B	405	-	-	1/13/13/18	-
2	C8E	E	402	-	-	5/12/12/18	-
2	C8E	B	403	-	-	2/11/11/18	-
2	C8E	A	511	-	-	0/5/5/18	-
2	C8E	F	410	-	-	1/10/10/18	-
2	C8E	A	507	-	-	3/14/14/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	E	401	-	-	6/17/17/18	-
2	C8E	B	402	-	-	2/7/7/18	-
2	C8E	C	406	-	-	5/10/10/18	-
2	C8E	D	501	-	-	3/8/8/18	-
2	C8E	F	403	-	-	2/6/6/18	-
2	C8E	F	407	-	-	3/7/7/18	-
2	C8E	D	506	-	-	0/8/8/18	-
2	C8E	A	508	-	-	1/6/6/18	-
2	C8E	F	404	-	-	1/4/4/18	-
2	C8E	A	514	-	-	0/7/7/18	-
2	C8E	B	411	-	-	1/9/9/18	-
2	C8E	F	406	-	-	2/6/6/18	-
2	C8E	D	508	-	-	3/12/12/18	-
2	C8E	B	410	-	-	2/9/9/18	-
2	C8E	D	505	-	-	7/18/18/18	-
2	C8E	B	401	-	-	5/18/18/18	-
2	C8E	A	502	-	-	2/8/8/18	-
2	C8E	A	510	-	-	6/10/10/18	-
2	C8E	D	507	-	-	4/12/12/18	-
2	C8E	F	408	-	-	3/5/5/18	-
2	C8E	D	502	-	-	2/6/6/18	-
2	C8E	A	501	-	-	10/18/18/18	-
2	C8E	A	512	-	-	1/7/7/18	-
2	C8E	A	505	-	-	5/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	505	C8E	O12-C13-C14-O15
2	D	501	C8E	O12-C13-C14-O15
2	F	410	C8E	O9-C10-C11-O12
2	E	402	C8E	O9-C10-C11-O12
2	C	407	C8E	O9-C10-C11-O12
2	A	502	C8E	C6-C7-C8-O9

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Mol	Chain	Res	Type	Atoms
2	A	515	C8E	C6-C7-C8-O9
2	A	501	C8E	C6-C7-C8-O9
2	C	407	C8E	O12-C13-C14-O15
2	A	506	C8E	O15-C16-C17-O18
2	B	412	C8E	O18-C19-C20-O21
2	C	404	C8E	O12-C13-C14-O15
2	E	402	C8E	C6-C7-C8-O9
2	A	510	C8E	C6-C7-C8-O9
2	F	411	C8E	C6-C7-C8-O9
2	B	409	C8E	C2-C3-C4-C5
2	B	403	C8E	C3-C4-C5-C6
2	B	408	C8E	C4-C5-C6-C7
2	A	501	C8E	O9-C10-C11-O12
2	B	403	C8E	C4-C5-C6-C7
2	C	404	C8E	C5-C6-C7-C8
2	C	405	C8E	C2-C3-C4-C5
2	F	411	C8E	C3-C4-C5-C6
2	A	505	C8E	O18-C19-C20-O21
2	B	410	C8E	C2-C3-C4-C5
2	A	515	C8E	C2-C3-C4-C5
2	A	506	C8E	O12-C13-C14-O15
2	F	411	C8E	C4-C5-C6-C7
2	C	405	C8E	C6-C7-C8-O9
2	C	407	C8E	C6-C7-C8-O9
2	E	406	C8E	C3-C4-C5-C6
2	C	406	C8E	C6-C7-C8-O9
2	D	505	C8E	C3-C4-C5-C6
2	B	409	C8E	C3-C4-C5-C6
2	C	407	C8E	O15-C16-C17-O18
2	F	405	C8E	C4-C5-C6-C7
2	C	404	C8E	C6-C7-C8-O9
2	D	505	C8E	O18-C19-C20-O21
2	F	403	C8E	O18-C19-C20-O21
2	F	407	C8E	C2-C3-C4-C5
2	D	508	C8E	O9-C10-C11-O12
2	A	501	C8E	C5-C6-C7-C8
2	E	403	C8E	C3-C4-C5-C6
2	A	510	C8E	C2-C3-C4-C5
2	E	406	C8E	C6-C7-C8-O9
2	B	412	C8E	O15-C16-C17-O18
2	A	507	C8E	C1-C2-C3-C4
2	F	407	C8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	508	C8E	C1-C2-C3-C4
2	F	405	C8E	C3-C4-C5-C6
2	C	406	C8E	C3-C4-C5-C6
2	B	408	C8E	C5-C6-C7-C8
2	B	401	C8E	C3-C4-C5-C6
2	A	510	C8E	C1-C2-C3-C4
2	D	505	C8E	O15-C16-C17-O18
2	E	402	C8E	C1-C2-C3-C4
2	A	509	C8E	C3-C4-C5-C6
2	A	507	C8E	C3-C4-C5-C6
2	C	403	C8E	C2-C3-C4-C5
2	C	404	C8E	C4-C5-C6-C7
2	A	510	C8E	O9-C10-C11-O12
2	C	406	C8E	C10-C11-O12-C13
2	A	501	C8E	C3-C4-C5-C6
2	F	409	C8E	C6-C7-C8-O9
2	F	406	C8E	C1-C2-C3-C4
2	B	402	C8E	C2-C3-C4-C5
2	F	408	C8E	C2-C3-C4-C5
2	A	502	C8E	C1-C2-C3-C4
2	F	408	C8E	C1-C2-C3-C4
2	B	401	C8E	C16-C17-O18-C19
2	C	404	C8E	C3-C4-C5-C6
2	B	410	C8E	C1-C2-C3-C4
2	D	508	C8E	C10-C11-O12-C13
2	A	506	C8E	C14-C13-O12-C11
2	B	405	C8E	C16-C17-O18-C19
2	F	411	C8E	C10-C11-O12-C13
2	A	506	C8E	C13-C14-O15-C16
2	E	401	C8E	C11-C10-O9-C8
2	E	402	C8E	O12-C13-C14-O15
2	E	401	C8E	O15-C16-C17-O18
2	E	401	C8E	C10-C11-O12-C13
2	A	507	C8E	C6-C7-C8-O9
2	F	407	C8E	C7-C8-O9-C10
2	A	501	C8E	C20-C19-O18-C17
2	C	406	C8E	C11-C10-O9-C8
2	A	505	C8E	C5-C6-C7-C8
2	A	505	C8E	C10-C11-O12-C13
2	C	405	C8E	O9-C10-C11-O12
2	E	406	C8E	C11-C10-O9-C8
2	F	405	C8E	C7-C8-O9-C10

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Mol	Chain	Res	Type	Atoms
2	A	509	C8E	C2-C3-C4-C5
2	A	515	C8E	C3-C4-C5-C6
2	D	505	C8E	C14-C13-O12-C11
2	B	402	C8E	C3-C4-C5-C6
2	B	404	C8E	C5-C6-C7-C8
2	E	401	C8E	C4-C5-C6-C7
2	D	502	C8E	C3-C4-C5-C6
2	D	507	C8E	C2-C3-C4-C5
2	F	408	C8E	C4-C5-C6-C7
2	F	411	C8E	C14-C13-O12-C11
2	F	406	C8E	C3-C4-C5-C6
2	A	506	C8E	O18-C19-C20-O21
2	C	407	C8E	C7-C8-O9-C10
2	E	402	C8E	C7-C8-O9-C10
2	F	404	C8E	C3-C4-C5-C6
2	B	411	C8E	C2-C3-C4-C5
2	D	502	C8E	C1-C2-C3-C4
2	E	406	C8E	C16-C17-O18-C19
2	F	411	C8E	O12-C13-C14-O15
2	D	501	C8E	C14-C13-O12-C11
2	A	515	C8E	C5-C6-C7-C8
2	E	401	C8E	C17-C16-O15-C14
2	C	406	C8E	O9-C10-C11-O12
2	C	404	C8E	C2-C3-C4-C5
2	E	401	C8E	C6-C7-C8-O9
2	A	506	C8E	C17-C16-O15-C14
2	B	401	C8E	C13-C14-O15-C16
2	A	501	C8E	C10-C11-O12-C13
2	C	407	C8E	C4-C5-C6-C7
2	A	510	C8E	C11-C10-O9-C8
2	A	509	C8E	C1-C2-C3-C4
2	F	409	C8E	C7-C8-O9-C10
2	D	505	C8E	C1-C2-C3-C4
2	A	501	C8E	O15-C16-C17-O18
2	B	408	C8E	C3-C4-C5-C6
2	B	408	C8E	C2-C3-C4-C5
2	B	401	C8E	O18-C19-C20-O21
2	D	507	C8E	O12-C13-C14-O15
2	B	401	C8E	O15-C16-C17-O18
2	D	508	C8E	C11-C10-O9-C8
2	A	505	C8E	C3-C4-C5-C6
2	A	501	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
2	A	501	C8E	C2-C3-C4-C5
2	D	505	C8E	O9-C10-C11-O12
2	A	505	C8E	O12-C13-C14-O15
2	A	512	C8E	O9-C10-C11-O12
2	A	501	C8E	C16-C17-O18-C19
2	D	507	C8E	O9-C10-C11-O12
2	D	501	C8E	O15-C16-C17-O18
2	F	403	C8E	C13-C14-O15-C16
2	E	406	C8E	O9-C10-C11-O12
2	A	515	C8E	C11-C10-O9-C8
2	E	406	C8E	O12-C13-C14-O15
2	D	507	C8E	C1-C2-C3-C4
2	A	510	C8E	C10-C11-O12-C13

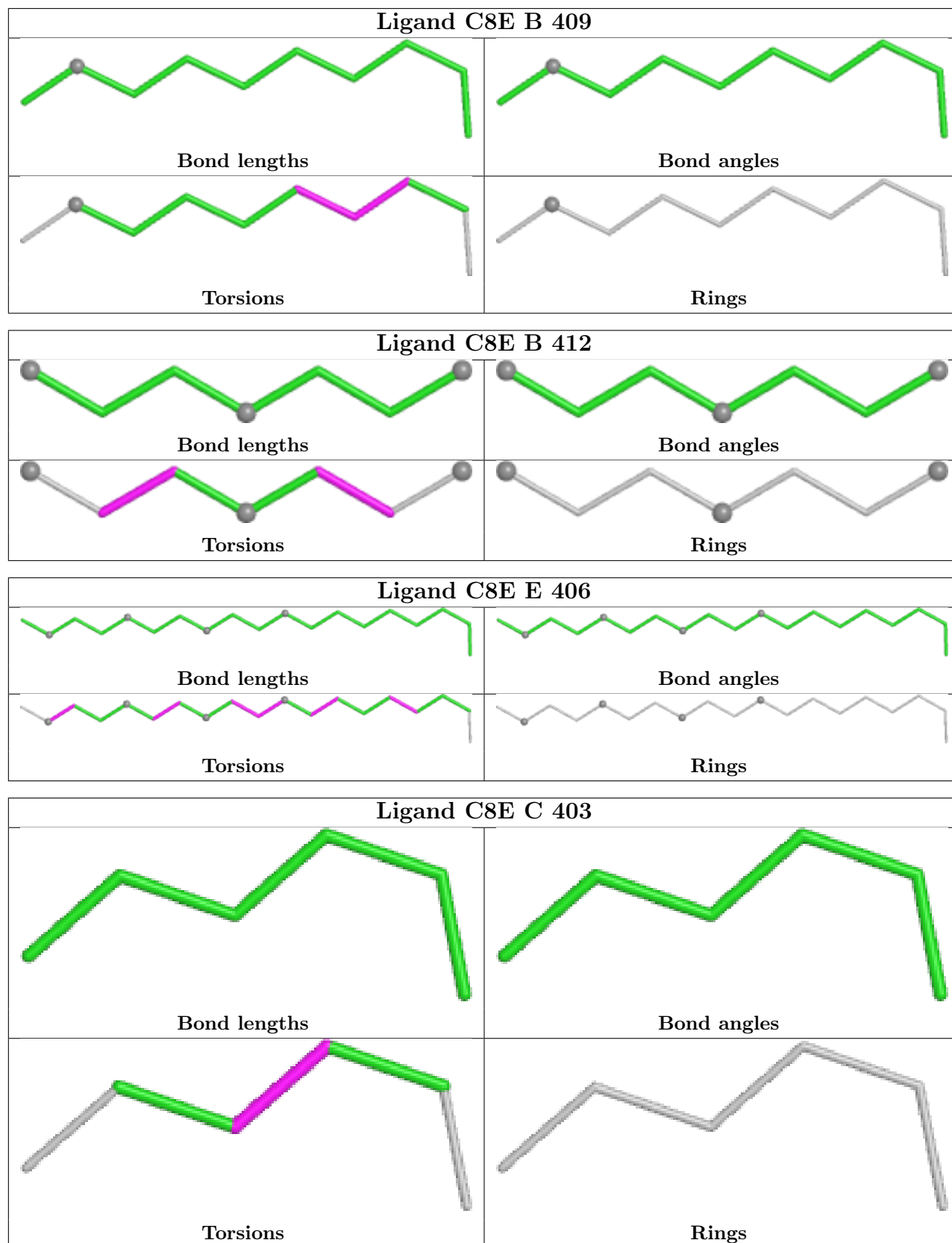
There are no ring outliers.

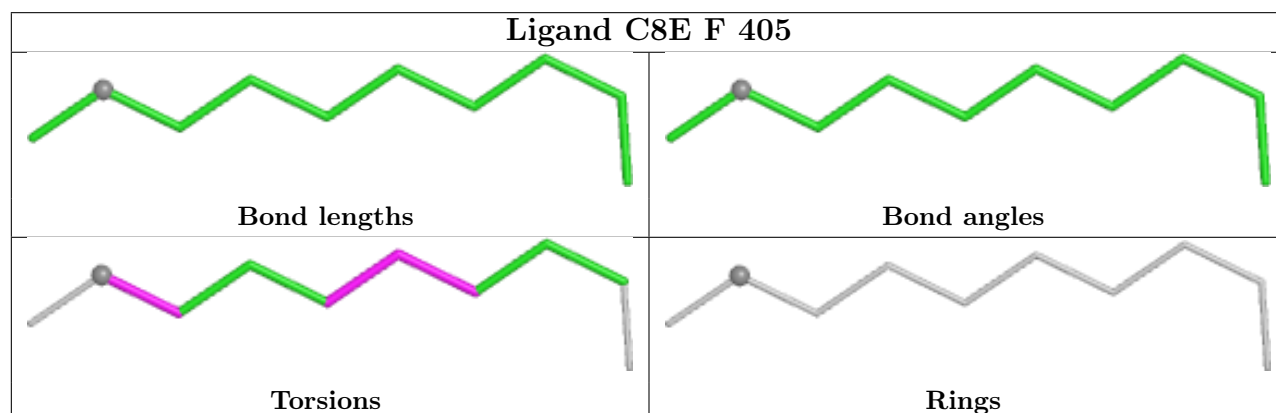
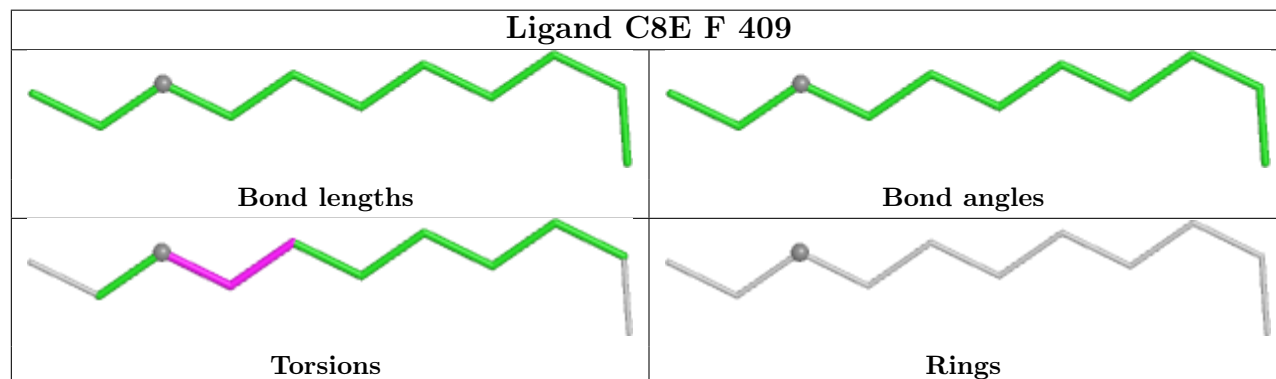
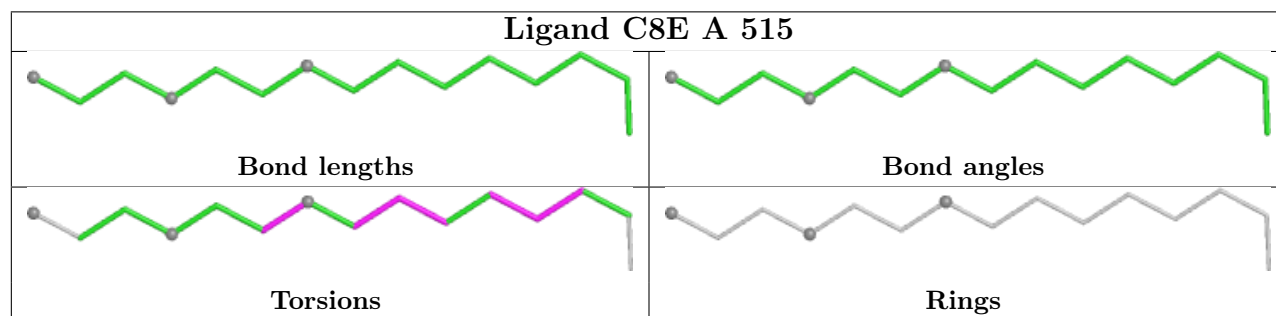
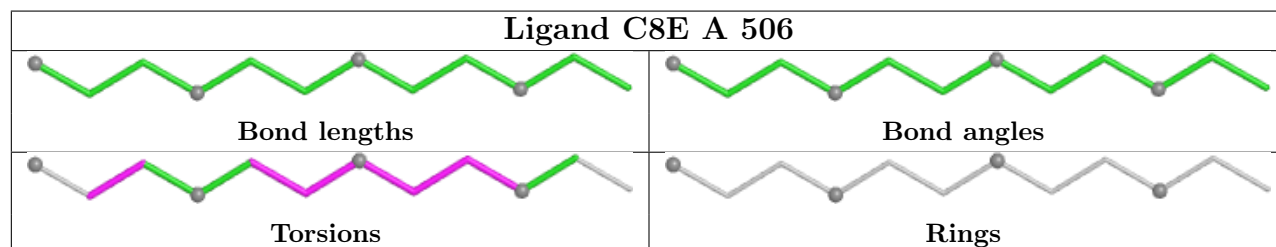
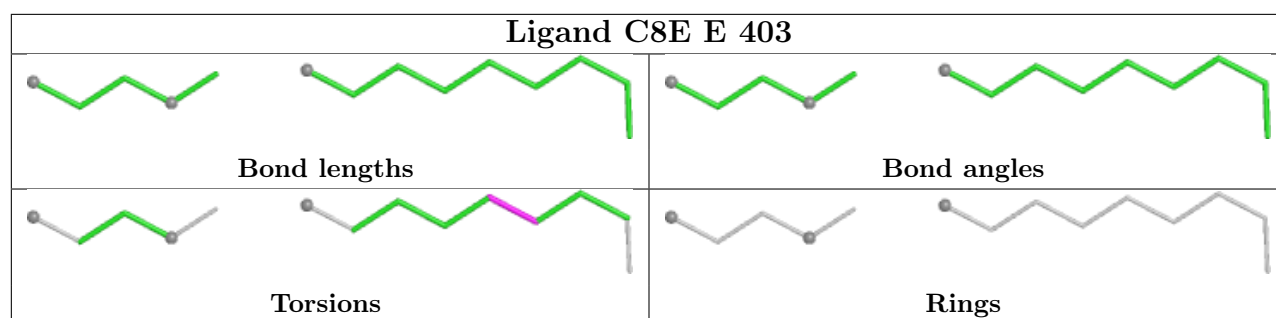
14 monomers are involved in 23 short contacts:

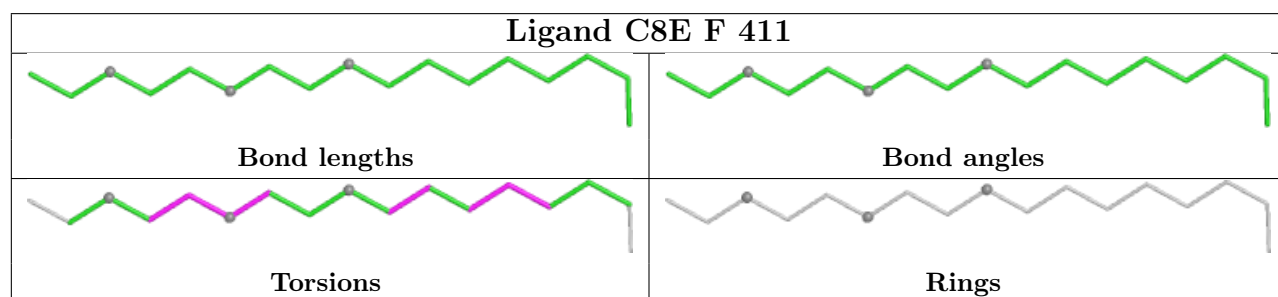
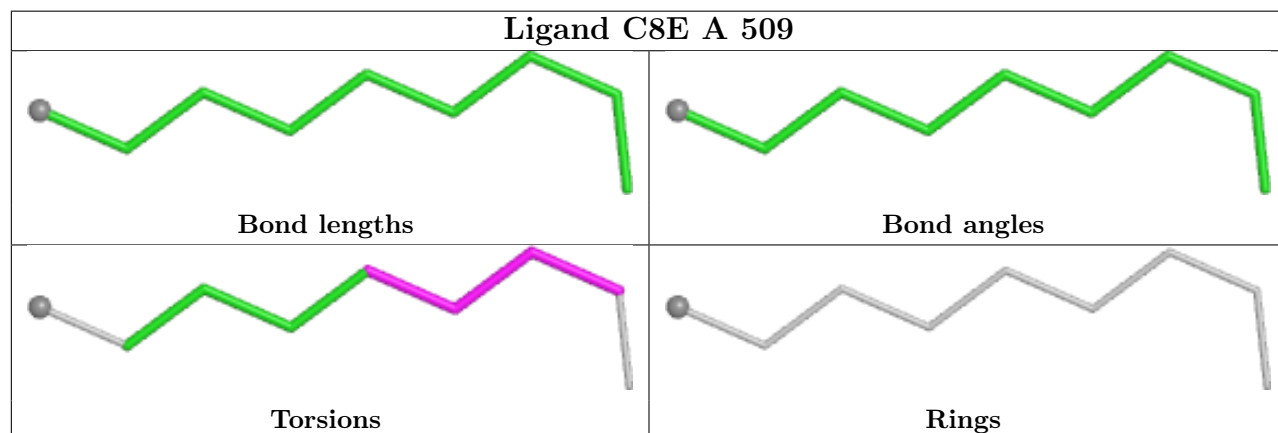
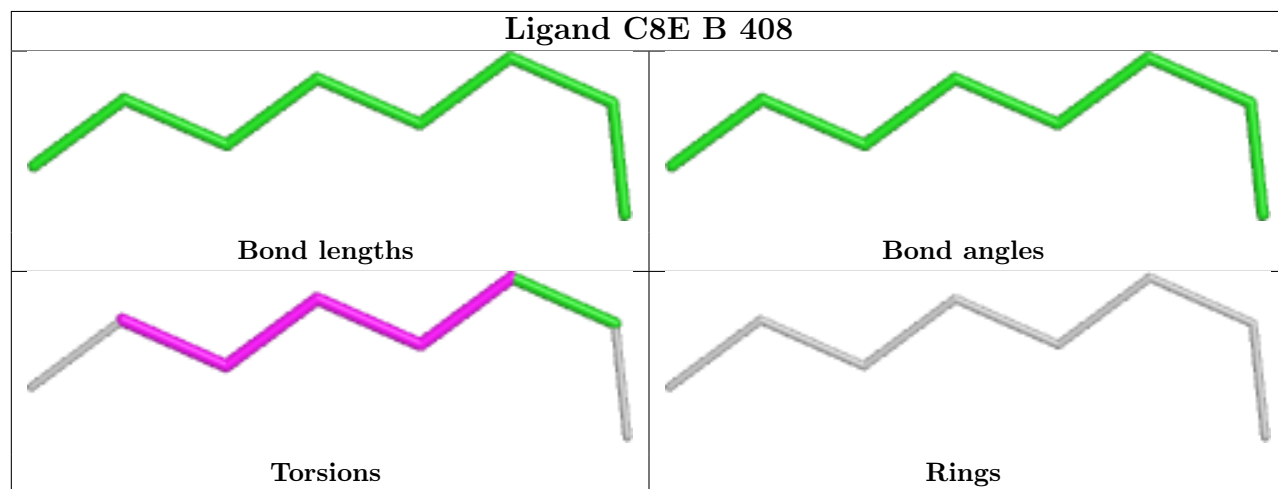
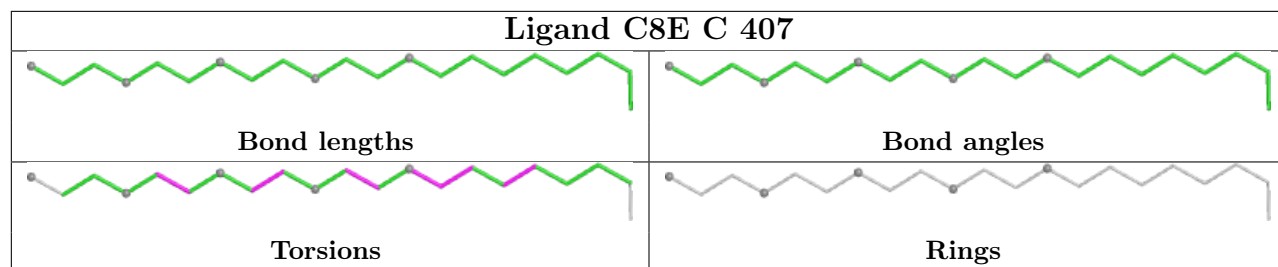
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	406	C8E	1	0
2	A	506	C8E	1	0
2	C	407	C8E	2	0
2	B	403	C8E	1	0
2	E	401	C8E	6	0
2	D	506	C8E	1	0
2	B	411	C8E	1	0
2	F	406	C8E	1	0
2	D	508	C8E	4	0
2	B	410	C8E	2	0
2	B	401	C8E	1	0
2	F	408	C8E	1	0
2	A	501	C8E	1	0
2	A	505	C8E	1	0

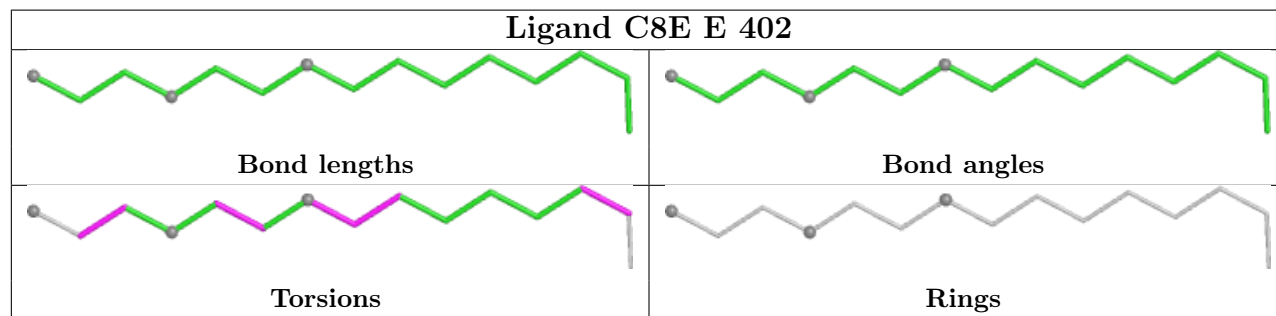
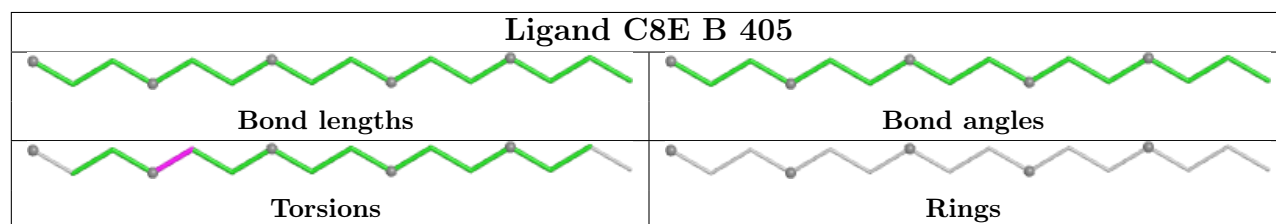
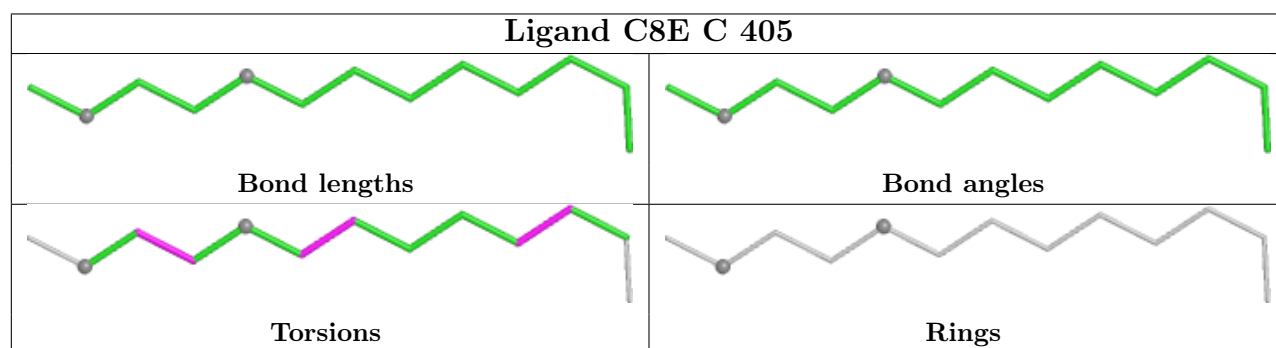
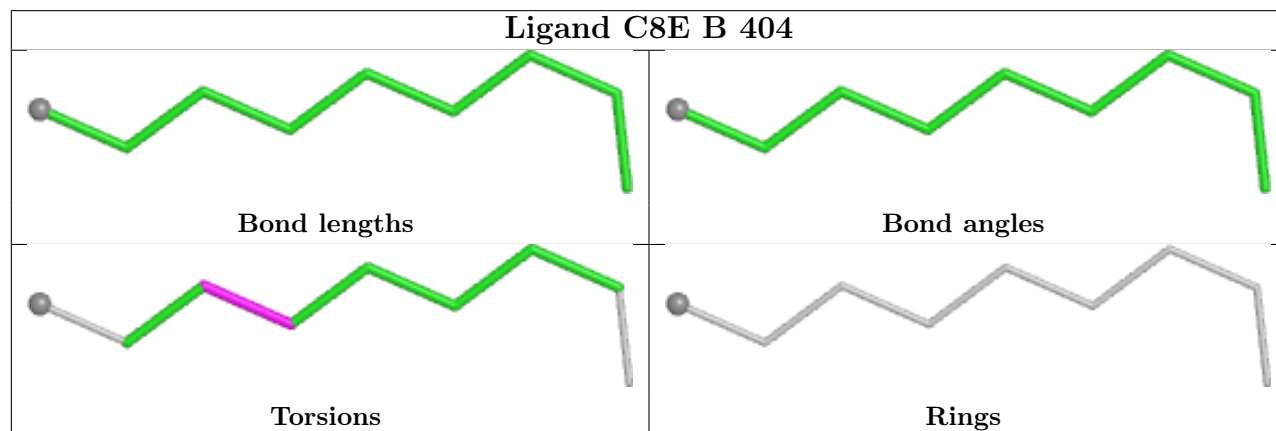
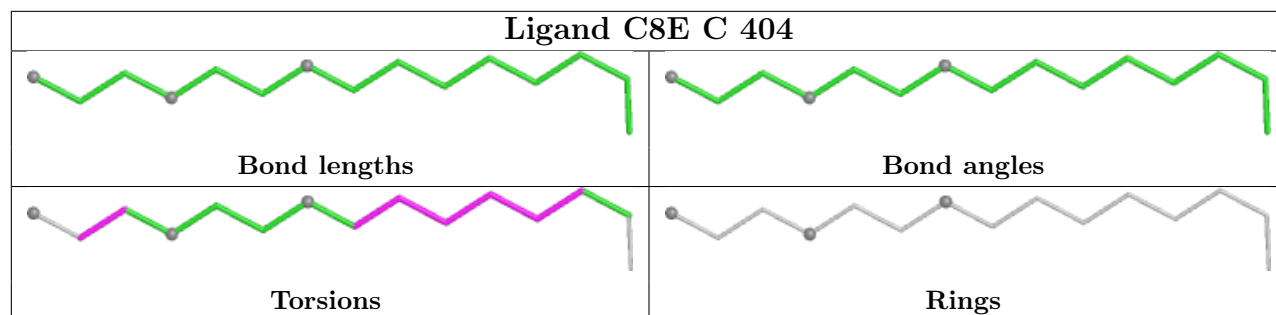
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

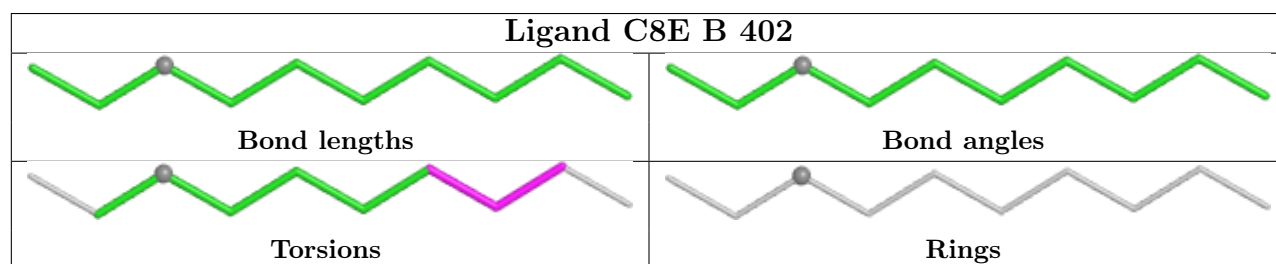
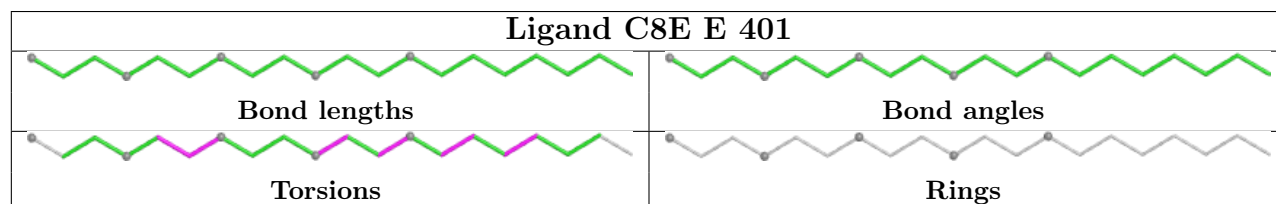
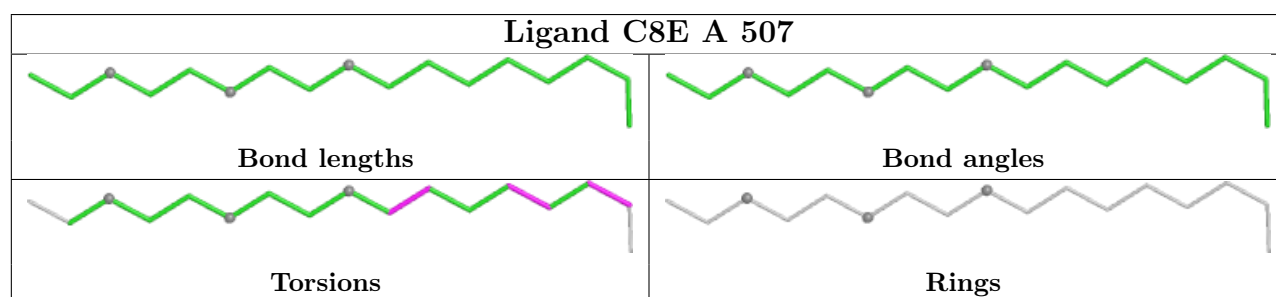
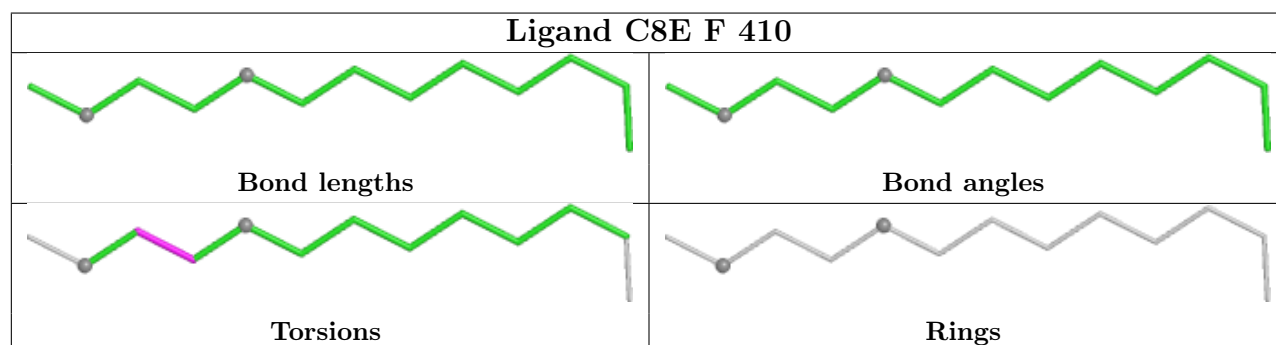
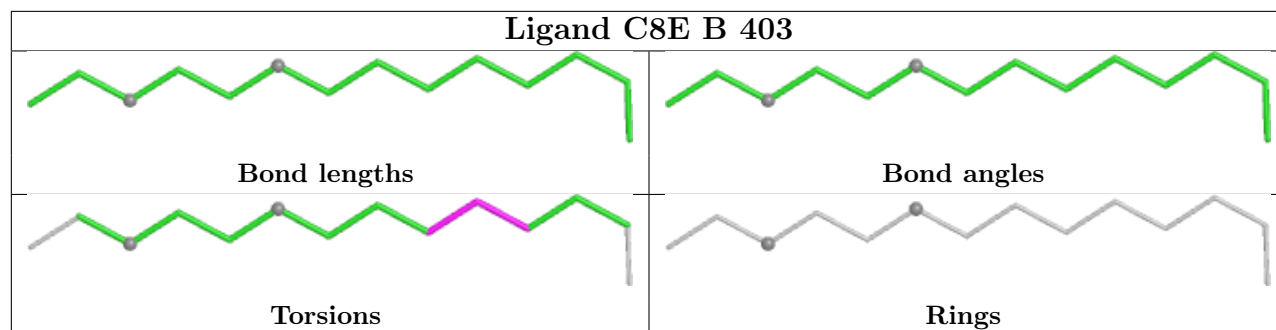
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

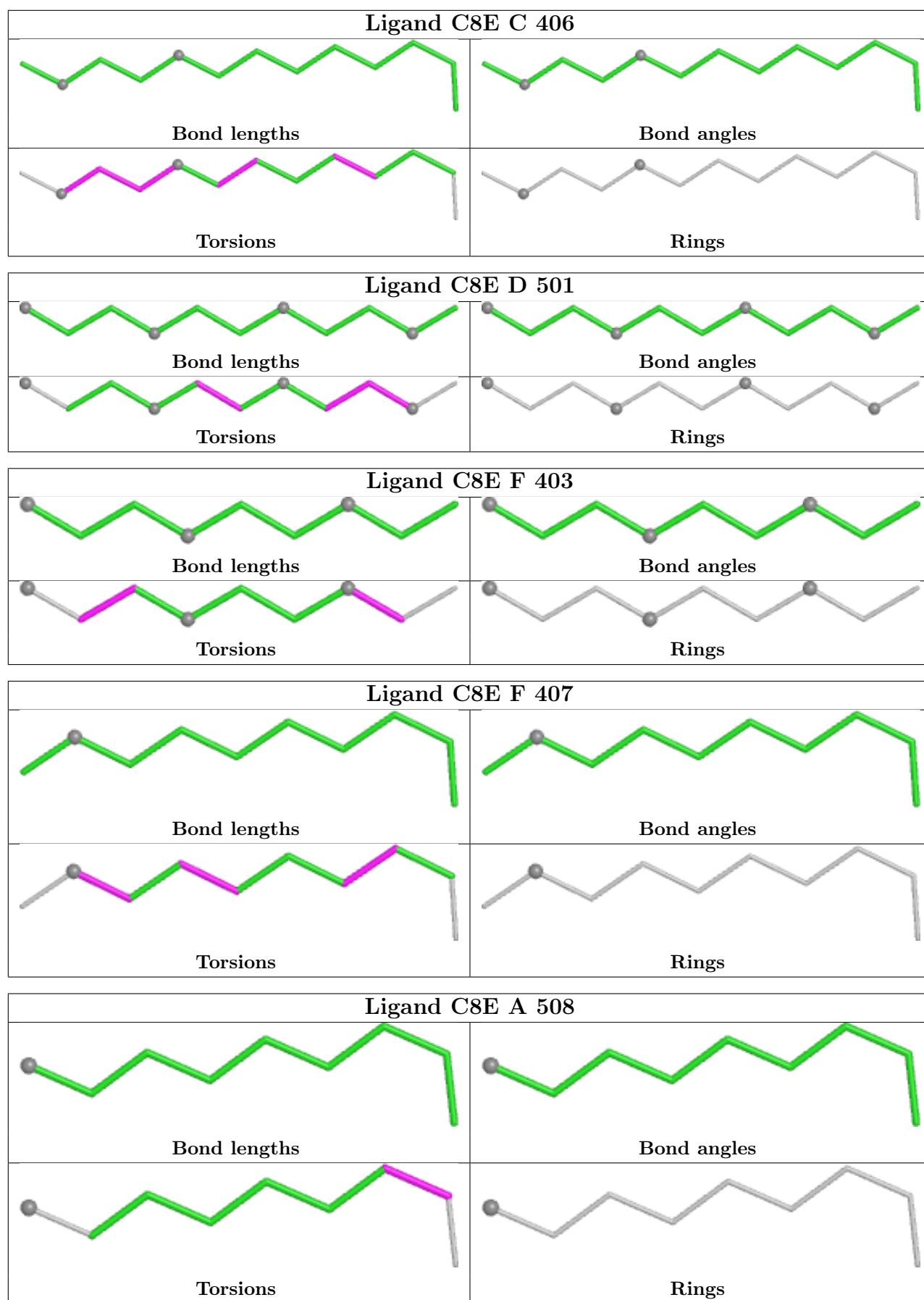


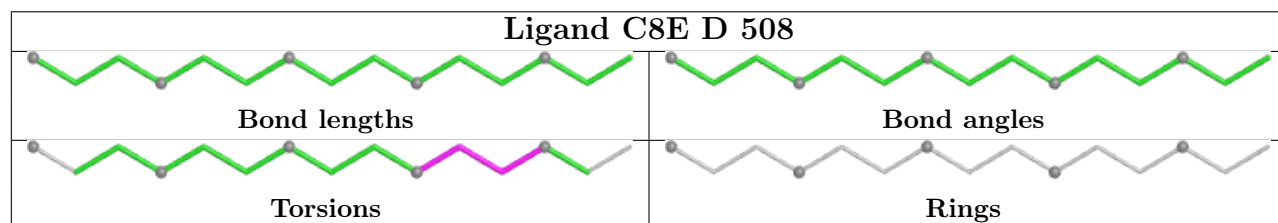
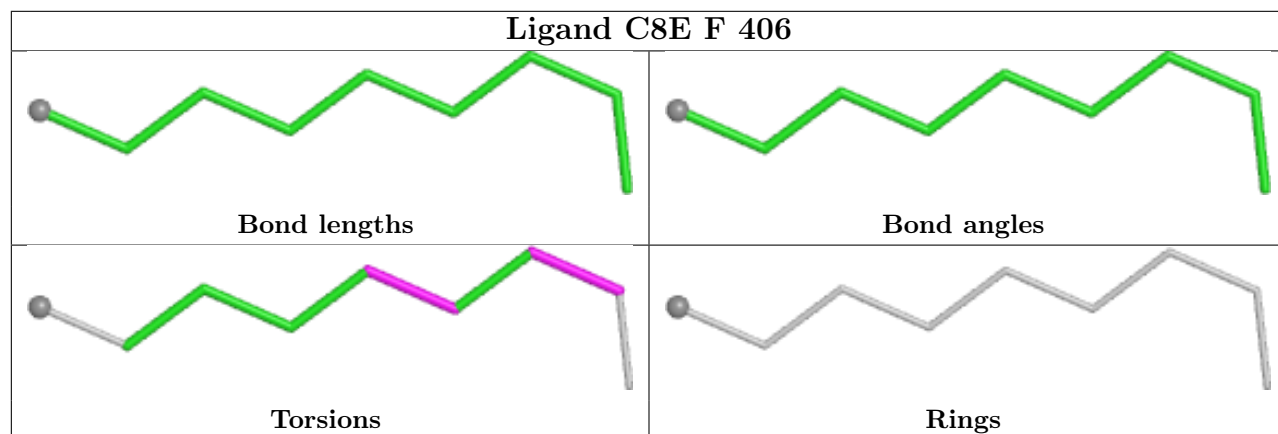
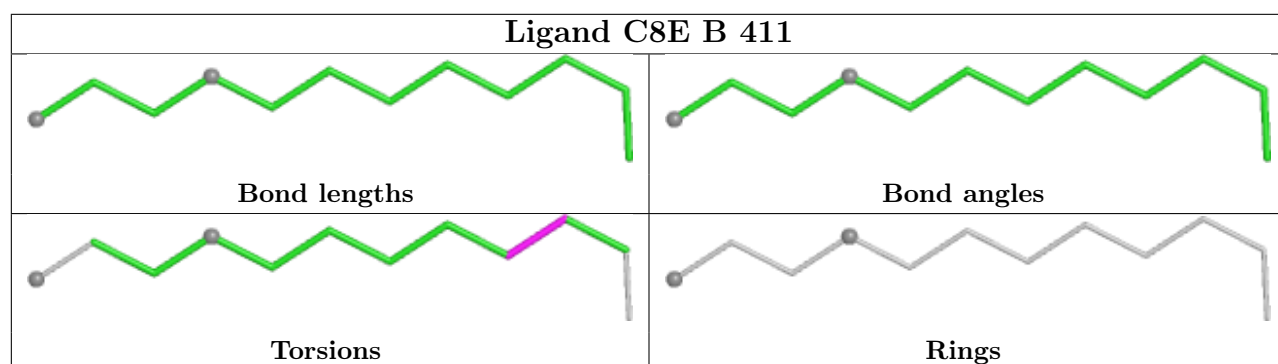
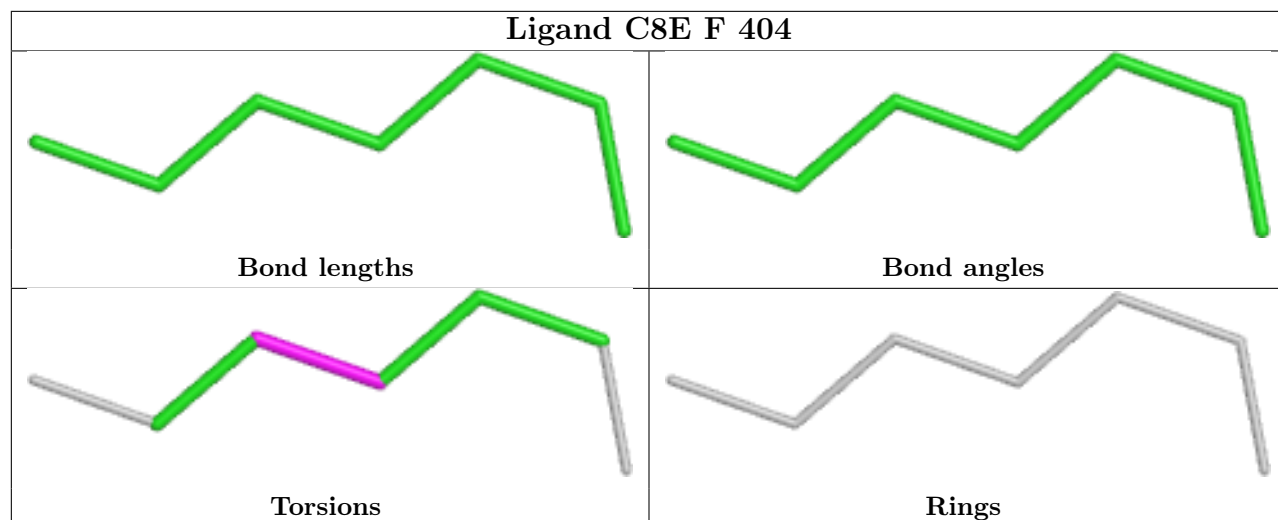


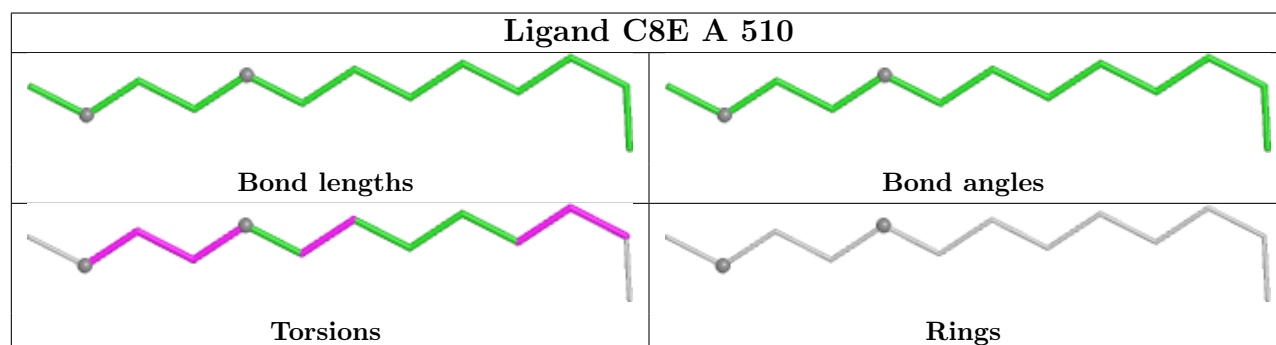
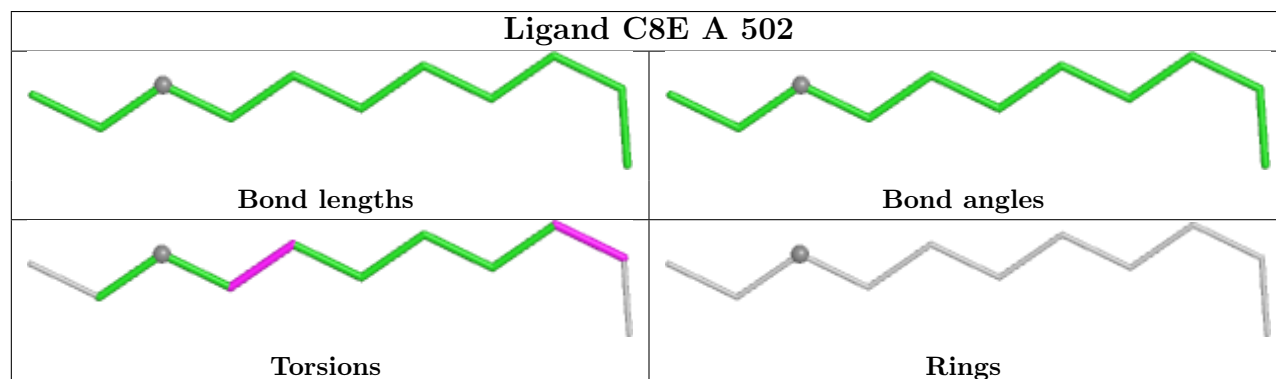
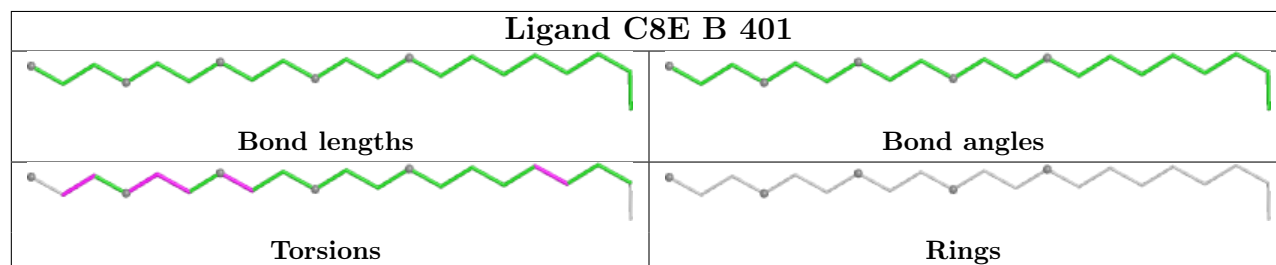
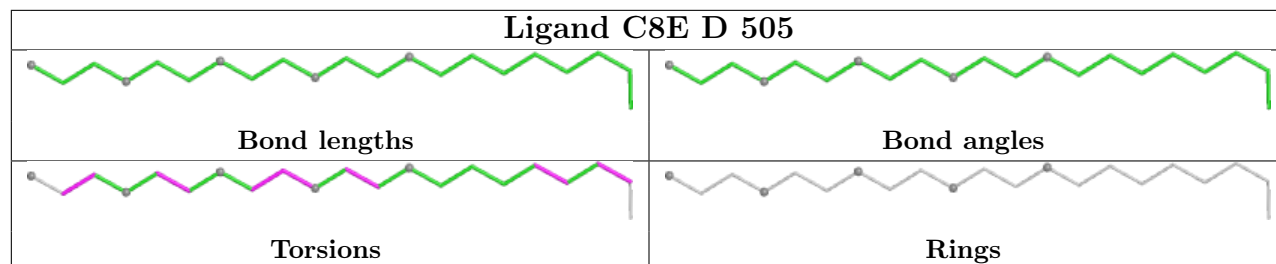
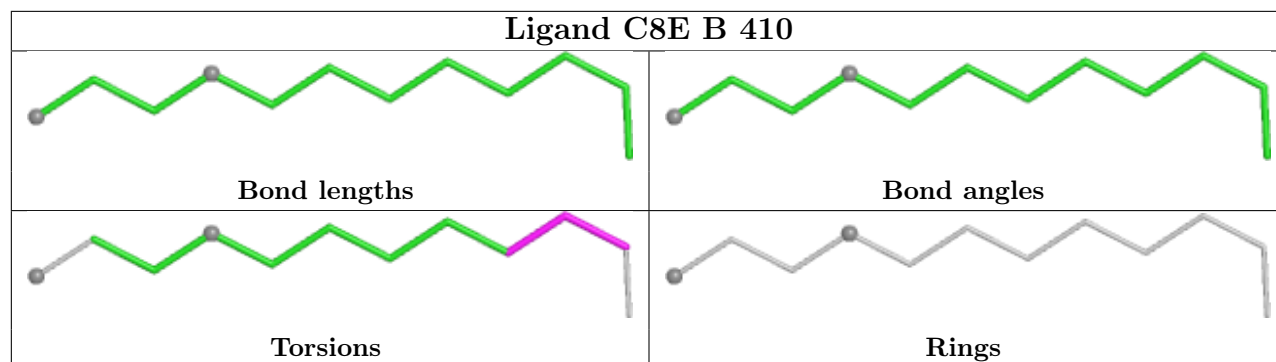


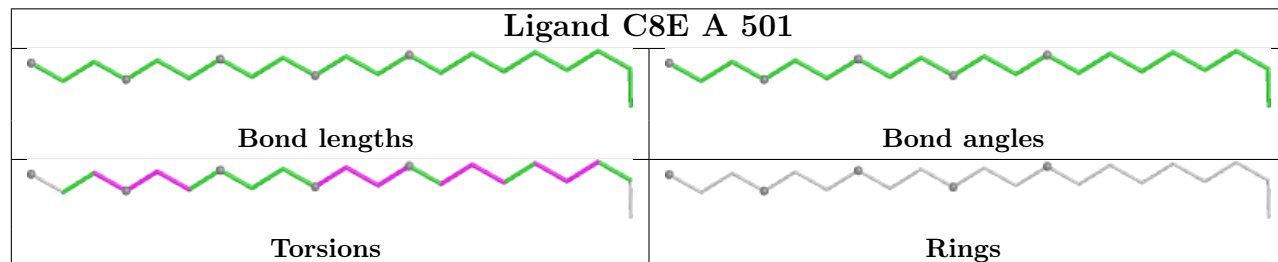
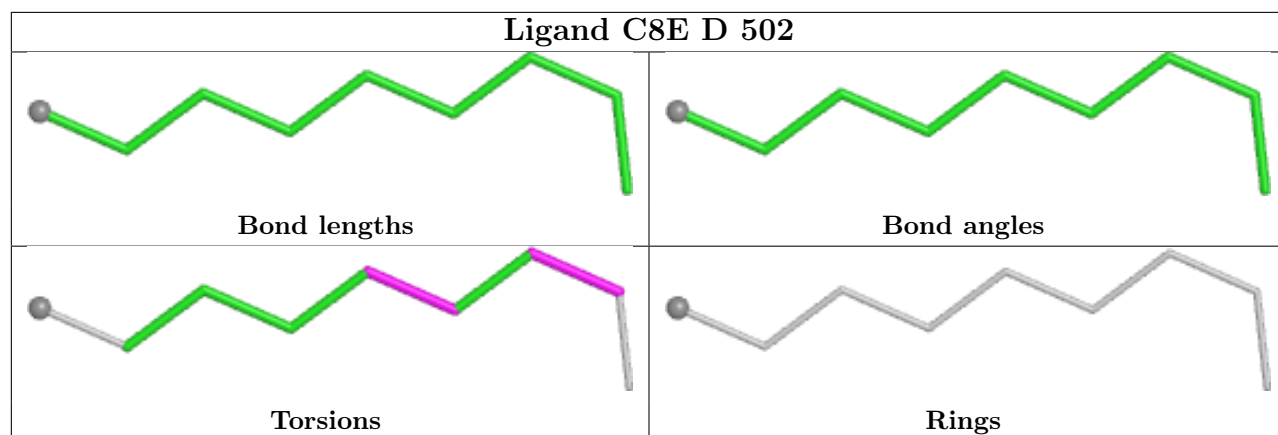
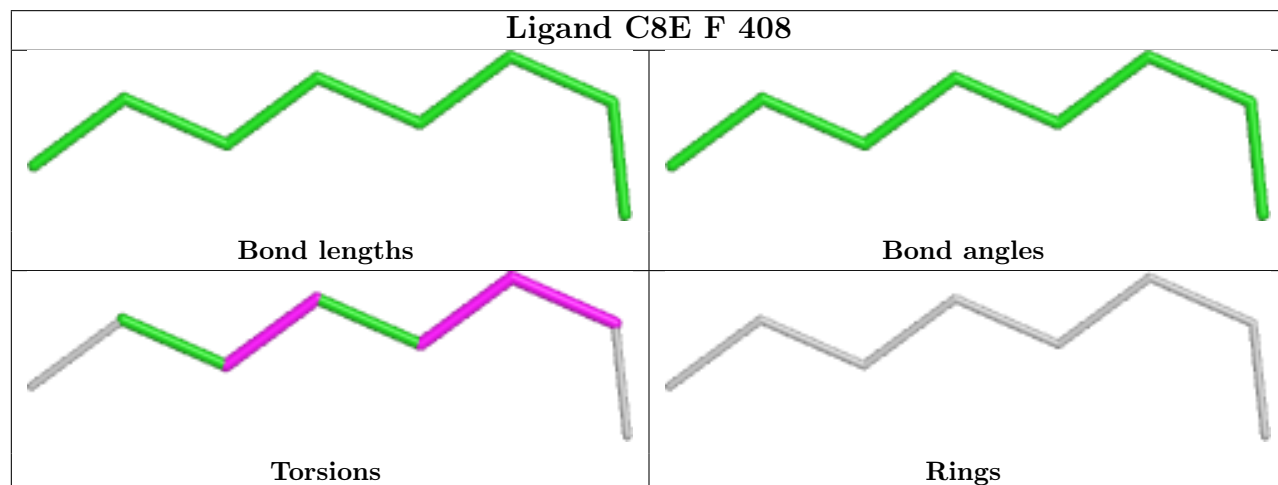
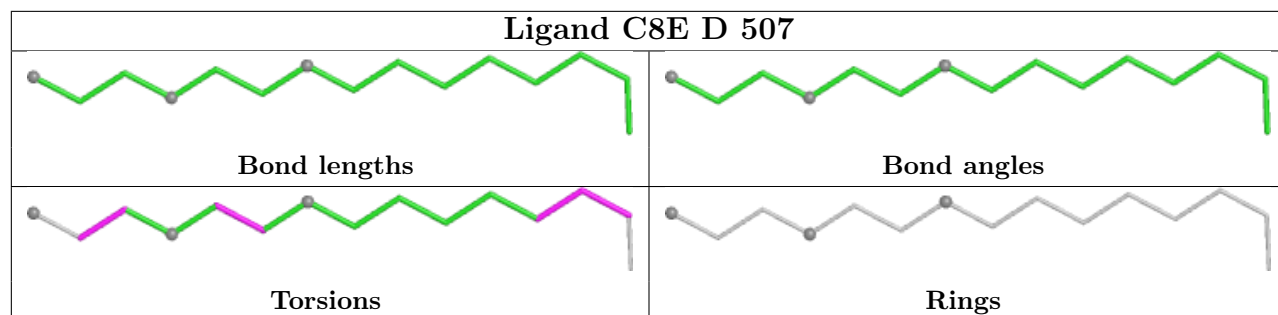


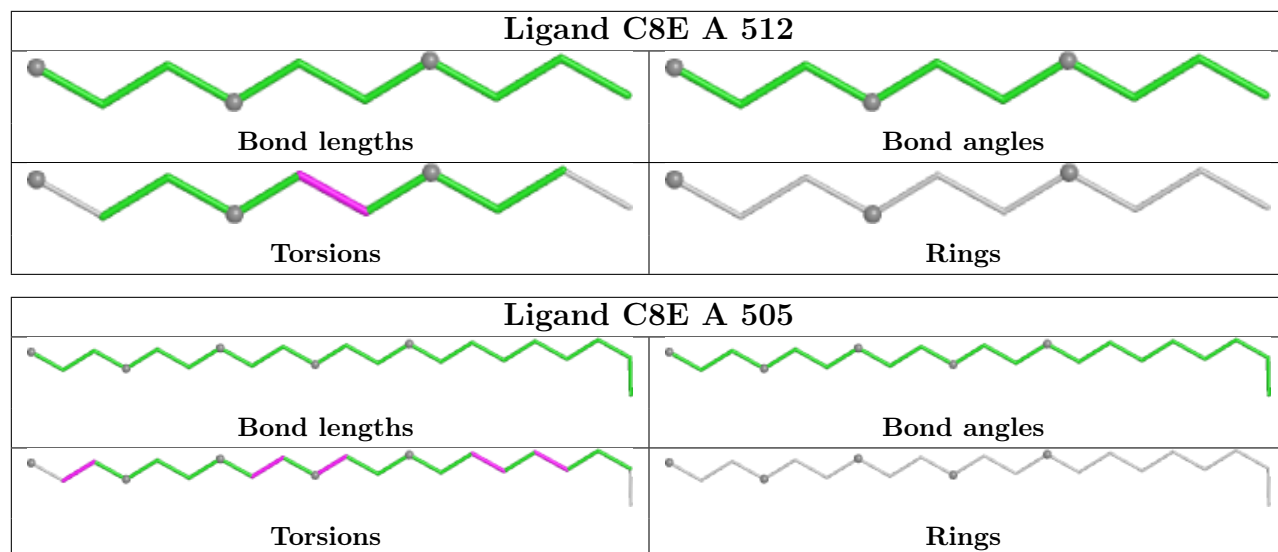












5.7 Other polymers [i](#)

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	346/346 (100%)	0.01	10 (2%) 53 61	14, 19, 30, 56	0
1	B	346/346 (100%)	0.05	12 (3%) 47 53	12, 20, 34, 53	0
1	C	346/346 (100%)	0.14	16 (4%) 37 43	13, 21, 34, 56	0
1	D	346/346 (100%)	0.07	19 (5%) 30 36	13, 20, 35, 58	1 (0%)
1	E	346/346 (100%)	0.12	20 (5%) 29 35	14, 20, 37, 52	0
1	F	346/346 (100%)	0.15	14 (4%) 42 48	14, 21, 34, 52	0
All	All	2076/2076 (100%)	0.09	91 (4%) 39 44	12, 20, 35, 58	1 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	TYR	9.9
1	A	115	ASP	8.2
1	D	187	TRP	8.0
1	A	117	TYR	7.8
1	A	118	GLY	7.7
1	F	116	THR	7.1
1	A	116	THR	7.1
1	B	117	TYR	6.8
1	B	115	ASP	6.3
1	E	86	ALA	6.3
1	C	187	TRP	6.1
1	C	117	TYR	5.9
1	E	117	TYR	5.8
1	C	186	ILE	5.6
1	F	187	TRP	5.6
1	B	187	TRP	5.4
1	D	116	THR	5.2
1	E	116	THR	5.2
1	D	186	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	115	ASP	5.0
1	D	117	TYR	5.0
1	B	116	THR	4.9
1	C	116	THR	4.8
1	F	115	ASP	4.7
1	C	113	GLY	4.2
1	E	140	GLY	4.2
1	D	115	ASP	4.0
1	A	114	ASP	3.7
1	E	115	ASP	3.7
1	F	186	ILE	3.5
1	E	84	GLY	3.3
1	E	141	LEU	3.3
1	C	147	PHE	3.2
1	B	7	ASP	3.2
1	D	7	ASP	3.2
1	D	188	ASP	3.2
1	E	85	ASP	3.1
1	F	114	ASP	3.1
1	E	188	ASP	3.1
1	B	114	ASP	3.0
1	C	345	PHE	3.0
1	B	188	ASP	2.9
1	D	141	LEU	2.9
1	F	184	TYR	2.9
1	D	322	ASP	2.9
1	D	12	ASP	2.8
1	A	194	PHE	2.8
1	C	118	GLY	2.8
1	C	114	ASP	2.8
1	D	114	ASP	2.8
1	F	188	ASP	2.8
1	E	114	ASP	2.7
1	C	188	ASP	2.7
1	E	187	TRP	2.7
1	D	83[A]	PHE	2.7
1	D	118	GLY	2.7
1	D	185	ASP	2.7
1	B	186	ILE	2.6
1	E	138	PHE	2.5
1	C	48	ASP	2.5
1	B	0	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	118	GLY	2.5
1	F	267	ASP	2.4
1	E	139	PHE	2.4
1	B	118	GLY	2.4
1	A	6	LYS	2.4
1	E	83	PHE	2.4
1	D	184	TYR	2.4
1	F	151	TYR	2.4
1	C	49	GLN	2.3
1	D	84	GLY	2.3
1	E	8	GLY	2.3
1	A	12	ASP	2.3
1	F	345	PHE	2.3
1	E	5	ASN	2.3
1	B	345	PHE	2.3
1	A	0	GLY	2.3
1	C	178	PHE	2.3
1	E	184	TYR	2.3
1	E	87	GLY	2.3
1	A	188	ASP	2.2
1	F	194	PHE	2.2
1	B	322	ASP	2.1
1	C	83	PHE	2.1
1	D	194	PHE	2.1
1	D	49	GLN	2.1
1	E	321	ASP	2.1
1	C	112	GLY	2.1
1	F	161	GLU	2.0
1	E	322	ASP	2.0
1	D	142	VAL	2.0

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 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(Å ²)	Q<0.9
2	C8E	A	514	10/21	0.67	0.26	49,50,51,51	0
2	C8E	F	409	11/21	0.71	0.25	43,44,44,44	0
2	C8E	A	507	17/21	0.74	0.21	33,38,43,43	0
2	C8E	F	410	13/21	0.74	0.26	47,50,53,53	0
2	C8E	F	411	17/21	0.74	0.23	42,49,50,50	0
2	C8E	A	511	8/21	0.75	0.24	37,37,37,37	0
2	C8E	A	512	10/21	0.75	0.26	57,58,59,59	0
2	C8E	C	406	13/21	0.76	0.20	41,45,47,47	0
2	C8E	A	515	15/21	0.76	0.25	53,54,56,56	0
2	C8E	B	404	9/21	0.76	0.27	46,47,49,49	0
2	C8E	B	405	16/21	0.76	0.23	55,57,57,57	0
2	C8E	B	401	21/21	0.78	0.24	53,57,60,60	0
2	C8E	B	402	10/21	0.78	0.21	41,41,42,42	0
2	C8E	D	505	21/21	0.79	0.21	39,44,52,52	0
2	C8E	A	501	21/21	0.80	0.19	41,47,49,50	0
2	C8E	F	404	7/21	0.80	0.20	38,38,40,40	0
2	C8E	F	407	10/21	0.80	0.18	40,40,41,41	0
2	C8E	A	510	13/21	0.81	0.18	38,41,44,44	0
2	C8E	F	405	10/21	0.81	0.20	32,33,36,36	0
2	C8E	B	408	8/21	0.81	0.21	41,42,42,42	0
2	C8E	F	408	8/21	0.81	0.20	39,41,42,43	0
2	C8E	E	401	20/21	0.81	0.18	37,39,46,46	0
2	C8E	E	406	19/21	0.81	0.21	41,46,51,51	0
2	C8E	F	403	9/21	0.81	0.23	56,56,57,57	0
2	C8E	C	407	21/21	0.82	0.21	47,48,49,49	0
2	C8E	D	506	11/21	0.82	0.25	47,48,49,49	0
2	C8E	B	412	7/21	0.83	0.19	47,47,48,48	0
2	C8E	C	404	15/21	0.83	0.20	45,46,51,52	0
2	C8E	F	406	9/21	0.84	0.20	54,54,54,54	0
2	C8E	D	502	9/21	0.84	0.19	44,45,46,47	0
2	C8E	A	506	12/21	0.84	0.19	40,41,44,45	0
2	C8E	A	505	21/21	0.85	0.16	33,38,40,41	0
2	C8E	C	405	13/21	0.85	0.20	45,48,50,51	0
2	C8E	D	507	15/21	0.85	0.17	43,43,45,45	0
2	C8E	B	403	14/21	0.85	0.16	41,41,44,45	0
2	C8E	E	402	15/21	0.85	0.17	41,42,45,45	0
2	C8E	E	403	14/21	0.85	0.17	39,40,53,53	0

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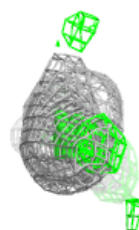
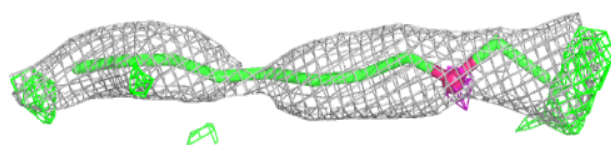
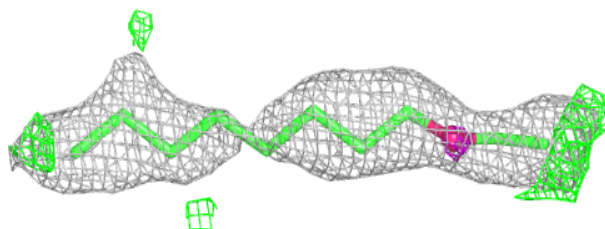
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	B	410	12/21	0.85	0.19	44,44,47,47	0
2	C8E	A	509	9/21	0.85	0.18	44,44,46,46	0
2	C8E	D	501	11/21	0.86	0.14	44,44,46,46	0
2	C8E	B	411	12/21	0.86	0.16	43,43,44,44	0
2	C8E	A	502	11/21	0.87	0.16	33,34,36,37	0
2	C8E	C	403	6/21	0.87	0.16	34,34,35,35	0
2	C8E	B	409	10/21	0.87	0.16	34,38,42,42	0
2	C8E	D	508	15/21	0.88	0.17	38,40,43,43	0
3	LI	C	401	1/1	0.88	0.36	8,8,8,8	0
2	C8E	A	508	9/21	0.91	0.15	35,35,37,38	0
3	LI	B	407	1/1	0.92	0.43	3,3,3,3	0
3	LI	F	401	1/1	0.92	0.44	3,3,3,3	0
3	LI	B	406	1/1	0.93	0.26	4,4,4,4	0
3	LI	E	404	1/1	0.93	0.33	4,4,4,4	0
3	LI	A	503	1/1	0.93	0.41	3,3,3,3	0
2	C8E	A	513	6/21	0.94	0.11	31,31,31,31	0
3	LI	F	402	1/1	0.94	0.23	3,3,3,3	0
3	LI	C	402	1/1	0.96	0.47	3,3,3,3	0
3	LI	A	504	1/1	0.96	0.47	3,3,3,3	0
3	LI	D	504	1/1	0.97	0.45	3,3,3,3	0
3	LI	D	503	1/1	0.97	0.36	3,3,3,3	0
3	LI	E	405	1/1	0.98	0.45	3,3,3,3	0

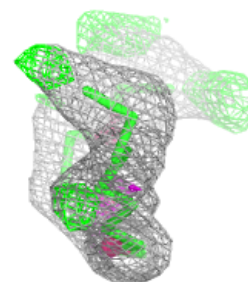
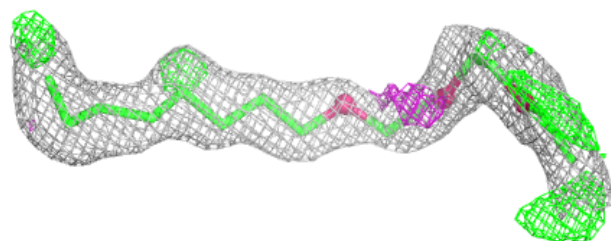
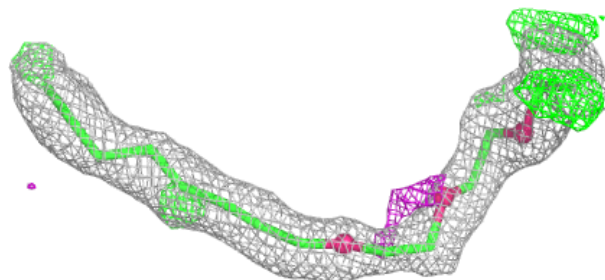
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E F 409:

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

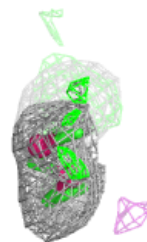
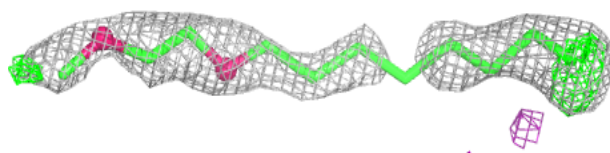
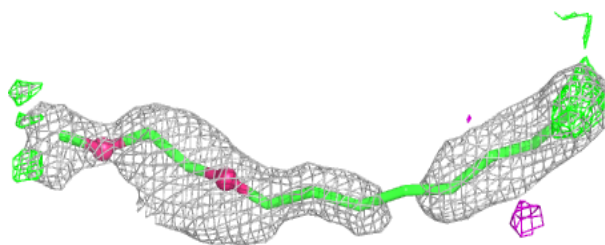
**Electron density around C8E A 507:**

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



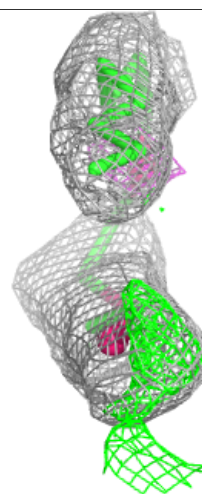
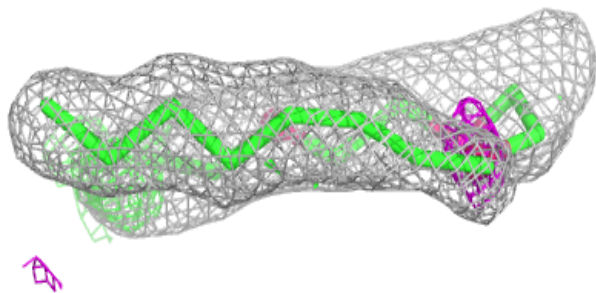
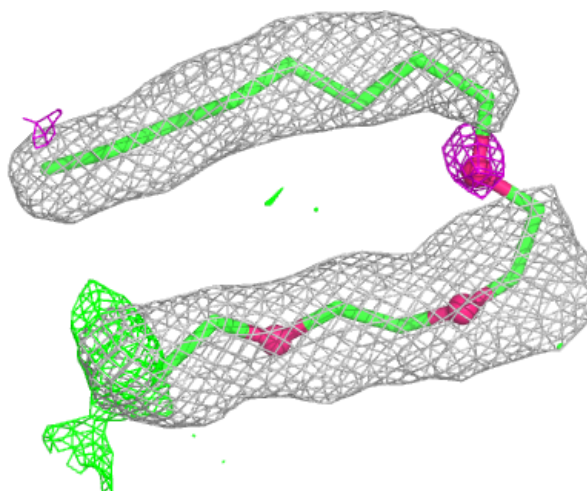
Electron density around C8E F 410:

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



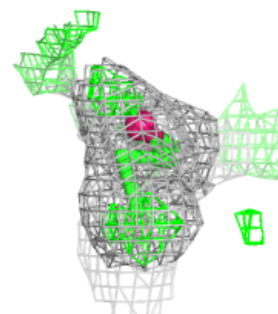
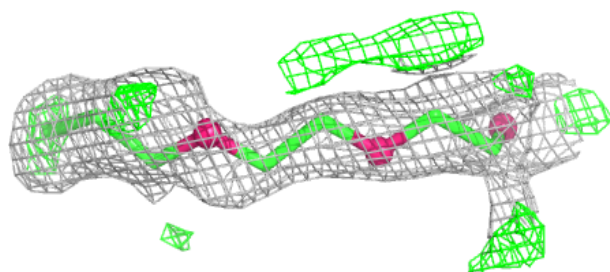
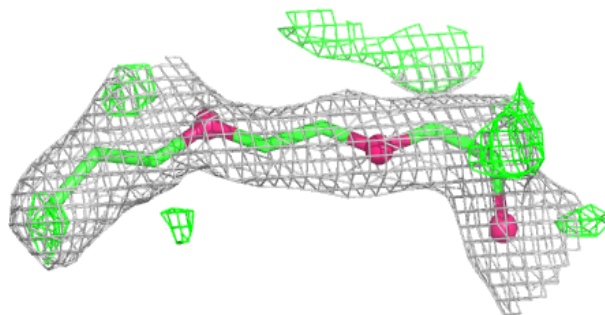
Electron density around C8E F 411:

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

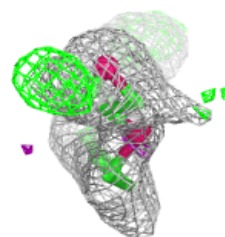
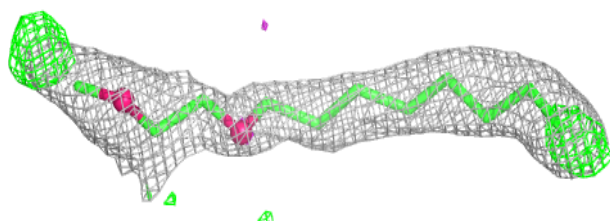
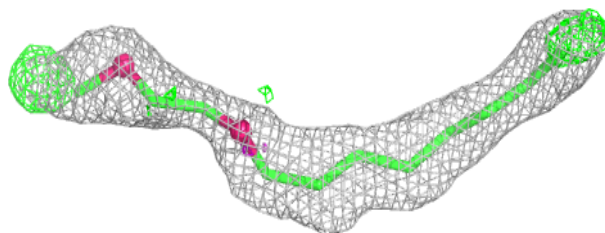


Electron density around C8E A 512:

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

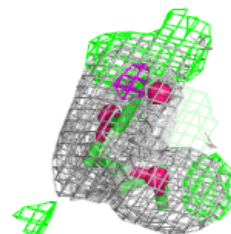
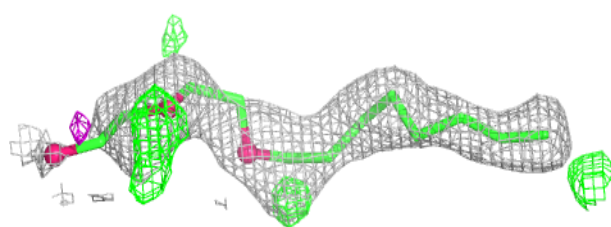
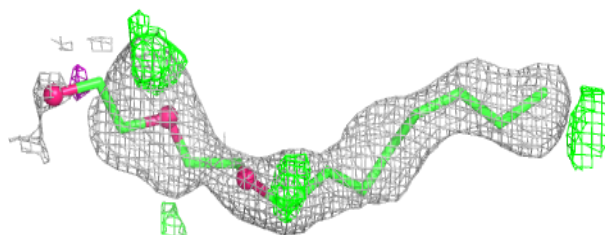
**Electron density around C8E C 406:**

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

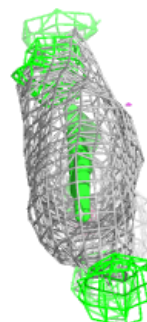
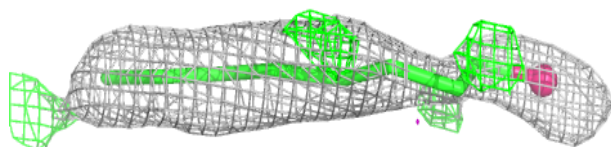
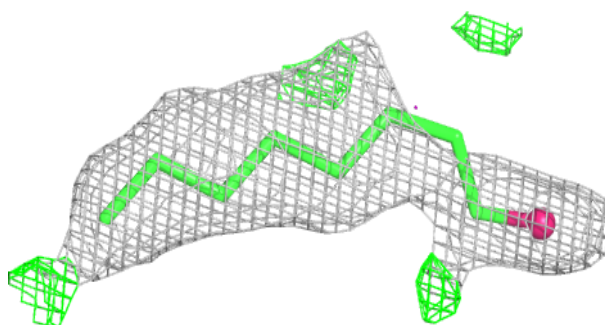


Electron density around C8E A 515:

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

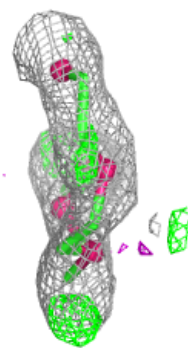
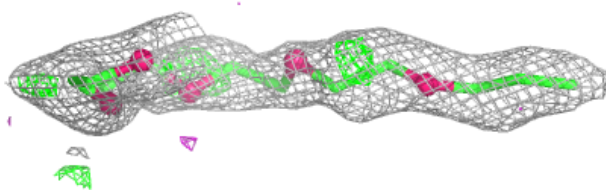
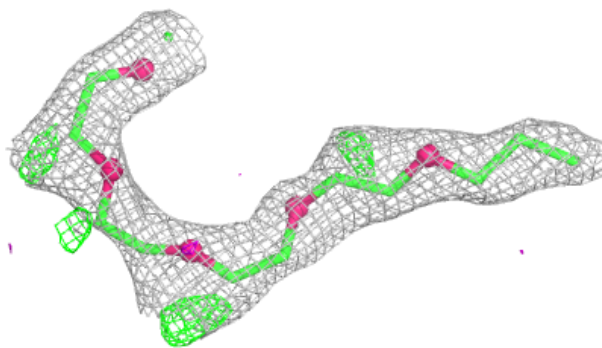
**Electron density around C8E B 404:**

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



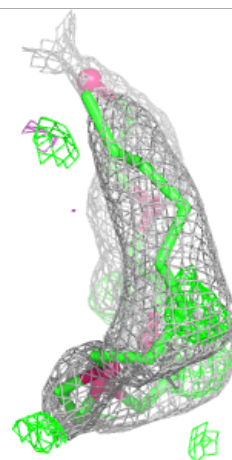
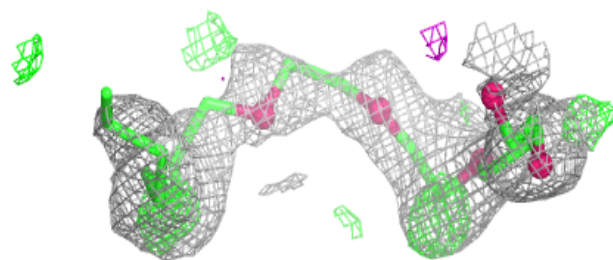
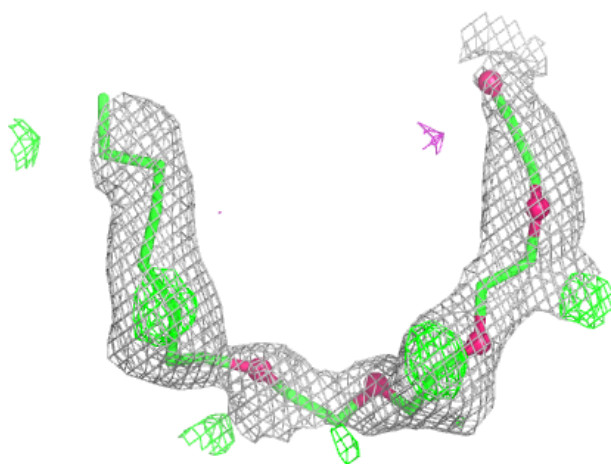
Electron density around C8E B 405:

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



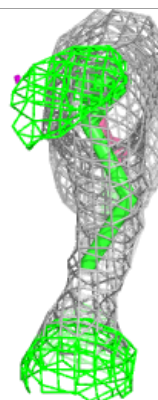
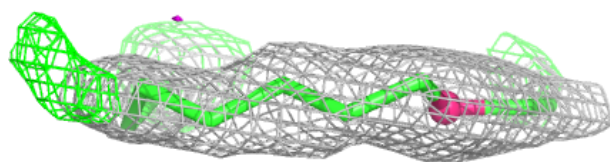
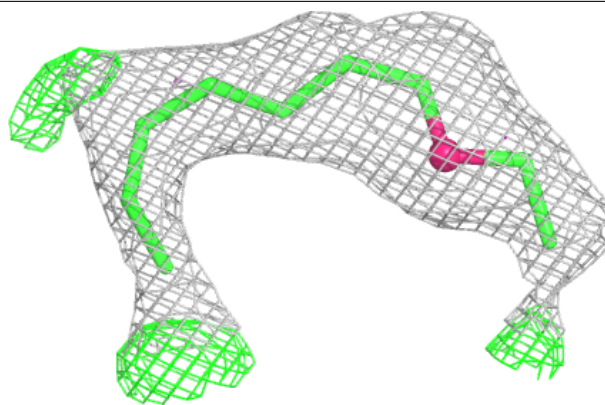
Electron density around C8E B 401:

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

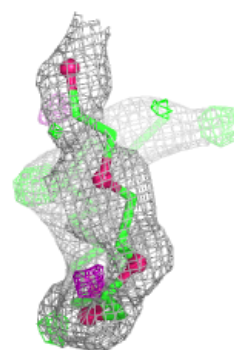
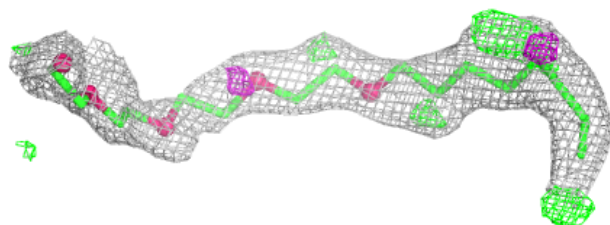
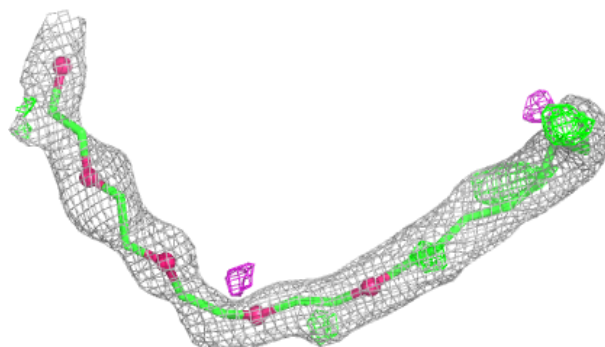


Electron density around C8E B 402:

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

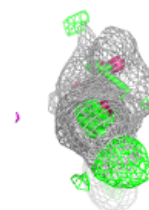
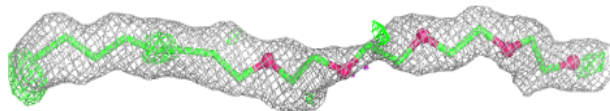
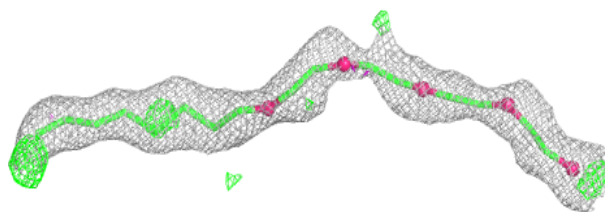
**Electron density around C8E D 505:**

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

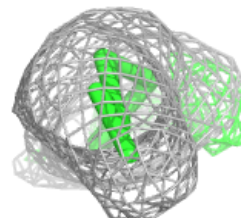
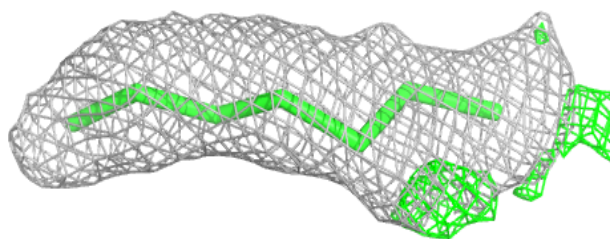
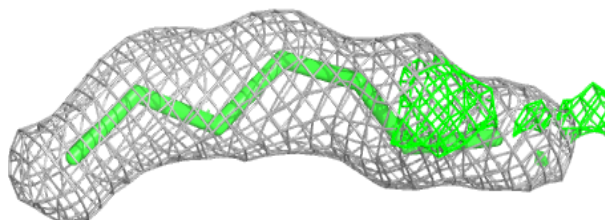


Electron density around C8E A 501:

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

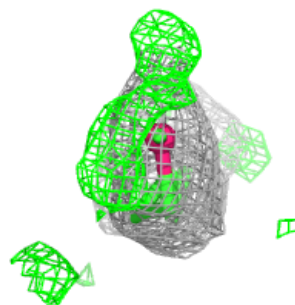
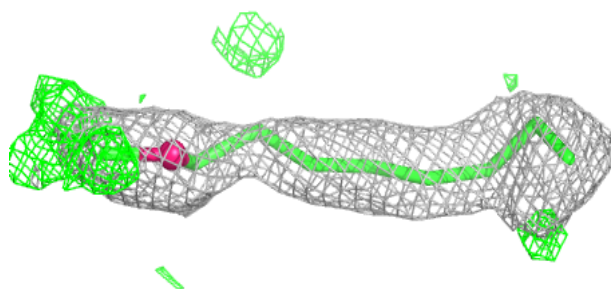
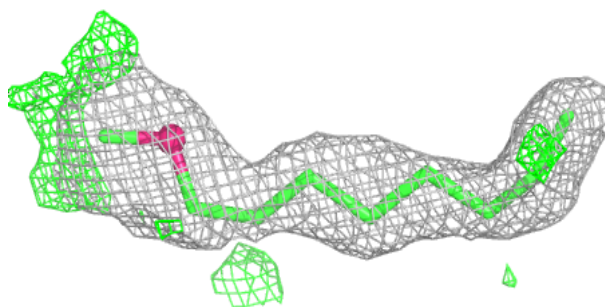
**Electron density around C8E F 404:**

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

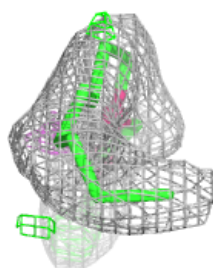
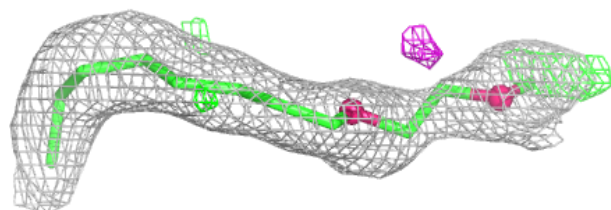
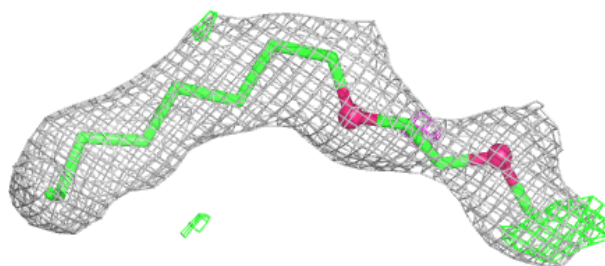


Electron density around C8E F 407:

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

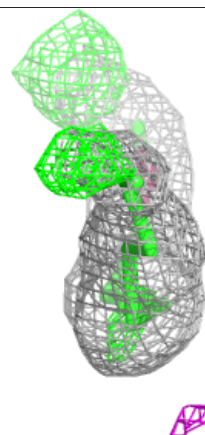
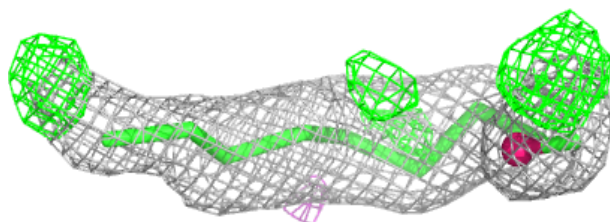
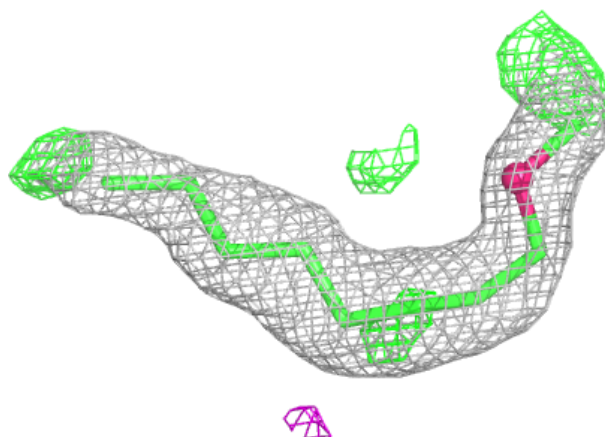
**Electron density around C8E A 510:**

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

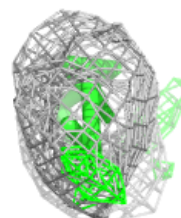
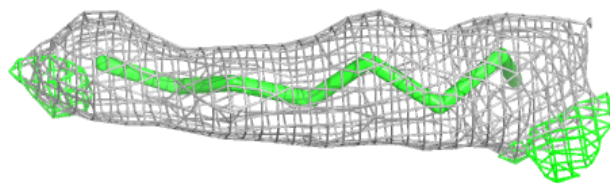
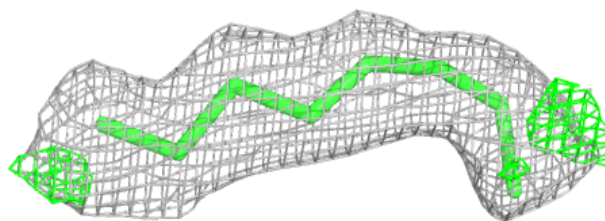


Electron density around C8E F 405:

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

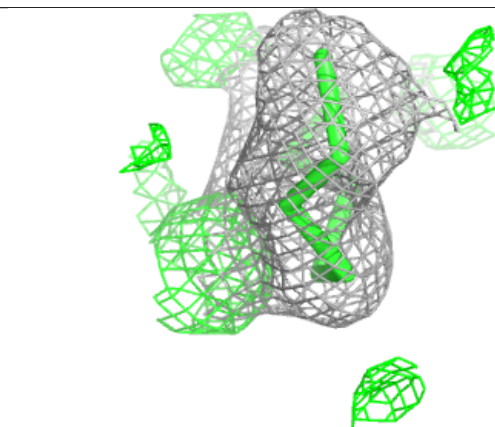
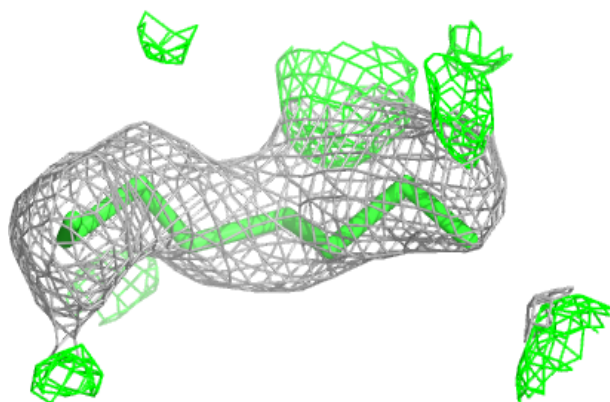
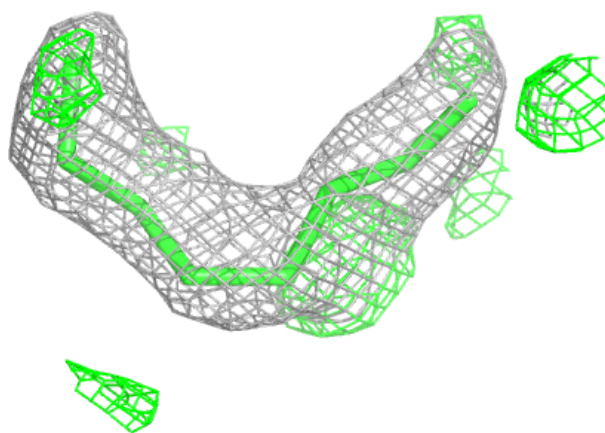
**Electron density around C8E B 408:**

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

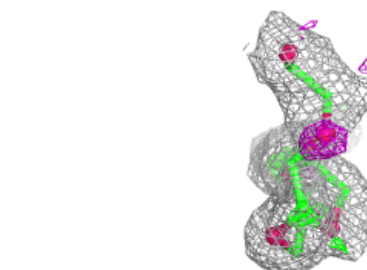
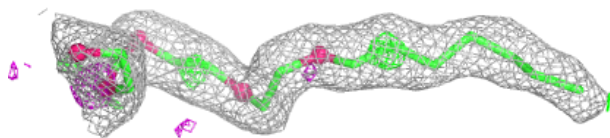
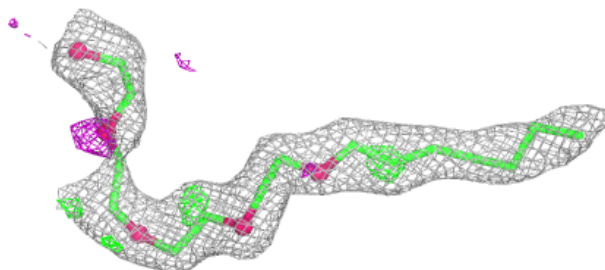


Electron density around C8E F 408:

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

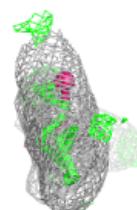
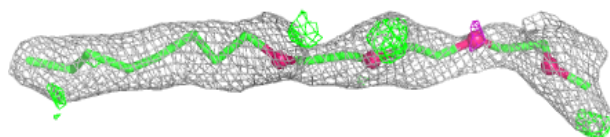
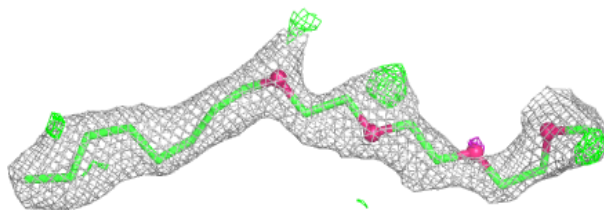
**Electron density around C8E E 401:**

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

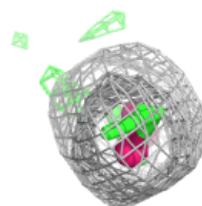
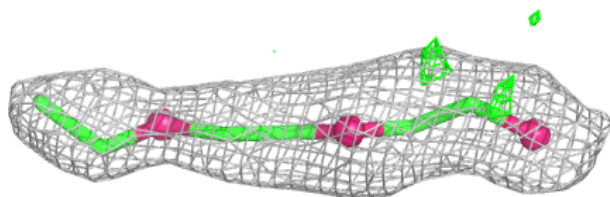
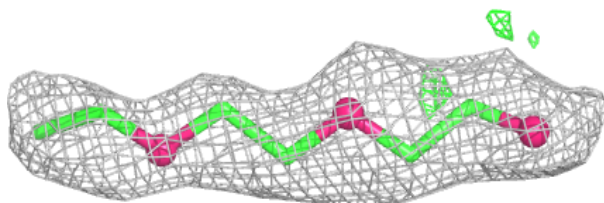


Electron density around C8E E 406:

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

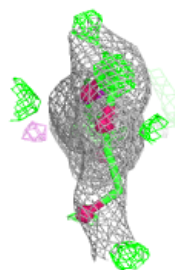
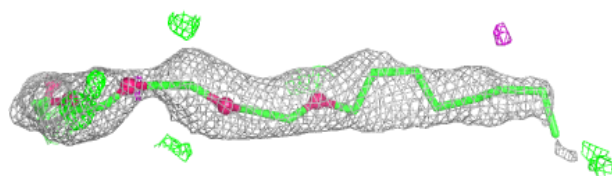
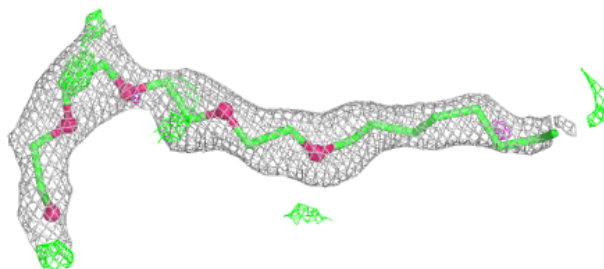
**Electron density around C8E F 403:**

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

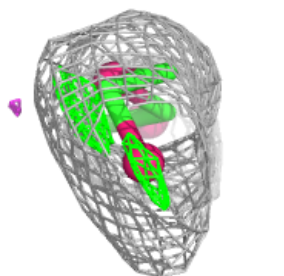
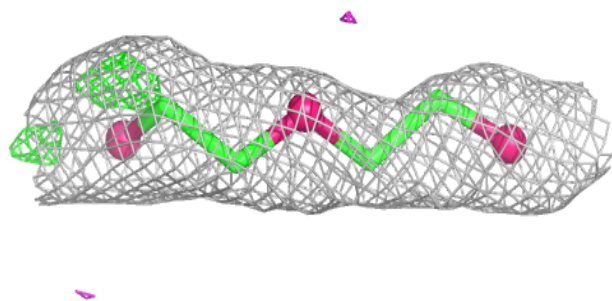
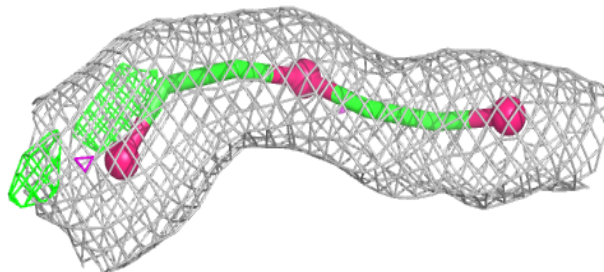


Electron density around C8E C 407:

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

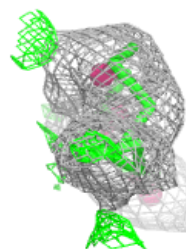
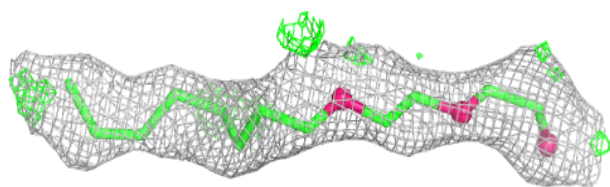
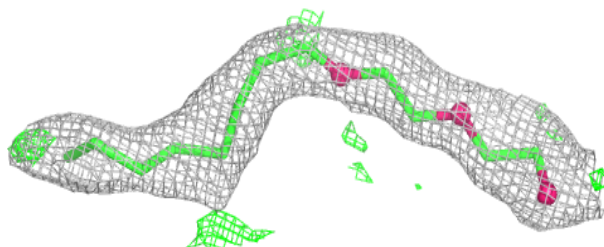
**Electron density around C8E B 412:**

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

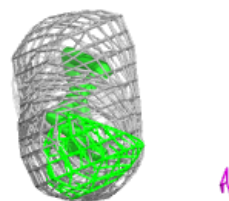
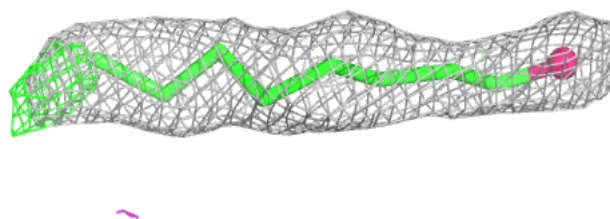
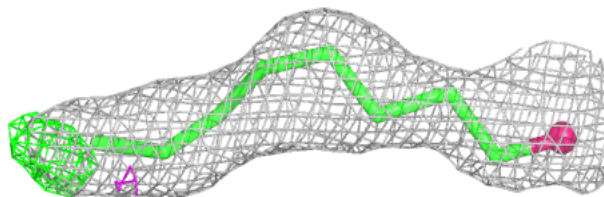


Electron density around C8E C 404:

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

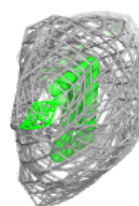
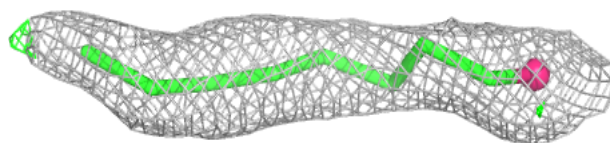
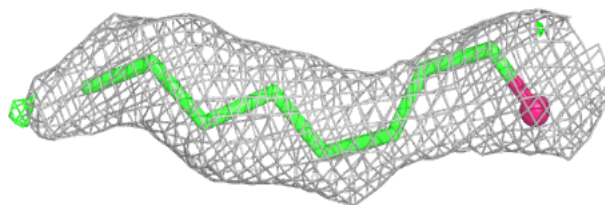
**Electron density around C8E F 406:**

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

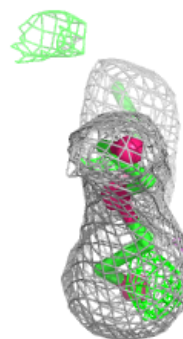
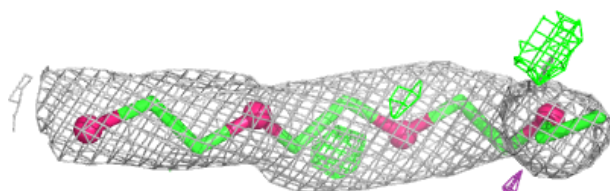
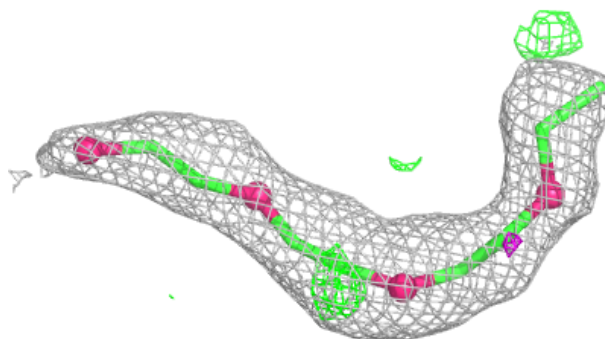


Electron density around C8E D 502:

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

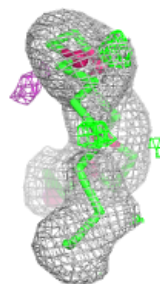
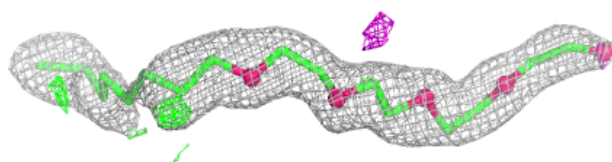
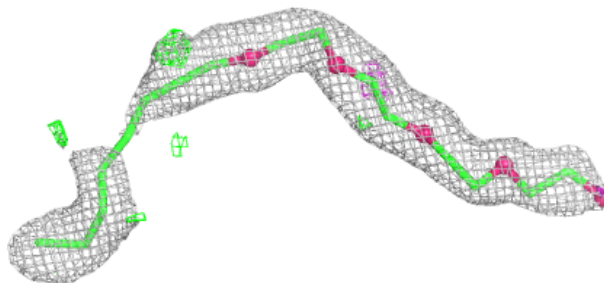
**Electron density around C8E A 506:**

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

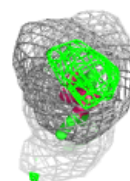
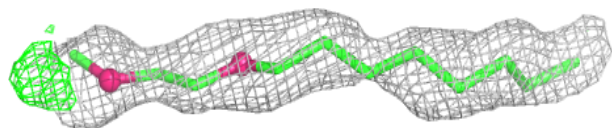
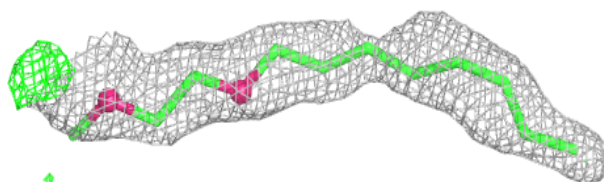


Electron density around C8E A 505:

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

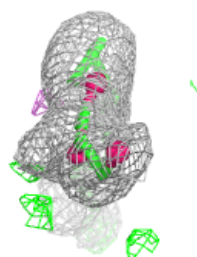
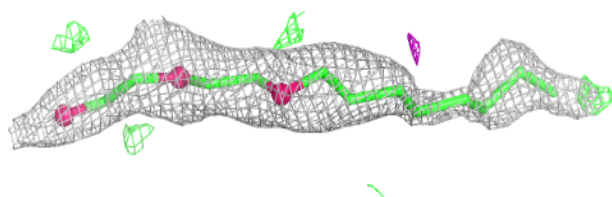
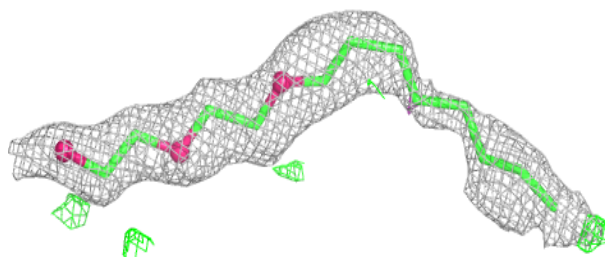
**Electron density around C8E C 405:**

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

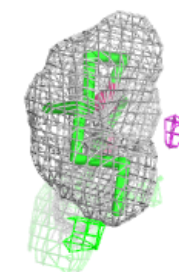
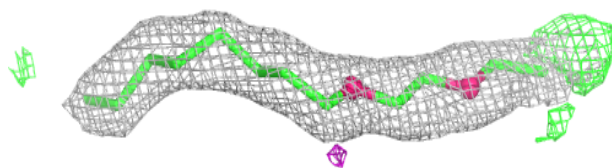
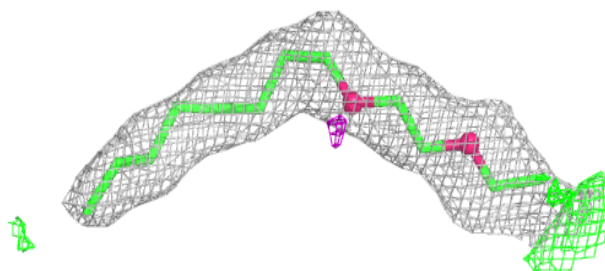


Electron density around C8E D 507:

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

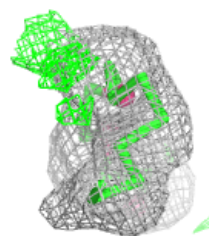
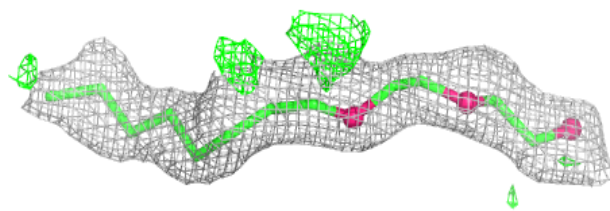
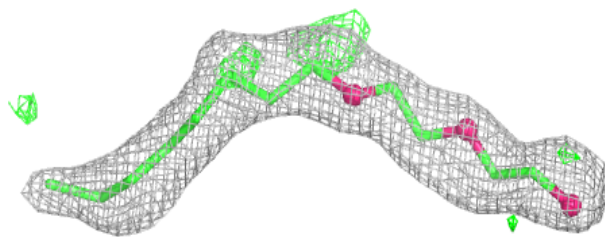
**Electron density around C8E B 403:**

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

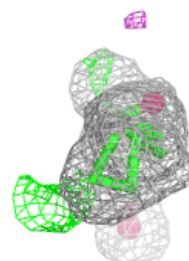
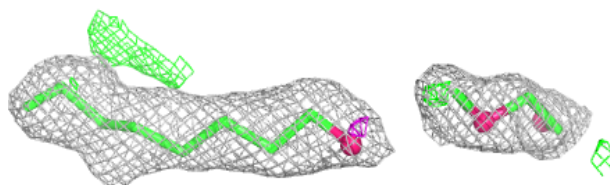
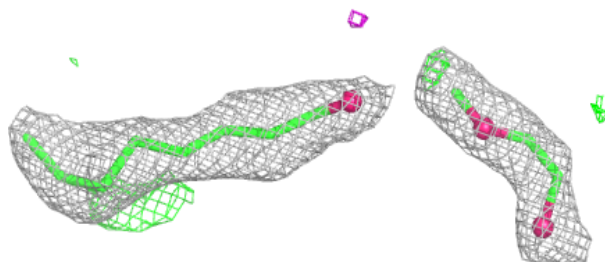


Electron density around C8E E 402:

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

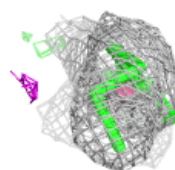
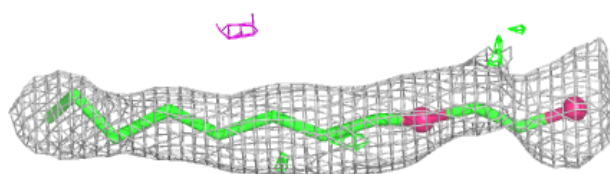
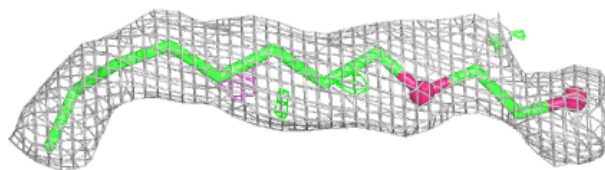
**Electron density around C8E E 403:**

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

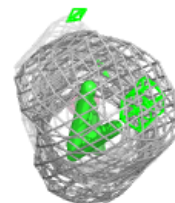
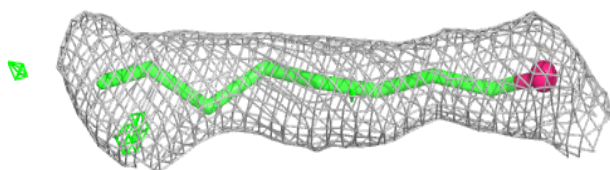
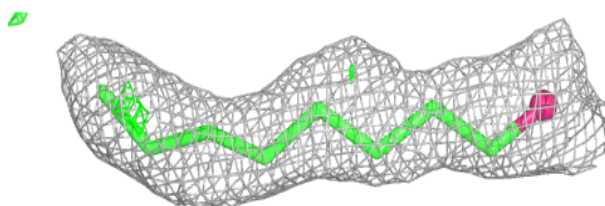


Electron density around C8E B 410:

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

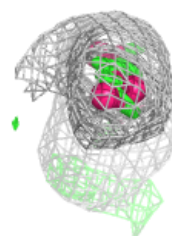
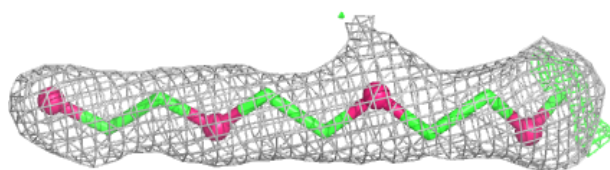
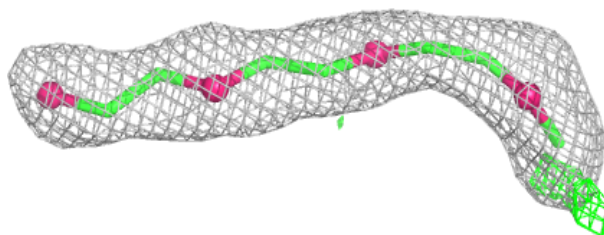
**Electron density around C8E A 509:**

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

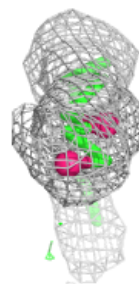
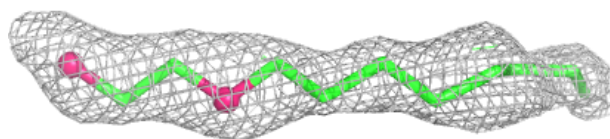
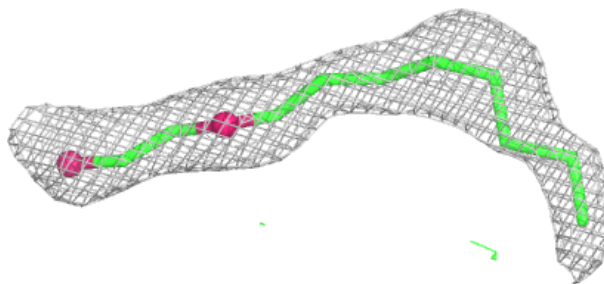


Electron density around C8E D 501:

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

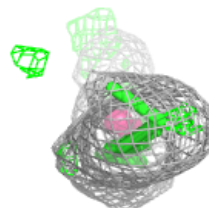
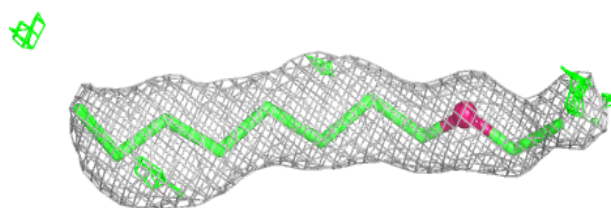
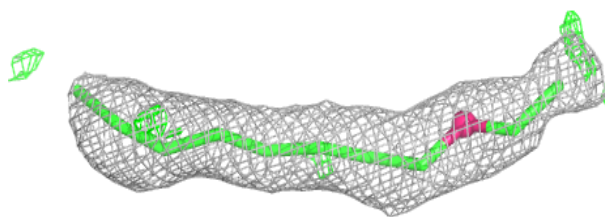
**Electron density around C8E B 411:**

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

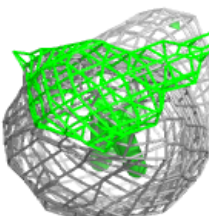
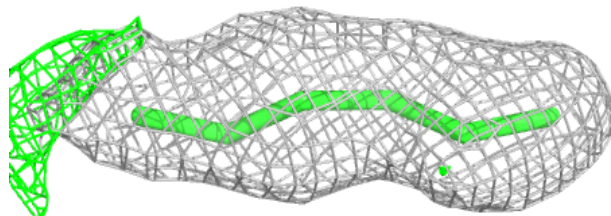
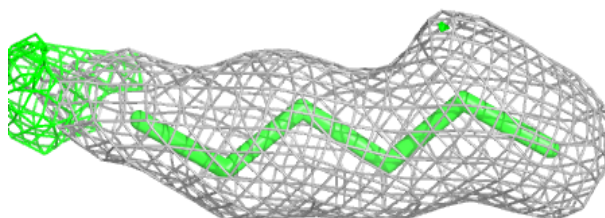


Electron density around C8E A 502:

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

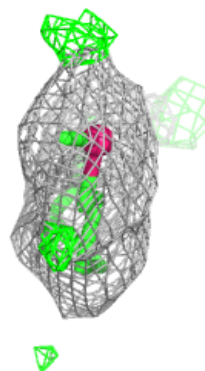
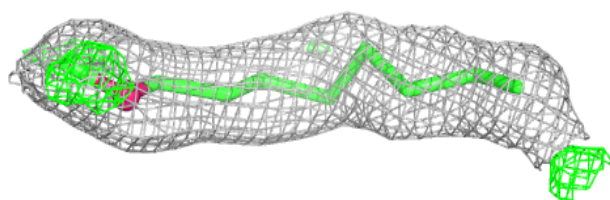
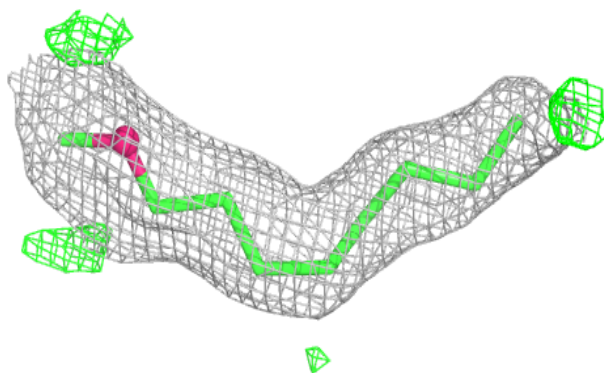
**Electron density around C8E C 403:**

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

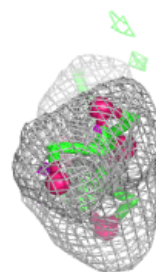
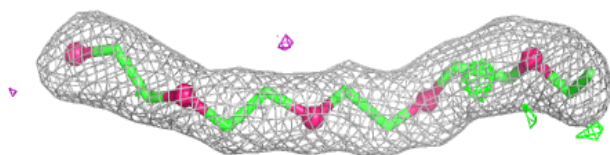
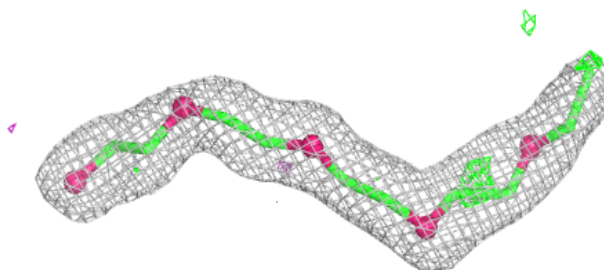


Electron density around C8E B 409:

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

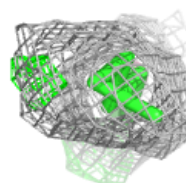
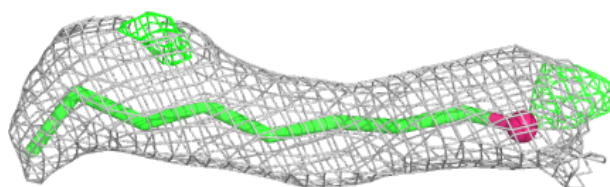
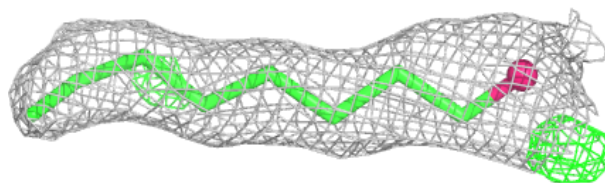
**Electron density around C8E D 508:**

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



Electron density around C8E A 508:

$2mF_o - DF_c$ (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.